Supporting Information

Development of in silico models for predicting P-Glycoprotein inhibitors based on a two-step approach for feature selection and its application to Chinese herbal medicine screening

Ming Yang, Jialei Chen, Xiufeng Shi, Liwen Xu, Zhijun Xi, Lisha You, Rui An*, and Xinhong Wang*

Contents

Table S1. All molecules and their structures & Reference of collected molecules.
Table S2. Descriptors calculated in the present work.
Table S3. Skewness of Box-Cox transformation for 28 continuous descriptors.
Table S4. Statistics of continuous descriptors for both data sets.
Table S5. The corrected p-values for each comparison between classifiers by a Wilcoxon signed rank test.
Table S6. Ranking information of our optimal descriptors by the rank-based feature selection methods.
Table S7. Classification performance with different Cutoff values of AD probability.
Table S8. Predictions by the developed models for Inside-AD compounds in TCMSP database.
Figure S1. Fitness evolution in different classifiers.
Figure S2. Accuracy curves of different rank-based feature selection methods for each classifier. (A) UST, (B) ReliefF, and (C) mRMR. UST, univariate statistical test.
Figure S3. Probability response curves for the optimal descriptors. (A) MLogP, (B) SpMAD_Dt, (C) ATSC1i, (D) LipoaffinityIndex, (E) SpMax4_Bhm, (F) SpMax1_Bhp, (G) SHBint8, (H) ATSC0p, (I) ASP.3, (J) SHBint3, (K) AATS5i, (L) SubFP84, (M) PubchemFP607, and (N) MACCSFP142. For the continuous descriptors (A-K), probability response curves were obtained by varying one specific descriptor from its minimum to maximum. For the binary fingerprint descriptors (L-N), probability response curves were obtained on the different quantile values of the continuous descriptors.
Figure S4. Distributions of continuous optimal descriptors for the combination of TCMSP database and modeling dataset. (A) MLogP, (B) SpMAD_Dt, (C) ATSC1i, (D) LipoaffinityIndex, (E) SpMax4_Bhm, (F) SpMax1_Bhp, (G) SHBint8, (H) ATSC0p, (I) ASP.3, (J) SHBint3, and (K) AATS5i

Table S1. All molecules and their structures

Compound_id	Database_id	Set	Class	Reference	Predicted by FDA	Predicted by SVM	Predicted by RanForest	Predicted by EM	SMILES
C1		Training	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1ccc2c(c1)c(=O)c(c(c1ccc(c(c1)OC)OC)o2)OC
C2		Training	noninhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	c1cc2c(c3c(sc2cc1N(C)C)cc(=[N+](C)C)cc3)c1sc(cc1)C(=S)N1CCCCC1
C3		Training	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1ccc(cc1OC)c1c(c(=O)c2ccc(cc2o1)O)O
C4		Training	noninhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	n1(n(c(c(c1=O)C(=O)c1ccccc1)C)CC(CNC(C)C)O)c1ccccc1
C5		Training	noninhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	n1(n(c(c(c1=O)C(=O)c1ccccc1)C)CC(CNCCC)O)c1ccccc1
C6		Training	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1(n(c(c(c1=O)C(=O)c1ccccc1)C)CC(CN(C(C)C)C(C)C)O)C
C7		Training	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1c(c(cc(c1)c1oc2c(c(=O)c1)c(c(c(c2)OC)OC)OC)OC)OC
C8		Training	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1c(cc(cc1)c1oc2c(c(=O)c1)c(c(c(c2)OC)OC)OC)OC
C9		Training	noninhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	N1(N=C(/C(=C(\CCc2ccccc2)/NCCC)/C1=O)C)c1ccccc1
C10		Training	noninhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	N1(N=C(/C(=C(\c2ccccc2)/N2CCN(CC2)c2ccccc2C)/C1=O)C)c1ccccc1
C11		Training	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1c2c(CC(=O)C1c1ccccc1)cc(cc2)OC
C12		Training	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(cc2c(c1)oc(cc2=O)c1ccccc1)OC
C13		Training	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1ccc2c(=O)cc(c3ccc(c(c3)OC)OC)oc2c1
C14		Training	noninhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)c1c(C(=O)Nc2ccccc2)c(c(n1CC[C@@H]1C[C@@H](O)CC(=O)O1)c1ccc(F)cc1)c1ccccc1
C15		Training	noninhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	c1(CCc2ccccc2OCc2cnccc2)cc(OC)ccc1
C16		Training	noninhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	COc1ccc(cc1OC)CCCN1CCC(CC1)Cc1ccccc1
C17		Training	noninhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	c1(c(C)n(CC(CN2CCN(CC2)c2c(cccc2)C)O)n(c1=O)c1ccccc1)C(=O)c1ccccc1
C18		Training	noninhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	c1c(cc2c(c1)C(=C1CCNCC1)c1c(CC2)cccn1)Cl
C19		Training	noninhibitor	59	inhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1C[C@@H]([C@@H]([C@H](O)CO[C@]2(O)O[C@@H](C[C@@H](C)[C@H](C)O)[C@H](C)[C@H]2O)[C@H](C)O)O[C@H]1C[C@@]2([C@H](C)[C@H](O)[C@@H](C)O2)C=C
C20		Training	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1C(CC(=O)c2c1c(c(cc2OC)OC)C)c1ccccc1
C21		Training	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1(=C(NC(=C(C1c1c(c(Cl)ccc1)Cl)C(=O)OCC)C)C)C(=O)OC
C22		Training	noninhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	O1C(=O)CC(O)[C@H](Cc2ccccc2)N(C)C(=O)[C@H](C(C)C)OC(=O)[C@@H](C)[C@H]1CCCCCCC
C23		Training	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@]12([C@@]([C@@](C(=O)CO)(CC[C@H]1[C@H]1[C@@H]([C@@]3(C(=CC(=O)CC3)CC1)C)[C@H](C2)O)O)C
C24		Training	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(CC(COc1ccc(cc1)CCOC)O)C(C)C
C25		Training	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@]123c4c5O[C@H]2[C@H](C=C[C@H]1[C@@H](Cc4ccc5O)N(CC3)C)O
C26		Training	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	o1c2c(c(=O)c(OC)c1c1ccc(O)cc1)c(O)c(OC)c(OC)c2
C27		Training	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(oc(c(c1=O)OC)c1ccc(c(c1)OC)OC)cc(cc2O)OC
C28		Training	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1cc2oc(cc(=O)c2c(OC)c1C)c1ccccc1
C29		Training	noninhibitor	59	inhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@]12([C@@H]([C@@]3([C@@H]([C@H]2O)OC3)OC(=O)C[C@H](C[C@@]2(C)[C+](C[C@@H](C2)OC(=O)[C@@H]([C@@H](NC(=O)c2cccc2)c2cccc2)O)C)[C@@H](C1=O)OC(=O)C)C)O)OC(=O)c1ccccc1)C
C30		Training	noninhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	O1[C@]2(C[C@@H]([C@@H](C[C@@H]([C@@H]([C@H]([C@@H](NC(C)C)[C@H](OC(=O)C)C[C@@H](C[C@@H](O)[C@@H]([C@@H]([C@@H]1C)O)O)O)C)O)C)O)C)O[C@@H](C2=O)C(C)C)C(C)C1
C31		Training	noninhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	C(=O)(c1c(n(nc1C)c1ccccc1)OCC(CN(C(C)C)C(C)C)O)c1ccccc1
C32		Training	noninhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	n1(n(c(c(c1=O)C(=O)CCc1ccccc1)C)CC(CNCCCC)O)c1ccccc1
C33		Training	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1(n(c(c(c1=O)c1sccc1)C)CC(CNC(C)C)O)c1ccccc1
C34		Training	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1(n(c(c(c1=O)c1sccc1)C)CC(CNCCC)O)c1ccccc1
C35		Training	noninhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	n1(n(c(c(c1=O)C(=O)CCc1ccccc1)C)CC(CNC(C)(C)C)O)c1ccccc1
C36		Training	noninhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	C(=O)(CCc1ccccc1)c1c(n(nc1C)c1ccccc1)NCCC
C37		Training	noninhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	c1(ccccc1CCc1ccccc1)OCc1cc(ccc1)OC
C38		Training	noninhibitor	59	inhibitor	noninhibitor	noninhibitor	noninhibitor	n1ccccc1COc1c(cccc1)CCc1ccccc1
C39		Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=O)NCCN1CCOCC1)Cl
C40		Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)Nc1ccc(cc1)Nc1ccccc1

C41	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)CNCCNCc1ccccc1
C42	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)C(=O)OCCCN(CCCOC(=O)/C=C/c1cc(c(c(c1)OC)OC)OC)C
C43	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)CN(C)C
C44	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C(=O)NCc1ccccc1
C45	Training	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@@](c1cc(c(c(c1)OC)OC)OC)(CCC[N+](CCc1ccc(c(c1)OC)OC)(C)C)C(C)C
C46	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cccc1)cc(cc2)Nc1ccccc1
C47	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc(c1C1N(Cc2cc(c(c(c2)OC)OC)OC)CCCN1Cc1cc(c(c(c1)OC)OC)OC)C)N(CCCl)CCCl
C48	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cccc1)nc1c(c2Nc2ccc(cc2)S(=O)(=O)N)c(ccc1C(=O)Nc1ccc(cc1)S(=O)(=O)Nc1cc(C)on1)Cl
C49	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1CN1CCCN(Cc2ccc(c(c2)OC)OC)C1c1ccc(cc1C)N(CCCl)CCCl)OC)OC
C50	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1CN1CCCN(Cc2ccc(c(c2)OC)OC)C1c1ccc(cc1Cl)N(CCCl)CCCl)OC)OC
C51	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c2c3c1C[C@@H]1[C@@]4(CCC(=O)[C@@H]([C@]34CCN1CC1CC1)O2)O)O
C52	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cccc1)[nH]c1c2C[C@@]2([C@@]34c5c(ccc(c5O[C@@H]14)O)C[C@@H]2N(CC3)CC1CC1)O
C53	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C1=NCC(=O)Nc2ccc(cc12)Cl
C54	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc2c(c1)/C(=C/[C@@H]1C3CCN(CC3)C1)/c1cc(ccc1S2)Cl
C55	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc(c1/C(=N/OCc1ccc(cc1Cl)Cl)/Cn1ccnc1)Cl)Cl
C56	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[C@H]([C@H](C)NCCC(=O)c1cccc(c1)OC)O
C57	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc(cc1)OCCN1CCC(CC1)n1c2ccccc2[nH]c1=O
C58	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c12c(cc(c(c1)OC)OC)c(Cc1ccc(c(c1)OC)OC)ncc2
C59	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C#CCOC[C@H]1CO[C@@](c2ccc(cc2Cl)Cl)(Cn2ccnc2)O1
C60	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(cc(c1F)N1CCN(CC1)C)n(cc(c2=O)C(=O)O)CC
C61	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl)O
C62	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)N(c1ccccc1O2)C(=O)CCl
C63	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)Cc1ccccc1OCCN(C)C
C64	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc(cc1)C1(c2ccccc2)CCC(CC1)NC(C)C
C65	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)OCCN([C@H](C)COc1ccccc1)C
C66	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(cc(c2)OC)N[C@@H](C)CCCN)nccc1
C67	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](C[N+](CCC)(C)C)O
C68	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=O)C)OC[C@H](CN1CCCCC1)O
C69	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(c(c1)C(=O)CC)OC[C@@H](CN1CCOCC1)O
C70	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc(c1[C@]1(Cn2cncn2)OC[C@@H](CCC)O1)Cl)Cl
C71	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(c(c1)OC(=O)NC)OC(C)C
C72	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc2c(cc1C[C@H](C)NC[C@H](c1ccc(c(c1)O)O)O)OCO2
C73	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cc(c(c1)OC)OC)nc(nc2N)N1CCN(CC=C)CC1
C74	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c([C@H](N[C@@H](N(CCO)CCO)O2)N(CC)CC)nc(nc1N(CC)CC)N(CCO)CCO
C75	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[C@@H]1C(Nc2c(c(nc(n2)N2CCOCC2)N(CCO)CCO)O1)N1CCOCC1
C76	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(nc(cn2)N2CCOCC2)nc(nc1N1CCOCC1)N1CCOCC1
C77	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(nc(c(n2)Cl)N(C)C)nc(nc1N(C)C)N1CCNCC1
C78	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)c1cc(=O)c2c(cc(cc2o1)OC1[C@@H](C([C@@H](C(CO)O1)O)O)O)O
C79	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c3c4c(c(c1O)C)O[C@@](C4=O)(C)O/C=C/[C@@H]([C@@H](C)[C@H]([C@H](C)C[C@H](C)[C@H]([C@H](/C=C/C=C(/C(=O)Nc(cc3OCC(=O)O)c2O)/C)C)O)O)OC(=O)C)OC
C80	Training	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(cc(c1)OC)[C@@H](c1ccc(cc1)C(=O)N(CC)CC)N1[C@@H](C)CN([C@H](C)C1)CCC
C81	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc(cc1)CC(=O)OCCN1CCN(CC1)CCOC(=O)Cc1ccccc1
C82	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc(cc1)[C@@H](C(=O)OCCCN1CCN(CCCOC(=O)[C@@H](c2ccccc2)CC)CC1)CC
C83	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C#CCN([C@H](C)Cc1ccccc1)C

C84	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	C1=C[C@H](C)C(CC[C@H](C[C@H](CC(=O)O)O)O)[C@@H]2C1=CC(C)CC2OC(=O)C(C)(C)CC
C85	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c(cc(c1F)F)F)C[C@H](CC(=O)N1Cc2n(c(C(F)(F)F)nn2)CC1)N
C86	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc(cc1)C[C@@H](c1ccccc1)C(=O)OCCN(CC)CC
C87	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1CS[C@@H](c1ccc(cc1Cl)Cl)Cn1ccnc1)Cl
C88	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1NC(=O)NC1CCCCC1)OC[C@@H](CNC(C)(C)C)O
C89	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	C(#CC(C)(C)C)/C=C/CN(Cc1c2c(ccc1)cccc2)C
C90	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1c2c(cc(c1OC)OC)[C@H]1CC(=O)[C@@H](CC(C)C)CN1CC2
C91	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1CN(c1ncccn1)CCN(C)C)OC
C92	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1cc(cc2c1c1ccc(cc1C2=O)OCCN(CC)CC)OCCN(CC)CC
C93	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc(c1[C@@H](Cn1ccnc1)OCc1ccsc1Cl)Cl)Cl
C94	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(c(c1)C)OC[C@@H](CNCCOc1ccc(cc1)C(=O)N)O
C95	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(cc(c1O)O)[C@@H](Cc1cc(c(c(c1)OC)OC)OC)NCC2
C96	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(c(c1)C1=NCc2n(c3ccc(cc13)Cl)c(C)nn2)Cl
C97	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(cc(c(c1OC)OC)OC)C(=O)N1CCOCC1
C98	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C(=C1CCN(CC1)CCOCCOCC(=O)O)c1ccccc1
C99	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(c(c1)N1CCN(CCCNc2cc(=O)n(c(=O)n2C)C)CC1)OC
C100	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(cc(cc1Cl)Cl)N1C(=O)[C@](C=C)(C)OC1=O
C101	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c12c(cccc1[nH]c1c2CCN2C[C@@H](C[C@]1(c1cc3c(cc1OC)N(C=O)[C@@H]1[C@@]43CCN[C@H]4[C@](C=CC3)(CC)[C@H](C[C@]1(C(=O)OC)O)OC(=O)C)C(=O)OC)C[C@@](CC)(C2)O
C102	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	C(=C\C(=C\COC(=O)CCCCCCCCCCCCCCC)\C)/C=C(/C=C/C1=C(C)CCCC1(C)C)\C
C103	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cccc2S(=O)(=O)NCCCCCCN)c(ccc1)Cl
C104	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cnc1)/C(=C\CN(C)C)/c1ccc(cc1)Br
C105	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc(c(c1)N1CCN(CCc2c(c3ccc(cc3)F)[nH]c(=O)o2)CC1)OC
C106	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1[N+](=O)[O-])OC(=O)N(C)C
C107	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C1(c2ccccc2)C(=O)NC(=O)N1
C108	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12cnc(nc1n(cc(c2=O)C(=O)O)CC)N1CCNCC1
C109	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cccc1)[nH]cc2C[C@@H](C(=O)O)N
C110	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(/C=C/C(=O)O)nc(c1)/C(=C/CN1CCCC1)/c1ccc(cc1)C
C111	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@H]([C@@H]([C@@H](CO)O)O)([C@@H](CO)O)O
C112	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)CCc1ccc(cc1)[C@H](Cn1ccnc1)O
C113	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc2c(c(c1)O)C(=O)C1=C([C@@]3(C(=O)C(=C([C@H]([C@@H]3C[C@H]1[C@]2(C)O)N(C)C)O)C(=O)NCN1CCCC1)O)O
C114	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc2c1[C@@H]1CC[C@@]3(C)[C@@H](CC[C@@H]3O)[C@H]1CC2)O
C115	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C[C@H]1[C@H]2[C@@H](C(=C)[C@H]([C@H]3/C=C/C[C@H](C)C[C@@](/C=C/[C@H]([C@]23C(=O)N1O)(C)O)O)C
C116	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1=C(C(=O)[C@@]2(CC(=C[C@@H]3[C@@H]4C(C)(C)[C@@]4([C@@H]([C@@H](C)[C@]3([C@H]12)O)O)O)CO)O)C
C117	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1=C(C(=O)[C@@]2(CC(=C[C@@H]3[C@@H]4C(C)(C)[C@@]4([C@@H]([C@@H](C)[C@]3([C@H]12)O)O)OC(=O)C)CO)O)C
C118	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c12c3cccc1C1=C[C@@H](C(=O)N[C@@H](CC)CO)CN([C@@H]1Cc2cn3C)C
C119	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(nc(n2)N(CCO)CCO)N2CC=CCC2)nc(nc1N1CC=CCC1)N(CCO)CCO
C120	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(nc(n2)N(CCO)CCO)N2CCCCC2)nc(nc1)N(CCO)CCO
C121	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(nc(n2)N(CCO)CCO)N(CCO)CCO)nc(nc1N(CCO)CCO)N(CCO)CCO
C122	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(nc(n2)NCCO)N2CCCCC2)nc(nc1N1CCCCC1)NCCO
C123	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	C(=C(C)C)CC/C(=C/CC/C(=C/CC/C(=C/CC/C(=C/CC/C(=C/CC/C(=C/CC/C(=C/CO)/C)/C)/C)/C)/C)/C)/C
C124	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc(cc1)[C@@](CCN1CCCCC1)([C@@H]1C[C@H]2C=C[C@@H]1C2)O
C125	Training	noninhibitor	61	noninhibitor	inhibitor	noninhibitor	noninhibitor	c1ccc(cc1)c1cccc(c1O)C(=O)OCCN(CC)CC
C126	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c2c(c1NCCNCCO)C(=O)c1c(c(ccc1O)O)C2=O)NCCNCCO

C127	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1[C@H](CNC)O)O)O
C128	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1C[C@@H]1c2cc(c(cc2CCN1C)O)O)O)O
C129	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc(c1)NC(=O)C(=O)N/N=C/c1ccc(c(c1)O)O)[N+](=O)[O-]
C130	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc2c1[C@@H]1C(=CC2)[C@H]2CCC(=O)[C@]2(C)CC1)O
C131	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(cc(c1O)O)[C@@H](C)NCC2
C132	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C[C@H](C(=O)N[C@@H](C(=O)N[C@H](C(=O)N[C@@H](C(=O)NCC(=O)N)C(C)C)C(C)C)CCC(=O)O)NC(=O)[C@@H](C)NC(=O)[C@H](Cc1ccc(cc1)O)N
C133	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1[C@H](CNC(C)(C)C)O)CO)O
C134	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=C(\C)/OP(=O)(OC)OC)\C(=O)OC
C135	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc(c1)[N+](=O)[O-])[C@@H]1C(=C(C)NC(=C1P1(=O)OCC(C)(C)CO1)C)C(=O)OCCCCCCCCCC
C136	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(ccc(c1)CCS(=O)(=O)c1ccccc1)[nH]cc2C[C@H]1CCCN1C
C137	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cc(cc1)OC)nc([nH]2)S(=O)(=O)Cc1c(c(c(cn1)C)OC)C
C138	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c(ccc1S(=O)(=O)N(C)C)N)C(=O)N1CCN(CC1)C
C139	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(ccnc2)c(ccc1)S(=O)(=O)N1[C@@H](C)CNCC1
C140	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(ccc(c1)CS(=O)(=O)NC)[nH]cc2CCN(C)C
C141	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cccc1)cc(cc2)S(=O)(=O)NCCCCN
C142	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccnc(c1)NS(=O)(=O)c1ccc(cc1)/N=N/c1cc(c(cc1)O)C(=O)O
C143	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc(cc1)c1ccc(cc1)[C@@H](C(=O)SCCN(CC)CC)CC
C144	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1[C@@H]([C@H](C)NCCCCCCCC)O)SC(C)C
C145	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(c(c1)OC[C@@H](CNC(C)C)O)SC
C146	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(cc(c1)S(=O)(=O)O)N)c(c(c(c2)S(=O)(=O)O)/N=N/c1ccc(cc1C)c1ccc(c(c1)C)/N=N/c1c(c2c(cc(cc2N)S(=O)(=O)O)cc1S(=O)(=O)O)O)O
C147	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)C(=O)N(C2=O)CSP(=S)(OC)OC
C148	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(nnnn1C)SCC1=C(C(=O)O)N2C(=O)[C@]([C@@H]2SC1)(NC(=O)C1S/C(=C(\C(=O)N)/C(=O)O)/S1)OC
C149	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc2c(c1)N(c1ccccc1S2)C[C@H]1CCN(C1)C
C150	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc2c(c1)N(c1ccccc1S2)CCCN(C)C
C151	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)S(=O)(=O)C)CCCN1CCC(C(=O)N)CC1
C152	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	C(#N)c1ccc2c(c1)N(c1ccccc1S2)CCCN1CCC(CC1)O
C153	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc2c(c1)N(c1c(cccn1)S2)CCCN1CCN(CC1)CCO
C154	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc2c(c1)C(c1ccccc1S2)C[C@@H]1CCCN(C1)C
C155	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)Nc1ccccc1[P+]12c2ccccc2Nc2ccccc12
C156	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c(C(=O)N[C@@H](C(=O)N[C@@H](C)[C@H]([C@@H](C(=O)N[C@@H](C(=O)NCCc2nc(cs2)c2nc(cs2)C(=O)NCCC[S+](C)C)[C@H](C)O)C)O)[C@H](c2c[nH]cn2)O[C@@H]2[C@H]([C@H]([C@@H]([C@@H](CO)O2)O)O)O[C@H]2[C@H]([C@H]([C@@H]([C@@H](CO)O2)O)OC(=O)N)O)nc([C@@H](CC(=O)N)NC[C@H](C(=O)N)N)nc1N)C
C157	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cccc1)[nH]cc2CCN
C158	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(#N)/C(=C/c1ccc(c(c1)O)O)/C(=S)N
C159	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)N1CCN(CCc2n[nH]nn2)CC1
C160	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(nc(c(c3ccccc3)n2)N)nc(nc1N)N
C161	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c12c(c(nc(n2)N2CCCCC2)N2CCCCC2)nc(nc1N1CCCCC1)N1CCCCC1
C162	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c12c(cccc1)c(c1ccccc1)nc(c2)N1CCNCC1
C163	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cccc1)nc1c(c2N)CCCC1
C164	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[C@H](c1ccccn1)CCN(C)C
C165	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)CN(c1ccccn1)CCN(C)C
C166	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)Cn1ccnc1
C167	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c12c(cccc1)oc(c2)C(=O)N1CCN(Cc2ccccc2)CC1
C168	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[C@H](c1nc(CCN(CC)CC)on1)CC
C169	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)c1nc(NCCN(CCCC)CCCC)on1

C170	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cc(cc1)O)sc(c2C(=O)c1ccc(cc1)OCCN1CCCCC1)c1ccc(cc1)O
C171	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(C2C(=C(C)NC(=C2C(=O)OCC(=O)O)C)C(=O)OCC(=O)O)sc1
C172	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)N(Cc1cccs1)CCN(C)C
C173	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[C@@H](c1ccc(cc1)Cl)N1CCNCC1
C174	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C(c1ccccc1)CN
C175	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(nc(n2)N2CCOCC2)N2CCOCC2)nc(nc1N1CCOCC1)N1CCOCC1
C176	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(ncn2)N2CCOCC2)nc(nc1N1CCOCC1)N1CCOCC1
C177	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1(=O)NCCO1
C178	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(CN1CCOCC1)N(C)C
C179	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c(nc(c(n1)Cl)N1CCCCCC1)N)C(=O)NC(=N)N
C180	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c(nc(c(n1)Cl)N(C(C)(C)C)C)N)C(=O)NC(=N)N
C181	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(cc(c1O)O)Sc1ccc(cc1N2CCCN(C)C)Cl
C182	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c(ccc1Cl)Cl)N1CCN(CCCNC(=O)C)CC1
C183	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=O)NCCN(CC)CC)NC(=O)C
C184	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	
C185	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1C2CC3CC1CC(C3)(C2)N
C186	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1[C@@H](C1CCCC1)OCCN(C)C)Br
C187	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c(ccc1OC(=O)NC)N(C)C)C
C188	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)CN(c1ccccc1)CC1=NCCN1
C189	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1CC(=O)N)OC[C@@H](CNC(C)C)O
C190	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1(=C([C@@H]([C@H](CO)O)OC1=O)O)O
C191	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(nc(nc(n1)Cl)NC(C)C)NCC
C192	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[C@H](C(=O)OC1C[C@H]2CC[C@H](C1)N2C)CO
C193	Training	noninhibitor	61	noninhibitor	inhibitor	noninhibitor	noninhibitor	c1ccnc(c1)N1CCN(CCCC(=O)c2ccc(cc2)F)CC1
C194	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=O)NCC[N+](CC)(CC)C)N=[N+]=[N-]
C195	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)CN(c1ccccc1)C1CCN(CC1)C
C196	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)CC1(CCCCCC1)OCCCN(C)C
C197	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C[C@@H](c1ccc(cc1)Cl)[C@H](C)NC(=O)/C=C/C(=O)O)Cl
C198	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(cc(c1O)OC)c1c3c(cc(c1OC)O)CCN([C@H]3C2)C
C199	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c12c3c(cccc3OC[C@@H](CNCCOc3ccc(cc3OC)O)O)[nH]c1cccc2
C200	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[C@H](c1ccc(cc1)Cl)N1CCN(CC1)CCOCC(=O)O
C201	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(c(cc2)OC)OC)c[n+](c2c1ccc1c2cc2c(c1)OCO2)C
C202	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1/C=C/C(=O)OC1C[C@](C(=O)O)(C[C@H]([C@H]1O)O)O)O)O
C203	Training	noninhibitor	61	noninhibitor	inhibitor	noninhibitor	noninhibitor	c12c(cc(cc1)Cl)nccc2N[C@@H](C)CCCN(CC)CC
C204	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccnc(c1)[C@@H](c1ccc(cc1)Cl)CCN(C)C
C205	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(cc(c(c1OC)OC)OC)/C=C/C(=O)N1CCN(CC(=O)OCC)CC1
C206	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(cc(c(c1OC)OC)OC)/C=C/C(=O)N1CCN(CC(=O)NC(C)C)CC1
C207	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(c(cc2Cl)CNCCCN(CC)CC)O)nccc1
C208	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C[C@](C)([C@H](C)CN(C)C)O)Cl
C209	Training	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)/C(=C(/c1ccccc1)\Cl)/c1ccc(cc1)OCCN(CC)CC
C210	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(c(c1)Cl)N=C1NCCN1)Cl
C211	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1=C2CC[C@@H]3[C@@H](C(=O)C[C@@]4(C)[C@H]3CC[C@@]4(C(=O)CO)O)[C@@]2(C)CCC1=O
C212	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	

C213	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc(cc1)C[C@H]1[C@@H]2[C@@H](C(=C)[C@H]([C@H]3/C=C/C[C@H](C)CCCC(=O)/C=C/C(=O)O[C@@]23C(=O)N1)O)C
C214	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C[C@H]1[C@H]2[C@@H](C(=C)[C@H]([C@H]3/C=C/CC(C(=O)[C@@]/(/C=C/[C@H]([C@]23C(=O)N1)OC(=O)C)(C)O)C)O)C
C215	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(c1ccc(cc1)Cl)C(Cl)(Cl)Cl)Cl
C216	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1c2c(cc(c1OC)OC)[C@H]1CC(=C(CC)CN1CC2)C[C@H]1c2cc(c(cc2CCN1)OC)OC
C217	Training	noninhibitor	61	noninhibitor	inhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)Cl)CCCNC
C218	Training	noninhibitor	61	noninhibitor	inhibitor	noninhibitor	noninhibitor	C(#N)c1ccc2c(c1)CO[C@]2(c1ccc(cc1)F)CCCNC
C219	Training	noninhibitor	61	noninhibitor	inhibitor	noninhibitor	noninhibitor	c1cc(c(cc1[C@H]1c2ccc(cc2CN(C1)C)OC)Cl)Cl
C220	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1(=C([C@@]2([C@H]3[C@@H]4C[C@H]([C@@H]3[C@]1(C2(Cl)Cl)Cl)[C@@H]1[C@H]4O1)Cl)Cl)Cl
C221	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)N(CC)CC
C222	Training	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c3cccc1[C@@H]1C[C@@H](C(=O)N[C@@]4(C(=O)N5[C@H](C(=O)N6[C@@H](CCC6)[C@]5(O)O4)Cc4ccccc4)C)CN([C@H]1Cc2c[nH]3)C
C223	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1c1cc(=O)c2c(cc(cc2o1)O[C@@H]1[C@H]([C@H]([C@@H]([C@@H](CO[C@H]2[C@H]([C@H]([C@@H]([C@H](C)O2)O)O)O)o1)O)O)O)O)O)O)OC
C224	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C(c1ccccc1)C(=O)N(C)C
C225	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[C@](c1ccccn1)(C)OCCN(C)C
C226	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1CO[C@@H](c1ccc(cc1Cl)Cl)Cn1ccnc1)Cl
C227	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc(c1[C@H](Cn1ccnc1)OCC=C)Cl)Cl
C228	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(nc(c1F)N1CCNCC1)n(cc(c2=O)C(=O)O)CC
C229	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)C1CCN(/C=N\CCCCCCCC)CC1
C230	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)(C(=O)N)CC[N+]1(CCCCC1)C
C231	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	C(#N)[C@H](c1cccc(c1)Oc1ccccc1)OC(=O)[C@H](c1ccc(cc1)Cl)C(C)C
C232	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C\1=C/C=C\C=C/C/)[C@@H](C[C@H](C[C@@H](C[C@@H](CC(CC(C[C@@H]([C@H](C(=O)O[C@H](C)[C@H](/C=C/C=C1)O)[C@H](CCCCC)O)O)O)O)O)O)O)O
C233	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1cc(c(cc1c1cc(=O)c2c(cc(cc2OCC(=O)N2CCN(Cc3ccc(c(c3OC)OC)OC)CC2)O)o1)O)OC
C234	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1c1cc(=O)c2c(cc(cc2o1)O[C@@H]1[C@H]([C@H]([C@@H]([C@@H](CO[C@H]2[C@H]([C@H]([C@@H]([C@H](C)O2)O)O)O)1)O)O)O)O)OCC(=O)N1CCN(Cc2ccc(c(c2OC)OC)OC)CC1)OC
C235	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(c(c(c1F)N1CCN(CC1)C)F)n(cc(c2=O)C(=O)O)CCF
C236	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1cc(c2c(c1)O[C@@H](CO)CO2)N1CCN(CC1)CCNC(=O)c1ccc(cc1)F
C237	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ncc1C(F)(F)F)Oc1ccc(cc1)O[C@@H](C(=O)OCCCC)C
C238	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(ccc1F)n1c(c(C(=O)OCC)nc1)CN(C2=O)C
C239	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[C@H](CCN(C)C)C1CCCCC1
C240	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cnc(nc1)N1CCN(CCCCN2C(=O)CC(C)(C)CC2=O)CC1
C241	Training	noninhibitor	61	noninhibitor	inhibitor	noninhibitor	noninhibitor	C(=C(C1CCCCC1)C1CCCCC1)[C@@H]1CCCCN1
C242	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1CCN)OC)OC
C243	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cc(c(c1)OC)OC)ncnc2N1CCN(C(=O)OCC(C)(C)O)CC1
C244	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1cc(c(c2c1[C@@H]([C@@H]1c3cc4c(cc3CCN1C)OCO4)OC2=O)OC)OC
C245	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(c(c3c1OCO3)OC)CN(CC2)C
C246	Training	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)Cl)CCCN1CCN(CC1)CCN1C(=O)N(CC1)C
C247	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(ccc(c1)OC)n(c(c2CC(=O)O)C)C(=O)c1ccc(cc1)Cl
C248	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)OC[C@@H](C)N[C@@H](C)[C@@H](c1ccc(cc1)O)O
C249	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(c(c1)[C@@]1(C(=O)CCCC1)NC)Cl
C250	Training	noninhibitor	61	noninhibitor	inhibitor	noninhibitor	noninhibitor	c1ccc(cc1)c1cc(cc(c1OCCN(CC)CC)Cl)Cl
C251	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1(C(C(C(C(C1Cl)Cl)Cl)Cl)Cl)Cl
C252	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(c(c1)c1ccc(cc1)Cn1c(c(nc1CCCC)Cl)CO)c1n[nH]nn1
C253	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	C1=C[C@H](C)C(CC[C@H](C[C@H](CC(=O)O)O)O)[C@@H]2C1=CC(C)CC2OC(=O)[C@@H](C)CC
C254	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C1(c2ccccc2)C(=O)N(CC(=O)O)[C@H](C)N1
C255	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cc(cc2Cl)nc(cc1)/C=C/c1cccc(c1)[C@H](SCCC(=O)N(CC)CC)SCCC(=O)O

C256	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=O)O)CCNC(=O)c1cc(ccc1OC)Cl
C257	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(c1ccc(cc1)OC)C(Cl)(Cl)Cl)OC
C258	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(C)OCCOC
C259	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(c(c1)C)OC[C@@H](C)N)C
C260	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c(nc(nc1Cl)NC)N1CCN(CC1)C)SC
C261	Training	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)Cc1ccccc1N1[C@H]2CN(CC1)C
C262	Training	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C12(C3(C4(C5(C(C1(C4(Cl)Cl)Cl)(C2(C(C35Cl)(Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl)Cl
C263	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1NCCN(C1)Cc1ccccc1
C264	Training	noninhibitor	60	inhibitor	noninhibitor	noninhibitor	noninhibitor	COc1c(OC)cc(/C=C/C2=C(NC(C)C)CN3CCN2CC3)cc1OC
C265	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[N]=C(N)N/N=C/c1c(Cl)cccc1Cl
C266	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CN1C2=C1C(N2)(c1ccccc1)c1ccccc1
C267	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1ccc(cc1)OC1=NCCc2ccccc12
C268	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[N]=C(N)NC(=O)Cc1c(Cl)cccc1Cl
C269	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[N]=C(N)N1CCc2ccccc2C1
C270	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)NC[C@H](COc1c(cc(cc1)NC(=O)C)C(=O)C)O
C271	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[C@@]1(C)CCc2c(C)c(O)c(C)c(C)c2O1
C272	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1c([C@H](CC(=O)C)c2ccc(cc2)[N+](=O)[O-])c(=O)c2ccccc2o1
C273	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ONC(=O)C
C274	Training	noninhibitor	60	noninhibitor	inhibitor	noninhibitor	noninhibitor	N(CC(=O)OCc1ccccc1)C(=O)[C@@H](CSC(=O)C)Cc1ccccc1
C275	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1cnc2c1c(=O)n(C)c(=O)n2C
C276	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN(C)c1c(C)n(C)n(c1=O)c1ccccc1
C277	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN1[C@H]2CC(C[C@@H]1[C@H]1O[C@@H]21)OC(=O)C(=C)c1ccccc1
C278	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)(C)NC[C@H](c1cc(cc(c1)OC(=O)N(C)C)OC(=O)N(C)C)O
C279	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NS(=O)(=O)c1cc2c(cc1C(F)(F)F)N[C@@H](Cc1ccccc1)NS2(=O)=O
C280	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1O[C@@H]2[C@H](OC(=O)c3cc(O)c(OC)c(O)c23)C(O)[C@@H]1O
C281	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C)CCc1ccccn1
C282	Training	noninhibitor	60	inhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1CC[C@@]2(C)[C@H](CC[C@@]3(C)[C@@H]2CC[C@@H]2[C@H]4[C@@H](CC[C@]4(CC[C@@]32C)C(=O)O)C(=C)C)C1(C)C
C283	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@]1(CC)C(=O)OCc2c1cc1n(Cc3c1nc1ccccc1c3)c2=O
C284	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1c(OC)c2c(C[C@@H]3N(CCc4cc5c(OCO5)cc34)C2)cc1
C285	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[C@@H](C(=O)N[C@H]1[C@@H]2SC(C)(C)[C@H](N2C1=O)C(=O)O)c1ccccc1
C286	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(CCCl)C(=O)N(CCCl)N=O
C287	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C1=C(Cl)CS[C@@H]2[C@H](NC(=O)[C@H](N)c3ccccc3)C(=O)N12
C288	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C1=C(COC(=O)C)CS[C@@H]2[C@@H](NC(=O)CSc3ccncc3)C(=O)N12
C289	Training	noninhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	N(CCCCN1CCN(CC1)c1ccccc1OC)C(=O)c1cc2ccccc2cc1
C290	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)c1nn(CC)c2cc3c(OCO3)cc2c1=O
C291	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C(C)(C)Oc1ccc(Cl)cc1
C292	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1c(OC)cc(cc1)C(=O)OC1C[C@@H]2CC[C@H](C1)N2C
C293	Training	noninhibitor	60	inhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1CC[C@@]2(COC)CN(CC)[C@H]3[C@]4(O)[C@@H](OC)[C@@H]2[C@]13[C@H]1C[C@@H]2[C@@H](OC)[C@@H]1[C@@]4(O)C[C@H]2OC
C294	Training	noninhibitor	60	inhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@]12C[C@H]3[C@@H](OC)[C@]1(O)[C@@]1(C[C@@H]3OC)OCO[C@]31[C@@H]([C@H]1[C@]42[C@H]2N(CC)C[C@]1(C)CC[C@@H]4OC)C(=O)C
C295	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1C(=O)OC(C)(C)C1=O
C296	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OS(=O)(=O)CN(C)c1c(C)n(C)n(c1=O)c1ccccc1
C297	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1[C@H]2[C@@H](C)c3cccc(O)c3C(=C2C(=O)[C@@]2(O)[C@H]1[C@H](N(C)C)C(=O)/C(=C(/O)\N)/C2=O)O
C298	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1cc(O)c2c(=O)cc(oc2c1)c1ccc(OC)cc1

C299	Training	noninhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	N([C@@H]1CCc2cc(OC)c(OC)c(OC)c2[C@H]2CCC(OC)C(=O)C[C@H]12)C(=O)C
C300	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=S)c1cc(CC)ncc1
C301	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1c2c(cc(OCC)cc2)C(=CC1(C)C)C
C302	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(CC)[C@@H](C)Cc1cc(ccc1)C(F)(F)F
C303	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1C[C@@]2(C)[C@@H](C[C@@H]3OC(C)(C)O[C@]23C(=O)COC(=O)C)[C@@H]2C[C@@H](F)C3=CC(=O)C=C[C@@]3(C)[C@@]12F
C304	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCC(=O)[C@]12OC(C)(C)O[C@@H]1C[C@@H]1[C@H]3C[C@@H](F)C4=CC(=O)C=C[C@@]4(C)[C@@H]3C(O)C[C@]21C
C305	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H](COc1cccc2c1n(C)c(=O)cc2OC)C(C)(C)O
C306	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CC1(CN)CCCCC1
C307	Training	noninhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	O[C@@H](C[C@@H](Cc1ccccc1)C(=O)N[C@H]1[C@H](O)Cc2ccccc12)CN1CCN(Cc2cccnc2)C[C@@H]1C(=O)NC(C)(C)C
C308	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(N1C[C@H]2CCC[C@H]2C1)C(=O)NS(=O)(=O)c1ccc(C)cc1
C309	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1cc(Cl)c(Cl)cc1OCC#CI
C310	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1c2ccccc2c2c1c(C)[nH]cc2
C311	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1N(C)CCc2cc3c(OCO3)cc12
C312	Training	noninhibitor	60	inhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=O)C(CCN(C(C)C)C(C)C)(c1ccccc1)c1ccccc1
C313	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[O-][N+](=O)O[C@H]1CO[C@H]2[C@H](CO[C@@H]12)O[N+](=O)[O-]
C314	Training	noninhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	[nH]1c(=O)n(CCN2CCC(CC2)C(=O)c2ccc(F)cc2)c(=O)c2ccccc12
C315	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(Cc1ccco1)c1[nH]cnc2c1ncn2
C316	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C(=O)c1c(C)onc1)c1ccc(cc1)C(F)(F)F
C317	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CC[C@H](NC(=O)c1ccc(cc1)NCC1CNc2c(N1C=O)c(=O)[nH]c(N)n2)C(=O)O
C318	Training	noninhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](C[C@H]1CCC[C@H](CC(=O)c2ccccc2)N1C)c1ccccc1
C319	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN(C)CCOC(=O)COc1ccc(Cl)cc1
C320	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN(CCCl)CCCl
C321	Training	noninhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Cc1cc(CN2CCN(CC2)[C@H](c2ccccc2)c2ccc(Cl)cc2)ccc1
C322	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)c1ccccc1Nc1c(Cl)ccc(C)c1Cl
C323	Training	noninhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	O[C@]1(CC[C@H]2[C@@H]3CCc4cc(OC)ccc4[C@H]3CC[C@@]12C)C#C
C324	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[C@@H]1[C@@H]2[C@H](SC1(C)C)[C@H](NC(=O)[C@H](N=C)c1ccccc1)C2=O
C325	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN(C)CCN(Cc1cccs1)c1ccccn1
C326	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN1CC[C@]23[C@@H]4[C@H]1Cc1c2c(c(cc1)OC)O[C@H]3C(=O)CC4
C327	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[C@H](CCS(=O)(=N)C)N
C328	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]([C@H](C)N)c1c(OC)ccc(OC)c1
C329	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc(N)c(nn1)c1c(Cl)c(Cl)ccc1
C330	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[C@@H](Cn1ccc(=O)c(O)c1)N
C331	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@]1(C)[C@H](C)C(=O)O[C@@H]2CCN3CC=C(COC(=O)[C@]1(C)O)C23
C332	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1cc(O)c2c(=O)c(O)c(oc2c1)c1cc(O)c(O)c(O)c1
C333	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1C(=C)[C@@H]2C[C@@]31[C@H]1C[C@H]4[C@@]5([C@H]1N(CC)C[C@]4(C)CC[C@H]5O)[C@@H]3C[C@H]2O
C334	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[C@@H](C)c1cc2c(cc1)cc(OC)cc2
C335	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1O[C@H](Oc2cc(O)c3C(=O)C[C@H](Oc3c2)c2ccc(O)cc2)[C@@H](O[C@H]2O[C@@H](C)[C@H](O)[C@@H](O)[C@H]2O)[C@H](O)[C@@H]1O
C336	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1O[C@H](O[C@H]2C(O)[C@@H](O[C@H]3O[C@@H](CN)[C@H](O)C[C@@H]3N)[C@H](C[C@@H]2N)N)[C@@H](O)[C@@H](N)[C@H]1O
C337	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C(=O)c1cnccc1)c1c(C)n(C)n(c1=O)c1ccccc1
C338	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H](CNC(C)C)c1cc(O)cc(O)c1
C339	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H](CCl)Cn1c(C)ncc1[N+](=O)[O-]
C340	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN(C)CCO[C@H](c1ccccc1)c1ccccc1C
C341	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)c1cc2c(cccc2)c(Cc2cc3ccccc3c(C(=O)O)c2O)c1O

C342	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1CCCC[C@@H]1[C@H](C(=O)OC)c1ccccc1
C343	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC1C@@H1O1C@@H](O[C@@H]2C(O)[C@@H](C1C@H](N[C@@H]2O[C@H]2O[C@H](CO)[C@@H](O)[C@@H](O)[C@H]2N)N)[C@H](O)[C@H]1O[C@@H]1O[C@H](CN)[C@H](O)[C@H](O)[C@@H]1N
C344	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C/C/1=C/CC[C@@]2(C)O[C@H]2[C@@H]2OC(=O)C(=C)[C@@H]2CC1
C345	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN1C(C)(C)CCCC1(C)C
C346	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C(=O)C)c1ccc(OCC)cc1
C347	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@]12C[C@@H]3O[C@@]43C(=O)O[C@H]([C@H]3OC(=O)[C@H]1[C@H]3C(=C)C)[C@@]24C
C348	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCOc1ccc(OCCCN2CCOCC2)cc1
C349	Training	noninhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	O[C@@H]1CC[C@]2(C)[C@H]3CC[C@@]4(C)[C@H](CC[C@H]4C(=O)C)[C@@H]3CC=C2C1
C350	Training	noninhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	OC(CCN1CCCCC1)(c1ccccc1)c1ccccc1
C351	Training	noninhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	CCN(CC)[C@H](C)CN1c2ccccc2Sc2c1cccc2
C352	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN1CCc2cc3c(OCO3)c3c2[C@@H]1Cc1ccccc31
C353	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1CCc2cc(OC)c(OC)cc2[C@H]1C
C354	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1O[C@@]23C[C@@H](C=CC2=C1)N1CCCC[C@@H]31
C355	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C1CCC(C)CC1)C(=O)N(CCCl)N=O
C356	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@]1(C)C(=C)C/C(=C\C)/C(=O)O[C@H]2CCN3CC=C(COC1=O)C23
C357	Training	noninhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	O[C@]12CC[C@H]3[C@H](C)[C@H]4CC[C@@H](C)CN4C[C@@H]3[C@@H]1C[C@@H]1[C@@H]2CC(=O)[C@@H]2CC(=O)CC[C@@]12C
C358	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1[C@@H](O[C@H]2[C@@H](C[C@@H](N)C@@H](O[C@H]3OC(=CC[C@@H]3N)CN)[C@@H]2O)N)OC[C@@](C)(O)[C@@H]1NC
C359	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1c(OC)c2nc3c(cco3)c(OC)c2cc1
C360	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@H](O)[C@@H](NC(=O)N(C)N=O)[C@@H](O)C1O
C361	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CCC(=O)Nc1ccc(cc1)S(=O)(=O)Nc1nccs1
C362	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ccc(cc1)S(=O)(=O)NC(=O)c1ccccc1
C363	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ccc(cc1)S(=O)(=O)Nc1nnc(Cl)cc1
C364	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ccc(cc1)S(=O)(=O)Nc1cc(OC)nc(OC)n1
C365	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ccc(cc1)S(=O)(=O)Nc1nc(C)cc(C)n1
C366	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ccc(cc1)S(=O)(=O)Nc1c(C)c(C)no1
C367	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc(nc2cc(OC)c(OC)cc12)N1CCN(CC1)C(=O)[C@H]1CCCO1
C368	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1c2ccccc2c2c1[C@@H]1C[C@@H]3[C@@H](CN1CC2)C(C)OC=C3C(=O)OC
C369	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=c1n2CCCCc2nc2ccccc12
C370	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)c1ccccc1S
C371	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(C#CCN1CCCC1)N1CCCC1
C372	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCC(=O)[C@]1(O)[C@@H](O)C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@]3(F)C(O)C[C@@]12C
C373	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NS(=O)(=O)c1c(Cl)cc2N[C@H](NS(=O)(=O)c2c1)C(Cl)Cl
C374	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CO[C@@H]1C=C2CCN(C)[C@H]2[C@H]2[C@@H]1OC(=O)c1cc3c(OCO3)cc21
C375	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@@H]([C@H](O)[C@H]1O)n1cnc2c1ncnc2N
C376	Training	noninhibitor	60	inhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@]1(C[C@@]2(CC)CCCN3CCc4c([C@H]23)n1c1ccccc41)C(=O)OC
C377	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C1=NCCCS1)c1c(C)cccc1C
C378	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1CC[C@H]2CN3CCc4c([nH]c5ccccc45)[C@H]3C[C@@H]2C1C(=O)O
C379	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C)C(=O)O/N=C/C(C)(C)SC
C380	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(CC)C(=O)Oc1ccccc1[N+](=O)[O-]
C381	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ClCC1(CCl)[C@@H]2C[C@H](C(Cl)(Cl)Cl)[C@@H]2Cl)/C/1=C/Cl
C382	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CCC(=O)O[C@H]1O[C@H]2O[C@@]3(C)CC[C@H]4[C@H](C)CC[C@@H]([C@H]1C)[C@@]24OO3
C383	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1cc2c3c(oc(=O)c4cc(O)c(O)c(oc2=O)c34)c1O
C384	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1CC(CCN2CCCCC2)Oc2ccccc12

C385	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)/C=C/c1cc(OC)c(O)cc1
C386	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(NC(=O)c1nn(C)cc1I)C(=C)c1ccnn1C
C387	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc(cc1)c1coc2cc(O)cc(O)c2c1=O
C388	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H](O)Cc1cc(OC)c(OC)cc1
C389	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C(=O)C(=O)N1CCCCCC1)/N=C/c1c(F)cccc1Cl
C390	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ccc(cc1)C(=O)OCCOCC
C391	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@@H](Oc2cccc3cc4c(C(=O)OC4)c(O)c23)[C@@H](O)[C@H](O)[C@@H]1O
C392	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN(C)c1ccc(cc1)c1nc(nc(n1)C(F)(F)F)C(F)(F)F
C393	Training	noninhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	N1[C@@H](N(c2ccc(CC)cc2)C(=O)c2ccccc12)c1ccc(OCc2ccccc2)cc1
C394	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N=C(CCC(=O)N)c1n[nH]c(=S)n1c1ccc(OC)cc1
C395	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C(=O)OC)c1[nH]c2c(cc(SCC)cc2)n1
C396	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=O)OC[C@](C)(CCC)COC(=O)NC(C)C
C397	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1C(=S)NC(=O)C(CC)([C@H](C)CCC)C1=O
C398	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C)CC(C)(C)c1ccccc1
C399	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C(C)(C)O/N=C(/C(=O)N[C@@H]1[C@H](C)N(C1=O)S(=O)(=O)O)\c1csc(n1)N
C400	Training	noninhibitor	60	inhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1c2c(c(c3c1cc[nH]c3)C)c1ccccc1n2
C401	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1cc(O)c2C(=O)C[C@@H](Oc2c1)c1cc(O)c(OC)cc1
C402	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NS(=O)(=O)c1c(Cl)ccc(c1)C(=O)N[C@@H]1[C@@H](C)Nc2ccccc12
C403	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc(cc1)C(=O)N/N=C/c1ccc(o1)[N+](=O)[O-]
C404	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1O)[C@H](CC)[C@H](CC)c1ccc(O)cc1
C405	Training	noninhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	O[C@]1(CC[C@@H]2[C@@H]3CCC4=CC(=O)CC[C@H]4[C@H]3CC[C@@]12C)C#C
C406	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1C(C(=O)c2ccccc12)c1ccccc1
C407	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]([C@H](C)N)c1ccccc1
C408	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[C@H]1N2[C@@H](SC1(C)C)C(NC(=O)[C@H](NC(=O)N1CCN(CC)C(=O)C1=O)c1ccccc1)C2=O
C409	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc(/C=C/c2cc(O)cc(O)c2)cc1
C410	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)c1c(OC(=O)C)cc(cc1)C(F)(F)F
C411	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1CC[C@@]2(C)[C@H](CC[C@]3(C)[C@@H]2CC=C2[C@@H]4[C@@H](C)[C@H](C)CC[C@]4(CC[C@]32C)C(=O)O)C1(C)C
C412	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1CCN=C1Cc1c(C)cc(cc1C)C(C)(C)C
C413	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1=NC2=NC(=NC(=O)C2=N1)c1ccccc1OCCC
C414	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1c(cccc1OC)/C=N/NC(=O)C(=O)NC(C)(C)C
C415	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCCC[C@@](C#N)(C(C)C)c1cc(OC)c(OC)cc1
C416	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCC(=O)[C@]1(O)CC(O[C@H]2C[C@@H](N)[C@H](O)[C@@H](C)O2)c2c(O)c3c(C(=O)c4cccc(OC)c4C3=O)c(O)c2C1
C417	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1C(O[C@@H]2[C@H]3COC(=O)[C@@H]3[C@@H](c3cc(OC)c(O)c(OC)c3)c3cc4c(OCO4)cc23)O[C@@H]2CO[C@@H](C)O[C@H]2C1O
C418	Training	noninhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	[nH]1c2cc(ccc2nc1c1ccc2[nH]c(nc2c1)c1ccc(OCC)cc1)N1CCN(C)CC1
C419	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1c(c(=O)n(n1C[C@H](CNC(C)C)O)c1ccccc1)C(=O)c1cccs1
C420	Training	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC1([C@@H](C(c2cc(ccc2O1)C#N)NC)O)C
C421	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c1(ccccc1CCc1cccc(c1)OC)OCc1cc(c(cc1)OC)OC
C422	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c1(ccccc1CCc1cccc(c1)OC)OCc1cc(cc(c1)OC)OC
C423	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c1(ccccc1CCc1cccc(c1)OC)OCc1cc(ccc1)OC
C424	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c1(ccccc1CCc1ccccc1)OCc1ccc(cc1)OC
C425	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c12N3CCCc1cc1c(c2CCC3)[se]c2c(c1c1sc(cc1)C(=S)N1CCOCC1)ccc(=[N+](C)C)c2
C426	Training	inhibitor	59	inhibitor	noninhibitor	inhibitor	inhibitor	n1ccc(cc1)COc1c(cccc1)CCc1ccccc1
C427	Training	inhibitor	59	noninhibitor	noninhibitor	inhibitor	noninhibitor	COc1c2c(=O)cc(oc2cc(c1)OC)c1cc(c(c(c1)OC)OC)OC

C428	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	N1(Cc2c(CC1)cc(c(c2)OC)OC)CCCC1=CCC(c2c1cccc2)OC
C429	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c1(OC)ccc2c(c1)/C(=C/CCN1Cc3c(CC1)cc(c(c3)OC)OC)/CCC2
C430	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	[C@H]1(CN(CC1)Cc1ccccc1)OC(=O)C1=C(NC(=C([C@@H]1c1cc([N+](=O)[O-])ccc1)C(=O)OC)C)C
C431	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c12ccc(N(C)C)cc1sc1c(c2c2ccccc2)ccc(=[N+](C)C)c1
C432	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	[C@H]1(C[C@@H](OC)C2=C([C@]3([C@@]([C@H](C2=O)OC)(Oc2c3c(c(c3c2[C@@H](C[C@H](O3)c2ccccc2)O)OC)OC)OC)OC)O1)c1ccccc1
C433	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c12n(c3c(nc1cc(/c(=N/C(C)C)/c2)Nc1ccc(Cl)cc1)cccc3)c1ccc(cc1)Cl
C434	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	C1(C(=C(NC(=C1C(=O)OCCN(c1ccccc1)Cc1ccccc1)C)C)P1(=O)OCC(CO1)(C)C)c1cc(ccc1)[N+](=O)[O-]
C435	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c12c(c(ccc1)OC)[nH]c1c(c2=O)cccc1C(=O)Nc1ccc(cc1)CCN1CCc2c(C1)cc(c(c2)OC)OC
C436	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	n1(c(=O)n(nc1)C(CC)C)c1ccc(N2CCN(c3ccc(OC[C@@H]4O[C@](c5c(cc(cc5)Cl)Cl)(Cn5ncnc5)OC4)cc3)CC2)cc1
C437	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c12ccc(N(C)C)cc1[se]c1c(c2c2ccccc2)ccc(=[N+](C)C)c1
C438	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	C\1=C(\[C@@H]([C@H](/C=C/C=C\2/[C@@]3([C@H](C(=O)O[C@@H]4C[C@H](C1)O[C@]1(C4)CC[C@@H]([C@@H](O1)[C@@H](CC)C)C)C=C([C@@H]([C@H]3OC2)O)C)O)C)O[C@@H]1O[C@@H]([C@@H]([C@H](C1)OC)O[C@H]1C[C@@H]([C@@H]([C@H](O1)C)O)OC)C)/C
C439	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	C1([C@H]2c3c(cccc3)[C@@H](c3c([C@@H]12)cccc3)N1CCN(CC1)C[C@H](COc1c2c(nccc2)ccc1)O)(F)F
C440	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	C1(C(=C(NC(=C1C(=O)OC)C)C)C(=O)OCCN1CCN(CC1)C(c1ccccc1)c1ccccc1)c1cc(ccc1)[N+](=O)[O-]
C441	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	N(c1c(cccc1)CCc1cccc(c1)OC)Cc1c(c(ccc1)OC)OC
C442	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	N(c1c(cccc1)CCc1cccc(c1)OC)Cc1cc(cc(c1)OC)OC
C443	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c1(ccccc1CCc1ccccc1)OCc1c(c(ccc1)OC)OC
C444	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	C1(=O)C2=CC[C@H](c3ccccc3)O[C@@]32[C@](C(=C1OC)OC)(c1c(c2c(c(c1OC)OC)O[C@H](C[C@@H]2O)c1ccccc1)O3)OC
C445	Training	inhibitor	59	noninhibitor	noninhibitor	inhibitor	noninhibitor	C1(=C(NC(=C(C1c1c([N+](=O)[O-])cccc1)C(=O)OC)C)C)C(=O)OCC(C)C
C446	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	O(c1cc(C(C(C)C)(CCCNCCc2cc(OC)c(OC)cc2)C#N)ccc1OC)C
C447	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)[C@@H]1C(=O)O[C@@H](C)/C(=N/[C@@H](C(C)C)C(=O)OC(C(C)C)/C(=N/[C@H](C(C)C)C(=O)OC(C)/C(=N/[C@@H](C(C)C)C(=O)OC(C(C)C)/C(=N/[C@H](C(C)C)C(=O)OC(C)/C(=N/[C@@H](C(C)C)C(=O)O[C@H](C(C)C)/C(=N/1)/O)/O)/O)/O)/O)/O
C448	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c1(c(cc2c(c1)CCN(C2)CCc1ccc(NC(=O)c2c(cccc2)NC(=O)c2ccccc2)cc1)OC)OC
C449	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	n1c2c(cccc2)cc(c1)C(=O)Nc1ccccc1C(=O)NC1C(CCCC1)N1CCN(CC1)c1ccccc1
C450	Training	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c1(ccccc1CCc1cccc(c1)OC)OCc1c(cccc1)OC
C451	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(=C\C[C@@H](C)[C@@H]([C@@H]1C(=O)N[C@@H](C(=O)N(CC(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@@H](C(=O)N[C@@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N1C)CC(C)C)C)CC(C)C)C)CC(C)C)C)C)CC(C)C)C(C)C)CC(C)C)C)C)CC)O)/C
C452	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C1=C2CC[C@H]3[C@H]4CC=C(C(=O)C)[C@]4(C)CC[C@H]3[C@@]2(C)CCC1=O
C453	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c3cccc1C1=C[C@@H](C(=O)N[C@@]4(C(=O)N5[C@H](C(=O)N6[C@@H](CCC6)[C@]5(O)O4)CC(C)C)C(C)C)CN([C@@H]1Cc2c([nH]3)Br)C
C454	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc2OC[C@@H](CN2CCN(C3c4ccccc4CCc4ccccc34)CC2)O)nccc1
C455	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc2O[C@H](CN2CCN(C(=O)C(Cc3ccccc3)Cc3ccccc3)CC2)O)nccc1
C456	Training	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1ccnc(c1)[C@@H](c1ccc(cc1)Cl)OCCN(C)C
C457	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)nc(c(=O)n2CCN(CC)CC)Cc1ccc(cc1)OC
C458	Training	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c12c(cccc1)[nH]c1c2CCN2[C@@H]3C(=C[C@@H](C[C@]13C(=O)OC)C2)CC
C459	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)Cl)C(=O)CCN(CC)CC
C460	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@H](c1ccccc1Cl)OCCN1CCN(Cc2ccccc2C)CC1
C461	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)Cl)CCCN(CC)CC
C462	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)/C(=C\CCN(C)C)/c1cc(ccc1S2)Cl
C463	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)cnc(c2)N1CCN(CCCC(=O)c2ccc(cc2)F)CC1
C464	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@@](c1ccc(cc1)Cl)(C)OCC[C@H]1CCCN1C
C465	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)/C=C/CN1CCN([C@@H](c2ccccc2)c2ccc(cc2)Cl)CC1
C466	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)CCc1ccc(cc1N2CCCN(C)C)Cl
C467	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@H](c1ccc(cc1)Cl)OCCN1CCCCC1
C468	Training	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)Cl)CCCCN
C469	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(c1ccc(cc1)F)CCCN1CCC(CC1)n1c2ccc(cc2[nH]c1=O)Cl)F
C470	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N=C(c1cc(ccc1S2)Cl)N1CCN(CC1)C

C471	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C=C[C@@]1(C)CC(=O)[C@]2([C@]3(C)[C@H](C(C)(C)CC[C@@H]3O)[C@@H]([C@@H]([C@]2(C)O1)OC(=O)C)O)O
C472	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@@H]1[C@@H]([C@@H](C)[C@@H]2C/C=C/C(=O)N[C@@H](C(=O)NC[C@H](C(=O)O[C@H](C(=O)O2)CC(C)C)C)Cc2ccc(c(c2)Cl)OC)O1
C473	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C[C@H]1C(=O)O[C@@H](C(=O)N2[C@H](C(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)NCC(=O)N([C@H](C(=O)N1)C(C)C)C)[C@H](C)CC)C)[C@@H](C)CC)C)CC(=O)OC(C)(C)C)C(C)C)C(C)C)C)CCCC2)C)O
C474	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C[C@H]1C(=O)O[C@H](C(=O)N2[C@H](C(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)NCC(=O)N([C@H](C(=O)N1)C(C)C)C)[C@H](C)CC)C)[C@@H](C)CC)C)CC(=O)OC(C)(C)C)C(C)C)C(C)C)C)CCCC2)C)OC
C475	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C[C@H]1C(=O)O[C@H](C(=O)N2[C@H](C(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)NCC(=O)N([C@H](C(=O)N1)C(C)C)C)[C@H](C)CC)C)[C@@H](C)CC)C)CC(=O)NC(C)(C)C)C(C)C)C(C)C)C)CCCC2)C)OC
C476	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C[C@H]1C(=O)O[C@H](C(=O)N2[C@H](C(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)NCC(=O)N([C@H](C(=O)N1)C(C)C)C)[C@H](C)CC)C)[C@@H](C)CC)C)CC(=O)N[C@@H](C(C)C)COC(C)(C)C)C(C)C)C(C)C)C)CCCC2)C)OC
C477	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C[C@H]1C(=O)O[C@@H](C(=O)N2[C@H](C(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)NCC(=O)N([C@H](C(=O)N1)C(C)C)C)[C@H](C)CC)C)[C@@H](C)CC)C)CC(=O)OCCC(C)C)C(C)C)C(C)C)C)CCCC2)C)OC
C478	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C1=C2CC[C@@H]3[C@@H]4CCC(=O)[C@@]4(C)CC[C@@H]3[C@@]2(C)CCC1=O
C479	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C[C@H]1C(=O)O[C@@H](C(=O)N2[C@H](C(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)NCC(=O)N([C@H](C(=O)N1)C(C)C)C)[C@H](C)CC)C)[C@@H](C)CC)C)CC(=O)NCC=C)C)C(C)C)C(C)C)C)CCCC2)C)OC
C480	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C[C@H]1C(=O)O[C@@H](C(=O)N2[C@H](C(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)NCC(=O)N([C@H](C(=O)N1)C(C)C)C)[C@H](C)CC)C)[C@@H](C)CC)C)CC(=O)NC13CC4CC(CC(C4)C3)C1)C)C(C)C)C(C)C)C)CCCC2)C)OC
C481	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C[C@H]1C(=O)O[C@@H](C(=O)N2[C@H](C(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)NCC(=O)N([C@H](C(=O)N1)C(C)C)C)[C@H](C)CC)C)[C@@H](C)CC)C)CC(=O)N1CCCCC1)C)C(C)C)C(C)C)C)CCCC2)C)OC
C482	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)COC[C@H](C(C)C)NC(=O)C[C@@H]1C(=O)N([C@@H](C(=O)N([C@@H](C(=O)NCC(=O)N([C@@H](C(=O)N[C@@H](C(=O)O[C@@H](C(=O)N2[C@@H](C(=O)N([C@@H](C(=O)N[C@@H](C(=O)N1C)C(C)C)C(C)C)C)CCCC2)C)Cc1ccc(cc1)OC)C(C)C)C)[C@@H](C)CC)C)[C@@H](C)CC)C
C483	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C[C@H]1C(=O)O[C@@H](C(=O)N2[C@H](C(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)NCC(=O)N([C@H](C(=O)N1)C(C)C)C)[C@H](C)CC)C)[C@@H](C)CC)C)CC(=O)N[C@@H](C(C)C)CO)C)C(C)C)C(C)C)C)CCCC2)C)OC
C484	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C[C@H]1C(=O)O[C@@H](C(=O)N2[C@H](C(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)NCC(=O)N([C@H](C(=O)N1)C(C)C)C)[C@H](C)CC)C)[C@@H](C)CC)C)CCCC(=O)OC(C)(C)C)C(C)C)C(C)C)C)CCCC2)C)OC
C485	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(=C\C[C@@H](C)[C@H]([C@H]1C(=O)N[C@H](C(=O)N(CC(=O)N([C@@H](C(=O)N[C@@H](C(=O)N([C@@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N1C)C(C)C)C)CC(C)C)C)CC(C)C)C)C)C)CC(C)C)C)C(C)C)CC(C)C)C)C)[C@H](C)O)O)/C
C486	Training	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@@H](c1cccc(c1)Oc1ccccc1)OC(=O)[C@H]1[C@H](C=C(Cl)Cl)C1(C)C
C487	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)/C(=C(\c1ccc(cc1)OCCN(C)C)/c1ccc(cc1)O)/CCCl
C488	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@](c1ccc(c(c1)OC)OC)(CC)CCCN(CCc1ccc(c(c1)OC)OC)C
C489	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)C(c1ccc(c(c1)C)C)(CCCN(CCc1ccc(c(c1)OC)OC)C)C(C)C
C490	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@@](c1ccc(c(c1)Cl)Cl)(CCCN(CCc1ccc(c(c1)OC)C)C)C(C)C
C491	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@](c1cc(cc(c1)OCC)OCC)(CCCN(CCc1cc(cc(c1)OCC)OCC)C)C(C)C
C492	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@@](c1cc(c(c(c1)OC)OC)OC)(CCCCCCCCCCCC)CCCN(CCc1ccc(cc1)OC)C
C493	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C1=C2CC[C@@H]3[C@@H]4CC[C@H](C(=O)CO)[C@@]4(C)CC[C@H]3[C@]2(C)CCC1=O
C494	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)/C(=C(\c1ccc(cc1)I)/c1ccc(cc1)OCCN(C)C)/CC
C495	Training	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1ccc(cc1)/C=C/c1cc(cc(=O)o1)OC
C496	Training	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1ccc2c(c1)C(c1ccc(c(c1)Cl)Cl)CC[C@@H]2N
C497	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C1(c2ccccc2)CCN(CC1)CCCOC(=O)C1=C(C)NC(=C(C(=O)OC)[C@H]1Cc1cccc(c1)[N+](=O)[O-])C
C498	Training	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1cc(c(cc1[N+](=O)[O-])Cl)OP(=S)(OC)OC
C499	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)NCCN1CCN(CCCC(c2ccc(cc2)F)c2ccc(cc2)F)CC1
C500	Training	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1cc2c(cc1CCC1CC(=CC(=O)O1)OC)OCO2
C501	Training	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1cc(cc(c1)Cl)CN1C(=O)NC(=S)N(Cc2cccc(c2)Cl)CC1
C502	Training	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1cc(ccc1C1C(=C(C)NC(=C1C(=O)C)C)C(=O)C)Cl
C503	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)c1ccc(cc1)OC[C@@H]1CO[C@@](c2ccc(cc2Cl)Cl)(Cn2ccnc2)O1
C504	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)/C(=C\CCN(C)C)/c1ccccc1OC2
C505	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)CCN[C@H](C)CC1CCCCC1
C506	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(c(c1)N1CCN(C[C@H](COc2cc(c(c(c2)OC)OC)OC)O)CC1)OC
C507	Training	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	C1(=C([C@@]2([C@H]3[C@@H]([C@@]1(C2(Cl)Cl)Cl)COS(=O)OC3)Cl)Cl)Cl
C508	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12ccccn2nc(c1[C@H]1C(=C(C)NC(=C1C(=O)OCCN(Cc1ccccc1)C)C)C(=O)OC)C(C)C
C509	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)OC1C[C@H]2CC[C@H](C1)N2CC
C510	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C(=O)N(CC)[C@@H]2Nc1ccc(cc1)OCCN1CCCCC1
C511	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@H]1C(=C)[C@@H]([C@@H]2[C@@](C(=O)[C@H](/C=C/C(C)(C)[C@@H]([C@@H]1OC(=O)C)OC(=O)C)C)(C[C@](C)([C@@H]2O)OC(=O)C)O)OC(=O)C(C)C
C512	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@H]1C(=C)[C@@H]([C@H]2[C@](C(=O)[C@H](/C=C/C(C)(C)[C@@H]([C@@H]1OC(=O)C)OC(=O)C)C)(C[C@H](C)[C@@H]2O)O)OC(=O)[C@H](C)CC
C513	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@H]1C(=C)[C@@H]([C@@H]2[C@@](C(=O)[C@H](/C=C/C(C)(C)[C@@H]([C@@H]1OC(=O)C)OC(=O)C)C)(C[C@H](C)[C@@H]2OC(=O)C)O)OC(=O)C(C)C

C514	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(cnc1)C(=O)O[C@@H]1[C@H]2[C@@](C(=O)[C@H](/C=C/C)C)(C[C@@H]([C@@H][C@H](C(=C)[C@@H]2O[C@](=O)C)OC(=O)[C](C)OC(=O)C)OC(=O)C)C)[C@@]1(C)OC(=O)C)O
C515	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(ccc(c1)OCCC(C)C)nccc2[C@@H]([C@@H]1C[C@@H]2CCN1C[C@H]2CC)O
C516	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@@H](C(=O)OCCN1[C@H](C)C(c2ccccc2)OCC1)CC
C517	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1c(c(ccc1OCC)OCC)N(C(=O)COc1ccc(cc1)OCCCC)CCN(CC)CC
C518	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(=O)C(C)C)OCCN1CCC(CC1)C(c1ccc(cc1)F)(c1ccc(cc1)F)O
C519	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1c1cc(=O)c2c(cc(cc2o1)OCC(=O)N1CCN(Cc2ccc(c(c2OC)OC)OC)CC1)O)O)OC
C520	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1[C@@H]1CC(=O)c2c(cc(cc2OC(=O)C(C)(C)C)OCC(=O)N2CCN(Cc3ccc(c(c3OC)OC)OC)CC2)O1)OC(=O)C(C)(C)C)OC
C521	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCN1CCCC(CC1)N1C(=O)c2ccccc2[C@@H](Cc2ccc(cc2)F)N1
C522	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(c(c1)N1CCN(CCCC(=O)c2ccc(cc2)F)CC1)OC
C523	Training	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1ccc(cc1)[C@H](CCNC)Oc1ccc(cc1)C(F)(F)F
C524	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C\1=C\[C@H]([C@@H](/C(=C/[C@@H](C)[C@@H]([C@@H](C[C@H](C)CC2=C(C(=O)C=C(C2=O)NC(=O)/C(=C1)/C)OC)OC)O)/C)OC(=O)N)OC
C525	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(=C(C)C)CC[C@]([C@H]1CC[C@]2(C)[C@H]1[C@H](C[C@H]1[C@]2(C)CC[C@@H](C(C)C)[C@H]3CC[C@@]21C)O[C@@H]1[C@H]([C@H]([C@@H](C(O)O1)O)O)O)O
C526	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1cccc(c1[nH]2)C(=O)Nc1ccc(cc1)OCCN(Cc1ccc(c(c1)OC)OC)C
C527	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(=O)NCCN1CCC(CC1)n1c2ccc(cc2[nH]c1=O)Cl)F
C528	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)CCc1ccccc1C2OC1CCN(CC1)C
C529	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1c(cc(c(c1OC)OC)OC)C(=O)OCCCN(CCN(CCCOC(=O)c1cc(c(c(c1)OC)OC)OC)C)C
C530	Training	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1/C=C/C(=N/N=C1NCC(C)(C)CN1)/C=C/c1ccc(cc1)C(F)(F)F)C(F)(F)F
C531	Training	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@H](c1ccc(cc1)Cl)N1CCN(CC1)CCOCCO
C532	Training	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1cc(c(c(c1)Cl)CO[C@@H](c1ccc(cc1Cl)Cl)Cn1ccnc1)Cl
C533	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@@H]1/C/2=C\[C@](C)([C@@H]([C@@H]([C@@H]([C@H](C(/C=C/[C@@H](C(=O)[C@]2(C[C@H]1C)OC(=O)C)C)C)OC(=O)C)OC(=O)C)OC(=O)C)O
C534	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C=C1[C@@H](CC(=O)C(/C=C/[C@H](C(=O)[C@]2(C[C@](C)([C@@H]([C@H]2[C@H]1OC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)C)(C)C)OC(=O)C
C535	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C=C1[C@@H]([C@H]2[C@@](C(=O)[C@H](C)[C@H]3[C@H](C(C)(C)C)C(C[C@H]1OC(=O)C(C)C)OC(=O)C(C)C)OC(=O)C)O3)(C)[C@](C)([C@@H]2OC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C
C536	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(cnc1)C(=O)O[C@@H]1C[C@H](C(=C)[C@@H]([C@H]2[C@@](C(=O)O[C@@H](/C=C/C1(C)C)C)(C[C@H](C)[C@@H]2OC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C
C537	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@@H]1[C@@H]2[C@](C[C@@]1(C)OC(=O)C)(C[C@H]([C@H](/C=C/C)(C)C)[C@@H]([C@@H]([C@H](C(=C)[C@@H]2OC(=O)C)OC(=O)C)(C)C)O)OC(=O)c1ccccc1)C)OC(=O)C)O
C538	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c2c(c1)Oc1ccccc1O2)C(=O)Nc1ccc(cc1)OCCN(CCc1ccc(c(c1)OC)OC)C
C539	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@@H]1/C/2=C\[C@@](C)([C@@H]1[C@H](C(/C=C/[C@@H](C(=O)[C@]2(C[C@@]1(C)O)OC(=O)C)C)C)OC(=O)C)OC(=O)C)OC(=O)C
C540	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@@H]1[C@H]2/C=C(/C)/[C@@H]([C@@H]([C@H](C(/C=C/[C@H](C)[C@@H]([C@]2(C[C@H]1C)OC(=O)C)OC(=O)C)C)C)OC(=O)C)OC(=O)C)O
C541	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C=C1[C@@H]([C@H]2[C@@](C(=O)[C@@H](/C=C/C(C)C)[C@@H]([C@@H]([C@H]1OC(=O)C(C)OC(=O)C)OC(=O)C)OC(=O)C)C[C@](C)([C@@H]2OC(=O)C)OC(=O)C)OC(=O)C
C542	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@@](c1ccc(c(c1)OC)OC)(CCCN(CCc1ccc(c(c1)Cl)Cl)C)C(C)C
C543	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)c1cc(=O)c2cccc(c2[nH]1)C(=O)Nc1ccc(cc1)OCCN(Cc1ccc(c(c1)OC)OC)C
C544	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@@](c1cc(c(c(c1)OC)OC)OC)(CCCN(CCc1cc(c(c(c1)OC)OC)OC)C)C(C)C
C545	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@@](c1ccc(c(c1OC)OC)OC)(CCCN(CCCCCCCCCC)C)C(C)C
C546	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1C[C@H]1c2cc(c(cc2CCN1C)OC)OC)OC)OC
C547	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(=O)CCCN1CCC(C(=O)c2ccc(cc2)F)CC1)F
C548	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CC(=O)N(c1ccc(cc1)Cl)C1CCN(C(C)C)CC1
C549	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C1(c2ccccc2)C(=O)N(CCCN2CCN(c3cccc(c3)Cl)CC2)[C@H](C)N1
C550	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)n1cccc(c1n2)C(=O)Nc1ccc(cc1)OCCN(CCc1ccc(c(c1)OC)OC)C
C551	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)/C(=C/c1ccc(cc1)C(C)(C)C)/c1ccc(cc1)OCCN(CC)CC
C552	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@H](c1ccc(cc1)OCCN(CC)CC)Cc1ccc(cc1)OC
C553	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1cccc(c1[nH]2)C(=O)Nc1ccc(cc1)OCCN(Cc1ccc(cc1)C)C
C554	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1C(=O)OCCCCN([C@@H](C)Cc1ccc(cc1)OC)CC)OC)OC
C555	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@@H](c1ccc(cc1)Cl)N1CCN(Cc2cccc(c2)C)CC1
C556	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C1=C2C(C)C[C@H]3[C@H]4CC[C@](C(=O)C)([C@]4(C)CC[C@H]3[C@@]2(C)CCC1=O)O

C557	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)(C(=O)CC)C[C@H](C)N(C)C
C558	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)Cl)CCCN1CCN(CC1)CCOC(=O)c1cc(c(c(c1)OC)OC)OC
C559	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C=C(c1cc(ccc1O2)OC)N1CCN(CC1)C
C560	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)nc(CCCN(CC[C@@H]1[C@H](c3ccc(cc3CC1OC(=O)COC)F)C(C)C)C)[nH]2
C561	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cc(c(c1)OC)OC)[nH]c(c2CCN1CCN(c2ccccc2OC)CC1)C
C562	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(c(c1)Cl)NC(=O)CN1C[C@@H](C(=O)N)N(CCCC(c2ccc(cc2)F)c2ccc(cc2)F)CC1)Cl
C563	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=CC(=O)OCCCN(CCCOC(=O)/C=C/c1cc(c(c(c1)OC)OC)OC)C)c1ccccc1
C564	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1c(cc(c(c1OC)OC)OC)/C=C\C(=O)O[C@H]1CC[C@@H](CC1)N([C@H]1CC[C@H](CC1)OC(=O)c1cc(c(c(c1)OC)OC)OC)C
C565	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc2)c(c2c(c1)cccc2)C(=O)OCCCN(CCCOC(=O)c1cc(c(c(c1)OC)OC)OC)C
C566	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1cccc(c1[nH]2)C(=O)Nc1ccc(cc1)OCCCN1Cc2cc(c(cc2CC1)OC)OC
C567	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)OC(=O)N1C=C[C@H](c2ccc(cc2)OC)C(=C1)C(=O)C
C568	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)OC(=O)N1C=C[C@H](c2ccc(cc2)C)C(=C1)C(=O)CC
C569	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)OC(=O)N1C=C[C@H](c2ccccc2OC)C(=C1)C(=O)CC
C570	Training	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1cc(ccc1[C@@H](C1(CCCCC1)O)CNC)OC
C571	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)/C(=C(/c1ccccc1)\CC)/c1ccc(cc1)OCCNC
C572	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)CCN(C(=O)CN(C(=O)CNCCC(C)C)CCc1ccc(cc1Cl)Cl)CC(=O)N
C573	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)OCCN(Cc1ccc(cc1)OC)CCN(Cc1ccc(cc1)OC)CCOC(=O)c1ccccc1
C574	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)c1c(c2ccc(cc2)Cl)c2c(CC(C)(C)CC2=O)n(c1=S)C1[C@@H]([C@H]([C@@H]([C@@H](COC(=O)C)O1)OC(=O)C)OC(=O)C)OC(=O)C
C575	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc2)c(ccc1)[C@@H](C(=O)OCCN1CCN(CC1)CCOC(=O)[C@H](c1c2c(ccc1)cccc2)C)C
C576	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc2)c(ccc1)OC[C@@H](CN1CCN(c2ccccc2OC)CC1)O
C577	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c3cccc1[C@]1(C[C@H](CN([C@@H]1Cc2cn3C)C)COC(=O)c1cc(cnc1)Br)OC
C578	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)n(c(CN1CCN(CC(=O)NC(C)C)CC1)n2)CCC(=O)c1ccccc1
C579	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1cccc(c1[nH]2)C(=O)Nc1ccc(cc1)CCCN(Cc1ccc(c(c1)OC)OC)C
C580	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)/C(=C(/c1ccc(cc1)OC)\c1ccc(cc1)OCCN1CCCC1)/[N+](=O)[O-]
C581	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(c2c1[C@@H]([C@@H]1c3c(cc4c(c3OC)OCO4)CCN1C)OC2=O)OC)OC
C582	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1cccc(c1[nH]2)C(=O)Nc1ccc(cc1)CCCCN(Cc1ccc(c(c1)OC)OC)C
C583	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#CCOC(=O)[C@](c1ccccc1)(C1CCCCC1)O)CN(CC)CC
C584	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)nc1c(c2NC(=O)Cc2ccccc2)CCN1Cc1ccccc1
C585	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(c(c1)CCNCC(=O)N(CC(=O)N(CC(=O)N)CCc1ccc(cc1Cl)Cl)CCc1ccc(cc1Cl)Cl)F
C586	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(cc(c1)OC)/C=N\OC[C@@H](CN1CCN(c2ccccc2OC)CC1)O
C587	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C(=Nc1ccccc1C2)N1CCN(CC1)C
C588	Training	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1cc(cc(c1)Cl)CN1C(=S)NC(=S)N(Cc2cccc(c2)Cl)CC1
C589	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1ccccc1O2)CCCCN1CCOCC1
C590	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1ccccc1O2)CCCN(CC)CC
C591	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1ccccc1O2)CCCN1CCCCC1
C592	Training	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1ccc(cc1)NC(=N)NC(=O)c1c(nc(c(n1)Cl)N)N
C593	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1cccc(c1[nH]2)C(=O)Nc1ccc(cc1)OCCCN(Cc1ccc(c(c1)OC)OC)C
C594	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(cc1CN1CCN(C/C=C(\C)/CC/C=C(\C)/CCC=C(C)C)CC1)OCO2
C595	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)/C(=C/CCN1CCN(CC1)CCO)/c1cc(ccc1OC2)Cl
C596	Training	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(=O)CCCN1CCC(C(=O)N)(CC1)N1CCCCC1)F
C597	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(cc1/C=C/C1[C@@H](c3ccc4c(c3)OCO4)C=C[C@H](C(=O)N3CCCCC3)[C@H]1C(=O)N1CCCCC1)OCO2
C598	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C(=C1CCN([C@@H]1C)CC)c1ccccc1CC2
C599	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C1(=O)C(=O)C[C@@]2(C)[C@@H](C1)CC[C@H]1[C@H]3CC[C@H](CC)[C@]3(C)CC[C@@H]21

C600	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C[C@H](C)NCCC(c1ccccc1)c1ccccc1
C601	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@H]1C(=O)O[C@@H]C[C@H](C(=O)N[C@@H](C(=O)N2[C@@H](C(=O)N[C@@H](C(=O)N3[C@@H](C(=O)N1)CC(=O)CC3)Cc1ccc(cc1)N(C)C)CC2)CC)NC(=O)c1c(cccn1)O
C602	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)(C(=O)OCCN(CC)CC)CCC
C603	Training	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1/C(=N\CCCC(=O)N)/c1cc(ccc1O)F)Cl
C604	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CN(C)C)O
C605	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CN(C(C)C)C(C)C)O
C606	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1cccc(c1[nH]2)C(=O)Nc1ccc(cc1)C/C=C/CN(Cc1ccc(c(c1)OC)OC)C
C607	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CNCc1ccccc1)O
C608	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CN1CCN(c2ccccc2C)CC1)O
C609	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CN1CCN(c2ccc(cc2)OC)CC1)O
C610	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CC[C@H](c1ccccc1OC[C@H](CN1CCN(c2ccc(cc2)F)CC1)O)O
C611	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1cc(ccc1)CCN1Cc3cc(c(cc3CC1)OC)OC)[nH]c1cccc(c1c2=O)OC
C612	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CC[C@@H](c1ccccc1OC[C@H](CN(C(C)C)C(C)C)O)O
C613	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CN1CCN(Cc2ccccc2)CC1)O
C614	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CN1CCN(c2ccc(cc2)F)CC1)O
C615	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CNc1ccc(cc1)C(=O)OC)O
C616	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CNc1ccc(cc1)C(F)(F)F)O
C617	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CN(Cc1ccccc1)CCC)O
C618	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C1(CCN(CC1)C[C@H](COc1ccccc1C(=O)CC)O)O
C619	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)N1CCN(C[C@@H](COc2ccccc2C(=O)CCc2ccccc2)O)CC1
C620	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CN1CCOCC1)O
C621	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CC[C@H](c1ccccc1OC[C@H](CN1CCCCC1)O)O
C622	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CC[C@@H](c1ccccc1OC[C@H](CN1CCOCC1)O)OC
C623	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc2)c(ccc1)CCC(=O)c1ccccc1OC[C@@H](CN1CCCCC1)O
C624	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc2)c(ccc1)CCC(=O)c1ccccc1OC[C@@H](CNCCC(c1ccccc1)c1ccccc1)O
C625	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)c1ccccc1OC[C@@H](CN1CCN(c2ccc(cc2)F)CC1)O
C626	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1cc(ccc1OC[C@@H](CN1CCN(Cc2ccccc2)CC1)O)O
C627	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1cc(ccc1OC[C@H](CNCCC)O)OCc1ccccc1
C628	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1cc(ccc1OC[C@@H](CN1CCCCC1)O)OCc1ccccc1
C629	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1cc(ccc1)CCCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1cccc(c1c2=O)OC
C630	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C=Cc1ccccc1C2CCCNC
C631	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(nc(nc1NCC=C)N1CCC(CC1)NC[C@@H]1c3ccccc3COc3ccccc13)n(cn2)CC=C
C632	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(nc(nc1NCC=C)N1CCC(CC1)NC[C@@H]1c3ccccc3CCc3cc(ccc13)OC)n(cn2)CC=C
C633	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cc(cc1)Cl)nc1c(cc(cc1)OC)c2N[C@H](C)CCCN(CC)CC
C634	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)CCc1ccccc1N2[C@H]1C2CCN(CC2)C1
C635	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(cc(c1[C@@]1(Cn2ccnc2)OC[C@H](COc2ccc(cc2)N2CCN(C(=O)OCC)CC2)O1)Cl)Cl
C636	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1ccc(cc1C)OCCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1cccc(c1c2=O)OC
C637	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(nc(c(c3ccccc3)n2)N2CCOCC2)nc(nc1N(CC)CCO)N1CCOCC1
C638	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(nc(c(c3ccccc3)n2)N2CCOCC2)nc(nc1N(Cc1ccccc1)CCO)N1CCOCC1
C639	Training	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c12c(c(nc(n2)N(CCOC)CCO)N(CC)CC)nc(nc1N(CC)CC)N(CCOC)CCO
C640	Training	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CNc1c(nc2c(n1)O[C@@H](N[C@@H]2N1CCSCC1)N1CCNCC1)Cl
C641	Training	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1ccc(cc1)C[C@@H](C)N[C@@H](C)COc1ccccc1
C642	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1c2c(c(c(c1OC)OC)OC)nnn(c2=O)C[C@@H](CN1CCOCC1)OC(=O)c1cc(c(c(c1)OC)OC)OC

C643	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cc(cc1)OC)[nH]c1c2CCN2[C@@H]1C[C@@H]1[C@H](C(=O)OC)[C@H](C(C[C@@H]1C2)OC(=O)c1cc(c(c(c1)OC)OC)OC)OC
C644	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1ccc(cc1C)OCCCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1cccc(c1c2=O)F
C645	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)COC(=O)CC[C@@H](C(=O)NCCCC[C@H](C(=O)OC)NC(=O)[C@@H](CC(=O)OCc1ccccc1)NC(=O)OC(C)(C)C)NC(=O)OC(C)(C)C
C646	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cc(cc1)F)onc2C1CCN(CCc2c(C)nc3CCCCn3c2=O)CC1
C647	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1c2c(cc(c1OC)OC)[C@H]1C[C@](C)(CC)[C@H](CC(C)C)CN1CC2
C648	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1CC[C@@H]1c2cc(c(cc2CCN1C)OC)OC)OC
C649	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C)CC[C@@H]1c2cc(c(cc2CCN1)OC)OC
C650	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1CC[C@H]1c2cc(c(cc2CCN1C)OC)OC)O
C651	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(cc1CC[C@@H]1c3cc(c(cc3CCN1C)OC)OC)OCO2
C652	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C1CCN(CC1)CCCN1C(=O)[C@](c2ccccc2)(c2ccc(cc2)OC)NC1=O
C653	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C\1(=N/OCOCCOC)/[C@H](C)C[C@](C)([C@@H](C(C)C([C@H](C(=O)O[C@H](CC)[C@](C)([C@@H]([C@H]1C)O)O)C)OC1C[C@](C)([C@H](C(C)O1)O)OC)OC1[C@@H]([C@H](C[C@@H](C)O1)N(C)C)O)O
C654	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)c(c1ccccc1O)nc(c2)N1CCN(CCCC(=O)c2ccc(cc2)F)CC1
C655	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)c(c1ccccc1)nc(c2/C=N/N1C(=O)OCC1)N1CCN(CC1)C
C656	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)cnc(c2)N1CCN(CCCC(=O)c2ccc(cc2)Br)CC1
C657	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(ccc(c1)N1CCN(CCCC(=O)c3ccc(cc3)F)CC1)c(C)nc(c2)C
C658	Training	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)(C(=O)NCCN(C)C)CCC
C659	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@H](C(=O)OCCN1CCN(CC1)CCOC(=O)c1ccc(cc1)OCCCC)CC
C660	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(c(c1)C)[C@@H](C(=O)OCCN1CCN(CC1)CCOC(=O)[C@H](c1ccccc1C)CC)CC
C661	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1[C@@H](C(=O)OCCN1CCN(CC1)CCOC(=O)[C@H](c1ccc(cc1)F)CC)CC)F
C662	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(c(c1)[C@H](C(=O)N1CCN(CC1)CCOC(=O)[C@@H](c1ccccc1Cl)CC)CC)Cl
C663	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@@H](C(=O)NCCN1CCN(CC1)CCNC(=O)[C@H](c1ccccc1)CC)CC
C664	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)NC(=O)OCCN1CCN(CC1)CCOC(=O)Nc1ccccc1
C665	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@@H](C(=O)OCCN(CC)CCN(CC)CCOC(=O)[C@H](c1ccccc1)CC)CC
C666	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1ccc(cc1OC)CCCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1cccc(c1c2=O)F
C667	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1[C@H](C(=O)OCCN1CCN(CC1)CCOC(=O)[C@@H](c1ccc(c(c1)OC)OC)CCC)CCC)OC)OC
C668	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)C(=O)OCCN1CCN(CC(=O)Nc2c(cccc2C)C)CC1
C669	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@](c1ccc(cc1)F)(CCCN(CCc1ccc(c(c1)OC)OC)C)C(C)C
C670	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(c(c1)N1CCN(C[C@@H](COc2cc3c(cc2)NC(=O)CC3)O)CC1)OCC
C671	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@H]1C(=O)[C@H]2C(C)(C)O[C@@]3([C@@H](C)C[C@@H]([C@H]([C@]13COC(=O)C)OC(=O)c1ccccc1)OC(=O)C)[C@H]2OC(=O)C
C672	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@H]1[C@]2([C@@]3([C@](C)(C[C@@H]([C@@H]2OC(=O)C)OC(=O)C)O)[C@@H]([C@H](C(C)(C)O3)[C@@H]1OC(=O)c1ccccc1)OC(=O)C)COC(=O)C
C673	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@H]1[C@@]2(C)[C@@]3([C@@](C)(C[C@@H]1OC(=O)C)O)[C@H]([C@H](C(C)(C)O3)[C@@H]([C@H]2OC(=O)c1ccccc1)OC(=O)c1ccccc1)OC(=O)C
C674	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@H]1C(=O)[C@H]2C(C)(C)O[C@@]3([C@@]1([C@@H]([C@H](C[C@@]3(C)O)OC(=O)c1ccccc1)OC(=O)c1ccccc1)COC(=O)C)[C@H]2OC(=O)C
C675	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1CCC)OC)OCC(=O)N1CCN(C(=O)COc2ccc(cc2OC)CCC)CC1
C676	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C\1=C/C=C(\C)/[C@H](C[C@@H]2CC[C@@H](C)[C@](C(=O)C(=O)N3[C@H](C(=O)O[C@H](CC(=O)[C@@H](/C=C(\C)/[C@H]([C@H](C(=O)[C@H](C)C[C@@H](/C=C1)C)OC)O)C)[C@H](C)C[C@@H]1CC[C@H]([C@@H](C1)OC)O)CCCC3)(O)O2)OC
C677	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1ccc(cc1OC)OCCCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1cccc(c1c2=O)C
C678	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)N1C2(C(=O)NC1)CCN(CC2)CCCOc1ccc(cc1)F
C679	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)N1C2(C(=O)NC1)CCN(CC/C=C(/c1ccc(cc1)F)\C)CC2
C680	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cc(cc1)OC)[nH]c1c2CCN2[C@H]1C[C@@H]1[C@@H](C(=O)OC)[C@@H](C(C[C@H]1C2)OC(=O)c1cc(c(c(c1)OC)OC(=O)OCC)OC)OC
C681	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@](c1cccc(c1)C(F)(F)F)(CCCN(CCc1ccc(c(c1)OC)OC)C)C(C)C
C682	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	[C@@H]1(C(=O)C[C@H](C)[C@]2(C)[C@@H]([C@H](C(=O)[C@H](C)C[C@](C)([C@@H]([C@H](C1=O)C)OC1[C@@H]([C@H](C[C@@H](C)O1)N(C)C)O)OC)C)N(C(=O)O2)CCCCn1cc(c2cccnc2)nc1)C
C683	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1ccc(cc1OC)CCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1cccc(c1c2=O)F
C684	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(cc(c1[C@@]1(Cn2cncn2)OC[C@H](COc2ccc(cc2)N2CCN(C(C)C)CC2)O1)Cl)Cl
C685	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)C[C@@H](C)NC(C)(C)C

C686	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)[C@@H](C([C@H](C)N2)OC(=O)c1ccc(cc1)C)N1CCCC1
C687	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)[C@@H](C([C@H](C)N2)OC(=O)c1ccc(cc1)C)N[C@H](C)CCCN(CC)CC
C688	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(cc2c1Cc1c(ccs1)C(=N2)C1CCN(CC1)C)Cl
C689	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12/C=C/3\C(=O)[C@]([C@H](C(=N3)/C=c/3\ccc(/c(=C/C4=N/C(=Cc(c(c1)C)[nH]2)/[C@@]([C4=O)(C)C1([C@@H]([C@H](C)CO1)O)OC(=O)C)/[nH]3)C)(C)[C@H]1[C@@H]([C@H](C)CO1)O)OC(=O)C
C690	Training	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1ccc(c(c1)C)N1CCN(CCCOc2ccccn2)CC1
C691	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(c1ccc(cc1)F)N(C1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1)CC)F
C692	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(c1ccc(cc1)F)NC1CCN(c2nc(nc(n2)NCCC)NCC=C)CC1)F
C693	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C(c1ccccc1O2)CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C694	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1cccc(c1n2C)C(=O)Nc1ccc(cc1)CCN(Cc1ccc(c(c1)OC)OC)C
C695	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)[C@H](c1ccc(cc1S(=O)(=O)N2C)Cl)CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C696	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)CCc1ccccc1C2CNC1CCN(c2nc(nc(n2)Cl)NCC=C)CC1
C697	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)CCc1ccccc1C2C(=O)NN1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C698	Training	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1cc(cc(c1)C(F)(F)F)C1(CCN(CCCC(=O)c2ccc(cc2)F)CC1)O
C699	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C1=C(c2ccc(cc2)OCCN(CC)CC)c2ccc(cc2CC1)OC
C700	Training	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@H](c1ccc(cc1)Cl)N1CCN(CC1)CCOCC(=O)N
C701	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=C1CCN(CC1)CCOCCOCC(=O)N)c1ccccc1
C702	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@](c1ccccc1)(c1ccc(c(c1)OC)OC)CCCNC1c2ccccc2CCc2ccccc12
C703	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1ccc(cc1)CCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1c(cccc1F)c2=O
C704	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@@](c1ccc(c(c1)OC)OC)(CCCNC(c1ccccc1)c1ccccc1)C(C)C
C705	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#CCNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1)C[C@@](C#N)(c1ccc(c(c1)OC)OC)C(C)C
C706	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@@](c1ccc(c(c1)OC)OC)(CCCNC1c2ccccc2c2ccccc12)C(C)C
C707	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)[nH]c1c2CCN2C[C@@H](C[C@]1(c1cc3c(cc1OC)N[C@@H]1[C@@]4(CCN3[C@@H]4[C@](C=CC3)(CC)[C@H]([C@@]1(C=O)OC)O)OC(=O)C)C(=O)OC)C(C)(C)C2)O
C708	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c2c(c1)c(=O)c1cccc(c1[nH]2)C(=O)Nc1ccc(cc1)CCN(Cc1ccc(c(c1)OC)OC)C)C
C709	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@@H]([C@@H](CN1CCN(C[C@H](c2ccccc2)OC)CC1)O)OC
C710	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C1(c2ccccc2)C(=O)N(C(=O)N1)CCCN1CCN(c2ccccc2)CC1
C711	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)n1c([C@H]3C[C@@]4(c5ccccc5N(C(=O)C)[C@H]4N3C(=O)[C@@H]1C)C(C=C)(C)C)n2
C712	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)N1CCN(CCCn2c3ccccc3[nH]c2=O)CC1
C713	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(nc(nc1NCC=C)N1CCC(CC1)NC[C@@H]1c3ccccc3C(=O)Nc3ccccc13)n(cn2)CC=C
C714	Training	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c1cc2c(c(c1)NCCCNCCO)C(=O)c1cccc(c1C2=O)NCCCNCCO
C715	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)nc(cc2)C(=O)N[C@H](C(=O)N[C@@H](Cc1ccccc1)[C@@H](CN1[C@H](C(=O)NC(C)(C)C)C[C@@H]2CCCC[C@@H]2C1)O)CC(=O)N
C716	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)C[C@H]1CCC[C@@H](C[C@@H](c2ccccc2)O)N1C
C717	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)(CCCN1CCCCC1)O
C718	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)CCc1ccccc1C2N1CCN(C[C@H](CNc2nc(nc(n2)NCC=C)NCC=C)O)CC1
C719	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1ccc(cc1)CCCCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1c(cccc1N)c2=O
C720	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)nccc2[C@H]([C@H]1C[C@@H]2CCN1CC2C=C)O
C721	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)[C@@H](C([C@H](C)N2C(=O)c1ccc(cc1)C)O)N1CCCC1
C722	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)[C@@H]([C@H]([C@H](C)N2C(=O)c1ccc(cc1)C)O)N[C@H](C)CCCN(CC)CC
C723	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CN[C@H]1c2ccccc2N(C(=O)c2ccc(cc2)C)[C@@H](C)[C@@H]1O
C724	Training	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c12c(cccc1)[nH]c1c2CCN2[C@H]1C[C@H]1[C@H](C(=O)OC)[C@H](CC[C@H]1C2)O
C725	Training	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	C1=C2CC[C@H]3[C@@H]4CC[C@@H]([C@@]4(C)CC[C@@H]3[C@@]2(C)CCC1=O)O
C726	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1ccc(cc1)CCCCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1ccc(cc1c2=O)OC
C727	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(c(nc(n2)N2CCN(CC2)C)N2CCCCC2)nc(nc1N1CCCCC1)N(CCO)CCO
C728	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(c(nc(n2)N(CCO)CCO)N2c3ccccc3CCC2)nc(nc1N1c2ccccc2CCC1)N(CCO)CCO

C729	Training	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c12c(c(nc(n2)N2CCCCC2)N(CCO)CCO)nc(nc1N(CCO)CCO)N1CCCCC1
C730	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(nc(c(c3ccccc3)n2)N2CCCCC2)nc(nc1N(CCO)CCO)N1CCCCC1
C731	Training	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	C(#N)c1c([nH]nc1/C(=C\c1cc(c(c(c1)C(C)(C)C)O)C(C)(C)C)/C#N)N
C732	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CN1[C@@H](c2nc3ccccc3c(=O)n2[C@@H]1c1ccc(c(c1)O)O)C
C733	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CN(CCOC(=O)C1=C(C)NC(=C([C@@H]1c1cccc(c1)[N+](=O)[O-])[P@@](=O)(N(C)C)OCC)C)C
C734	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)OCCCN(CCN(CCCOc1ccccc1)S(=O)(=O)c1ccccc1)S(=O)(=O)c1ccccc1
C735	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)CCc1ccccc1C12c2ccccc2CN1C
C736	Training	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c12c(cc(cc1)OC)nc([nH]2)[S@@](=O)Cc1c(c(c(cn1)C)OC)C
C737	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc2)c(ccc1)N(C(=S)Sc1nc2c(cccc2)o1)C
C738	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1[C@@H](CCCCCN1Cc2cc(c(cc2CC1)OC)OC)SCCCCC)OC)OC
C739	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C)S[C@H](c1ccc(c(c1)OC)OC)CCCCCN1Cc2cc(c(cc2CC1)OC)OC
C740	Training	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	C(=C(C)C)CC/C(=C/CC/C(=C/CSC[C@@H](C(=O)NC)NC(=O)C)/C)/C
C741	Training	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	C(=C(C)C)CC/C(=C/CC/C(=C/CSC[C@@H](C(=O)OC)NC(=O)C)/C)/C
C742	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)SC[C@@H]([C@@H](CN1[C@H](C(=O)NC(C)(C)C)C[C@H]2CCCC[C@H]2C1)O)NC(=O)c1cccc(c1C)O
C743	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1cccc(c1[nH]2)C(=O)Nc1ccc(cc1)SCCCN(Cc1ccc(c(c1)OC)OC)C
C744	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(nc(c(n2)SCc2ccccc2)N(C)C)nc(nc1N(C)C)N1CCNCC1
C745	Training	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1CN1C(=O)N[C@H](N(Cc2ccc(cc2)Cl)CC1)SC)Cl
C746	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cc(c(c1)OC)OC)[nH]c(c2CCN1CCN(c2ccccc2)CC1)C(=O)OCC
C747	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@@](c1ccc(c(c1)OC)OC)(CCCCCCN1Cc2cc(c(cc2CC1)OC)OC)Sc1ccc(cc1)C
C748	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@](c1ccc(c(c1)OC)OC)(CCCCCN1Cc2cc(c(cc2CC1)OC)OC)Sc1ccc(cc1)C
C749	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@@](c1ccc(c(c1)OC)OC)(CCCCCN1Cc2cc(c(cc2C1)OC)OC)SC1CCCCC1
C750	Training	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1ccc(c(c1)CC=C)OC[C@@H](CNC(C)C)O
C751	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)OC)C[C@@H](C)CN1CCC(CC1)O
C752	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)C(=O)C)C[C@@H](C)N(C)C
C753	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)[S@](=O)C)CC[C@@H]1CCCCN1C
C754	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)C(=O)C)CCCN(C)C
C755	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)C(=O)C)CCCN1CCC(C(=O)c2ccc(cc2)F)CC1
C756	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)C(F)(F)F)CCCN1CCCN(C2CC2)CC1
C757	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)S(=O)(=O)N(C)C)CCCN1CCN(CC1)C
C758	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C(=CCCN(C)C)c1ccccc1CC2
C759	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)C(=O)CC)CCCN1CCN(CC1)CCO
C760	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1ccccc1S2)CCN1CCCC1
C761	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)c1ccc2c(c1)C1=C(c3ccccc3S2)CCN(CC1)C
C762	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1cccc(c1s2)C(=O)Nc1ccc(cc1)OCCN(CCc1ccc(c(c1)OC)OC)C
C763	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(cc1C(F)(F)F)/C(=C/CCN1CCN(CC1)CCO)/c1ccc(cc1S2)F
C764	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@H]1C(=S)N(C(=C(C(=O)C)[C@@H]1c1ccc(cc1)OC)c1ccccc1)C1[C@@H]([C@H]([C@@H]([C@@H](COC(=O)C)O1)OC(=O)C)OC(=O)C)OC(=O)C
C765	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@H]1C(=S)N(C(=C[C@@H]1c1ccccc1)c1ccccc1)C1[C@@H]([C@H]([C@@H]([C@@H](COC(=O)C)O1)OC(=O)C)OC(=O)C)OC(=O)C
C766	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c3c(ccc1)CCc1ccccc1n3cc2CN(Cc1ccccc1)C
C767	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(=C(c1ccc(cc1)OC)CN(C)C)c1ccc(cc1)OC)OC
C768	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(nc(nc1N1CCC(CC1)NCC1c3ccccc3CCc3ccccc13)NCC=C)n(cn2)CC=C
C769	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)CCc1ccccc1C2CNC1CCN(c2nc(nc(n2)N(C)C)N(C)C)CC1
C770	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)CCc1ccccc1C2NC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C771	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(c(c1)C)C(c1c(cccc1C)C)CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1)C

C772	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C773	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)[C@H]1c3ccccc3[C@]2(CC1)CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C774	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C=Cc1ccccc1C2CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C775	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)CCc1ccccc1C2CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C776	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)CCc1ccccc1C2CN1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C777	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)CCc1ccccc1C2CNC1CCN(c2nc(nc(n2)NCCC)NCC=C)CC1
C778	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)CCNC1CCN(c2nc(nc(n2)NCCC)NCC=C)CC1
C779	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C1=Nc2cccnc2N(c2ccccc12)CCCN(C)C
C780	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C(=C(C2)CCN(C)C)[C@H](c1ccccn1)C
C781	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)oc(c2CCc1ccccc1)C(=O)CN1CCN(c2ccccc2OC)CC1
C782	Training	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c12c(c(ccc1)[C@H]1C(=C(C)NC(=C1C(=O)OC(C)C)C)C(=O)OC)non2
C783	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C(=C1CCN(CC1)C)c1ccsc1CC2
C784	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)N(C1Cc2ccccc2C1)CCCN(CC)CC
C785	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C(=C1CCN(CC1)CCOCCOCCO)c1ccsc1C(=O)C2
C786	Training	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1c(csc1)[C@@H](C(=O)OCCN1CCCCCC1)C1CCCCC1
C787	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC1Cc2ccc(c(c2c2cc(ccc2CCN1C)OC)O)OC
C788	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C[C@@H]1C(=O)N([C@@H](C(=O)N2[C@@H](C(=O)N[C@@H](C(=O)N([C@@H](C(=O)N[C@@H](C(=O)N([C@@H](C(=O)O[C@@H](C(=O)N([C@@H](C(=O)N1)C(C)C)C)[C@@H](C)CC)C(C)(C)O)C)CC(C)C)C(C)C)C)[C@@H](C)CC)CCC2)Cc1ccccc1)C
C789	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(Cc1ccc(cc1)Cl)nn(c2=O)C1CCCN(CC1)C
C790	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(c(c1)[C@H]1C(=C(C)NC(=C1C(=O)OCCNC(=O)c1ccc(cc1)N=[N+]=[N-])C)C(=O)OCC)C(F)(F)F
C791	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(=C\C[C@@H](C)[C@H]([C@H]1C(=O)N[C@@H](C(=O)N(CC(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@@H](C(=O)N1C)C(C)C)C)CC(C)C)C)CC(C)C)C)C)C)CC(C)C)C)C(C)C)CC(C)C)C)C)CC)OC(=O)C)/C
C792	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C1(c2ccccc2)CC[N+](CC1)(CCCOC(=O)C1=C(C)NC(=C(C(=O)OCC)[C@@H]1c1cccc(c1)[N+](=O)[O-])C)C
C793	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(nc(c(c3ccccc3)n2)N2C[C@H](C)O[C@H](C)C2)nc(nc1N(CC(C)(C)O)CCO)N1C[C@H](C)O[C@H](C)C1
C794	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(/C=C/C(=O)OC(C)C)nc(c1)/C(=C/CN1CCCC1)/c1ccc(cc1)C
C795	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(/C=C/C(=O)N2CCCC2)nc(c1)/C(=C/CN1CCCC1)/c1ccc(cc1)C
C796	Training	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)N(C(=O)/C=C/c1cccc(/C(=C/CN2CCCC2)/c2ccc(cc2)C)n1)C
C797	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1ccc(CCN(C)CC#CCN2C(=O)[C@H]3[C@H](C4c5ccccc5C3c3ccccc43)C2=O)cc1OC
C798	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1ccc(CCN(C)CCCN2C(=O)[C@@H]3[C@H](C4c5ccccc5C3c3ccccc43)C2=O)cc1OC
C799	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCCCC[C@@H]1[C@@H](C(=O)O[C@H](C(=O)N([C@H](C(CC(=O)O1)OCOC)Cc1ccccc1)C)C(C)C)C
C800	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC1COC(=O)C[C@H]([C@@H](N(C(=O)[C@@H](OC1=O)C(C)C)C)Cc1ccccc1)O
C801	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCCCC[C@@H]1[C@@H](C(=O)O[C@H](C(=O)N([C@H](CCC(=O)O1)Cc1ccccc1)C)C(C)C)C
C802	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCCCC[C@@H]1[C@@H](C(=O)OC(C(=O)N([C@H](C(CC(=O)O1)OCOC)Cc1ccccc1)C)(C)C)C
C803	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCC[C@@H]1[C@@H](C(=O)OCC(=O)N([C@H](C(CC(=O)O1)OCOC)Cc1ccccc1)C)C
C804	Training	inhibitor	60	noninhibitor	inhibitor	inhibitor	inhibitor	CN([C@@H](Cc1ccccc1)[C@@H](CC(=O)OC)OCOC)C(=O)OCc1ccccc1
C805	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCCCC[C@@H]1[C@@H](C(=O)OCC(=O)N([C@H](C(CC(=O)O1)O)Cc1ccccc1)C)C
C806	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCCCCC1CC(=O)O[C@H](C(=O)N([C@H](C(CC(=O)O1)O)Cc1ccccc1)C)C(C)C
C807	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	C[C@H]1[C@H](OC(=O)C[C@H]([C@@H](N(C(=O)[C@@H](OC1=O)C(C)C)C)Cc1ccccc1)OCOC)C
C808	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1ccccc1n2CCCCN1CCCCC1
C809	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc2c1n(c1ccccc1c2=O)CCCCN1CCCCC1
C810	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc2c1n(c1ccccc1c2=O)CCCCN1CCOCC1
C811	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc2c1n(c1ccccc1c2=O)CCCCN(CCO)CCO
C812	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1ccccc1n2CCCCN1CCN(CC1)CCO
C813	Training	inhibitor	60	inhibitor	noninhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1ccccc1n2CCCCl
C814	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1ccccc1n2CCCN1CCOCC1

C815	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1ccccc1n2CCCN(CCO)CCO
C816	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc2c1n(c1ccccc1c2=O)CCCN1CCN(CC1)CCO
C817	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc2c1n(c1ccccc1c2=O)CCCCCl
C818	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN1CCN(CC1)CCCCn1c2ccccc2c(=O)c2c1cccc2
C819	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN1CCN(CC1)CCCCn1c2ccccc2c(=O)c2c1c(ccc2)OC
C820	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)CCC(=O)OC)c1ccc(cc1)N(C)C
C821	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)C(=O)OC)c1ccc(cc1)N(C)C
C822	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)CCCCOC)c1ccc(cc1)N(C)C
C823	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCOC/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)N(C)C)c1ccc(cc1)N(C)C
C824	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/COCCOC)c1ccc(cc1)N(C)C
C825	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/COc1ccccc1)c1ccc(cc1)N(C)C
C826	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCC(=O)OC/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)N(C)C)c1ccc(cc1)N(C)C
C827	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/CN1CCOCC1)c1ccc(cc1)N(C)C
C828	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCCCn1c(c(nc1c1ccc(cc1)C(=O)OC)c1ccc(cc1)N(C)C)c1ccc(cc1)N(C)C
C829	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/C(=O)O)c1ccc(cc1)N(C)C
C830	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/C(=O)OC)c1ccc(cc1)N(C)C
C831	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)O)c1ccc(cc1)N(C)C
C832	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)c1ccc(cc1)c1c(n(c(n1)c1ccc(cc1)C(=O)O)CCc1ccccc1)c1ccc(cc1)N(C)C
C833	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCN(CC)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/C(=O)OC)c1ccc(cc1)N
C834	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)Nc1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/C(=O)OC)c1ccc(cc1)NC
C835	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCOC/C=C\c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)N1CCOCC1)c1ccc(cc1)N1CCOCC1
C836	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCOC/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)NC)c1ccc(cc1)N(C)C
C837	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCOC/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)NC)c1ccc(cc1)N1CCCC1
C838	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCN(CC)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/C(=O)OC)c1ccc(cc1)N(CC)CC
C839	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCNc1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/COCC)c1ccc(cc1)NC(C)C
C840	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCN(CCC)c1ccc(cc1)c1c[nH]c(n1)c1ccc(cc1)/C=C/COCC
C841	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCOC/C=C/c1ccc(cc1)c1[nH]c(cn1)c1ccc(cc1)NCC(C)C
C842	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)N(CC=C)CC=C)c1ccc(cc1)N(CC=C)CC=C
C843	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CNc1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/C(=O)OC)c1ccc(cc1)N(C)C
C844	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCN(CCC)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/C(=O)OC)c1ccc(cc1)NC
C845	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2CCN(CCc3ccc(NC(=O)c4ccccc4[N+](=O)[O-])cc3)Cc2cc1OC
C846	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Nc1ccccc1C(=O)Nc1ccc(CCN2CCc3ccccc3C2)cc1
C847	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	[O-][N+](=O)c1ccc(cc1)C(=O)Nc1ccc(CCN2CCc3ccccc3C2)cc1
C848	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2CCN(CCc3ccc(NC(=O)c4ccc(N)cc4)cc3)Cc2cc1OC
C849	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2CCN(CCc3ccc(NC(=O)c4cnc5ccccc5c4)cc3)Cc2cc1OC
C850	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1ccc(cc1OC)C(=O)Nc1ccc(CCN2CCc3cc(OC)c(OC)cc3C2)cc1
C851	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2CCN(CCc3ccc(NC(=O)c4cc(OC)c(OC)cc4[N+](=O)[O-])cc3)Cc2cc1OC
C852	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2CCN(CCc3ccc(NC(=O)c4ccnc5ccccc45)cc3)Cc2cc1OC
C853	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2CCN(CCc3ccc(NC(=O)c4cccc(Br)c4)cc3)Cc2cc1OC
C854	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2CCN(CCc3ccc(NC(=O)c4cccc5ccccc45)cc3)Cc2cc1OC
C855	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2CCN(CCc3ccc(NC(=O)c4cccnc4)cc3)Cc2cc1OC
C856	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O=C(Nc1ccccc1C(=O)Nc1ccc(CCN2CCc3ccccc3C2)cc1)c1cnc2ccccc2c1
C857	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1c1cc(=O)c2c(cc(cc2o1)O)O)OCCOCCOCCOCCO

C858	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Oc1ccc2[nH]cc(CCCCN3CCC(=CC3)c3ccccc3)c2c1
C859	Training	inhibitor	60	noninhibitor	inhibitor	inhibitor	inhibitor	Oc1cc(CCCCC)cc(O)c1[C@H]1C=C(C)CC[C@H]1C(=C)C
C860	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1c(ccc2c1sc(c1ccc(cc1)S(=O)(=O)CCCC)c2C(=O)c1ccc(OCCN2CCCCC2)cc1)OS(=O)(=O)CCCC
C861	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	N(c1ccc(cc1)C1=N[C@@H]2CCN(C)C[C@@H]2c2c1cc(OC)c(OC)c2)S(=O)(=O)c1ccc(C)cc1
C862	Training	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	NS(=O)(=O)c1c(Cl)cc2NC(=NS(=O)(=O)c2c1)CSCc1ccccc1
C863	Training	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	OC(=O)C1=C(COC(=O)C)CS[C@H]2[C@@H](NC(=O)/C(=N/OC)/c3csc(n3)N)C(=O)N12
C864	Training	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	O[C@H](COC(=O)N)COc1ccc(Cl)cc1
C865	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H]1C[C@H](CCn2c(C(C)C)c(C(=O)Nc3ccccc3)c(c2c2ccc(F)cc2)c2ccccc2)OC(=O)C1
C866	Training	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	Oc1c(OC)cc2CCN3Cc4c(C[C@H]3c2c1)ccc(OC)c4O
C867	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@]12O[C@@](NC(=O)[C@@H]3CN(C)[C@@H]4Cc5c[nH]c6cccc(c56)C4=C3)(C(C)C)C(=O)N1[C@@H](Cc1ccccc1)C(=O)N1CCCC21
C868	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@]12O[C@@](NC(=O)[C@@H]3CN(C)[C@@H]4Cc5c[nH]c6cccc(c56)C4=C3)(C(C)C)C(=O)N1[C@@H](CC(C)C)C(=O)N1CCCC21
C869	Training	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	[nH]1c2=CC(=O)C=Cc2c2CCNC(=c12)C
C870	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1c(OC)cc(C[C@@H]2N(C)CCc3cc(OC)c(OC)cc23)c(Br)c1
C871	Training	inhibitor	60	inhibitor	noninhibitor	inhibitor	inhibitor	O[C@@H]1CC[C@@]2(C)[C@@H](CCC3[C@@H]4CC[C@@H]([C@H](C)CCC(=O)O)[C@@]4(C)CC[C@H]23)C1
C872	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H]1C[C@H](CC[C@H]2[C@@H](C)C=CC3=C[C@@H](C)C[C@@H](OC(=O)[C@H](C)CC)[C@H]23)OC(=O)C1
C873	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	N([C@@H]1CN(C)[C@@H]2Cc3c[nH]c4cccc(c34)C2=C1)C(=O)N(CC)CC
C874	Training	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	NCc1ccc(cc1)S(=O)(=O)N
C875	Training	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	OCC(=O)[C@]1(O)CC[C@@H]2[C@@H]3C[C@@H](C)C4=CC(=O)C=C[C@]4(C)[C@@H]3C(O)C[C@]12C
C876	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@]1(CC[C@@H]2[C@H]3CCC4=CC(=O)CCC4=C3[C@H](C[C@@]12C)c1ccc(cc1)N(C)C)C#CC
C877	Training	inhibitor	60	noninhibitor	inhibitor	inhibitor	inhibitor	N1CCCCC1CC(C1CCCCC1)C1CCCCC1
C878	Training	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	C1CCn2nnnc2CC1
C879	Training	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	N(CCN(CC)CC)C(=O)c1c(OC)ccc(c1)S(=O)(=O)C
C880	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Oc1cc2c(O)c(c1)NC(=O)/C(=C/C=C[C@@H](C)[C@@H](OC(=O)N)/C(=C/[C@@H](C)[C@H](OC)[C@H](C[C@@H](C)[C@H]2OC)OC)/C)/C
C881	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H]1[C@@H](C)/C=C(\C)/[C@H](OC(=O)N)[C@@H](OC)/C=C/C=C(\C)/C(=O)NC2=CC(=O)C(=C(C[C@H](C)C[C@@H]1OC)C2=O)NCC=C
C882	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	OCCOCCN1CCN(CC1)C1=Nc2ccccc2Sc2ccccc12
C883	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	N1C(=C([C@@H](c2cccc(c2)[N+](=O)[O-])C(=C1C)C(=O)O[C@H]1CCCN(Cc2ccccc2)C1)C(=O)OC)C
C884	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1cccc2c1oc(cc2=O)C(=O)Nc1cc(OC)c(OC)cc1c1nnn(n1)c1ccc(CCN2CCc3cc(OC)c(OC)cc3C2)cc1
C885	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	OC[C@H]1Oc2c(OC1c1ccc(OC)c(OC)c1)cc(cc2)c1c(O)c(=O)c2c(O)cc(OC)cc2o1
C886	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	OC[C@H]1Oc2c(OC1c1ccc(OC)c(OC)c1)cc(cc2)c1c(OC)c(=O)c2c(O)cc(O)cc2o1
C887	Training	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	OC[C@H]1Oc2c(OC1c1ccc(O)c(O)c1)cc(cc2)c1c(O)c(=O)c2c(O)cc(O)cc2o1
C888	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	OC[C@@H]1Oc2ccc(cc2OC1c1ccc(O)c(OC)c1)[C@H]1Oc2c(C(=O)[C@@H]1O)c(O)cc(OCc1ccccc1)c2
C889	Training	inhibitor	60	noninhibitor	inhibitor	inhibitor	inhibitor	OC[C@H]1Oc2c(OC1c1ccc(O)c(OC)c1)cc(cc2)c1c(O)c(=O)c2c(O)cc(O)cc2o1
C890	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	OC[C@H]1Oc2c(OC1c1ccc(O)c(OC)c1)cc(cc2)c1c(OC)c(=O)c2c(O)cc(OC)cc2o1
C891	Training	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	CC(=O)Oc1c(O)cc2oc(cc(=O)c2c1O)c1ccccc1
C892	Training	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	COc1c(OC)c(O)c2c(=O)cc(oc2c1)c1ccccc1
C893	Training	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	Oc1c2c(=O)cc(oc2cc2c1OCO2)c1ccccc1
C894	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1c2c(=O)cc(oc2cc2c1OC(O2)(c1ccccc1)c1ccccc1)c1ccccc1
C895	Training	inhibitor	60	noninhibitor	inhibitor	inhibitor	inhibitor	CCCOc1c(O)cc2oc(cc(=O)c2c1O)c1ccccc1
C896	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCOc1c(OC)cc2oc(cc(=O)c2c1OC)c1ccccc1
C897	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCOc1c(OCCC)c(O)c2c(=O)cc(oc2c1)c1ccccc1
C898	Training	inhibitor	60	noninhibitor	inhibitor	inhibitor	inhibitor	CCOc1c(OCC)c(O)c2c(=O)cc(oc2c1)c1ccccc1
C899	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCCCCCCOc1c(OCCCCCCCCC)c(O)c2c(=O)cc(oc2c1)c1ccccc1
C900	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCCOc1c(OCCCCC)c(O)c2c(=O)cc(oc2c1)c1ccccc1

C901	Training	inhibitor	60	noninhibitor	inhibitor	inhibitor	inhibitor	CC(=O)Oc1c(OC(=O)C)c(OC(=O)C)c2c(=O)cc(oc2c1)c1ccccc1
C902	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCCOc1c(OCCCCC)c(OC)c2c(=O)cc(oc2c1)c1ccccc1
C903	Training	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	Oc1c(CNCC)cc(cc1)Nc1ccnc2cc(Cl)ccc12
C904	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCOc1c(OCCCC)c(OC)c2c(=O)cc(oc2c1)c1ccccc1
C905	Training	inhibitor	60	noninhibitor	inhibitor	inhibitor	inhibitor	COc1c(OC(=O)C)c(OC)c2c(=O)cc(oc2c1)c1ccccc1
C906	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC(=O)Oc1c(OCc2ccccc2)cc2oc(cc(=O)c2c1OC(=O)C)c1ccccc1
C907	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC(=O)Oc1c(OCc2ccccc2)c(O)c2c(=O)cc(oc2c1)c1ccccc1
C908	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1c(cccc1)C(=O)CCc1ccccc1)CN1CCN(CC1)c1cccc(C)c1C
C909	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Clc1c(cccc1)c1nc2c(cccc2)c(n1)N1CCCC1
C910	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cccc1)C(=O)CCc1ccccc1)CN(CCC)C(=O)c1ccccc1
C911	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cccc1)C(=O)Cc1cccc2c1cccc2)CN1CCC(O)(CC1)c1ccccc1
C912	Training	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	O[C@H](COc1c(cc(C)cc1)C(=O)C)CN1CCCCC1
C913	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cccc1)C(=O)CCc1ccccc1)CN[C@@H](c1ccccc1)C(C)(C)C
C914	Training	inhibitor	60	noninhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1cccc2c1C(=C)CC2=O)CN1CCCCC1
C915	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1cccc2c1C(=O)[C@H](C2=C)c1ccccc1)CN1CCCCC1
C916	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1cccc2c1C(=O)[C@@H](C2=C)c1ccccc1)CN1CCN(CC1)c1cccc(C)c1C
C917	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1cccc(c1)C(=O)C)CN1CCN(CC1)c1c(C)c(C)ccc1
C918	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	C([C@@H]1Oc2ccccc2[C@H]1Cc1ccccc1)N1CCCCC1
C919	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	N(C(=O)c1ccc(OCCCC)cc1)c1cc2c(cc1)nc(SCc1c(C)c(C(=O)C)c(C)cc1C)s2
C920	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	N(C(=O)CCc1ccccc1)c1cc2c(cc1)nc(SCc1c(C)c(C(=O)C)c(C)cc1C)s2
C921	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1ccc(cc1)C(=O)CCc1ccccc1)CN1CCN(CC1)c1cccc(C)c1C
C922	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1c(cccc1)C(=O)C)CN1CCN(CC1)c1ccccc1C
C923	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1c(ccc(C)c1)C(=O)C)CN1CCN(CC1)c1ccccc1C
C924	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1c(cc(Cl)c(Cl)c1)C(=O)C)CN1CCN(CC1)c1ccccc1C
C925	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(ccc(OC)c1)C(=O)CCc1ccc(cc1)N(C)C)CN1CCN(CC1)c1ccccc1C
C926	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1ccc(cc1)C(=O)C)CNCCC(c1ccccc1)c1ccccc1
C927	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1cc(ccc1)C(=O)CCc1ccccc1)CN1CCN(CC1)c1ccccc1C
C928	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1cc(ccc1)C(=O)CCc1ccccc1)CNCCC(c1ccccc1)c1ccccc1
C929	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1cc(ccc1)C(=O)CCc1ccccc1)CN1CCOCC1
C930	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1c(cccc1)C(=O)CCc1ccccc1)CN1CCCCC1
C931	Training	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	O[C@@H](COc1c(cccc1)C(=O)CC)CN1CCCCC1
C932	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cccc1)C(=O)CCc1ccccc1)CN1CCN(CC1)c1ccccc1
C933	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1c(cccc1)C(=O)CCc1ccccc1)CN(C)CCC
C934	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cccc1)C(=O)CCc1ccccc1)CN1CCC(O)(CC1)c1ccccc1
C935	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	C(Cc1c(CCc2ccccc2)c2c(o1)cccc2)N1CCCCC1
C936	Training	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	O[C@H](CNCCC)c1c(CC)c2c(o1)cccc2
C937	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cccc1)C(=O)CCc1ccccc1)CN1CCC(Cc2ccccc2)CC1
C938	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1cccc2c1cccn2)CN1CCN(CC1)C1c2ccccc2[C@H]2[C@H](c3c1cccc3)C2(F)F
C939	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1ccc(cc1)C(=O)CCc1ccccc1)CN1CCOCC1
C940	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1ccccc1[C@H](CCc1ccccc1)OC)CN(CCC)CCC
C941	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1ccccc1C(=O)CCc1ccccc1)CNCC(c1ccccc1)c1ccccc1
C942	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O=C(CCc1ccccc1)c1ccccc1OCCCN1CCCCC1
C943	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O=C(CCc1ccccc1)c1ccccc1OCCN1CCCCC1

C944	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O=C(CCc1ccccc1)c1ccccc1OCCCCCN1CCCCC1
C945	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O=C(CCc1ccccc1)c1ccccc1OCCCCCCN1CCCCC1
C946	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O=C(CCc1ccccc1)c1ccccc1OCCCCCCCCN1CCCCC1
C947	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1c(cccc1)[C@H](CCc1ccccc1)OC)CNCCCC(c1ccccc1)c1ccccc1
C948	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cc(O)cc1)C(=O)CCc1ccccc1)CN1CCCCC1
C949	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1c(cccc1)C(=O)CCc1ccccc1)CNCCCC(c1ccccc1)c1ccccc1
C950	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cccc1)C(=O)CCc1ccccc1)CNC1CCCCC1
C951	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	N1[C@H](N(c2ccc(cc2)C(C)(C)C)C(=O)c2ccccc12)c1ccc2OCOc2c1
C952	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	N1[C@@H](N(c2ccc(CC)cc2)C(=O)c2ccccc12)c1ccc(OCC(C)C)cc1
C953	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	N1[C@@H](N(c2ccc(cc2)[C@H](C)CC)C(=O)c2ccccc12)c1ccc(cc1)C(C)C
C954	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cc(O)cc1)C(=O)CCc1ccccc1)CN(C(C)C)C(C)C
C955	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cccc1)C(=O)C)CN1CCC(O)(CC1)c1ccccc1
C956	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cccc1)C(=O)CCc1ccc(Cl)cc1)CN1CCN(CC1)c1c(C)cccc1
C957	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1c(cc(c(c1)OCC[C@H](CN1CCN(CC1)c1c(cccc1)C)O)C(=O)CCc1ccccc1)OC
C958	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1c(cc(C)cc1)C(=O)CCc1ccccc1)CN1CCN(CC1)c1ccccc1C
C959	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O=C(CCc1ccccc1)c1c(OCCCCN2CCOCC2)cccc1
C960	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	C[C@H]1CC[C@@H]2COC3=C([C@H]2C1)C(=O)C1=C([C@H]2C[C@@H](C)CC[C@H]2C(C)(C)O1)C3=O
C961	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCN3CCN(CC3)c3cc(Cl)ccc3)cccc2)c1
C962	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCCN3CCN(CC3)c3cc(ccc3)C(F)(F)F)cccc2)c1
C963	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCN3CCN(CC3)c3c(OC)cccc3)cccc2)c1
C964	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCCCN3CCN(CC3)c3c(OC)cccc3)cccc2)c1
C965	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCN3CCN(CC3)c3ccc(F)cc3)cccc2)c1
C966	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCCN3CCN(CC3)c3ccc(F)cc3)cccc2)c1
C967	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCCCN3CCN(CC3)c3ccc(F)cc3)cccc2)c1
C968	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCN3CCN(CC3)c3ncccn3)cccc2)c1
C969	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCCN3CCN(CC3)c3ncccn3)cccc2)c1
C970	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCN3CCc4ccccc4C3)cccc2)c1
C971	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCCCN3CCc4ccccc4C3)cccc2)c1
C972	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCN3CCc4cc(OC)c(OC)cc4C3)cccc2)c1
C973	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	N([C@H](C)c1ccccc1)C(=O)Nc1ccc(S[C@@H]2CC3=CC(=O)CC[C@]3(C)[C@H]3CC[C@]4(C)[C@H](CC[C@H]4C(=O)C)[C@H]23)cc1
C974	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	OCC12[C@@H]3C4[C@H]1N([C@@H]1C([C@H](N3C(=O)OC)C1(CO)[C@@H]4c1ccccc1)[C@@H]2c1ccccc1)C(=O)OC
C975	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	OCC12[C@H]3C4[C@@H]1N([C@H]1C([C@@H](N3C(=O)OC(C)(C)C)C1(CO)[C@H]4c1ccccc1)[C@@H]2c1ccccc1)C(=O)OC(C)(C)C
C976	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	OCC12[C@@H]3C4[C@H]1N(Cc1ccccc1)[C@@H]1C([C@H](N3Cc3ccccc3)C1(CO)[C@H]4c1ccccc1)[C@H]2c1ccccc1
C977	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)CCCOc1nn(Cc2ccccc2)c2c1cccc2
C978	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@]12OC(C)(NC(=O)[C@H]3C[C@H]4[C@@H](Cc5c[nH]c6cccc4c56)N(C)C3)C(=O)N1[C@@H](Cc1ccccc1)C(=O)N1CCC[C@@H]21
C979	Training	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	Oc1c(cc(C)c(CC2=NCCN2)c1C)C(C)(C)C
C980	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC(=O)S[C@@H]1CC2=CC(=O)CC[C@@]2(C)[C@@H]2CC[C@@]3(C)[C@H](CC[C@@]43CCC(=O)O4)[C@H]12
C981	Training	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	Nc1ccc(cc1)c1cc(cc(c1)C(F)(F)F)C(F)(F)F
C982	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1ccccc1C(=O)C)CN1CCN(CC1)c1cccc(C)c1C
C983	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cc(OC)cc1)C(=O)C)CN1CCN(CC1)c1ccccc1C
C984	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	[nH]1c2cc(OC)ccc2c2c1[C@H]1C[C@H]3[C@@H](C[C@@H](OC(=O)/C=C/c4cc(OC)c(OC)c(OC)c4)[C@@H](OC)C3C(=O)OC)CN1CC2
C985	Training	inhibitor	60	noninhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1c(cccc1)C(=O)c1ccccc1)CN(CC)CC
C986	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](CN1CCN(CC1)c1cccc(OC)c1)c1c(CCc2ccccc2)c2c(o1)cccc2

C987	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cc(Oc2ccccc2)cc1)C(=O)CCc1ccccc1)CN1CCCCC1
C988	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCCN3CCc4cc(OC)c(OC)cc4C3)cccc2)c1
C989	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCCN3CCN(C)CC3)cccc2)c1
C990	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	N(CC)C(=O)Nc1ccc(S[C@@H]2CC3=CC(=O)CC[C@]3(C)[C@@H]3CC[C@@]4(C)[C@H](CC[C@@H]4C(=O)C)[C@H]23)cc1
C991	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Cc1cccc(c1NC(=O)c1ccc(cc1)C(C)C)C(=O)NCCN1CCc2cc(c(cc2C1)OC)OC
C992	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)c1ccc(cc1)C(=O)Nc1cccc(c1C(=O)NCCN1CCc2cc(c(cc2C1)OC)OC)Cl
C993	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCNC(=O)c1ccccc1NC(=O)c1ccc(cc1)OCc1ccccc1
C994	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCc1ccc(cc1)NC(=O)c1ccccc1NC(=O)c1ccsc1
C995	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCc1ccc(cc1)NC(=O)c1ccccc1NC(=O)c1ccoc1
C996	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Cc1ccc(cc1C)C(=O)Nc1ccccc1C(=O)Nc1ccc(cc1)CCN1CCc2cc(c(cc2C1)OC)OC
C997	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCc1ccc(cc1)NC(=O)c1ccccc1NC(=O)c1ccc2ccccc2n1
C998	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCC(=O)c1cnc(cn1)C(=O)Nc1ccccc1C(=O)Nc1ccc(cc1)CCN1CCc2cc(c(cc2C1)OC)OC
C999	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCNC(=O)c1ccccc1NC(=O)c1ccc2ccccc2c1
C1000	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCc1ccc(cc1)NC(=O)c1ccccc1NC(=O)c1cc2c(nc1)CCCC2
C1001	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCNC(=O)c1ccccc1NC(=O)c1ccc(cc1)C1CCCCC1
C1002	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(CCc1ccc(cc1)NC(=O)c1ccccc1NC(=O)c1cc2ccccc2nc1)Cc1ccc(c(c1)F)F
C1003	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(CCc1ccc(cc1)NC(=O)c1ccccc1NC(=O)c1cc2ccccc2nc1)Cc1ccc(c(c1)OC)O
C1004	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)(C)c1ccc(cc1)C(=O)Nc1ccccc1C(=O)NCCN1CCc2cc(c(cc2C1)OC)OC
C1005	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)c1ccc(cc1)C(=O)Nc1ccc(cc1C(=O)NCCN1CCc2cc(c(cc2C1)OC)OC)Cl
C1006	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCNC(=O)c1ccccc1NC(=O)c1cc2ccccc2cn1
C1007	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCc1ccc(cc1)C(=O)Nc1ccccc1C(=O)NCCN1CCc2cc(c(cc2C1)OC)OC
C1008	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCNC(=O)c1ccccc1NC(=O)c1ccc(cc1)Br
C1009	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCNC(=O)c1ccccc1NC(=O)c1ccc(cc1)Cc1ccccc1
C1010	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCc1ccc(cc1)NC(=O)c1ccccc1NC(=O)c1cccnc1
C1011	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCc1ccc(cc1)NC(=O)c1ccccc1NC(=O)c1cnccn1
C1012	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1ccc(cc1OC)CN1CCc2ccc(cc2C1)NC(=O)c1ccccc1NC(=O)c1cnc2ccccc2n1
C1013	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(CCc1ccc(cc1)NC(=O)c1ccccc1NC(=O)c1cc2ccccc2nc1)CCc1ccc(c(c1)OC)OC
C1014	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Cc1nc(cs1)C(=O)Nc1ccccc1C(=O)Nc1ccc(cc1)CCN1CCc2cc(c(cc2C1)OC)OC
C1015	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCNc1c2c(c(c3n2CCCC3)C#N)ncn1
C1016	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCCN1CCN(CC1)c1c2c(c(c3n2CCCC3)C#N)ncn1
C1017	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(c(c1)CCN1CCN(CC1)c1c2c(c(c3n2CCCC3)C#N)ncn1)Cl
C1018	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(cc(c1)Cl)CCN1CCN(CC1)c1c2c(c(c3n2CCCC3)C#N)ncn1
C1019	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(cc(c1)[N+](=O)[O-])CCN1CCN(CC1)c1c2c(c(c3n2CCCC3)C#N)ncn1
C1020	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1CCN1CCN(CC1)c1c2c(c(c3n2CCCC3)C#N)ncn1)F)F
C1021	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1CCN1CCN(CC1)c1c2c(c(c3n2CCCC3)C#N)nc(n1)c1ccncc1)F)F
C1022	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCN1CCN(CC1)c1c2c(c(c3n2CCCC3)C(=O)c2ccccc2)ncn1
C1023	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Cc1nc(no1)c1c2n(c3c1ncnc3N1CCN(CC1)CCc1ccccc1)CCCC2
C1024	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(c1OC)CNC(=O)c1c2n(c3c1ncnc3N1CCN(CC1)CCc1ccc(c(c1)F)F)CCCC2
C1025	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccnc(c1)CNC(=O)c1c2n(c3c1ncnc3N1CCN(CC1)CCc1ccc(c(c1)F)F)CCCC2
C1026	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CO[C@@H](CCc1ccccc1)c1ccccc1OC[C@H](CN1CCN(CC1)c1ccc(cc1)F)O
C1027	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)N(C[C@H](COc1ccccc1C(=O)CCc1cccc2c1cccc2)O)C(C)C
C1028	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccc(cc1)OC[C@H](CN1CCCCC1)O
C1029	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1cc(ccc1OC[C@@H](CN1CCN(CC1)Cc1ccccc1)O)OCc1ccccc1

C1030	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC(=O)c1ccc(cc1)OC[C@H](CN1CCN(CC1)c1ccc(cc1)F)O
C1031	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCN(CC)C[C@H](COc1ccccc1C(=O)CCc1ccccc1)O
C1032	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CN1CCCC1)O
C1033	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1ccccc1N1CCN(CC1)C[C@@H](COc1ccccc1C(=O)CCc1ccccc1)O
C1034	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Cc1c(c(=O)n(n1C[C@@H](CN(C(C)C)C(C)C)O)c1ccccc1)C(=O)c1ccccc1
C1035	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCNC[C@@H](Cn1c(c(c(=O)n1c1ccccc1)C(=O)CCc1ccccc1)C)O
C1036	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Cc1c(c(=O)n(n1C[C@@H](CNC(C)C)O)c1ccccc1)C(=O)CCc1ccccc1
C1037	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	OC[C@]1(O)O[C@H]([C@H]2C[C@H](C)[C@H](O2)[C@]2(CC)CC[C@@H](O2)[C@]2(C)CC[C@@]3(C[C@@H](O)[C@@H](C)C(O3)[C@H](C)[C@@H](OC)[C@@H](C)C(=O)O)O2)C(C)C[C@@H]1C
C1038	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Cc1ccccc1N1CCN(CC1)C[C@@H](Cn1c(c(c(=O)n1c1ccccc1)C(=O)CCc1ccccc1)C)O
C1039	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Cc1c(c(n(n1)c1ccccc1)OC[C@H](CN(C(C)C)C(C)C)O)C(=O)c1ccccc1
C1040	Training	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC1([C@@H](C(c2cc(ccc2O1)C#N)N(Cc1ccccc1)CC(=O)OC(C)(C)C)O)C
C1041	Test	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c1(ccccc1CCc1ccccc1)OCc1cc(c(cc1)OC)OC
C1042	Test	noninhibitor	59	inhibitor	noninhibitor	noninhibitor	noninhibitor	n1cccc(c1)COc1c(cccc1)CCc1ccccc1
C1043	Test	noninhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	n1(n(c(c(c1=O)C(=O)c1ccccc1)C)CC(CNC(C)(C)C)O)c1ccccc1
C1044	Test	noninhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	n1(n(c(c(c1=O)C(=O)c1ccccc1)C)CC(CN(C(C)C)C(C)C)O)c1ccccc1
C1045	Test	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1c1cc(=O)c2c(cc(cc2o1)O)O)O)O
C1046	Test	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1c2c(=O)cc(oc2cc(c1)OC)c1ccc(cc1)OC
C1047	Test	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c1(ccccc1CCc1ccccc1)OCc1cc(cc(c1)OC)OC
C1048	Test	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	o1c(c(OC)c(=O)c2c1cc(OC)cc2O)c1cc(O)c(OC)cc1
C1049	Test	noninhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccccc1CCc1ccccc1OCc1ccccc1
C1050	Test	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(Nc1cc(c(OCC(CNC(C)(C)C)O)cc1)C(=O)C)N(CC)CC
C1051	Test	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1SC([C@@H](NC(=O)[C@@H](NC(=O)CNC(=O)[C@H](NC(=O)[C@@H](N)Cc2ccc(O)cc2)C1(C)C)Cc1ccccc1)C(=O)O)(C)C
C1052	Test	noninhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	[C@@H]1([C@@H](C(=O)O[C@@H]([C@]([C@@H]([C@@H](C(=O)[C@@H](C[C@]([C@@H]([C@H]1C)O[C@H]1[C@H]([C@H](C[C@@H](O1)C)N(C)C)O)(O)C)C)C)O)(O)C)CC)C)O[C@H]1C[C@]([C@@H]([C@@H](O1)C)O)(OC)C
C1053	Test	noninhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	[C@@]12([C@@]([C@H]([C@H]([C@@H]3[C@@]1([C@H](CCC3(C)C)O)C)O)OC(=O)C)(O[C@](CC2=O)(C=C)C)C)O
C1054	Test	noninhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	C1Cc2c([C@]1(C#N)CCCN(CCc1ccc(c(c1)OC)OC)C)ccc(c2OC)OC
C1055	Test	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c1(ccccc1CCc1cccc(c1)OC)OCc1ccc(cc1)OC
C1056	Test	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(ccc(c1)CCNC(=O)NC(C)C)OCC(O)CNC(C)C
C1057	Test	noninhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	N1([C@@H](C[C@H]2[C@H](C1)CCCC2)C(=O)NC(C)(C)C)C[C@@H]([C@@H](Cc1ccccc1)NC(=O)[C@@H](NC(=O)c1nc2c(cc1)cccc2)CC(=O)N)O
C1058	Test	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c12N3CCCc1cc1c(c2CCC3)[se]c2c(c1c1sc(cc1)C(=S)N1CCCCC1)ccc(=[N+](C)C)c2
C1059	Test	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c(c(c2c(c1)OC(c1ccccc1)CC2=O)O)C)OC
C1060	Test	noninhibitor	59	noninhibitor	noninhibitor	inhibitor	noninhibitor	COc1ccc(cc1)c1cc(=O)c2c(OC)c(OC)c(OC)c(OC)c2o1
C1061	Test	noninhibitor	59	inhibitor	noninhibitor	inhibitor	inhibitor	c1(ccccc1)[P+](c1ccccc1)(c1ccccc1)c1ccccc1
C1062	Test	noninhibitor	59	noninhibitor	noninhibitor	inhibitor	noninhibitor	C(=O)(c1c(n(nc1C)C)OCC(CN(C(C)C)C(C)C)O)c1ccccc1
C1063	Test	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c12C=C3C4C(c1sc1c(c2c2ccccc2)ccc(=[N+](C)C)c1)CCCN4CCC3
C1064	Test	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c12C=C3C4C(c1[se]c1c(c2c2ccccc2)ccc(=[N+](C)C)c1)CCCN4CCC3
C1065	Test	inhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	c1cc2c(c3c([se]c2cc1N(C)C)cc(=[N+](C)C)cc3)c1sc(cc1)C(=S)N1CCCCC1
C1066	Test	inhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	n1ccc(cc1)COc1c(cccc1)CCc1cccc(c1)OC
C1067	Test	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c2c(c1)/C(=C/CCN1Cc3c(CC1)cc(c(c3)OC)OC)/CCC2)OC
C1068	Test	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	[C@@H]1(C(=C(NC(=C1C(=O)OC)C)C)C(=O)OC1CN(Cc2ccccc2)CCC1)c1cc(ccc1)[N+](=O)[O-]
C1069	Test	inhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1CCN(CCCNC(=O)c2c(OCC)cccc2)CC1
C1070	Test	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	C1(C(=O)N(c2c(S[C@H]1c1ccc(cc1)OC)cccc2)CCN(C)C)OC(=O)C
C1071	Test	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c1(C(C#N)(C(C)C)CCCN(CCc2cc(c(cc2)OC)OC)C)cc(c(c(c1)OC)OC)OC
C1072	Test	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	N(c1c(cccc1)CCc1cccc(c1)OC)Cc1cc(ccc1)OC

C1073	Test	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	N(c1c(cccc1)CCc1cccc(c1)OC)Cc1cc(c(cc1)OC)OC
C1074	Test	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	C1(=O)C2=CC[C@H](c3ccccc3)O[C@@]32[C@](C(=C1OC)OC)(c1c(c2c(c(c1OC)OC)O[C@H](C[C@@H]2OC)c1ccccc1)O3)OC
C1075	Test	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	C1(=C(NC(=C([C@@H]1c1cccc(c1)[N+](=O)[O-])C(=O)OC)C)C)C(=O)OCCCN1CCC(CC1)(c1ccccc1)c1ccccc1
C1076	Test	inhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1(=C(NC(=C(C1c1cc([N+](=O)[O-])ccc1)C(=O)OC)C#N)C)C(=O)OC(C)C
C1077	Test	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	C1(=O)[C@@H](N(C(=O)[C@@H](N(C(=O)[C@@H](N(C(=O)[C@H](NC(=O)[C@@H](NC(=O)[C@@H](N(C(=O)[C@@H](NC(=O)[C@@H](N(C(=O)CN(C(=O)[C@@H](NC(=O)[C@@H](N1C)C(=O)[C@H](C)C/C=C/C)C(C)C)C)CC(C)C)C(C)C)CC(C)C)C)C)CC(C)C)CC(C)C)C(C)C
C1078	Test	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c1(ccccc1CCc1cccc(c1)OC)OCc1c(c(ccc1)OC)OC
C1079	Test	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c1(c(cc2c(c1)CCN(CCc1ccc(cc1)NC(=O)c1c(cccc1)NC(=O)c1cc3c(nc1)cccc3)C2)OC)OC
C1080	Test	noninhibitor	59	noninhibitor	noninhibitor	inhibitor	noninhibitor	C(=O)(c1c(n(nc1C)c1ccccc1)NCCC)c1ccccc1
C1081	Test	inhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	c1(ccccc1CCc1ccccc1)OCc1c(cccc1)OC
C1082	Test	noninhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	n1(n(c(c(c1=O)C(=O)CCc1ccccc1)C)CC(CNC(C)C)O)c1ccccc1
C1083	Test	noninhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	n1(n(c(c(c1=O)C(=O)CCc1ccccc1)C)CC(CNCCC)O)c1ccccc1
C1084	Test	noninhibitor	59	noninhibitor	noninhibitor	inhibitor	noninhibitor	n1(n(c(c(c1=O)c1sccc1)C)CC(CNC(C)(C)C)O)c1ccccc1
C1085	Test	noninhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	c1(ccccc1CCc1cccc(c1)OC)OCc1ccccc1
C1086	Test	noninhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	n1(n(c(c(c1=O)C(=O)CCc1ccccc1)C)CC(CN1CCN(CC1)c1ccccc1C)O)c1ccccc1
C1087	Test	noninhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c12N3CCCc1cc1c(c2CCC3)sc2c(c1c1sc(cc1)C(=S)N1CCOCC1)ccc(=[N+](C)C)c2
C1088	Test	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1(N=C(/C(=C(\c2ccccc2)/NCCC)/C1=O)C)C
C1089	Test	noninhibitor	59	inhibitor	inhibitor	noninhibitor	inhibitor	n1ccccc1COc1c(cccc1)CCc1cccc(c1)OC
C1090	Test	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1cc(c2oc3ccccc3c(=O)c2)ccc1OC
C1091	Test	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c(c(c2c(c1OC)oc(c(c2=O)OC)c1cc(c(cc1)OC)OC)OC)OC)OC
C1092	Test	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1c(oc2cc(cc(c2c1=O)O)O)c1cc(c(c(c1)OC)OC)OC
C1093	Test	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc(c1)[C@H]1[C@@H]([C@@H]([C@@H](CO)O1)O)O)C(=O)N
C1094	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=O)N1CCN(CC(=O)N2CCOCC2)CC1)OC
C1095	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCN(C1CCCCC1)CC
C1096	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)OC1C[C@@H]2CC[C@H](C1)N2C
C1097	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cccc2)c(ccc1)Nc1ccccc1
C1098	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(C(=O)C=CC2=O)nc2c1CCC2
C1099	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(ccc(c2)NC(=O)/C=C/c2ccccc2)[n+](c(cc1)/C=C/c1ccc(cc1)C(CCCl)CCCl)CC
C1100	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)nc(cc2C(=O)NCCCNCCNC(=O)c1cccc(c1OCc1ccccc1)OCc1ccccc1)c1ccccc1
C1101	Test	noninhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c1cc(c(cc1CN1CCCN(Cc2ccc(c(c2)OC)OC)C1c1ccc(cc1)N(CCCl)CCCl)OC)OC
C1102	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CN(c1ccccc1)C[C@H](COCC(C)C)N1CCCC1
C1103	Test	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c12c(cccc2)c(ccc1)CN(C/C=C/c1ccccc1)C
C1104	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c2c3c1C[C@@H]1[C@@]4(CC[C@@H]([C@@H]([C@]34CCN1CC1CCC1)O2)O)O)O
C1105	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c2c3c1C[C@@H]1[C@@]4(CCC(=O)[C@@H]([C@]34CCN1CC=C)O2)O)O
C1106	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[C@@H]1c2cccc(c2CN(C1)C)N
C1107	Test	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc(c1)OC[C@@H](CNCCc1ccc(c(c1)OC)OC)O)C
C1108	Test	noninhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c12c(c(cc(c2)O[C@@H]2C[C@@H]([C@@H]([C@@H](C)O2)OC(=O)C)O[C@H]2C[C@@H]([C@@H]([C@H](C)O2)OC)O)O)c(c2c(c1)C[C@@H]([C@H](C2=O)O[C@@H]1C[C@H]([C@H]([C@H](C)O1)O)O[C@H]1C[C@@H]([C@H]([C@H](C)O1)O)O[C@H]1C[C@@H]([C@H]([C@H](C)O1)OC(=O)C(C)C)OC)[C@H](C(=O)[C@@H]([C@H](C)O)O)OC)O
C1109	Test	noninhibitor	61	noninhibitor	inhibitor	noninhibitor	noninhibitor	c1cc(cc(c1/C(=C(\C)/n1ccnc1)/OCCOc1ccc(cc1)Cl)Cl)Cl
C1110	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1c2c(cc(c1OCCN(CC)CC)OCCN(CC)CC)oc(=O)cc2C
C1111	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(cc3c1OCO3)n(cc(c2=O)C(=O)O)CC
C1112	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(c(c1)OCC=C)OC[C@@H](CNC(C)C)O
C1113	Test	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(C[C@@H](C[N+](C)(C)C)OC(=O)CCCCCCCCCCCCCCC)O
C1114	Test	noninhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	C1CCC(CC1)C(C[C@H]1CCCCN1)C1CCCCC1
C1115	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)CCN

C1116	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1N1CCN(CCCN(C)C)CC1)NC(=O)C
C1117	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C1(c2ccccc2)C(=O)O[C@H](CCN2CCCCC2)O1
C1118	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1[C@H](C(=O)O)C)Cl)N1CC=CC1
C1119	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(c(c1)C)OC[C@H](CNCCn1cc(c(=O)[nH]c1=O)C)O
C1120	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(c(c1)Nc1cc(nc(n1)SCC(=O)O)Cl)C)C
C1121	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](C[N+](CC)(CC)C)O
C1122	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)/C(=N\CC(C)C)/N1CCN(CCCCCC)CC1
C1123	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](C[N+](C(C)C)(C(C)C)C)O
C1124	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(c(c1)C(=O)C)OC[C@H](CN1CCCCC1)O
C1125	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(ncnc1N(C)C)n(cn2)[C@H]1[C@@H]([C@@H]([C@@H](CO)O1)NC(=O)[C@H](Cc1ccc(cc1)OC)N)O
C1126	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccnc(c1)N(Cc1ccc(cc1)OC)CCN(C)C
C1127	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@H](c1ccc(cc1)Cl)N1CCN(Cc2ccc(cc2)C(C)(C)C)CC1
C1128	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(nc(n2)N(CCO)CCO)N2CCOCC2)nc(nc1N1CCOCC1)N(CCO)CCO
C1129	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(ncn2)N2CCOCC2)ncnc1N1CCOCC1
C1130	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(nc(c(n2)Cl)N2CCOCC2)nc(nc1N1CCOCC1)N1CCNCC1
C1131	Test	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1cc(cc2c1C[C@@H]1[C@H]3CCCC[C@]23CCN1C)OC
C1132	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cc(cc1)OC)[nH]c1c2CCN2[C@@H]1C[C@@H]1[C@H](C(=O)O)C([C@@H](C[C@@H]1C2)O)OC
C1133	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc2)c(ccc1)C(=O)N(CCCC)CCN(CC)CC
C1134	Test	noninhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c12c3c4c(c(c1O)C)O(C@)(C4=O)C)O/C=C/[C@@H]([C@@H](C)[C@H]([C@H](C)C[C@H](C)[C@H](C)[C@H])/C=C/C(C(=O)Nc(cc3O)c2O)/C)C)O)O)OC(=O)C)OC
C1135	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@@H](C(=O)OCCN1CCN(CCC(=O)c2ccc(cc2)OC)CC1)CC
C1136	Test	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc(cc1)CCC(=O)OCCN1CCN(CC1)CCOC(=O)CCc1ccccc1
C1137	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@H](C(=O)OCCN(CCCN(CCOC(=O)[C@H](c1ccccc1)CC)C)C)CC
C1138	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)NC(=O)c1ccccc1OCCN(CC)CC
C1139	Test	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c1cnc(nc1)N1CCN(CCCCN2C(=O)CC3(CC2=O)CCCC3)CC1
C1140	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[C@H](C(=O)OC1C[C@@H]2[C@@H]3[C@H]([C@H](C1)N2C)O3)CO
C1141	Test	noninhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	C1=C([C@H]2CC[C@@]3([C@H]4CC[C@]5(C[C@H](CC[C@@]5(C=O)[C@H]4CC[C@]23C)O)O)O)COC1=O
C1142	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc(c1)Cl)Nc1c2c(c(C)nc2nc[nH]1)C
C1143	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C1=C2CC[C@H]3[C@@H]4C[C@@H](C)[C@H](C(=O)C)[C@]4(C)CC[C@H]3[C@]2(C)CCC1=O
C1144	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(ccc1Cl)sc(=O)n2CC(=O)N1CCN(CC1)CCO
C1145	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)N[C@@H](C(Cl)(Cl)Cl)N1CCN(CC1)[C@H](C(Cl)(Cl)Cl)NC=O
C1146	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(c(c(c1)OC)OC)OC)nc(nc2N)N1CCN(C(=O)OCC(C)(C)O)CC1
C1147	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(c(c1C(=O)OCC[N+](CC)(CC)CC)OC)OC)OC
C1148	Test	noninhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1cc(cc(c1[C@@]1(Cn2ccnc2)OC[C@H](CSc2ccc(cc2)NC(=O)OCC)O1)Cl)Cl
C1149	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CC(=O)N([C@H]1CC[C@]2(CCCO2)C[C@@H]1N1CCCC1)C
C1150	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C1=C(c2ccc(cc2)OCCN(CC)CC)c2ccc(cc2C1)OC
C1151	Test	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	[illegible]
C1152	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(ccc(c2)S(=O)(=O)NCCCCN)c(ccc1)Cl
C1153	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)c1ccc(cc1)CC[C@H](C)CC(=O)OCCN(C)C
C1154	Test	noninhibitor	61	noninhibitor	inhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[C@@H](c1c(c2ccccc2oc1=O)O)CC(=O)C
C1155	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(ccc(c1)C[C@H]1COC(=O)N1)[nH]cc2CCN(C)C
C1156	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c3c(ccc1)c(=O)n(c(=O)c3cc(c2)[N+](=O)[O-])CCN1CCCC1
C1157	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)n1c(=O)cc(C)n1C
C1158	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C1=NCC(=O)Nc2ccc(cc12)[N+](=O)[O-]

C1159	Test	noninhibitor	61	noninhibitor	inhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)c(=O)[nH]c1cccnc1n2C(=O)CN1CCN(CC1)C
C1160	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12cnc(nc1n(cc(c2=O)C(=O)O)CC)N1CCCC1
C1161	Test	noninhibitor	61	noninhibitor	inhibitor	noninhibitor	noninhibitor	CCCCCCCCCCCCCCCC[C@@H]([C@H](CO)N)O
C1162	Test	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C(c1ccccc1)(C1CCN(CCC[C@H](c2ccc(cc2)C(C(=O)O)(C)C)O)CC1)O
C1163	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(C[C@@H](C[N+](C)(C)C)O)O
C1164	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)N1CCN(C[C@@H](CO)O)CC1
C1165	Test	noninhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1cc(ccc1[C@H](C1(CCCCC1)O)CN(C)C)O
C1166	Test	noninhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	C1=C2C[C@H](CC[C@@]2(C)[C@@H]2CC[C@]3(C)[C@@H](CC[C@@]3(C(=O)C)O)[C@@H]2C1)O
C1167	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C(=CCCN[C@@H](C)Cc1ccc(c(c1)OC)OC)c1ccccc1CC2
C1168	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(nc(n2)N(CCO)CCO)N2CCC[C@H](C2)O)nc(nc1N1CCC[C@H](C1)O)N(CCO)CCO
C1169	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1=C2[C@@H]3CC(C)(C)CC[C@]3(C(=O)O)CC[C@@]2(C)[C@]2(C)CC[C@H]3[C@](C)(CC[C@@H](C3(C)C)O)[C@H]2C1
C1170	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc2c1[C@@H]1CC[C@@]3(C)[C@@H](C[C@H](C3O)O)[C@H]1CC2)O
C1171	Test	noninhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	C1=C(C(=O)[C@@]2(CC(=C[C@@H]3[C@@H]4C(C)(C)[C@@]4([C@@H]([C@@H](C)[C@]3([C@H]12)O)O)OC(=O)CCC)CO)O)C
C1172	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C(=C1CCN(CC1)C)c1ccccc1C2O
C1173	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(=C(C)C)CC1=C([C@]2(C(=O)[C@](C1=O)(CC=C(C)C)C[C@H](CC=C(C)C)[C@@]2(C)CCC=C(C)C)CC(C)C)O
C1174	Test	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c12c3cccc1C1=C[C@@H](C(=O)N[C@@H](C)CO)CN([C@H]1Cc2c[nH]3)C
C1175	Test	noninhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c12c(c(nc(n2)N(CCO)C)N2CCCCC2)nc(nc1N1CCCCC1)N(CCO)C
C1176	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(nc(n2)N(CCO)CCO)N)nc(nc1N)N(CCO)CCO
C1177	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(c(nc(n2)N2CC[N+](CC2)(C)C)N2CCCCC2)nc(nc1N1CCCCC1)N(CCO)CCO
C1178	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C=Cc1ccccc1N2CCCN1CCN(CC1)CCO
C1179	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@](CCN1CCCCC1)(C1CCCCC1)O
C1180	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)c(=O)n1c(/C(=C\c3ccc(c(c3)O)O)/OCC1)n2
C1181	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc2c3c(c1)CCN([C@@H]3Cc1ccc(c(c21)O)O)C
C1182	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C[C@H](C)NC[C@@H](c1cc(cc(c1)O)O)O)O
C1183	Test	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c12c3c4c(c5c1c(c(cc2OC)O)C(=O)C(=C5C[C@@H](C)OC(=O)c1ccccc1)OC)C(=C(C(=O)c4c(cc3OC)O)OC)C[C@@H](C)OC(=O)Oc1ccc(cc1)O
C1184	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CN1[C@H](c2nc3ccccc3c(=O)n2[C@H]1c1cccc(c1)O)C
C1185	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1[C@H](CNCCCCCCNC[C@@H](c1ccc(c(c1)O)O)O)O)O)O)O
C1186	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1C[C@@H]1c2cc(c(cc2CCN1)O)O)O)O
C1187	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1CC[C@H](C)NCCc1ccc(c(c1)O)O)O
C1188	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc2c1[C@@H]1CC[C@@]3(C(=O)CC[C@H]3[C@@H]1CC2)C)O
C1189	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(ccc(c2)O)c2c(cc1)[C@H]1CCC(=O)[C@@]1(C)CC2
C1190	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)CC[C@H](C)N[C@@H](C)[C@H](c1ccc(cc1)O)O
C1191	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1CCN[C@@H](C)[C@@H](c1ccc(cc1)O)O)O
C1192	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C1=C2CC[C@H]3[C@@H]4CC[C@]([C@]4(C)CC[C@@H]3[C@@]2(C)CCC1=O)O
C1193	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCN(CCN(C(=O)C(c1ccccc1)(c1ccccc1)OCC)C)C
C1194	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=N\OC(=O)NC)/C(C)(C)S(=O)(=O)C
C1195	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(ccnc2)c(ccc1)S(=O)(=O)NCCNC(=N)N
C1196	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1CCN[C@@H](C)[C@H](c1ccc(c(c1)NS(=O)(=O)C)O)O)OC
C1197	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C1(C(=O)N(c2ccccc2)N(c2ccccc2)C1=O)CC[S@](=O)c1ccccc1
C1198	Test	noninhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1OC[C@@H](CNCCCCCCCCC)O)SC(C)C
C1199	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cc(c(c1)OC)OC)nc(nc2N)N1CCN(C(=O)c2nnc(o2)SC)CC1
C1200	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=C(C)C)CC/C(=C/CC/C(=C/CSC[C@@H](C(=O)O)N)/C)/C
C1201	Test	noninhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c12c(c(ccc2S(=O)(=O)O)NC(=O)c2ccc(c(c2)NC(=O)c2cccc(c2NC(=O)Nc2cc(ccc2C)C(=O)Nc2cc(ccc2C)C(=O)Nc2c3c(cc(cc3S(=O)(=O)O)S(=O)(=O)O)c(cc2)S(=O)(=O)O)c(cc(c1)S(=O)(=O)O)S(=O)(=O)O

C1202	Test	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c12c3c(cccc3OC[C@H](CNCCOc3ccccc3OC)O)[nH]c1cccc2
C1203	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=N\OC(=O)NC)(\C)/SC
C1204	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1=CCC(=CC1)[C@H](C(=O)N[C@@H]1C(=O)N2C(=C(C)CS[C@@H]12)C(=O)O)N
C1205	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1ccccc1S2)C[C@@H](C)CN(C)C
C1206	Test	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc2c(c1)N(c1c(cccn1)S2)CCCN(C)C
C1207	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C[C@@H](C)NCCC1c2ccccc2Sc2ccccc12
C1208	Test	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C(c1ccccc1)C[C@H](C)[N+](CC)(C)C
C1209	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c3c(c(c4c(c3C)c[n+](cc4)CCN(CC)CC)C)[nH]c1cccc2
C1210	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(cc[n+](c1)C)c1cc[n+](cc1)C
C1211	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cccc1)[nH]cc2CN(C)C
C1212	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(#N)c1c([nH]nc1c1c2c(cccc2)[nH]c1)N
C1213	Test	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc(c(c1)C)N1CCN(CCc2n3c(CCCC3)nn2)CC1
C1214	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(nc(n2)N(C)C)N2CCCCC2)nc(nc1N1CCCCC1)N(C)C
C1215	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cccc2)nc2c(c1)cccc2
C1216	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cccc1)nc(cc2)N1CCNCC1
C1217	Test	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cccc1)nc1c(c2N)CCN1C1CCCCC1
C1218	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)Cc1ccccn1
C1219	Test	noninhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c12c(cccc1)oc(c2CC)[C@H](CNCCC)O
C1220	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccnc(c1)N(Cc1ccsc1)CCN(C)C
C1221	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc[n+](cc1)CC1=C(C(=O)O)N2C(=O)[C@H]([C@@H]2SC1)NC(=O)/C(=N\OC(C(=O)O)(C)C)/c1csc(n1)N
C1222	Test	noninhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1ccc(cc1)N(C1CCN(CC1)C)Cc1cccs1
C1223	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1CN(c1nccs1)CCN(C)C)OC
C1224	Test	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)Cl)CCN
C1225	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c2c(c1C(=O)C)OCCO2)OC[C@@H](CN1CCN(C(=O)/C=C/c2cc(c(c(c2)OC)OC)OC)CC1)O
C1226	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)/C=C/CN1CCN(C(c2ccccc2)c2ccccc2)CC1
C1227	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)n(c(CN1CCN(C/C=C/c3ccccc3)CC1)n2)CCC(=O)c1ccccc1
C1228	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)n(c(CN1CCCC1)n2)Cc1ccc(cc1)Cl
C1229	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)/C(=C\CCN1CCN(CC1)CCO)/c1cc(ccc1S2)Cl
C1230	Test	inhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc2c(c1)C(=C1CCN(CC1)C)c1cc(ccc1O2)Cl
C1231	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)/C(=C/CCN1CCN(CCC(=O)NC)CC1)/c1cc(ccc1S2)Cl
C1232	Test	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc2c1c(c(c(=O)o2)Cl)C)OP(=S)(OCC)OCC
C1233	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C=Cc1ccccc1/C/2=C/CCN(C)C
C1234	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cc(cc1)Cl)ncc(c2N[C@H](C)CCCN(CC)CC)C
C1235	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(c2nc(c(=O)c(c(=O)c3ccc(Cl)cc3)n2C)C)=O)C(=O)N[C@H](C)CCCN(CC)CC
C1236	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(c2nc(c(=O)c(c(=O)c3ccc(Cl)cc3)n2C)C)=O)C(=O)N[C@H](C)CCCN(CC)CC
C1237	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(c2nc(c(=O)c(c(=O)c3ccc(Cl)cc3)n2C)C)=O)C(=O)N[C@H](C)CCCN(CC)CC
C1238	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(c2nc(c(=O)c(c(=O)c3ccc(Cl)cc3)n2C)C)=O)C(=O)N[C@H](C)CCCN(CC)CC
C1239	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(c2nc(c(=O)c(c(=O)c3ccc(Cl)cc3)n2C)C)=O)C(=O)N[C@H](C)CCCN(CC)CC
C1240	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(c2nc(c(=O)c(c(=O)c3ccc(Cl)cc3)n2C)C)=O)C(=O)N[C@H](C)CCCN(CC)CC
C1241	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(c2nc(c(=O)c(c(=O)c3ccc(Cl)cc3)n2C)C)=O)C(=O)N[C@H](C)CCCN(CC)CC
C1242	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(NC(=O)C1[C@H]2C(=O)N[C@H](C=O)NC(=O)NC(=O)N[C@H](C=O)NC(=O)OCC)C(=O)N2CCC)CCCCC3)CCc2ccc(cc2)OCC)CCC)C[C@@H](CCC)C)cc1
C1243	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(cc1C(c1ccccc1)NC(=O)C[C@H](C=O)N[C@@H](C=O)NC(=O)N[C@H](C=O)NC(=O)OCC)C(=O)N[C@@H](C=O)N[C@@H](C=O)N[C@@H](C=O)NC(=O)[C@@H](CCC)C)C(=O)N[C@@H](CCC)C)C(=O)N[C@@H](CCC)C)C(=O)N[C@@H](CCC)C
C1244	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(c2nc(c(=O)c(c(=O)c3ccc(Cl)cc3)n2C)C)=O)C(=O)N[C@H](C)CCCN(CC)CC

C1245	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C[C@H]1C(=O)O[C@@H](C(=O)N2[C@H](C(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)NCC(=O)N([C@H](C(=O)N1)C(C)C)C)[C@H](C)CC)C)[C@@H](C)CC)C)CC(=O)N1[C@H](CCC1)COC(C)(C)C)C(C)C)C(C)C)C)CCCC2)C)OC
C1246	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)/C(=C(\c1ccc(cc1)OCCN(C)C)/c1ccc(cc1)O)/CC
C1247	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C[C@H]1C(=O)O[C@@H](C(=O)N2[C@H](C(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)NCC(=O)N([C@H](C(=O)N1)C(C)C)C)[C@H](C)CC)C)[C@@H](C)CC)C)CCOC(=O)C)C)C(C)C)C(C)C)C)CCCC2)C)OC
C1248	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C[C@H]1C(=O)O[C@@H](C(=O)N2[C@H](C(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)NCC(=O)N([C@H](C(=O)N1)C(C)C)C)[C@H](C)CC)C)[C@@H](C)CC)C)C/C=C/C(=O)OC(C)(C)C)C)C(C)C)C(C)C)C)CCCC2)C)OC
C1249	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(=C\C[C@@H](C)[C@H]([C@H]1C(=O)N[C@@H](C(=O)N(CC(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@@H](C(=O)N1C)C(C)C)C)CC(C)C)C)CC(C)C)C)C)CC(C)C)C)C(C)C)CC(C)C)C)C)CC)O)/C
C1250	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(=C\C[C@@H](C)[C@H]([C@H]1C(=O)N[C@H](C(=O)N(CC(=O)N([C@@H](C(=O)N[C@@H](C(=O)N([C@@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N1C)C(C)C)C)CC(C)C)C)CC(C)C)C)C)CC(C)C)C)C(C)C)CC(C)C)C)C)CCC)O)/C
C1251	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C[C@H]1[C@H]2[C@H](C)[C@]3(C)[C@H]([C@@H]4/C=C/C[C@@H](C(=O)[C@@](/C=C/OC(=O)O[C@@]24C(=O)N1)(C)O)C)O3
C1252	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@](c1ccc(c(c1)OC)OC)(Cc1ccccc1)CCCN(CCc1ccc(c(c1)OC)OC)C
C1253	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@](c1ccc(cc1)OC)(CCN(CCc1ccc(c(c1)OC)OC)C)C(C)C
C1254	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@@](c1cc(cc(c1)OC)OC)(CCCN(CCc1cc(cc(c1)OC)OC)C)C(C)C
C1255	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C1(c2ccccc2)CCN(CC1)CCCOC(=O)C1=C(C)NC(=C(C(=O)OC)[C@@H]1c1ccc(c(c1)OC)OC)C
C1256	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(Cc1ccc(cc1)Cl)nn(c2=O)C1CCCNCC1
C1257	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@@](c1ccc(c(c1)OC)OC)(CCCN(CCc1cccc(c1)OC)C)C(C)C
C1258	Test	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	C1=C(C(=O)[C@@]2(CC(=C[C@@H]3[C@H]4C(C)(C)[C@@]4([C@@H]([C@@H](C)[C@]3([C@H]12)O)OC(=O)CCC)OC(=O)CCC)CO)O)C
C1259	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)nc1c(c2NC(=O)CN2CCCCC2)CCN1Cc1ccccc1
C1260	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1c(cc(c(c1OC)OC)OC)C(=O)OCCCN1CCCN(CCCOC(=O)c2cc(c(c(c2)OC)OC)OC)CC1
C1261	Test	inhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C(c1ccccc1)OC1CCN(CC1)C
C1262	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C1(c2ccccc2)C(=O)N(CC)C[C@@H]1CCN1CCOCC1
C1263	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C(=O)N(c1ccc(cc1)[C@H](C)CC)[C@@H](c1ccc(cc1)OC)N2
C1264	Test	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(#CC(=O)Nc1cc2c(cc1)ncnc2Nc1cccc(c1)Br)C
C1265	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)OC1CCN(CCCC(=O)c2ccc(cc2)C(C)(C)C)CC1
C1266	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@@](c1ccccc1)(CCCN(CCc1ccccc1)C)C(C)C
C1267	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)[C@@H](C)CN1CCN(C[C@H](c2ccccc2)OCC)CC1
C1268	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@H](CCN1CCN(C[C@@H](c2ccccc2)OC)CC1)O
C1269	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c3cccc1C1=C[C@@H](C(=O)N[C@@]4(C(=O)N5[C@H](C(=O)N6[C@@H](CCC6)[C@@]5(O)O4)Cc4ccccc4)C(C)C)CN([C@@H]1Cc2c[nH]3)C
C1270	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c3cccc1C1=C[C@@H](C(=O)N[C@@]4(C(=O)N5[C@H](C(=O)N6[C@@H](CCC6)[C@@]5(O)O4)CC(C)C)C(C)C)CN([C@@H]1Cc2c[nH]3)C
C1271	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c3cccc1C1=C[C@@H](C(=O)N[C@@]4(C(=O)N5[C@H](C(=O)N6[C@H](CCC6)[C@]5(O)O4)Cc4ccccc4)C)CN([C@@H]1Cc2c[nH]3)C
C1272	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C1(=O)[C@H](C)C[C@](C)([C@@H]([C@@H](C)C([C@H](C(=O)O[C@H](CC)[C@](C)([C@@H]([C@H]1C)O)O)C)O[C@@H]1C[C@](C)([C@H]([C@H](C)O1)O)OC)O[C@@H]1[C@H]([C@@H](C[C@H](C)O1)N(C)C)O)O
C1273	Test	inhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OCCN(CC)CC
C1274	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@H]1C(=C)[C@@H]([C@@H]2[C@@](C(=O)[C@H](/C=C/C(C)(C)[C@@H]([C@@H]1OC(=O)C)OC(=O)C)C)(C[C@](C)([C@@H]2O)OC(=O)C)O)OC(=O)[C@@H](C)CC
C1275	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@H]1C(=C)[C@@H]([C@@H]2[C@@](C(=O)[C@H](/C=C/C(C)(C)[C@@H]([C@@H]1OC(=O)C)OC(=O)C)C)(C[C@](C)([C@@H]2O)OC(=O)C)O)OC(=O)c1cccnc1
C1276	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)cc(cc2)CN1CCC(CC1)C(c1ccc(cc1)F)c1ccc(cc1)F
C1277	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@@H]1[C@H]2[C@@](C(=O)[C@H](/C=C/C(C)(C)[C@@H]([C@@H]([C@H](C(=C)[C@@H]2OC(=O)C)OC(=O)C(C)C)OC(=O)C)OC(=O)C)C)(C[C@@H]1C)O
C1278	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(cnc1)C(=O)O[C@H]1C(/C=C/[C@@H](C(=O)[C@]2(C[C@](C)([C@@H]([C@@H]2[C@H](C(=C)[C@@H]([C@@H]1OC(=O)C)OC(=O)C)OC(=O)C(C)C)OC(=O)C)OC(=O)c1cccnc1)OC(=O)C)C)(C)C
C1279	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@H](C(=O)OCCN1CCN(CC1)CCOC(=O)[C@H](c1ccccc1)CC)CC
C1280	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)CCN[C@H](c1ccccc1)C
C1281	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)Sc1ccc(cc1)CO[C@@H](c1ccc(cc1Cl)Cl)Cn1ccnc1
C1282	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(c(c1)C1C(=C(C)N(C(=C1C(=O)OCC)C)CCN1CCOCC1)C(=O)OCC)C(F)(F)F
C1283	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)(C(=O)N(C)C)CCN1CCC(c2ccc(c(c2)C(F)(F)F)Cl)(CC1)O
C1284	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C(=Nc1cc(ccc1C2)F)N1CCN(CC1)C
C1285	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(c(c1)CCNCC1CCC(CC1)CNc1ccccc1Cl)Cl
C1286	Test	inhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc(c(c1)C1=NCC(=O)N(c2ccc(cc12)Cl)CCN(CC)CC)F
C1287	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)N1C2(C(=O)NC1)CCN(CCCC(c1ccc(cc1)F)c1ccc(cc1)F)CC2

C1288	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C=CCNC1=C2C(=O)C(=CC1=O)NC(=O)/C(=C/C=C\[C@H]([C@@H]\/C(=C/[C@@H](C)[C@@H]([C@@H](C[C@H](C)C2)OC)O)/C)OC(=O)N)OC)/C
C1289	Test	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=C/C)/CCC[C@](C)(C)C(=O)[C@H]2CC[C@@H]3[C@@]4(C)CC[C@@H](C)C[C@H]4CC[C@H]3CC[C@H]2C(=O)O)O
C1290	Test	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c1c2c(cc(c1OC)OC)C[C@H]1c3c(cc(c(c23)OC)OC)CCN1C
C1291	Test	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)C(=O)c1c(c(c3c(c1O)C[C@](C(=O)C)(C[C@@H]3O[C@H]1C[C@@H]([C@@H](C(C)O1)O)N)O)O)C2=O
C1292	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(cnc1)c1ccnc(n1)Nc1cc(ccc1C)NC(=O)c1ccc(cc1)CN1CCN(CC1)C
C1293	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1cccc(c1o2)C(=O)Nc1ccc(cc1)OCCN(CCc1ccc(c(c1)OC)OC)C
C1294	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C\=C/C@@H](C@@H](C\=C/C@@H](C@@H](C@@H](C(C)C@@H](C@@H](CCC)O)OC\=O)C@@H](C=C)C@@H](C@@H](C@@H](C@)C/C=C)CO)O)O)C@@H](C@@H](C@@H](C)OC)O)C@@H](C@@H](C@@H](C)O)O)OC)OC
C1295	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)OCC(=O)O[C@@H]1[C@H]2[C@@](C=O)[C@H](/C=C/C)(C)C[C@@H][C@@H]([C@H](C=C)[C@@H]2OC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)C[C@@]1(C)OC(=O)C)O
C1295	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@@H]1[C@H]2[C@@](C=O)[C@H](/C=C/C)(C)C[C@@H][C@@H]([C@H](C=C)[C@@H]2OC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)C[C@@]1(C)OC(=O)C)O
C1296	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@@H]1[C@H]2[C@](C)(O)[C@@]1(C)OC(=O)C)[C@H]([C@H](/C=C/C)(C)C[C@@H][C@@H]([C@H](C=C)[C@@H]2OC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)O
C1297	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@@H]1[C@H]2[C@](C)(O)[C@@]1(C)OC(=O)C)[C@H]([C@H](/C=C/C)(C)C[C@@H][C@@H]([C@H](C=C)[C@@H]2OC(=O)C)OC(=O)C)OC(=O)C)O)c1ccccc1)C)OC(=O)C)O
C1298	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@@H]1[C@H]2[C@](C[C@@]1(C)OC(=O)C)[C@H]([C@H](/C=C/C)(C)C)[C@@H][C@@H]([C@H](C=C)[C@@H]2OC(=O)C)OC(=O)C)(C)C)O)OC(=O)C)OC(=O)C)O
C1299	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@@H]1/C/2=C\[C@@](C)([C@@H][C@@H]([C@H]([C@H](C(/C=C/[C@H](C)[C@@H]([C@@H]2[C@]2([C@H]1C)OC(=O)C)OC(=O)C)C)OC(=O)C)OC(=O)C)O
C1300	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@@H]1/C/2=C\[C@@](C)([C@@H][C@@H]([C@H]([C@H](C(/C=C/[C@@H](C=O)[C@@]2([C@H]1C)OC(=O)C)C)OC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C
C1301	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C=C1[C@@H](C[C@H](C(/C=C/[C@H](C(=O)[C@]2([C@](C)([C@H][C@@H]([C@H]2[C@H]1OC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)C)C)OC(=O)C)OC(=O)C
C1302	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@@](c1ccc(c(c1)Cl)Cl)(CCCN(CCc1ccc(c(c1)OC)OC)C)C(C)C
C1303	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@](c1ccc(c(c1OC)OC)OC)(CCCN(CCc1ccccc1)C)C(C)C
C1304	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@@](c1ccc(c(c1OC)OC)OC)(CCCN(CCCCCCCC)C)C(C)C
C1305	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@@](c1ccc(c(c1OC)OC)OC)(CCCN(CCCCCCCCCCCC)C)C(C)C
C1306	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc2OC[C@@H](CN2CCN(C3c4ccccc4[C@H]4C[C@H]4c4ccccc34)CC2)O)nccc1
C1307	Test	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1cc(ccc1CN1C(=O)NC(=S)N(Cc2ccc(cc2)Cl)CC1)Cl
C1308	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)nc1c(cccc1C(=O)Nc1ccc(cc1)OCCN(Cc1ccc(c(c1)OC)OC)C)n2
C1309	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(c(c1)C)NC(=O)CN1CCN(CCCC(c2ccc(cc2)F)c2ccc(cc2)F)CC1)C
C1310	Test	inhibitor	61	noninhibitor	inhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[C@@H](c1ccc(cc1)Cl)OCCN1CCOCC1
C1311	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C1CCN(CC1)CCCN1C(=O)C(c2ccccc2)(c2ccccc2)N[C@H]1C
C1312	Test	inhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc(cc1)C1(c2ccccc2)C(=O)N(C(=O)N1)CCCN1CCOCC1
C1313	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C1CCN(CC1)CCCN1C(=O)C(c2ccccc2)(c2ccccc2)NC1=O
C1314	Test	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C1(c2ccccc2)C(=O)N(C(=O)N1)CCC(=O)N
C1315	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@](c1ccc(c(c1)OC)OC)(CCCNCc1c2c(cc3c1cccc3)cccc2)C(C)C
C1316	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C\1=C\[C@@H](C)[C@@H](/C(=C/[C@@H](C)[C@@H]([C@@H](C[C@H](C)C(C2=CC(=O)C=C(C2=O)NC(=O)/C(=C1)/C)OC)OC)O)/C)OC(=O)N
C1317	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)N1CCN(CC1)CCOC(=O)C1=C(C)NC(=C(C(=O)OC)[C@@H]1c1ccccc(c1)[N+](=O)[O-])C
C1318	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C1c3ccccc3C2(CC1)CCCNC
C1319	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C1=C2C(=C[C@@H]3[C@H]4CC[C@](C(=O)C)([C@@]4(C)CC[C@H]3[C@@]2(C)CCC1=O)OC(=O)C)C
C1320	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)CCNCCCOC(=O)c1cc(c(c(c1)OC)OC)OC
C1321	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c3cccc1[C@@H]1C[C@@H](CNC(=O)OCc4ccccc4)CN([C@H]1Cc2cn3C)C
C1322	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CN(CC)CCOc1ccc(cc1)NC(=O)c1cccc2c1[nH]c1ccccc1c2=O
C1323	Test	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc2c(cc1/C=C/[C@H]1CC(=CC(=O)O1)OC)OCO2
C1324	Test	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c12c(cc(cc1)OC)[nH]c1c2CCN2[C@@H]1C[C@H]1[C@H](C(=O)OC)[C@H](C(C[C@@H]1C2)OC)OC
C1325	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#C[C@]1(CC[C@H]2[C@H]3C(=C4C(=CC(=O)CC4)CC3)[C@@H](c3ccc(cc3)N(C)C)C[C@]12C)O)C
C1326	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(=O)C1CCN(CC1)CCCn1c2ccc(cc2[nH]c1=O)Cl)F
C1327	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1cccc(c1[nH]2)C(=O)Nc1ccc(cc1)OCCCN(CCc1ccc(c(c1)OC)OC)C
C1328	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(=O)(C@H)(C)[C@@H]([C@H](C)C)C1[C@H](C)[C@H](C[C@]2(CC1C@)(C)[C@H]3CC[C@@](CC)([C@@H]4[C@@H](C)C[C@@H](C3[C@@H](C)[C@@H](C)[C@@](CO)(O)O5)O4)O3)(O2)O1)O)OC)O
C1329	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)N([C@@H]1Cc2ccccc2[C@H]1OC)CCCN(CC)CC
C1330	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc2)c(c2c(c1)cccc2)C(=O)OCCCCCN(CCCCCOC(=O)/C=C/c1ccc(c(c1)OC)OC)C

C1331	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)c1ccc(cc1)/C=C/C(=O)OCCCN(CCCOC(=O)/C=C/c1cc(c(c(c1)OC)OC)OC)C
C1332	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(c1ccc(cc1)OC)C(=O)OCCCN(CCCOC(=O)/C=C/c1cc(c(c(c1)OC)OC)OC)C)OC
C1333	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc2)c(c2c(c1)cccc2)C(=O)OC1CCC(CC1)N(C1CCC(CC1)OC(=O)c1cc(c(c(c1)OC)OC)OC)C
C1334	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1c(cc(c(c1OC)OC)OC)/C=C/C(=O)OCCCN(CCCOC(=O)c1cc(c(c(c1)OC)OC)OC)C
C1335	Test	inhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1cc(c(cc1C[C@@H]1c2cc(c(cc2CCN1)OC)OC)OC)OC
C1336	Test	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc2c(c(c1)OC)C(=O)c1c(c(c3c(c1O)[C@H](C[C@](C(=O)C)(C3)O)O[C@H]1C[C@@H]([C@@H]([C@H](C)O1)O)NC(=O)C)O)C2=O
C1337	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)OC(=O)N1C=C[C@H](c2ccc(cc2)OC)C(=C1)C(=O)CC
C1338	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)OC(=O)N1C=C[C@H](c2ccc(cc2)C)C(=C1)C(=O)C
C1339	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)OC(=O)N1C=C[C@H](c2ccccc2OC)C(=C1)C(=O)C
C1340	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)/C(=C(/c1ccccc1)\CCCl)/c1ccc(cc1)OCCNC
C1341	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1cccc(c1[nH]2)C(=O)Nc1ccc(cc1)CN(Cc1ccc(c(c1)OC)OC)C
C1342	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)[C@@H](c1ccc(cc1)OCCN(CC)CC)C(c1ccc(cc1)OC)C(=O)O2
C1343	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)COc1cc(cc(c1OCc1ccccc1)OCc1ccccc1)C(=O)OCCN(CC)CC
C1344	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1c(cc(C)nc1C)c1c(cc2c(c1F)n(cc1c2nn(c1=O)C1CCC(CC1)N(C)C)C1CC1)F
C1345	Test	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)c(=O)cc(c1ccc(c(c1OC)OC)OC)o2
C1346	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1cccc(c1[nH]2)C(=O)Nc1ccc(cc1)CCN(Cc1ccc(c(c1)OC)OC)C
C1347	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C1=C(c2ccc(cc2)OCCN2CCCC2)c2ccc(cc2CC1)OC
C1348	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CN(CCOC(=O)C1=C(C)NC(=C(C(=O)OC)[C@@H]1c1cccc(c1)[N+](=O)[O-])C)C
C1349	Test	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1cc(cc(c1)[N+](=O)[O-])C1C(=C(C)NC(=C1C(=O)OCCOCC)C)C(=O)OCCOCC
C1350	Test	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[C@H](CCN)Oc1ccc(cc1)C(F)(F)F
C1351	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C(=CCCNC)c1ccccc1CC2
C1352	Test	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cc(c(c1)OC)OC)ncnc2Nc1cccc(c1)Br
C1353	Test	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1[S@]2=O)Cl)CCCN(C)C
C1354	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cc(c(c1)OC)OC)[nH]c(c2CCN1CCN(c2ccccc2)CC1)C
C1355	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(c1ccc(cc1)F)CCCN1CCC(c2ccc(c(c2)C(F)(F)F)Cl)(CC1)O)F
C1356	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1CCNCC(=O)N(CC(=O)N(CC(=O)N)CCc1ccc(cc1Cl)Cl)CCc1ccc(cc1Cl)Cl)F
C1357	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1cccc(c1[nH]2)C(=O)Nc1ccc(cc1)CCCCCN(Cc1ccc(c(c1)OC)OC)C
C1358	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1ccccc1O2)CCCCN1CCCCC1
C1359	Test	inhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc2c(c1)N(c1ccccc1O2)C(=O)CN1CCCCC1
C1360	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1ccccc1O2)CCCN(CCO)CCO
C1361	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1ccccc1O2)CCCN1CCOCC1
C1362	Test	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(ccc1OC(=O)NC)N([C@H]1[C@@]2(C)CCN1C)C
C1363	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=C1CCN(CC1)CCOCCOCCO)c1ccccc1
C1364	Test	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c1ccc(cc1)/C(=C\1/CCN(CC)C1)/c1ccc(cc1)F
C1365	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1cccc(c1[nH]2)C(=O)Nc1ccc(cc1)/C=C/CN(Cc1ccc(c(c1)OC)OC)C
C1366	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)Cl)CCCN1CCN(CC1)C
C1367	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CNCCC)O
C1368	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CN(CCC)C)O
C1369	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CN1CCCC1)O
C1370	Test	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CCC)O
C1371	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CN(CC)CC)O
C1372	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CN1CCCCC1)O
C1373	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccc(cc1)OC[C@H](CN1CCN(c2ccc(cc2)F)CC1)O

C1374	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccc(cc1)OC[C@@H](CN(C(C)C)C(C)C)O
C1375	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CC[C@@H](c1ccccc1OC[C@@H](CN(C(C)C)C(C)C)O)OC
C1376	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CNc1ccccc1)O
C1377	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CNc1ccc(cc1)[N+](=O)[O-])O
C1378	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)N(CCC)C[C@H](COc1ccccc1C(=O)CCc1ccccc1)O
C1379	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(c(c1)CCN1Cc2cc(c(cc2CC1)OC)OC)NC(=O)c1cccc2c1[nH]c1cccc(c1c2=O)OC
C1380	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CN1CCC(c2ccccc2)(CC1)O)O
C1381	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CC[C@@H](c1ccccc1OC[C@H](CN1CCCCC1)O)OC
C1382	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CC[C@@H](c1ccccc1OC[C@@H](CNCCC(c1ccccc1)c1ccccc1)O)OC
C1383	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C1(CCN(CC1)C[C@H](COc1ccccc1C(=O)C)O)O
C1384	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1cc(ccc1)CCCN1Cc3cc(c(cc3CC1)OC)OC)[nH]c1cccc(c1c2=O)OC
C1385	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc2)c(ccc1)CCC(=O)c1ccccc1OC[C@H](CN(C(C)C)C(C)C)O
C1386	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc2)c(ccc1)CCC(=O)c1ccccc1OC[C@H](CN1CCOCC1)O
C1387	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc2)c(ccc1)CCC(=O)c1ccccc1OC[C@H](CN1CCC(c2ccccc2)(CC1)O)O
C1388	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)c1ccccc1OC[C@H](CN1CCC(c2ccccc2)(CC1)O)O
C1389	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1cc(ccc1OC[C@@H](CN(C(C)C)C(C)C)O)OCc1ccccc1
C1390	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1cc(ccc1OC[C@H](CN1CCN(Cc2ccccc2)CC1)O)OCc1ccccc1
C1391	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CC[C@@H](c1ccccc1OC[C@@H](CN1CCN(c2ccc(cc2)F)CC1)O)OC
C1392	Test	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@@](C(=O)O[C@@H]1CCCN(C1)C)(C1CCCCC1)O
C1393	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C[C@@](c1ccccc1)([C@@H](C)CN(C)C)OC(=O)CC
C1394	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(nc(nc1N1CCC(CC1)NC[C@H]1c3ccccc3COc3ccccc13)NCC=C)n(cn2)CC=C
C1395	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(nc(nc1NCC=C)N1CCC(CC1)NCC(c1ccc(cc1)F)c1ccc(cc1)F)n(cn2)CC=C
C1396	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1ccc(cc1C)OCCCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1cccc(c1c2=O)C
C1397	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(ccc(c1)OC)nccc2[C@@H]([C@H]1C[C@@H]2CCN1C[C@H]2C=C)O
C1398	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(cc(c1[C@@]1(Cn2ccnc2)OC[C@@H](COc2ccc(cc2)n2ccnc2)O1)Cl)Cl
C1399	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(cc(c1[C@@]1(Cn2ccnn2)OC[C@H](COc2ccc(cc2)N2CCN(C(=O)C)CC2)O1)Cl)Cl
C1400	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)n(c(=O)[nH]2)C1CCN(CCCCc2ccc(cc2)F)CC1
C1401	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(nc(c(c3ccccc3)n2)N2[C@H](C)COCC2)nc(nc1N(C[C@@H](C)O)CCO)N1[C@@H](C)COCC1
C1402	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(nc(c(c3ccccc3)n2)N2CCOCC2)nc(nc1N1CCOCC1)N1CCOCC1
C1403	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(nc(c(c3ccccc3)n2)N2CCOCC2)nc(nc1N(CCO)C)N1CCOCC1
C1404	Test	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1ccc(cc1)[C@H]([C@H]1CNCCO1)Oc1ccccc1OCC
C1405	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cc(cc1)OC)[nH]c1c2CCN2[C@@H]1C[C@H]1[C@H](C(=O)OC)[C@H](C(C[C@@H]1C2)OC(=O)/C=C/c1cc(c(c(c1)OC)OC)OC)OC
C1406	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)COC(=O)C[C@H](C(=O)N[C@H](C(=O)OC(C)(C)C)CCCCNC(=O)OCc1ccccc1)NC(=O)OC(C)(C)C
C1407	Test	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1CN1C(=S)NC(=S)N(Cc2ccc(cc2)Cl)CC1)Cl
C1408	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c3c4c(c(c1O)C)O[C@@]1(C4=O)C/C=C/[C@@H](C[C@@H]1[C@H](C[C@H]3C)[C@H]2C)C(=O)Nc(c(3O)/C=N/N1CCN(CC1)c2O)/C)C)O)OC(=O)C)OC
C1409	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)C[C@@H]1c2ccccc2C(=Nc2cc(ccc12)Cl)C1CCN(CC1)C
C1410	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1CC[C@H]1c2cc(c(cc2CCN1)OC)OC)OC
C1411	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1CC[C@H]1c2cc(c(cc2CCN1C)OC)OC)OC)OC
C1412	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1ccc(cc1C)CCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1cccc(c1c2=O)F
C1413	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1CC)CC[C@H]1c2cc(c(cc2CCN1C)OC)OC
C1414	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(c1ccc(cc1)F)CNC1CCN(Cc2nc(nc(n2)NCC=C)NCC=C)CC1)F
C1415	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(c(c1)N1CCN(C[C@@H](COc2cc3c(cc2)N(C(=O)C3)C)O)CC1)OC
C1416	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(c(c1)N1CCN(C[C@H](COc2cc3c(cc2)NC(=O)CC3)O)CC1)OC

C1417	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)c(c1ccccc1OC)nc(c2)N1CCN(CCCC(=O)c2ccc(cc2)F)CC1
C1418	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1ccc(cc1OC)OCCCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1cccc(c1c2=O)F
C1419	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)c(c1ccccc1)nc(c2)N1CCN(CC1)CCN1C(=O)OCC1
C1420	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)c(C)nc(c2)N1CCN(CCCC(=O)c2ccc(cc2)F)CC1
C1421	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(ccc(c1)N1CCN(CCCC(=O)c3ccc(cc3)Cl)CC1)cnc(c2)C
C1422	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(ccc(c1)N1CCN(CCCC(=O)c3ccc(cc3)F)CC1)cnc(c2)Cl
C1423	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(ccc(c1)N1CCN(CCCC(=O)c3ccc(cc3)F)CC1)cnc(c2)C
C1424	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(cc2c1[C@@H](c1c(cc(cc1Br)Cl)C2)C1CCN(C(=O)CC2CCC(C(=O)C)CC2)CC1)Br
C1425	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	[C@@H]1(C(=O)N[C@H](C(=O)N(C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N[C@H](C(=O)N[C@@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N1C)C(C)C)C)CC(C)C)C)CC(C)C)C)C)CC(C)C)C(C)C)C)CC(C)C)C)C(C)C)C(=O)[C@H](C)C/C=C/C
C1426	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1ccc(cc1CC)OCCCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1cccc(c1c2=O)F
C1427	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@@H](C(=O)OCCN1CCN(CC1)CCOc1ccc(cc1)OC)CC
C1428	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@H](C(=O)OCCN1CCN(C(=O)c2cc(c(c(c2)OC)OC)OC)CC1)CC
C1429	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@@H](C(=O)OCCN1CCN(CC(=O)Nc2c(cccc2C)C)CC1)CC
C1430	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@@H](C(=O)OCCN1CCN(CCC(=O)Nc2c(cccc2C)C)CC1)CC
C1431	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cccc(c1)[C@@H](C(=O)OCCN1CCN(CC1)CCOC(=O)[C@H](c1ccccc1F)CC)C)F
C1432	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1[C@@H](C(=O)OCCN1CCN(CC1)CCOC(=O)[C@@H](c1ccc(cc1)Cl)CC)CC)Cl
C1433	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cccc(c1)[C@@H](C(=O)OCCN1CCN(CC1)CCOC(=O)[C@@H](c1ccccc1Cl)CC)CC)Cl
C1434	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1ccc(cc1OC)CCCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1cccc(c1c2=O)OC
C1435	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1[C@@H](C(=O)OCCN1CCN(CC1)CCOC(=O)[C@@H](c1ccc(c(c1)OC)OC)CC)CC)OC)OC
C1436	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@@H](C(=O)OCCN1CCN(CC1)CCOC(=O)[C@H](c1ccccc1)CCC)CCC
C1437	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)C(=O)OCCN1CCN(CC1)CCOC(=O)C(c1ccccc1)c1ccccc1
C1438	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@H](C(=O)OCCN(CCN(CCOC(=O)[C@H](c1ccccc1)CC)C)C)CC
C1439	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)O[C@@H](C(=O)OCCN1CCN(CC1)CCOC(=O)[C@@H](CC)Oc1ccccc1)CC
C1440	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@@H](C(=O)NCCCN1CCN(CCCNC(=O)[C@H](c2ccccc2)CC)CC1)CC
C1441	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1[C@@H](C(=O)OCCN1CCN(CC1)CCOC(=O)[C@H](c1ccc(c(c1)OC)OC)CCCC)CCCC)OC)OC
C1442	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@@H](C(=O)OCCN1CCCN(CC1)CCOC(=O)[C@@H](c1ccccc1)CC)CC
C1443	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)(C(=O)OCCN1CCN(CC1)CCOC(=O)C(c1ccccc1)(c1ccccc1)C)C
C1444	Test	inhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1cc(ccc1C[C@H](C)N(CC)CCCC(=O)C1CCCCC1)OC
C1445	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1ccc(cc1C)CCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1cccc(c1c2=O)C
C1446	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@H]1[C@]2([C@@]3([C@H](C)C[C@@H]([C@@H]2OC(=O)C)OC(=O)C)[C@@H]([C@H](C(C)(C)O3)[C@@H]1OC(=O)c1ccccc1)OC(=O)C)COC(=O)C
C1447	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)O[C@H]1[C@@]2(C)[C@@]3([C@](C)(C[C@@H]([C@@H]2OC(=O)c2ccccc2)OC(=O)c2ccccc2)O)[C@@H]([C@H](C(C)(C)O3)[C@@H]1O)OC(=O)C
C1448	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@](c1ccc(cc1)Cl)(C)OCCN1CCCCCC1
C1449	Test	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1[C@@H]1C(CO)Oc2ccc(cc2O1)[C@@H]1[C@H](C(=O)c2c(cc(cc2O1)O)O)O)OC)O
C1450	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cc3c(c1)OCO3)[nH]cc2CCN1CCN(c2ccccc2OC)CC1
C1451	Test	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c1c(cc(c(c1OC)OC)OC)C(=O)OCCCCCCCCN(CC)CC
C1452	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C=CC[C@@H]1/C=C(\C)/C[C@H](C)CC([C@@H]2[C@H](C[C@@H](C)[C@@](C(=O)C(=O)N3[C@H](C(=O)O[C@H](/C(=C/C4CC[C@H](C(C4)OC)O)/C)[C@H](C)[C@H](CC1=O)O)CCCC3)(O)O2)OC)OC
C1453	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1[C@@H]1c2ccc(cc2[C@@H](C1)N1CCN(CC1)CCO)C(F)(F)F)F
C1454	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(C)(C)CC)OCCCCCCN1CCN(c2ccc(c(c2)Cl)C)CC1
C1455	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1ccc(cc1)CCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1c(cc(cc1OC)OC)c2=O
C1456	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(c1ccc(cc1)F)NC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1)F
C1457	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(c1ccc(cc1)F)N(C1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1)CC=C)F
C1458	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cccc(c1)C)[C@H](c1cc(cc(c1)OC)OC)CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C1459	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1[C@H](C1CCCCC1)CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1)F

C1460	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)[C@H](c1ccccc1OC2)CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C1461	Test	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1cc(cc(c1)Cl)CN1C(=O)N[C@H](N(Cc2cccc(c2)Cl)CC1)SC
C1462	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)CCc1ccccc1C2CNC1CCN(c2nc(nc(n2)OC)NCC=C)CC1
C1463	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)CCc1cc(ccc1[C@H]2CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1)OC
C1464	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(c1ccc(cc1)F)N1CCN(CC1)Nc1nc(nc(n1)NCC=C)NCC=C)F
C1465	Test	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@](CC)(COC(=O)c1cc(c(c(c1)OC)OC)OC)N(C)C
C1466	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)CCc1ccccc1N2C[C@@H](C)CN(C)C
C1467	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C)[C@@](c1ccc(cc1)OCCN(CC)CC)(Cc1ccc(cc1)Cl)O
C1468	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1ccc(cc1)CCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1c(cccc1[N+](=O)[O-])c2=O
C1469	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C=Cc1c(cccn1)[C@@H]2OC1C[C@H]2CC[C@@H](C1)N2C
C1470	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C1=C2C[C@H](CC[C@]2(C)[C@@H]2CC[C@@]3(C(=O)CC[C@H]3[C@@H]2C1)C)OCCN(CC)CC
C1471	Test	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=C1CCN(CC(=O)N)CC1)c1ccc(cc1)Cl
C1472	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=C1CCN(CC1)CCOCC(=O)N)c1ccc(cc1)OC
C1473	Test	inhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	C1(=O)[C@H](C(C)C)NC(=O)[C@H](C(C)C)OC(=O)[C@H](C)OC(=O)[C@@H](C(C)C)NC(=O)[C@@H](C(C)C)OC(=O)[C@@H](C(C)C)NC(=O)[C@H](C)OC(=O)[C@@H](C(C)C)NC(=O)[C@@H](C(C)C)OC(=O)[C@@H](C(C)C)NC(=O)[C@@H](C)OC(=O)[C@H](C(C)C)N1
C1474	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#CCNCC(c1ccccc1)c1ccccc1)C[C@@](C#N)(c1ccc(c(c1)OC)OC)C(C)C
C1475	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@@](c1ccc(c(c1)OC)OC)(CCCNC1c2ccccc2CCc2ccccc12)C(C)C
C1476	Test	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC[C@@H](c1ccc(c(c1)OC)OC)N(C)C
C1477	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(cc2c1[C@]13CCN4[C@@H]1[C@](C=CC4)(CC)[C@H]([C@](C(=O)OC)([C@H]3N2C)O)OC(=O)C)OC
C1478	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(=C\C[C@@H](C)[C@H]([C@H]1C(=O)N[C@@H](C(=O)N(CC(=O)N([C@H](C(=O)N[C@H](C(=O)N([C@@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@H](C(=O)N([C@@H](C(=O)N1C)[C@@H](C)CC)C)CC(C)C)C)CC(C)C)C)C)CC(C)C)C)C(C)C)CC(C)C)C)[C@H](C)O)O)/C
C1479	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)/C=c\1/c(=O)[nH]/c(=C\c2cccc(c2)C(=O)Nc2ccc(cc2)CCN2Cc3cc(c(cc3CC2)OC)OC)/c(=O)n1C
C1480	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)c1ccc(cc1)/C=C/C(=O)O[C@H]1C[C@@H]2[C@@]([C@H]3[C@]1(C(=O)[C@@H](C1=C(C)[C@H](C[C@](C1(C)C)([C@H]3OC(=O)c1ccccc1)O)OC(=O)C)OC(=O)C)C)(CO2)OC(=O)C
C1481	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C1(c2ccccc2)C(=O)N(CCCN2CCN(c3ccccc3)CC2)[C@H](C)N1
C1482	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)c1cc(=O)n(CCCN2CCN(c3ccccn3)CC2)n1c1ccccc1
C1483	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)n1c([C@H]3C[C@@]4(c5ccccc5N(C(=O)C)[C@H]4N3C(=O)C1)C(C=C)(C)C)n2
C1484	Test	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)N(C(=O)CC(C)C)[C@H](C(=O)N2)CC
C1485	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1ccc(cc1)CCN(Cc1ccc(c(c1)OC)OC)C)[nH]c1c(cccc1OC)c2=O
C1486	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)(C1CCN(CCC[C@@H](c2ccc(cc2)C(C)(C)C)O)CC1)O
C1487	Test	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)C[C@H](CNC(C)C)O
C1488	Test	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c12c(c(nc(n2)N(C[C@H](C)O)CCO)N2CCCCC2)nc(nc1N1CCCCC1)N(C[C@@H](C)O)CCO
C1489	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CN1CCN([C@H]2c3ccccc3N(C(=O)c3ccc(cc3)C)[C@@H](C)[C@@H]2O)CC1
C1490	Test	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	C1(=O)CC[C@H]2[C@H]3CC[C@H]4C[C@@H](CC[C@]4(C)[C@H]3CC[C@@]12C)O
C1491	Test	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(nc(n2)N(CCO)CCO)N2CCCC2)nc(nc1N1CCCC1)N(CCO)CCO
C1492	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(c(nc(n2)N2CCCCC2)N2CCCCC2)nc(nc1N1CCCCC1)N(CCO)CCO
C1493	Test	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(ncn2)N2CCCCC2)nc(nc1N1CCCCC1)N(CCO)CCO
C1494	Test	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@](CCN1CCCC1)(C1CCCCC1)O
C1495	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1cc(c(c(c1)CN1CCCCC1)O)CN1CCCCC1)(C)C
C1496	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(c(c1)C(=O)Nc1ccc(cc1)CCN1Cc3cc(c(cc3CC1)OC)OC)[nH]c1c(cccc1F)c2=O
C1497	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(c(c1)C)N1CCN([C@@H]2Cc3ccc(cc3CC2)O)CC1
C1498	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(cc2c1C[C@@H]1[C@@H](C)[C@@]2(C)CCN1CC=C(C)C)O
C1499	Test	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1/C(=C(/c1ccc(cc1)O)\CC)/CC)O
C1500	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CN(c1ccccc1)CCOC(=O)C1=C(C)NC(=C([C@@H]1c1cccc(c1)[N+](=O)[O-])P1(=O)OCC(C)(C)CO1)C
C1501	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CN(c1ccccc1)[C@]1(C)[C@@H](C(=O)O)[C@H](c2cccc(c2CC)[N+](=O)[O-])C(=C(C)N1CCN1CCOCC1)P1(=O)OCC(C)(C)CO1
C1502	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@H]1[C@H](CCCN1)NCc1cc(ccc1OC)N(C)S(=O)(=O)C

C1503	Test	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1ccc(cc1)C[C@@H]([C@@H](CN(CC(C)C)S(=O)(=O)c1ccc(cc1)N)O)NC(=O)O[C@H]1CCOC1
C1504	Test	inhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c12c(ccc(c1)NS(=O)(=O)C)[nH]c(c2)C(=O)N1CCN(c2cc(ccn2)NC(C)C)CC1
C1505	Test	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c1ccc(cc1)CC[C@@H](/C=C/S(=O)(=O)c1ccccc1)NC(=O)[C@H](Cc1ccccc1)NC(=O)N1CCOCC1
C1506	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C)S[C@H](c1ccc(c(c1)OCCc1cnc[nH]1)OC)CCCCCCN1Cc2cc(c(cc2CC1)OC)OC
C1507	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1[C@@H](CCCCCN1Cc2cc(c(cc2CC1)OC)OC)SC1CCCCC1)OC)OC
C1508	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C)S[C@H](c1ccc2c(c1)OCO2)CCCCCN1Cc2cc(c(cc2CC1)OC)OC
C1509	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)SC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C1510	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(c1ccc(cc1)F)N1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1)F
C1511	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(=C(C)C)CC/C(=C/CC/C(=C/CC/C(=C/CSC[C@@H](C(=O)OC)N)/C)/C)/C
C1512	Test	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	C(=C(C)C)CC/C(=C/CC/C(=C/CSC[C@H](C(=O)N)NC(=O)C)/C)/C
C1513	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)n(c(=O)[nH]2)CCCCN1CCN(c2ccccc2SCCC)CC1
C1514	Test	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c12c(c(ncn2)SCc2ccccc2)nc(nc1N1CCOCC1)N1CCNCC1
C1515	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@@](c1ccc(c(c1)OC)OC)(CCCCCCCCN1Cc2cc(c(cc2CC1)OC)OC)Sc1ccc(cc1)C
C1516	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@@](c1ccc(c(c1)OC)OC)(CCCCCN1Cc2cc(c(cc2CC1)OC)OC)SC1CCCCC1
C1517	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@](c1ccc(c(c1)OC)OC)(CCCCCN1Cc2cc(c(cc2C1)OC)OC)Sc1ccc(cc1)C
C1518	Test	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c1ccc(cc1)C1(CCCN(CCc2ccc(c(c2)OC)OC)C)S(=O)(=O)CCCS1(=O)=O
C1519	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)NC(=O)OCCN(C(=O)N1c2ccccc2Sc2ccc(cc12)OC)CCOC(=O)Nc1ccccc1
C1520	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)C(=O)C)[C@@H](C)CN(C)C
C1521	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)OC)C[C@@H](C)CN(C)C
C1522	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1ccccc1S2)C[C@@H](C)CN1CCN(CC1)CCOCCO
C1523	Test	inhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc2c(c1)N(c1ccccc1S2)C[C@@H](C)N(C)C
C1524	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1ccccc1S2)C[C@@H]1C2CCN(CC2)C1
C1525	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)S(=O)(=O)C)CC[C@@H]1CCCCN1C
C1526	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)SC)CC[C@@H]1CCCCN1C
C1527	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)C(F)(F)F)CCCN1CCC(C(=O)c2ccc(cc2)F)CC1
C1528	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)C(=O)CCC)CCCN1CCN(CC1)C
C1529	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)C(F)(F)F)CCCN1CCN(C2CC2)CC1
C1530	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)C(=O)C)CCCN1CCN(CC1)CCO
C1531	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c2c(c1)Sc1ccccc1N2)C(=O)Nc1ccc(cc1)OCCN(CCc1ccc(c(c1)OC)OC)C
C1532	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)/C(=C/CCN1CCN(CC1)C)/c1cc(ccc1S2)S(=O)(=O)N(C)C
C1533	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N=C(c1cc(ccc1S2)C)N1CCN(CC1)C
C1534	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C(=C1CCN(CC1)C)c1ccccc1S2
C1535	Test	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1ccc(c(c1)[C@H]1C(=C(C)NC(=C1C(=O)OCC)COCCN)C(=O)OC)Cl
C1536	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@H]1C(=S)N(C(=C[C@@H]1c1ccco1)c1ccccc1)C1[C@@H]([C@H]([C@@H]([C@@H](COC(=O)C)O1)OC(=O)C)OC(=O)C)OC(=O)C
C1537	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)c1c(c2ccc(cc2)OC)c2c(CC(C)(C)CC2=O)n(c1=S)C1[C@@H]([C@H]([C@@H]([C@@H](COC(=O)C)O1)OC(=O)C)OC(=O)C)OC(=O)C
C1538	Test	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1CN1C(=S)NC(=S)N(Cc2ccc(c(c2)OC)OC)CC1)OC)OC
C1539	Test	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1[N+](=O)[O-])OP(=S)(OC)OC
C1540	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)CCC1=C(C[Cl+]C=C1)N2CCCN(C)C
C1541	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12ccn(c1nc(nc2NCC=C)N1CCC(CC1)NCC1c2ccccc2CCc2ccccc12)CC=C
C1542	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(nc(nc1NCC=C)N1CCC(CC1)NCC(c1ccccc1)c1ccccc1)n(cn2)CC=C
C1543	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(nc(nc1NCC=C)N1CCC(CC1)NCC1c3ccccc3CCc3ccccc13)n(cn2)CC=C
C1544	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(nc(nc1NCC=C)N1CCC(CC1)NCC1c3ccccc3CCc3ccccc13)n(cn2)CCC
C1545	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc2)c(ccc1)CNC1CCN(c2nc3c(c(n2)NCC=C)ncn3CC=C)CC1

C1546	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(nc(nc1NCCC)N1CCC(CC1)NCC1c3ccccc3CCc3ccccc13)n(cn2)CCC
C1547	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)N1CCN(CC1)/N=C/c1cccc(C)n1
C1548	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)CCc1ccccc1C2CNC1CCN(c2nc(nc(n2)NCC=C)NCC)CC1
C1549	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)CN(C1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1)C
C1550	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)NC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C1551	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c1ccccc1C2CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C1552	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)CCNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C1553	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(c1ccc(cc1)F)CCCN1CCN(C(=O)NCC)CC1)F
C1554	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)CCc1ccccc1C2CNN1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1
C1555	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)CNC1CCN(c2nc(nc(n2)NCCC)NCC=C)CC1
C1556	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(ccc(c1)CN1CCN(C(c3ccccc3)c3ccccc3)CC1)n(c(CCCC)n2)CC
C1557	Test	inhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccnc(c1)/C(=C/CN1CCCC1)/c1ccc(cc1)C
C1558	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)c1ccc(cc1)[C@H](c1ccccc1)n1ccnc1
C1559	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C1=C2CC(=O)CC[C@]2(C)[C@H]2CC[C@]3(C(=O)CC[C@H]3[C@H]2C1)C
C1560	Test	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(ccc1)CC)oc(c2)[C@H](CNC(C)(C)C)O
C1561	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)oc(c2CCc1ccccc1)[C@H](CN1CCN(c2ccccc2OC)CC1)O
C1562	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)oc(c2CCc1ccccc1)CCNC(C)C
C1563	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(c1ccccc1)Cc1nc(CCN2CCCCC2)on1
C1564	Test	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c12c(c(ccc1)C1C(=C(C)NC(=C1C(=O)OCC)C)C(=O)OCC)non2
C1565	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C(=C1CCN(CC1)C)c1ccsc1C(=O)C2
C1566	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cc(cc1)NC(=O)c1ccc(cc1)C(C)(C)C)sc(n2)SCc1c(cc(c(c1C)C(=O)C)C)C
C1567	Test	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1cc(C2C(=C(C)NC(=C2C(=O)OCC(=O)OCC)C)C(=O)OCC(=O)OCC)sc1
C1568	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(cc(c1OC)OC)CNCC2
C1569	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)CCNC2
C1570	Test	inhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	C1=C2CC[C@@H]3[C@H]4CC[C@](C(=O)CO)([C@@]4(C)CC[C@H]3[C@@]2(C)CCC1=O)O
C1571	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc(c1)OC)CN(C)C
C1572	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)CN1CC=CC1
C1573	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)CCN1CCCCC1
C1574	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)N1CCNCC1
C1575	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(nc(n2)N2CCOCC2)N2CCOCC2)nc(nc1)N1CCOCC1
C1576	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1CNC(=N)NC(=O)c1c(nc(c(n1)Cl)N)N)Cl)Cl
C1577	Test	noninhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1c2c(ccc1O)Sc1cc(c(cc1N2CCCN(C)C)Cl)O
C1578	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c(nc(c(n1)Cl)N(CC(C)C)C)N)C(=O)NC(=N)N
C1579	Test	noninhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1cc(cc2c1N(c1cc(ccc1S2)Cl)CCCN(C)C)O
C1580	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)c1c(c(C(C)C)n(c1c1ccc(cc1)F)CC[C@H](C[C@H](CC(=O)OC)O)O)C(=O)Nc1ccccc1
C1581	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1(c(c2c(c(c1O)C)CC[C@@](C)(CCC[C@H](C)CCC[C@H](C)CCCC(C)C)O2)C)C
C1582	Test	noninhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1ccc(cc1)C(c1ccccc1)(C(=O)N)C[C@H](C)N(C)C
C1583	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cc(cc1)Cl)nccc2Nc1cc(c(cc1)O)CN(CC)CC
C1584	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=O)OCCN(CC)CCN(CC)CC)N
C1585	Test	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	C\1=C/C=C/C=C/C=C/[C@@H](C[C@H]2[C@@H](C(=O)O)[C@H](C[C@@](C[C@H](C[C@@H]([C@H](CC[C@@H](C[C@@H](CC(=O)O[C@@H](C)[C@@H](C)[C@H]([C@@H](/C=C/C=C/C=C1)C)O)O)O)O)O)O)(O)O2)O)O[C@H]1[C@H]([C@H]([C@@H]([C@H](C)O1)O)N)O
C1586	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc(c1C1(Cn2cncn2)OCCO1)Cl)Cl
C1587	Test	noninhibitor	61	noninhibitor	inhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C(c1ccccc1)(C(=O)OCCN(CC)CC)O
C1588	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1c2c(cc(c1OC)OC)[C@@H]1C[C@@H]([C@@H](C(=O)N(CC)CC)CN1CC2)OC(=O)C

C1589	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(c(cc1)OC)OC)c[n+]1c(c2)c2cc3c(cc2CC1)OCO3
C1590	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1c2c(cc(c1OC)OC)[C@@H](CCCC[C@@H]1c3cc(c(cc3CCN1)OC)OC)NCC2
C1591	Test	noninhibitor	61	noninhibitor	inhibitor	noninhibitor	noninhibitor	c1cc(ccc1c1ccc(cc1)OCCN1CCCC1)C(F)(F)F
C1592	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccnc(c1)[C@H](c1ccc(cc1)Br)CCN(C)C
C1593	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(=CC(=O)OC1/C(=C/C(=O)OC)/C[C@H]2[C@H]([C@@H](CO)OC(=O)C[C@@H](C[C@@H]3CC[C@@H](C[C@](C[C@@H]4CC(=CC(=O)OC)/C[C@H](/C=C/C(C)(C)C[C@]1(O)[C@]2(O4)(O)O3)OC(=O)C(O)(C)C)C(=O)OC)C(=O)OC)O)O)O)C=C/CCC
C1594	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)Cl)C(=O)CCN1C[C@@H]2CCCN2CC1
C1595	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(cc(c(c1OC)C(=O)CCCN1CCCC1)OC)OC
C1596	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[C@@H](C(=O)OCCN(CC)CC)CC
C1597	Test	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(ccc(c1C(=O)O)NC)oc(CC1[C@@H](C)CC[C@]3([C@H](C)C[C@@H](C)C([C@H](C(=O)c4ccc[nH]4)C)O3)O1)n2
C1598	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cccc2)c(ccc1)OC(=O)NC
C1599	Test	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c12c3c(cccc3OC[C@H](CNCCOc3ccccc3O)O)[nH]c1cccc2
C1600	Test	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c12c3c(cccc3OC[C@H](CNCCOc3cc(ccc3OC)O)O)[nH]c1cccc2
C1601	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[C@@](c1ccccc1Cl)(CCN(C)C)O
C1602	Test	noninhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1ccc(cc1)[C@H](c1ccc(cc1)Cl)N1CCN(CC1)C
C1603	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccnc(c1)N(Cc1ccc(cc1)Cl)CCN(C)C
C1604	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(cc(c(c1OC)OC)OC)/C=C\C(=O)N1CCN(CC(=O)O)CC1
C1605	Test	noninhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1c(cc(c(c1OC)OC)OC)/C=C/C(=O)N1CCN(CC(=O)N2CCCC2)CC1
C1606	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(cc(c(c1OC)OC)OC)/C=C/C(=O)N
C1607	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)c1ccc2c(c1)CO[C@]2(c1ccc(cc1)F)CCCN(C)C
C1608	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)C=Cc1ccccc1C2C(=O)N
C1609	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=O)N(c1ccc(cc1)OC)CCCC(=O)O)Cl
C1610	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)CN1CCC(CC1)NC(=O)c1cc(c(cc1OC)N)Cl
C1611	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cc(cc1)Cl)nccc2N[C@@H](C)CCCNCCO
C1612	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(cc2c1[C@@H]1CC[C@@]3(C(=O)[C@@H](C[C@H]3[C@H]1CC2)Cl)C)OC
C1613	Test	noninhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c12c(cc(c(c2)OC)OC)cc[n+]2c1cc1c(cc(c(c1)OC)OC)c2C
C1614	Test	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(c1)COc1ccc(cc1)[C@@H](C(=O)N2C[C@H](C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N[C@@H]3CCCC[C@@H]3C2)C(=O)O)C(C)C)C(C)C)CCCC2)C
C1615	Test	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C[C@@H](C(=O)N[C@@H](C(=O)N[C@@H](C(=O)N[C@@H](C(=O)N[C@@H](C(=O)N[C@@H](C(=O)N[C@@H](C(=O)N[C@@H](C(=O)N[C@@H](C(=O)N[C@@H](C(=O)N[C@@H](C(=O)N[C@@H]3CCCC[C@@H]3C2)C(=O)O)C(C)C)C(C)C)CCCC2)C
C1616	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)Nc1cc2c(c/c/1=N\C1CCCCC1)n(c1ccccc1)c1ccccc1n2
C1617	Test	noninhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c1ccc(cc1)C[C@H]1[C@H]2C(=C(C)[C@H]([C@H]3/C=C/CC(C(=O)[C@@]/(/C=C/[C@H]([C@]23C(=O)N1)OC(=O)C)(C)O)C)O)C
C1618	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C[C@H]1[C@H]2[C@@H](C(=C)[C@H]([C@H]3/C=C/CC(C)C[C@@]/(/C=C/[C@H]([C@@]23C(=O)N1)OC(=O)C)(C)O)O)C
C1619	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1CCN(CCC[C@@](c1ccc(c(c1)OC)OC)(C(C)C)N)C)OC)OC
C1620	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=C(Cl)Cl)c1ccc(cc1)Cl)Cl
C1621	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)[nH]c1c2CCN2[C@H]1C([C@@H]1C(C(=O)OC)[C@H](CC[C@H]1C2)O)OC(=O)c1ccccc1
C1622	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)C(=O)N(C2=O)[C@H](CCl)SP(=S)(OCC)OCC
C1623	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)CNCc1ccccc1
C1624	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)OC[C@@H](CN1CCN(C[C@@H]3COc4ccccc4O3)CC1)O2
C1625	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)Cl)CCCN
C1626	Test	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(cc(c1F)N1CCN(CC1)C)n(c1ccc(cc1)F)cc(c2=O)C(=O)O
C1627	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1c1cc(=O)c2c(cc(cc2o1)O)O)O)OC
C1628	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C(c1ccccc1)OCC1=NCCN1
C1629	Test	noninhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@@](c1ccccn1)(C(=O)N)CCN(C(C)C)C(C)C
C1630	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)n(c(=O)[nH]2)CCCN1CCC(CC1)n1c2ccc(cc2[nH]c1=O)Cl
C1631	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc2c(c(c1)OC)C(=O)c1c(c(c3c(c1O)[C@H](C[C@](C(=O)CO)(C3)O)O[C@@H]1C[C@@H]([C@@H](C(C)O1)O)N)O)C2=O

C1632	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(/C=C/C(=O)N2CCCCC2)nc(c1)/C(=C/CN1CCCC1)/c1ccc(cc1)C
C1633	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@@H](C(=O)OCCN(CC)CC)C1CCCCC1
C1634	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c2c(c1)OCCO2)N1CCNCC1
C1635	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)CN(c1ccccc1)CC
C1636	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C(=C(CC)CN)c1ccccc1
C1637	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1CCN(CCCN1C(=O)c2cc(c(cc2C1)OC)OC)C)OC)OC
C1638	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(nc(nc1)N)n(cn2)CCC(COC(=O)C)COC(=O)C
C1639	Test	noninhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1ccc(cc1)C(c1ccccc1)(C(=O)N)CCN1CCCCC1
C1640	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1c1c(c(=O)c2ccc(cc2o1)O)O)O)O
C1641	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1c1cc(=O)c2c(cc(cc2o1)OC1[C@@H](C([C@@H](C(CO)O1)O)O)O)OCC(=O)N1CCN(Cc2ccc(c(c2OC)OC)OC)CC1)OC
C1642	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1c1cc(=O)c2c(cc(cc2o1)O)O)OCC(=O)N1CCN(Cc2ccc(c(c2OC)OC)OC)CC1)OC
C1643	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1[C@@H]1CC(=O)c2c(cc(cc2O1)OCC(=O)N1CC[N+](Cc2ccc(c(c2OC)OC)OC)(CC1)C)O)O)OC
C1644	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(c(c1)Cl)/C=N/NC(=N)N)Cl
C1645	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(c(c1)Cl)CC(=O)NC(=N)N)Cl
C1646	Test	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc(cc1)CN(c1ccccc1)CCN1CCCC1
C1647	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cc(cc1)c1[nH]c3c(cc(cc3)N3CCN(CC3)C)n1)nc(c1ccc(cc1)OCC)[nH]2
C1648	Test	noninhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@@H](c1ccc(cc1)Cl)N1CCCN(CC1)C
C1649	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(/C=C/C(=O)N2CCOCC2)nc(c1)/C(=C/CN1CCCC1)/c1ccc(cc1)C
C1650	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c2c3c1C[C@@H]1[C@@H]4CCC(=O)[C@@H]([C@]34CCN1C)O2)O
C1651	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)c1noc(=N)n1CCN(CC)CC
C1652	Test	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c12c(cccc1)n(cn2)CC[C@H](C)NC[C@H](c1ccc(c(c1)OC)O)O
C1653	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(ccnc1)C(=O)NN
C1654	Test	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CN1CCN(CCc2c(c3ccc(cc3)F)[nH]c(=O)o2)CC1
C1655	Test	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(/C=C/C(=O)OCC)nc(c1)/C(=C/CN1CCCC1)/c1ccc(cc1)C
C1656	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[C@@H]([C@H]1CCCCN1)OC(=O)C
C1657	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1c1cc(=O)c2c(cc(cc2o1)O)O)O)OC1[C@@H](C([C@@H](C(CO)O1)O)O)O
C1658	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C1(c2ccccc2)C(=O)N(C(=O)N1)CC(=O)O
C1659	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)C1(c2ccccc2)C(=O)N(C(=O)N1)CCC(=O)O
C1660	Test	noninhibitor	61	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc2c(c1)C1=C(c3ccccc3O2)CCN(CC1)C
C1661	Test	noninhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)[C@](c1ccc(cc1)Cl)(C)O[C@H](C)CN(C)C
C1662	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)C(=NCC2)COc1ccc(cc1)OC
C1663	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)CC(C)(C)NC
C1664	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(N)OCC(C)(CCC)COC(=O)N
C1665	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c(cc(c1Cl)N)OC)C(=O)NCCN(CC)CC
C1666	Test	noninhibitor	61	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1cc(cc(c1[C@H](Cn1ccnc1)OCc1ccc(cc1Cl)Cl)Cl)Cl
C1667	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1(=C(C(=O)C2=C(C1=O)N1[C@@]([C@@H]2COC(=O)N)([C@@H]2[C@H](C1)N2)OC)N)C
C1668	Test	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1CC/N=C\1/CCCN1C)OC)OC
C1669	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H](COc1ccc(cc1)NC(=O)C)CNC(C)C
C1670	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1ccc(CCN(C)CCN2C(=O)[C@H]3[C@@H](C4c5ccccc5C3c3ccccc43)C2=O)cc1OC
C1671	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC1COC(=O)C[C@H]([C@H](N(C(=O)[C@@H](OC1=O)C(C)C)C)Cc1ccccc1)OCOC
C1672	Test	inhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	CCCCCCC[C@@H]1[C@@H](C(=O)O[C@H](C(=O)N([C@H](C(CC(=O)O1)O)Cc1ccccc1)C)C(C)C)C
C1673	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCCCC[C@@H]1[C@@H](C(=O)OC(C(=O)N([C@H](C(CC(=O)O1)O)Cc1ccccc1)C)(C)C)C
C1674	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCC[C@@H]1[C@@H](C(=O)OCC(=O)N([C@H](C(CC(=O)O1)O)Cc1ccccc1)C)C

C1675	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCCCC[C@@H]1[C@@H](C(=O)O[C@H](C(=O)N([C@H](C(CC(=O)O1)O)Cc1ccccc1)C)C)C
C1676	Test	inhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN([C@@H](Cc1ccccc1)[C@@H](CC(=O)OC)O)C(=O)OCc1ccccc1
C1677	Test	inhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCCC[C@H]([C@H](C)C(=O)O[C@@H](C(C)C)C(=O)OC)O
C1678	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCCCC[C@@H]1[C@@H](C(=O)O[C@H](C(=O)N([C@H](C(CC(=O)O1)OCOC)Cc1ccccc1)C)C)C
C1679	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCCCC[C@@H]1[C@@H](C(=O)OCC(=O)N([C@H](C(CC(=O)O1)OCOC)Cc1ccccc1)C)C
C1680	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCCCCC1CC(=O)O[C@H](C(=O)N([C@H](C(CC(=O)O1)OCOC)Cc1ccccc1)C)C(C)C
C1681	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	C[C@H]1[C@H](OC(=O)C[C@H]([C@@H](N(C(=O)[C@@H](OC1=O)C(C)C)C)Cc1ccccc1)O)C
C1682	Test	noninhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	O[C@H]1CC[C@H]2CN3CCc4c([nH]c5ccccc45)[C@H]3C[C@@H]2C1C(=O)OC
C1683	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1ccccc1n2CCCCN1CCOCC1
C1684	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1ccccc1n2CCCCN(CCO)CCO
C1685	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc2c1n(c1ccccc1c2=O)CCCCN1CCN(CC1)CCO
C1686	Test	inhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1cccc2c1[nH]c1ccccc1c2=O
C1687	Test	inhibitor	60	inhibitor	noninhibitor	inhibitor	inhibitor	COc1cccc2c1n(c1ccccc1c2=O)CCCCl
C1688	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN1CCN(CC1)CCCn1c2ccccc2c(=O)c2c1cccc2
C1689	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN1CCN(CC1)CCCn1c2ccccc2c(=O)c2c1c(ccc2)OC
C1690	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1ccccc1n2CCCN1CCCCC1
C1691	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc2c1n(c1ccccc1c2=O)CCCN1CCCCC1
C1692	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc2c1n(c1ccccc1c2=O)CCCN1CCOCC1
C1693	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc2c1n(c1ccccc1c2=O)CCCN(CCO)CCO
C1694	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(=O)c1ccccc1n2CCCN1CCN(CC1)CCO
C1695	Test	inhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	c1ccc2c(c1)c(=O)c1ccccc1n2CCCCCl
C1696	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/C#N)c1ccc(cc1)N(C)C
C1697	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/COC)c1ccc(cc1)N(C)C
C1698	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)CCCOC)c1ccc(cc1)N(C)C
C1699	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)[C@@H]1C[C@@H]1C(=O)OC)c1ccc(cc1)N(C)C
C1700	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/COCc1ccccc1)c1ccc(cc1)N(C)C
C1701	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCN(CC)C(=O)OC/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)N(C)C)c1ccc(cc1)N(C)C
C1702	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)C/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)N(C)C)c1ccc(cc1)N(C)C
C1703	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/CN1CCCCC1)c1ccc(cc1)N(C)C
C1704	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCCCn1c(c(nc1c1ccc(cc1)C(=O)O)c1ccc(cc1)N(C)C)c1ccc(cc1)N(C)C
C1705	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)c1ccc(cc1)c1c(n(c(n1)c1ccc(cc1)O)CCc1ccccc1)c1ccc(cc1)N(C)C
C1706	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CNc1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/C(=O)OC)c1ccc(cc1)NC
C1707	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCOC/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)N(C)C)c1ccc(cc1)N(C)C
C1708	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCN(CC)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/COCC)c1ccc(cc1)N(CC)CC
C1709	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCN(CC)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/COCC)c1ccc(cc1)NC
C1710	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCOC/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)NC)c1ccc(cc1)NC(C)C
C1711	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCOC/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)F)c1ccc(cc1)NC(C)C
C1712	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCN(CC)c1ccc(cc1)c1c[nH]c(n1)c1ccc(cc1)/C=C/COCC
C1713	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCOC/C=C/c1ccc(cc1)c1[nH]c(cn1)c1ccc(cc1)N1CCOCC1
C1714	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCOC/C=C/c1ccc(cc1)c1[nH]c(cn1)c1ccc(cc1)NC(C)C
C1715	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)/C=C/c1ccc(cc1)c1[nH]c(c(n1)c1ccc(cc1)N1CCCC1)c1ccc(cc1)N1CCCC1
C1716	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCN(CC)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/C(=O)OC)c1ccc(cc1)NC
C1717	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@]12O[C@@](NC(=O)[C@@H]3CN(C)[C@@H]4Cc5c(Br)[nH]c6cccc(c56)C4=C3)(C(C)C)C(=O)N1[C@@H](CC(C)C)C(=O)N1CCCC21

C1718	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCN(CCCC)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/C(=O)OC)c1ccc(cc1)NC
C1719	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)c1ccc(cc1)c1c([nH]c(n1)c1ccc(cc1)/C=C/C(=O)OC)c1ccc(cc1)N
C1720	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O=C(N[C@@H]1CCCC[C@@H]1N1CCN(CC1)c1ccccc1)c1ccccc1NC(=O)c1cnc2ccccc2c1
C1721	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	[O-][N+](=O)c1ccccc1C(=O)Nc1ccc(CCN2CCc3ccccc3C2)cc1
C1722	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2CCN(CCc3ccc(NC(=O)c4ccccc4N)cc3)Cc2cc1OC
C1723	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2CCN(CCc3ccc(NC(=O)c4ccc(cc4)[N+](=O)[O-])cc3)Cc2cc1OC
C1724	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Nc1ccc(cc1)C(=O)Nc1ccc(CCN2CCc3ccccc3C2)cc1
C1725	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O=C(Nc1ccc(CCN2CCc3ccccc3C2)cc1)c1cnc2ccccc2c1
C1726	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2CCN(CCc3ccc(NC(=O)c4ccccc4Br)cc3)Cc2cc1OC
C1727	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)COCCN1CCN(CC1)[C@@H](c1ccccc1)c1ccc(Cl)cc1
C1728	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2CCN(CCc3ccc(NC(=O)c4ccc5ccccc5c4)cc3)Cc2cc1OC
C1729	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2CCN(CCc3ccc(NC(=O)c4cnc5ccccc5n4)cc3)Cc2cc1OC
C1730	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2CCN(CCc3ccc(NC(=O)c4cc5ccccc5cn4)cc3)Cc2cc1OC
C1731	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2CCN(CCc3ccc(NC(=O)c4ccc(Br)cc4)cc3)Cc2cc1OC
C1732	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2CCN(CCc3ccc(NC(=O)c4ccc5ncccc5c4)cc3)Cc2cc1OC
C1733	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2CCN(CCc3ccc(NC(=O)c4ccccc4NC(=O)c4ccc(C)cc4)cc3)Cc2cc1OC
C1734	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ClNCc1ccccc1Cl
C1735	Test	noninhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	CCN(CC)CCOC(=O)C(c1ccccc1)c1ccccc1
C1736	Test	noninhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	CN(C)CCCOC1(CCCCC1)Cc1ccccc1
C1737	Test	noninhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	C[C@H](NC1=C(C=C1)O)[C@@H](Cc1ccc(Cl)cc1)c1ccc(Cl)cc1
C1738	Test	noninhibitor	60	inhibitor	noninhibitor	inhibitor	inhibitor	COc1c(OC)cc(/C=C/C2=C(CN3CCN2CC3)N2CCCC2)cc1OC
C1739	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C1=NCCN1)c1c(Cl)cccc1Cl
C1740	Test	noninhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COC1CC2CC3N(CCC4CC(OC)C(OC)CC34)C(C)C2CC1OC
C1741	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(c1ccc(OC#N)cc1)c1ccc(OC#N)cc1
C1742	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1ccc(cc1)C(OCCN(C)C)c1ccccc1
C1743	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COCCCNCc1cc(OC)c(OC)c(OC)c1
C1744	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(NC)c(NCC[C@H](O)CCC)nc(nc1[C@@H](NCCN(CCO)CCO)N1CCCC(O)C1)N(CCO)CCO
C1745	Test	noninhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	CCN(CC)CCOC(=O)[C@H](Cc1ccccc1)c1ccccc1
C1746	Test	noninhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC[C@@H](c1ccccc1)/C/1=C(/OCCCN2CCN(CCCO1)CC2)\[C@H](CC)c1ccccc1
C1747	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCCCCCCNSc1cccc2c(Cl)cccc12
C1748	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1CN(CCN1CCc1[nH]nnn1)c1ccccc1
C1749	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1c2O[C@H]3C(=O)CC[C@@]4(O)[C@@H]5Cc(cc1)c2[C@]34CCN5CC1CC1
C1750	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C)CC[C@H](c1ccccc1)c1ccccn1
C1751	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H]1C(=C[C@@H]2C(=O)O[C@@H]3C[C@H](C/C=C/C[C@H](/C=C/C=C/4\CO[C@H]1[C@@]24O)C)C)O[C@]1(C3)C/C(=N/OC)/[C@H](C)C(O1)/C(=C/C(C)C)/C)C
C1752	Test	inhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCC(=O)[C@]1(O)CC[C@@H]2[C@@H]3CCC4=CC(=O)CC[C@H]4[C@@H]3C(=O)C[C@]12C
C1753	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	C1(c2ccccc2C2C(c3c1cccc3)C2(F)F)N1CCN(CC1)C[C@@H](COc1c2c(ccc1)nccc2)O
C1754	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCOc1c(OC)cc2c(c1)[C@H]1CN(C)CC[C@H]1N=C2c1ccc(cc1)C(=O)N(C(C)C)C(C)C
C1755	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc(cc1)NC(=O)C
C1756	Test	noninhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	NS(=O)(=O)c1c(Cl)cc2N[C@H](CSCC=C)NS(=O)(=O)c2c1
C1757	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@@H](O[C@H]2[C@@H](C[C@@H](N)[C@H](O[C@H]3O[C@@H](CN)[C@@H](O)[C@H](O)[C@@H]3O)[C@@H]2O)NC(=O)[C@@H](O)CCN)[C@@H](O)[C@H](N)[C@@H]1O
C1758	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[C@H]1N2[C@@H](SC1(C)C)[C@@H](NC(=O)[C@@H](N)c1ccc(O)cc1)C2=O
C1759	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1cc(c[nH]c1=O)c1ccncc1
C1760	Test	noninhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Oc1c(cccc1NC=O)C(=O)N[C@@H]1[C@H](C)OC(=O)[C@@H](CCCCCC)[C@H](OC(=O)CC(C)C)[C@H](C)OC1=O

C1761	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc(cc1)[N+](=O)[O-]
C1762	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H](O)[C@@H]1OC(=C(O)C1=O)O
C1763	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1CC(=C2[C@H]([C@@H]3OC(=O)[C@H](C)[C@H]13)C(=CC2=O)C)C
C1764	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[C@@H]1N2[C@H](SC1(C)C)C(NC(=O)[C@@H](NC(=O)N1CCNC1=O)c1ccccc1)C2=O
C1765	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H](CC[C@H]1[C@H](C)C=CC2=C[C@@H](O)C[C@H](OC(=O)[C@H](C)CC)[C@H]12)C[C@@H](O)CC(=O)O
C1766	Test	noninhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	C1C[C@@H]2C([C@@]3(C1=CC(=C)C=C3)C)([C@H](C[C@]1([C@H]2C[C@@H]([C@@]1(C(=O)CO)O)C)C)O)F
C1767	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H](COc1ccc(CCOCC2CC2)cc1)CNC(C)C
C1768	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN1CCc2cc3c(OCO3)cc2[C@@H]1[C@H]1OC(=O)c2c1ccc1c2OCO1
C1769	Test	noninhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC(=O)Oc1ccc(cc1)C(c1ccc(OC(=O)C)cc1)c1ccccn1
C1770	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CS(=O)(=O)OCCCCOS(=O)(=O)C
C1771	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	[nH]1c2cc(OC)ccc2c2c1[C@H]1C[C@@H]3[C@@H](C[C@H](OC(=O)c4cc(OC)c(OC)c(OC)c4)[C@H](OC)C3C(=O)OC)CN1CC2
C1772	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1c(Br)cc(C(=O)NCCN(CC)CC)c(OC)c1
C1773	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C(=O)[C@@H]1CCCCN1CCCC)c1c(C)cccc1C
C1774	Test	noninhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	N1[C@@H]2N(C)CC[C@@]3([C@H]4Nc5c(cccc5)[C@@]23CCN4C)c2ccccc12
C1775	Test	inhibitor	60	inhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CCC(=O)O[C@@H]1CC[C@]2(C)[C@H](CC[C@@]3(C)[C@@H]2C(=O)C=C2[C@@H]4C[C@](C)(CC[C@@]4(C)CC[C@]32C)C(=O)O)C1(C)C
C1776	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C1=C(CSc2nnnn2C)CS[C@@H]2N1C(=O)[C@]2(OC)NC(=O)CSCC#N
C1777	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C1=C(COC(=O)N)CS[C@H]2N1C(=O)[C@H]2NC(=O)/C(=N/OC)/c1ccco1
C1778	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=N)c1cc(=O)c(=O)c2=c1[nH]c1c(o2)cc(cc1)N(CC)CC
C1779	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C1=C(COC(=O)C)CS[C@H]2[C@@H](NC(=O)Cc3cccs3)C(=O)N12
C1780	Test	inhibitor	60	inhibitor	noninhibitor	inhibitor	inhibitor	O[C@@H]1CC[C@@]2(C)[C@H](C1)C[C@H](O)C1[C@@H]3CC[C@@H]([C@H](C)CCC(=O)O)[C@@]3(C)CC[C@H]21
C1781	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN1[C@H](c2ccc(Cl)cc2)S(=O)(=O)CCC1=O
C1782	Test	noninhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1ccc(cc1)C(=C(c1ccc(OC)cc1)c1ccc(OC)cc1)Cl
C1783	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(CCC)C(=O)NS(=O)(=O)c1ccc(Cl)cc1
C1784	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@]1(NC(=O)c2ccccc12)c1cc(c(Cl)cc1)S(=O)(=O)N
C1785	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NS(=O)(=O)c1c(Cl)cc2NC=NS(=O)(=O)c2c1
C1786	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1C=CC(=O)c2c1ccc1c2ccc2ccccc12
C1787	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N([C@@H]1CCSC1=O)C(=O)C
C1788	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H](CNC(C)(C)C)c1cc(Cl)c(N)c(Cl)c1
C1789	Test	inhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1[C@@H](O[C@@H]([C@@H](NC(=O)[C@H]2C[C@@H](CCC)CN2C)[C@@H](C)Cl)[C@@H](O)[C@@H]1O)SC
C1790	Test	noninhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	OC1C[C@]2(C)[C@H](C[C@@H](C)[C@]2(OC(=O)CC)C(=O)CCl)[C@H]2CCC3=CC(=O)C=C[C@@]3(C)[C@@]12F
C1791	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NS(=O)(=O)c1c(Cl)ccc(c1)C(=O)NN1[C@H](C)CCC[C@H]1C
C1792	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C#CCN(C)CCCOc1c(Cl)cc(Cl)cc1
C1793	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCC(=O)[C@]1(O)CC[C@@H]2[C@H]3CCC4=CC(=O)CC[C@@]4(C)[C@@H]3C(O)C[C@]12C
C1794	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H](CC1CC(=O)NC(=O)C1)[C@H]1CC(C)C[C@@H](C)C1=O
C1795	Test	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	OC1C[C@@]2(C)[C@H](C[C@H](C)[C@]2(O)C(=O)COC(=O)C)[C@H]2CCC3=CC(=O)C=C[C@@]3(C)[C@]12F
C1796	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ON(CCCCCNC(=O)CCC(=O)N(O)CCCCCNC(=O)CCC(=O)N(O)CCCCCN)C(=O)C
C1797	Test	noninhibitor	60	inhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1[C@@H]2C34[C@H]5C[C@@H]6[C@@H](OC)[C@H]5[C@@]5(C[C@H]6OC)OCO[C@@]15[C@@H]3N(CC)C[C@@]2(COC)CC[C@H]4OC
C1798	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H]1C[C@@H](CC[C@H]2[C@H](C)C=CC3=C[C@@H](C)C[C@H](OC(=O)C(C)C)CC)[C@H]23)OC(=O)C1
C1799	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1[C@H]2C[C@@H]3[C@H](N(C)C)C(=O)/C(=C(/O)\N)/C(=O)[C@]3(O)C(=O)C2=C(O)c2c(O)ccc(Cl)c12
C1800	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C(=O)OCC)C1=C(N2CC2)C(=O)C(=C(N2CC2)C1=O)NC(=O)OCC
C1801	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCN(CC)C(=O)N1CCN(C)CC1
C1802	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc(cc1)/C(=C(/CC)\c1ccc(O)cc1)/CC
C1803	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc(cc1)/C(=C/C)/C(=C/C)/c1ccc(O)cc1

C1804	Test	inhibitor	60	noninhibitor	inhibitor	inhibitor	inhibitor	N(C(=O)OC[C@@H](CN1CCCCC1)OC(=O)Nc1ccccc1)c1ccccc1
C1805	Test	noninhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	O[C@H](CN(CC(C)C)S(=O)(=O)c1ccc(cc1)N)[C@@H](Cc1ccccc1)NC(=O)O[C@H]1CCOC1
C1806	Test	noninhibitor	60	inhibitor	noninhibitor	noninhibitor	noninhibitor	CC[C@@]12CCCN3CCc4c([C@H]13)n(c1ccccc41)C(=O)C2
C1807	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1[C@H](C(Oc2cc(cc(c12)O)O)c1cc(c(cc1)O)O)O
C1808	Test	noninhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@]12O[C@@](NC(=O)[C@@H]3CN(C)[C@H]4Cc5c[nH]c6cccc(c56)C4=C3)(C)C)C(=O)N1[C@@H](C(C)C)C(=O)N1CCC[C@@H]21
C1809	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C)C(=O)Oc1ccc2N(C)[C@H]3N(C)CC[C@@]3(C)c2c1
C1810	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CN(CC(=O)O)CC(=O)Nc1c(CC)cccc1CC
C1811	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H](COc1c(OC)c2nc3c(cco3)c(OC)c2cc1)C(C)(C)O
C1812	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[C@@H](C)c1cc(Oc2ccccc2)ccc1
C1813	Test	inhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H](CN[C@H](C)Cc1ccc(O)cc1)c1cc(O)cc(O)c1
C1814	Test	inhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	Clc1ccc(OCC(=O)N2CCN(Cc3cc4c(OCO4)cc3)CC2)cc1
C1815	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Cc1c(oc2c(cccc2c1=O)C(=O)OCCN1CCCCC1)c1ccccc1
C1816	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCC(=O)[C@]1(O)CC[C@@H]2[C@H]3CCC4=CC(=O)CC[C@@]4(C)[C@]3(F)C(O)C[C@]12C
C1817	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN(C)CCOC(c1ccccc1)c1ccccc1
C1818	Test	noninhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	OC1C[C@@]2(C)[C@H](CC[C@]2(O)C(=O)C)[C@H]2C[C@H](C)C3=CC(=O)C=C[C@@]3(C)[C@]12F
C1819	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CC[C@H](NC(=O)c1ccc(cc1)NCc1cnc2nc([nH]c(=O)c2n1)N)C(=O)O
C1820	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[O-][N+](=O)c1ccc(o1)/C=N/N1C[C@H](CN2CCOCC2)OC1=O
C1821	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)c1cc(c(Cl)cc1NCc1ccco1)S(=O)(=O)N
C1822	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1C[C@@H]2Oc3c(OC)ccc4c3[C@@]2(CCN(C)C4)C=C1
C1823	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1=c2c(=C3C1=CC(=O)C=C3)ccnc2C
C1824	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCC(CO)OCn1cnc2c1nc([nH]c2=O)N
C1825	Test	noninhibitor	60	inhibitor	noninhibitor	noninhibitor	noninhibitor	N1C(=O)[C@@]2([C@@H]3OC[C@@H]4[C@@H]5[C@H]2[C@]([C@H]4C3)(CN5C)C=C)c2ccccc12
C1826	Test	noninhibitor	60	inhibitor	noninhibitor	noninhibitor	noninhibitor	Cn1c2ccccc2c(=O)cc1c1cc2c(OCO2)cc1
C1827	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H](O)COc1ccccc1OC
C1828	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC(=O)N1CCN(CC1)c1ccc(OC[C@@H]2CO[C@](Cn3ccnc3)(O2)c2ccc(Cl)cc2Cl)cc1
C1829	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1c2ccccc2c2c1[C@@H](C)NCC2
C1830	Test	noninhibitor	60	noninhibitor	inhibitor	noninhibitor	noninhibitor	O[C@H]1C[C@]2(C)[C@H](C[C@H]3OC(C)(C)O[C@@]23C(=O)CCl)[C@H]2CCC3=CC(=O)CC[C@@]3(C)[C@@]12F
C1831	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1CCN2CC=C(COC(=O)[C@@](O)(C(C)C)[C@H](C)OC)C12
C1832	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCCN1CCN(CCS(=O)(=O)O)CC1
C1833	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1CCC2=c3ccc(OC)cc3=NC2=C1C
C1834	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1[C@@H](C)O[C@@H](OC[C@H]2O[C@@H](Oc3cc(O)c4C(=O)C[C@H](Oc4c3)c3cc(O)c(OC)cc3)[C@@H](O)[C@@H](O)[C@@H]2O)[C@@H](O)[C@@H]1O
C1835	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1C=C2CCN(C)[C@H]2[C@H]2[C@H]1OC(=O)c1cc3c(OCO3)cc21
C1836	Test	inhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	COc1c(OC)c2c(cc1)[C@H](OC2=O)[C@@H]1N(C)CCc2cc3c(OCO3)cc12
C1837	Test	noninhibitor	60	inhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]([C@@H](C)N1CCC(Cc2ccccc2)CC1)c1ccc(O)cc1
C1838	Test	noninhibitor	60	inhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1c2c(C[C@@H]3N(C)CCc4cc(OC)c(OC)c2c34)ccc1OC
C1839	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C(C)C)c1c(C)n(C)n(c1=O)c1ccccc1
C1840	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O(C@H)(C@H)2C(O)(C@H)(O[C@@H]3O(C@@H)(CN)(C@@H)(O)(C@@H)(O)[C@H]3O)(C@@H)(C[C@@H]2N)N)(C@H)(O)(C@H)(N)(C@H)1O
C1841	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1[C@@H]2C[C@@H]3[C@H]1[C@](O)(C[C@@H]2OC)[C@H]1C[C@H]2[C@]43[C@H]1N(CC)C[C@]2(C)CC[C@H]4O
C1842	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COC1=CC(=O)O[C@H](C1)/C=C/c1ccccc1
C1843	Test	noninhibitor	60	noninhibitor	inhibitor	noninhibitor	noninhibitor	O[C@H](COc1cccc2c1CCCC2=O)CNC(C)(C)C
C1844	Test	noninhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@]1(CC[C@@H]2[C@@H]3CCC4=CC(=O)CC[C@H]4[C@H]3CC[C@@]12CC)C#C
C1845	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)c1cn(CC)c2c(cc(F)c(N3CCN[C@H](C)C3)c2F)c1=O
C1846	Test	noninhibitor	60	noninhibitor	inhibitor	inhibitor	inhibitor	CCN(CC)CCOCCOC(=O)C1(CCCC1)c1ccccc1

C1847	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN1c2ccc(Cl)cc2C(=NCC1=O)c1ccccc1
C1848	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1C=C2CCN3Cc4cc5c(OCO5)cc4[C@@H]([C@H]23)[C@@H]1O
C1849	Test	inhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1CN(C)[C@H]2Cc3c[nH]c4cccc(c34)C2=C1
C1850	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1C(=O)C[C@@](C)(CC)C1=O
C1851	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(CCN(CC)CC)C(=O)COc1ccc(OC)cc1
C1852	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OS(=O)(=O)CCS
C1853	Test	inhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H](CNC)c1cc(OC)c(O)cc1
C1854	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1ccn(C)c1=S
C1855	Test	inhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	CN1CCCC(CC2c3ccccc3Sc3c2cccc3)C1
C1856	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H](COC(=O)N)COc1ccccc1OC
C1857	Test	noninhibitor	60	inhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H](CC)NC(=O)[C@H]1CN(C)[C@@H]2Cc3c[nH]c4cccc(c34)C2=C1
C1858	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCCn1c(C)ncc1[N+](=O)[O-]
C1859	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ClC(Cl)[C@H](c1ccc(Cl)cc1)c1ccccc1Cl
C1860	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CC/C(=C/Cc1c(O)c2c(COC2=O)c(C)c1OC)/C
C1861	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C[C@@H](NC(=O)C)C(=O)O
C1862	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@H](O)[C@@H](NC(=O)C)[C@@H](O[C@@H](C)C(=O)O)C1O
C1863	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1[C@H](C)CCC[C@@H]1C
C1864	Test	inhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc(cc1)[C@H]1CC(=O)c2c(O)cc(O)cc2O1
C1865	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1[C@@H](CN)O[C@@H](O[C@H]2[C@@H](O)[C@@H](O)[C@@H](C[C@H]2N)N)[C@H](N)[C@H]1O
C1866	Test	noninhibitor	60	inhibitor	noninhibitor	noninhibitor	noninhibitor	CN1CCO[C@@H](c2ccccc2)c2c(C1)cccc2
C1867	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)c1c(nccc1)Nc1cccc(c1)C(F)(F)F
C1868	Test	noninhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	[nH]1c2ccccc2c2c1[C@H]1[C@H]3CC[C@@H]([C@H]4CCCNC34)N1CC2
C1869	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]([C@H](C)N)c1cc(O)c(O)cc1
C1870	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCN(CC)CCc1nc(no1)c1ccccc1
C1871	Test	noninhibitor	60	inhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H](CC(=O)O)[C@@H](CC(C)C)NC(=O)[C@@H](C)NC(=O)C[C@@H](O)[C@H](CC(C)C)NC(=O)[C@@H](NC(=O)[C@H](NC(=O)CC(C)C)C(C)C)C(C)C
C1872	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc(N)c(cc1)/N=N/c1ccccc1
C1873	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1c(OC)cc(cc1)C(=O)OC1C[C@H]2CC[C@@H](C1)N2C
C1874	Test	noninhibitor	60	noninhibitor	inhibitor	noninhibitor	noninhibitor	N(Cc1cnccc1)C(=O)c1cc(C(=O)NCc2cnccc2)c(OC)cc1
C1875	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O/C(=C\1/N(C)S(=O)(=O)c2ccccc2C1=O)/Nc1ccccn1
C1876	Test	noninhibitor	60	inhibitor	noninhibitor	inhibitor	inhibitor	O[C@@H]1[C@H]2COC(=O)C2[C@@H](c2cc(OC)c(OC)c(OC)c2)c2c1cc1OCOc1c2
C1877	Test	noninhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Oc1c(cc(SC(C)(C)Sc2cc(c(O)c(c2)C(C)(C)C)C(C)(C)C)cc1C(C)(C)C)C(C)(C)C
C1878	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1c(=O)cc(CCC)[nH]c1=S
C1879	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=O)c1nccnc1
C1880	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCc1cnc(C)c(O)c1CO
C1881	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1c(C#N)c(=O)n(C)cc1
C1882	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ccc(cc1)S(=O)(=O)Nc1nccc(C)n1
C1883	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCC(=O)[C@]1(O)CC[C@@H]2[C@@H]3CCC4=CC(=O)C=C[C@@]4(C)[C@@H]3C(=O)C[C@@]12C
C1884	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ccc(cc1)S(=O)(=O)Nc1ncc(OC)cn1
C1885	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ccc(cc1)S(=O)(=O)Nc1nnc(C)s1
C1886	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ccc(cc1)S(=O)(=O)Nc1ccccn1
C1887	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ccc(cc1)S(=O)(=O)Nc1cc2nccnc2cc1
C1888	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1c2cccnc2nc1c1c(OC)cc(cc1)S(=O)C
C1889	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[C@H](C)c1ccc(cc1)C(=O)c1cccs1

C1890	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CCC(=O)OCC1(CCCC)C(=O)N(N(C1=O)c1ccccc1)c1ccccc1
C1891	Test	noninhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	[nH]1c2cc(OC)ccc2c2c1[C@H]1C[C@H]3[C@H](C[C@@H](OC(=O)c4cc(OC)c(OC(=O)OCC)c(OC)c4)[C@@H](OC)C3C(=O)OC)CN1CC2
C1892	Test	noninhibitor	60	inhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1[C@H]2[C@@H]3N4C[C@@]5(C)C[C@H](OC(=O)c6ccccc6)[C@@H](OC(=O)C)[C@]63[C@@H]5[C@H]4C[C@@]32CC(=C)[C@H]1[C@H](OC(=O)C)[C@@H]63
C1893	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H](CNC(C)(C)C)c1cc(O)cc(O)c1
C1894	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1CCN=C1[C@H]1CCCc2ccccc12
C1895	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1CN2C[C@H](N=C2S1)c1ccccc1
C1896	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1CCC2=Nc3ccccc3CN2C1
C1897	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1c2ccccc2nc1c1cscn1
C1898	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NS(=O)(=O)c1ccc(OC)c(c1)C(=O)NC[C@@H]1CCCN1CC
C1899	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCS(=O)(=O)CCn1c(C)ncc1[N+](=O)[O-]
C1900	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(N1CCCCCC1)C(=O)NS(=O)(=O)c1ccc(C)cc1
C1901	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[C@@H](Cc1cc(I)c(Oc2cc(I)c(O)cc2)c(I)c1)N
C1902	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1CCN(Cc2c(OC)c(OC)c(OC)cc2)CC1
C1903	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN1C(=O)OC(C)(C)C1=O
C1904	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1cc2c(o1)c(C)c1oc(=O)cc(C)c1c2
C1905	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Fc1ccc(cc1)C(OCCN1CCN(CCCc2ccccc2)CC1)c1ccc(F)cc1
C1906	Test	noninhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	O[C@H]1[C@@H](O)[C@]2(O)[C@H](C[C@@]34O[C@@]5(O)[C@H](CC[C@@H]23)[C@]4(C)CC[C@@H]5OC(=O)c2cc(OC)c(OC)cc2)[C@@H]2CN3C[C@@H](C)CC1[C@H]3[C@@](C)(O)[C@@H]12
C1907	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCOC(=O)C1=C[C@@]2(CC)CCCN3CCc4c([C@@H]23)n1c1ccccc41
C1908	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H]1[C@H](C)/C=C(\C)/[C@@H](OC(=O)N)[C@H](OC)/C=C/C=C(\C)/C(=O)NC2=CC(=O)C(=C(C[C@H](C)C[C@@H]1OC)C2=O)OC
C1909	Test	inhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1c2c(cc(C)s2)C(=Nc2ccccc12)N1CCN(C)CC1
C1910	Test	inhibitor	60	noninhibitor	inhibitor	inhibitor	inhibitor	N(/N=C(/C=C/c1ccc(cc1)C(F)(F)F)\C=C\c1ccc(cc1)C(F)(F)F)C1=NCC(C)(C)CN1
C1911	Test	noninhibitor	60	noninhibitor	inhibitor	inhibitor	inhibitor	CC1(C)[C@H](C=C(Cl)Cl)[C@H]1C(=O)OCc1cc(Oc2ccccc2)ccc1
C1912	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(SCCN(C2)C(=O)CCN2CCC(Cc3ccccc3)CC2)cc1
C1913	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCCCCCCCCCCC(CCCN(C)CCc1cc(OC)ccc1)(C#N)c1cc(OC)ccc1
C1914	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	n1c(NCCc2cccc(OC)c2OC)nc(c2c1cc(OC)c(OC)c2)N1CCc2cc(OC)c(OC)cc2C1
C1915	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	n1c(c2c(nc1NCCc1ccc(c(c1)OC)OC)ccc(c2)C)N(Cc1ccccc1)C
C1916	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	OC[C@H]1Oc2c(OC1c1ccc(OC)c(OC)c1)cc(cc2)c1c(OC)c(=O)c2c(O)cc(OC)cc2o1
C1917	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	OC[C@H]1Oc2c(OC1c1ccc(OC)c(OC)c1)cc(cc2)c1c(O)c(=O)c2c(OC)cc(OC)cc2o1
C1918	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	OC[C@H]1Oc2c(OC1c1ccc(O)c(OC)c1)cc(cc2)c1c(O)c(=O)c2c(O)cc(OCc3ccccc3)cc2o1
C1919	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	OC[C@H]1Oc2c(OC1c1ccc(O)c(OC)c1)cc(cc2)c1c(O)c(=O)c2c(O)cc(OC)cc2o1
C1920	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	OC[C@H]1Oc2c(OC1c1ccc(OC)c(OC)c1)cc(cc2)c1c(O)c(=O)c2c(O)cc(O)cc2o1
C1921	Test	inhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1c(OC)c(OC)c2c(=O)cc(oc2c1)c1ccccc1
C1922	Test	inhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1c2c(=O)cc(oc2cc2c1OCO2)c1ccccc1
C1923	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1(c2c(cc(c1OC(=O)C)Oc1ccccc1)oc(cc2=O)c1ccccc1)OC(=O)C
C1924	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1(c2c(cc(c1Oc1ccccc1)O)oc(cc2=O)c1ccccc1)O
C1925	Test	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	CCOc1c(O)cc2oc(cc(=O)c2c1O)c1ccccc1
C1926	Test	inhibitor	60	noninhibitor	inhibitor	inhibitor	inhibitor	CC(=O)Oc1c(OC(=O)C)c(O)c2c(=O)cc(oc2c1)c1ccccc1
C1927	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc(cc1)c1coc2cc(O)ccc2c1=O
C1928	Test	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	CCOc1c(OC)cc2oc(cc(=O)c2c1O)c1ccccc1
C1929	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCOc1c(OCCCC)c(O)c2c(=O)cc(oc2c1)c1ccccc1
C1930	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCCCOc1c(OCCCCCC)c(OC)c2c(=O)cc(oc2c1)c1ccccc1
C1931	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCOc1c(OCC)c(OC)c2c(=O)cc(oc2c1)c1ccccc1
C1932	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC(=O)Oc1c(OC(=O)C)c(OCc2ccccc2)c2c(=O)cc(oc2c1)c1ccccc1

C1933	Test	inhibitor	60	noninhibitor	inhibitor	noninhibitor	noninhibitor	CC(=O)Oc1c(OC(=O)C)c(Br)c2oc(cc(=O)c2c1O)c1ccccc1
C1934	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1c2C(=O)C=C(C(=O)c2cc(C)c1)c1c(C)cc2C(=O)C=CC(=O)c2c1O
C1935	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cccc1)C(=O)CC)CN1CCC(O)(CC1)c1ccccc1
C1936	Test	inhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H](COc1cc(ccc1)C(=O)C)CN1CCCCC1
C1937	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1cc(ccc1)C(=O)C)CN1CCN(CC1)c1ccc(F)cc1
C1938	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1c(cccc1)C(=O)CCc1ccccc1)CN1CCN(CC1)C(=O)c1ccccc1
C1939	Test	inhibitor	60	noninhibitor	inhibitor	noninhibitor	noninhibitor	O[C@H](COc1ccc(OC)cc1)CN1CCN(CC1)c1ccc(F)cc1
C1940	Test	inhibitor	60	inhibitor	noninhibitor	inhibitor	inhibitor	NC1=C(C#N)[C@H](c2c(O1)n[nH]c2c1ccc(C)cc1)c1ccc(cc1)N(C)C
C1941	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cccc1)C(=O)CCc1ccccc1)CN[C@H](C(C)C)c1ccccc1
C1942	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cc(Cl)c(Cl)c1)C(=O)CCc1ccccc1)CN1CCN(CC1)c1ccccc1C
C1943	Test	inhibitor	60	noninhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1cccc2c1C(=O)CC2=C)CN1CCCCC1
C1944	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1cccc2c1C(=C)[C@H](C2=O)c1ccccc1)CN1CCCCC1
C1945	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)COc1ccccc1C(=O)CCc1ccccc1
C1946	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1cccc(c1)C(=O)C)CN1CCN(CC1)c1c(C)cccc1
C1947	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1ccccc1C(=O)C)CN1CCN(CC1)c1c(C)c(C)ccc1
C1948	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O=C([C@@H]1Oc2ccccc2[C@H]1Cc1ccccc1)N1CCCCC1
C1949	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H]1[C@@H](Oc2c1cccc2)C(=O)N1CCCCC1
C1950	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	N(C(=O)c1cccc2c1cccc2)c1cc2c(cc1)nc(SCc1c(C)c(C(=O)C)c(C)cc1C)s2
C1951	Test	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	N(C(=O)C1=C(C)NC(=S)N[C@H]1c1cccs1)c1c(OCC)cccc1
C1952	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1(cc(ccc1C(=O)CCc1ccccc1)OC)OCC(=O)CN1CCN(CC1)c1c(cccc1)C
C1953	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cc(C)cc1)C(=O)C)CN1CCN(CC1)c1ccccc1C
C1954	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1ccc(cc1)C(=O)CCc1ccccc1)CNCCC(c1ccccc1)c1ccccc1
C1955	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(/N=C/c1cccnc1)c1nnc(nn1)n1nc(C)cc1C
C1956	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1c(cccc1)C(=O)CCc1ccc(cc1)N(C)C)CN1CCN(CC1)c1ccccc1C
C1957	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cccc1)C(=O)CCc1ccccc1)CN(C(C)C)C(C)C
C1958	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c(cc1)OC[C@@H](CN1CCN(CC1)c1c(cccc1)OC)O)C(=O)CCc1ccccc1
C1959	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cccc1)C(=O)CCc1ccccc1)CN1CCN(CC1)c1cccc(OC)c1
C1960	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H](C(Cl)(Cl)Cl)P(=O)(OC)OC
C1961	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cccc1)C(=O)CCc1ccccc1)CN1CCN(CC1)c1ccc(OC)cc1
C1962	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cccc1)C(=O)CCc1ccccc1)CN1CCN(CC1)c1ccccc1C
C1963	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cccc1)C(=O)CCc1ccccc1)CN1CCOCC1
C1964	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1ccc(cc1)C(=O)CCc1ccccc1)CN1CCCCC1
C1965	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](CNCCC)c1c(CCc2ccccc2)c2c(o1)cccc2
C1966	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H](COc1cc(ccc1)C(=O)C)CN1CCOCC1
C1967	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1c(cc(O)cc1)C(=O)CCc1ccccc1)CN(CCC)CCC
C1968	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1cc(ccc1)C(=O)CCc1ccccc1)CN1CCCCC1
C1969	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1ccc(cc1)C(=O)CCc1ccccc1)CN(CCC)CCC
C1970	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1ccccc1[C@@H](O)CCc1ccccc1)CN(CCC)CCC
C1971	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1ccccc1C(=O)CCc1cccc2c1cccc2)CNCCC(c1ccccc1)c1ccccc1
C1972	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](CN1CCN(CC1)C(c1ccccc1)c1ccccc1)c1cc(OC)c(OC)cc1
C1973	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O=C(CCc1ccccc1)c1ccccc1OCCCCN1CCCCC1
C1974	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1c(cccc1)[C@@H](O)CCc1ccccc1)CN1CCOCC1
C1975	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1c(cc(Oc2ccccc2)cc1)C(=O)CCc1ccccc1)CNC(C)C

C1976	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	N1[C@@H](N(c2ccc(Oc3ccccc3)cc2)C(=O)c2c1cccc2)c1ccc(OC)cc1
C1977	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	N1[C@H](N(c2ccc(Cl)cc2)C(=O)c2c1cccc2)c1ccc(cc1)[C@@H](C)CC
C1978	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCSc1nc2c(c(=O)n1CC=C)C1(CCCC1)Cc1c2cccc1
C1979	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cccc1)[C@H](CCc1ccccc1)OC(C)C)CN1CCCCC1
C1980	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cccc1)C(=O)C)CN1CCC(Cc2ccccc2)CC1
C1981	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1c(cccc1)C(=O)CCc1ccc(OC)cc1)CN1CCN(CC1)c1c(C)cccc1
C1982	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC(=O)O[C@H](COc1c(cccc1)C(=O)CCc1ccccc1)CN1CCCCC1
C1983	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cc(Cl)cc1)C(=O)CCc1ccccc1)CN1CCN(CC1)c1ccccc1C
C1984	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cccc1)C(=O)CCc1ccccc1)CN(C(=O)CC)c1ccccc1
C1985	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Fc1ccc(cc1)N1CCN(CCCCOc2c(cccc2)C(=O)CCc2ccccc2)CC1
C1986	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](CN1C[C@@H]2CCCC[C@H]2CC1C(=O)NC(C)(C)C)[C@H](Cc1ccccc1)NC(=O)[C@@H](CC(=O)N)NC(=O)c1nc2ccccc2cc1
C1987	Test	inhibitor	60	inhibitor	noninhibitor	inhibitor	inhibitor	COc1ccc2[C@@H]3[C@H](COc2c1)C(C)(C)OC1=C3C(=O)C(=O)C2=C1OC(C)(C)[C@H]1COc3cc(OC)ccc3[C@@H]21
C1988	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCN3CCN(C)CC3)cccc2)c1
C1989	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCN3CCc4cc(OC)c(OC)cc4C3)cccc2)c1
C1990	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCN3CCN(CC3)c3cc(Cl)ccc3)cccc2)c1
C1991	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCCN3CCN(CC3)c3cc(Cl)ccc3)cccc2)c1
C1992	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCCCN3CCN(CC3)c3cc(Cl)ccc3)cccc2)c1
C1993	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCN3CCN(CC3)c3cc(ccc3)C(F)(F)F)cccc2)c1
C1994	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCCN3CCN(CC3)c3c(OC)cccc3)cccc2)c1
C1995	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCN3CCN(CC3)c3ccc(F)cc3)cccc2)c1
C1996	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCN3CCN(CC3)c3ncccn3)cccc2)c1
C1997	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCCCN3CCN(CC3)c3ncccn3)cccc2)c1
C1998	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCCCN3CCN(C)CC3)cccc2)c1
C1999	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCN3CCc4ccccc4C3)cccc2)c1
C2000	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCCN3CCc4ccccc4C3)cccc2)c1
C2001	Test	inhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CC[C@H](NC(=O)c1ccc(Cl)c(Cl)c1)C(=O)N(CCCCC)CCCOC
C2002	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	OCC12[C@H]3C4[C@H](C5[C@@H](N([C@H]14)C(=O)Oc1ccccc1)C([C@H]2c1ccccc1)[C@@H]5N3C(=O)Oc1ccccc1)CO)c1ccccc1
C2003	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)Cc1ccccc1Nc1c(Cl)cccc1Cl
C2004	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCCO/N=C(/CCCCOC)\c1ccc(cc1)C(F)(F)F
C2005	Test	inhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1C(=O)CCc2c1ccc(OCCCCc1nnnn1C1CCCCC1)c2
C2006	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)/C=C/c1cc(O)c(O)cc1
C2007	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C1=C(CSc2nnc(C)s2)CS[C@H]2N1C(=O)[C@@H]2NC(=O)Cn1cnnn1
C2008	Test	inhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1c2nc(Cl)nc2n(C)c(=O)n1C
C2009	Test	noninhibitor	60	noninhibitor	inhibitor	noninhibitor	noninhibitor	Oc1c(Cc2c(O)oc3ccccc3c2=O)c(=O)c2ccccc2o1
C2010	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCCNC(=O)Cn1ccnc1[N+](=O)[O-]
C2011	Test	inhibitor	60	inhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]([C@@H](C)CCc1c(C(=O)O)c(O)c(C)cc1)[C@@H](C)C(=O)[C@@H](CC)[C@H]1O[C@@](CC)(C[C@H]1C)[C@@H]1CC[C@@](O)(CC)[C@@H](C)O1
C2012	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(Cc1ccccc1)c1ncnc2c1[nH]cn2
C2013	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	On1ccccc1=S
C2014	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[N]=C(N)c1ccc(OCCCCCOc2ccc(cc2)C(=N)N)cc1
C2015	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@]1(O)[C@H](C)C/C(=C\C)/C(=O)O[C@H]2CCN3CC=C(COC1=O)C23
C2016	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1CCN2C[C@H]3C[C@@H](CN4CCCC[C@H]34)C2C1
C2017	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	OC1C[C@]2(C)[C@H](C[C@H](C)[C@]2(OC(=O)c2ccco2)C(=O)CCl)[C@H]2CCC3=CC(=O)C=C[C@@]3(C)[C@]12Cl
C2018	Test	noninhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	N([C@@H](C(C)C)C(=O)O[C@@H](C#N)c1cc(Oc2ccccc2)ccc1)c1c(Cl)cc(cc1)C(F)(F)F

C2019	Test	inhibitor	60	noninhibitor	inhibitor	inhibitor	inhibitor	CCCOc1c(OC)cc2oc(cc(=O)c2c1O)c1ccccc1
C2020	Test	inhibitor	60	noninhibitor	inhibitor	inhibitor	inhibitor	COc1c2c(=O)cc(oc2cc(OC(=O)C)c1OC(=O)C)c1ccccc1
C2021	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1c(cc(C(=O)C)c(C)c1)C(=O)C)CN1CCN(CC1)c1ccccc1C
C2022	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1cc(ccc1)C(=O)CCc1ccccc1)CN1CCN(CC1)c1cccc(C)c1C
C2023	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H](COc1ccccc1C(=O)CCc1ccccc1)CNC(c1ccccc1)c1ccccc1
C2024	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O=C(CCc1ccccc1)c1ccccc1OCCCCCCCN1CCCCC1
C2025	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1c(cc(Oc2ccccc2)cc1)C(=O)CCc1ccccc1)CN1CCN(Cc2ccccc2)CC1
C2026	Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C)CCC[C@@](C#N)(C(C)C)c1cc(OC)c(OC)cc1
C2027	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1c(cccc1)C(=O)CCc1ccc(C)cc1)CN1CCN(CC1)c1c(C)cccc1
C2028	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCCCN3CCc4cc(OC)c(OC)cc4C3)cccc2)c1
C2029	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(CCc2c(OCCCN3CCN(C)CC3)cccc2)c1
C2030	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	N(CCCl)C(=O)Nc1ccc(S[C@@H]2CC3=CC(=O)CC[C@]3(C)[C@H]3CC[C@@]4(C)[C@H](CC[C@H]4C(=O)C)[C@H]23)cc1
C2031	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCCCCc1ccc(cc1)C(=O)Nc1ccccc1C(=O)NCCN1CCc2cc(c(cc2C1)OC)OC
C2032	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)c1ccc(cc1)C(=O)Nc1c(cccc1Cl)C(=O)NCCN1CCc2cc(c(cc2C1)OC)OC
C2033	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCNC(=O)c1ccccc1NC(=O)c1ccc(cc1)Oc1ccccc1
C2034	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCNC(=O)c1ccccc1NC(=O)c1ccc(cc1)C(=O)c1ccccc1
C2035	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)c1ccc(cc1)C(=O)Nc1cc(ccc1C(=O)NCCN1CCc2cc(c(cc2C1)OC)OC)N
C2036	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCNC(=O)c1ccccc1NC(=O)c1ccc(cc1)OC1CCCCC1
C2037	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCc1ccc(cc1)NC(=O)c1ccccc1NC(=O)c1cccc2c1cccc2
C2038	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCNC(=O)c1ccccc1NC(=O)c1ccc(cc1)c1ccccc1
C2039	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCc1ccc(cc1)NC(=O)c1ccccc1NC(=O)c1cccs1
C2040	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Oc1c(OC)cc(cc1)[C@@](CCCN(C)CCc1cc(OC)c(OC)cc1)(C#N)C(C)C
C2041	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCc1ccc(cc1)NC(=O)c1ccccc1NC(=O)c1cc2ccccc2o1
C2042	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)Cc1ccc(cc1)NC(=O)c1ccccc1NC(=O)c1cc2ccccc2nc1
C2043	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(CCc1ccc(cc1)NC(=O)c1ccccc1NC(=O)c1cnc2ccccc2n1)Cc1ccc(c(c1)OC)OC
C2044	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CN(CCc1ccc(cc1)NC(=O)c1ccccc1NC(=O)c1cc2ccccc2nc1)Cc1ccc(c(c1)O)OC
C2045	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Cc1cnc(cn1)C(=O)Nc1ccccc1C(=O)Nc1cccc(c1)CCN1CCc2cc(c(cc2C1)OC)OC
C2046	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)c1ccc(cc1)C(=O)Nc1cc(ccc1C(=O)NCCN1CCc2cc(c(cc2C1)OC)OC)Cl
C2047	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCNC(=O)c1ccccc1NC(=O)c1ccc2ccccc2n1
C2048	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(cc1OC)CN(CC2)CCc1ccc(cc1)NC(=O)c1ccccc1NC(=O)c1ccccn1
C2049	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(c1)C(=O)Nc1ccccc1C(=O)Nc1ccc(cc1)CCN1CCc2cc(c(cc2C1)OC)OC
C2050	Test	inhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)CS(=O)(=O)Nc1c2c(c(c3n2CCCC3)C#N)ncn1
C2051	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)c(c[nH]2)CCN1CCN(CC1)c1c2c(c(c3n2CCCC3)C#N)ncn1
C2052	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCN1CCN(CC1)c1c2c(c(c3n2CCCC3)C#N)ncn1
C2053	Test	inhibitor	60	noninhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CS(=O)(=O)N1CCN(CC1)c1c2c(c(c3n2CCCC3)C#N)ncn1
C2054	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)CN1CCN(CC1)c1c2c(c(c3n2CCCC3)C#N)ncn1
C2055	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1CCN1CCN(CC1)c1c2c(c(c3n2CCCC3)C#N)ncn1)Cl
C2056	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1CCN1CCN(CC1)c1c2c(c(c3n2CCCC3)C#N)ncn1)[N+](=O)[O-]
C2057	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COc1cccc(c1)CCN1CCN(CC1)c1c2c(c(c3n2CCCC3)C#N)ncn1
C2058	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCN1CCN(CC1)c1c2c(c(c3n2CCCC3)C#N)nc(n1)I
C2059	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCN1CCN(CC1)c1c2c(c(c3n2CCCC3)C#N)nc(n1)c1ccccc1
C2060	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CC(=O)Nc1ccc(cc1)c1nc2c(c3n(c2c(n1)N1CCN(CC1)CCc1ccccc1)CCCC3)C#N
C2061	Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Cc1ccccc1c1nc2c(c3n(c2c(n1)N1CCN(CC1)CCc1ccc(c(c1)F)F)CCCC3)C#N

C2062		Test	noninhibitor	60	inhibitor	noninhibitor	inhibitor	inhibitor	[nH]1cc(CCS(=O)(=O)c2ccccc2)c2cc(C[C@@H]3CCCN3C)ccc12
C2063		Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)c1c2n(c3c1ncnc3N1CCN(CC1)CCc1ccccc1)CCCC2
C2064		Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	Cc1c(sc(n1)c1c2n(c3c1ncnc3N1CCN(CC1)CCc1ccccc1)CCCC2)C
C2065		Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCNC(=O)c1c2n(c3c1ncnc3N1CCN(CC1)CCc1ccc(c(c1)F)F)CCCC2
C2066		Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(cnc1)NC(=O)c1c2n(c3c1ncnc3N1CCN(CC1)CCc1ccc(c(c1)F)F)CCCC2
C2067		Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccc(cc1)OC[C@H](CN1CCOCC1)O
C2068		Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1cc(ccc1OC[C@H](CN1CCCCC1)O)OCc1ccccc1
C2069		Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)c1ccc(cc1)OC[C@H](CN1CCOCC1)O
C2070		Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CN1CCN(CC1)Cc1ccccc1)O
C2071		Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@H](CNCCC(c1ccccc1)c1ccccc1)O
C2072		Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)CCC(=O)c1ccccc1OC[C@@H](CNCC(c1ccccc1)c1ccccc1)O
C2073		Test	inhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	Cc1ccccc1N1CCN(CC1)C[C@@H](Cn1c(C)c(c(=O)n1c1ccccc1)C(=O)c1ccccc1)O
C2074		Test	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCNC[C@H](Cn1c(c(c(=O)n1c1ccccc1)C(=O)c1cccs1)C)O
C2075		Test	inhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	CCCCNC[C@H](Cn1c(c(c(=O)n1c1ccccc1)C(=O)CCc1ccccc1)C)O
C2076		Test	inhibitor	60	inhibitor	inhibitor	noninhibitor	inhibitor	Cc1c(c(=O)n(n1C[C@H](CNC(C)(C)C)O)c1ccccc1)C(=O)CCc1ccccc1
C2077		Test	inhibitor	60	noninhibitor	noninhibitor	inhibitor	noninhibitor	Cc1c(c(n(n1)C)OC[C@H](CN(C(C)C)C(C)C)O)C(=O)c1ccccc1
C2078		Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCN(CC)CCC[C@H](C)N[C@H]1c2ccccc2N([C@H]([C@@H]1O)C)C(=O)c1ccc(cc1)C
C2079		Test	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	CCN(CC)CCC[C@H](C)N[C@H]1c2ccccc2N[C@H]([C@@H]1OC(=O)c1ccc(cc1)C)C
C2080	M1114707	External Validation	inhibitor	35,59	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2cc(cnc2cc1)C(=O)Nc1c(cccc1)C(=O)NC[C@H]1N(CCC1)CCc1ccc(c(c1)OC)OC
C2081	M416446	External Validation	noninhibitor	44,59	inhibitor	inhibitor	inhibitor	inhibitor	N1(Cc2c(CC1)cc(c(c2)OC)OC)CCCC1=CCCc2c1ccc(c2)OC
C2082	M416674	External Validation	noninhibitor	44,59	inhibitor	inhibitor	inhibitor	inhibitor	N1(Cc2c(CC1)cc(c(c2)OC)OC)CCCC1=CCCc2c1cc(cc2)OC
C2083	M4311	External Validation	noninhibitor	2,11,59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(=O)n(nnn1CC)CCN1CCC(N(C(=O)CC)c2ccccc2)(CC1)COC
C2084	M385	External Validation	noninhibitor	3,39,59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(=C(\NC)/NCCSCc1nc[nH]c1C)/C#N
C2085	M11310	External Validation	noninhibitor	39,43,59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@]12([C@H]([C@H]3[C@@]([C@@]4(C(=CC(=O)C=C4)CC3)C)([C@H](C2)O)F)C[C@H]([C@@]1(C(=O)CO)O)C)C
C2086	M4817	External Validation	noninhibitor	59	inhibitor	noninhibitor	noninhibitor	noninhibitor	OCCN(c1nc(N2CCCCC2)c2nc(nc(N3CCCCC3)c2n1)N(CCO)CCO)CCO
C2087	M337	External Validation	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(C(=O)c3c(C1=O)cccc3OC)c(c1c(c2O)C[C@](C[C@@H]1OC1CC([C@@H](C(O1)C)O)N)(C(=O)CO)O)O
C2088	M11744	External Validation	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@H]12[C@@H](c3c([C@H]([C@H]1C(=O)OC2)c1cc(c(c(c1)OC)O)OC)cc1c(c3)OCO1)OC1[C@@H]([C@H]2[C@H](O1)CO[C@H](O2)C)O)O
C2089	M10030	External Validation	noninhibitor	59	noninhibitor	noninhibitor	inhibitor	noninhibitor	C(c1ccc(OC(c2ccccc2)CCNC)cc1)(F)(F)F
C2090	M759062	External Validation	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(nc([nH]1)S(=O)Cc1c(c(ccn1)OCC(F)(F)F)C)cccc2
C2091	M15572	External Validation	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	o1c2c(c(c(c(c2c(=O)cc1c1cc(c(cc1)OC)OC)OC)OC)OC)OC
C2092	M714865	External Validation	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(c2c(c1)/C(=C/CCN1CCCCC1)/CCC2)OC
C2093	M10658	External Validation	noninhibitor	59	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1(nc2c([nH]1)ccc(c2)OC)S(=O)Cc1c(c(c(cn1)C)OC)C
C2094	M4596	External Validation	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1c(nc2c1ccc(c2)OC(F)F)S(=O)Cc1nccc(c1OC)OC
C2095	M7106	External Validation	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(N1CCCCC1)/C=C/C=C/c1cc2c(OCO2)cc1
C2096	M10801	External Validation	noninhibitor	39,59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C12=C[C@H](C[C@@H]([C@@H]1[C@@H](CC[C@H](C[C@H](CC(=O)O)O)O)[C@H](C=C2)C)OC(=O)[C@H](CC)C)O
C2097	M383	External Validation	noninhibitor	39,59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(OCC(CNC(C)C)O)cccc1cccc2
C2098	M10658	External Validation	noninhibitor	59	noninhibitor	noninhibitor	inhibitor	noninhibitor	COc1ccc2nc([nH]c2c1)S(=O)Cc1ncc(C)c(OC)c1C
C2099	M11820	External Validation	noninhibitor	3,39,59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[N+](=O)(/C=C(/NC)\NCCSCc1oc(cc1)CN(C)C)[O-]
C2100	M11648	External Validation	noninhibitor	59	noninhibitor	noninhibitor	inhibitor	noninhibitor	c12[C@H](c3cc(c(cc3)Cl)Cl)CCC(c1cccc2)NC
C2101	M574073	External Validation	inhibitor	6,59	inhibitor	inhibitor	inhibitor	inhibitor	c1cccc2c1C1C(c3c(C2N2CCN(CC2)C[C@@H](O)COc2cccc4c2cccn4)cccc3)C1(Cl)Cl
C2102	M1114632	External Validation	inhibitor	59	inhibitor	inhibitor	inhibitor	inhibitor	c12N3CCCc1cc1c(c2CCC3)sc2c(c1c1sc(cc1)C(=S)N1CCCCC1)ccc(=[N+](C)C)c2
C2103	M522288	External Validation	inhibitor	44,59	inhibitor	inhibitor	inhibitor	inhibitor	N1(Cc2c(CC1)cc(c(c2)OC)OC)CCC=C1CCCCC1
C2104	M414890	External Validation	inhibitor	44,59	inhibitor	inhibitor	inhibitor	inhibitor	N1(Cc2c(CC1)cc(c(c2)OC)OC)CCCC1c2c(cc(c(c2)OC)OC)CCC1

C2105	M414475	External Validation	inhibitor	44,59	inhibitor	inhibitor	inhibitor	inhibitor	N1(Cc2c(CC1)cc(c(c2)OC)OC)CCCC1c2c(c(ccc2)OC)CCC1
C2106	M414891	External Validation	inhibitor	44,59	inhibitor	inhibitor	inhibitor	inhibitor	N1(Cc2c(CC1)cc(c(c2)OC)OC)CCCC1c2c(cc(cc2)OC)CCC1
C2107	M520483	External Validation	inhibitor	44,59	inhibitor	inhibitor	inhibitor	inhibitor	N1(Cc2c(CC1)cc(c(c2)OC)OC)CCCC1c2c(ccc(c2)OC)CCC1
C2108	M3575	External Validation	inhibitor	2,3,59	inhibitor	inhibitor	inhibitor	inhibitor	n1(c2c(nc1NC1CCN(CC1)CCc1ccc(cc1)OC)cccc2)Cc1ccc(cc1)F
C2109	M207452	External Validation	inhibitor	6,59	inhibitor	inhibitor	inhibitor	inhibitor	c1cccc(c1)C(c1ccccc1)C(=O)N1CCN(CC1)CC(O)COc1c2cccnc2ccc1
C2110	M399601	External Validation	inhibitor	35,59	inhibitor	inhibitor	inhibitor	inhibitor	n1c2c(cccc2)cc(c1)C(=O)Nc1cc(c(cc1C(=O)Nc1ccc(cc1)N1CCN(CC1)Cc1cc(c(cc1)OC)OC)OC)OC
C2111	M424626	External Validation	inhibitor	35,59	inhibitor	inhibitor	inhibitor	inhibitor	n1c2c(cccc2)cc(c1)C(=O)Nc1ccccc1C(=O)Nc1ccc(cc1)N1CCN(CC1)Cc1cc(c(cc1)OC)OC
C2112	M8963	External Validation	inhibitor	38,59	inhibitor	inhibitor	inhibitor	inhibitor	c1(cccc(c1C)O)C(=O)N[C@@H]([C@@H](O)CN1[C@@H](C[C@H]2[C@H](C1)CCCC2)C(=O)NC(C)(C)C)CSc1ccccc1
C2113	M196073	External Validation	inhibitor	44,59	inhibitor	inhibitor	inhibitor	inhibitor	N1(CCN(CC1)CCCC1c2c(c(ccc2)OC)CCC1)C1CCCCC1
C2114	M2145	External Validation	inhibitor	4,59	inhibitor	inhibitor	inhibitor	inhibitor	[C@@](c1cc(c(cc1)OC)OC)(CCCN(CCc1cc(c(cc1)OC)OC)C)(C(C)C)C#N
C2115	M451514	External Validation	inhibitor	4,59	inhibitor	inhibitor	inhibitor	inhibitor	Brc1c2[C@@H](C3CCN(CC3)C(=O)CC3CCN(CC3)C(=O)N)c3ncc(Br)cc3CCc2cc(Cl)c1
C2116	M481924	External Validation	inhibitor	7,59	inhibitor	inhibitor	inhibitor	inhibitor	n1cc(cc2ccccc12)C(=O)Nc1c(cc(c(c1)OC)OC)C(=O)Nc1ccc(cc1)CCN1Cc2c(CC1)cc(c(c2)OC)OC
C2117	M9654	External Validation	noninhibitor	59	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1c(oc2cc(cc(c2c1=O)O)O)c1cc(c(cc1)O)O
C2118	M13905	External Validation	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc(c1c1c(c(=O)c2c(cc(cc2o1)O)O)O)O)O
C2119	M271	External Validation	noninhibitor	3,61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc(c1)OC(=O)N(C)C)[N+](C)(C)C
C2120	M7899	External Validation	noninhibitor	39,61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(cc(c1F)N1CCNCC1)n(cc(c2=O)C(=O)O)CC
C2121	M3466	External Validation	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c3c(c(c1F)N1CCN(CC1)C)OC[C@H](C)n3cc(c2=O)C(=O)O
C2122	M481423	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(cnc1)CCCC(CCCc1cccnc1)OC(=O)C1CCCCN1C(=O)C(=O)c1cc(c(c(c1)OC)OC)OC
C2123	M13019	External Validation	noninhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C(c1ccccc1O2)C(=O)OCC[N+](C(C)C)(C(C)C)C
C2124	M1010501	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cc(c(c1)OC)OC)nc(nc2N1Cc2cc(c(cc2CC1)OC)OC)NCCc1ccc(c(c1)OC)OC
C2125	M1017600	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cc(c(c1)OC)OC)nc(nc2NCCc1cccc(c1OC)OC)NCCc1cccc(c1OC)OC
C2126	M4339	External Validation	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(cc(c(c1OC)OC)OC)Cc1cnc(nc1N)N
C2127	M407175	External Validation	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1[C@@H](C1(CCCCC1)O)CN(C)C)OC
C2128	M1017602	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(ccc(c1)N(C)C)nc(nc2N1Cc2cc(c(cc2CC1)OC)OC)NCCc1ccc(c(c1)OC)OC
C2129	M1017599	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1C)nc(nc2N(Cc1ccccc1)C)NCCc1ccc(c(c1)OC)OC
C2130	M14503	External Validation	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=O)c1c(cc(CC(=O)O)n1C)C)Cl
C2131	M8074	External Validation	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1=C2CC[C@H]3[C@@H]4CC[C@H](C(=O)CO)[C@@]4(C)C[C@@H]([C@@H]3[C@@]2(C)CCC1=O)O
C2132	M12589	External Validation	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1C[C@@H](C(=O)O)N)O)O
C2133	M10352	External Validation	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)CC[C@@H](C)NC[C@H](c1ccc(c(c1)C(=O)N)O)O
C2134	M15782	External Validation	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1[C@H](C(=O)N[C@@H]1C(=O)N2C(=C(CS[C@H]12)CSc1nnnn1C)C(=O)O)NC(=O)N1C(=O)C(=O)N(CC)CC1)O
C2135	M3421	External Validation	noninhibitor	61	inhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cccc1)c(c(cc2)OCC)C(=O)N[C@@H]1C(=O)N2[C@@H](C(=O)O)C(C)(C)S[C@H]12
C2136	M60683	External Validation	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCC[N+](CCCC)(CCCC)C
C2137	M120545	External Validation	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c1cc2ccc1C[C@H]1c3c(cc4c(c3Oc3cc5c(cc3OC)CCN([C@@H]5Cc3ccc(c(c3)O2)OC)C)OCO4)CCN1C
C2138	M5051	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)C=Cc1ccccc1C2=C1CCN(CC1)C
C2139	M12057	External Validation	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c12c(cccc1)oc(c2C(=O)c1cc(c(c(c1)I)OCCNCC)I)CCCC
C2140	M3717	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)CCc1ccccc1N2CCCNC
C2141	M8819	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)nc(cc2C(=O)NCCN(CC)CC)OCCCC
C2142	M1106438	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)C1=C(C)NC(=C(C(=O)c2ccccc2)C1c1ccccc1)C
C2143	M1106440	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)C1=C(C)NC(=C(C(=O)c2ccccc2)C1c1ccccc1[N+](=O)[O-])C
C2144	M1106441	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)C1=C(C)NC(=C(C(=O)c2ccccc2)C1c1cccc(c1)Oc1ccccc1)C
C2145	M1106449	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C(=O)C1=C(C)NC(=C(C(=O)c2ccccc2)C1c1cccc(c1)Cl)C
C2146	M10190	External Validation	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(c(c1)Cl)Cl)[C@@H]1C(=C(C)NC(=C1C(=O)OCC)C)C(=O)OC
C2147	M10476	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)/C=C/CN1CCN(C(c2ccc(cc2)F)c2ccc(cc2)F)CC1

C2148	M1402	External Validation	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1/C(=N/OCCN)/CCCCOC)C(F)(F)F
C2149	M347099	External Validation	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c12c(ccnc2)c(ccc1)S(=O)(=O)NCCNC/C=C/c1ccc(cc1)Br
C2150	M6297	External Validation	inhibitor	61	noninhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(=O)CCCN1CCC(c2ccc(cc2)Cl)(CC1)O)F
C2151	M664	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)CCc1ccccc1N2CCCN(C)C
C2152	M15534	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc2OC[C@@H](CN2CCN(C3c4ccccc4[C@@H]4[C@H](c5ccccc35)C4(F)F)CC2)O)nccc1
C2153	M5615	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)C[C@@H](C[C@@H]([C@H](Cc1ccccc1)NC(=O)COc1c(cccc1C)C)O)NC(=O)[C@H](C(C)C)N1C(=O)NCCC1
C2154	M12976	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N=C(c1cc(ccc1O2)Cl)N1CCN(CC1)C
C2155	M15678	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C1=C2C(C)C[C@H]3[C@@H]4CC[C@](C(=O)C)([C@@]4(C)CC[C@@H]3[C@@]2(C)CCC1=O)OC(=O)C
C2156	M1018138	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)N1C2(C(=O)N(CC(C)C)C1)CCN(CC2)C[C@](c1ccc(cc1)F)(C)C1OCCO1
C2157	M11920	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)OCCn1c(CC)nn(c1=O)CCCN1CCN(c2cccc(c2)Cl)CC1
C2158	M4202	External Validation	inhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(c(c1)C1C(=C(C)NC(=C1C(=O)OC)C)C(=O)OC)[N+](=O)[O-]
C2159	M1017597	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	C(#N)[C@](c1cc(c(c(c1)OC)OC)OC)(CCCNCCc1ccc(c(c1)OC)OC)C(C)C
C2160	M380650	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1c1c(c2ccc(cc2)NC(C)C)[nH]c(c2ccc(cc2)/C=C/COCC)n1)NC(C)C
C2161	M9705	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)Cl)CCCN1CCN(CC1)CCO
C2162	M13856	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)n(c(=O)[nH]2)C1CCN(CCCC(c2ccc(cc2)F)c2ccc(cc2)F)CC1
C2163	M7381	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)/C(=C(/c1ccccc1)\CC)/c1ccc(cc1)OCCN(C)C
C2164	M52793	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1c2c(ccc(c1OC)Oc1cc(c(cc1C[C@@H]1c3cc(c(cc3CCN1C)OC)OC)OC)OC)C[C@@H]1c3c(cc(c(c23)OC)OC)CCN1C
C2165	M12877	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc(cc1)/C(=C(/c1ccccc1)\CCCl)/c1ccc(cc1)OCCN(C)C
C2166	M328406	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1C(c1ccc(cc1)F)CNC1CCN(c2nc(nc(n2)NCC=C)NCC=C)CC1)F
C2167	M13959	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1c1c(CC(=O)N(C)C)n2c(ccc(c2)C)n1)C
C2168	M1106477	External Validation	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c1ccc(cc1)P(=CC(=O)c1ccccc1c1ccccc1C(=O)C=P(c1ccccc1)(c1ccccc1)c1ccccc1)(c1ccccc1)c1ccccc1
C2169	M91186	External Validation	inhibitor	61	inhibitor	noninhibitor	inhibitor	inhibitor	c1cc(c(cc1CCN(CCCC1(c2ccc(c(c2)OC)OC)S(=O)(=O)CCCS1(=O)=O)C)OC)OC
C2170	M1083101	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)cc(cc2)C1(CCCN(CCc2ccc(c(c2)OC)OC)C)SCCCS1
C2171	M1017612	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1cc(ccc1S2)SCC)CCCN1CCN(CC1)C
C2172	M7367	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)/C(=C/CCN1CCN(CC1)CCO)/c1cc(ccc1S2)C(F)(F)F
C2173	M9482	External Validation	inhibitor	61	noninhibitor	inhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)N=C(c1cc(ccc1O2)Cl)N1CCNCC1
C2174	M237104	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cccc1)oc(c2CCc1ccccc1)CCNCCC
C2175	M1017603	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cc(cc1)OS(=O)(=O)CCCC)sc(c2C(=O)c1ccc(cc1)OCCN1CCCCC1)c1ccc(cc1)OS(=O)(=O)CCCC
C2176	M1017604	External Validation	inhibitor	61	inhibitor	inhibitor	inhibitor	inhibitor	c12c(cc(cc1)OS(=O)(=O)CCCCCC)sc(c2C(=O)c1ccc(cc1)OCCN1CCCCC1)c1ccc(cc1)OS(=O)(=O)CCCCCC
C2177	M3384	External Validation	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c(ccc1NC(=O)CCC)OC[C@@H](CNC(C)C)O)C(=O)C
C2178	M13199	External Validation	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c(nc(c(n1)Cl)N)N)C(=O)NC(=N)N
C2179	M2557	External Validation	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)C=Cc1ccccc1N2C(=O)N
C2180	M10890	External Validation	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(ccc1Cl)oc(=O)[nH]2
C2181	M7123	External Validation	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(cc(c1F)N1CCNCC1)n(cc(c2=O)C(=O)O)C1CC1
C2182	M5328	External Validation	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)CCN(C(=N)N)C2
C2183	M9679	External Validation	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc(c1C(Cn1cncn1)(Cn1cncn1)O)F)F
C2184	M7455	External Validation	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(c(c1)C)NC(=O)CN(CC)CC)C
C2185	M3335	External Validation	noninhibitor	61	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[C@]1(C(=O)N(C(=O)N1)C)CC
C2186	M1007070	External Validation	inhibitor	4	inhibitor	inhibitor	inhibitor	inhibitor	C[C@@H]1[C@@H](OC(=O)/C=C/C=C/c2ccccc2)[C@@]2(O[C@]3(O[C@@H]2C2C4O[C@@]4(CO)[C@@H](O)[C@@]4(O)[C@@H](C=C(C)C4=O)[C@@]12O3)c1ccccc1)C(=C)C
C2187	M10071	External Validation	inhibitor	2, 3, 11	inhibitor	inhibitor	inhibitor	inhibitor	COc1c(OC)cc2c(N)nc(nc2c1)N1CCN(CC1)C(=O)C1COc2ccccc2O1
C2188	M1010568	External Validation	inhibitor	2, 3, 56	inhibitor	inhibitor	inhibitor	inhibitor	COc1ccc(cc1)c1c(C#N)c(=S)n(C2OC(COC(=O)C)C(OC(=O)C)C(OC(=O)C)C2OC(=O)C)c2c1C(=O)CC(C)(C)C2
C2189	M1016888	External Validation	inhibitor	4, 56	inhibitor	noninhibitor	inhibitor	inhibitor	COC1=CC(=O)c2c3c1c1C(=CC(=O)c4c1c(c(CC(C)OC(=O)c1ccccc1)c(OC)c4O)c3c(CC(C)OC(=O)Oc1ccc(O)cc1)c(OC)c2O)OC
C2190	M1016889	External Validation	inhibitor	4, 56	inhibitor	noninhibitor	inhibitor	inhibitor	CO[C@]1(C)[C@H]([C@@H]2O[C@@]1(C)n1c3ccccc3c3c4CNC(=O)c4c4c5ccccc5n2c4c13)N(C)C(=O)c1ccccc1

C2191	M1016890	External Validation	inhibitor	4, 5, 7, 8, 11, 17, 56	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)C1C(c2cc(ccc2)[N+](=O)[O-])C(=C(C)N[C@]1(C)c1ccc(cc1)N1CCN(CC1)C(c1ccccc1)c1ccccc1)C(=O)OC=C
C2192	M1017596	External Validation	inhibitor	10	inhibitor	noninhibitor	noninhibitor	noninhibitor	OC(CNCCOc1ccccc1O)COc1cccc2c1c1ccccc1[nH]2
C2193	M1017611	External Validation	inhibitor	5, 8, 11, 17	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)c1cnc2n1CCc1ccccc1C2=C1CCN(CCc2ccc(OCc3nc4ccccc4cc3)cc2)CC1
C2194	M1017635	External Validation	inhibitor	13	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)[N+](C)(CC(O)COc1ccccc1C(=O)CCc1ccccc1)C(C)C
C2195	M1017636	External Validation	inhibitor	13	inhibitor	inhibitor	noninhibitor	inhibitor	CCC[N+](C)(C)CC(O)COc1ccccc1C(=O)CCc1ccccc1
C2196	M1017637	External Validation	inhibitor	13	inhibitor	inhibitor	inhibitor	inhibitor	C[N+]1(C[C@@H](O)COc2ccccc2C(=O)CCc2ccccc2)CCCCC1
C2197	M1017638	External Validation	inhibitor	13	inhibitor	inhibitor	inhibitor	inhibitor	CC[N+](C)(CC)CC(O)COc1ccccc1C(=O)CCc1ccccc1
C2198	M1018137	External Validation	inhibitor	2, 3	inhibitor	inhibitor	inhibitor	inhibitor	COc1ccc(cc1)c1c(O[C@@H]2O[C@@H](C)[C@H](O)[C@@H](O)[C@H]2O)c(=O)c2c(O)cc(O)c(CC=C(C)C)c2o1
C2199	M1018139	External Validation	inhibitor	2, 3	inhibitor	inhibitor	inhibitor	inhibitor	CC(=O)OCC1OC(C(OC(=O)C)C(OC(=O)C)C1OC(=O)C)N1C(=C(C#N)C(C=C1c1ccccc1)c1ccco1)S
C2200	M1018140	External Validation	inhibitor	2, 3	inhibitor	inhibitor	inhibitor	inhibitor	CC(=O)OCC1OC(C(OC(=O)C)C(OC(=O)C)C1OC(=O)C)n1c(=S)c(C#N)c(c2ccc(Cl)cc2)c2c1CC(C)(C)CC2=O
C2201	M1018141	External Validation	inhibitor	2, 3	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCC1OC(C(O)C(O)C1O)N1C(=C(C#N)C(C=C1c1ccccc1)c1ccco1)S
C2202	M1018142	External Validation	inhibitor	2, 3	noninhibitor	noninhibitor	inhibitor	noninhibitor	OCC1OC(C(O)C(O)C1O)N1C(=C(C#N)C(C=C1c1ccccc1)c1ccccc1)S
C2203	M1018143	External Validation	inhibitor	2, 3	inhibitor	inhibitor	inhibitor	inhibitor	CC(=O)OCC1OC(C(OC(=O)C)C(OC(=O)C)C1OC(=O)C)N1C(=C(C#N)C(C=C1c1ccccc1)c1ccccc1)S
C2204	M1018328	External Validation	inhibitor	2, 3, 4	noninhibitor	inhibitor	noninhibitor	noninhibitor	CC(=CCc1c(O)cc(O)c2c1oc(c(O)c2=O)c1ccccc1)C
C2205	M1050678	External Validation	inhibitor	54	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1ccc(NC(=S)N/N=C/2\C(=O)Nc3c2cc(I)cc3)cc1
C2206	M1050680	External Validation	inhibitor	54	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1ccc(NC(=S)N/N=C/c2ccccn2)cc1
C2207	M10573	External Validation	inhibitor	4, 53	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1cc(O)c2c(=O)c(O)c(oc2c1)c1ccc(OC)cc1
C2208	M109311	External Validation	inhibitor	15	inhibitor	inhibitor	inhibitor	inhibitor	C[C@@H]1C[C@H]2[C@@H]3CC=C4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1C(=O)C
C2209	M109583	External Validation	inhibitor	8, 11	inhibitor	noninhibitor	inhibitor	inhibitor	CC(C)CN(C[C@@H](O)[C@@H](Cc1ccccc1)NC(=O)O[C@H]1CO[C@H]2OCC[C@@H]12)S(=O)(=O)c1ccc(N)cc1
C2210	M1106431	External Validation	inhibitor	4	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)C1CN=C2N1CCc1c(cccc1)C2=C1CCN(CCc2ccc(OCc3nc4c(cccc4)cc3)cc2)CC1
C2211	M1106437	External Validation	inhibitor	18	noninhibitor	inhibitor	noninhibitor	noninhibitor	CCOC(=O)C1C(COCCNC2=NCCN2)NC(=C(C1c1c(Cl)cccc1)C(=O)OC)C
C2212	M1106439	External Validation	noninhibitor	19	inhibitor	inhibitor	inhibitor	inhibitor	CC1=C(C(c2cc(ccc2)[N+](=O)[O-])C(=C(C)N1)C(=O)c1ccccc1)C(=O)c1ccccc1
C2213	M1106445	External Validation	inhibitor	19	inhibitor	inhibitor	inhibitor	inhibitor	CSc1ccc(cc1)C1C(=C(C)NC(=C1C(=O)c1ccccc1)C)C(=O)c1ccccc1
C2214	M1106446	External Validation	noninhibitor	19	inhibitor	inhibitor	inhibitor	inhibitor	COc1c(cccc1)C1C(=C(C)NC(=C1C(=O)c1ccccc1)C)C(=O)c1ccccc1
C2215	M1106448	External Validation	noninhibitor	19	inhibitor	inhibitor	inhibitor	inhibitor	CC1=C(C(c2c(Cl)cccc2)C(=C(C)N1)C(=O)c1ccccc1)C(=O)c1ccccc1
C2216	M1106450	External Validation	noninhibitor	19	inhibitor	inhibitor	inhibitor	inhibitor	CC1=C(C(c2ccc(Cl)cc2)C(=C(C)N1)C(=O)c1ccccc1)C(=O)c1ccccc1
C2217	M1106452	External Validation	noninhibitor	19	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc(cc(OC)c1OC)C1C(=C(C)NC(=C1C(=O)c1ccccc1)C)C(=O)c1ccccc1
C2218	M1106453	External Validation	inhibitor	20, 21	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)C(=O)c1ccc(OCCCN2CCC(CC2)C(O)(c2ccc(F)cc2)c2ccc(F)cc2)cc1
C2219	M1106457	External Validation	inhibitor	22	inhibitor	inhibitor	inhibitor	inhibitor	COc1c(C)c2c(cc1)[C@@]1(C)CCC3[C@@H](C)[C@@]4(OC(C)(C)[C@@H](C)[C@H]4O)O[C@]13C=C2
C2220	M1106459	External Validation	inhibitor	4	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc(/C=C/C(=O)O[C@@H]2[C@H](O)[C@@H]3C[C@H](C[C@H]2N3C)OC(=O)c2cc(OC)c(OC)c(OC)c2)cc(OC)c1OC
C2221	M1106469	External Validation	inhibitor	23	inhibitor	inhibitor	inhibitor	inhibitor	CCOC(=O)c1c[n+](ccc1c1ccc(OC)cc1)C(=O)Oc1ccccc1
C2222	M1106470	External Validation	inhibitor	23	inhibitor	inhibitor	inhibitor	inhibitor	CCOC(=O)c1c(cc[n+](c1)C(=O)Oc1ccccc1)c1ccccc1OC
C2223	M1106471	External Validation	inhibitor	23	inhibitor	inhibitor	inhibitor	inhibitor	CCOC(=O)c1c[n+](ccc1c1ccc(C)cc1)C(=O)Oc1ccccc1
C2224	M1106472	External Validation	inhibitor	23	inhibitor	inhibitor	noninhibitor	inhibitor	COc1ccc(cc1)c1cc[n+](cc1C(=O)C)C(=O)Oc1ccccc1
C2225	M1106473	External Validation	inhibitor	23	inhibitor	inhibitor	inhibitor	inhibitor	COc1ccccc1c1cc[n+](cc1C(=O)C)C(=O)Oc1ccccc1
C2226	M1106474	External Validation	inhibitor	23	inhibitor	inhibitor	inhibitor	inhibitor	CC(=O)c1c[n+](ccc1c1ccc(C)cc1)C(=O)Oc1ccccc1
C2227	M1106478	External Validation	inhibitor	2, 24	inhibitor	inhibitor	inhibitor	inhibitor	COc1ccc(cc1)C1C(=C(S)N(C2OC(COC(=O)C)C(OC(=O)C)C(OC(=O)C)C2OC(=O)C)C(=C1C(=O)C)c1ccccc1)C#N
C2228	M1107346	External Validation	inhibitor	24	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(CC3N(C)CCc4cc(OC)c(OC)c2c34)cc1Oc1cc(OC)c(OC)cc1Cc1c2CN(C)CCc2cc(OC)c1OC
C2229	M1107348	External Validation	inhibitor	24	inhibitor	inhibitor	inhibitor	inhibitor	C[C@H]1C(COC(=O)C)O[C@H]([C@H](OC(=O)C)[C@H]1OC(=O)C)N1C(=C(C#N)C(C=C1c1ccccc1)c1ccco1)S
C2230	M1107349	External Validation	inhibitor	24	inhibitor	inhibitor	inhibitor	inhibitor	COc1ccc(cc1)C1=C(C#N)C(=S)N(C2CC(COC(=O)C)C(OC(=O)C)C(OC(=O)C)C2OC(=O)C)C2CC(C)(C)CC(=O)C12
C2231	M1107350	External Validation	inhibitor	24	inhibitor	inhibitor	inhibitor	inhibitor	CC(=O)OCC1CC(C(OC(=O)C)C(OC(=O)C)C1OC(=O)C)N1C2CC(C)(C)CC(=O)C2C(=C(C#N)C1=S)c1ccc(Cl)cc1
C2232	M1107353	External Validation	inhibitor	24	inhibitor	inhibitor	inhibitor	inhibitor	C[C@H]1C(COC(=O)C)O[C@H]([C@H](OC(=O)C)[C@H]1OC(=O)C)N1C(=C(C#N)C(C=C1c1ccccc1)c1ccccc1)S
C2233	M1107367	External Validation	inhibitor	4, 9, 14, 30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)C1=C(C)NC(=C(C1c1cc(ccc1)[N+](=O)[O-])C(=O)OCCCN1CCC(CC1)(c1ccccc1)c1ccccc1)C

C2234	M1107375	External Validation	noninhibitor	25	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc(O)c(cc1C1CC(=O)c2c(O)cc(O)c(CC=C(C)C)c2O1)C(C)(C)C=C
C2235	M1107376	External Validation	inhibitor	25	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1c(C)c(O)c(C)c(O)c1C(=O)/C=C\c1ccccc1
C2236	M1107377	External Validation	noninhibitor	25	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCc1cc2c(cc1)C1COc3cc(O)ccc3C1O2
C2237	M1107378	External Validation	inhibitor	5	noninhibitor	inhibitor	inhibitor	inhibitor	O=C(Nc1cc2c(cc1)c(=O)cc(o2)c1[nH]nnn1)c1ccc(OCCCCc2ccccc2)cc1
C2238	M1107379	External Validation	inhibitor	5	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc(cc(OC)c1OC)C(=O)C(=O)N(C)[C@@H](Cc1ccc(Cl)cc1)C(=O)N(Cc1ccccc1)C(CCc1ccncc1)CCc1ccncc1
C2239	M1107380	External Validation	inhibitor	5	inhibitor	inhibitor	inhibitor	inhibitor	CC(=O)OC(C)(C)[C@H]1CC[C@@]2(C)(O1)[C@@H](O)CC[C@]1(C)(O)[C@H]1CC[C@H]2O[C@H](CC[C@]2(C)O1)[C@]1(C)CC[C@@H](Br)C(C)(C)O1
C2240	M1107383	External Validation	inhibitor	5	noninhibitor	noninhibitor	noninhibitor	noninhibitor	BrC1=CCn2ccccc2=C1Br
C2241	M1107384	External Validation	inhibitor	5	noninhibitor	inhibitor	inhibitor	inhibitor	CCCC1=C(C(=O)CC(C)(C)C1)[C@@]1(CCCC(C)(C)C1)C#N
C2242	M1107385	External Validation	inhibitor	5	noninhibitor	noninhibitor	inhibitor	noninhibitor	Cc1cc(C)c(c(C)c1)S(=O)(=O)c1ccc(cc1)C(C)(C)C
C2243	M1107386	External Validation	inhibitor	5	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1SC2SCCSC2S1
C2244	M1107391	External Validation	inhibitor	5	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1c(OC)c(OC)c(OC)c(OC)c1OC
C2245	M1107394	External Validation	inhibitor	5	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nnc(Cc2nnc(N)s2)s1
C2246	M1107397	External Validation	inhibitor	5	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1cc2c(s1)sc(Cl)c2
C2247	M1107403	External Validation	inhibitor	5	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1cc(=O)oc2c1cc(c(O)c2)[N+](=O)[O-]
C2248	M1107404	External Validation	inhibitor	5	inhibitor	noninhibitor	inhibitor	inhibitor	CC(C)C1COC2C(N1)c1c(OC2(C)C)ccc(c1)C#N
C2249	M1107405	External Validation	inhibitor	5	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)NC1C(OC(=O)c2ccc(C)cc2)C(C)Nc2c1cccc2
C2250	M1107408	External Validation	inhibitor	5	inhibitor	noninhibitor	inhibitor	inhibitor	CC(C)NCC(O)c1c(CCc2ccc(F)cc2)c2c(s1)cccc2
C2251	M1107409	External Validation	inhibitor	5	inhibitor	inhibitor	inhibitor	inhibitor	C(CN1CCCCC1)CN1c2c(Sc3c1ccc1ccccc31)cccc2
C2252	M1107410	External Validation	inhibitor	5	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)N(CC(O)COc1cccc(c1)C(=O)c1ccccc1)C(C)C
C2253	M1107417	External Validation	inhibitor	5	inhibitor	inhibitor	inhibitor	inhibitor	CCOC(=O)/C=C(/C)\C=C/C=C\Cc1cc2c(cc1)C(C)(C)CCC2(C)C
C2254	M1107427	External Validation	inhibitor	26	inhibitor	inhibitor	inhibitor	inhibitor	CC1(C)Oc2ccc(cc2C([C@H]1O)N1CCN(Cc2ccccc2)CC1)C#N
C2255	M1107428	External Validation	inhibitor	26	inhibitor	inhibitor	inhibitor	inhibitor	CCN(CC)CCCC[C@@H](C)N[C@H]1[C@@H](O)[C@@H](C)N(C(=O)c2ccc(C)cc2)c2ccccc12
C2256	M1114515	External Validation	inhibitor	28	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)C(=O)O[C@H]1C2[C@@H](O)C@](C)(C[C@]2(O)C(=O)[C@H](C)/C=C/C(C)(C)[C@@H](OC(=O)C)[C@@H](OC(=O)C)[C@H](OC(=O)c2ccccc2)C1=C)OC(=O)C
C2257	M1114516	External Validation	inhibitor	28	inhibitor	inhibitor	inhibitor	inhibitor	CCC(C)C(=O)O[C@H]1C2[C@@H](O)[C@](C)(C[C@]2(O)C(=O)[C@H](C)/C=C/C(C)(C)[C@@H](OC(=O)C)[C@@H](OC(=O)C)[C@H](OC(=O)c2ccccc2)C1=C)OC(=O)C
C2258	M1114517	External Validation	inhibitor	28	inhibitor	inhibitor	inhibitor	inhibitor	C[C@@H]1/C=C/C(C)(C)[C@@H](OC(=O)C)[C@@H](OC(=O)C)[C@H](OC(=O)c2ccccc2)C(=C/[C@@H](OC(=O)c2ccccc2)C2[C@@H](O)[C@](C)(C[C@]2(O)C1=O)OC(=O)C
C2259	M1114518	External Validation	inhibitor	28	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)C(=O)O[C@H]1[C@@H]2[C@@H](O)[C@@H](C)C[C@@]2(O)C(=O)[C@H](C)/C=C/C(C)(C)[C@@H](OC(=O)C)[C@@H](OC(=O)C)[C@@H](OC(=O)c2ccccc2)C1=C
C2260	M1114519	External Validation	inhibitor	28	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)C(=O)O[C@H]1[C@@H]2[C@@H](OC(=O)C)[C@@H](C)C[C@@]2(O)C(=O)[C@H](C)/C=C/C(C)(C)[C@@H](OC(=O)C)[C@@H](OC(=O)C)[C@@H](OC(=O)c2ccccc2)C1=C
C2261	M1114520	External Validation	inhibitor	28	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)C(=O)O[C@H]1[C@@H]2[C@@H](OC(=O)C)[C@@](C)(O)C[C@@]2(O)C(=O)[C@H](C)/C=C/C(C)(C)[C@@H](OC(=O)C)[C@@H](OC(=O)C)[C@@H](OC(=O)c2ccccc2)C1=C
C2262	M1114521	External Validation	inhibitor	28	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)C(=O)O[C@H]1[C@H](OC(=O)C)[C@H](OC(=O)C)C(C)(C)/C=C/[C@@H](C)C(=O)[C@@]2(O)C[C@](C)(OC(=O)C)[C@H](OC(=O)c3ccccc3)C2[C@H](OC(=O)C)C1=C
C2263	M1114522	External Validation	inhibitor	28	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)C(=O)O[C@H]1[C@H](OC(=O)C)[C@H](OC(=O)C)C(C)(C)/C=C\[C@@H](C)C(=O)[C@@]2(O)C[C@](C)(OC(=O)C)[C@H](OC(=O)c3ccccn3)C2[C@H](OC(=O)C)C1=C
C2264	M1114523	External Validation	inhibitor	28	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)C(=O)O[C@H]1[C@H](OC(=O)C)[C@H](OC(=O)C)C(C)(C)/C=C\[C@@H](C)C(=O)[C@@]2(O)C[C@H](C)[C@H](OC(=O)c3ccccc3)C2[C@H](OC(=O)C)C1=C
C2265	M1114524	External Validation	inhibitor	28	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)C(=O)O[C@H]1C2[C@@H](OC(=O)C)[C@](C)(C[C@]2(O)C(=O)C)[C@H](C)/C=C/C(C)(C)[C@@H](OC(=O)c2ccccc2)[C@@H](OC(=O)C)[C@H](OC(=O)C)C1=C)OC(=O)c1ccccc1
C2266	M1114556	External Validation	inhibitor	29	inhibitor	inhibitor	inhibitor	inhibitor	C[C@@H]1/C=C/C(C)(C)[C@@H](OC(=O)c2ccccc2)[C@@H](OC(=O)C)[C@H](OC(=O)C)C(=C[C@@H](OC(=O)C)C2[C@@H](OC(=O)c3ccccc3)[C@](C)(C[C@]2(O)[C@@H]1OC(=O)OC(=O)C
C2267	M1114557	External Validation	inhibitor	29	inhibitor	inhibitor	inhibitor	inhibitor	CCC(C)C(=O)O[C@H]1[C@H](O)[C@H](OC(=O)c2ccccc2)C(C)(C)/C=C\[C@@H](C)C(=O)[C@@]2(O)C[C@](C)(OC(=O)C)[C@H](OC(=O)c3ccccc3)C2[C@H](OC(=O)C)C1=C
C2268	M1114558	External Validation	inhibitor	29	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)C(=O)O[C@H]1[C@H]2[C@@H](OC(=O)C)[C@@](C)(C[C@]2(O)C(=O)[C@H](OC(=O)C)[C@@H](C)/C=C/C(C)(C)[C@H](OC(=O)C)[C@@H](OC(=O)C)[C@@H](OC(=O)c2ccccc2)C1=C)OC(=O)C
C2269	M1114559	External Validation	inhibitor	29	inhibitor	inhibitor	inhibitor	inhibitor	C[C@H]1C[C@@]2(OC(=O)C)C([C@H]1OC(=O)C)[C@H](OC(=O)C)C(=C)[C@H](C[C@H](OC(=O)C)C(C)(C)/C=C/[C@@H](C)C2=O)OC(=O)C
C2270	M1114560	External Validation	inhibitor	29	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)C(=O)O[C@H]1[C@H](O)[C@H](OC(=O)c2ccccc2)C(C)(C)/C=C/[C@@H](C)C(=O)[C@@]2(O)C[C@](C)(OC(=O)C)[C@H](OC(=O)c3ccccc3)C2[C@H](OC(=O)C)C1=C
C2271	M1114561	External Validation	inhibitor	29	inhibitor	inhibitor	inhibitor	inhibitor	C[C@@H]1/C=C/C(C)(C)[C@@H](OC(=O)C)[C@@H](O)[C@H](OC(=O)C)C(=C)[C@@H](OC(=O)C)C2[C@@H](OC(=O)c3ccccc3)[C@](C)(C[C@]2(O)[C@@H]1OC(=O)OC(=O)C
C2272	M1114562	External Validation	inhibitor	29	inhibitor	inhibitor	inhibitor	inhibitor	C[C@H]1/C=C/C(C)(C)[C@H](C[C@H](OC(=O)C)C(=C)[C@@H](OC(=O)C)C2[C@@H](OC(=O)C)[C@](C)(C[C@]2(OC(=O)C)C1=O)OC(=O)C)OC(=O)c1ccccc1
C2273	M1114565	External Validation	inhibitor	4, 58	inhibitor	inhibitor	inhibitor	inhibitor	C(C[C@H](C[C@H](NC(C)=O)[C@@H](CC(=O)C[C@H](CC(=O)OC)C(C)(C)C=C[C@@H](C)C=O)[C@@H](NC(=O)[C@H](C)C(C)(C)C=C)C(=O)[C@@H](CCCCCNC(=O)[C@H](C)C(C)(C)C=C)C(=O)OC)C(=O)OC)C(=O)OC
C2274	M1114595	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)C1=C(C)NC(=C(C1c1ccc(OC)cc1)C(=O)OCCCN1CCC(CC1)(c1ccccc1)c1ccccc1)C
C2275	M1114596	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	CCOc1ccc(cc1)C1C(=C(C)NC(=C1C(=O)OCCCN1CCC(CC1)(c1ccccc1)c1ccccc1)C)C(=O)OC
C2276	M1114597	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)C1=C(C)NC(=C(C1c1ccc(cc1)N(C)C)C(=O)OCCCN1CCC(CC1)(c1ccccc1)c1ccccc1)C

C2277	M1114598	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)C1=C(C)NC(=C(C1c1ccc(OCc2ccccc2)cc1)C(=O)OCCCN1CCC(CC1)(c1ccccc1)c1ccccc1)C
C2278	M1114600	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)C1=C(C)NC(=C(C1c1ccc(OC(=O)C)cc1)C(=O)OCCCN1CCC(CC1)(c1ccccc1)c1ccccc1)C
C2279	M1114602	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)C1=C(C)NC(=C(C1c1ccc(cc1)C(=O)OCc1ccccc1)C(=O)OCCCN1CCC(CC1)(c1ccccc1)c1ccccc1)C
C2280	M1114603	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)C1=C(C)NC(=C(C1c1ccc(C)cc1)C(=O)OCCCN1CCC(CC1)(c1ccccc1)c1ccccc1)C
C2281	M1114604	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)C1=C(C)NC(=C(C1c1cc(O)ccc1)C(=O)OCCCN1CCC(CC1)(c1ccccc1)c1ccccc1)C
C2282	M1114605	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)C1=C(C)NC(=C(C1c1cc(C)c(O)cc1)C(=O)OCCCN1CCC(CC1)(c1ccccc1)c1ccccc1)C
C2283	M1114606	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)C1=C(C)NC(=C(C1c1cc(OC)c(OC)cc1)C(=O)OCCCN1CCC(CC1)(c1ccccc1)c1ccccc1)C
C2284	M1114607	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)C1=C(C)NC(=C(C1c1cc2c(OCCO2)cc1)C(=O)OCCCN1CCC(CC1)(c1ccccc1)c1ccccc1)C
C2285	M1114608	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)C1=C(C)NC(=C(C1c1cc2c(OCO2)cc1)C(=O)OCCCN1CCC(CC1)(c1ccccc1)c1ccccc1)C
C2286	M1114609	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)c1c(c2ccc(OC)cc2)c(C(=O)OCCCN2CCC(CC2)(c2ccccc2)c2ccccc2)c(C)nc1C
C2287	M1114610	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	CCOc1ccc(cc1)c1c(C(=O)OC)c(C)nc(C)c1C(=O)OCCCN1CCC(CC1)(c1ccccc1)c1ccccc1
C2288	M1114611	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)c1c(c2ccc(cc2)N(C)C)c(C(=O)OCCCN2CCC(CC2)(c2ccccc2)c2ccccc2)c(C)nc1C
C2289	M1114612	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)c1c(c2ccc(OCc3ccccc3)cc2)c(C(=O)OCCCN2CCC(CC2)(c2ccccc2)c2ccccc2)c(C)nc1C
C2290	M1114613	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)c1c(c2ccc(NC(=O)C)cc2)c(C(=O)OCCCN2CCC(CC2)(c2ccccc2)c2ccccc2)c(C)nc1C
C2291	M1114614	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)c1c(c2ccc(cc2)C(=O)OCc2ccccc2)c(C(=O)OCCCN2CCC(CC2)(c2ccccc2)c2ccccc2)c(C)nc1C
C2292	M1114615	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)c1c(c2cc(OC)c(OC)cc2)c(C(=O)OCCCN2CCC(CC2)(c2ccccc2)c2ccccc2)c(C)nc1C
C2293	M1114616	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)c1c(c2cc3c(OCCO3)cc2)c(C(=O)OCCCN2CCC(CC2)(c2ccccc2)c2ccccc2)c(C)nc1C
C2294	M1114617	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)c1c(c2cc3c(OCO3)cc2)c(C(=O)OCCCN2CCC(CC2)(c2ccccc2)c2ccccc2)c(C)nc1C
C2295	M1114705	External Validation	inhibitor	33	inhibitor	inhibitor	noninhibitor	inhibitor	CC(C)C(=O)OC(C)(C)C1Cc2c(O1)ccc1c2oc(=O)cc1
C2296	M1114706	External Validation	inhibitor	34	inhibitor	inhibitor	inhibitor	inhibitor	COc1c2Oc3ccc(C[C@@H]4N(C)CCc5cc(OC)c(Oc6c(OC)c(OC)c(Br)c7c6[C@H](Cc(cc1)c2)N(C)CC7)cc45)cc3
C2297	M1114708	External Validation	inhibitor	35	inhibitor	inhibitor	inhibitor	inhibitor	O=C(Nc1ccccc1C(=O)N[C@H]1CCCC[C@@H]1N1CCN(CC1)c1ccccc1)c1cc2c(cccc2)nc1
C2298	M1114709	External Validation	inhibitor	4	inhibitor	inhibitor	inhibitor	inhibitor	CC1=C(C(c2cc(ccc2)[N+](=O)[O-])C(=C(C)N1CCN1CCOCC1)P1(=O)OCC(C)(C)CO1)C(=O)OCCN(Cc1ccccc1)c1ccccc1
C2299	M1114710	External Validation	inhibitor	4	noninhibitor	noninhibitor	inhibitor	noninhibitor	COC(=O)[C@]1(O)C[C@@H]2O[C@]1(C)n1c3ccccc3c3c4CNC(=O)c4c4c5ccccc5n2c4c13
C2300	M1114711	External Validation	inhibitor	4	noninhibitor	inhibitor	noninhibitor	noninhibitor	CC(=CCc1c(O)cc2oc(c(O)c(=O)c2c1O)c1ccccc1)C
C2301	M1114712	External Validation	inhibitor	4	noninhibitor	inhibitor	inhibitor	inhibitor	CO[C@H]1[C@H](C[C@H]2O[C@@]1(C)n1c3ccccc3c3c4CN(Cc5ccccc5)C(=O)c4c4c5ccccc5n2c4c13)N(C)C(=O)c1ccccc1
C2302	M1114716	External Validation	inhibitor	36	inhibitor	inhibitor	inhibitor	inhibitor	C[C@H]1C[C@]2(OC(=O)C)C(/C=C(\C)/[C@H](OC(=O)C)C(OC(=O)C)C(=O)C(C)(C)/C=C\[C@H](C)C2=O)[C@@H]1OOc1ccccc1
C2303	M1114717	External Validation	inhibitor	36	inhibitor	inhibitor	inhibitor	inhibitor	C[C@H]1C[C@]2(OC(=O)C)C(/C=C(/C)\[C@H](OC(=O)C)[C@@H](OC(=O)C)C(=O)C(C)(C)C/C=C(/C)\C2=O)[C@@H]1OOc1ccccc1
C2304	M1114718	External Validation	inhibitor	36	inhibitor	inhibitor	inhibitor	inhibitor	C[C@H]1C[C@]2(OC(=O)C)C(/C=C(/C)/[C@H](O)C[C@@H](O)C(C)(C)/C=C/[C@@H](C)[C@@H]2OC(=O)C)[C@@H]1OOc1ccccc1
C2305	M1114719	External Validation	inhibitor	36	inhibitor	inhibitor	inhibitor	inhibitor	C[C@H]1C[C@]2(OC(=O)C)C(/C=C(/C)/[C@@H](CC(=O)C(C)(C)/C=C/C(C)[C@@H]2OC(=O)COOc2ccccc2)[C@@H]1OOc1ccccc1
C2306	M1114720	External Validation	inhibitor	36	inhibitor	inhibitor	inhibitor	inhibitor	CC1C[C@]2(O)C(/C=C(/C)\C(CC(OC(=O)C)C(C)(C)/C=C/C(C)C2OC(=O)C)OC(=O)c2ccccc2)C1OC(=O)C
C2307	M1114721	External Validation	inhibitor	36	inhibitor	inhibitor	inhibitor	inhibitor	C[C@H]1C[C@]2(OC(=O)C)C(/C=C(\C)/[C@@H](CC(=O)C(C)(C)/C=C/C(C)[C@@H]2OC(=O)COOC(=O)C)[C@@H]1OOc1ccccc1
C2308	M1114723	External Validation	inhibitor	36	inhibitor	inhibitor	inhibitor	inhibitor	CCC/C=C\C=C/C(=O)O[C@H]1C[C@H]2[C@@H](/C=C(\C)/C(=O)[C@]3(C[C@@H](C)[C@@H](O)[C@@H]3/C=C\1/C)OC(=O)C)C2(C)C
C2309	M1114750	External Validation	inhibitor	20	inhibitor	inhibitor	noninhibitor	inhibitor	COc1c(O)ccc(c1)C(O)CNCCCCCCOCCCCc1ccccc1
C2310	M1114751	External Validation	inhibitor	20	inhibitor	inhibitor	inhibitor	inhibitor	N#CC(COc1cccc2c1cccn2)CN1CCN(CC1)C1c2c(CCc3c1cccc3)cccc2
C2311	M11544	External Validation	inhibitor	2, 3, 4, 53	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1cc(O)c2c(oc(c(O)c2=O)c2ccccc2)c1
C2312	M117181	External Validation	inhibitor	6	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)[C@@]1(NC(=O)[C@@H]2C[C@H]3[C@@H](Cc4c[nH]c5cccc3c45)N(C)C2)O[C@@]2(O)[C@@H]3CCCN3C(=O)[C@H](Cc3ccccc3)N2C1=O
C2313	M11763	External Validation	inhibitor	2, 3, 4, 8, 11	inhibitor	inhibitor	inhibitor	inhibitor	CC#C[C@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CCC4=C3[C@H](C[C@]12C)c1ccc(cc1)N(C)C
C2314	M120818	External Validation	inhibitor	5	inhibitor	noninhibitor	noninhibitor	noninhibitor	CN(C)CCNC(=O)c1cccc2cc3c(cccc3)nc12
C2315	M12202	External Validation	inhibitor	23	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)c1cccnc1
C2316	M12733	External Validation	inhibitor	17, 32	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc(S)c2[nH]cnc2n1
C2317	M12859	External Validation	inhibitor	5	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCOC(=O)C
C2318	M12987	External Validation	inhibitor	2, 3, 11	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H]1C[C@H]2O[C@@H]2[C@H]2[C@H](OC(=O)C)CC(=O)O[C@@H]2C(C=CC=C(C[C@H]3O[C@H]2CC=O)O[C@H]3C)C(=O)O[C@H]1C[C@H]2O[C@H]3[C@H](OC(=O)C)C2[C@H]4NC)C
C2319	M1303	External Validation	noninhibitor	2, 3, 4, 11, 39	inhibitor	noninhibitor	noninhibitor	noninhibitor	CCC(=O)[C@H]1CC[C@H]2[C@H]3CC=C4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]12C)OC(=O)CC(C)(C)C(=O)O[C@H]1CC[C@]2(C)C(=CC1)CC[C@H]1[C@@H]2CC=C2[C@]1(C)CC[C@H](O)C2

C2320	M130974	External Validation	inhibitor	4, 5, 6, 7, 8, 11, 12, 17, 38, 44, 50, 51, 55, 56	inhibitor	inhibitor	inhibitor	inhibitor	COC1CCCC2C1NC1C(CCCC1C(=O)Nc1ccc(CCN3CCc4cc(OC)c(OC)cc4C3)cc1)C2=O
C2321	M132899	External Validation	inhibitor	17	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)C/C=C/C(=O)N[C@H]1C/O[C@@H](O)[C@@H](C)[C@H](O)[C@H]2O[C@@H]([C@@H](O)[C@@H]2O)N2CCC(=O)NC2=O)O[C@@H]1O[C@H]1O[C@@H](CO)[C@@H](O)[C@H](O)[C@H]1NC(=O)C
C2322	M136	External Validation	inhibitor	2, 11, 51	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H]1[C@@H]1O[C@H]2[C@@H]([C@@H](C)[C@@H]1O[C@H]3O[C@@H](C)[C@@H](O)[C@@H]3OC(=O)C)C3([C@@H](C(=O)O[C@@H]1CC)[C@@H]2O)C=O)[C@@H](C)[C@@H](C)[C@@H](C)[C@@H]3C)C=O)[C@@H](C)[C@@H](C)[C@@H](C)[C@@H]1NC)C
C2323	M13899	External Validation	inhibitor	5	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1ccccc1
C2324	M139686	External Validation	inhibitor	4	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1c(oc2cc(O)cc(O)c2c1=O)c1ccccc1
C2325	M1400	External Validation	inhibitor	6	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@]12O[C@@]([NC(=O)[C@@H]3C=C4c5c6c([nH]cc6C[C@@H]4N(C)C3)ccc5)(C(=O)N1[C@H](C(=O)N1CCC[C@H]21)Cc1ccccc1)C
C2326	M140091	External Validation	inhibitor	17	noninhibitor	noninhibitor	inhibitor	noninhibitor	COc1c(O)cc2CCN[C@]3(CS[C@H]4[C@H]5[C@@H]6N(C)[C@@H](Cc7c6c(O)c(OC)c(C)c7)(C@H](O)N5[C@H](COC3=O)c3c5OCOc5c(C)c(OC(=O)C)c43)c2c1
C2327	M14240	External Validation	inhibitor	11	inhibitor	noninhibitor	inhibitor	inhibitor	COc1c(cc(Cl)cc1)C(=O)NCCc1ccc(cc1)S(=O)(=O)NC(=O)NC1CCCCC1
C2328	M14245	External Validation	inhibitor	5	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ClCCOCCCl
C2329	M14424	External Validation	inhibitor	3, 11	inhibitor	inhibitor	inhibitor	inhibitor	N1c2c(N=c3ccccc3=C1N1CCN(C)CC1)ccc(Cl)c2
C2330	M14566	External Validation	noninhibitor	33	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=c1oc2cc3c(cco3)cc2cc1
C2331	M15634	External Validation	inhibitor	41	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1ccc(cc1)c1coc2cc(O)cc(O)c2c1=O
C2332	M15790	External Validation	inhibitor	2, 3, 8, 9, 11, 12, 14, 31, 38, 55, 58	inhibitor	inhibitor	inhibitor	inhibitor	CC[C@]1(O)C[C@H]2CN(C1)CCc1c[nH]c3c1cccc3)[C@@]2(C(=O)OC)c1cc2c(cc1OC)N(C)[C@@H]1[C@@]2[C2CN2CC=C[C@](CC)([C@@H][32][C@@H](OC(=O)C)[C@]1(O)C(=O)OC
C2333	M159520	External Validation	inhibitor	42	inhibitor	inhibitor	inhibitor	inhibitor	CS(=O)(=O)CCNCc1ccc(o1)c1ccc2ncnc(Nc3cc(Cl)c(OCc4cc(F)ccc4)cc3)c2c1
C2334	M17181	External Validation	inhibitor	11	inhibitor	inhibitor	noninhibitor	inhibitor	COc1cc2c(cc1OC)C1CC(=O)C(CC(C)C)CN1CC2
C2335	M17314	External Validation	inhibitor	5	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1cc(C)[nH]n1
C2336	M18063	External Validation	noninhibitor	33	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc2ccc(=O)oc2c1
C2337	M1808	External Validation	inhibitor	2, 3, 11, 40	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCN(CCC)S(=O)(=O)c1ccc(cc1)C(=O)O
C2338	M18589	External Validation	inhibitor	5	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ClCC1CO1
C2339	M204304	External Validation	inhibitor	26	inhibitor	inhibitor	inhibitor	inhibitor	CCN(CC)CCCC(C)N[C@@H]1[C@@H](OC(=O)c2ccc(C)cc2)[C@H](C)Nc2c1cccc2
C2340	M21220	External Validation	noninhibitor	33	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=c1oc2c3ccoc3ccc2cc1
C2341	M2167	External Validation	inhibitor	4, 7	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc2cc3c(nc2cc1N(C)C)cc(cc3)N(C)C
C2342	M2191	External Validation	inhibitor	2, 3, 41	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(/C=C/c1ccccc1)c1ccccc1
C2343	M221729	External Validation	inhibitor	30	inhibitor	inhibitor	inhibitor	inhibitor	COC(=O)c1c(c2cc(ccc2)[N+](=O)[O-])c(C(=O)OCCCN2CCC(CC2)(c2ccccc2)c2ccccc2)c(C)nc1C
C2344	M231436	External Validation	inhibitor	2, 3, 11	inhibitor	inhibitor	inhibitor	inhibitor	OC1=C(C2CCC(CC2)c2ccc(Cl)cc2)C(=O)C(=O)c2c1cccc2
C2345	M238029	External Validation	inhibitor	13, 27	inhibitor	inhibitor	inhibitor	inhibitor	CC(=O)c1ccccc1OCC(O)CN1CCN(CC1)c1ccc(F)cc1
C2346	M241860	External Validation	inhibitor	13	inhibitor	inhibitor	inhibitor	inhibitor	OC(COc1cccc(c1)C(=O)CCc1ccccc1)CN1CCN(CC1)c1ccc(F)cc1
C2347	M242896	External Validation	inhibitor	13, 27	inhibitor	inhibitor	inhibitor	inhibitor	OC(COc1ccccc1C(O)CCc1ccccc1)CN1CCN(CC1)c1ccc(F)cc1
C2348	M2433	External Validation	inhibitor	46	inhibitor	noninhibitor	inhibitor	inhibitor	OC(=O)c1c(OCC)cc(cc1)CC(=O)N[C@H](c1ccccc1N1CCCCC1)CC(C)C
C2349	M243462	External Validation	inhibitor	13	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)c1ccc(OCC(O)CN2CCCCC2)cc1
C2350	M243860	External Validation	inhibitor	47	noninhibitor	inhibitor	inhibitor	inhibitor	CCCNCC(O)COc1ccc(O)cc1C(=O)CCc1ccccc1
C2351	M244636	External Validation	inhibitor	13	inhibitor	inhibitor	inhibitor	inhibitor	OC(COc1ccc(cc1)C(=O)CCc1ccccc1)CN1CCN(CC1)c1ccc(F)cc1
C2352	M246106	External Validation	noninhibitor	11	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC[C@@H](N1CCCC1=O)C(=O)N
C2353	M278334	External Validation	inhibitor	47	noninhibitor	inhibitor	noninhibitor	noninhibitor	NCC(O)COc1ccccc1C(=O)CCc1ccccc1
C2354	M287111	External Validation	inhibitor	2, 3, 4	inhibitor	inhibitor	inhibitor	inhibitor	CC(=CCC/C(=C\Cc1c2oc(cc(=O)c2c(O)cc1O)c1ccccc1)/C)C
C2355	M28754	External Validation	inhibitor	20, 21	inhibitor	inhibitor	inhibitor	inhibitor	OCCN1CCCN(CCCN2c3ccccc3Sc3ccc(cc23)C(F)(F)F)CC1
C2356	M3235	External Validation	inhibitor	46	inhibitor	inhibitor	noninhibitor	inhibitor	OCc1c(O)ccc(c1)[C@@H](O)CNCCCCCCOCCCCc1ccccc1
C2357	M323684	External Validation	inhibitor	48	inhibitor	inhibitor	inhibitor	inhibitor	OC(COc1c2cccnc2ccc1)CN1CCN(CC1)C1c2c(cccc2)C2C(c3c1cccc3)C2(F)F
C2358	M3320	External Validation	inhibitor	5	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1CNCCN1
C2359	M336538	External Validation	inhibitor	13, 27	inhibitor	inhibitor	inhibitor	inhibitor	CCN(CC)CC(O)COc1ccccc1C(=O)CCc1ccccc1
C2360	M33913	External Validation	inhibitor	5	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1cc2c([nH]cc2CN(C)C)cc1
C2361	M339254	External Validation	inhibitor	13, 27	inhibitor	inhibitor	inhibitor	inhibitor	OC(COc1ccccc1C(=O)CCc1ccccc1)CN1CCOCC1
C2362	M3466	External Validation	inhibitor	2, 3, 4, 7, 11	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1c(N2CCN(CC2)C)c2OCC(n3c2c(c1)c(=O)c(c3)C(=O)O)C

C2363	M35592	External Validation	inhibitor	10	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)NCC(O)COc1c(cc(NC(=O)C)cc1)C(=O)C
C2364	M359933	External Validation	inhibitor	45	inhibitor	inhibitor	inhibitor	inhibitor	CCC(=O)N(CC(O)COc1ccccc1C(=O)CCc1ccccc1)Cc1ccccc1
C2365	M360620	External Validation	inhibitor	45	inhibitor	inhibitor	inhibitor	inhibitor	CCCN(CC(O)COc1ccccc1C(=O)CCc1ccccc1)C(=O)c1ccccc1
C2366	M3676	External Validation	inhibitor	6, 8, 11, 37, 55	inhibitor	inhibitor	inhibitor	inhibitor	[nH]1c(nc2ccccc12)CCCN(C)CC[C@@]1(OC(=O)COC)CCc2c(ccc(F)c2)[C@@H]1C(C)C
C2367	M369416	External Validation	inhibitor	13, 27, 45	inhibitor	inhibitor	inhibitor	inhibitor	OC(COc1ccccc1C(=O)CCc1ccccc1)CN1CCCCC1
C2368	M4045	External Validation	noninhibitor	49	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ccc(cc1)C(=O)NCC(=O)O
C2369	M4147	External Validation	noninhibitor	43	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H]1CC2=CC[C@H]3[C@@H]4CC[C@H]([C@H](C)CCCC(C)C)[C@@]4(C)CC[C@@H]3[C@@]2(C)CC1
C2370	M4175	External Validation	noninhibitor	11	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C(=O)OC)c1[nH]c2c(n1)cc(SCCC)cc2
C2371	M4466	External Validation	noninhibitor	33	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1c(O)cc2ccc(=O)oc2c1
C2372	M4517	External Validation	inhibitor	4	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCCC[C@H](Nc1c2ncccc2cc(OC)c1)C
C2373	M465811	External Validation	inhibitor	52	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)(C)NC(=O)[C@H]1CN(Cc2cc3c(occ3)nc2)CCN1C[C@@H](O)C[C@@H](Cc1ccccc1)C(=O)N[C@@H]1[C@@H](O)Cc2ccccc12
C2374	M478798	External Validation	inhibitor	45	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1ccccc1C(=O)CCc1ccccc1)CN1CCN(Cc2ccccc2)CC1
C2375	M479134	External Validation	inhibitor	13, 45	inhibitor	inhibitor	inhibitor	inhibitor	OC(COc1ccccc1C(=O)CCc1ccccc1)CN1CCC(O)(CC1)c1ccccc1
C2376	M481020	External Validation	inhibitor	4	inhibitor	inhibitor	inhibitor	inhibitor	CC(=CCc1c(O)c2c(oc(cc2=O)c2ccccc2)c(CC=C(C)C)c1O)C
C2377	M500998	External Validation	inhibitor	45	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](COc1ccccc1C(=O)CCc1ccccc1)CN1CCN(CC1)C(=O)c1ccccc1
C2378	M502737	External Validation	inhibitor	54	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[O-][N+](=O)c1cc2c(NC(=O)/C/2=N\NC(=S)Nc2ccccc2)cc1
C2379	M51114	External Validation	inhibitor	2, 11, 12	inhibitor	inhibitor	inhibitor	inhibitor	C[NH+](C)CCC=C1c2c(CCc3c1cccc3)cccc2
C2380	M5346	External Validation	inhibitor	6, 51, 56	inhibitor	inhibitor	inhibitor	inhibitor	O[C@]1(CC)CN2C[C@@H](C1)C[C@@](C(=O)OC)(c1c(c3ccccc3[nH]1)CC2)c1c(OC)cc2N(C)[C@@H]3[C@]4(c2c1)CCN1CC=C[C@](CC)([C@@H]41)[C@@H](OC(=O)C)[C@]3(O)C(=O)OC
C2381	M536263	External Validation	inhibitor	4	noninhibitor	inhibitor	inhibitor	inhibitor	COc1c(oc2c(c(O)cc(O)c2c1=O)C(C)(C)C=C)c1ccccc1
C2382	M550284	External Validation	inhibitor	25	inhibitor	inhibitor	inhibitor	inhibitor	CC(=CCc1c2OCC(C(=O)c2c(O)cc1O)c1cc(c(O)cc1O)C(C)(C)C=C)C
C2383	M55376	External Validation	noninhibitor	11	inhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)n1c(/C=C\[C@H](O)C[C@H](O)CC(=O)O)c(c2ccccc12)c1ccc(F)cc1
C2384	M559899	External Validation	inhibitor	54	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1ccc(NC(=S)N/N=C/2\C(=O)Nc3c2ccc2ccccc32)cc1
C2385	M56146	External Validation	noninhibitor	33	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCC1O[C@@H](Oc2c(O)cc3oc(=O)ccc3c2)C(O)C(O)[C@@H]1O
C2386	M5652	External Validation	noninhibitor	11	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1CO[C@@H]2[C@H](O)CO[C@H]12
C2387	M573329	External Validation	inhibitor	54	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1ccc(NC(=S)N/N=C/2\C(=O)Nc3c2cc(cc3)[N+](=O)[O-])cc1
C2388	M577760	External Validation	inhibitor	54	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1ccc(NC(=S)N/N=C/2\C(=O)Nc3c2cc(Br)cc3)cc1
C2389	M594356	External Validation	inhibitor	25	inhibitor	noninhibitor	inhibitor	inhibitor	CC(=CCc1c2OC(CC(=O)c2c(O)cc1O)c1cc(c(O)cc1O)C(C)(C)C=C)C
C2390	M6112	External Validation	inhibitor	37	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cn(cn1)C[C@H](OCc1ccc(Cl)cc1)c1c(Cl)cc(Cl)cc1
C2391	M614377	External Validation	inhibitor	4	inhibitor	inhibitor	inhibitor	inhibitor	CC(=CCC/C(=C\Cc1c(O)cc2oc(cc(=O)c2c1O)c1ccccc1)/C)C
C2392	M617543	External Validation	inhibitor	5	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)(CO)NCC(=O)N1[C@@H](CC[C@@H]1C#N)C#N
C2393	M61964	External Validation	inhibitor	2, 4, 9, 38, 41	inhibitor	inhibitor	inhibitor	inhibitor	CC[C@H]1NC(=O)[C@@H]([C@@H](O)[C@@H](C)C/C=C/C)N(C)C(=O)[C@@H](C(C)C)N(C)C(=O)[C@@H](CC(C)C)N(C)C(=O)[C@@H](CC(C)C)N(C)C(=O)[C@@H](C)NC(=O)[C@@H](C)NC(=O)[C@@H](CC(C)C)N(C)C(=O)[C@@H](NC(=O)[C@@H](CC(C)C)N(C)C(=O)CN(C)C1=O)C(C)C
C2394	M630270	External Validation	noninhibitor	44	inhibitor	inhibitor	inhibitor	inhibitor	COc1cc2c(CN(CCCC3=CCCc4c(OC)cccc34)CC2)cc1OC
C2395	M646585	External Validation	inhibitor	13	inhibitor	inhibitor	inhibitor	inhibitor	CCC(=O)c1ccccc1OCC(O)CN1CCC(O)(CC1)c1ccccc1
C2396	M64805	External Validation	noninhibitor	39	inhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)[C@@H](NC(=O)[C@@H](CCCN=C(N)N)NC(=O)[C@@H](N)CC(=O)N)C(=O)N[C@H](Cc1ccc(O)cc1)C(=O)N[C@H](C(C)C)C(=O)N[C@@H](Cc1c[nH]cn1)C(=O)N1CCC[C@@H]1C(=O)N[C@@H](Cc1ccccc1)C(=O)O
C2397	M6496	External Validation	inhibitor	6	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@]12O[C@@](NC(=O)[C@H]3CN(C)[C@@H]4Cc5c[nH]c6cccc(c56)[C@H]4C3)(C(=O)N1[C@H](C(=O)N1CCC[C@@H]21)Cc1ccccc1)C
C2398	M66671	External Validation	inhibitor	6	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)[C@]1(NC(=O)C2CN(C)C3Cc4c[nH]c5cccc(c45)C3=C2)O[C@]2(O)C3CCCN3C(=O)C(Cc3ccccc3)N2C1=O
C2399	M66672	External Validation	inhibitor	6	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)CC1N2C(=O)[C@](NC(=O)C3CN(C)C4Cc5c[nH]c6cccc(c56)C4=C3)(O[C@]2(O)C2CCCN2C1=O)C(C)C
C2400	M667908	External Validation	noninhibitor	25	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1cc(/C=C\c2ccc(O)cc2)cc(OC)c1
C2401	M66946	External Validation	inhibitor	6	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)[C@@H]1N2C(=O)[C@](NC(=O)[C@H]3CN(C)[C@@H]4Cc5c[nH]c6cccc(c56)C4=C3)(O[C@@]2(O)[C@@H]2CCCN2C1=O)C(C)C
C2402	M684340	External Validation	inhibitor	54	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=S)N/N=C/c1c(N)cccn1
C2403	M68614	External Validation	noninhibitor	43	inhibitor	inhibitor	inhibitor	inhibitor	CC(=O)C1=CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C
C2404	M6922	External Validation	inhibitor	57, 1	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[C@@]1(C)CC[C@]2(C)CC[C@@]3(C(=CC(=O)[C@@H]4[C@@]5(C)CC[C@H](O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]2C1)C
C2405	M6959	External Validation	inhibitor	11	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H]1[C@@H](O[C@H]2[C@@H](C)[C@@H](O[C@H]3O[C@@H](C)[C@@H](O)[C@@](OC)(C)C3)[C@@H](C(=O)O[C@@H](CC)[C@@](O)(C)[C@H](O)[C@@H](N(C)C[C@@H](C)C[C@@]2(O)C)C)C)O[C@@H](C)C[C@@H]1N(C)C

C2406	M700622	External Validation	inhibitor	11	inhibitor	inhibitor	inhibitor	inhibitor	CC[C@@H]1OC(=O)[C@@H](C)C(=O)[C@@H](C)[C@@H](O[C@@H]2O[C@@H](C)C[C@@H](C[C@@H]2O)N(C)C)[C@@](C)(C[C@@H](C)C(=O)[C@@H](C)[C@@H]2N(CCCCa3cac(c3)c3cccc3)C(=O)O[C@]12C)OC
C2407	M70826	External Validation	inhibitor	2, 3, 4, 8, 9, 16, 56	inhibitor	inhibitor	inhibitor	inhibitor	CC[C@]12C=CCN3CC[C@]4([C@H]13)[C@@H](N(C)c1c4ccc(OC)c1)[C@](O)([C@@H]2OC(=O)C)C(=O)OC
C2408	M71140	External Validation	inhibitor	57, 1	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](CCC=C(C)C)CC=O
C2409	M759047	External Validation	inhibitor	3, 6, 11, 12, 56	inhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)O[C@H]1C2=C(C[C@@H](C[C@@](O)([C@@H]O[C@H](C(=O)c3ccccc3)[C@H]2[C@]4(CO[C@@H]4C[C@@H](O)[C@@]3(C)C1=O)OC(=O)C)C2(C)OC(=O)[C@@H](O)[C@@H]NC(=O)c1ccccc1)c1ccccc1
C2410	M759064	External Validation	inhibitor	2, 4, 11, 38, 51	inhibitor	inhibitor	inhibitor	inhibitor	CC[C@@H](C)n1ncn(c1=O)c1ccc(cc1)N1CCN(CC1)c1ccc(OC[C@H]2CO[C@@](Cn3cncn3)(O2)c2c(Cl)cc(Cl)cc2)cc1
C2411	M759092	External Validation	inhibitor	46	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1c(C)c(C)c(/C=C/C(=C/C=C/C(=C\C(=O)O)/C)/C)c(C)c1
C2412	M7948	External Validation	noninhibitor	2, 3, 11, 55, 56	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@H]12CC[C@](O)(C(=O)CO)[C@@]1(C)C[C@H](O)[C@H]1[C@H]2CCC2=CC(=O)C=C[C@]12C
C2413	M8381	External Validation	inhibitor	2, 6, 11, 38	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@]12O[C@@](NC(=O)[C@@H]3C=C4c5c6c([nH]c(Br)c6C[C@H]4N(C)C3)ccc5)(C(=O)N1[C@H](C(=O)N1CCC[C@@H]21)CC(C)C)C(C)C
C2414	M9083	External Validation	inhibitor	2, 3, 4, 9, 11, 56	inhibitor	inhibitor	inhibitor	inhibitor	C(c(c@@H](C[C@@H]([C@@H]([C@@H]([C@@H]CC(=O)[C@H](C)/C=C/C)[C@@H](O)[C@@H](OC)C(=O)[C@H](C)C[C@H](C)/C=C/C=C/C)C)[C@@H]([C@@H](C[C@@H](C)[C@@H](O)(O)O3)C(=O)C(=O)N3CCCCC3[C@H]2C=O)O2)OCC(C)(C)C
C2415	M9249	External Validation	inhibitor	4	inhibitor	inhibitor	inhibitor	inhibitor	CN(C)CCCn1cc(c2c1cccc2)C1=C(C(=O)NC1=O)c1c[nH]c2c1cccc2
C2416	M9472	External Validation	inhibitor	2, 4, 6, 8, 11, 12, 14, 38, 51, 55, 56	inhibitor	inhibitor	inhibitor	inhibitor	CC(C)(C)NC(=O)[C@H]1C[C@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@@H](Cc1ccccc1)NC(=O)[C@@H](CC(=O)N)NC(=O)c1ccc2ccccc2n1
C2417	M9537	External Validation	inhibitor	46	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H]1C/C(=C/C=C\2/CCC[C@@]3(C)[C@H]2CC[C@@H]3[C@H](C)CCCC(C)C)/C(=C)CC1
C2418	M9557	External Validation	inhibitor	2, 3, 20, 21	inhibitor	inhibitor	inhibitor	inhibitor	N1C(=C(C(=O)OC)[C@H](c2cc(ccc2)[N+](=O)[O-])C(=C1C)C(=O)O[C@H]1CN(Cc2ccccc2)CCC1)C
C2419	M98515	External Validation	inhibitor	5	inhibitor	inhibitor	inhibitor	inhibitor	CC(=O)[C@@]1(O)CC[C@H]2[C@@H]3C=C(C)C4=CC(=O)CC[C@@H]4[C@H]3CC[C@]12C
C2420	M9862	External Validation	inhibitor	46	inhibitor	noninhibitor	inhibitor	inhibitor	CCCc1nc2c(cc(cc2C)c2nc3c(cccc3)n2C)n1Cc1ccc(cc1)c1ccccc1C(=O)O
C2421	M5097	External Validation	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(CCCC)C(=O)NS(=O)(=O)c1ccc(C)cc1
C2422	M2469	External Validation	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CC[C@H](NC(=O)c1ccc(cc1)N(C)Cc1cnc2nc(nc(N)c2n1)N)C(=O)O
C2423	M1156	External Validation	inhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cn1cnc2c1c(=O)n(CCCCC(=O)C)c(=O)n2C
C2424	M2026	External Validation	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	N1CN(c2ccccc2)C2(CCN(CCCC(=O)c3ccc(F)cc3)CC2)C1=O
C2425	M10163	External Validation	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cn1cnc2c1c(=O)n(C)c(=O)n2C
C2426	M11671	External Validation	inhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=c1cc(oc2ccccc12)c1ccccc1
C2427	M654531	External Validation	inhibitor	60	inhibitor	inhibitor	inhibitor	inhibitor	N1C(=C([C@@H](c2cccc(c2)[N+](=O)[O-])C(=C1C)C(=O)OCCN(C)Cc1ccccc1)C(=O)OC)C
C2428	M6004	External Validation	noninhibitor	60	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc(cc1)c1cc(=O)c2c(O)cc(O)cc2o1
C2429	DB00104	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)[C@H]1NC(=O)[C@@H]([C@@H](O)C)NC(=O)[C@@H]1NC(=O)[C@@H](Cc2c[nH]c3c2cccc3)NC(=O)[C@@H](Cc2ccccc2)NC(=O)[C@@H](NC(=O)[C@@H]([C@@H](O)C)NC(=O)[C@@H](Cc2ccccc2)N(CSSC1)CCCCN)NC(=O)[C@@H](CO)[C@@H](O)C
C2430	DB00119	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C(=O)C
C2431	DB00125	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(O)[C@@H](N)CCCNC(=N)N
C2432	DB00132	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CCCCCCC/C=C\C/C=C\C/C=C\CC
C2433	DB00140	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(nc3c(cc(c(c3)C)C)n2C[C@@H]([C@@H]([C@@H](CO)O)O)O)c(=O)[nH]c(=O)n1
C2434	DB00141	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)[C@@H]([C@H]([C@@H]([C@@H]([C@H](O)CO)O)O)O)NC(=O)C
C2435	DB00143	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	SC[C@H](NC(=O)CC[C@H](N)C(=O)O)C(=O)NCC(=O)O
C2436	DB00147	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1c(c(CO)cnc1C)C=O
C2437	DB00148	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CN(C)C(=N)N
C2438	DB00152	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	s1c(c([n+](Cc2c(nc(nc2)C)N)c1)C)CCO
C2439	DB00154	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CCCCCC/C=C\C/C=C\C/C=C\CCCCC
C2440	DB00159	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=C\C/C=C\C/C=C\C/C=C\CC)\C/C=C\CCCC(=O)O
C2441	DB00168	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(C[C@@H](C(=O)N[C@@H](Cc1ccccc1)C(=O)OC)N)O
C2442	DB00179	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1cc(C[C@@H]([C@@H](Cc2cc(O)c(O)cc2)C)C)ccc1O
C2443	DB00184	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1(C(CCC1)c1cccnc1)C
C2444	DB00186	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1cc2C(=NC(O)C(=O)Nc2cc1)c1c(Cl)cccc1
C2445	DB00189	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(C(C=CCl)(C#C)O)C
C2446	DB00190	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(c(c1)O)O)C[C@](C(=O)O)(C)NN
C2447	DB00191	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(Cc1ccccc1)(C)C
C2448	DB00202	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(CC[N+](C)(C)C)C(=O)CCC(=O)OCC[N+](C)(C)C

C2449	DB00205	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1ccc(c2c(nc(nc2N)N)CC)cc1
C2450	DB00208	DrugBank	inhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c(CN2CCc3sccc3C2)cccc1
C2451	DB00221	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(C(NC(C)C)CC)c1cc(O)c(O)cc1
C2452	DB00225	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[O-]C(=O)CN(CCN(CC(=O)NC)CC(=O)[O-])CCN(CC(=O)NC)CC(=O)[O-]
C2453	DB00226	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1C2(OCC1CN=C(N)N)CCCCC2
C2454	DB00228	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ClC(F)C(F)(F)OC(F)F
C2455	DB00230	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C[C@H](CC(C)C)CN
C2456	DB00232	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ClCC1N(S(=O)(=O)c2c(N1)cc(Cl)c(S(=O)(=O)N)c2)C
C2457	DB00240	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	C1=C[C@]2(C(=CC1=O)C[C@H]([C@@H]1[C@@H]2[C@H](C[C@]2([C@H]1C[C@H]([C@@]2(C(=O)CO)O)C)C)O)Cl)C
C2458	DB00242	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1nc2n([C@@H]3O[C@@H]([C@@H](O)C3)CO)cnc2c(n1)N
C2459	DB00249	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Ic1cn([C@@H]2O[C@@H]([C@@H](O)C2)CO)c(=O)[nH]c1=O
C2460	DB00250	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(c1ccc(N)cc1)c1ccc(N)cc1
C2461	DB00254	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@H]12[C@](C(=C3[C@H]([C@@H]2O)[C@H](c2c(C3=O)c(ccc2)O)C)O)(C(=O)C(=C([C@H]1N(C)C)O)C(=O)N)O
C2462	DB00258	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[O-]C(=O)C
C2463	DB00259	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(N)c1ccc(N)cc1
C2464	DB00260	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1C[C@@H](N)C(=O)N1
C2465	DB00266	DrugBank	noninhibitor	62	noninhibitor	inhibitor	noninhibitor	noninhibitor	c1(c(c2c(oc1=O)cccc2)O)Cc1c(c2c(oc1=O)cccc2)O
C2466	DB00270	DrugBank	inhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	O(C(=O)C1=C(NC(=C(C1c1c2nonc2ccc1)C(=O)OC)C)C)C(C)C
C2467	DB00271	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Ic1c(NC(=O)C)c(I)c(c(I)c1NC(=O)C)C(=O)O
C2468	DB00272	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1nccc1CCN
C2469	DB00274	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N(C(=O)[C@@]2(OC)NC(=O)CSCC#N)C(=C(C1)CSc1n(nnn1)C)C(=O)O
C2470	DB00279	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Ic1cc(C[C@H](N)C(=O)O)cc(I)c1Oc1cc(I)c(O)cc1
C2471	DB00280	DrugBank	noninhibitor	62	inhibitor	noninhibitor	inhibitor	inhibitor	n1ccccc1C(CCN(C(C)C)C(C)C)(C(=O)N)c1ccccc1
C2472	DB00290	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[illegible]
C2473	DB00291	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ClCCN(c1ccc(CCCC(=O)O)cc1)CCCl
C2474	DB00292	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(n(cnc1)[C@@H](c1ccccc1)C)C(=O)OCC
C2475	DB00293	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	s1c(N(Cc2cc3c([nH]c(nc3=O)C)cc2)C)ccc1C(=O)N[C@@H](CCC(=O)O)C(=O)O
C2476	DB00301	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c(c2noc(c2C(=O)N[C@H]2[C@H]3SC([C@@H](N3C2=O)C(=O)O)(C)C)C)c(F)ccc1
C2477	DB00302	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1C[C@H](CC[C@@H]1C(=O)O)CN
C2478	DB00303	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1(=C([C@@H]([C@H]2N1C(=O)[C@@H]2[C@H](O)C)C)S[C@@H]1CN[C@@H](C1)C(=O)Nc1cccc(c1)C(=O)O)C(=O)O
C2479	DB00322	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1cn([C@@H]2O[C@@H]([C@@H](O)C2)CO)c(=O)[nH]c1=O
C2480	DB00326	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]([C@H](O)[C@H](O)CO)[C@@H](O)C(O)C(=O)[O-]
C2481	DB00330	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N([C@H](CO)CC)CCN[C@H](CO)CC
C2482	DB00331	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=N)NC(=N)N(C)C
C2483	DB00336	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	o1c(ccc1[N+](=O)[O-])/C=N/NC(=O)N
C2484	DB00350	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(N2CCCCC2)cc([n+](c(n1)N)[O-])N
C2485	DB00353	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(N[C@@H](CC)CO)[C@H]1CN([C@H]2C(=C1)c1c3c(C2)c[nH]c3ccc1)C
C2486	DB00359	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(Nc1ncccn1)c1ccc(N)cc1
C2487	DB00368	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H](c1cc(O)c(O)cc1)CN
C2488	DB00375	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(CCNCCN)CCNCCN
C2489	DB00379	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(CC(N)C)c1c(cccc1C)C
C2490	DB00388	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H](CNC)c1cc(O)ccc1
C2491	DB00391	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(N)c1cc(C(=O)NCC2N(CCC2)CC)c(OC)cc1

C2492	DB00393	DrugBank	inhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	O(C(=O)C1=C(NC(=C(C1c1cc([N+](=O)[O-])ccc1)C(=O)OCCOC)C)C)C(C)C
C2493	DB00395	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(CC(CCC)(COC(=O)N)C)C(=O)NC(C)C
C2494	DB00403	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	[C@H](/C=N/NC(=O)N[C@@H]2[C@H](O)[C@H](O)[C@@H](CO)O[C@H]2n2nc(=O)n(C)c(=O)n2)O[C@H]1[C@H](O)[C@@H](CO)O[C@H]1n2cccc2)[C@H](O)[C@H]1O
C2495	DB00411	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C([N+](C)(C)C)COC(=O)N
C2496	DB00417	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N([C@H](C1(C)C)C(=O)O)C(=O)[C@H]2NC(=O)COc1ccccc1
C2497	DB00423	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(CC(O)COC(=O)N)c1c(OC)cccc1
C2498	DB00429	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1[C@H](O)[C@H](C/C=C\CCCC(=O)[O-])[C@H]([C@H]1O)/C=C/[C@](CCCCC)(O)C
C2499	DB00430	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N12C(=O)[C@H]([C@H]1SCC(=C2C(=O)O)CSc1n(nnn1)C)NC(=O)[C@H](NC(=O)c1c(cc(nc1)C)O)c1ccc(cc1)O
C2500	DB00432	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	FC(F)(F)c1cn([C@@H]2O[C@@H]([C@@H](O)C2)CO)c(=O)[nH]c1=O
C2501	DB00437	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=c1ncnc2[nH][nH]cc12
C2502	DB00441	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	FC1(F)[C@H](O)[C@H](O[C@H]1n1ccc(nc1=O)N)CO
C2503	DB00442	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1[C@H](C(=C)[C@@H](n2c3[nH]c(nc(=O)c3nc2)N)C1)CO
C2504	DB00443	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	F[C@@]12[C@H]([C@H]3[C@@]([C@](O)([C@H](C3)C)C(=O)CO)(C[C@@H]1O)C)CCC1=CC(=O)C=C[C@]21C
C2505	DB00444	DrugBank	noninhibitor	62	inhibitor	noninhibitor	inhibitor	inhibitor	s1c([C@H]2O[C@H]3[C@@H](O)[C@@H](O)[C@@H]O[C@H]4[C@@H]5[C@@H]([C@@H](c6c4cc4OCOc4c6)c4cc(OC)c(O)c(OC)c4)C(=O)OC5)O[C@@H]3CO2)ccc1
C2506	DB00446	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(ccc(c1)[N+](=O)[O-])[C@H]([C@H](NC(=O)C(Cl)Cl)CO)O
C2507	DB00451	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Ic1cc(C[C@H](N)C(=O)O)cc(I)c1Oc1cc(I)c(O)c(I)c1
C2508	DB00456	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N(C(=O)[C@H]2NC(=O)Cc2sccc2)C(=C(C1)COC(=O)C)C(=O)O
C2509	DB00462	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C12C(O2)[C@H]2[N+]([C@H]1C[C@@H](C2)OC(=O)[C@@H](c1ccccc1)CO)(C)C
C2510	DB00465	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C1CCn2c1ccc2C(=O)c1ccccc1
C2511	DB00471	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1cc2nc(/C=C/c3cc([C@H](SCC4(CC4)CC(=O)O)CCc4c(C(O)(C)C)ccccc4)ccc3)ccc2cc1
C2512	DB00478	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(C12CC3CC(C1)CC(C2)C3)C
C2513	DB00485	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c(c2noc(c2C(=O)N[C@H]2[C@H]3SC([C@@H](N3C2=O)C(=O)O)(C)C)C)c(Cl)ccc1
C2514	DB00489	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(Nc1ccc(C(O)CNC(C)C)cc1)C
C2515	DB00495	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@@H](n2cc(c(=O)[nH]c2=O)C)C[C@H](N=[N+]=[N-])[C@H]1CO
C2516	DB00499	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	FC(F)(F)c1cc(NC(=O)C(C)C)ccc1[N+](=O)[O-]
C2517	DB00500	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(c1n(c(cc1)CC(=O)O)C)c1ccc(cc1)C
C2518	DB00507	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	s1c(NC(=O)c2c(OC(=O)C)cccc2)ncc1[N+](=O)[O-]
C2519	DB00509	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc(c(c(c1)I)Oc1cc(I)c(O)c(c1)I)I)C[C@H](C(=O)O)N
C2520	DB00512	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2cc1c3c1c4c5cc(ccc5[C@@H]5[C@@H]6[C@@H](C[C@@H]7[C@@]6(CC[C@@H]8[C@]7(CC[C@@H](C8)O)C)C)C(=O)O[C@@H]5C4)C(=O)O[C@@H]3C2)C(=O)O1
C2521	DB00520	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@H]1[C@H]([C@H]2[C@@H](CCN2C(=O)[C@@H](N)C(=O)[C@@H](N)C(=O)[C@@H]2NC(=O)[C@@H](C(C)C)NC(=O)[C@@H](C1)NC(=O)CCCCCCCCC)C(C)C)C)C)[C@H](C2O)[C@@H]([C@H](c1ccccc1)O)O)O[C@@H](CC(=O)O)N
C2522	DB00523	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)/C=C(/C=C/C=C(\C=C\C1=C(CCCC1(C)C)C)/C)\C
C2523	DB00528	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	O(C(CN(CCC(c1ccccc1)c1ccccc1)C)(C)C)C(=O)C1=C(NC(=C(C1c1cc([N+](=O)[O-])ccc1)C(=O)OC)C)C
C2524	DB00534	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[Hg](Cl)CC(OC)CNC(=O)N
C2525	DB00535	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N(C(=O)[C@H]2NC(=O)/C(=N\O)/c2nc(sc2)N)C(=C(C1)C=C)C(=O)O
C2526	DB00536	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=N)N
C2527	DB00544	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1c(=O)[nH]c(=O)[nH]c1
C2528	DB00548	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CCCCCCCC(=O)O
C2529	DB00552	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@H]1(C[C@@H]([C@H](O1)CO)O)n1c2N=CNC[C@H](c2nc1)O
C2530	DB00556	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	FC(C(C(F)(F)F)(F)F)(F)F
C2531	DB00558	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@H]([C@H](NC(=O)C)[C@@H](N=C(N)N)C=C1C(=O)O)[C@H](O)[C@H](O)CO
C2532	DB00567	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N(C(=O)[C@H]2NC(=O)[C@H](N)c2ccccc2)C(=C(C1)C)C(=O)O
C2533	DB00573	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(c1cc(C(C)C(=O)O)ccc1)c1ccccc1
C2534	DB00578	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N([C@H](C1(C)C)C(=O)O)C(=O)[C@H]2NC(=O)C(c1ccccc1)C(=O)O

C2535	DB00581	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O([C@H]1[C@H](O)[C@@](O[C@@H]1CO)(O)CO)[C@@H]1O[C@@H]([C@H](O)[C@H](O)[C@H]1O)CO
C2536	DB00583	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H](C[N+](C)(C)C)CC(=O)[O-]
C2537	DB00585	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(CCN/C(=C/[N+](=O)[O-])/NC)Cc1nc(sc1)CN(C)C
C2538	DB00587	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	s1cc(nc1/C=C/c1cc(NC(=O)CC(CC)(CC)C(=O)O)ccc1)C1CCC1
C2539	DB00595	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@H]12[C@](C(=C3[C@H]([C@@H]1O)[C@](c1c(C3=O)c(ccc1)O)(C)O)O)(C(=O)C(=C([C@H]2N(C)C)O)C(=O)N)O
C2540	DB00597	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(CN1CCN(CCN(CCN(CC1)CC(=O)[O-])CC(=O)[O-])CC(=O)[O-])C
C2541	DB00598	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(CNC(CCc1ccccc1)C)c1cc(c(O)cc1)C(=O)N
C2542	DB00602	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	C\[C@@H]([C@H](O[C@@](C)(C[C@@H]\C(=C/c1ccc(cc1)O)/C)[C@H]2CC(=C)[C@H](CC2)O)C)/C=C/C=C(/C)C\[C@@H]([C@H](C)C(=O)O)O
C2543	DB00606	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1cc2NC(NS(=O)(=O)c2cc1S(=O)(=O)N)C1C2CC(C1)C=C2
C2544	DB00616	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(C1(C[C@H](C(=O)Oc2ccc3c(c2)CCC3)COCCOC)CCCC1)N[C@H]1CC[C@@H](C(=O)O)CC1
C2545	DB00618	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(C1=C([C@@H](N(C)C)[C@H]2[C@](C(=C3[C@H](C2)[C@@H](c2c(C3=O)c(ccc2Cl)O)O)O)(C1=O)O)O)N
C2546	DB00620	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	F[C@@]12[C@H]([C@H]3[C@@]([C@](O)([C@H](O)C3)C(=O)CO)(C[C@@H]1O)C)CCC1=CC(=O)C=C[C@]21C
C2547	DB00622	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	O(C(=O)C1=C(NC(=C(C1c1cc([N+](=O)[O-])ccc1)C(=O)OC)C)C)CCN(Cc1ccccc1)C
C2548	DB00626	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	\C1C(\[nH]\N=C1C\[nH]\N[C@@H](C)C[C@@H](C)c1ccc(cc1)OC)=C/[nH]\N=C1C\[nH]\N[C@@H](C)C[C@@H](C)c1ccc(cc1)OC
C2549	DB00628	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1cc2C(=NC(C(=O)Nc2cc1)C(=O)O)c1ccccc1
C2550	DB00629	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c(c(Cl)ccc1)C=NN=C(N)N
C2551	DB00631	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1nc2n([C@@H]3O[C@@H]([C@@H](O)[C@@H]3F)CO)cnc2c(n1)N
C2552	DB00632	DrugBank	noninhibitor	62	inhibitor	inhibitor	noninhibitor	inhibitor	OCCCCCCCCCCCCCCCCCCCCCCC
C2553	DB00633	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1c([C@H](c2cccc(c2C)C)C)c[nH]c1
C2554	DB00634	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(NC(=O)C)c1ccc(N)cc1
C2555	DB00650	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=c1nc([nH]c2NC[C@@H](N(c12)C=O)CNc1ccc(cc1)C(=O)N[C@@H](CCC(=O)O)C(=O)O)N
C2556	DB00655	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1[C@@]2([C@H]([C@H]3[C@H](CC2)c2c(CC3)cc(O)cc2)CC1)C
C2557	DB00657	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C1(C(C2CC1CC2)(C)C)C)C
C2558	DB00659	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(O)CCCNC(=O)C
C2559	DB00660	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1C(CNC1=O)COc1cc(cc(c1)C)C
C2560	DB00664	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(Nc1nccnc1OC)c1ccc(N)cc1
C2561	DB00665	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	FC(F)(F)c1cc(N2C(=O)C(NC2=O)(C)C)ccc1[N+](=O)[O-]
C2562	DB00667	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1c(CCN)cnc1
C2563	DB00671	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1CC(=C(N2[C@H]1[C@@H](C2=O)NC(=O)/C(=N\OCC(=O)O)/c1csc(n1)N)C(=O)O)C=C
C2564	DB00682	DrugBank	noninhibitor	62	noninhibitor	inhibitor	noninhibitor	noninhibitor	c1cccc2c1c(c(C(c1ccccc1)CC(=O)C)c(=O)o2)O
C2565	DB00685	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1c(N2C[C@H]3[C@H](C3N)C2)nc2n(cc(c(=O)c2c1)C(=O)O)c1c(F)cc(F)cc1
C2566	DB00687	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	F[C@]12[C@H]([C@H]3[C@@]([C@](O)(CC3)C(=O)CO)(C[C@@H]2O)C)CCC2=CC(=O)CC[C@]12C
C2567	DB00688	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	O1CCN(CC1)CCOC(=O)CC/C(=C/Cc1c(OC)c(c2c(c1O)C(=O)OC2)C)/C
C2568	DB00689	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N(C(=O)[C@H]2NC(=O)[C@H](N)c2ccccc2)C(=C(C1)COC(=O)C)C(=O)O
C2569	DB00693	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1C2(c3c(C1=O)cccc3)c1c(Oc3c2ccc(O)c3)cc(O)cc1
C2570	DB00698	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	o1c(/C=N\N2CC(=O)NC2=O)ccc1[N+](=O)[O-]
C2571	DB00700	DrugBank	inhibitor	62	inhibitor	inhibitor	noninhibitor	inhibitor	[C@@H]12[C@]3(O1)[C@]1(CCC(=O)C=C1C[C@H]([C@H]3[C@H]1[C@](C2)([C@]2(CC1)OC(=O)CC2)C)C(=O)OC)C
C2572	DB00703	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(N)c1s/c(=N\C(=O)C)/n(n1)C
C2573	DB00712	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1c(ccc(C(C)C(=O)O)c1)c1ccccc1
C2574	DB00713	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N([C@H](C1(C)C)C(=O)O)C(=O)[C@H]2NC(=O)c1c(noc1C)c1ccccc1
C2575	DB00721	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(CCN(CC)CC)C(=O)c1ccc(N)cc1
C2576	DB00726	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	N1(CC(CN(C)C)C)c2c(CCc3c1cccc3)cccc2
C2577	DB00731	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cccc(c1)C[C@H](C(=O)O)NC(=O)[C@H]1CCC(CC1)C(C)C

C2578	DB00733	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc[n+](C)c(c1)/C=N/O
C2579	DB00738	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(CCCCCOc1ccc(cc1)C(=N)N)c1ccc(cc1)C(=N)N
C2580	DB00739	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N([C@H](C1(C)C)C(=O)O)C(=O)[C@H]2N1C(N[C@@H](C1=O)c1ccccc1)(C)C
C2581	DB00745	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(C(c1ccccc1)c1ccccc1)CC(=O)N
C2582	DB00747	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@H]12C[C@@H](C[C@H]([C@@H]3[C@H]1O3)N2C)OC(=O)[C@H](CO)c1ccccc1
C2583	DB00749	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1C(c2[nH]c3c(c2CC1)cccc3CC)(CC)CC(=O)O
C2584	DB00750	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(Nc1c(cccc1)C)C(NCCC)C
C2585	DB00753	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ClC(OC(F)F)C(F)(F)F
C2586	DB00754	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1N(C(=O)NC1c1ccccc1)CC
C2587	DB00755	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C=C(C=CC=C(C=CC1=C(CCCC1(C)C)C)C)C)C
C2588	DB00756	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c(Cc2c(O)c(Cl)cc(Cl)c2Cl)c(O)c(Cl)cc1Cl
C2589	DB00766	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@H]2N([C@H](/C/1=C/CO)C(=O)O)C(=O)C2
C2590	DB00770	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1[C@@H]([C@@H](CCCCCCC(=O)O)C(=O)C1)C=C[C@@H](O)CCCCC
C2591	DB00779	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=c1c2c(n(CC)cc1C(=O)O)nc(cc2)C
C2592	DB00780	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(N)CCc1ccccc1
C2593	DB00781	DrugBank	noninhibitor	62	inhibitor	noninhibitor	inhibitor	inhibitor	CCC(C)CCCCC(=O)NC(CCN)C(=O)NC(C(C)O)C(=O)NC(CCN)C(=O)NC1CCNC(=O)C(NC(=O)C(CCN)NC(=O)C(CCN)NC(=O)C(CC(C)C)NC(=O)C(Cc2cccc2)NC(=O)C(CCN)NC1=O)C(C)O
C2594	DB00784	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)c1c(Nc2c(c(ccc2)C)C)cccc1
C2595	DB00789	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[O-]C(=O)CN(CCN(CC(=O)O)CC(=O)[O-])CCN(CC(=O)O)CC(=O)[O-]
C2596	DB00796	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(c1n(Cc2ccc(cc2)c2c(cccc2)c2n[nH]nn2)c2c(n1)cccc2C(=O)O)CC
C2597	DB00797	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1C(=NCC1)Cc1ccccc1
C2598	DB00800	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c2c(C(CNCC2)c2ccc(O)cc2)cc(O)c1O
C2599	DB00808	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c(S(=O)(=O)N)cc(C(=O)NN2C(Cc3c2cccc3)C)cc1
C2600	DB00809	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(N(Cc1ccncc1)CC)C(c1ccccc1)CO
C2601	DB00816	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(CNC(C)C)c1cc(O)cc(O)c1
C2602	DB00818	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1c(C(C)C)cccc1C(C)C
C2603	DB00819	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(N)c1sc(NC(=O)C)nn1
C2604	DB00821	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1cc2c3c([nH]c2cc1)cc(C(C)C(=O)O)cc3
C2605	DB00825	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1[C@@H](CC[C@H](C1)C)C(C)C
C2606	DB00841	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1cc(CCNC(CCc2ccc(O)cc2)C)ccc1O
C2607	DB00842	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1cc2C(=NC(O)C(=O)Nc2cc1)c1ccccc1
C2608	DB00851	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1[nH]c(c(n1)C(=O)N)/N=N/N(C)C
C2609	DB00853	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=c1n2c(nnn1C)c(nc2)C(=O)N
C2610	DB00856	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1ccc(OCC(O)CO)cc1
C2611	DB00861	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1c(c2cc(c(O)cc2)C(=O)O)ccc(F)c1
C2612	DB00865	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(C[C@@H](N(Cc2ccccc2)C)C)ccccc1
C2613	DB00869	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	c12c([C@H](C[C@@H](S1(=O)=O)C)NCC)cc(s2)S(=O)(=O)N
C2614	DB00871	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(CNC(C)(C)C)c1cc(O)cc(O)c1
C2615	DB00875	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	c12ccccc1SC1C(C2=CCCN2CCN(CC2)CCO)C=C(C=C1)C(F)(F)F
C2616	DB00876	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	n1(Cc2ccc(cc2)C(=O)O)c(/C=C(/C(=O)O)\Cc2sccc2)cnc1CCCC
C2617	DB00877	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	C1[C@@H]2N(CCC1)C(=O)[C@@]1(O)[C@@]3(O)[C@@H](CC)C[C@H](C)C[C@H](OC)/C=C/C=C/C=C/[C@H](C)C[C@H](C)[C@@H](O[C@]4(C[C@H](OC)[C@H](C)[C@H](O)[C@H](C)CC4=O)[C@H](C)C[C@@H](C)[C@H](C)[C@@H](C)OC)O[C@]3(C)O1)OC)C(C)C)O)OC)C(C)C)O)OC)C(C)C)O
C2618	DB00879	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1C[C@H](O[C@H]1CO)n1cc(F)c(nc1=O)N
C2619	DB00887	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(N)c1c(Oc2ccccc2)c(NCCCC)cc(c1)C(=O)O
C2620	DB00905	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H]1[C@@H]([C@H]([C@H](O)C1)/C=C/[C@@H](O)CCc1ccccc1)C/C=C\CCCC(=O)NCC

C2621	DB00909	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(N)Cc1noc2c1cccc2
C2622	DB00917	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1[C@@H]([C@H](C(=O)C1)C/C=C\CCCC(=O)O)/C=C/[C@@H](O)CCCCC
C2623	DB00918	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	S(=O)(=O)(N1CCCC1)Cc1cc2c(CCN(C)C)c[nH]c2cc1
C2624	DB00923	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N(C(=O)[C@H]2NC(=O)Cc2c(CN)cccc2)C(=C(C1)CSc1n(nnn1)CC(=O)O)C(=O)O
C2625	DB00931	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@]12[C@@H]([C@@H](O)[C@H]3C(=C1O)C(=O)c1c(C3=C)cccc1O)[C@H](N(C)C)C(=O)C(C2=O)C(=O)N
C2626	DB00937	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(C(N(CC)CC)C)c1ccccc1
C2627	DB00943	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@@H](n2ccc(nc2=O)N)CC[C@H]1CO
C2628	DB00945	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(c1c(cccc1)C(=O)O)C(=O)C
C2629	DB00946	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cccc2c1oc(=O)c(c2O)C(c1ccccc1)CC
C2630	DB00948	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N([C@H](C1(C)C)C(=O)O)C(=O)[C@H]2NC(=O)[C@H](NC(=O)N1CCN(S(=O)(=O)C)C1=O)c1ccccc1
C2631	DB00949	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(CC(c1ccccc1)COC(=O)N)C(=O)N
C2632	DB00960	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(CC(O)CNC(C)C)c1c2c([nH]cc2)ccc1
C2633	DB00964	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c(NC2=NCCN2)c(Cl)cc(N)c1
C2634	DB00974	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CN(CCN(CC(=O)O)CC(=O)O)CC(=O)O
C2635	DB00977	DrugBank	noninhibitor	62	inhibitor	inhibitor	noninhibitor	inhibitor	O[C@@]1([C@@]2([C@H]([C@@H]3CCc4c(ccc(O)c4)[C@H]3CC2)CC1)C)C#C
C2636	DB00978	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1c(N2CC(NCC2)C)c(F)cc2c1n(CC)cc(c2=O)C(=O)O
C2637	DB00982	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C\C(=O)O)/C)/C)C)(C)C
C2638	DB00983	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(CNC(Cc1ccc(OC)cc1)C)c1cc(NC=O)c(O)cc1
C2639	DB00986	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	O(C1C[N+](CC1)(C)C)C(=O)C(O)(C1CCCC1)c1ccccc1
C2640	DB00988	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1cc(CCN)ccc1O
C2641	DB00991	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	o1c(c(nc1CCC(=O)O)c1ccccc1)c1ccccc1
C2642	DB00994	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H](C[C@H](O[C@H]2O[C@@H](C[C@@H](O)[C@@H]2O)[C@@H]2O[C@H]2N)CN[C@H]N)[C@H]1O[C@H]1O[C@@H](C[C@@H](O)[C@H]2O[C@@H](C[C@@H]2O)[C@@H]1O)[C@H]2NCN)[C@H]1O)CO
C2643	DB00999	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c(S(=O)(=O)N)cc2S(=O)(=O)NCNc2c1
C2644	DB01000	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N([C@H](C1(C)C)C(=O)O)C(=O)[C@H]2NC(=O)C1(N)CCCCC1
C2645	DB01001	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(CNC(C)(C)C)c1cc(c(O)cc1)CO
C2646	DB01006	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1(ncnc1)C(c1ccc(cc1)C#N)c1ccc(cc1)C#N
C2647	DB01009	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C(c1cc(ccc1)C(=O)c1ccccc1)C
C2648	DB01010	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1cc([N+](CC)(C)C)ccc1
C2649	DB01015	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(Nc1noc(c1)C)c1ccc(N)cc1
C2650	DB01019	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(C(C[N+](C)(C)C)C)C(=O)N
C2651	DB01021	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ClC(Cl)C1NS(=O)(=O)c2c(N1)cc(Cl)c(S(=O)(=O)N)c2
C2652	DB01022	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	c12C(=O)C(=C(C(=O)c1cccc2)C/C=C(/CCC[C@@H](CCC[C@@H](CCCC(C)C)C)C)\C)C
C2653	DB01026	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	c1(cc(c(cc1)C1(OCC(COc2ccc(cc2)N2CCN(CC2)C(=O)C)O1)Cn1ccnc1)Cl)Cl
C2654	DB01028	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ClC(Cl)C(F)(F)OC
C2655	DB01031	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(C1(CCCCC1)C#C)C(=O)N
C2656	DB01033	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S=c1nc[nH]c2nc[nH]c12
C2657	DB01035	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(NCCN(CC)CC)c1ccc(N)cc1
C2658	DB01042	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(N(CCCl)CCCl)ccc(cc1)C[C@@H](C(=O)O)N
C2659	DB01046	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	FC(F)([C@@]1(O[C@H]2[C@@H]([C@@H](C(=O)C2)CCCCCCC(=O)O)CC1)O)CCCC
C2660	DB01050	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C(c1ccc(CC(C)C)cc1)C
C2661	DB01053	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N([C@H](C1(C)C)C(=O)O)C(=O)[C@H]2NC(=O)Cc1ccccc1
C2662	DB01056	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(Nc1c(cccc1C)C)C(N)C
C2663	DB01057	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(P(=O)(OCC)OCC)CC[N+](C)(C)C

C2664	DB01061	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[C@H](C(=O)N[C@@H]1C(=O)N2[C@@H]1SC([C@@H]2C(=O)O)(C)C)NC(=O)N1C(=O)NCC1
C2665	DB01064	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(CNC(C)C)c1cc(O)c(O)cc1
C2666	DB01068	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c(C2=NCC(=O)Nc3c2cc([N+](=O)[O-])cc3)cccc1
C2667	DB01071	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	S1c2c(N(CC3C4CCN(C3)CC4)c3c1cccc3)cccc2
C2668	DB01080	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CCC(N)C=C
C2669	DB01085	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1C[C@@H]([C@H](CC)C1=O)Cc1n(cnc1)C
C2670	DB01093	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(C)C
C2671	DB01099	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1c([nH]c(=O)nc1)N
C2672	DB01112	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@H]12N(C(=C(CS1)COC(=O)N)C(=O)O)C(=O)[C@H]2NC(=O)/C(=N\OC)/c1occc1
C2673	DB01121	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(NC(=O)N)Cc1ccccc1
C2674	DB01123	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1c2c(cc3c1cc(N)cc3)ccc(N)c2
C2675	DB01131	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1ccc(NC(=N/C(=N/C(C)C)/N)N)cc1
C2676	DB01140	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@H]12N(C(=C(CS1)C)C(=O)O)C(=O)[C@H]2NC(=O)[C@@H](c1ccc(cc1)O)N
C2677	DB01142	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	C1(=CCCN(C)C)c2c(COc3c1cccc3)cccc2
C2678	DB01145	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(c1ccc(NCS(=O)O)cc1)c1ccc(NCS(=O)O)cc1
C2679	DB01147	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c(c2noc(c2C(=O)N[C@H]2[C@H]3SC([C@@H](N3C2=O)C(=O)O)(C)C)C)cccc1
C2680	DB01150	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N12[C@@H]([C@@H](C2=O)NC(=O)[C@H](N)c2ccc(cc2)O)SCC(=C1C(=O)O)C=CC
C2681	DB01156	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1cc(C(=O)C(NC(C)(C)C)C)ccc1
C2682	DB01158	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Brc1c(C[N+](CC)(C)C)cccc1
C2683	DB01159	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	BrC(Cl)C(F)(F)F
C2684	DB01160	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1[C@@H]([C@H]([C@H](O)C1)/C=C/[C@@H](O)CCCCC)C/C=C\CCCC(=O)O
C2685	DB01161	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c(C(=O)OCCN(CC)CC)ccc(N)c1
C2686	DB01168	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(NC(C)C)c1ccc(CNNC)cc1
C2687	DB01187	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Ic1c(C(CCCCCCCCC(=O)OCC)C)cccc1
C2688	DB01189	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	FC(OC(F)F)C(F)(F)F
C2689	DB01192	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@@H]2[C@]34[C@](O)([C@H](N(CC3)C)Cc3c4c1c(O)cc3)CCC2=O
C2690	DB01193	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(CC(O)CNC(C)C)c1c(cc(NC(=O)CCC)cc1)C(=O)C
C2691	DB01199	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	O1c2c3[C@H]([N+](CCc3cc(OC)c2O)(C)C)Cc2cc(Oc3cc4[C@@H](N(CCc4cc3OC)C)Cc3ccc1cc3)c(O)cc2
C2692	DB01206	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ClCCN(N=O)C(=O)NC1CCCCC1
C2693	DB01208	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1c2n(C3CC3)cc(c(=O)c2c(N)c(F)c1N1C[C@@H](N[C@@H](C1)C)C)C(=O)O
C2694	DB01209	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1[C@H]2Cc3ccc(cc3[C@]([C@H]2N)(CCCC1)C)O
C2695	DB01219	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1(=O)NC(=O)CN1N=Cc1oc(cc1)c1ccc([N+](=O)[O-])cc1
C2696	DB01238	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	Clc1c(N2CCN(CC2)CCCCOc2cc3NC(=O)CCc3cc2)cccc1Cl
C2697	DB01239	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	c1cccc2c1C(=CCCN(C)C)c1c(S2)ccc(c1)Cl
C2698	DB01240	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@@H]2[C@@H]([C@H]([C@H](O)C2)/C=C/[C@@H](O)CCCCC)CC1=CCCCC(=O)O
C2699	DB01241	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(CCCC(C)C)C(=O)O)c1c(ccc(c1)C)C
C2700	DB01243	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c2c(nccc2)c(O)c(Cl)c1
C2701	DB01247	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	o1nc(C(=O)NNCc2ccccc2)cc1C
C2702	DB01250	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc(c(cc1)O)C(=O)O)/N=N/c1cc(c(cc1)O)C(=O)O
C2703	DB01255	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccccc1C[C@@H](NC(=O)[C@H](CCCCN)N)C
C2704	DB01262	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@@H]([C@@H](O)C[C@@H]1n1c(=O)nc(nc1)N)CO
C2705	DB01265	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@H](n2cc(c(=O)[nH]c2=O)C)C[C@@H](O)[C@@H]1CO
C2706	DB01274	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H](CN[C@@H](Cc1ccc(OC)cc1)C)c1cc(NC=O)c(O)cc1

C2707	DB01275	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(N)c1nncc2c1cccc2
C2708	DB01288	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(CNC(Cc1ccc(O)cc1)C)c1cc(O)cc(O)c1
C2709	DB01291	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(CNC(C)(C)C)c1nc(c(O)cc1)CO
C2710	DB01296	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@@H]([C@@H](O)[C@H](O)[C@@H](N)C1O)CO
C2711	DB01297	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(Nc1ccc(OCC(CNC(C)C)O)cc1)C
C2712	DB01298	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(Nc1nc(=O)n(CC)cc1)c1ccc(N)cc1
C2713	DB01299	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(Nc1ncnc(OC)c1OC)c1ccc(N)cc1
C2714	DB01303	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(n(c(=O)n(c1=O)C)C)nc[n-]2
C2715	DB01321	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	O[C@H]1[C@H](N/C/C)[C@@H](O)[C@@H](O/C@@H]1/C)O[C@H]1[C@H](CO)[C@@H](O)/C=C/C=C/[C@H](OC)=O)[C@@H](OC)=O)/C)[C@@H]1OC)C)CC=O)[C@@H]1O[C@H]([C@H](OC)=O)CC(/C)C)[C@@H](O)C1=)C
C2716	DB01325	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c(S(=O)(=O)N)cc2c(NC(NC2=O)CC)c1
C2717	DB01326	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N(C(=O)[C@H]2NC(=O)[C@H](O)c2ccccc2)C(=C(C1)CSc1n(nnn1)C)C(=O)O
C2718	DB01327	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@H]12N(C(=C(CS1)CSc1nnc(s1)C)C(=O)O)C(=O)[C@H]2NC(=O)Cn1cnnn1
C2719	DB01329	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N(C(=O)[C@H]2NC(=O)C(NC(=O)N2CCN(C(=O)C2=O)CC)c2ccc(O)cc2)C(=C(C1)CSc1n(nnn1)C)C(=O)O
C2720	DB01331	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N(C(=O)[C@@]2(OC)NC(=O)Cc2sccc2)C(=C(C1)COC(=O)N)C(=O)O
C2721	DB01332	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N(C(=O)[C@H]2NC(=O)/C(=N\OC)/c2nc(sc2)N)C(=CC1)C(=O)O
C2722	DB01333	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N(C(=O)[C@H]2NC(=O)[C@H](N)C2=CCC=CC2)C(=C(C1)C)C(=O)O
C2723	DB01362	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Ic1c(N(CC(O)CO)C(=O)C)c(I)c(c(I)c1C(=O)NCC(O)CO)C(=O)NCC(O)CO
C2724	DB01366	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]([C@@H](NC(C)C)CC)c1c2c([nH]c(=O)cc2)c(O)cc1
C2725	DB01390	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[O-]
C2726	DB01397	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(c(c1)C(=O)[O-])O
C2727	DB01399	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(c1c(cccc1)C(=O)O)C(=O)c1c(O)cccc1
C2728	DB01403	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)N(c1c(S2)ccc(c1)OC)C[C@@H](CN(C)C)C
C2729	DB01407	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1cc(C(O)CNC(C)(C)C)cc(Cl)c1N
C2730	DB01408	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(CNC(C)(C)C)c1cc(OC(=O)N(C)C)cc(OC(=O)N(C)C)c1
C2731	DB01410	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	O1[C@]2[C@@]3([C@H]([C@H]4[C@H]([C@@H](O)C3)[C@@]3(C(=CC(=O)C=C3)CC4)C)C[C@H]2OC1C1CCCCC1)C)C(=O)COC(=O)C(C)C
C2732	DB01412	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=c1[nH]c(=O)n(c2ncn(c12)C)C
C2733	DB01415	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@H]12N(C(=CCS1)C(=O)O)C(=O)[C@H]2NC(=O)/C(=C\CC(=O)O)/c1csc(n1)N
C2734	DB01419	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	FC(F)(F)c1cc(N2CCN(CC2)CCOC(=O)c2c(Nc3c4c(ncc3)cc(cc4)C(F)(F)F)cccc2)ccc1
C2735	DB01421	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H](C[C@H](O[C@H]2O[C@@H]([C@@H](O)[C@@H]2O[C@H]2N)CO[C@H]N)C[C@@H]N)[C@H]1O[C@H]1O[C@@H]([C@@H](O[C@H]2O[C@@H]([C@@H]2O[C@H]O)[C@H]2NCN)[C@H]1O)CO
C2736	DB01577	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N([C@H](Cc1ccccc1)C)C
C2737	DB01583	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Ic1cc(C[C@H](N)C(=O)[O-])cc(I)c1Oc1cc(I)c(O)c(I)c1
C2738	DB01589	DrugBank	inhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1cc2c(N(CC(F)(F)F)C(=S)CN=C2c2c(F)cccc2)cc1
C2739	DB01591	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	O([C@@H]1C2CCN(C1)CC2)C(=O)N1[C@H](c2c(CC1)cccc2)c1ccccc1
C2740	DB01598	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(C1=C(N2[C@@H]([C@H](C2=O)[C@H](O)C)C1)C(=O)O)CC/N=C/N
C2741	DB01602	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N([C@H](C1(C)C)C(=O)OC(OC(=O)OCC)C)C(=O)[C@H]2NC(=O)[C@H](N)c1ccccc1
C2742	DB01603	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N([C@H](C1(C)C)C(=O)O)C(=O)[C@H]2NC(=O)c1c(OC)cccc1OC
C2743	DB01604	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N([C@H](C1(C)C)C(=O)OCOC(=O)C(C)(C)C)C(=O)[C@H]2NC(=O)[C@H](N)c1ccccc1
C2744	DB01606	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1(=O)(=O)[C@]([C@@H](N2[C@H]1CC2=O)C(=O)O)(Cn1nncc1)C
C2745	DB01607	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1[C@H]2N([C@H](C1(C)C)C(=O)O)C(=O)[C@H]2NC(=O)[C@@H](c1ccsc1)C(=O)O
C2746	DB01609	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1c(nn(c1c1ccccc1O)c1ccc(cc1)C(=O)O)c1ccccc1O
C2747	DB01610	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(C(COC(=O)[C@@H](N)C(C)C)CO)Cn1c2[nH]c(nc(=O)c2nc1)N
C2748	DB01620	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(CCC(c1ccccc1)c1ncccc1)(C)C
C2749	DB01625	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	O=C(N)C(CC[N+](C(C)C)(C(C)C)C)(c1ccccc1)c1ccccc1

C2750	DB01626	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(Cc1ccccc1)(CC#C)C
C2751	DB02187	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc2c(cc1)[C@@H]1C(=CC2)[C@H]2[C@](CC1)(C(=O)CC2)C)O
C2752	DB02546	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(Nc1ccccc1)CCCCCCC(=O)NO
C2753	DB02638	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1SCJC@@H](NCj=O)CNCj=O)CNCj=O)CNJCj=O)NJC@@H](Cj=O)NJC@@H](Cj=O)NJC@@H](Cj=O)NJC@@H](Cj=O)NJCj@@H](CCCCJCj=O)NJCCj=O)NJCJ)CCj=O)NJCCCj=O)NJCc1ccccc1)Cc1ccc(O)cc1
C2754	DB04572	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	P(=S)(N1CC1)(N1CC1)N1CC1
C2755	DB04573	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1[C@@]2([C@H]([C@H]3[C@H](CC2)c2c(CC3)cc(O)cc2)C[C@H]1O)C
C2756	DB04794	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	n1(C(c2ccc(cc2)c2ccccc2)c2ccccc2)ccnc1
C2757	DB04835	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	FC1(F)CCC(C(=O)N[C@@H](CCN2[C@H]3CC(n4c(nnc4C)C(C)C)C[C@@H]2CC3)c2ccccc2)CC1
C2758	DB04877	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	O(C(=O)[C@]12[C@H]3N(C[C@H](C1)C[C@@H]3CC)CCc1c2[nH]c2c1cc(OC)c(c2)[C@H]1C[C@@H]2C([C@H](N(C/C/2=C/C)C)Cc2c1[nH]c1c2cccc1)C(=O)OC)C
C2759	DB04878	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@]1(C[C@H](NC(CO)CO)[C@H](O)[C@@H](O)[C@@H]1O)CO
C2760	DB04880	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(c1ccc(C(=O)c2[nH]c(=O)[nH]c2C)cc1)C
C2761	DB04894	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12cccc1[nH]cc2C[C@H]1C(=O)N[C@@H](C(=O)N[C@@H](C(=O)N[C@@H](CSSC[C@H](NC(=O)[C@@H](N[C@@H](C(=O)N1)Cc1ccc(cc1)O)C(=O)N[C@@H](C(=O)N[C@@H](C(=O)N[C@@H]1Cc1ccc(cc1)O)C(=O)N[C@@H](C(=O)N[C@@H](C(=O)N[C@@H]1Cc1c[nH]c2ccccc12)C(C)C)CCCCN
C2762	DB04896	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(N(CC)CC)[C@]1([C@H](C1)CN)c1ccccc1
C2763	DB04946	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	Fc1cc2onc(C3CCN(CC3)CCCOc3c(OC)cc(cc3)C(=O)C)c2cc1
C2764	DB04948	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c(OC(C2=NCCN2)C)c(Cl)ccc1
C2765	DB05039	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	O[C@@H](CNC1Cc2c(C1)cc(c(c2)CC)CC)c1c2c([nH]c(=O)cc2)c(O)cc1
C2766	DB05245	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)([N-]c1ncccn1)c1ccc(N)cc1
C2767	DB05246	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1N(C(=O)CC1(c1ccccc1)C)C
C2768	DB05521	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	O=C(N[C@@H](CCC)C(=O)C(=O)NC1CC1)[C@H]1N(C[C@@H]2[C@H]1CCC2)C(=O)[C@H](NC(=O)[C@@H](NC(=O)c1nccnc1)C1CCCCC1)C(C)(C)C
C2769	DB06147	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ccc(cc1)S(=O)(=O)Nc1nccs1
C2770	DB06196	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	s1sC1C@@H](NC(=O)CNC(=O)[C@H](NC[C@@H](C2)C(=O)[C@H]2NCCC2)C(=O)[C@H](NC(=O)[C@H](NCCCN=C)NQCCCN=C)NQCCCN=C)NJC(=O)[C@H](C(=O)N2[C@@H](C(=O)N3[C@@H](C[C@H](C=O)NJC(=O)[C@H](CCCN=C)NJQCC(=O)[C@H](CCCC)C)cdC2ssss3)CO)ssc1
C2771	DB06201	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1c(Cn2nnc(c2)C(=O)N)c(F)ccc1
C2772	DB06204	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1cc([C@@H]([C@H](CN(C)C)C)CC)ccc1
C2773	DB06210	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc(c1)C(=O)O)c1cccc(c1O)N/N=C\1/C(=NN(C1=O)c1cc(c(cc1)C)C)C
C2774	DB06213	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@@H](n2c3nc(nc(N)c3nc2)n2ncc(c2)C(=O)NC)[C@H](O)[C@H](O)[C@H]1CO
C2775	DB06216	DrugBank	noninhibitor	62	noninhibitor	inhibitor	noninhibitor	noninhibitor	Clc1cc2C3C(CN(C3)C)c3c(Oc2cc1)cccc3
C2776	DB06268	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c(onc1C)NS(=O)(=O)c1c(scc1)C(=O)Cc1c(cc2OCOc2c1)C
C2777	DB06288	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(c1cc(C(=O)NCC2N(CCC2)CC)c(OC)cc1N)CC
C2778	DB06616	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	c1c(c(c2c(n1)cc(c(c2)OC)OCCCN1CCN(CC1)C)Nc1c(cc(c(c1)OC)Cl)Cl)C#N
C2779	DB06623	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1ccc(CNc2nc(N)c(NC(=O)OCC)cc2)cc1
C2780	DB06637	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cnccc1N
C2781	DB06689	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
C2782	DB06703	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1([C@@H]([C@@H](CO)O)CO)CCN(CCN(CCN(CC1)CC(=O)[O-])CC(=O)[O-])CC(=O)[O-]
C2783	DB06709	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C[N+](C)(C)C)OC(=O)C
C2784	DB06714	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(CC1CCCCC1)NC
C2785	DB06725	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1sc2c(S(=O)(=O)N(/C(=C(/O)\Nc3ncccc3)/C2=O)C)c1
C2786	DB06768	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(C(C)O)[O-]
C2787	DB06771	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1c(c(Cl)c2c(c1)c(=O)c(C(=O)O)cn2C1CC1)N1CCCC[C@@H](N)C1
C2788	DB06800	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	[C@]123[C@@]4([C@H]([N+](CC5CC5)(CC3)C)Cc3c1c(O[C@H]2C(=O)CC4)c(cc3)O)O
C2789	DB06803	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1[N+](=O)[O-])Cl)NC(=O)c1c(ccc(c1)Cl)O
C2790	DB06813	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(O)[C@@H](NC(=O)c1ccc(cc1)C(CC#C)Cc1nc2c(nc1)nc(nc2N)N)CCC(=O)O
C2791	DB08604	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(c1c(cc(cc1)Cl)Cl)c1c(cc(cc1)Cl)O
C2792	DB08795	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(cccc1)[C@H](C(=O)N[C@H]1[C@@H]2N(C1=O)[C@H](C(S2)(C)C)C(=O)O)N=[N+]=[N-]

C2793	DB08798	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(Nc1oc(c(n1)C)C)c1ccc(N)cc1
C2794	DB08823	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	[C@@H]1([C@H](O[C@@H](CC1)O[C@H]1[C@@H](C(=O)C2=C[C@@H]3[C@H]4[C@@H](C=C[C@@H]3[C@H]2CC(=O)O[C@H](CCC1)CC)C[C@H](C4)O[C@H]1C[C@@H]([C@H]([C@H]([C@H]1OC)OC)OC)C)C)C)N(C)C
C2795	DB08826	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1(ccc(=O)c(c1C)O)C
C2796	DB08828	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1cccc(n1)c1cc(ccc1Cl)NC(=O)c1ccc(cc1Cl)S(=O)(=O)C
C2797	DB08835	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[C@@H](CCC(=O)O)NC(=O)C[C@@H](C(=O)O)NC(=O)C
C2798	DB08860	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(O)C[C@H](O)C[C@H](O)/C=C/c1c(c2ccccc2nc1C1CC1)c1ccc(F)cc1
C2799	DB08868	DrugBank	noninhibitor	62	noninhibitor	inhibitor	noninhibitor	noninhibitor	c1cc(ccc1CCCCCCCC)CCC(CO)(CO)N
C2800	DB08887	DrugBank	noninhibitor	62	inhibitor	inhibitor	noninhibitor	inhibitor	C(OC(=O)CCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CC)C
C2801	DB08890	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(CC[C@@H]1NC(=O)[C@H]2NC(=O)[C@H](CSSC[C@@H]3NC(=O)[C@@H](NC(=O)[C@H](Cc4ccc(cc4)O)NC1=O)CSSC[C@H](NC(=O)CNC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H]1N(C(=O)[C@@H](NC3=O)CC(=O)N)CCC1)C)CSSC2)[C@H](O)C)C(=O)N[C@@H](Cc1ccc(cc1)O)C(=O)O)N)O
C2802	DB08893	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cccc(c1)[C@H](CNCCc1ccc(cc1)NC(=O)Cc1csc(n1)N)O
C2803	DB08901	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	N1(CCN(CC1)C)Cc1c(cc(cc1)NC(=O)c1cc(c(cc1)C)C#Cc1cnc2n1nccc2)C(F)(F)F
C2804	DB08907	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	[C@@H]1([C@@H]([C@H]([C@@H](O[C@@H]1CO)c1ccc(c(c1)Cc1sc(cc1)c1ccc(cc1)F)C)O)O)O
C2805	DB08918	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[C@]1(C(=O)N(CC)CC)C[C@H]1CN
C2806	DB01783	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C(=O)C(C(CO)(C)C)O)CCC(=O)O
C2807	DB01230	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1C(c2ccccc2)C(=O)N=C1N
C2808	DB01442	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1c2cc(CC(N)C)cc(OC)c2OC1
C2809	DB01446	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1c2c(c(CC(N)C)c1)cccc2
C2810	DB01447	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1C(C(N=C1N)C)c1ccccc1
C2811	DB01454	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1c2cc(CC(NC)C)ccc2OC1
C2812	DB01460	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(CCc1c2c([nH]c1)cccc2)(CC)CC
C2813	DB01465	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(c1c(CC(N)C)cc(OC)cc1)C
C2814	DB01472	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(c1ccc(CC(N)C)cc1)C
C2815	DB01484	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Brc1c(OC)cc(CC(N)C)c(OC)c1
C2816	DB01487	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(c1cc(C(CC)(CC)CNC(=O)CCCO)ccc1)C
C2817	DB01490	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1C(CN=C1N)c1ccccc1
C2818	DB01494	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[O-]C(=O)C[N+](C)(C)C
C2819	DB01506	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC1(CCCCC1)c1ccccc1
C2820	DB01509	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1c2cc(CC(N)C)ccc2OC1
C2821	DB01512	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@@H]2[C@]34[C@](O)([C@H](N(CC3)C)Cc3c4c1c(O)cc3)CC[C@@H]2O
C2822	DB01525	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1[C@@H]([C@@H]2N([C@@H](CC2)C1)C)C(=O)O
C2823	DB01528	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(c1c(CC(N)C)cc(OC)c(c1)C)C
C2824	DB01531	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1C2C34C(C(N(CC3)C)Cc3c4c1c(O)cc3)CCC2
C2825	DB01534	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ClC(Cl)(Cl)C(OC(CC(O)(C)C)C)O
C2826	DB01556	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1ccc(CC(N)(C)C)cc1
C2827	DB01565	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@@H]2[C@]34[C@H]([C@H](N(CC3)C)Cc3c4c1c(O)cc3)CC[C@@H]2O
C2828	DB04836	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CCCCCC[NH2+]C1c2c(CCc3c1cccc3)cccc2
C2829	DB00311	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(N)c1sc2c(n1)ccc(OCC)c2
C2830	DB00365	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1c(N2CC(NCC2)C)cc2n(C3CC3)cc(c(=O)c2c1C)C(=O)O
C2831	DB00414	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(NC(=O)NC1CCCCC1)c1ccc(cc1)C(=O)C
C2832	DB00447	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N12C(=O)[C@H]([C@H]2CCC(=C1C(=O)O)Cl)NC(=O)[C@H](N)c1ccccc1
C2833	DB00532	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1N(C(=O)NC1(CC)c1ccccc1)C
C2834	DB00580	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(N)c1ccc(c2c(noc2C)c2ccccc2)cc1
C2835	DB01079	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCc1cc2c(N=C/C/2=C\NN/C(=N/CCCCC)/N)cc1

C2836	DB01405	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1c(N2CC(NCC2)C)cc2n(cc(c(=O)c2c1)C(=O)O)c1c(F)cc(F)cc1
C2837	DB04812	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1ccc(c2oc3c(n2)cc(C(C)C(=O)O)cc3)cc1
C2838	DB04813	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c(O)c(Sc2c(O)c(Cl)cc(Cl)c2)cc(Cl)c1
C2839	DB04816	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1c2c(C(=O)c3c1c(O)ccc3)cccc2O
C2840	DB04817	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)([O-])CN(c1c(n(n(c1=O)c1ccccc1)C)C)C
C2841	DB04818	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(NNC(C)C)c1ccncc1
C2842	DB04823	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1Nc2c(C1(c1ccc(O)cc1)c1ccc(O)cc1)cccc2
C2843	DB04831	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c(ccc(OCC(=O)O)c1Cl)C(=O)c1sccc1
C2844	DB04832	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Brc1ccc(C(=CCN(C)C)c2cccnc2)cc1
C2845	DB04834	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	O([C@H]1[C@@]2([C@H]([C@H]3[C@@H]([C@@]4([C@H]([CC3)C[C@H](OC(=O)C)[C@@H](N3CCCCC3)C4)C)CC2)C[C@@H]1[N+](CCCCC1)CC=C)C)C(=O)CC
C2846	DB08878	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1c(c2c(nc1N)ncc(n2)CNc1ccc(C(=O)N[C@H](C(=O)O)CCC(=O)O)cc1)N
C2847	DB01873	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	C[C@H]1CCC/C(=C\C[C@@H](OC(=O)C[C@@H](O)C(C)(C)C(=O)[C@@H](C)[C@@H]1O)/C(=C/c1csc(C)n1)/C)/C
C2848	DB03010	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	C[C@H]1CCC[C@]2(C)O[C@H]2C[C@H](OC(=O)C[C@@H](O)C(C)(C)C(=O)[C@@H](C)[C@@H]1O)/C(=C/c1csc(C)n1)/C
C2849	DB03516	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=c1[nH]c(=O)[nH]cc1C#C
C2850	DB04335	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@@H](n2c3[nH]cnc(=O)c3nc2)[C@H](O)[C@H](O)[C@H]1CO
C2851	DB04853	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@@H](n2c3nc(N/N=C/C4CCCCC4)nc(N)c3nc2)[C@H](O)[C@H](O)[C@H]1CO
C2852	DB04858	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	On1c2c([n+]([O-])nc1=N)cccc2
C2853	DB04874	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1c(cccc1)C
C2854	DB04879	DrugBank	noninhibitor	62	inhibitor	inhibitor	noninhibitor	inhibitor	Clc1ccc(Nc2nnc(c3c2cccc3)Cc2ccncc2)cc1
C2855	DB04882	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1C(n2c3c(c4c2cc(O)cc4)c2c(c4c3[nH]c3c4ccc(O)c3)c(=O)n(NC(CO)CO)c2=O)[C@H](O)[C@@H](O)[C@H](O)[C@H]1CO
C2856	DB04883	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(C([C@H](Oc1nc(OC)cc(OC)n1)C(=O)O)(c1ccccc1)c1ccccc1)C
C2857	DB04889	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1CC2(C(C2)C1)c1ccc(cc1)C
C2858	DB04903	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	Clc1nc2nc(N3C(CC(=O)CCC(C)C)c4c(C3=O)cccc4)ccc2cc1
C2859	DB04908	DrugBank	inhibitor	62	inhibitor	inhibitor	noninhibitor	inhibitor	FC(F)(F)c1cc(N2CCN(CC2)CCn2c3c([nH]c2=O)cccc3)ccc1
C2860	DB04910	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(c1cc2[nH]c(nc2cc1)NC(=O)OC)CCC
C2861	DB04911	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	O=n1c2ccccc2[n+]([O-])c(/C=C/c2ccc(N(CCO)CCO)cc2)c1C
C2862	DB04926	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC1(CC(CC(C1)(C)C)(C)C)C
C2863	DB04936	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]([C@H](O)CO)[C@H](O)C(=O)CO
C2864	DB04944	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@@H](n2c(N)c(nc2)C(=O)N)[C@H](O)[C@H](O)[C@H]1CO
C2865	DB04954	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@@H](n2c3ncnc(N[C@@H]4CCOC4)c3nc2)[C@H](O)[C@H](O)[C@H]1CO
C2866	DB04996	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC1CCCCC1
C2867	DB05016	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1c(c2onc(n2)c2cc(ccc2)C(=O)O)cccc1
C2868	DB05057	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1CCC(NC(=O)CSCC(=O)O)C1=O
C2869	DB05095	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1ncn(c1c1cc(F)c(OC)cc1)c1ccc(S(=O)(=O)N)cc1
C2870	DB05219	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(c1ccc(cc1)Oc1ccc2c(c1)COB2O)N
C2871	DB05229	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@@H]2[C@@H]([C@H]([C@H](O)C2)/C=C/[C@@H](O)C(CC#CC)C)c2c1c(ccc2)CCCC(=O)[O-]
C2872	DB05262	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=c1[nH]c(=O)nc2[nH][nH]cc12
C2873	DB05289	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1c(ccc([C@@H](C)C(=O)O)c1)c1ccccc1
C2874	DB05298	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	s1c(nc(c2nc(ccc2)C(=O)O)c1)c1cc(OCC)c(OCC)cc1
C2875	DB05347	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(Cn1c2[nH]c(nc(=O)c2nc1)N)CCO
C2876	DB05366	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	O([C@]1([C@@]2([C@H]([C@H]3C(=C4C(=CC(=O)CC4)CC3)[C@H](C2)c2ccc(N(C)C)cc2)CC1)C)C(=O)C)C(=O)C
C2877	DB05383	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[NH3+]N=C(N)N
C2878	DB05398	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[O-]C(=O)C[N+](CCCCCCCCCCCC)(C)C

C2879	DB05409	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(C(=O)CCCO[N+](=O)[O-])c1ccc(NC(=O)C)cc1
C2880	DB05413	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	[illegible]
C2881	DB05424	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	Clc1cc(Nc2ncnc3c2cc(NC(=O)C=C)c(OCCCN2CCOCC2)c3)ccc1F
C2882	DB05446	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(CC(NC(=O)CCC(N)C(=O)O)C(=O)NCC(=O)O)CO
C2883	DB05448	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(Sc1[nH]ccn1)C(CC)C
C2884	DB05482	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1Cc2c([C@@](O)(CC)C1=O)cc1n(Cc3c1nc1c(c3CC)cc(O)cc1)c2=O
C2885	DB05490	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	[illegible]
C2886	DB05791	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	BrC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
C2887	DB05817	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ClCCN(S(=O)(=O)C)N(S(=O)(=O)C)C(=O)NC
C2888	DB05837	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S=c1n([C@@]2(O[C@@H]([C@@H](O)[C@@H]2O)CO)O)ccc(n1)N
C2889	DB05838	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	Clc1c(C(=O)N2CCC[C@@H](c3c2cccc3)CC(=O)NC(C)C)ccc(N2CCCC2)c1
C2890	DB05855	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(CC/C=C/c1cccnc1)C
C2891	DB05861	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(N)c1cc2c(nc1)cccc2
C2892	DB06614	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1[C@H]([C@H](N=C(N)N)C[C@@H]1C(=O)O)C(NC(=O)C)C(CC)CC
C2893	DB08831	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@@H]([C@H]([C@@H](CC1O)O)O)CO
C2894	DB08919	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	N1(CCN(CC1)CC/C=C/1\c2cc(ccc2Sc2ccccc12)Cl)CCOC(=O)C
C2895	DB08920	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	c1ccc2c(c1)/C(=C/CCN1CCN(CC1)CCOC(=O)CCCCCCCCC)/c1c(S2)ccc(c1)Cl
C2896	DB01134	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	O=C(C1C2(C(C3C(C4(C(=CC(=O)CC4)CC3)C)CC2)CC1)C)COC(=O)C(C)(C)C
C2897	DB01527	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c(CC(N)(C)C)cccc1
C2898	DB01629	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@H]([C@H](O)[C@@H]1O)n1cc(F)c(=O)[nH]c1=O
C2899	DB01633	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[illegible]
C2900	DB01634	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](C[C@H]1C=C(NNc2ccccn2)C(=CC1=O)O)C(=O)O
C2901	DB01637	DrugBank	noninhibitor	62	inhibitor	inhibitor	noninhibitor	inhibitor	CC(C)CCC[C@H](C)CCC[C@H](C)CCC[C@H](C)CCO
C2902	DB01641	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@H](O)[C@H](N)C1=N/C(=C\c2c[nH]c3cccc(N)c23)/C(=O)N1CC(=O)O
C2903	DB01642	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CO[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O
C2904	DB01644	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(O)cc2Oc3cc(O)ccc3C(c12)CCC(=O)O
C2905	DB01646	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N[C@@H](CCSC)C(=O)O
C2906	DB01648	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CO[C@@H]1O[C@H](CO)[C@@H](S)[C@H](O)[C@H]1O
C2907	DB01649	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[illegible]
C2908	DB01653	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]([C@@H](N)C1=N/C(=C\c2c3c([nH]c2)cccc3)/C(=O)N1CCO)C
C2909	DB01661	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	[illegible]
C2910	DB01665	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC1N=c2ccccc2=N1
C2911	DB01670	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCOC(=O)C
C2912	DB01684	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H](O)CSO
C2913	DB01685	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cnccc1c1nc(n[nH]1)c1cc(ncc1)C#N
C2914	DB01686	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN(C)/C(=N/CCC[C@H](N)C(=O)O)/N
C2915	DB01689	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c(ccc1)CC(=O)Nc1cc(c(c(c1)C)S(=O)(=O)NCC(=O)O)C)C
C2916	DB01692	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H](CS)[C@H](O)CS
C2917	DB01695	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ONC(=O)CCCP(=O)([O-])[O-]
C2918	DB01698	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[illegible]
C2919	DB01699	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C/C=C(\N)/CCC(=O)O
C2920	DB01701	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@H](Cl)CCl
C2921	DB01706	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1nc(Br)nc2[nH]cnc12

C2922	DB01711	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCc1c(F)c(F)c(F)c(F)c1F
C2923	DB01716	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N[C@H]1[C@H](O)C[C@@](CC=C)(O[C@@H]1[C@@H](O)[C@H](O)CO)C(=O)O
C2924	DB01720	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)/C(=C/c1ccc(Oc2ccccc2Br)cc1)/NC(=O)c1ccccc1
C2925	DB01734	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc2c(cc1)cc(c(c2)NC(=O)C(=O)O)C(=O)O
C2926	DB01737	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N([C@@H](Cc1cccc(c1)C(=N)N)C(=O)OC)C(=O)CNS(=O)(=O)c1ccc(C)cc1
C2927	DB01740	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCc1nc(N)[se]c1CCC
C2928	DB01742	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@H]1CCCN(C1)C(=O)C
C2929	DB01743	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@H](O)[C@H](NC(=O)[C@@H](NC(=O)[C@@H](CCCN)[S(=O)(=O)O])[C@@H](CCCNC(=N)N)C(=O)[C@@H]1CCCN1C(=O)[C@@H](NC(=O)[C@@H](CCCN)C(=O)[C@@H](CCCN)N)C(=O)[C@@H](CO)NC(=O)[C@@H](CCCN)C(=O)[C@@H](CCCN)N)C(=O)[C@@H](CO)NC(=O)[C@@H](CCCN)N)C(=O)O
C2930	DB01749	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COCCOC
C2931	DB01750	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cccc1cccc2)CC(=O)O
C2932	DB01751	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)Cc1cc(I)c(Oc2cc(I)c(O)c(I)c2)c(I)c1
C2933	DB01752	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCSC[C@@H]1O[C@H]([C@H](O)[C@H]1O)n1cnc2c1ncnc2N)C(=O)O
C2934	DB01754	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(c(c(c(=O)n2C)O)O)ccc1
C2935	DB01755	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC[C@@H](C)[C@H](N)C(=O)NS(=O)(=O)NC[C@@H]1O[C@H]([C@H](O)[C@H]1O)n1cnc2c1ncnc2N
C2936	DB01759	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCc1cc(=O)c(O)co1
C2937	DB01760	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1nccnc1C(C)C
C2938	DB01762	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)CC(=O)O
C2939	DB01763	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=S)c1ccc[n+]([c1)[C@@H]1O[C@@H](COP(=O)([O-])OP(=O)(O)OC[C@@H]2O[C@H]([C@H](OP(=O)(O)O)[C@H]2O)n2cnc3c2ncnc3N)[C@H](O)[C@H]1O
C2940	DB01768	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N[C@H]1[C@H](O)C[C@](O[C@@H]1[C@@H](O)[C@H](O)CO)(Oc1ccc2c(C)cc(=O)oc2c1)C(=O)O
C2941	DB01775	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCC(=O)CO
C2942	DB01778	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cn1c(=O)n(C)c2[nH]c(N)nc2c1=O
C2943	DB01782	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc2c(cc1)c(=O)c1c3c(ccc1)[nH]nc23
C2944	DB01784	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NS(=O)(=O)c1ccc(F)cc1
C2945	DB01789	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@H]1C=C(CO)C[C@@H](O)[C@@H]1O
C2946	DB01793	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1C1=C(C(=O)NC1=O)Nc1ccc(c(c1)C(=O)O)Cl)Cl
C2947	DB01803	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[N+](C)(C)CCS
C2948	DB01808	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CS[AsH]O)C(=O)O
C2949	DB01816	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1CCN2C[C@H](O)[C@@H](O)[C@H](O)[C@H]12
C2950	DB01817	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](O[C@H](O)C[C@H](N)C(=O)O)[C@@H](N)C(=O)O
C2951	DB01821	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCC[C@@H](NC(=O)[C@@H](N)CCCNC(=N)N[N+](=O)[O-])C(=O)N
C2952	DB01823	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@]2(NC(=O)NC2=O)[C@H](O)[C@@H](O)[C@@H]1O
C2953	DB01824	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	N[C@@H](O)O[C@H]1Cc2ccccc2C1[C@H]1CN[C@](C[C@@H](O)[C@@H](Cc2ccccc2)NC(=O)O[C@@H]2CCOC2)(Cc2ccccc2)C1=O
C2954	DB01825	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(C)c2[nH]c(N)nc(=O)c2cc1
C2955	DB01826	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCC[N+]#[C-]
C2956	DB01827	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(N)c1c(F)c(c(c(c1F)F)OC)F
C2957	DB01833	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCONC(=N)N)C(=O)O
C2958	DB01835	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=N)NCC[C@@H](F)C[C@H](N)C(=O)O
C2959	DB01839	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(O)CO
C2960	DB01841	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@H]1C[C@H](O)[C@@H](O)[C@H](O)O1
C2961	DB01843	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NN1C(=O)N[C@]2(O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)C1=O
C2962	DB01845	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCc1ccccc1
C2963	DB01848	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C[C@@H]([C@@H](O[Ca])C(=O)O)C(=O)O
C2964	DB01849	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1CCNC(=O)N1

C2965	DB01856	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CCCCCC(=O)O
C2966	DB01862	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)S[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O
C2967	DB01868	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@H](NC(=O)CCCC[C@@H](NC(=O)C[NH3+])C(=O)[O-])P(=O)[O-]
C2968	DB01870	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@@H](S)[C@H](O)[C@@H](O)[C@@H]1S
C2969	DB01875	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=c1[nH]c(=O)c2[nH]nnc2[nH]1
C2970	DB01881	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](O)C[C@@](C)(O)CO
C2971	DB01884	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1CN(CC1)C(=O)[C@H](C(C)C)N
C2972	DB01885	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1OC(=O)[C@@H](O)[C@@H](O)[C@@H]1O
C2973	DB01904	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H](O)[C@@H](O)[C@H](O)CO
C2974	DB01906	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc(O)c2nn(nc2n1)c1cccc(c1)C(=O)O
C2975	DB01909	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[illegible]
C2976	DB01910	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@H](CC[C@@H](N)C(=O)O)C[C@@H]1O[C@H]([C@H](O)[C@H]1O)n1cnc2c1ncnc2N
C2977	DB01914	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H](O)[C@H](O)[C@@H](O)[C@@H](O)C=O
C2978	DB01917	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCCCCN
C2979	DB01919	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCC=O
C2980	DB01921	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O/N=C/1\NC[C@@H](O)[C@H](O)[C@H]1O
C2981	DB01925	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c(O)c(O)ccc1)c1c(cccc1)Cl
C2982	DB01929	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(nc(nc2c1c(c(cc2)N)[Cl](=O)=O)N)N
C2983	DB01930	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)(CO)[C@@H](O)C(=O)[O-]
C2984	DB01936	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@H](O)[C@@H](O)[C@@H]1O
C2985	DB01938	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cccc2c1cc(cc2)NC(=O)[C@H](N)Cc1[nH]cnc1
C2986	DB01940	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	Oc1ccc(cc1)C(=O)N[C@H]1CNCCC[C@H]1OC(=O)c1ccc(cc1)C(=O)c1ccccc1O
C2987	DB01949	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CNC(=O)[C@@H](N)C(C)(C)C
C2988	DB01950	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(sc(cn1)[N+](=O)[O-])NC(=O)NCc1ccc(cc1)OC
C2989	DB01952	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cn2cnc3[nH]cnc3c2n1
C2990	DB01954	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc(c(cc1)OC)OC1CCCC1)[C@H]1CC(=O)NC1
C2991	DB01955	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCCCCO
C2992	DB01956	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCCS(=O)(=O)O
C2993	DB01973	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](COS(=O)(=O)Cc1ccccc1)C(=O)O
C2994	DB01974	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CS[C@@H]1NOC(=C1)[C@@H](N)C(=O)O)C(=O)O
C2995	DB01976	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1cccc2c1cc1ccccc1c2
C2996	DB01977	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N=C(N)c1ccc2cc(ccc2c1)C(=O)Nc1ccccc1
C2997	DB01978	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cn1c[n+](C)c2c1nc(N)nc2O
C2998	DB01979	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CO[C@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@@H]1O
C2999	DB01980	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(I)cc1)C[C@@H](N)C(=O)NO
C3000	DB01985	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N[C@@H](CCCNC(=N)N)C(=O)O
C3001	DB01986	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1c(N)cccc1F
C3002	DB02002	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=C)C(=O)N
C3003	DB02005	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C/C=C/C(=O)C(=O)O
C3004	DB02016	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	CN(CCCCCCOc1ccc(c(F)c1)C(=O)c1ccc(Br)cc1)CC=C
C3005	DB02017	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1O[C@@H](O[C@H]2[C@H](O)[C@@H](O)c3nccn3[C@H]2CO)[C@@H](O)[C@H](O)[C@H]1O
C3006	DB02019	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc2c(c(c1)O)C(=O)c1c(C2)ccc(c1O)CC(=O)O
C3007	DB02020	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(=O)n(c(=O)c3c1c(ccc3)ccc2)CC(=O)O

C3008	DB02021	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=O)[C@H]1C[C@]2(NC(=O)NC2=O)c2cc(F)ccc2O1
C3009	DB02025	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)[C@@H](NC(=O)[C@H](CS)NC(=O)CCC[C@H](N)C(=O)O)C(=O)O
C3010	DB02026	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN(Cc1coc2c1c(N)nc(N)n2)c1ccc(cc1)C(=O)N[C@H](CCC(=O)O)C(=O)O
C3011	DB02027	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCCNC[C@@H](N)CCCNC(=N)N[N+](=O)[O-]
C3012	DB02033	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	Oc1c([C@@H](C2CC2)c2cccc(NS(=O)(=O)c3ccccc3)c2)c(=O)oc2c1CCCCCC2
C3013	DB02034	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1CCCN2C[C@@H](O)[C@@H](O)[C@H]12
C3014	DB02036	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1Nc2ccccc2S[C@@H]1CC(=O)NO
C3015	DB02041	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ccc2c(=O)[nH][nH]c(=O)c2c1
C3016	DB02044	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(cccc1CNC(=N)C)CN
C3017	DB02045	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCN
C3018	DB02055	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCNS(=O)(=O)c1ccccc1
C3019	DB02056	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(CCC/C=C\C[C@H]1[C@H](CC(=O)[C@@H]1/C=C/[C@H](CCCCC)O)O)O
C3020	DB02060	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1CCCCC1
C3021	DB02066	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CNc1ncnc2c([nH]nc12)[C@@H]1O[C@@H](CO)[C@H](O)[C@H]1O
C3022	DB02067	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc2c(N(C=O)[C@H](CNc3ccc(cc3)C(=O)N[C@H](CCC(=O)N[C@@H](CCC(=O)N[C@H](CCC(=O)O)C(=O)O)C(=O)O)C(=O)O)CN2)c(=O)[nH]1
C3023	DB02068	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[NH3+]CCCCC(=O)O
C3024	DB02069	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=O)NCc1ccccc1F)S(=O)(=O)N
C3025	DB02070	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CC(=O)c1ccccc1N)C(=O)O
C3026	DB02072	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1Cc2c(CC1)c(c(s2)NC(=O)C(=O)O)C(=O)O
C3027	DB02077	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCCNC(=N)N[N+](=O)[O-])C(=O)N[C@H]1CN[C@@H](C1)C(=O)N
C3028	DB02079	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NOCC(=O)O
C3029	DB02087	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NS(=O)(=O)c1cc(F)cc(F)c1
C3030	DB02091	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1sc(c(n1)C)c1nc(ncc1)N
C3031	DB02095	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1Nc2ccccc2C1=O
C3032	DB02096	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1n(cnc1C(=O)N)[C@@H](CO)CCc1ccccc1
C3033	DB02100	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CO[C@H]1O[C@H](CO)[C@H](O)[C@H](O)[C@H]1O
C3034	DB02102	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	Nc1cc(CN2[C@@H](Cc3ccccc3)[C@H](O)[C@@H](O)[C@H](Cc3ccccc3)N(Cc3cc(N)ccc3)[C@@H]2O)ccc1
C3035	DB02105	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1cc(cc(c1O)[N+](=O)[O-])[N+](=O)[O-]
C3036	DB02107	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)C[C@@H](C)N
C3037	DB02108	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCC=N
C3038	DB02113	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1c2c(ncnc2nc1)C
C3039	DB02119	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc2c(N=C(CO)CN2)c(=O)[nH]1
C3040	DB02120	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@H]1C=C(CO)[C@@H](O)[C@H](O)[C@@H]1O
C3041	DB02121	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCC(=O)N
C3042	DB02124	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@H]1[C@H](O)C=CC=C1C(=O)O
C3043	DB02125	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1[C@@H]2C[C@H]3C[C@@H](C2)C[C@@H]1C3
C3044	DB02127	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	P(=O)(OC(C)C)(OC(C)C)C
C3045	DB02130	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1cc(ccc1O)C(=O)[O-]
C3046	DB02132	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc2c(cc1Cl)n(c(=O)n(c2=O)Cc1c(cc(cc1)Br)F)CC(=O)O
C3047	DB02134	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c([nH]c(=O)[nH]c1=O)nc[nH]2
C3048	DB02143	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)NC(=N)NO
C3049	DB02144	DrugBank	noninhibitor	62	inhibitor	inhibitor	noninhibitor	inhibitor	CCCCCCCCCCCCCCCC(=O)OC[C@@H](COP(=O)([O-])O[C@@H]1[C@@H](O)[C@H](O)[C@@H](O)[C@H](O)[C@H]1O)OC(=O)CCCCCCC/C=C/CCCCCCCC
C3050	DB02145	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCO

C3051	DB02146	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCNc1nc(NC(C)C)nc(SC[C@@H](NC(=O)CC[C@H](N)C(=O)O)C(=O)NCC(=O)O)n1
C3052	DB02148	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)[C@@H](N)COCc1ccccc1
C3053	DB02156	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C(=O)CS(=O)(=O)O
C3054	DB02158	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CSC[C@H]1N[C@H]([C@H](O)[C@@H]1O)c1c[nH]c2[C@H](N)NC=Nc12
C3055	DB02168	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Brc1ncnc2[nH]cnc12
C3056	DB02172	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1N[C@@H](CO)[C@H](O)[C@H]1O
C3057	DB02179	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1)C(F)(F)F)Nc1c(cccc1)C(=O)O
C3058	DB02185	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1C(=O)N(c2c(O1)cc(cc2)OC)O
C3059	DB02190	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C[C@@H](C(=O)O)C(=O)C(=O)O
C3060	DB02192	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCCc1ccccc1
C3061	DB02202	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](O)CCO
C3062	DB02203	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)(O)C#N
C3063	DB02207	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[O-][N+](=O)c1cccc2c[nH]nc12
C3064	DB02210	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCCCCCCO
C3065	DB02214	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H](O)[C@H](O)[C@@H](O)Cn1c(=O)c(=O)[nH]c2c1[nH]c(=O)[nH]c2=O
C3066	DB02215	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N([C@@H](CC(C)C)C(=O)O)C(=O)c1occc1
C3067	DB02219	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OS(=O)(=O)CCCNC1CCCCC1
C3068	DB02221	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=O)NCc1c(cc(cc1F)F)F)S(=O)(=O)N
C3069	DB02222	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@H](Cn1cnc2c1nc(N)nc2N)OCP(=O)([O-])[O-]
C3070	DB02224	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1[C@H](Oc2cc(O)cc(O)c2C1=O)c1ccc(O)c(O)c1
C3071	DB02227	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1CO[C@@H](C[C@@H]1O)C(=O)O
C3072	DB02235	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[S@](=O)CC[C@@H](N)C(=O)O
C3073	DB02236	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCC(=O)N[C@@H]1O[C@@H](COP(=O)([O-])[O-])[C@H](O)[C@H]1O
C3074	DB02238	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CSCCC(=O)C(=O)O
C3075	DB02239	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)CCC(=O)O
C3076	DB02245	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc2c(CC=N2)c(=O)[nH]1
C3077	DB02247	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1CC(=C(C(=O)O)N[C@@H]1[C@@H](C(=O)O)NC(=O)Cc1cccs1)C
C3078	DB02248	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H]1C[C@H](N[C@@H]1C(=O)O)S(=O)(=O)O
C3079	DB02251	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)c1ccccc1C(=O)CCC(=O)O
C3080	DB02254	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1c(CCOP(=O)([O-])[O-])sc[n+]1Cc1cnc(nc1N)C(F)(F)F
C3081	DB02255	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ONC(=O)C[C@H](C(=O)N[C@H](C(=O)NC)Cc1c[nH]c2ccccc12)CC(C)C
C3082	DB02256	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@@H](C[C@@H]1O)n1ccc(=O)[nH]c1=O
C3083	DB02258	DrugBank	noninhibitor	62	inhibitor	noninhibitor	inhibitor	inhibitor	CC1(C)CCC(C)(C)c2cc(ccc12)/C(=N\O)/c1ccc2cc(ccc2c1)C(=O)O
C3084	DB02259	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCc1c(C(=O)c2cc(Br)c(O)c(Br)c2)c2c(o1)cc(cc2)S(=O)(=O)Nc1ccc(cc1)S(=O)(=O)N
C3085	DB02260	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(CCC(=O)O)CCC(=O)CCC(=O)O
C3086	DB02265	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC[Si](C)(C)C
C3087	DB02266	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccccc1Nc1cc(ccc1)C(F)(F)F)C(=O)O
C3088	DB02267	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCCNC(=N)N[C@H](CC(=O)O)C(=O)O)C(=O)O
C3089	DB02274	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@H](N)C(=O)CCCCCC(=O)O
C3090	DB02277	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1ccc(NC(=O)Nc2n(nc(C(C)(C)C)c2)C)cc1
C3091	DB02278	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1c(N)[nH]c(=O)c2N=C(C(C)(C)Nc12)O
C3092	DB02282	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CSC[C@@H]1O[C@H]([C@H](O)[C@H]1O)n1cnc2c1ncnc2N
C3093	DB02283	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1)NCCS(=O)(=O)O

C3094	DB02286	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](Cc1c[nH]c2cccc(N)c12)C(=O)O
C3095	DB02296	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)CCO
C3096	DB02301	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc(=O)c2c([nH]1)N=C[C@@H]1CN(CN21)c1ccc(cc1)C(=O)N[C@H](CCC(=O)O)C(=O)O
C3097	DB02302	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN/C(=N\C)/NCCC[C@H](N)C(=O)O
C3098	DB02303	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	I[C@@H]1CNC(=O)NC1=O
C3099	DB02304	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCC[C@H](O)/C=C/C1=C(C/C=C/CCCC(=O)O)C(=O)CC1
C3100	DB02305	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1OC(=C[C@@H](O)[C@@H]1O)C(=O)O
C3101	DB02307	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=O)[C@@H](CC(=O)O)NC(=O)[C@@H](Cc1ccccc1)N[C@@H](CCc1ccccc1)C(=O)O
C3102	DB02311	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CSC[S@](=O)C
C3103	DB02318	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@@H](F)[C@H](F)[C@@H](O)[C@@H]1O
C3104	DB02320	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N[C@H]1O[C@@H](CO)[C@H](O)[C@@H](O)[C@@H]1O
C3105	DB02321	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCSC[C@H]1O[C@H](O)[C@@H](O)[C@@H]1O)C(=O)O
C3106	DB02323	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1C[C@@H](CCCCCCCCC(=O)OC[C@@H]1O[C@H]([C@H](O)[C@H]1O)n1cnc3c1ncnc3N)[C@H]2O
C3107	DB02326	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)C[C@@H](C(=O)O)C(=O)NO
C3108	DB02334	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H](CS(=O)(=O)O)C(=O)O
C3109	DB02335	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC1=NCCS1
C3110	DB02356	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@H](CO)[C@@H]1N=C(Cc2c[nH]cn2)C(=O)N1CCO
C3111	DB02364	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCOP(=O)(OCC)OC[C@@H](N)C(=O)O
C3112	DB02365	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1cccc2ccc3cccnc3c12
C3113	DB02374	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1Cn2ccnc2[C@@H](O)[C@@H]1O
C3114	DB02377	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc2[nH]cnc2c(=O)[nH]1
C3115	DB02381	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCNC(=N)NO)C(=O)O
C3116	DB02394	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@]12O[C@H]1C[C@H](O)[C@@H](O)[C@H]2O
C3117	DB02396	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCNC
C3118	DB02397	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N[C@H]1[C@H](O)[C@@H](O)[C@H](CO)O[C@H]1OC[C@@H](N)C(=O)O
C3119	DB02402	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(nc(n1)N)N)c(ccc2)Oc1ccc(cc1)OC
C3120	DB02403	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ccccc1F
C3121	DB02405	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(O)CCCCCCCCCCCBr
C3122	DB02408	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1CC1NCC([C@@H](N)CCCC)(O)O
C3123	DB02424	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	CO[C@@H]1C[C@@H](C)CC2=C(OC)C(=O)C=C(NC(=O)/C(=C\C=C/[C@@H](OC)[C@H](OC(=O)N)/C(=C\[C@H](C)[C@H]1O)/C)/C)C2=O
C3124	DB02425	DrugBank	noninhibitor	62	inhibitor	inhibitor	noninhibitor	inhibitor	CCCCCCCCCCCCCCCCCOC(=O)CCCCCCC
C3125	DB02429	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=O)NCc1ccc(cc1)F)S(=O)(=O)N
C3126	DB02436	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCNC(=O)[C@@H](Cc1ccc(OC(C(=O)O)C(=O)O)cc1)NC(=O)N[C@H](Cc1ccccc1)C(=O)O
C3127	DB02437	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@H](CO)CCCCNC(=O)O
C3128	DB02441	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1c(CCCC)[nH]c2c(=O)[nH][nH]c(=O)c12
C3129	DB02446	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCC(=O)NO)C(=O)O
C3130	DB02447	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@]2(NC(=O)N(O)C2=O)[C@H](O)[C@@H](O)[C@@H]1O
C3131	DB02448	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CCCCCCCCCCCC
C3132	DB02458	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCC(=O)N[C@H](CSc1ccc(cc1[N+](=O)[O-])[N+](=O)[O-])C(=O)NCC(=O)O)C(=O)O
C3133	DB02459	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=N)Nc1ccc(cc1)C(=O)O
C3134	DB02472	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1O[C@H]([C@H](O)[C@H]1O)N1CNc2c(O)ncnc12
C3135	DB02475	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=N)NCCC[C@@H](N1CCC1=O)C(=O)O
C3136	DB02477	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	Cc1nccn1CCCCc1ccc(CC(=O)N[C@H](CO)C(=O)N[C@H](CCCCN)C(=O)NCCC2CCCCC2)cc1

C3137	DB02481	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=CNCc1ccccc1
C3138	DB02486	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCCSSCCO
C3139	DB02489	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cn1cnc2c1nc(N)nc2O
C3140	DB02490	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN(CC(=O)O)C(N)N
C3141	DB02501	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=N)NCCC[C@@H](NC(=O)CCC(=O)O)C(=O)O
C3142	DB02502	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc2c(nc(O)n2[C@H]2C[C@@H](O)[C@H](CO)O2)c(=O)[nH]1
C3143	DB02506	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(O)[C@@H](C)[C@@H](N)CC[C@@H](C)C[C@H](C)[C@@H](OC)Cc1ccccc1
C3144	DB02511	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](Cc1c(O)cc(O)c(c1)N/C(=C/C=O)/COc1ccc2ccccc2c1)C(=O)O
C3145	DB02513	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)c1ccc(C)cc1O
C3146	DB02520	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCN(CC)C(=S)S
C3147	DB02521	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1c2cc(O)cc(O)c2C(=O)C=C1O
C3148	DB02523	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[S+](CCON)C[C@@H]1O[C@H]([C@H](O)[C@H]1O)n1cnc2c1ncnc2N
C3149	DB02525	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1N/C(=N\O)/[C@@H](O)[C@@H](O)[C@@H]1O
C3150	DB02528	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@H](Cc1cn(cn1)c1[nH]nnn1)C=O
C3151	DB02529	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCN(CC)C(=O)[C@H]1O[C@H](C[C@@H](N)[C@@H]1NC(=O)C)C(=O)O
C3152	DB02532	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(N)ccc2nc(N)nc(c2c1)N
C3153	DB02534	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccccc1CC=C
C3154	DB02536	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H](O)C=O
C3155	DB02537	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1ccc(OC/C(=C/C=O)/Nc2cc(C[C@H](N)C(=O)O)c(O)cc2O)cc1
C3156	DB02539	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCSC(=N)N
C3157	DB02541	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[NH3+]CCCCO
C3158	DB02551	DrugBank	noninhibitor	62	inhibitor	noninhibitor	inhibitor	inhibitor	CC[C@H]1CNCc2c1cc(NC(=O)c1ccc3cc(ccc3c1)C(=N)N)cc2
C3159	DB02553	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCCCCNCCCNC(=O)CNC(=O)[C@@H](CSSC[C@@H](NC(=O)CC[C@@H](N)C(=O)O)C(=O)NCC(=O)NCCCNCCCCN)NC(=O)CC[C@H](N)C(=O)O
C3160	DB02558	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C([C@@H](Cc1ccccc1)S)N[C@H](C(=O)N[C@H](C(=O)O)C)Cc1ccccc1
C3161	DB02561	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@]1(O)OC[C@H](O)[C@@H](O)[C@@H]1O
C3162	DB02562	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@H](O)[C@H](O)[C@H]1CNC2=NC(=NC(=O)C2=N1)N
C3163	DB02568	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc(=O)c2c([nH]1)c(Cc1cnccc1)c[nH]2
C3164	DB02576	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](O)C[NH3+]
C3165	DB02578	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@H](NC(=O)[C@@H](C)NC(=O)CCCC[C@@H](NC(=O)C[NH3+])C(=O)[O-])C(=O)O
C3166	DB02582	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=C)[C@H](NC(=O)[C@H](CS)NC(=O)CCC[C@H](N)C(=O)O)C(=O)O
C3167	DB02586	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1ccc(c2ccc3c(ccnc3c12)C)C
C3168	DB02589	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC[Se]C(=N)N
C3169	DB02591	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1cc2[nH]cnc2cc1C
C3170	DB02593	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc2c(c(c1O)C(=O)O)c(=O)c1c(o2)C[C@@H](O[C@H]1OC)C)O
C3171	DB02594	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc(=O)n(cc1)[C@H]1C[C@@H](O)[C@H](CO)O1
C3172	DB02597	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S[C@@H](CCCCC)C(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H](C)C(=O)O
C3173	DB02598	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N[C@@H](Cc1cc(I)c(O)c(I)c1)C(=O)NCC(=O)O
C3174	DB02606	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC[C@@H](C)O
C3175	DB02608	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N[C@@H](CO)[C@@H](O)c1ccc(cc1)[N+](=O)[O-]
C3176	DB02610	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=O)NCc1c(c(c(c(c1F)F)F)F)F)S(=O)(=O)N
C3177	DB02613	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[N+]([O-])(C)(C)CCCCCCCCCC
C3178	DB02614	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(C(NC(=O)C)B(O)O)c1cccc(C(=O)O)c1
C3179	DB02619	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCCCCCCCCCCCCCBr

C3180	DB02620	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)NCCSSCCNC(=O)[C@H]1CC[C@@H](CC1)NC(=O)c1nccnc1C(=O)O
C3181	DB02621	DrugBank	noninhibitor	62	noninhibitor	inhibitor	inhibitor	inhibitor	S1C[C@H](NC1=O)[C@@]1(O[C@@H]2CC[C@H](/C=C\C=C/CC/C(=C\C(=O)O[C@H](C2)C1)/C)C)O
C3182	DB02624	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H]1CCOC1=O
C3183	DB02625	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCC[C@@H](CN(O)C=O)C(=O)O
C3184	DB02626	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ON(C(=O)C)CCC[C@@H]1NC(=O)[C@@H](NC(=O)CNC(=O)[C@H](NC(=O)CNC(=O)[C@@H](NC1=O)CCCN(O)C(=O)C)Cc1ccccc1)CCCN(O)C(=O)C
C3185	DB02637	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C(=O)CC(=O)[O-]
C3186	DB02639	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1cc(=O)oc2cc(O[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)ccc12
C3187	DB02643	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(CC[N+](C)(C)CCCCCCCCCCCC)S(=O)(=O)O
C3188	DB02645	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1O[C@H](OCC[C@@H]2CO2)[C@@H](O)[C@H](O)[C@H]1O
C3189	DB02646	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCN=O
C3190	DB02647	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(C2CC2)cc([nH]n1)NC(=O)c1ccccc1
C3191	DB02660	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(N)O/N=C(\C)/c1ccc(OC)c(c1)OC1CCCC1
C3192	DB02662	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1I)C(=O)O)NC(=O)C(=O)O
C3193	DB02668	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	Cc1ccccc1CNC(=O)[C@H]1N(CSC1(C)C)C(=O)[C@@H](O)[C@@H](Cc1ccccc1)NC(=O)c1cccc(O)c1C
C3194	DB02669	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	S[C@@H](Cc1ccccc1)C(=O)NCC(=O)N1[C@H](CC[C@H]1C(=O)O)c1ccccc1
C3195	DB02670	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1C[C@H](O)[C@@H](O)[C@H](O)O1
C3196	DB02671	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cn1cc[nH+]c1
C3197	DB02675	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@H](C(=O)O)c1ccc(O[C@H]2O[C@@H](CO)[C@H](O)[C@@H](O)[C@H]2O[C@H]2O[C@@H](CO)[C@H](O)[C@@H](O)[C@@H]2O)cc1
C3198	DB02676	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCC(CO)(CO)NCCCNC(CO)(CO)CO
C3199	DB02678	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@H]1[C@H](O)O[C@H](CO)[C@H](O)[C@@H]1O
C3200	DB02680	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[O-][N+](=O)c1cc(ccc1)[N+](=O)[O-]
C3201	DB02684	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@H](CS)C(=O)NS(=O)(=O)OC[C@@H]1O[C@H]([C@H](O)[C@H]1O)n1cnc2c1ncnc2N
C3202	DB02690	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(O)c2nc(C)[nH]c(=O)c2ccc1
C3203	DB02693	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1CSSC[C@@H]1O
C3204	DB02697	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)[C@@H](N)C(=O)NO
C3205	DB02706	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)/C(=N\C(=O)[C@H](CS)CCc1ccccc1)/c1ccc(Cn2cnnn2)s1
C3206	DB02712	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(F)ccc2OCC[C@@]3(C(=O)NC(=O)N3)c2c1
C3207	DB02718	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc(=O)c2c([nH]1)N=C[C@@H](CNc1ccc(cc1)C(=O)N[C@H](CCC(=O)O)C(=O)O)N2C=O
C3208	DB02720	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=O)[C@H]1O[C@@H](CO)[C@H](O)[C@@H](O)[C@@H]1O
C3209	DB02727	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCNC(=N)NO
C3210	DB02730	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CS[C@H]1[C@@H](CO)O[C@@H](O)[C@H](O)[C@@H]1O
C3211	DB02731	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S([Hg]CC)c1ccccc1C(=O)O
C3212	DB02734	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1OC(=C[C@@H](O)[C@@H]1O)C(=O)O
C3213	DB02742	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1[C@@H](O)[C@H](O)[C@@H](O)[C@@H]2NC(=O)C(=O)N12
C3214	DB02745	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1O[C@H]([C@H](O)[C@H]1O)n1ccc(=O)[nH]c1=O
C3215	DB02747	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@H](N[C@H](CCc1ccccc1)C(=O)N[C@H](CCCNC(=[NH2+])N)C(=O)Nc1ccccc1)C(=O)O
C3216	DB02751	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=N)NCC(=O)O
C3217	DB02752	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(ccc(c1)S(=O)(=O)N1CCC[C@@H]1C(=O)O)C
C3218	DB02753	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1O[C@H]([C@H](O)[C@H]1O)n1cnc2c1nc[nH]c2=[SeH]
C3219	DB02763	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)c1cc(S)ccc1[N+](=O)[O-]
C3220	DB02764	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCC
C3221	DB02767	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(C[C@@H](CCCCCCCCCCC)O)O
C3222	DB02768	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)(C)OC=O

C3223	DB02772	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1O[C@H](O[C@@]2(CO)O[C@@H](CO)[C@H](O)[C@H]2O)[C@@H](O)[C@H](O)[C@H]1O
C3224	DB02773	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1cc(ccc1OCCC)CC(=O)O
C3225	DB02774	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCCCO
C3226	DB02776	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCCCCCCCCCCCCS(=O)(=O)O
C3227	DB02784	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H](NC(=O)CCNC(=O)CBr)C(=O)NCCc1ccc(NC(=O)C(=O)O)cc1
C3228	DB02786	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1C[C@](O)(C=C(F)[C@@H]1O)C(=O)O
C3229	DB02787	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](O)N[C@H](CO)[C@H](O)[C@@H](O)[C@H](O)CO
C3230	DB02788	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](O)C(=O)C
C3231	DB02792	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	CN[C@H](C(C)C)C(=O)N[C@@H](C@H]3O)c2ccc(O)c3ccc4oc(O)c5ccc(cc5C)[C@H]3[C@H](C@H]2C2C@@]3C)NC(=O)O[C@@H]3C)[C@](=O)N[C@H](CC(=O)N)C1=O)c1ccc(O)c(-)c1-c(=O)oc(O)cc1[C@@H]3NC5=O)[C@H]3O)c(O)c3Oc4[C@]2o2
C3232	DB02797	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OB(O)c1cccc(c1)[N+](=O)[O-]
C3233	DB02800	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc(=O)c2c([nH]1)N=C[C@@H](CNc1ccc(cc1)C(=O)N[C@H](CCC(=O)O)C(=O)O)N2CO
C3234	DB02801	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1C[C@](O)(C=C[C@@H]1O)C(=O)O
C3235	DB02803	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H](O)Cc1ccccc1
C3236	DB02809	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1cc(Cc2c[nH+]c(N)nc2N)cc(OCCC[C@@H](CCC(=O)[O-])C(=O)[O-])c1Br
C3237	DB02812	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N1C[C@@H](O)C[C@H]1C(=O)N[C@H](CCCNC(=N)N)C(=O)c1nc2c(s1)cccc2
C3238	DB02813	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N[C@@H]1[C@@H](O)[C@H](O)[C@@H](CO)OC1=O
C3239	DB02815	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1C=Cc2ccccc12
C3240	DB02816	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cn1cc(nn1)[C@@H]1SC=C(NC=C1C=O)C(=O)O
C3241	DB02821	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NOCC[C@@H](N)C(=O)O
C3242	DB02822	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCc1ccc(Br)cc1
C3243	DB02828	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CCC(=O)CF
C3244	DB02833	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc(C)c(s1)c1nc(ncc1)Nc1cccc(c1)[N+](=O)[O-]
C3245	DB02834	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c(ccc1F)C(=O)NCc1nc2c(s1)c(F)cc(F)c2F)OCC(=O)O
C3246	DB02840	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2OCOc2ccc1c1c(C(=O)O)[nH]nc1c1cc(CC)c(O)cc1O
C3247	DB02844	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCCCCC/C(=C\CN)/SC[C@@H]1O[C@H]([C@H](O)[C@H]1O)n1cnc2c1ncnc2N
C3248	DB02847	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](O)[C@@](C)(O)CN
C3249	DB02852	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@H](/C=C/C=C(\C)/[C@H]1CN[C@@H]([C@H]1CC(=O)O)C(=O)O)C(=O)O
C3250	DB02856	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCOC(=O)NC
C3251	DB02861	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=O)NCc1cc(c(c(c1)F)F)F)S(=O)(=O)N
C3252	DB02862	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1[C@H](O)[C@@H](O)[C@H](O)c2nc(cn12)c1ccccc1
C3253	DB02869	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(C[C@@H](N)CCc1ccccc1)S(=O)(=O)c1ccccc1
C3254	DB02880	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](NC(=O)c1cc(F)ccc1O)c1ccc(Br)cc1
C3255	DB02881	DrugBank	noninhibitor	62	noninhibitor	inhibitor	inhibitor	inhibitor	CC(C)c1cc(Sc2ccc(O)c(c2)C(C)C)ccc1O
C3256	DB02891	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1cccc2c1n1cn[nH+]c1s2
C3257	DB02895	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S/C=C/C[S@](=O)CC=C
C3258	DB02896	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CSc1ncnc2c1ncn2[C@@H]1O[C@@H](CO)[C@H](O)[C@H]1O
C3259	DB02898	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc(OC[C@H]2CCC(=O)N2)c2[nH]cnc2n1
C3260	DB02899	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N([C@@H](CCSC)C(=O)O)C(=O)O
C3261	DB02904	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC[C@H](CO)C(=O)O
C3262	DB02906	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(O)C[C@H]1C(C)(C)[C@H](C)C(=O)C1
C3263	DB02909	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	o1c(C(=O)O)ccc1c1ccccc1Cl
C3264	DB02911	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1c(N)nc(N)c2c1NC[C@H](N2)c1ccccc1
C3265	DB02916	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ncnc2c1ncn2[C@@H]1O[C@@H](COS(=O)(=O)N)[C@H](O)[C@H]1O

C3266	DB02921	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1cn(c(=O)[nH]c1=O)[C@@]12C[C@H](O)[C@@H](CO)[C@@H]1C2
C3267	DB02923	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c(c(cc1)O)O)c1ccccc1
C3268	DB02933	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CSC[C@H]1O[C@H]([C@H](O)[C@@H]1O)n1ccc2c(N)ncnc12
C3269	DB02934	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](O)[C@@H]1O[C@H]([C@H](O)[C@H]1O)n1cnc2c1ncnc2C
C3270	DB02937	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ncnc2c1ncn2[C@@H]1O[C@@H](COP(=O)(O)OP(=O)(O)C[As](O)(O)O)[C@H](O)[C@H]1O
C3271	DB02938	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCCC(=O)O
C3272	DB02943	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1ccc(CSC[C@@H](NC(=O)CCCN)C(=O)NCC(=O)O)cc1
C3273	DB02946	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC[C@@]1([C@H](C)C1(Cl)Cl)C(=O)N[C@@H](C)c1ccc(Cl)cc1
C3274	DB02947	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc(F)nc2c1ncn2[C@H]1C[C@@H](O)[C@H](CO)O1
C3275	DB02951	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCC(=O)C(=O)O
C3276	DB02954	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ON(CC(=O)O)C(=O)O
C3277	DB02964	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@]2(NC(=S)NC2=O)[C@H](O)[C@@H](O)[C@@H]1O
C3278	DB02967	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCN1C(=O)C=CC1=O
C3279	DB02968	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC1(C)S[C@H](N[C@H]1C(=O)[O-])[C@@H](NC(=O)Cc1ccccc1)C(=O)OC[C@@H](N)C(=O)[O-]
C3280	DB02969	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1c(CCO)scn1
C3281	DB02970	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCc1ccccc1N
C3282	DB02971	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCCOCC[C@@H](N)C(=O)O
C3283	DB02972	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC[C@H](N)Cc1ccccc1
C3284	DB02979	DrugBank	noninhibitor	62	noninhibitor	inhibitor	noninhibitor	noninhibitor	CS/C(=N/CCCCCCCCCCCCCCC/N=C(\N)/SC)/N
C3285	DB02982	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCC/C=C/C=C/CCCCCCCCCO
C3286	DB02983	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OS(=O)(=O)c1ccc([Hg])cc1
C3287	DB02985	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc2[nH]c(I)nc2c(=O)[nH]1
C3288	DB02986	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1(S(=O)(=O)N)ccc(s1)S(=O)(=O)NCc1cccs1
C3289	DB02988	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N=C(Cc1c[nH]c2ccccc12)C(=O)O
C3290	DB02991	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N/C(=N\c1ccc(cc1)C(F)(F)F)/SCC
C3291	DB02993	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1nc2c(o1)nc(N)[nH]c2=O
C3292	DB02996	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(O)[C@@H](CS)CC(C)C
C3293	DB03003	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCC(=O)N[C@H](CS(=O)(=O)O)C(=O)NCC(=O)O)C(=O)O
C3294	DB03004	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[S@](=O)C[C@H](N1[C@H](S)[C@@H](NC(=O)CCC[C@H](N)C(=O)O)C1=O)C(=O)O
C3295	DB03007	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC/C=C/C[C@H]1[C@H](CCCCCCCC(=O)O)C=CC1=O
C3296	DB03008	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@]1(F)O[C@H](F)[C@@H](O)[C@H](O)[C@H]1O
C3297	DB03015	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1O[C@H]([C@H](O)[C@H]1O)n1c[nH+]c2c1N=CN[C@@H]2O
C3298	DB03019	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nccc(n1)c1c(Cl)sc(Cl)c1
C3299	DB03024	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)[C@@H](C)Cc1csc(n1)N
C3300	DB03025	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCC[C@H](O)C=C
C3301	DB03029	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1ccccc1C
C3302	DB03030	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	s1c(ccc1)c1ncn(c1)Cc1ccc(cc1)C
C3303	DB03032	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCCCCSC[C@@H](NC(=O)CC[C@H](N)C(=O)O)C(=O)NCC(=O)O
C3304	DB03034	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@H]1COc2c(N3CCN(C)CC3)c(F)cc3c2n1cc(C(=O)O)c3=O
C3305	DB03035	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c2c(c(cc1)[N+](=O)[O-])C(=O)c1c(C2=O)c(ccc1)O)O
C3306	DB03037	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc2c(c(c1)O)C(=O)c1c(C2=O)ccc(c1O)CC(=O)O
C3307	DB03039	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=O)NCc1cc(ccc1F)F)S(=O)(=O)N
C3308	DB03044	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	Cc1ccc(cc1)n1nc(cc1NC(=O)Nc1ccc(OCCN2CCOCC2)c2c1cccc2)C(C)(C)C

C3309	DB03056	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1CCCCN1C1CCNCC1
C3310	DB03057	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=CCC=O
C3311	DB03058	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ccccc1CO
C3312	DB03061	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCC[C@H](C)NC=O
C3313	DB03065	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1n(cc2cccc(c12)[N+](=O)[O-])C(=N)N
C3314	DB03068	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@H]([C@H](O)[C@@H]1O)n1cccnc1=O
C3315	DB03071	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](N)c1nc(C)c(O)n1CC(=O)O
C3316	DB03074	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc2[nH]cc(C#N)c2c(=O)[nH]1
C3317	DB03087	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC[C@@H](C)c1nccs1
C3318	DB03090	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCN[C@H](Cc1ccccc1)C=O
C3319	DB03092	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCC1=C[C@H](O)[C@@H](O)[C@H](O)[C@H]1O
C3320	DB03094	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@H](N)[C@H]1N[C@@H](CN)C(=O)N1CC(=O)O
C3321	DB03096	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCCN1CCOCC1
C3322	DB03102	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1Cc2c(CC1)c(c(s2)NC(=O)C(=O)O)C(=O)O
C3323	DB03106	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1[C@H](O)[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1O
C3324	DB03118	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1nc(nn1)/C(=C\C(=O)c1c2cc(ccc2[nH]c1)Cl)/O
C3325	DB03119	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCC
C3326	DB03120	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1ccc(cc1)S(=O)(=O)O
C3327	DB03124	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)[C@H](CC(=O)O)NC(=O)c1ccc(cc1)CNS(=O)(=O)c1cc(c(cc1)O)C(=O)O
C3328	DB03125	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH+]1c(N)nc(N)c(c1)Cc1cc(c(c(c1)OC)OC)OC
C3329	DB03128	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)OCC[N+](C)(C)C
C3330	DB03130	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCC(=O)N[C@H](CS[C@H](O)OCc1ccc(cc1)[N+](=O)[O-])C(=O)NCC(=O)O)C(=O)O
C3331	DB03132	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc2nc(sc2cc1)SCCCS(=O)(=O)O
C3332	DB03133	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1ccc2[nH]c(nc2c1)[C@H]1O[C@@H](CO)[C@H](O)[C@@H](O)[C@@H]1O
C3333	DB03142	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1O[C@@H](O)[C@H](O)[C@H]1O
C3334	DB03143	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCCCCCO
C3335	DB03149	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)C(N)Cc1ccccc1
C3336	DB03153	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ncnc2c1N=NC2
C3337	DB03154	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(c1ccc2ccc(cc2c1)C(F)(F)P(=O)(O)O)(F)(F)P(=O)(O)O
C3338	DB03172	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ncnc2c1ccn2[C@@H]1O[C@@H](CO)[C@H](O)[C@H]1O
C3339	DB03175	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCO
C3340	DB03176	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)Cc1cc(c(Oc2ccc(O)c(c2)C(C)C)c(c1)Cl)Cl
C3341	DB03177	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1cc2c(cc1)nc[nH]2
C3342	DB03185	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1O[C@H]([C@H](O)[C@H]1O)n1cccc[nH]c1=O
C3343	DB03187	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCSCC[C@@H](CCCCC(=O)O)SSCCO
C3344	DB03188	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1O[C@H](O)[C@@H](O)[C@H](O)[C@H]1S
C3345	DB03193	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCCCCCCCCCCCCCCC(=O)O
C3346	DB03204	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1ncc(CN)c(N)n1
C3347	DB03205	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)c1cc(C(=O)O)c2c(n1)C(=O)C(=O)c1cc([nH]c21)C(=O)O
C3348	DB03206	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1NC[C@@H](O)[C@H](O)[C@H]1O
C3349	DB03207	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc2CN([C@H](Cc2cc1)C(=O)O)S(=O)(=O)c1ccc(c2ccccc2)cc1
C3350	DB03218	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)NC(=O)N[C@H]1O[C@@H](CO)[C@H](O)[C@@H](O)[C@@H]1O
C3351	DB03223	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[N+](C)(C)[C@@H](CCc1[nH]cc(C[C@H](N)C(=O)O)n1)C(=O)N

C3352	DB03226	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCC(F)(F)F
C3353	DB03228	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc(c(cc1[N+](=O)[O-])[N+](=O)[O-])C(=O)N)N(CCCl)CCCl
C3354	DB03229	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)CC(=O)C(=O)O
C3355	DB03236	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCCC(=O)NCC[C@H](N)C(=O)O
C3356	DB03238	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1cc(F)cc(F)c1
C3357	DB03241	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCC[C@@H](N)C=O
C3358	DB03242	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ccc(O[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)cc1
C3359	DB03243	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[NH3+]Cc1ccc(F)cc1
C3360	DB03246	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1O[C@H](O)[C@H](O)[C@H]1O
C3361	DB03250	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@H]1([C@H](O)[C@@H](O)[C@H](O)[C@H](O1)CO)c1nc2cc(ccc2s1)C
C3362	DB03256	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc(=O)c2c(NC[C@H](CNc3ccc(cc3)C(=O)N[C@H](CCC(=O)O)C(=O)O)N2C=O)[nH]1
C3363	DB03259	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c(O)c(O)ccc1)c1c(cccc1Cl)Cl
C3364	DB03263	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1O[C@H](S[C@H]2[C@@H](CO)O[C@H](O)[C@@H](O)[C@@H]2O)[C@@H](O)[C@H](O)[C@H]1O
C3365	DB03266	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=CCCCC=O
C3366	DB03270	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NS(=O)(=O)c1c(F)cccc1F
C3367	DB03272	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cn1nc(c2cc(C(=O)O)c(Cl)cc2F)c(Br)c1C(F)(F)F
C3368	DB03274	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H]1O[C@@H](C[C@@H]1O)n1ccc(=O)[nH]c1=O
C3369	DB03275	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@H](CS)C(=O)N
C3370	DB03284	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1COC(=C[C@H]1O)C(=O)O
C3371	DB03285	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc(cc1)/C=C/C(=O)c1ccc(O)cc1O
C3372	DB03286	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](O)[C@@]1(O[C@@H](CO)[C@H](O)[C@@H](O)[C@@H]1O)N=[N+]=[N-]
C3373	DB03287	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1ncc(COP(=O)(O)O)c(CN[C@H](/C=C/OCCN)C(=O)O)c1O
C3374	DB03288	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c([nH]c(c1)C(=O)NC[C@H](N(C1CCCC1)CCO)O)ccc(c2)Cl
C3375	DB03291	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H]1[C@@H](CO)O[C@@H](O)[C@H](O)[C@H]1O
C3376	DB03293	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cn1c(=O)[nH]c2c1[nH]c(=O)[nH]c2=O
C3377	DB03294	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(c1ccc2n(C)sc(=O)c2c1)N
C3378	DB03295	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCCCCNCCCNC(=O)CNC(=O)[C@@H](CS)NC(=O)CC[C@H](N)C(=O)O
C3379	DB03297	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OS(=O)Cc1ccccc1
C3380	DB03301	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1cccc(CC=C)c1O
C3381	DB03304	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCc1c[nH]c2nc(N)[nH]c(=O)c12
C3382	DB03307	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ncnc(c1)Nc1ccc(cc1)S(=O)(=O)N
C3383	DB03308	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)C[C@H](N)C(=O)NO
C3384	DB03309	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OS(=O)(=O)CCNC1CCCCC1
C3385	DB03310	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@H](CCC(=O)N[C@H](CSSC[C@@H](NC(=O)CC[C@@H](N)C(=O)O)C(=O)NCC(=O)O)C(=O)NCC(=O)O)C(=O)O
C3386	DB03311	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCc1c(C(=O)c2cc(Br)c(O)c(Br)c2)c2c(o1)cc(cc2)S(=O)(=O)Nc1ccc(cc1)S(=O)(=O)Nc1nccs1
C3387	DB03313	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)OCC1=C(N2[C@@H](SC1)[C@H](NC(=O)CCC[C@H]([NH3+])C(=O)O)C2=O)C(=O)O
C3388	DB03316	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1COCCO1
C3389	DB03319	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)(C)c1c(C[C@@H]([NH3+])C(=O)[O-])c([O-])no1
C3390	DB03321	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N[C@@H]1[C@@H](N)C=C(O[C@H]1[C@H](O)[C@@H](O)CO)C(=O)O
C3391	DB03330	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCC(=O)N[C@H](CS[C@H](O)N(O)c1ccc(I)cc1)C(=O)NCC(=O)O)C(=O)O
C3392	DB03332	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc2c(N3[C@H](CN2)COC3=O)c(=O)[nH]1
C3393	DB03333	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	S(=O)(=O)(N)c1ccc(cc1)NC(=S)OCCc1ccsc1
C3394	DB03335	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](O)CBr

C3395	DB03337	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=N)c1ccc(cc1)NC(=O)Nc1ccc(cc1)Oc1ccccc1
C3396	DB03346	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1cc(cc(Cl)c1O)c1cc(Cl)c(O)c(Cl)c1
C3397	DB03347	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	P(=O)(OCC)(OCC)OCC
C3398	DB03354	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1nnc(o1)[C@H]1O[C@@H](CO)[C@H](O)[C@@H](O)[C@@H]1O
C3399	DB03359	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[N+](C)(C)c1cccc(c1)C(O)(O)C(F)(F)F
C3400	DB03360	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N1CCC[C@@H]1C(=O)O
C3401	DB03367	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	s1c(cc(c1)c1ccc(cc1)c1ccncc1)C(=O)N[C@H](CC(=O)O)c1ccccc1
C3402	DB03369	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc2c(cc1)c1c(cc2N)cccc1
C3403	DB03371	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CC[C@@H](O)O[C@H]1O[C@H](CO)[C@@H](O)[C@@]1(O)F)C(=O)O
C3404	DB03376	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](N)C(=O)NS(=O)(=O)OC[C@@H]1O[C@H]([C@H](O)[C@H]1O)n1cnc2c1ncnc2N
C3405	DB03381	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCCCCCCCCCCCC=O
C3406	DB03382	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](C[S+]=O)C(=O)O
C3407	DB03384	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1cc2c(cc1)[nH]c(c2)C(=O)NCCS
C3408	DB03387	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)N(O)C(=O)C(=O)O
C3409	DB03391	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CSCC[C@@H](N)C1=N/C(=C\c2ccc(O)cc2)/C(=O)N1CC=O
C3410	DB03399	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC[N+]#C
C3411	DB03406	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CO[C@H]1O[C@@H](CO)[C@H](S)[C@@H](O)[C@@H]1O
C3412	DB03407	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc(cc1O)[N+](=O)[O-]
C3413	DB03410	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1cc(=O)c2ccccc2o1
C3414	DB03411	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1NC[C@H](O)[C@H]1O
C3415	DB03414	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H]1S[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O
C3416	DB03417	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)(C)NC(=O)N1CCN(CC1)C(=O)N[C@H]([C@@H](CCCNC(=N)N)C=O)C(=O)O
C3417	DB03420	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N[C@H]1[C@@H](C[C@@H](O[C@H]1[C@H](O)[C@@H](O)CO)C(=O)O)NC(=N)N
C3418	DB03423	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CC[Se]C[C@@H]1O[C@H]([C@H](O)[C@H]1O)n1cnc2c1ncnc2N)C(=O)O
C3419	DB03424	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)C[C@@H](NC(=O)[C@@H](O)[C@H](N)Cc1ccccc1)C(=O)O
C3420	DB03427	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCCC(=O)N[C@H](CS)C(=O)N[C@H](C=C)C(=O)O)C(=O)O
C3421	DB03437	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CO/N=C(/C(=O)N[C@H](C=O)[C@@H]1N[C@H](C(=O)O)C(C)(C)S1)\c1csc(N)n1
C3422	DB03438	DrugBank	noninhibitor	62	noninhibitor	inhibitor	noninhibitor	noninhibitor	CCCCCCCCCCCCCCCCC(=O)OC[C@H](O)COP(=O)([O-])OC[C@H](O)CO
C3423	DB03440	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(O)CNC(=O)CCCCCCCCCCCCCCC
C3424	DB03442	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1cc(ccc1n1nc(C)c(/N=N/c2cc(ccc2C(=O)O)S(=O)(=O)O)c1O)S(=O)(=O)O
C3425	DB03446	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@H]1(Oc2cccc(c2)C(=O)NCc2ccccc2)[C@@H](O)[C@@H](O)[C@@H](O)[C@@H](O1)CO
C3426	DB03450	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1CC(=C(C(=O)O)N[C@H]1[C@@H](C=O)NC(=O)Cc1cccs1)CC(=O)OC
C3427	DB03455	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(O)[C@H](NOCCS)c1c[nH]c2ccccc12
C3428	DB03458	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN(CC[C@H](N)C(=O)O)C[C@H]1O[C@H]([C@H](O)[C@@H]1O)n1cnc2c(N)ncnc12
C3429	DB03462	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1c[nH]c(=O)[nH]c1=O
C3430	DB03467	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(cc(c2c1O[C@@H](CC2=O)c1ccc(cc1)O)O)O
C3431	DB03468	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc2c1CCNC2)S(=O)(=O)N
C3432	DB03470	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCC(=O)N[C@H](CS)C(=O)NCC(=O)NCCCCNCCCNC(=O)CNC(=O)[C@H](CS)NC(=O)CC[C@@H](N)C(=O)O)C(=O)O
C3433	DB03471	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CC[C@H](CCc1ccccc1)NC(=O)CCCCCCc1ccccc1
C3434	DB03474	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc(Nc2cc(cc3c2c(O)c(/N=N/c2ccccc2S(=O)(=O)O)c(c3)S(=O)(=O)O)S(=O)(=O)O)nc(N)n1
C3435	DB03475	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c(cc(c1)C(=O)O)NC(CC)CC)N1C(CCC1=O)(CO)CO
C3436	DB03476	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc2c(cc1)cc(cc2)C(=N)N)[C@H]1[C@H](c2ccccc2)C1
C3437	DB03477	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c2ccc(cc2)Br)n(c2ccc(cc2)S(=O)(=O)N)nc1C(F)(F)F

C3438	DB03479	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN1C(=O)N[C@]2(O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)C1=O
C3439	DB03480	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1c(nc2ccc(F)cc2c1C(=O)O)c1ccc(cc1)c1ccccc1
C3440	DB03487	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H]1CC(=O)NC1=O
C3441	DB03490	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1nc2c(c1c1ccncc1)Cc1c2cccc1
C3442	DB03498	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[O-]P(=O)([O-])CS
C3443	DB03499	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H](CC(=O)O)C(=O)[O-]
C3444	DB03500	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCCCCCCCCCCCCCCCCCCCC(=O)O
C3445	DB03505	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(N)ccc2nc(N)nc(O)c2c1
C3446	DB03509	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc2c(c(c1)C(=O)N)nc(cn2)c1ccc(cc1)Cl
C3447	DB03515	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc2c(cc1)c1c(cc2)[C@H]2[C@](CC1)(C(=O)CC2)C)O
C3448	DB03518	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@](O)(CCO)CC(=O)[O-]
C3449	DB03520	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1nc(Cl)c2[nH]cnc2n1
C3450	DB03522	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CC(=O)OCC(=O)O)C(=O)O
C3451	DB03523	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1c(nc2ccc(F)cc2c1C(=O)O)c1ccc(cc1)c1ccccc1F
C3452	DB03526	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1(S(=O)(=O)N)ccc(s1)S(=O)(=O)NCc1ccc(cc1)OC
C3453	DB03533	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1N[C@H]2NC(=O)N[C@H]2N1
C3454	DB03536	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(N[C@@H](CCCNC(N)N)C(=O)N[C@@H](C)C(=O)C)OCc1ccccc1
C3455	DB03539	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1[C@H](O)[C@@H](O)[C@H]2N=C(O[C@@H]12)N=C
C3456	DB03540	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1C[C@@H]2CC[C@H]1C2
C3457	DB03541	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1c(N)nc(=O)c2cc(ccc12)CN(c1ccc(cc1)C(=O)N[C@@H](CCC(=O)O)C(=O)O)CC#C
C3458	DB03542	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1[C@H](O)[C@@H](O)[C@H](OP(=O)([O-])[O-])[C@@H](O)[C@@H]1O
C3459	DB03546	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H]1N[C@H](N)[C@@H](CCC[C@@H](c2ccc(cc2)C(=O)N[C@H](CCC(=O)O)C(=O)O)C(O)(O)C(F)(F)F)C(=O)N1
C3460	DB03548	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H](O)[C@@H]1O[C@](O)(C[C@H](O)[C@H]1O)C(=O)O
C3461	DB03549	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(CCCC[C@H]1[C@@H]2[C@H](CS1)NC(=O)N2)Nc1ccc(cc1)[N+](=O)[O-]
C3462	DB03550	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC1(C)S[C@H]2[C@H](NC(=O)CCC[C@H](N)C(=O)O)C(=O)N2[C@@H]1C(=O)O
C3463	DB03554	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Ic1c[nH]c(=O)[nH]c1=O
C3464	DB03558	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CCNC(=O)[C@@H]1CCCN1S(=O)(=O)c1ccc(cc1)C(=O)N[C@H](CCC(=O)O)C(=O)O
C3465	DB03564	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](O)CC(C)(C)O
C3466	DB03567	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N[C@H]1[C@H](O)O[C@H](CO)[C@H](O)[C@@H]1O
C3467	DB03569	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1OC(=C[C@H](O)[C@@H]1O)C(=O)O
C3468	DB03570	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[N+](CO)(CO)CO
C3469	DB03573	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(O)C[C@H](O)C(=O)N[C@H](CCc1ccccc1)C(=O)NCCC(C)C
C3470	DB03578	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)C(=O)N
C3471	DB03587	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)C=O
C3472	DB03589	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C(=O)C(=O)O
C3473	DB03596	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=O)NCC(CC)c1cc2cc[nH]c2cc1)S(=O)(=O)N
C3474	DB03597	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCC(=O)N[C@H](CSCc1ccccc1I)C(=O)NCC(=O)O)C(=O)O
C3475	DB03600	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(CCCCCCCCC)O
C3476	DB03601	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc(cc1)[C@@H]1CC(=O)c2ccc(O)cc2O1
C3477	DB03602	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCC(=O)N[C@H](CSCc1ccccc1)C(=O)NCC(=O)O)C(=O)O
C3478	DB03604	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)Cc1cc(I)c(Oc2ccc(O)c(I)c2)c(I)c1
C3479	DB03605	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[C@@H](Cc1ccccc1)N(Cc1cccc(c1)C(F)(F)F)C(=O)c1ccc(Cl)cc1Cl
C3480	DB03608	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(cc1)C(=N)N)N/N=N/c1ccc(cc1)C(=N)N

C3481	DB03609	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc2c(ncn2[C@H]2O[C@H](CO)C[C@@H]2O)c(=O)[nH]1
C3482	DB03615	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC[C@@H]1O[C@H](O[C@H]2[C@H](N)C[C@H](N[C@@H](O)[C@@H]2O[C@@H]2O[C@@H](CO)[C@H](O)[C@H]2O)[C@@H](N)[C@H](O)[C@H]1O
C3483	DB03623	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(ccnc1)ccc1c2cc(cn1)c1ccc(cc1)O
C3484	DB03624	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](N)[C@@H](CCCCCC(=O)O)NC(=O)O
C3485	DB03627	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1[C@H]2C[C@H]3C[C@@H]1C[C@@H](C2)C3
C3486	DB03630	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	SCc1ccccc1I
C3487	DB03631	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CC1=CC(=N)C(=CC1=O)O)C(=O)O
C3488	DB03635	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCS(=O)(=O)O
C3489	DB03636	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCC(=O)N
C3490	DB03651	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1c(cc(cc1[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]
C3491	DB03654	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@H](C=O)CSSCCC
C3492	DB03655	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCC(CC)[C@@H](NC(=O)C)[C@@H]1[C@@H](O)[C@@H](C[C@H]1NC(=N)N)C(=O)O
C3493	DB03659	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCN
C3494	DB03661	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CS(=O)(=O)O)C(=O)O
C3495	DB03667	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c(cccc1)O)C(=O)NOC(=O)C
C3496	DB03669	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCCc1ccc(F)cc1
C3497	DB03670	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C(=O)Nc1c(C(=O)O)c2c(CNCC2)s1
C3498	DB03671	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	C[C@]12CC[C@H](O)C[C@@H]1CC[C@@H]1[C@@H]2C[C@@H](O)[C@]2(C)[C@H](CC[C@@]12O)C1=CC(=O)OC1
C3499	DB03675	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC[C@](C)(O)[C@H](O)C(=O)O
C3500	DB03680	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(C(=O)[O-])C(=O)[O-]
C3501	DB03683	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C[C@H](CN(C=O)O)C(=O)O)C
C3502	DB03686	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCC(=O)N[C@H](CSCc1ccc(cc1)[N+](=O)[O-])C(=O)NCC(=O)O)C(=O)O
C3503	DB03691	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(O)C[C@H](O)C(=O)N[C@@H](CCc1ccccc1)C(=O)NCCC(C)C
C3504	DB03693	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1nccc2c(Cl)ccc(c12)S(=O)(=O)NCCN
C3505	DB03697	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCCCCNC(=O)c1ccc(cc1)S(=O)(=O)N
C3506	DB03704	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(CCCCCCCCCCC(=O)O)O
C3507	DB03706	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCC(=O)N[C@H](CS[C@H](CO)COc1ccc(cc1)[N+](=O)[O-])C(=O)NCC(=O)O)C(=O)O
C3508	DB03709	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCCN(CCO)CC(=O)O
C3509	DB03719	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCNC(=O)[C@@H]1O[C@H]([C@H](O)[C@H]1O)n1cnc2c1ncnc2N
C3510	DB03722	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1cccc2c1CCNC2=O
C3511	DB03727	DrugBank	noninhibitor	62	inhibitor	noninhibitor	inhibitor	inhibitor	Cc1c2Cc3[nH]c(Cc4[nH]c(Cc5[nH]c(Cc([nH]2)c1CCC(=O)O)c(C)c5CCC(=O)O)c(C)c4CCC(=O)O)c(C)c3CCC(=O)O
C3512	DB03729	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1[nH]c2ccc(O)cc2n1
C3513	DB03730	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cn1cnc2c1[n+](C)cnc2N
C3514	DB03733	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ClCCCl
C3515	DB03735	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1ncnc2c1ncn2[C@H]1C[C@@H](O)[C@H](CO)O1
C3516	DB03736	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](CC1CC1)C=O
C3517	DB03737	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1c(C#C[C@@H](O)[C@@H](N)[C@H](O)C)c2c(NC(=O)/C/2=C\c2c(OC)cc[nH]2)cc1
C3518	DB03739	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O/N=C/1\C[C@](O)(C[C@H](O)[C@H]1O)C(=O)O
C3519	DB03744	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(c1ccccc1)[C@@H](C(=O)N1CC(C(=O)O)C1)NC(=O)c1cc2c(ccc(Cl)c2)[nH]1
C3520	DB03746	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@H]1C=C(C[C@@H](O)[C@@H]1O)C(=O)[O-]
C3521	DB03747	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC1=N[C@H]2[C@H](O[C@@H](CO)[C@H](O)[C@H]2O)S1
C3522	DB03749	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1cc(O)c(CC)cc1c1n[nH]cc1c1c[nH]cn1
C3523	DB03756	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	CC/C=C/C/C=C/C/C=C/C/C=C/C/C=C/C/C=C/CCC(=O)O

C3524	DB03758	DrugBank	noninhibitor	62	noninhibitor	inhibitor	noninhibitor	noninhibitor	C1(=O)[C@@H]2C(=O)CC(=O)[C@H]([C@@H]2CC(=O)CCCC[C@@H]2[C@@H](C[C@@H](C)O1)O2)Cl
C3525	DB03760	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(O)CCCC[C@H](CCS)S
C3526	DB03763	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cn1cc([C@H]2C[C@@H](O)[C@H](CO)O2)c(=O)[nH]c1=O
C3527	DB03764	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1cc(OO)ccc1O
C3528	DB03775	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1(=O)N[C@@H]([C@@H](N1)C)CCCCCC(=O)O
C3529	DB03776	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](O)C=O
C3530	DB03780	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc2ccccc2c(=O)[nH]1
C3531	DB03781	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[C@@H](C)Oc1ccc(cc1)Oc1ccc(Cl)cc1Cl
C3532	DB03789	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cn1cc[nH+]c1C
C3533	DB03796	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCCCCCCCCCCCC(=O)O
C3534	DB03801	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCCCNC(=O)O)C(=O)O
C3535	DB03804	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@@H](n2cc(c(=O)[nH]c2=O)c2ccc(s2)Br)C[C@@H]1O
C3536	DB03808	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(cc1)OCCCCCCOc1ccc(cc1)C(=N)N)C(=N)N
C3537	DB03817	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCC[C@H](N)C(=O)O
C3538	DB03819	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ONC(=O)c1ccccc1O
C3539	DB03820	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC1(C)S[C@H]2[C@H](NC(=O)CCCC[C@@H](NC(=O)C[NH3+])C(=O)[O-])C(=O)N2[C@@H]1C(=O)[O-]
C3540	DB03823	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H]1Cc2c(O)cc(O)cc2O[C@H]1c1cc(O)c(O)c(O)c1
C3541	DB03835	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)NN1C(=O)N[C@]2(O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)C1=O
C3542	DB03842	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC1=CC=CC(=C)[C@H]1N
C3543	DB03844	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=O)NCc1c(cccc1F)F)S(=O)(=O)N
C3544	DB03845	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1cn([C@@H]2C[C@H](N=[N+]=[N-])[C@@H](COP(=O)([O-])OP(=O)([O-])OP(=O)([O-])OP(=O)([O-])OC[C@@H]3O[C@H]([C@H](O)[C@H]3O)n3cnc4c3ncnc4N)O2)c(=O)[nH]c1=O
C3545	DB03851	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CCCn1c2ccccc2c2c1cccc2
C3546	DB03856	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCCC[C@@](N)(C(F)F)C(=O)O
C3547	DB03858	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)CSC[C@H](N)C(=O)O
C3548	DB03859	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@@H](S)[C@H](O)[C@@H](O)[C@@H]1O
C3549	DB03861	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N[C@@H]1NC[C@@H](CO)[C@H](O)[C@H]1O
C3550	DB03864	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H](O)CS
C3551	DB03867	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](Cc1ccc(O)c(c1)[N+](=O)[O-])C(=O)O
C3552	DB03869	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@H](CO)C(=O)NS(=O)(=O)OC[C@@H]1O[C@H]([C@H](O)[C@H]1O)n1cnc2c1ncnc2N
C3553	DB03870	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1O[C@@H](O[C@@H]2[C@@H](O)CO[C@H](O)[C@H]2O)[C@H](O)[C@H]1O
C3554	DB03872	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@H]1O[C@H](O)CC[C@H]1O
C3555	DB03883	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H](O)[C@H](O)[C@@H](O)Cn1c(=O)c(CCC(=O)O)nc2c1[nH]c(=O)[nH]c2=O
C3556	DB03884	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(O)C(=O)Cc1ccccc1
C3557	DB03885	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCC(=O)N[C@H](CSCc1cccc2c1cccc2)C(=O)NCC(=O)O)C(=O)O
C3558	DB03886	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@H](O)[C@@H](O)c1cnc2nc(N)[nH]c(=O)c2n1
C3559	DB03889	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCC(=O)N[C@H](CS[C@H](O)N(O)c1ccc(Br)cc1)C(=O)NCC(=O)O)C(=O)O
C3560	DB03900	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)(C)O
C3561	DB03901	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C[C@H]1CCC(=O)N1
C3562	DB03910	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(Cc1cc(ccc1)CCSC(=N)N)SC(=N)N
C3563	DB03914	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](O)[C@@H](N)C1=N/C(=C\c2c[nH]c3ccccc23)/C(=O)N1CC=O
C3564	DB03919	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCNC(=O)OC
C3565	DB03920	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CNC(=C)C(=O)O
C3566	DB03924	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c2c(c(cc1)O)C(=O)c1c(C2=O)c(ccc1N)N)O

C3567	DB03927	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@H](NC(=O)CCCC[C@@H](NC(=O)C[NH3+])C(=O)[O-])C(=O)O
C3568	DB03938	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC1=C(N2[C@@H](SC1)[C@H](NC(=O)CCC[C@H](N)C(=O)O)C2=O)C(=O)O
C3569	DB03939	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1NC(=O)NC=C1
C3570	DB03941	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCCCc1ccc(O)cc1
C3571	DB03947	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H](O)[C@H](O)C(=O)CO
C3572	DB03962	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=O)c1ccc[n+](c1)[C@@H]1O[C@@H](COP(=O)([O-])OP(=O)(O)OC[C@@H]2O[C@H]([C@H](OP(=O)(O)O)[C@H]2O)n2c(Br)nc3c2ncnc3N)[C@H](O)[C@H]1O
C3573	DB03964	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H](C(=O)[O-])/C(=C/C(=O)[O-])/C(=O)[O-]
C3574	DB03972	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@H]1Oc2ccccc2[C@@H](O)S1
C3575	DB03977	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[N+](C)(C)CCCC[C@@H](N)C(=O)O
C3576	DB03989	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1O[C@H](O)[C@@H](O)[C@H](O)[C@H]1O
C3577	DB03991	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N[C@@H]1[C@@H](O)C=C(O[C@H]1[C@H](O)[C@@H](O)CO)C(=O)O
C3578	DB03995	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	[illegible]
C3579	DB03998	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCC1=N/C(=C\c2ccc(O)cc2)/C(=O)N1CC=O
C3580	DB04001	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12cc(c(cc1cc[nH]2)C(=O)O)NC(=O)C(=O)O
C3581	DB04002	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(cc1)S(=O)(=O)N)C(=O)NCCCCNCS
C3582	DB04010	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12nc([nH]c1cccc2C(=O)N)c1cc(OC)ccc1
C3583	DB04013	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COC(=O)N[C@]1(O[C@@H](CO)[C@H](O)[C@@H](O)[C@@H]1O)C(=O)N
C3584	DB04014	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1C(=O)Cc2c(c3c1cccc3)[nH]c1c2cc(cc1)[N+](=O)[O-]
C3585	DB04018	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)SC(=N)N
C3586	DB04028	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@H]1O[C@H](O)[C@@H](O)C[C@H]1O
C3587	DB04035	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	B(O)(O)CNC(=O)/C(=N\OC(C)(C)C(=O)O)/c1csc(N)n1
C3588	DB04039	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(CC(=O)CCCCCCCCCCCCC)O
C3589	DB04044	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc(c1C(=O)O)C(=O)O)Oc1c(cccc1)NC(=O)c1cc(ccc1)[N+](=O)[O-]
C3590	DB04046	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CO[C@@H]1O[C@H](CO)[C@H](O)[C@H](O)[C@H]1O
C3591	DB04049	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	Oc1ccc(CC(=O)Nc2ncc(nc2Cc2ccccc2)c2ccc(O)cc2)cc1
C3592	DB04050	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCC[N+]#[C-]
C3593	DB04065	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C=O)(C1CCCC1)C1CCC1
C3594	DB04069	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2CCc3ccccc3c2nnc1N
C3595	DB04074	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)C(=O)C(=O)O
C3596	DB04076	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=c1[nH]cnc2[nH]cnc12
C3597	DB04077	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCC(O)CO
C3598	DB04079	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCC[C@H](O)[C@@H](O)CO
C3599	DB04081	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	CN[C@@H]1C[C@H](C)S(=O)(=O)c2c1cc(s2)S(=O)(=O)N
C3600	DB04082	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(OCCCCCCCCCC)O
C3601	DB04084	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@@H](O)[C@H](F)[C@@H](O)[C@@H]1O
C3602	DB04089	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1(S(=O)(=O)N)cc2[C@@H](O)CN(Cc3cccs3)S(=O)(=O)c2s1
C3603	DB04091	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CO[C@H]1O[C@@H](C)[C@H](O)[C@@H](O)[C@@H]1O
C3604	DB04092	DrugBank	noninhibitor	62	inhibitor	inhibitor	noninhibitor	inhibitor	C[C@H](NC(=O)[C@@H]1CCCN1C(=O)[C@@H]1CCCN1C(=O)[C@@H](O)[C@H](N)Cc1ccccc1)C(=O)N
C3605	DB04093	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCCCCCCC=O
C3606	DB04094	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)CCO
C3607	DB04096	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1N[C@H](O)[C@@H](O)[C@H](O)[C@@H]1O[C@H]1O[C@@H](CO)[C@H](O)[C@@H](O)[C@@H]1O
C3608	DB04098	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)c1cccc(O)c1C(=O)c1c(O)cc(cc1O)C(=O)O[C@@H]1CCCNC[C@H]1NC(=O)c1ccc(O)cc1
C3609	DB04101	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1sc(c(n1)C)c1nc(ncc1)N/C=N\O

C3610	DB04102	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H]1[C@@H](O)[C@H](CO)O[C@H]1n1cnc2c1ncnc2N
C3611	DB04104	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cn1cnc(N)c2ncnc12
C3612	DB04108	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCSCC[C@@H]([C@@H](C(=O)N[C@H](c1cccc2c1cccc2)C)O)N
C3613	DB04111	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	CN[C@@H](CC(C)C)C(=O)N[C@H]1[C@@H](O)c2cc(Cl)c(Oc3c(O[C@H]4O[C@@H](CO)[C@@H](O)[C@@H](O)[C@@H]4O)c4cc(c3)[C@@H](NC(=O)[C@@H](CC(=O)N)NC1=O)C(=O)N[C@H]1C(=O)N[C@H]([C@@H](O[C@H]3C[C@](C)(N)C(=O)[C@H](C)O3)c3cc(Cl)c(O4)cc3)C(=O)N[C@H](C(=O)O)c3cc(c(O)cc(O)c3)c3c(O)ccc1c3)cc2
C3614	DB04113	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=CN1CCCCC1
C3615	DB04128	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H](O)[C@H](O)[C@@H](O)CNc1c(N=O)c(=O)[nH]c(=O)[nH]1
C3616	DB04130	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1ccc2[nH]cnc2c1
C3617	DB04132	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCCSC[C@@H](NC(=O)CC[C@H]([NH3+])C(=O)O)C(=O)NCC(=O)O
C3618	DB04133	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1CC(=C(C(=O)O)N[C@H]1[C@@H](C=O)NC(=O)Cc1cccs1)C
C3619	DB04147	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[N+]([O-])(C)(C)CCCCCCCCCCCC
C3620	DB04153	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCC(=O)N[C@H](CSCO)C(=O)NCC(=O)O)C(=O)O
C3621	DB04161	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCC(=O)N
C3622	DB04162	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H](O)[C@H](O)[C@@H](O)CNc1c(c(=O)[nH]c(=O)[nH]1)[N+](=O)[O-]
C3623	DB04163	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(nc(n1)N)N)c(ccc2)Sc1ccccc1
C3624	DB04165	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCC(CCC)C(=O)N
C3625	DB04168	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc(c(Br)c(O)n1)c1ccccc1
C3626	DB04169	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1cc(N)c2c(=O)[nH][nH]c(=O)c2c1
C3627	DB04173	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1O[C@@](O)(CO)[C@H](O)[C@H]1O
C3628	DB04174	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N[C@H]1[C@@H](O[C@H](CO)[C@H](O)[C@@H]1O[C@@](C)(OP(=O)(O)O)C(=O)O)OP(=O)(O)OP(=O)(O)OC[C@@H]1O[C@H]([C@H](O)[C@H]1O)n1ccc(=O)[nH]c1=O
C3629	DB04180	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=O)NCc1c(cc(cc1)F)F)S(=O)(=O)N
C3630	DB04181	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CO/N=C(/C(=O)N[C@H](C=O)[C@H]1NC(=C(CS1)CC(=O)OC)C(=O)O)\c1csc(N)n1
C3631	DB04182	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCSC[C@H](O)[C@H](O)C(=O)CO)C(=O)O
C3632	DB04187	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCC(=O)N[C@H](CS[C@H]1[C@H](O)c2ccccc2c2ccccc12)C(=O)NCC(=O)O)C(=O)O
C3633	DB04189	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=N)NCCC[C@@H](NCCC(=O)O)C(=O)O
C3634	DB04197	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N/C(=N\CCC[NH3+])/NO
C3635	DB04201	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ncnc2c1ncn2[C@@H]1O[C@@H](COP(=O)([O-])OC(=O)[C@H]([NH3+])Cc2c[nH]cn2)[C@H](O)[C@H]1O
C3636	DB04203	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1ccc(cc1[Hg])S(=O)(=O)N
C3637	DB04208	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(C(=O)O)Cc1cc(OC)c(cc1)OC
C3638	DB04211	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N[C@H]1[C@H](O)[C@@H](F)[C@@H](O[C@H]1[C@H](O)[C@@H](O)CO)C(=O)O
C3639	DB04221	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCCCCCC[N+](C)(C)CCCCCCCCCC
C3640	DB04222	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CSC[S@](=O)C[C@H](CO)NC(=O)/C=C/c1c(C)[nH]c(=O)[nH]c1=O
C3641	DB04224	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCCCC/C=C/CCCCCCCC(=O)O
C3642	DB04227	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N[C@@H]1[C@@H](O)C=C(O[C@H]1[C@H](O)[C@@H](O)CN)C(=O)O
C3643	DB04229	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CN(CCN(CC(=O)O)CC(=O)NCCS)CCN(CC(=O)O)CC(=O)NCCS
C3644	DB04237	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(CCO)(CCO)CCO
C3645	DB04250	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCC(=O)SCC[N+](C)(C)C
C3646	DB04253	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c(cc(c1[N+](=O)[O-])N1CC1)C(=O)N)[N+](=O)[O-]
C3647	DB04257	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCC/C=C/CCCCCCCC(=O)O
C3648	DB04262	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H](O)[C@H](O)[C@@H](O)Cn1c(O)c(CCC(=O)O)nc2c(=O)[nH]c(=O)nc12
C3649	DB04265	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N[C@H]1[C@H](O)C[C@](O)(O[C@@H]1[C@@H](O)[C@@H](O)CO)C(=O)O
C3650	DB04274	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc2C(=O)C[C@H](Oc2c1)c1ccccc1
C3651	DB04281	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	O=C1/C(=C\2/CCC(CC2)c2ccc(Cl)cc2)/C(=C(O)c2ccccc12)O
C3652	DB04283	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1nc(Br)nc2[nH]cnc12

C3653	DB04284	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[N+]1(C)CCC[C@@H]1C(=O)O
C3654	DB04287	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CC[C@H](Cc1ccc(OCc2ccccc2)cc1)NC(=O)CCCCCCc1ccccc1
C3655	DB04293	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](C(=O)N[C@@H]1[C@H]2CCC(=C(N2C1=O)C(=O)O)Cl)c1ccccc1
C3656	DB04300	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1[C@H](OP(=O)(O)O)[C@@H](OP(=O)(O)O)[C@H](O)[C@@H](OP(=O)(O)O)[C@@H]1OP(=O)(O)O
C3657	DB04303	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CO[C@H]1[C@H](O)[C@@H](O)[C@H](O)O[C@@H]1C(=O)O
C3658	DB04306	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(c(nc(n1)N)N)c(ccc2)Sc1ccc(cc1)C
C3659	DB04312	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCc1cccc(F)c1F
C3660	DB04318	DrugBank	noninhibitor	62	inhibitor	noninhibitor	inhibitor	inhibitor	NC(=O)[C@@H](Cc1c[nH]c2ccccc12)NC(=O)[C@@H](CCCc1ccccc1)C[P@](=O)(O)[C@@H](Cc1ccccc1)NC(=O)OCc1ccccc1
C3661	DB04320	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCC(=C)Br
C3662	DB04323	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CS[C@@H]1C[C@@H](ON1)[C@@H](N)C(=O)O)C(=O)O
C3663	DB04325	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[NH3+]CCc1ccccc1
C3664	DB04330	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1ccc2C(=O)[C@]3(O[C@@H]([C@H]([C@@H]3C(=O)O)C(=O)Nc3ccc(cc3)c3csnn3)c3ccc(Cl)c(Cl)c3)C(=O)c2c1
C3665	DB04334	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CC1=CC(=O)C(=CC1=O)O)C(=O)O
C3666	DB04336	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N=C(N)c1ccc(cc1)NC(=O)Nc1ccc(cc1)Cl
C3667	DB04340	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[O-]C(=O)c1ccccc1OP(=O)[O-]
C3668	DB04341	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCC(=O)N[C@H](CSCc1cccc(I)c1)C(=O)NCC(=O)O)C(=O)O
C3669	DB04345	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1c(=O)[nH]c(=O)c2c1nc1c(n2)cc(C)c(C)c1
C3670	DB04346	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@]1(O)OC[C@@H](O)C1(O)O
C3671	DB04349	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](O)CO
C3672	DB04350	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N/C(=N/CCC[C@@H]1NC(=O)[C@H](CCCC(=O)O)NC(=O)[C@H](Cc2cnc[nH]2)N2[C@H](O)C[C@H](NC(=O)[C@H]3CCCN3C1=O)C2=O)/N
C3673	DB04351	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[O-]C(=O)C/C(=C/C(=O)[O-])/C(=O)[O-]
C3674	DB04359	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OS(=O)(=O)C=C
C3675	DB04361	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN=N
C3676	DB04362	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1c(CCO[P@](=O)([O-])O[P@](=O)([O-])OC[C@H]2O[C@@H]([C@@H](O)[C@@H]2O)n2cnc3c2ncnc3N)sc(n1)C(=O)[O-]
C3677	DB04363	DrugBank	noninhibitor	62	inhibitor	noninhibitor	inhibitor	inhibitor	CCC1=C(C)C(=O)N/C/1=C/C1=N/C(=C\c2[nH]c(/C=C/3\NC(=O)C(=C3CC)C)c(CCC(=O)O)c2C)/C(=C1CCC(=O)O)C
C3678	DB04367	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC1=N/C(=C/2\CCNC(=O)c3[nH]ccc23)/C(=O)N1
C3679	DB04369	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OB1OCCO1
C3680	DB04374	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1nnc(c1SC(CCCCC)CCCCC)C(=O)O
C3681	DB04375	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN1[C@H](CNc2ccc(cc2)C(=O)N[C@H](CCC(=O)O)C(=O)O)CNc2c1c(=O)[nH]c(N)n2
C3682	DB04377	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(O)(CC(=O)O)CC(=O)O
C3683	DB04382	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1O[C@H](O)C[C@H](O)[C@H]1O
C3684	DB04385	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1cc(=O)n(cc1)[C@@H]1O[C@@H](CO)[C@H](O)[C@H]1O
C3685	DB04386	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@]1(OC[C@H]2O[C@@H](O)[C@H](O)[C@@H](O)[C@H]2O1)C(=O)O
C3686	DB04393	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(ccc(c1O)Oc1ccc(cc1)Cl)Cl
C3687	DB04394	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(c1ccc(N2C(=O)CCC2)c([N+](=O)[O-])c1)N
C3688	DB04396	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@@H](S[C@H]2O[C@@H](CO)[C@H](O)[C@@H](O)[C@@H]2O)[C@H](O)[C@@H](O)[C@@H]1O
C3689	DB04401	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[N+](C)(C)CC=O
C3690	DB04404	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN(C)C1=N[C@@H]2[C@@H](O)[C@@H](O)[C@H](CO)[C@@H]2O1
C3691	DB04409	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc(cc2cc(ccc12)S(=O)(=O)[O-])S(=O)(=O)[O-])S(=O)(=O)[O-]
C3692	DB04410	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[NH3+]CCCc1ccccc1
C3693	DB04426	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CO[C@H]1O[C@@H](CO)[C@H](O)[C@@H](O)[C@@H]1NC(=O)C
C3694	DB04429	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc(cc1)[C@@H]1CC(=O)c2ccccc2O1
C3695	DB04431	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	CN[N+]([O-])(=O)c1cc(c(c(c1[N+]([O-])(=O)=O)N(C)C)[N+]([O-])(=O)=O)[N+]([O-])(=O)=O

C3696	DB04432	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(F)c(c(F)c([nH+]c1Oc1cc(ccc1)C(=N)N)Oc1cccc(c1)C(=N)N)C
C3697	DB04437	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CSCC(=O)Nc1cc2c(nccc2)c2c1cccn2)C(=O)O
C3698	DB04440	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H]1O[C@H]([C@H](O)[C@H]1O)n1c[nH+]c2c1ncnc2
C3699	DB04441	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc(F)nc2c1ncn2[C@@H]1O[C@@H](CO)[C@H](O)[C@H]1O
C3700	DB04448	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCc1ccc(F)cc1F
C3701	DB04449	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1cc(cc(O)c1O)/C=C/C(O)O
C3702	DB04450	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@H]1(SCCCCCCC)[C@H](O)[C@@H](O)[C@H](O)[C@H](O1)CO
C3703	DB04451	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN1CCN(CC1)C=O
C3704	DB04452	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1c2c(N)cc(C)nc2ccc1NC(=O)Nc1cc2c(N)cc(C)nc2cc1
C3705	DB04458	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](NC(=O)[C@@]1([C@H](C)C1(Cl)Cl)[S@@](=O)C)c1ccc(Br)cc1
C3706	DB04459	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c(Cl)c2ccccc2c(=O)o1
C3707	DB04461	DrugBank	noninhibitor	62	inhibitor	noninhibitor	inhibitor	inhibitor	Cc1c2Cc3[nH]c(Cc4[nH]c(Cc5[nH]c(Cc([nH]2)c1CCC(=O)O)c(C)c5CCC(=O)O)c(C)c4CCC(=O)O)c(CCC(=O)O)c3C
C3708	DB04462	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Brc1c(Br)c(Br)c2[nH]nnc2c1Br
C3709	DB04471	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	Oc1ccc2[C@H](N(CCc2c1)c1ccccc1)c1ccc(OCCN2CCCCC2)cc1
C3710	DB04472	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C([C@H](O)c1ccc(cc1)[N+](=O)[O-])N=[N+]=[N-]
C3711	DB04474	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cccc2cccc(S(=O)(=O)O)c12)Nc1ccccc1
C3712	DB04485	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1cn([C@H]2C[C@@H](O)[C@H](CO)O2)c(=O)[nH]c1=O
C3713	DB04486	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCCCCCC[C@H](N)C(=O)O
C3714	DB04488	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)OC[C@@H]1CS[C@H]2[C@H](NC(=O)CCCC[C@@H](NC(=O)C[NH3+])C(=O)[O-])C(=O)N2[C@H]1C(=O)[O-]
C3715	DB04489	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=N)NCCS[C@@H](CC(=O)O)C(=O)O
C3716	DB04491	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)OP(=O)OC(C)C
C3717	DB04503	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1CN([C@H](C1)C(=O)O)S(=O)(=O)c1ccc(cc1)C(=O)N[C@@H](CCC(=O)O)C(=O)O
C3718	DB04508	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CO[C@H]1O[C@@H](C=S)[C@H](O)[C@@H](O)[C@@H]1O
C3719	DB04509	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	C[N@+]1(CC[C@]23[C@H]4Oc5c(O)ccc(C[C@@H]1[C@]2(O)CCC4=O)c35)CC=C
C3720	DB04511	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CCC(=O)N[C@@H](C(=O)O)CCSC
C3721	DB04512	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1c(c(ncc1)OC)CC(C)C
C3722	DB04515	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CO[C@H]1[C@@H](O)O[C@@H](C)[C@H](O)[C@H]1O
C3723	DB04517	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC1=N[C@H](CC2=NCC(=C2CC(=O)O)CCC(=O)O)C(=C1CC(=O)O)CCC(=O)O
C3724	DB04519	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCCCC(=O)O
C3725	DB04521	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCC[C@H]1O[C@@H](O)C[C@@H]1SC[C@@H](NC(=O)CC[C@H](N)C(=O)O)C(=O)NCC(=O)O
C3726	DB04526	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H](O)[C@@H]1O[C@H](O)[C@@H](O)[C@H](O)[C@H]1O
C3727	DB04528	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc(cc1[N+](=O)[O-])[N+](=O)[O-]
C3728	DB04529	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	CN[C@H](C(C)C)C(=O)N[C@@H](C)[C@H](O)c1ccc(cc1)S(=O)(=O)Nc1ccccc1C[C@@H](C(=O)N[C@@H](CC(=O)O)C(=O)O)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H](CC(=O)N)NC(=O)c1ccc(cc1)c1ccccc1)CCC(=O)O)C(C)C
C3729	DB04532	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2[nH]ccc2c1
C3730	DB04543	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(CSc2ncc[nH]2)c2nc(N)[nH]c(=O)c2cc1N
C3731	DB04544	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N[C@@]1(O[C@@H](CO)[C@H](O)[C@@H](O)[C@@H]1O)C(=O)N
C3732	DB04545	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1CNC[C@@H](O)[C@@H]1O
C3733	DB04549	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=O)NCc1c(c(c(cc1)F)F)F)S(=O)(=O)N
C3734	DB04553	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCC(=O)C(=O)O
C3735	DB04556	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1[C@@H](N(C)C)C)O
C3736	DB04557	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCC/C=C/C/C=C/C/C=C/C/C=C/CCCC(=O)O
C3737	DB04559	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1ccc(cc1)NC(=N)NO
C3738	DB04560	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(CCC(=O)CCC(=O)CCC(=O)O)O

C3739	DB04564	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1OC(=O)[C@H](O)[C@@H](O)[C@@H]1O
C3740	DB04565	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)Nc1ccc(cc1NC(=O)CO)C(=O)O
C3741	DB04567	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@H](O)[C@@H](N)C1=N/C(=C\c2ccc(O)cc2)/C(=O)N1CC=O
C3742	DB04569	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=COCc1ccccc1
C3743	DB04580	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cn1c(=O)ccc2ccccc12
C3744	DB04588	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c(cc(O)c(c1)c1[nH]ncc1C(=O)NCc1ccc(cc1)S(=O)(=O)N)O
C3745	DB04591	DrugBank	inhibitor	62	noninhibitor	inhibitor	noninhibitor	noninhibitor	C1CN[C@H](CC1)C(F)(F)CNc1c2c(ccn1)oc(n2)Cc1ccccc1n1ncnc1
C3746	DB04592	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCCC(=C)Br
C3747	DB04593	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N=C(N)CC[C@H](NC(=O)[C@H](NS(=O)(=O)Cc1cc(ccc1)C(=O)O)[C@H](C)CC)C(=O)NCc1ccc(cc1)C(=N)N
C3748	DB04596	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@]1(OC[C@H]2O[C@@H](O[C@H]3[C@H](O)[C@@H](O)[C@H](O)O[C@@H]3C(=O)O)[C@@H](O)[C@@H](O)[C@@H]2O1)C(=O)O
C3749	DB04597	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@]1(OC[C@H]2O[C@@H](O)[C@@H](O)[C@@H](O)[C@@H]2O1)C(=O)O
C3750	DB04599	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1N(CCC1)C(=O)c1ccc(OC)cc1
C3751	DB04604	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@@H](n2cc(c3c(ncnc23)N)I)[C@H](O)[C@@H]1O
C3752	DB04605	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1cccc2c1ccnc2
C3753	DB04608	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc2c(c1)c1c([nH]2)cc(c2c1c(=O)[nH]c2=O)c1ccccc1
C3754	DB04610	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1c(=O)c2N=C(CO)[C@@](CCc3ccccc3)(C)Nc2nc1N
C3755	DB04619	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)c1ccccc1
C3756	DB04622	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)NCCc1cnc[nH]1
C3757	DB04624	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1c2c(O)c(c(cc2C(=O)c2c1c(O)ccc2)CC(=O)OC)[C@H](O)C[C@@H](O)CC
C3758	DB04626	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN[C@H]1[C@@H](O)[C@H]2O[C@@H](O[C@H]3[C@@H](N)C[C@@H](N)[C@H](O)[C@@H]3O)[C@@H](N)C[C@@H]2O[C@@H]1O[C@H]1O[C@H](CO)[C@@H](N)[C@H](O)[C@@H]1O
C3759	DB04627	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@@H]2[C@@H](Oc3nc(=O)ccn23)[C@@H]1O
C3760	DB04634	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[C@H](C)NC(=O)OCc1ccccc1
C3761	DB04637	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCCCCCCBr
C3762	DB04638	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1c(cc(O)c(c1)C(C)(C)C)C(C)(C)C
C3763	DB04640	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=S(=O)(O)c1ccc2cc(ccc2c1)S(=O)(=O)O
C3764	DB04643	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(Cl)cc1Cl)C(=O)NC(=O)Nc1ccc(OCCCC(=O)O)cc1Cl
C3765	DB04644	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(Cl)cc1Cl)C(=O)NC(=O)Nc1ccc(OCCCC(=O)O)c(c1C)C
C3766	DB04645	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(Cl)cc1Cl)C(=O)NC(=O)Nc1cccc(OCCCCC(=O)O)c1C
C3767	DB04648	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCCCSC[C@H](N)CO
C3768	DB04654	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=CCCCC1CCNCC1
C3769	DB04655	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1c(nc(c(c1C)c1cc(c(cc1)Cl)Cl)N)N
C3770	DB04665	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=c1oc2ccccc2cc1
C3771	DB04676	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN(C)c1cccc2c1cccc2S(=O)(=O)NCCCC[C@H](N)C(=O)O
C3772	DB04677	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C=CCN(C)[C@H](C)Cc1ccccc1
C3773	DB04687	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COP(=S)(O)OC
C3774	DB04694	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@@H](O)[C@@H](O)[C@@H]1O[C@@H]([C@H](F)[C@H](O)[C@H]1O)C(=O)O
C3775	DB04698	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=S(=O)(N=c1[nH]nn[nH]1)c1cc2c(cc1)oc1ccccc1c2=O
C3776	DB04700	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCC(=O)N[C@@H](CS(=O)O)C(=O)NCC(=O)O)C(=O)O
C3777	DB04701	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CSC[C@H](NC(=O)CC[C@H](N)C(=O)O)C(=O)NCC(=O)O
C3778	DB04723	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NC(=Nc1cccc(c1)[C@@H](CS)C(=O)O)N
C3779	DB04746	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCC/C=C\C=C\CCCCCCCCC(=O)O
C3780	DB04747	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC/C=C\C=C\C=C\CCCCCCCCCC(=O)O
C3781	DB04749	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	SCCC(=O)SCCC=O

C3782	DB04750	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)c1cc(C(=O)O)c(cc1)c1c2cc(F)c(=O)cc2oc2cc(O)c(F)cc12
C3783	DB04756	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1c(OOO)c(Cl)cc(c1)Nc1ccccc1C(=O)O
C3784	DB04758	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N=C(N)c1ccc(CNC(=O)[C@H](CCC(=O)N)NC(=O)[C@@H](Cc2c[nH]c3ccccc23)NS(=O)(=O)CC)cc1
C3785	DB04761	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc(C(=O)NCc2cccnc2)ncn1)C(=O)NCc1cnccc1
C3786	DB04767	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N=C(N)c1ccc(CNC(=O)[C@H](CCSC)NC(=O)[C@H](NS(=O)(=O)CCC)[C@H](C)O)cc1
C3787	DB04776	DrugBank	noninhibitor	62	noninhibitor	inhibitor	noninhibitor	noninhibitor	OC[C@@H](CC)Nc1nc2n(C(C)C)cnc2c(n1)N(Cc1ccccc1)C
C3788	DB04777	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[O-][N+](=O)c1ccc(cc1)[C@@H]1CO1
C3789	DB04778	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@@H](N[C@@H](NCC(O)O)Nc1ccc(CN)cc1)c1ccccc1
C3790	DB04782	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[O-][N+](=O)c1ccc(cc1)[C@H]1CO1
C3791	DB04789	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN1[C@@H](CNc2ccc(cc2)C(=O)N[C@@H](CCC(=O)O)C(=O)O)CNc2c1c(=O)nc(N)[nH]2
C3792	DB04790	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N=C(N)c1cccc(O[C@@H]2CO[C@@H]3[C@@H](Oc4cccc(C(=N)N)c4)CO[C@H]23)c1
C3793	DB04791	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N=C(c1ccc(cc1)O[C@H]1CO[C@H]2[C@@H]1OC[C@H]2Oc1cccc(c1)C(=N)N)N
C3794	DB04792	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N=C(N)c1ccc(O[C@@H]2CO[C@@H]3[C@@H](Oc4ccc(C(=N)N)cc4)CO[C@H]23)cc1
C3795	DB04793	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(O[C@@H]2CO[C@@H]3[C@@H](Oc4cccc(C(=N)N)c4)CO[C@H]23)cc1)C(=N)N
C3796	DB04799	DrugBank	noninhibitor	62	noninhibitor	inhibitor	inhibitor	inhibitor	c1nc2c(C(=O)C(=C(C2=O)CCCCCCCCCCC)O)s1
C3797	DB04800	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cn1nc(cc1NS(=O)(=O)O)c1ccccc1
C3798	DB04801	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCC/C=C\CCCCCCCCCC(=O)O
C3799	DB04806	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H]1O[C@H](Oc2c[nH]c3c2c(Cl)c(Br)cc3)[C@@H](O)[C@@H](O)[C@@H]1O
C3800	DB06832	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c2c(cc1O)nc(o2)c1ccc(c(c1)F)O)C=C
C3801	DB06836	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=S(=O)(NCCO)c1c(Cl)ccc(c1)c1c(C)[nH]/c(=N/C(=O)C)/s1
C3802	DB06837	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cccc2c1C[C@H]([C@H]2NC(=O)[C@H](Cc1cccc(c1)O)CC(=O)NO)O
C3803	DB06839	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCOC(=O)N[C@H](C(=O)O)CC(C)C
C3804	DB06840	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CCCCN)B(OCC)OCC
C3805	DB06842	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCOc1c(OC)ccc(C[C@H]2NC(=O)NC2)c1
C3806	DB06857	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c(Cl)cc(cc1)NC(=O)c1cc(C)cc(I)c1O)C(=N)N
C3807	DB06861	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(CCCC(=N)N)[C@H]([C@H]1CCC[C@@H]1O)C=O
C3808	DB06862	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)c1c(ccc(c1)S(=O)(=O)NCCS)O
C3809	DB06864	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(O)[C@H]1[C@@H](C=CC=C1C(=O)CCC(=O)O)O
C3810	DB06865	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(CCCC(=N)N)C([C@H]1c2c(C[C@@H]1O)ccc(c2)c1ccc(cc1)O)C(=O)O
C3811	DB06866	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(CCCC(=N)N)C([C@H]1c2c(C[C@@H]1O)cc(cc2)c1cc(ccc1)OC)C(=O)O
C3812	DB06871	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C[C@]12CCc3c4ccc(O)cc4ccc3[C@@H]1CC[C@@]2(C)O
C3813	DB06875	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c(cc(cc1)c1cc2c(c(c1)C#N)cc(cc2)O)F)O
C3814	DB06877	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CN(C)C(=O)c1cc(c[nH]1)c1n[nH]cc1c1ccccc1
C3815	DB06884	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(Cc1ccc(cc1)C(C)C)NC(=O)c1ccc(cc1)O
C3816	DB06890	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(C(CC)c1ccccc1)Nc1ccncc1
C3817	DB06891	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(N)c1nnc(s1)NS(=O)(=O)c1cc(c(c(c1)Cl)N)F
C3818	DB06893	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=S(=O)(O)CCCCCCCCCC
C3819	DB06894	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OCCCCCCCCCCCC
C3820	DB06902	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc(cc1)C(C)(C)c1ccccc1
C3821	DB06907	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(cc(c1)C(=O)O)oc(c1c(cccc1Cl)Cl)n2
C3822	DB06912	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=CCCC/C=C(\CC/C=C(\CCC=O)/C=O)/C=O
C3823	DB06913	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(cc(cc1C(F)(F)F)N[C@@H](C(C(=O)N)C#N)S)C(F)(F)F
C3824	DB06917	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1ccc(cc1)C(=O)c1ccncc1

C3825	DB06922	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	c12ccccc1cccc2CC(C(=O)O)N1C(=O)c2cc(C(=O)O)ccc2C1=O
C3826	DB06924	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccccc1C[C@@H](C(=O)O)C[N+](=O)[O-]
C3827	DB06929	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1([C@H](C(=O)NCc2ccc(C(=N)N)cc2)CCC1)C(=O)CCC
C3828	DB06934	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccccc1[C@H](O)CCCl
C3829	DB06935	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(O)c1ccc(cc1)c1c(F)cccc1F
C3830	DB06937	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc2c(cc1)c(no2)c1c(cc(cc1)O)O)O
C3831	DB06947	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1([C@H](C(=O)NCc2ccc(C(=N)N)cc2)CCC1)C(=O)[C@H](N)CC
C3832	DB06949	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1c2ccccc2ccc1C(=O)N/N=C/c1cc(Br)c(O)c(Br)c1O
C3833	DB06950	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(Cl)ccc1C(=O)N/N=C/c1cc(Br)c(O)c(Br)c1O
C3834	DB06952	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[C@@]1(O)Oc2c(C=C1)cccc2
C3835	DB06956	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(C)c1ccc(cc1)NC(=O)c1cn[nH]c1c1cc(Cl)c(O)cc1O
C3836	DB06972	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	[C@]12(CCCN2C(=O)C(=C1C#N)c1cc(cc(c1)Cl)Cl)Cc1ccc(cc1)C#N
C3837	DB06973	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc(cc1)C(C)(C)c1ccc(cc1)O
C3838	DB06976	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12[C@H]3N(C(=O)c1cccc2NC(=O)Nc1cc([nH]n1)[C@@H]1CCCN1)CCC3
C3839	DB06978	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1ccc(cc1)C(=O)N/N=C/c1cc(Br)c(O)c(Br)c1O
C3840	DB06979	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCCCCCCCCSc1[nH]nnc1C(=O)O
C3841	DB06980	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[C@@H](CCCC)c1c2ccccc2[nH]c1
C3842	DB06981	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C(CCC)c1c2ccccc2[nH]c1
C3843	DB06990	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc(=O)[nH]c(=O)[nH]1)/C=N/OCCO/N=C/c1ccc(C(=O)O)cc1
C3844	DB06993	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@H]([C@@H](C(=O)N1C[C@H](CC1)F)N)(CC1CC1)[C@@H]1N[C@H](NO1)c1ccc(cc1F)S(=O)(=O)C
C3845	DB06994	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C([C@@H](C(=C1CCCC1)F)N)(CC1CC1)c1nc(no1)c1ccc(cc1Cl)S(=O)(=O)C
C3846	DB06998	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(CN1C(=S)S[C@H](Cc2cc(OCC)c(c(Br)c2Br)O)C1=O)O
C3847	DB07003	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2O[C@@H](C)CN=C(N)c2sc1
C3848	DB07009	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc2c(cc1)nc(o2)c1c2c(ccc1)c(ccc2)O)O
C3849	DB07010	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cccc(c1)c1c[nH]nc1c1c[nH]c(c1)C(=O)NCc1ccccc1)Cl
C3850	DB07011	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	c1c2OCOc2ccc1CN1C[C@H](CCC1)Oc1ccc(cc1)n1ccnc1
C3851	DB07012	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1c[nH]c2cc3nc(N)[nH]c(=O)c3cc12
C3852	DB07023	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(cc1)C(CNC(=N)N)OC(=O)c1cccnc1)B1OC[C@H](O1)CO
C3853	DB07033	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1(=O)C(=c2c(=N1)ccc(c2)O)[C@@H](C)c1ccc[nH]1
C3854	DB07037	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccnc2c(NC[C@H](CN)O)ccc(c12)[N+](=O)[O-]
C3855	DB07038	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1CCCCC1Nc1ccccc1C(=O)O
C3856	DB07044	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1c(Br)cccc1C(=O)N/N=C/c1cc(Br)c(O)c(Br)c1O
C3857	DB07045	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(Cl)c(Cl)ccc1CNc1nc2c(N)ncnc2n1[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O
C3858	DB07050	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccccc1S(=O)(=O)Nc1sc(nn1)S(=O)(=O)N
C3859	DB07052	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCSC[C@H]1O[C@H]([C@@H]([C@@H]1O)O)n1cnc2c1ncnc2N
C3860	DB07055	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1c2ccccc2C(=O)N1CCc1nnn[nH]1
C3861	DB07057	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1C[C@@H](CN1c1c(O)cccc1)C(=O)O
C3862	DB07066	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1cc2cc([nH]c2s1)C(=O)N[C@@H]1Cc2ccccc2NC1=O
C3863	DB07067	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@H](C(=O)N1CCCC1)([C@@H](c1nc(c2ccc(cc2)S(=O)(=O)C)no1)C)N
C3864	DB07071	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(cc1)B1O[C@@H](CO1)CO)CCNC(=N)N
C3865	DB07076	DrugBank	noninhibitor	62	inhibitor	noninhibitor	inhibitor	inhibitor	N=C(N)c1cc2ccc(cc2cc1)C(=O)Nc1cccc(OC2CCCC2)c1
C3866	DB07077	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(cc1)B1O[C@@H](CO1)CO)NC(=N)N
C3867	DB07093	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12nc(Cn3c(=O)n(CC(=O)O)ccc3=O)sc1ccc(Cl)c2

C3868	DB07094	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCc1sc(cc1)c1sccc1
C3869	DB07095	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	O=C(NCc1ccc(C(=N)N)cc1)[C@@H]1CCCN1C(=O)CCC1CCCC1
C3870	DB07098	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(Br)ccc1C(=O)N/N=C/c1cc(Br)c(O)c(Br)c1O
C3871	DB07099	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccccc1COc1ccc(cc1)NC(=O)CN
C3872	DB07102	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccccc1COc1ccc(cc1)NC(=O)CC[C@@H](C(=O)O)N
C3873	DB07106	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=N)(SCCCCN(C)C)N
C3874	DB07109	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1ccc(cc1O)/C=C/C(=O)O
C3875	DB07111	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CC[C@@H](/C=C/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CC)O
C3876	DB07115	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(Cl)ccc1CN(C)S(=O)(=O)c1ccc(cc1)S(=O)(=O)N
C3877	DB07118	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc2oc(=O)cc(C)c12)O
C3878	DB07119	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c(c2c(cc1)cc(cc2)c1ccc(cc1)O)Cl)O
C3879	DB07125	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(C(=O)O)ccc1c1cnc2ccc(nn12)N[C@H](CC)CO
C3880	DB07127	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=S(=O)(O)Nc1ccc(cc1)CC(c1noc(C)n1)(c1noc(C)n1)Cc1ccccc1
C3881	DB07134	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)c1c(c(N2CC(=O)NS2(=O)=O)cs1)Cl
C3882	DB07139	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c2sc(CCC(=O)O)cc2)cccc1[N+](=O)[O-]
C3883	DB07146	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	c1nc2c(c(c1)NCCN1CCNCC1)c(c(o2)c1ccccc1)c1ccccc1
C3884	DB07148	DrugBank	inhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1nc(c(=O)n2c1C=C[C@H]2C(=O)N1CCCC1)OCc1ccc(cc1)F
C3885	DB07150	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2c(c1)c(ccc2c1ccc(cc1)O)/C=N/O
C3886	DB07151	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1N=C(c2cc(C)c(O)cc2)CC(=N1)c1ccccc1
C3887	DB07156	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	c1cc(ccc1CN1CCCC1)N/C=C\1/c2cc(ccc2C(=O)NC1=O)Br
C3888	DB07161	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12cc(ccc2[nH]nc1N)c1ccccc1
C3889	DB07163	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCCNc1cc(c2ccc[nH]2)c2c(=O)[nH]c3ccc(F)c1c23
C3890	DB07168	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc(nc(n1)Nc1ccc(cc1)CC#N)NC)Nc1cc(C2CC2)[nH]n1
C3891	DB07169	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(NN1C(=S)S[C@H](Cc2ccc(c(c2)Cl)Cl)C1=O)c1sccc1
C3892	DB07170	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1[C@H](O)[C@@H](CF)O[C@H]1n1cnc2c1ncnc2N
C3893	DB07171	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(CCO)CC(CCCCO)CCO
C3894	DB07172	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC/C=C\C/C=C\C/C=C\C/C=C\C=C\[C@@H](CCCC(=O)O)O
C3895	DB07173	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1c(c2c(nc1)n(cc2I)[C@H]1[C@@H]([C@@H]([C@H](O1)C)O)O)N
C3896	DB07176	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2c(c1S(=O)(=O)O)cccc2N
C3897	DB07177	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCC(=O)/C=C/[C@@H]1[C@H](O)CC(=O)[C@H]1C/C=C/CCCC(=O)O
C3898	DB07187	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(S(=O)(=O)c2oc3ccc(Cl)cc3c2C)n[nH]c(=O)c1
C3899	DB07193	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1cc(F)c(cc1F)[C@H]1Cc2n(C[C@@H]1N)c1ccc(cc1n2)S(=O)(=O)C
C3900	DB07207	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc2c(c1)nc([nH]2)c1c(O)c([nH]n1)c1ccccc1)C(=N)N
C3901	DB07212	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12ccc(cc1c(ccc2)NC(=O)c1cccc(c1C)O)C(=N)N
C3902	DB07226	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1ccccc1c1c2c(=O)[nH]c(=O)c2c2c(c1)[nH]c1c2cc(cc1)NC=O
C3903	DB07227	DrugBank	inhibitor	62	inhibitor	inhibitor	noninhibitor	inhibitor	N1(CCN(C(=O)C1)c1cc(ccc1)Cl)Cc1n(Cc2ccc(cc2)C#N)cnc1
C3904	DB07230	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc2c(cc1)C(=C(C2=O)c1ccc(cc1)O)Br)O
C3905	DB07231	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(Cc1ccccc1)C(=O)[C@H]1O[C@@H]1C(=O)N[C@H](C(=O)N1[C@H](C(=O)O)CCC1)[C@H](CC)C
C3906	DB07232	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c(cccc1nc([C@]1(CCCN1C)C)[nH]2)C(=O)N
C3907	DB07233	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(cc(c1)C)c(c[nH]2)C[C@H](C(=O)O)NS(=O)(=O)c1ccc(cc1)OCC#CC
C3908	DB07235	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	O=C(c1sc(cc1)c1ccnc(n1)NC)N[C@H](CN)Cc1ccc(Cl)cc1Cl
C3909	DB07236	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc2c(cc1)cc(cc2)O)c1c2c(on1)cc(cc2)O
C3910	DB07252	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(nccc(Nc2c3OCOc3ccc2Cl)n1)Nc1cccc(S(=O)(=O)N)c1

C3911	DB07253	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(c1nccc(Nc2c3OCOc3ccc2Cl)n1)c1cccc(S(=O)(=O)C)c1
C3912	DB07254	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(c1nccc(Nc2c3OCOc3ccc2Cl)n1)c1cccc(NS(=O)(=O)C)c1
C3913	DB07259	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(cc1)CN)c1cccs1
C3914	DB07262	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N=C(N)NC(=N)SCc1cc(ccc1)C(F)(F)F
C3915	DB07264	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c2c(c[nH]n2)c2cccc(c2)Cl)cc(C(=O)N[C@@H](c2ccc(F)c(Cl)c2)CO)[nH]1
C3916	DB07267	DrugBank	noninhibitor	62	inhibitor	inhibitor	noninhibitor	inhibitor	Cc1cccc(n1)c1nc(c2ccccc2n1)Nc1ccncc1
C3917	DB07268	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(nc(ccn1)Nc1c(cccc1)C(=O)N)Nc1cccc(c1)O
C3918	DB07270	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc(c1Cl)S(=O)(=O)Nc1nc2cc(cc(c2o1)c1cc(ccc1)N)OC)Cl
C3919	DB07273	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1cc(c(cc1Cl)N)S(=O)(=O)N1CCC[C@H]1C(=O)O
C3920	DB07280	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	c1nc(c(c(n1)N)c1ccc(cc1)N(C)C)C#Cc1cnc(cc1)N1CCOCC1
C3921	DB07285	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1ccc(cc1)S(=O)(=O)[C@@H](C(F)F)CC(=O)O
C3922	DB07287	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	Clc1cc(Cl)c(cc1)Oc1ccc(cc1O)Cc1ncccc1
C3923	DB07291	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N#Cc1cnn(c1N)c1ccc(Cl)cc1
C3924	DB07292	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc(cc1)c1csc(n1)N
C3925	DB07297	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	c1nc2c(c(n1)NCCN1CCNCC1)c(c(o2)c1ccccc1)c1ccccc1
C3926	DB07301	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12ccccc1c1ccccc1[nH]2
C3927	DB07305	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)c1oc(cc1)c1ccc([N+](=O)[O-])cc1Cl
C3928	DB07308	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(O)c1oc(cc1)Cc1ccccc1Cl
C3929	DB07309	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1ccc(cc1)S(=O)(=O)Nc1ccc(cc1C(=O)O)Br
C3930	DB07311	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(cc(c1)Cl)NC(=O)Nc1nc(cnc1)OCCCCCO2
C3931	DB07312	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc(c1Cl)S(=O)(=O)Nc1nc2cc(Cl)ccc2o1)Cl
C3932	DB07313	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)S(=O)(=O)Nc1ccc(cc1C(=O)O)C
C3933	DB07314	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ncc(nc1)NC(=O)Nc1cc(c(cc1OC)OC)Cl)C#N
C3934	DB07315	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(NC(=O)c2[nH]c3c(c2)cc(cc3)Cl)ccc(cc1)[C@H](CO)O
C3935	DB07324	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cn(c(=O)o1)NCc1c(cccc1)C#Cc1cc(nc(n1)N)C
C3936	DB07331	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(Cc1ccc([N+](=O)[O-])cc1)O
C3937	DB07343	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(Oc2nc(Nc3ccc(cc3)C#N)nc(N)n2)c(Cl)cccc1Cl
C3938	DB07346	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(C)c1c(ccc(CCN)c1)O
C3939	DB07347	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(S(=O)(=O)F)ccc1CCN
C3940	DB07348	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1C[C@@H]2[C@@H](C1)[C@H](/C=C/C(=O)O[C@H](CCC/C=C/2)C)O
C3941	DB07349	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H](O)COP(=O)([O-])OC[C@@H](COC(=O)CCCC)OC(=O)CCCCCCC
C3942	DB07354	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(cc(c1OC)OC)c[nH+]c1c2Cc2c1cc1c(c2)OCO1
C3943	DB07355	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(cccc1C(=O)O)OCCCCCCC
C3944	DB07357	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@H]1(OCCCCCC)[C@H](O)[C@H]([C@@H](O)[C@H](O1)CO)N
C3945	DB07358	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c(cc(c1)Sc1nncn1C)C(=O)Nc1nc(cs1)C)N
C3946	DB07371	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CCc1c2ccccc2c(c2c1cccc2)C
C3947	DB07372	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12ccccc1cc1ccccc1c2
C3948	DB07374	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(ccc(c1)C[C@@H]1[C@@H]([C@H](CN1)O)OC(=O)C)OC
C3949	DB07377	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(C)(C)SCC[C@@H](N)[C@H](O)C(=O)NNC(=O)c1cccc(c1)Cl
C3950	DB07378	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@H]1(OCCCCCCCC)[C@H](O)[C@H]([C@@H](O)[C@H](O1)CO)N
C3951	DB07383	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(=O)N[C@H](C(C(F)(F)F)(O)O)Cc1ccccc1
C3952	DB07384	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1(C(=O)C)[C@H](C(=O)O)CCCC1
C3953	DB07387	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCS(=O)(=O)CCC(=O)O

C3954	DB07395	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c(cc(C(=O)NC(=O)Nc2ccc(cc2OC(F)(F)F)C(=O)O)c(Cl)c1)F)F
C3955	DB07397	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2NC(=O)COc2ccc1CNC(=O)c1nc2c(c(=O)[nH]1)c1c(s2)CCC[C@H]1CC(=O)N
C3956	DB07410	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12ccccc1oc1c2cccc1c1cc(ccc1)CC(P(=O)(O)O)(P(=O)(O)O)O
C3957	DB07412	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCc1ccccc1c1ccccc1
C3958	DB07413	DrugBank	noninhibitor	62	noninhibitor	inhibitor	noninhibitor	noninhibitor	C(CCCCCCCNCCSC[C@H]1O[C@H]([C@@H]([C@@H]1O)O)n1cnc2c1ncnc2N)CC
C3959	DB07431	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc2c(cc1OC)c1c(C(=O)N[C@@H](CN1)CN)s2
C3960	DB07434	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	ONC(=O)C(Cc1ccccc1)C(=O)N[C@@H](C)C(=O)NCC(=O)Nc1ccc(cc1)[N+](=O)[O-]
C3961	DB07435	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc2ccc3c4c(cc5ccc1c2c35)[C@@H](O)[C@H](O)[C@H](O)C4
C3962	DB07436	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)N[C@H](CC)c1ccccc1
C3963	DB07440	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)(C)c1ccc(cc1)S(=O)(=O)O
C3964	DB07444	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=c1[nH]c(=O)c2c1c(C)cc1c2c2cc(C)ccc2n1CCCN
C3965	DB07445	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccncc1C(=O)N/N=C/c1cc(Br)c(O)c(Br)c1O
C3966	DB07446	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(O)[C@@H](CC(C)C)NS(=O)(=O)c1ccc(cc1)c1ccccc1
C3967	DB07449	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(N)[C@H](CCCNC(=N)C)NC(=O)c1ccccc1
C3968	DB07451	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Brc1cnc(cc1)NC(=O)N[C@H]1C[C@H]1c1c(F)ccc(c1O)C(=O)CC
C3969	DB07452	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1c2cc3c(cc2nc1N)nc(N)[nH]c3=O
C3970	DB07459	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1c(cccc1)CNC(=O)c1ccc(cc1)Oc1ccccc1
C3971	DB07463	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1nc2c([nH]cc2CN2C[C@@H]([C@@H](O)C2)CSCCCC)c(N)n1
C3972	DB07464	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(C(NC(=O)C)B(O)O)c1cccc(C(=O)O)c1O
C3973	DB07466	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C([C@@H](B(O)O)NC(=O)Cc1ccccc1)c1cccc(C(=O)O)c1
C3974	DB07467	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=S(=O)(N)c1cc(ccc1Cl)C(=O)NN1[C@@H](C)Cc2c1cccc2
C3975	DB07473	DrugBank	noninhibitor	62	inhibitor	noninhibitor	inhibitor	inhibitor	S1[C@]2(N([C@@H](C1)C(=O)OC)C(=O)c1c2cccc1)c1ccccc1
C3976	DB07476	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NS(=O)(=O)c1ccc(cc1)NC(=O)c1ccccc1S
C3977	DB07477	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(C(=O)O)c1ccc(cc1)c1ccccc1
C3978	DB07478	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc(O)c(O)cc1)c1ccccc1
C3979	DB07479	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1[C@@H](O)[C@@H](O)[C@H](O)c2ccc3ccc4ccccc4c3c12
C3980	DB07482	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1[C@H](C(=O)N2CCC[C@H]2B(O)O)CCC1
C3981	DB07483	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c(ccc1)S(=O)O)c1ccccc1
C3982	DB07484	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccccc1C[C@@H](C(=O)O)CC(O)(O)C[N+](=O)[O-]
C3983	DB07487	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2O[C@H](CP(=O)[O-])CCc2cc(c1)C
C3984	DB07492	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(N[C@H](CO)[C@H](O)c1ccc([N+](=O)[O-])cc1)C(Br)Br
C3985	DB07496	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(C(=O)Nc1ccccc1)c1ccccc1
C3986	DB07497	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)CCCC[C@@H]1SC[C@@H]2NC(=O)N[C@H]12
C3987	DB07498	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(cc(c1)c1nc(CCCC(=O)O)on1)[N+](=O)[O-]
C3988	DB07499	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1scnc1c1scc(C(=O)NCCCCNC(=N)N)n1
C3989	DB07502	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc2c(cc1O)onc2c1cc(c(cc1O)O)Br
C3990	DB07503	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1(=O)NC(=O)S/C/1=C\c1cc2c(cc1)OC(O2)(F)F
C3991	DB07510	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)/C(=C(/F)\C=C\C(=O)c1ccc(cc1)F)/O
C3992	DB07522	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](Cc1ccccc1)[C@H](O)CNS(=O)(=O)c1ccc2ccccc2c1
C3993	DB07524	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(c1ccccc1)c1c[nH]c2c1cccn2
C3994	DB07527	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1cc(C)c(c(C)c1C)S(=O)(=O)NC[C@@H](O)[C@@H](N)Cc1ccccc1
C3995	DB07531	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=S(=O)(N)c1ccc(cc1)c1oc(cc1)/C=C/1\SC(=O)NC1=O
C3996	DB07532	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(CCCCC)N[C@H](C(=O)O)CCO

C3997	DB07534	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=S(=O)(N)c1ccc(cc1)c1oc(cc1)/C=C/1\SC(=N)NC1=O
C3998	DB07538	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=S(=O)(N)c1c(C(F)(F)F)cc(cc1)c1oc(cc1)/C=C/1\SC(=N)NC1=O
C3999	DB07539	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(O)c1ccc(cc1)c1oc(cc1)/C=C/1\SC(=N)NC1=O
C4000	DB07542	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CC1CCCCC1)[C@@H](O)CC(CC(C)C)C(=O)O
C4001	DB07543	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@@H](CNC(C)C)COc1cccc2c1c1c([nH]2)cccc1
C4002	DB07544	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	FC(F)(F)c1ccccc1S(=O)(=O)NNC(=O)c1cc2c(o1)ccc(c2)Cl
C4003	DB07573	DrugBank	inhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1ccc(C)c(OC[C@@H](O)CN2CCOCC2)c1
C4004	DB07574	DrugBank	noninhibitor	62	inhibitor	inhibitor	noninhibitor	inhibitor	O=C(CS)N[C@@H]1c2cc(=O)c(ccc2c2c(CC1)cc(c(c2OC)OC)OC)OC
C4005	DB07575	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C([C@H](N)C(O)[C@@H](N)Cc1ccccc1)c1ccccc1
C4006	DB07577	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1c(nc(c(c1N)c1ccccc1)CC)N
C4007	DB07588	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12ccccc1[nH]cc2c1c(C(=O)O)[nH]c(C(=O)O)c1c1c2ccccc2[nH]c1
C4008	DB07590	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)[C@@H](N)CSCCC(=O)c1cc(c(cc1)Cl)Cl
C4009	DB07591	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(Nc1nccs1)C(=O)NC1CCCC1
C4010	DB07594	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1c2OCCOc2ccc1c1c(C)n[nH]c1c1cc(CC)c(O)cc1O
C4011	DB07597	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@H]1([C@H](CCc2ccccc12)N)O
C4012	DB07598	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@H]2N(CCC2)C(=O)c2c1cc1c(c2)OCCO1
C4013	DB07599	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CO/N=C(\C(=O)NCB(O)O)/c1csc(N)n1
C4014	DB07602	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccccc1Nc1c2cc(ccc2ncn1)NC(=O)CCSC[C@@H](C(=O)O)N
C4015	DB07603	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C([C@@H](C(=O)O)NC(=O)CCCCC)CS
C4016	DB07608	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1c(Cl)cccc1[C@H](CCN)C(=O)Nc1cc2c(cc1)[nH]nc2NC(=O)c1ccccc1
C4017	DB07609	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cccnc1)c1ccc(o1)CN(C)C
C4018	DB07610	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1ccc2c(c1O)cccc2
C4019	DB07613	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c2cc(no2)c2ccccc2)n[nH]c1
C4020	DB07614	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c2sc(nc2)c2ccccc2)n[nH]c1
C4021	DB07616	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c2cc(c(cc2)F)C)nc(sc1)Nc1cc(c(cc1)C(=O)O)O
C4022	DB07621	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccncc1c1ccc(o1)CN
C4023	DB07623	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cnccc1SSc1ccncc1
C4024	DB07627	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccccc1NC(=S)N[C@@H](CC(C)C)C(=O)N[C@@H]1CO[C@@H](C1)O
C4025	DB07632	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=S(=O)(N)c1sc(nn1)c1ccccc1Cl
C4026	DB07636	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC1=C(C(=O)c2c(scn2)C1=O)CCCCCCC
C4027	DB07639	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	C(N)(N)c1cc2cc(ccc2cc1)CC(C(=O)OCC)c1ccc(cc1)O[C@@H]1CNCC1
C4028	DB07641	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CP(=O)(CCCCCCCCCC)C
C4029	DB07645	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(O)CCCCCCCCC(=O)O
C4030	DB07646	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[N+]([O-])(C)(C)CCCCCCCCCCC
C4031	DB07650	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCCCCCCOC=O
C4032	DB07658	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	B([C@H](CCCCN)NC(=O)[C@@H]1CCCN1C(=O)[C@@H](Cc1ccccc1)NC(=O)C)(O)O
C4033	DB07659	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	B([C@H](CCCCCN)NC(=O)[C@@H]1CCCN1C(=O)[C@@H](Cc1ccccc1)NC(=O)C)(O)O
C4034	DB07660	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	B([C@H](CCCN)NC(=O)[C@@H]1CCCN1C(=O)[C@@H](Cc1ccccc1)NC(=O)C)(O)O
C4035	DB07663	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1c2c(cc(cc2)C(=O)O)C(=O)N1[C@@H](C(=O)O)Cc1ccc(O)cc1
C4036	DB07664	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1cccc(F)c1NC(=S)n1nc(nc1N)Nc1ccc(cc1)S(=O)(=O)N
C4037	DB07666	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1(cc(c(cc1[C@H]1CN(C[C@@H]1N)c1cc(c2cccc(c2)S(=O)(=O)C)ncn1)F)F)F
C4038	DB07668	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(/C(=C/c1c(cc(cc1)N(CC)CC)O)/C)O
C4039	DB07672	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1)[Si](C)(C)[C@@H]1CC[N@@+](CC1)([O-])C

C4040	DB07681	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)([O-])CCCCCCCCCCCC
C4041	DB07683	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc2c(cc1)c1c(s2)cccc1)S(=O)(=O)N[C@@H](C(C)C)C(=O)O
C4042	DB07686	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=S(=O)(N)c1ccc(cc1)Nc1n2ncnc2nc(c1)NC1CCCCC1
C4043	DB07687	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=S(=O)(N)c1ccc(cc1)Nc1n2ncnc2nc(c1)N[C@H]1CC[C@H](N)CC1
C4044	DB07693	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1cccc(C)c1C(=O)Nc1cc(Br)c(O)c(Br)c1
C4045	DB07694	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(Br)c(O)c(Br)cc1NC(=O)c1cc(Cl)ccc1Cl
C4046	DB07695	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1cc(cc(c1O)C)C(=O)Nc1cc(Br)c(O)c(Br)c1
C4047	DB07702	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@H]12CC[C@]3(C)[C@H](O)[C@H](O)C[C@H]3[C@@H]1CCc1cc(O)ccc21
C4048	DB07706	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(cc(c1O)O)CC[C@H]1[C@H]3[C@](CC[C@H]21)([C@H](CC3)O)C
C4049	DB07715	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(O)cc(O)cc2C(=O)c3cc(C)cc(O)c3C(=O)c12
C4050	DB07723	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1c2ccc(cc2c(CCC(=O)O)c1)OC
C4051	DB07724	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(Cc1cn(c2c1cc(cc2)OC)S(=O)(=O)c1ccc(cc1)OC)C(=O)O
C4052	DB07726	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)(C)c1cc(O)ccc1O
C4053	DB07730	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1(=CC(=O)NS1(=O)=O)c1cccc(c1)O
C4054	DB07742	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1C(=O)NCc1cccc(c1F)F)S(=O)(=O)N
C4055	DB07746	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCc1ccc(c(c1C)C(=O)O)NS(=O)(=O)c1ccc(cc1)F
C4056	DB07754	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1ccc(cc1)CSC[C@@H](C(=O)O)NC(=O)N[C@H](C(=O)O)CCC(=O)O
C4057	DB07756	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1c2c(c(c(c1C)CSCc1cc(ccc1)C(C(F)(F)F)(O)O)N)c(ccc2)F
C4058	DB07758	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	o1c(C(=O)O)ccc1c1c(ccc(c1)Cl)Cl
C4059	DB07760	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)c1cccc(c1)/C=N/OCCO/N=C/c1[nH]c(=O)[nH]c(=O)c1
C4060	DB07762	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c(cc(c1)C(=O)O)NC(=O)C(CC)CC)NC(=O)C
C4061	DB07764	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(O)cc2Oc3cc(O)ccc3C(c2cc1)c1ccccc1C(=O)O
C4062	DB07775	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C\1(=C\c2c(c(c(c(c2)Br)O)Br)O)/C(=O)c2c(cc(cc2O1)O)O
C4063	DB07794	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cn2c(cc1)c(c(n2)c1ccccc1)c1cc2c(nn1)[nH]nc2N
C4064	DB07802	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Brc1c(=O)oc2c(c1C)ccc(c2Br)O
C4065	DB07803	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)c1c[nH]c(n1)c1ccccc1
C4066	DB07805	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	FC(F)(F)c1ccc(cc1)NC(=O)C(C)(C)CCl
C4067	DB07808	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1ccc(F)c(c1)NC(=O)[C@H]1[C@H](C1)C(=O)O
C4068	DB07812	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	C([C@H](c1ccccc1)NC(=O)c1ccc(c2ccnc3c2cc[nH]3)s1)N
C4069	DB07818	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(NO)/C=C/c1c(Cl)cc(cc1)Cl
C4070	DB07819	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(NO)/C=C/c1ccc(Cl)cc1
C4071	DB07821	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CC(C)(C)[C@@H](C)OP(=O)C
C4072	DB07823	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1N([C@H](C(=O)O)C)C(=O)[C@H]2[C@@H]1[C@H]1CC[C@H]2C1
C4073	DB07824	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=c1c(CC)c(C)[nH]n1c1[nH]nnn1
C4074	DB07825	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(C)c1ccc(cc1)N1C(=O)C[C@@H](C1)C(=O)O
C4075	DB07827	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	n1(c2c(c(=O)n(Cc3ccc(C(=O)O)cc3)c1=O)cc(cc2)C#CCc1ccccc1)C
C4076	DB07837	DrugBank	noninhibitor	62	inhibitor	noninhibitor	inhibitor	inhibitor	c1cccc2ccc(c3cc4c([nH]cc4c4ccc(cc4)CC(=O)O)nc3)cc12
C4077	DB07852	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(c1nn(c(n1)C)c1cc(cc(c1)Cl)Cl)O
C4078	DB07855	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](c1ccccc1)c1ccc(cc1)c1ncnc2[nH]cnc12
C4079	DB07857	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCC(c1ccc(Cl)cc1)c1ccc(cc1)c1c[nH]nc1
C4080	DB07858	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NCC(c1ccc(Cl)cc1)c1ccc(cc1)c1cn[nH]c1
C4081	DB07860	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1[C@@H](c1ccccc1)CN)Cl
C4082	DB07861	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	O=C(NO)[C@@H](Cc1ccc2ccccc2c1)NS(=O)(=O)c1ccc2ccccc2c1

C4083	DB07863	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1ccc([N+](=O)[O-])cc1C(=O)Nc1ccccc1
C4084	DB07887	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(cc1)B1O[C@@H](CO1)CO)CNC(=N)N
C4085	DB07888	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COC(=O)C[C@@H]1ON=C(C1)c1ccc(O)cc1
C4086	DB07900	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(O)C(=O)[C@H]([C@@H](CC(C)C)C=O)O
C4087	DB07906	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1[C@H](CO)NCc2cc(ccc12)[N+](=O)[O-]
C4088	DB07907	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCC[C@H](O)C(=O)O
C4089	DB07908	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c(=O)oc2cc(ccc2c1C)O)CCO
C4090	DB07911	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cccc(c1)C(=O)C/C=C/C(=O)C(=O)[O-]
C4091	DB07913	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@H](C(=O)C)CCc1ccccc1
C4092	DB07916	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C[C@H](CC(=O)O)NC(=O)[C@H](c1sccc1)CCCCNC(=O)c1nc2c(cc1)cccc2O
C4093	DB07921	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=S(=O)(NCC(=O)N=O)c1ccc(cc1)F
C4094	DB07922	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(N=O)CNS(=O)(=O)c1ccccc1
C4095	DB07927	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(S(=O)(=O)c1ccsc1C(=O)O)c1c(cc(cc1)C(=O)O)O
C4096	DB07930	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(CCCCCCC[C@@H](O)CC(=O)O)C
C4097	DB07939	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	SCCC(=O)N[C@H](C)C(=O)O
C4098	DB07959	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cccc2c(c3[nH]c4ccccc4n3)n[nH]c12
C4099	DB07968	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	COc1ccc(O)cc1NC(=O)NC(=O)c1ccc(F)cc1Cl
C4100	DB07973	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(cc1)cc(n2Cc1cccc(c1)OC)C(=O)NC1CCN(CC1)C(C)C
C4101	DB07974	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	c1cc2c(cc1)cc(n2CC(=O)Nc1ccc(cc1)Cl)C(=O)NC1CCN(CC1)C(C)C
C4102	DB07978	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)C1=C(C=CC1)C(=O)Nc1c(F)c(F)c(c(F)c1F)c1cc(OC(F)(F)F)ccc1
C4103	DB07979	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(O)C(=N)Cc1cc(O)c(O)cc1
C4104	DB07981	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	c1c(ccc2c1c(c(C)n2C(=O)c1ccc(cc1)Cl)CC(=O)N[C@@H](CO)CC)OC
C4105	DB07983	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	n1(c(c(c2cc(ccc12)OC)CC(=O)O)C)C(=O)c1ccc(cc1)I
C4106	DB07984	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	c1c(ccc2c1c(c(C)n2C(=O)c1ccc(Cl)cc1)CC(=O)N[C@@H](CC)CO)OC
C4107	DB07985	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(cc1C(=N)N)[C@@H](CCc1ccc(C(=N)N)cc1)CC(=O)OC
C4108	DB07992	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O(c1c[nH]c2c1cccc2)S(=O)(=O)O
C4109	DB07999	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12ccccc1c1C(=O)N(CC(=O)O)S(=O)(=O)c1c(C(=O)OCC(=O)O)c2
C4110	DB08000	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12c3C(=O)N(CC(=O)O)S(=O)(=O)c3c(C(=O)O)cc1cccc2
C4111	DB08003	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@H]1(CC(=O)NS1(=O)=O)c1ccc(cc1)C[C@@H](C(=O)N)NC(=O)[C@@H](NC(=O)C)Cc1ccccc1
C4112	DB08004	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC[C@H](C(C)C)Nc1ccc2n(n1)c(cn2)c1cc(ccc1)N
C4113	DB08007	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C([C@H](O)CNC(=O)NCc1ccccc1)O
C4114	DB08018	DrugBank	noninhibitor	62	noninhibitor	inhibitor	inhibitor	inhibitor	c1cc(Cl)ccc1CNCCN[C@@H]1CNC[C@@H]1Cc1cc(cc(N)n1)C
C4115	DB08019	DrugBank	noninhibitor	62	noninhibitor	inhibitor	inhibitor	inhibitor	c1c(cc(nc1N)C[C@@H]1[C@H](CNC1)NCCNCc1cccc(c1)Cl)C
C4116	DB08021	DrugBank	inhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1cccc(NC(=O)c2ccc(o2)Br)c1N1CCN(CC1)CC#C
C4117	DB08031	DrugBank	noninhibitor	62	inhibitor	noninhibitor	inhibitor	inhibitor	CC(NC(=O)c1ccc2c(n3c(c4c(cccc4)OCC3)c2C2CCCCC2)c1)(C(=O)O)C
C4118	DB08034	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(=C\c1c(OC)ccc2ccccc12)/NC(=O)c1cc(c(cc1)O)O
C4119	DB08036	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1NC(=O)c2c1c1c([nH]c3c1cccc3)c1c2c2c([nH]1)cccc2
C4120	DB08038	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccccc1C[C@H](NC(=O)[C@H](C)NC(=O)[C@H](C)N)[C@H](O)C
C4121	DB08040	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(NO)CC(C(=O)N[C@@H](C)C(=O)O)Cc1ccccc1
C4122	DB08048	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1cc(O)ccc1c1c2ccc(O)cc2[nH]n1
C4123	DB08049	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=c1oc2c(O)c(O)ccc2c(c1)c1ccccc1
C4124	DB08050	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccccc1)CCCC(=O)C(=O)O
C4125	DB08059	DrugBank	inhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@H]1(OC(=O)c2c3[C@]1(C1=C(C(=O)c3oc2)[C@H]2[C@@](C[C@H]1OC(=O)C)(C)C(=O)CC2)C)COC

C4126	DB08060	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(CC(=O)c1c(cccc1)N)C(=O)O
C4127	DB08061	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1nc(cc1C1CCNCC1)c1ccc(cc1)Cl
C4128	DB08062	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CSc1nnc([nH]1)c1ccc(Cl)cc1
C4129	DB08065	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(n[nH]1)c1nc2ccccc2[nH]1
C4130	DB08068	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	Clc1ccc(cc1COc1cnccc1)NC(=O)C1=C[C@H](F)C[C@H](C1)N1CCOCC1
C4131	DB08069	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nn1c(=S)[nH]nc1c1ccccc1C
C4132	DB08070	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1n[nH]cc1c1ccc(CCN)cc1
C4133	DB08077	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc(cc(c1)Cl)Cl)NC(=O)Nc1ccc(cc1)OC(C)(C)C(=O)O
C4134	DB08080	DrugBank	noninhibitor	62	noninhibitor	inhibitor	noninhibitor	noninhibitor	O=C1N[C@@H](CS1)[C@@]1(O)C[C@@H]2OC(=O)/C=C(\CC/C=C\[C@H](CC[C@H](C2)O1)C)/C
C4135	DB08082	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(NCCO)c1ccc(Cl)cc1
C4136	DB08083	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1scnc1c1[nH]c2ccc(S(=O)(=O)N)cc2n1
C4137	DB08095	DrugBank	noninhibitor	62	noninhibitor	inhibitor	noninhibitor	noninhibitor	N(C(=O)Nc1c(Cl)cccc1)(c1ccc(cc1)OC)c1ccnc(n1)N[C@@H](C)C(C)(C)O
C4138	DB08098	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(c2nnc(SCC(=O)O)o2)o1)[N+](=O)[O-]
C4139	DB08100	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1cc(cc(c1O)C)/C=C/c1ccccc1
C4140	DB08101	DrugBank	noninhibitor	62	noninhibitor	inhibitor	noninhibitor	noninhibitor	c1c(Br)c(O)c(Br)cc1/C=C/c1ccccc1
C4141	DB08102	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(Br)c(O)c(Br)cc1c1ccccc1
C4142	DB08104	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(Br)c(O)c(Br)cc1NC(=O)c1ccccc1
C4143	DB08105	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=S(=O)(N[C@H](C(=O)O)CCC(=O)O)c1ccc2cc(ccc2c1)OCCCC
C4144	DB08106	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=S(=O)(N[C@@H](C(=O)O)CCC(=O)O)c1ccc2c(c1)ccc(c2)OCCCC
C4145	DB08107	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=S(=O)(N[C@@H](C(=O)O)CCC(=O)O)c1ccc2cc(ccc2c1)OCCCCC
C4146	DB08108	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N#Cc1ccc(cc1)COc1ccc2c(c1)ccc(c2)S(=O)(=O)N[C@@H](C(=O)O)CCC(=O)O
C4147	DB08109	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCO[C@@H]1CCC[C@@H]2C1=C(C(=O)O)N[C@@H]2[C@@H](CC)C=O
C4148	DB08113	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12ccccc1[nH]nc2c1ccncc1
C4149	DB08114	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccccc1Cc1sc(nc1)N
C4150	DB08120	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(N)CCCC[C@@H](S)CCS
C4151	DB08131	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(ccc(c1)C(=O)N[C@@H](C(C)C)C(=O)O)CCc1c[nH]c2c1c(=O)[nH]c(n2)N
C4152	DB08134	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	NS(=O)(=O)c1ccc(Nc2cncc(Cl)n2)cc1
C4153	DB08135	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(Nc1ccccc1)c1cc[nH]n1
C4154	DB08147	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccc(N(Cc2ccccc2)Cc2ccccc2)cc1C(=O)CC(=O)C(=O)O
C4155	DB08151	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccccc1C1=NO[C@@]2(C1)O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O
C4156	DB08155	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(cc1)CCNC(=O)C)S(=O)(=O)N
C4157	DB08157	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(cc1)CCC(=O)OCC)S(=O)(=O)N
C4158	DB08159	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cccc2c1c1c(n(c2=O)CCCC(=O)O)c2c(C1=O)cccc2
C4159	DB08161	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccccc1CCC[C@@H](C(=O)O)CS
C4160	DB08168	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1cc2c(c(cc(=O)o2)C)cc1
C4161	DB08171	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(O)CCCCCCCCCCS
C4162	DB08173	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	c1(ccc(s1)C(=O)NCCNC(=O)c1ccc(cc1)n1ccccc1=O)Cl
C4163	DB08179	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(OC)c1c(O)cc(cc1C)Oc1cc(cc(c1O)O)C
C4164	DB08191	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(cccc1)c1cc2c(c[nH]c2nc1)c1ccc(C(=O)O)cc1
C4165	DB08192	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(O)c1c(C(C)C)sc(n1)[C@H]1NCc2c(C1)cccc2
C4166	DB08193	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(Cc1cc([N+](=O)[O-])ccc1)O
C4167	DB08194	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc(C)c2c(n1)CCSC2
C4168	DB08199	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(N[C@@H](CS)C(=O)NCC(=O)O)OCc1ccccc1

C4169	DB08202	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(cc1)NC(=S)NN1CCN(C)CC1)S(=O)(=O)N
C4170	DB08205	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1cc(cc(c1O)C)c1oc2ccccc2n1
C4171	DB08206	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(Br)c(O)c(Br)cc1c1oc2ccccc2n1
C4172	DB08211	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Brc1cc2c(cc1)[nH]c(C(=O)N)c2S(=O)(=O)N1CCCC1
C4173	DB08212	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cnc(cc1)NC(=S)N[C@@H]1C[C@@H]1c1c(ccc(c1O)C(=O)C)OC)C#N
C4174	DB08220	DrugBank	noninhibitor	62	inhibitor	noninhibitor	inhibitor	inhibitor	C1CC(=CC2=CC[C@@H]3[C@@H]([C@@]12C)CC[C@]1([C@H]3CC[C@@H]1C(=O)c1ccc(cc1)O)C)C(=O)O
C4175	DB08224	DrugBank	noninhibitor	62	noninhibitor	inhibitor	noninhibitor	noninhibitor	O[C@@H]1C[C@@H](OC(=O)C1)CC[C@H]1[C@@H](C)C=CC2=CCC[C@H](O)[C@H]12
C4176	DB08230	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=c1c2c(O)cc(O)cc2oc(c1)c1cc(O)c(O)c(c1)O
C4177	DB08231	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(O)CCCCCCCCCCCCC
C4178	DB08235	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Cc1[nH]c2ccccc2c1CCNC(=O)c1cccs1
C4179	DB08236	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(Br)cccc1[C@@H]1SCC(=O)N1c1cc(ccc1O)Cl
C4180	DB08238	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(O)c1cc2cccc(c2cc1)N
C4181	DB08251	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(cncc1C(=O)N[C@@H](CC(=O)O)C=O)c1ccc(cc1)C(=O)O
C4182	DB08253	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](Cc1cccc2ccccc12)C(=O)N
C4183	DB08254	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(O)c1cc2ccccc2cc1
C4184	DB08255	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@H]12[C@@H]([C@H]([C@@H]([C@@H](CO)O1)O)O)N=C(CCC)S2
C4185	DB08257	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1(NC(=O)NCCCC(=O)O)CCCCC1
C4186	DB08258	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1(NC(=O)NCCCCCC(=O)O)CCCCC1
C4187	DB08259	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1(NC(=O)NCCCCCCC(=O)O)CCCCC1
C4188	DB08261	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2c(ccc(c2C(=O)O[C@H]2[C@@H](C=C[C@@H]2O)O)O)c(cc1OC)C
C4189	DB08264	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1[C@@H](O)C=Cc2c1cccc2
C4190	DB08273	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc([N+](=O)[O-])c(O)c(I)c1)CC(=O)NCCCCCC(=O)[O-]
C4191	DB08274	DrugBank	noninhibitor	62	noninhibitor	inhibitor	inhibitor	inhibitor	c1(c(=O)oc2c(c1O)CCCCC2)[C@H](c1ccccc1)CC
C4192	DB08288	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](CC1CCCCC1)[C@@H](O)C(=O)OC(C)C
C4193	DB08289	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[N+]1(CCCCC1)([O-])CCc1ccc(cc1)NC(=O)CCCC(=O)O
C4194	DB08294	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc(c(cc1O)[N+](=O)[O-])CC(=O)O
C4195	DB08295	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc([N+](=O)[O-])c(O)cc1)CC(=O)NCCCCCC(=O)[O-]
C4196	DB08299	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(c2cc3cccnc3c(n2)c2cc(ccc2)[N+](=O)[O-])cc1)C(=O)O
C4197	DB08301	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(N)c1ccc(NC(=O)NS(=O)(=O)c2ccc(C)cc2)cc1
C4198	DB08314	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Brc1cc(ccc1)C(=O)c1oc(N)nc1
C4199	DB08319	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c(ccc1)S(=O)O)c1ccccc1O
C4200	DB08331	DrugBank	noninhibitor	62	noninhibitor	inhibitor	noninhibitor	noninhibitor	c1(ccc(cc1)Nc1ccc(cc1)Nc1[nH]ccn1)Nc1[nH]ccn1
C4201	DB08356	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1nc(c(c1C)c1ccc(cc1)OC)c1c(cc(cc1)O)O
C4202	DB08365	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c2c(c(=O)[nH]c2=O)c2c(c(C(=O)NCCO)n(C)c12)Br)c1c(cccc1)Cl
C4203	DB08366	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@@H]2[C@@H]3[C@](CCC(=O)Nc4c(O)c(C(=O)O)ccc4O)(C(=O)CC[C@]43C[C@@H](C2)[C@@]1(C4)C)C
C4204	DB08368	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CC[C@@H](C(=O)O)C[C@H](C(=O)O)C[C@H](C)C(=O)O
C4205	DB08371	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@H](C(=O)O)Cc1ccc(cc1)C(=O)c1ccccc1
C4206	DB08374	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@H](C(=O)CCl)Cc1ccccc1
C4207	DB08375	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C([C@H]([C@@H]1N=C(C(=C)CS1)C(=O)O)NC(=O)/C(=N\OC)/c1csc(n1)N)O
C4208	DB08378	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(cc1)N[C@H](CCC(=O)O)O)N1C(=O)CCC1=O
C4209	DB08381	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cccc2c1c1c(cc2)cccc1
C4210	DB08383	DrugBank	noninhibitor	62	inhibitor	noninhibitor	inhibitor	inhibitor	c1c(ccc(c1)OC)c1c(c2ccc(cc2)OC)[nH]c(c2cccs2)n1
C4211	DB08396	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccccc1C1=N/C(=C\NC/C=C/C(=O)O)/C(=O)O1

C4212	DB08399	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc(cc(c1)/C=C/c1cc(c(cc1)O)O)O)O
C4213	DB08401	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)CC/C(=N\OC[C@@H](C(=O)O)NC(=O)COc1ccccc1)/C(=O)O
C4214	DB08402	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1cc(Cl)c(cc1)C(=O)Nc1ccc(cc1C(=O)O)Oc1ncccn1
C4215	DB08410	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(cc1)[N+](=O)[O-])CNC(=O)CCCC(=O)NCC(=O)O
C4216	DB08420	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(c1cc(ccc1)C#N)C(NC(=O)[C@H]1N(CCC1)C(=O)[C@@H](Cc1ccccc1)N)B(O)O
C4217	DB08421	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1[C@@H](CCCC1)C(=O)NC(C)(C)C
C4218	DB08424	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1c(cnn1c1ccc(F)cc1)C(=O)c1cccc(OC[C@@H](O)CO)c1
C4219	DB08427	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@]1(C=C[C@H](O)C=C1)(C(=O)O)CC(=O)C(=O)O
C4220	DB08445	DrugBank	noninhibitor	62	noninhibitor	inhibitor	noninhibitor	noninhibitor	n1c(ccc(c2cc(N3C[C@@H]([C@@H](c4cc(c(F)cc4F)F)C3)N)ncn2)c1)OC
C4221	DB08451	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=S(=O)(C)Nc1cccc2c1nccc2
C4222	DB08454	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccccc1c1nc(c2c(n1)cccc2)Nc1cc(C)[nH]n1
C4223	DB08455	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc(c(c(c1)C)/C=C/C(=C/C=C/[C@H](CC(=O)O)C)/C)C)O
C4224	DB08456	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C([C@@H](N)CSSCC1=C(C([N+](=O)C1(C)C)(C)C)c1ccccc1)O
C4225	DB08470	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(F)ccc1c1[nH]c(nn1)c1ccccc1
C4226	DB08473	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c12cc(Cl)c(Cl)cc1ncn2[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O
C4227	DB08476	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@H]1CCCCCCCCCNC1=O
C4228	DB08478	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(c(c1)NC(=N)NC(=N)N)Cl)C(F)(F)F
C4229	DB08479	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(cc(cc(c1)NC(=N)NC(=N)N)OC)OC
C4230	DB08480	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C=C/C=N/[C@@H]1CCc2c1cccc2O
C4231	DB08485	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(O)[C@@]1(O)C[C@@H](O)[C@H](O)C(=C1)c1cccc(c1)Sc1ccccc1
C4232	DB08489	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	C(=O)(NO)C[C@H](C(=O)N[C@@H]1C(=O)NCCCCCCn2cc(C1)c1c2cccc1)CC(C)C
C4233	DB08492	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(O)/C=C/c1ccccc1C#CCCCCCC
C4234	DB08493	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(O)C[C@H](C(=O)N[C@@H]1C(=O)NCCCCCCn2cc(C1)c1c2cccc1)CC(C)C
C4235	DB08500	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c2ccccc2ccc1[C@@H]1C[C@]2(ON1)O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O
C4236	DB08503	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(C)ccc1[C@@H]1C[C@]2(ON1)O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O
C4237	DB08511	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(N)nc2cc3nc(C)[nH]c3cc2c(=O)[nH]1
C4238	DB08512	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc2cc3[nH]c(NCc4c5ccccc5ccc4)nc3cc2c(=O)[nH]1
C4239	DB08513	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(cc1)Nc1nc(c(cn1)C(=O)N)Nc1cccc(c1)C)CC(=O)O
C4240	DB08514	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[nH]1c2c(nc1NCc1cccs1)cc1c(c(=O)[nH]c(N)n1)c2
C4241	DB08515	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1O[C@@]2(C)[C@H](C(=O)N[C@@]2([C@H]([C@@H]2C=CCCC2)O)C=O)C1
C4242	DB08523	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1)CCCN(O)CO
C4243	DB08525	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(nc(ccc1)CCCN(O)C=O)C
C4244	DB08528	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1c(c(c(cc1)S(=O)(=O)c1cc(cc(c1)C)C)C#N)N
C4245	DB08540	DrugBank	inhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1(=Nc2c(cccc2)SC1)N1CCN(CC1)c1nc(cs1)C(=O)OCC
C4246	DB08541	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1c2C(=O)C3=C(O[C@@H](CC3=Cc2ccc1)CC(=O)O)C
C4247	DB08554	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@H](C(=O)O)(CCC)NC(=O)CCC(=O)O
C4248	DB08558	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@H]1([C@@H]([C@H]([C@@H]([C@@H](CO)O1)O)O)O)SCCCCCCCC
C4249	DB08562	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccccc1/C=C/c1ccc(cc1)NC(=O)CCCC(=O)O
C4250	DB08570	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(O)c1cc(O)c(NC(=O)C)c([N+](=O)[O-])c1
C4251	DB08573	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N(c1ccc(cc1)Cl)S(=O)(=O)c1c(scc1)C(=O)O
C4252	DB08574	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@H]1(SC(=NC1=O)S)Cc1ccc(cc1)C(F)(F)F
C4253	DB08575	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	SC[C@H](c1nc2c([nH]1)cc[nH+]c2)Cc1ccccc1
C4254	DB08577	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1C(=O)/C(=C\c2[nH]cc(c2CCC(=O)O)C)/c2ccccc12

C4255	DB08578	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Brc1cnc(cc1)NC(=O)CCC(=O)O
C4256	DB08587	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(c(cc(cc1OC)/C=C/C(=O)O)OC)O
C4257	DB08589	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(OC)c1cc(OC)c(c(c1)OC)O
C4258	DB08593	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccccc1N1S(=O)(=O)NC(=O)C1
C4259	DB08599	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=S(=O)(N[C@H](C)C(=O)O)c1ccc(cc1)OC
C4260	DB08603	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(=O)(=O)(c1ccc(cc1)C)N[C@H](C(=O)CCl)CCCCN
C4261	DB08605	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	s1c(C)cc2c1C=NN(B2O)S(=O)(=O)CCC
C4262	DB08606	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1nc(c2c(c(CN3C[C@H](CSC)[C@H](C3)O)c[nH]2)n1)N
C4263	DB08621	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(Cl)(Cl)C(=O)N[C@H](CO)[C@H](O)c1ccc(cc1)S(=O)(=O)C
C4264	DB08623	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S1CC(=C)[C@@H](C(=O)O)N=C1[C@@H](C(=O)O)NC(=O)Cc1cccs1
C4265	DB08626	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	SC[C@H](C(=O)NCC(=O)O)Cc1ccccc1
C4266	DB08629	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N1(CCCN2CCC[C@@H]12)C[C@H](CC(C)C)N
C4267	DB08636	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(C(=O)O)/C=C/c1ccccc1O
C4268	DB08637	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(C(=O)O)/C=C/c1ccccc1OC
C4269	DB08640	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)[C@H]([C@H](C(=O)O)CNS(=O)(=O)c1ccc(cc1)C)CC
C4270	DB08646	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	N[C@@H](Cc1c2c([nH]c1)c(c(cc2)NNc1ccccc1)O)C=O
C4271	DB08650	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1=C[C@@H](O)[C@H]2C[C@]1(C(=O)O)C[C@H](O2)C(=O)O
C4272	DB08654	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O[C@H]1c2ccccc2CC[C@@H]1N
C4273	DB08656	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	C(=O)(c1c(C)ccc(c1)N)N[C@H](C)c1c2c(ccc1)cccc2
C4274	DB08657	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(Nc1sc(Sc2ncccc2)cn1)NCc1nc(c[nH]1)c1ccc(cc1)OCC(=O)O
C4275	DB08659	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1ccccc1c1c2cc(S(=O)(=O)N)ccc2[nH]c1C(=O)NN
C4276	DB08660	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1c2c(O)ccc(O)c2C(=O)c2c1ccc(O)c2O
C4277	DB08661	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C1CCCN1C[C@@H]1O[C@@H](C[C@H]1O)n1cc(C)c(=O)[nH]c1=O
C4278	DB08662	DrugBank	noninhibitor	62	noninhibitor	inhibitor	inhibitor	inhibitor	c1(c(=O)oc2c(c1O)cccc2)[C@H](c1ccc(cc1)Br)C(C)C
C4279	DB08668	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(O)c1cccc(c1)/N=N/C1=C(N)N=NC1=N
C4280	DB08673	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=S(=O)(N)c1ccc(Nc2sc(cn2)C(C)C)cc1
C4281	DB08678	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=S(=O)(O)Nc1ccc(CC)cc1
C4282	DB08683	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	inhibitor	noninhibitor	[nH]1c(=O)c2c3c4c(cccc4)n4c3c3n(c5c(cccc5)c3c2c1=O)[C@H]1O[C@@H]4CC1
C4283	DB08684	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	CCCCCCCCCCOC(=O)S
C4284	DB08686	DrugBank	noninhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	c1(c(=O)oc2c(c1O)CCCCCC2)[C@H](c1ccccc1)CC
C4285	DB08695	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[N+](=O)(c1ccc(c2n[nH]cc2)cc1)[O-]
C4286	DB08705	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(c(cc1Br)c1[nH]c(=O)c(c(c1)c1ccccc1)C#N)O
C4287	DB08706	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(ccc1[C@@H](C(=O)O)NC1=NC(=O)/C(=C/c2ccc(o2)CC)/S1)F
C4288	DB08709	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(O)c1c2[nH]c(c(c3ccccc3)c2ccc1)c1ccccc1
C4289	DB08711	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(c(c1)OC)O)C(=O)OC
C4290	DB08712	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(O)CCCCCCCCCCOC(=O)S
C4291	DB08718	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Oc1c(O)cc(cc1)c1sccc1CC
C4292	DB08731	DrugBank	noninhibitor	62	inhibitor	noninhibitor	noninhibitor	noninhibitor	c12ccccc1cccc2CC(CC(=O)O)N1C(=O)c2cc(C(=O)O)ccc2C1=O
C4293	DB08735	DrugBank	noninhibitor	62	noninhibitor	inhibitor	noninhibitor	noninhibitor	c12c(c(C(C[C@H](C)O)c3ccccc3)c(=O)oc2cccc1)O
C4294	DB08736	DrugBank	noninhibitor	62	noninhibitor	inhibitor	noninhibitor	noninhibitor	c12c(c(C(C[C@@H](C)O)c3ccccc3)c(=O)oc2cccc1)O
C4295	DB08740	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[C@@H](N)([C@@H](O)[C@@H](O)CC(C)C)CC1CCCCC1
C4296	DB08750	DrugBank	inhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Fc1cccc2c1C(=NC1(N2)CCN(CC1)C(=O)c1ccc(CN)cc1)N
C4297	DB08754	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(O)ccc(CCNC(=O)/C=C/c2ccc(O)c(O)c2)cc1

C4298	DB08756	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C([C@H]1CC[C@@H](CC1)[C@@H](C)N)Nc1ccncc1
C4299	DB08757	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1ccccc1c1oc(cc1)C(=O)NN
C4300	DB08758	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1n2ccc3ccccc3c2nc1C(=O)NN
C4301	DB08760	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(Cl)ccc1O[C@H](C(=O)O)Cc1ccccc1
C4302	DB08761	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C1[C@H](Cc2ccc(O)cc2)NC(=O)[C@@H](N1)Cc1ccc(O)cc1
C4303	DB08764	DrugBank	inhibitor	62	inhibitor	inhibitor	inhibitor	inhibitor	C1CN(C)CCC1COc1cc2c(cc1OC)/c(=N/c1ccc(Br)cc1F)/nc[nH]2
C4304	DB08767	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=C(N)Cc1ccc(OC)cc1
C4305	DB08772	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(=O)c2c(c(nn1Cc1nc3c(ccc(c3)C(F)(F)F)s1)CC(=O)O)cccc2
C4306	DB08773	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(O)cc2sc(c3ccc(O)cc3)cc12
C4307	DB08775	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	C(=O)(N[C@@H](Cc1ccc(cc1)O)C(=O)N[C@@H](C)C(=O)C)OCc1ccccc1
C4308	DB08777	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=c1c2c3CCCCc3sc2nc[nH]1
C4309	DB08782	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1(ccc(cc1)CCN)S(=O)(=O)N
C4310	DB08783	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[Se](=O)(Cc1ccc(cc1)C[C@H](NC(=O)OC(C)(C)C)C(=O)OC)O
C4311	DB08784	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	c1cc(Cl)ccc1Nc1ncccc1C(=O)O
C4312	DB08785	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O=c1oc2ccccc2c(C)c1
C4313	DB08786	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Nc1nc(cc(C)n1)OCCOC
C4314	DB08787	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	Clc1ccc(c(c1)Cl)c1nc(ncc1/N=N/c1ccccc1)N
C4315	DB08790	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	OC(=O)c1cnn(c1)c1ccccc1
C4316	DB08805	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	S(Cc1nc[nH]c1C)CCNC(=S)NC
C4317	DB08830	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	O1[C@@H](C(=O)C(=O)C1=O)C(O)CO
C4318	DB08837	DrugBank	noninhibitor	62	noninhibitor	noninhibitor	noninhibitor	noninhibitor	[N+](CC)(CC)(CC)CC

Table S1 Reference of collected molecules

Reference No.	Title	Journal reference	Authors
1	Inhibition of P-glycoprotein-mediated transport by terpenoids contained in herbal medicines and natural products.	Food and chemical toxicology : an international journal published for the British Industrial Biological Research Association, 2006; 44 (12); 2033-9	Yoshida, N; Koizumi, M; Adachi, I; Kawakami, J;
2	Classification of substrates and inhibitors of P-glycoprotein using unsupervised machine learning approach	Journal of chemical information and modeling, 2005; 45 (3); 750-7	Wang, YH; Li, Y; Yang, SL; Yang, L;
3	Computational models for identifying potential P-glycoprotein substrates and inhibitors.	Molecular pharmaceutics, 2006; 3 (1); 33-44	Crivori, P; Reinach, B; Pezzetta, D; Poggesi, I;
4	Structure-activity relationship: analyses of p-glycoprotein substrates and inhibitors	Journal of clinical pharmacy and therapeutics, 2003; 28 (3); 203-28	Wang, RB; Kuo, CL; Lien, LL; Lien, EJ;
5	Similarity-Based Descriptors (SIBAR) as Tool for QSAR Studies on P-Glycoprotein Inhibitors: Influence of the Reference Set	QSAR and Combinatorial Science, 2007; 26 (5); 669–678	Zdrazil, B.; Kaiser, D.; Kopp, S.; Chiba, P.; Ecker, G.;
6	Three-dimensional quantitative structure-activity relationships of inhibitors of P-glycoprotein.	Molecular pharmacology, 2002; 61 (5); 964-73	Ekins, S; Kim, RB; Leake, BF; Dantzig, AH; Schuetz, EG; Lan, LB; Yasuda, K; Shepard, RL; Winter, MA; Schuetz, JD; Wikel, JH; Wrighton, SA;
7	Overlapping ligand specificity of P-glycoprotein and serum alpha(1)-acid glycoprotein: evidences and potential implications.	Current drug metabolism, 2007; 8 (6); 563-93	Zsila, F;
8	Recent advances in molecular modeling and medicinal chemistry aspects of phospho-glycoprotein.	Current drug metabolism, 2006; 7 (2); 205-17	Srinivas, E; Murthy, JN; Rao, AR; Sastry, GN;
9	Structure-activity relationships of multidrug resistance reversers.	Current medicinal chemistry, 2001; 8 (6); 685-713	Wiese, M; Pajeva, IK;
10	Application of three-dimensional quantitative structure-activity relationships of P-glycoprotein inhibitors and substrates.	Molecular pharmacology, 2002; 61 (5); 974-81	Ekins, S; Kim, RB; Leake, BF; Dantzig, AH; Schuetz, EG; Lan, LB; Yasuda, K; Shepard, RL; Winter, MA; Schuetz, JD; Wikel, JH; Wrighton, SA;
11	Clinical manual of drug interaction principles for medical practice	American Psychiatric Publishing,Inc.2009; (); 608	Wynn, H.; Oesterheld, R.; Cozza, L.; Armstrong, C.;
12	From MDR to MXR: new understanding of multidrug resistance systems, their properties and clinical significance.	Cellular and molecular life sciences : CMLS, 2001; 58 (7); 931-59	Litman, T; Druley, TE; Stein, WD; Bates, SE;
13	Structure-activity relationship studies of propafenone analogs based on P-glycoprotein ATPase activity measurements.	Biochemical pharmacology, 1999; 58 (9); 1447-56	Schmid, D; Ecker, G; Kopp, S; Hitzler, M; Chiba, P;
14	Drug transporters and their role in multidrug resistance of neoplastic cells.	General physiology and biophysics, 2001; 20 (3); 215-37	Kvackajová-Kisucká, J; Barancik, M; Breier, A;
15	Comparison of steroid substrates and inhibitors of P-glycoprotein by 3D-QSAR analysis	Journal of Molecular Structure, 2005; 733 (1-3); 111-118	Li, Y.; Wang, Y.; Yang, L.; Zhang, S.; Liu, C.; Yang, S.;
16	Physical-chemical properties shared by compounds that modulate multidrug resistance in human leukemic cells.	Molecular pharmacology, 1988; 33 (4); 454-62	Zamora, JM; Pearce, HL; Beck, WT;
17	Strategies for overcoming ABC-transporters-mediated multidrug resistance (MDR) of tumor cells.	Acta biochimica Polonica, 2005; 52 (3); 609-27	Borowski, E; Bontemps-Gracz, MM; Piwkowska, A;
18	Reversal of p-glycoprotein-mediated multidrug resistance by CJX1, an amlodipine derivative, in doxorubicin-resistant human myelogenous leukemia (K562/DOX) cells.	Life sciences, 2005; 77 (18); 2221-32	Ji, BS; He, L; Liu, GQ;
19	3,5-dibenzoyl-1,4-dihydropyridines: synthesis and MDR reversal in tumor cells.	Bioorganic & medicinal chemistry, 2002; 10 (4); 1051-5	Kawase, M; Shah, A; Gaveriya, H; Motohashi, N; Sakagami, H; Varga, A; Molnár, J;

20	Lead identification for modulators of multidrug resistance based on in silico screening with a pharmacophoric feature model.	Archiv der Pharmazie, 2004; 337 (6); 317-27	Langer, T; Eder, M; Hoffmann, RD; Chiba, P; Ecker, GF;
21	Development of modulators of multidrug resistance: A pharmacoinformatic approach*	Pure and Applied Chemistry, 2004; 76 (5); 997–1005	Ecker, G.; Chiba, P.;
22	Agariblazeispirols A and B, an unprecedented skeleton from the cultured mycelia of the fungus, Agaricus blazei	Tetrahedron letters, 2003; 44 (43); 7975-7979	Hirotani, M.; Hirotani, S.; Takayanagi, H.; Komiyama, K.; Yoshikawa, T.;
23	Structure-activity relationships of novel N-acyloxy-1,4-dihydropyridines as P-glycoprotein inhibitors	Bioorganic & medicinal chemistry, 2007; 15 (15); 5110-3	Voigt, B; Coburger, C; Monár, J; Hilgeroth, A;
24	P-glycoprotein substrates and antagonists cluster into two distinct groups.	Molecular pharmacology, 1997; 51 (6); 1024-33	Scala, S; Akhmed, N; Rao, US; Paull, K; Lan, LB; Dickstein, B; Lee, JS; Elgemeie, GH; Stein, WD; Bates, SE;
25	Phenolic metabolites of Dalea versicolor that enhance antibiotic activity against model pathogenic bacteria.	Journal of natural products, 2004; 67 (3); 481-4	Belofsky, G; Percivill, D; Lewis, K; Tegos, GP; Ekart, J;
26	Synthesis and in vitro multidrug resistance modulating activity of a series of dihydrobenzopyrans and tetrahydroquinolines.	Journal of Medicinal Chemistry, 1999; 42 (11); 1921-6	Hiessböck, R; Wolf, C; Richter, E; Hitzler, M; Chiba, P; Kratzel, M; Ecker, G;
27	Structural requirements for activity of propafenone-type modulators in P-glycoprotein-mediated multidrug resistance.	Molecular pharmacology, 1996; 49 (6); 1122-30	Chiba, P; Ecker, G; Schmid, D; Drach, J; Tell, B; Goldenberg, S; Gekeler, V;
28	Jatrophane diterpenes as P-glycoprotein inhibitors. First insights of structure-activity relationships and discovery of a new, powerful lead.	Journal of Medicinal Chemistry, 2003; 46 (15); 3395-402	Corea, G; Fattorusso, E; Lanzotti, V; Taglialatela-Scafati, O; Appendino, G; Ballero, M; Simon, PN; Dumontet, C; Di Pietro, A;
29	Jatrophane diterpenes as modulators of multidrug resistance. Advances of structure-activity relationships and discovery of the potent lead pepluanin A.	Journal of Medicinal Chemistry, 2004; 47 (4); 988-92	Corea, G; Fattorusso, E; Lanzotti, V; Motti, R; Simon, PN; Dumontet, C; Di Pietro, A;
30	New 4-aryl-1,4-dihydropyridines and 4-arylpyridines as P-glycoprotein inhibitors.	Drug metabolism and disposition: the biological fate of chemicals, 2005; 33 (3); 321-8	Zhou, XF; Zhang, L; Tseng, E; Scott-Ramsay, E; Schentag, JJ; Coburn, RA; Morris, ME;
31	Studies of interactions between uracil-based hybrid molecules and P-glycoprotein--search for multidrug resistance modulators.	Bioorganic & medicinal chemistry, 2006; 14 (21); 7183-6	Singh, P; Paul, K;
32	Covalent inhibitors of P-glycoprotein ATPase activity.	The Journal of biological chemistry, 1994; 269 (12); 8986-92	al-Shawi, MK; Urbatsch, IL; Senior, AE;
33	Inhibition of P-glycoprotein transport function and reversion of MDR1 multidrug resistance by cnidiadin.	Cancer chemotherapy and pharmacology, 2005; 56 (2); 173-81	Barthomeuf, C; Grassi, J; Demeule, M; Fournier, C; Boivin, D; Béliveau, R;
34	Reversal of multidrug resistance of cancer through inhibition of P-glycoprotein by 5-bromotetrandrine.	Cancer chemotherapy and pharmacology, 2005; 55 (2); 179-88	Jin, J; Wang, FP; Wei, H; Liu, G;
35	In vitro activity of novel dual action MDR anthranilamide modulators with inhibitory activity on CYP-450 (Part 2).	Bioorganic & medicinal chemistry, 2007; 15 (11); 3854-68	Labrie, P; Maddaford, SP; Lacroix, J; Catalano, C; Lee, DK; Rakhit, S; Gaudreault, RC;
36	Discovery of a new series of jatrophane and lathyrane diterpenes as potent and specific P-glycoprotein modulators.	Organic & biomolecular chemistry, 2008; 6 (10); 1756-62	Barile, E; Borriello, M; Di Pietro, A; Doreau, A; Fattorusso, C; Fattorusso, E; Lanzotti, V;
37	Pharmacophore-Based Screening as a Clue for the Discovery of New P-Glycoprotein Inhibitors	Advances in Bioinformatics Advances in Soft Computing, 2010; 74 (); 175-180	Palmeira A.,; Rodrigues F.,; Sousa E.,; Pinto M.,; Vasconcelos M.H.,; Fernandes, M.;
38	Drugs as P-glycoprotein substrates, inhibitors, and inducers.	Drug metabolism reviews, 2002; 34 (1-2); 47-54	Kim, RB;
39	Many P-glycoprotein substrates do not inhibit the transport process across cell membranes.	Xenobiotica; the fate of foreign compounds in biological systems, 2003; 33 (2); 131-40	Barecki-Roach, M; Wang, EJ; Johnson, WW;
40	Evaluation of a vincristine resistant Caco-2 cell line for use in a calcein AM extrusion screening assay for P-glycoprotein interaction.	European journal of pharmaceutical sciences : official journal of the European Federation for Pharmaceutical Sciences, 2001; 12 (3); 205-14	Eneroth, A; Aström, E; Hoogstraate, J; Schrenk, D; Conrad, S; Kauffmann, HM; Gjellan, K;
41	Interactions between the flavonoid biochanin A and P-glycoprotein substrates in rats: in vitro and in vivo.	Journal of pharmaceutical sciences, 2010; 99 (1); 430-41	Zhang, S; Sagawa, K; Arnold, RD; Tseng, E; Wang, X; Morris, ME;

42	The role of efflux and uptake transporters in [N-{3-chloro-4-[(3-fluorobenzyl)oxy]phenyl}-6-[5-({[2-(methylsulfonyl)ethyl]amino}methyl)-2-furyl]-4-quinazolinamine (GW572016, lapatinib) disposition and drug interactions.	Drug metabolism and disposition: the biological fate of chemicals, 2008; 36 (4); 695-701	Polli, JW; Humphreys, JE; Harmon, KA; Castellino, S; O'Mara, MJ; Olson, KL; John-Williams, LS; Koch, KM; Serabjit-Singh, CJ;
43	Steroid treatment, accumulation, and antagonism of P-glycoprotein in multidrug-resistant cells.	Biochemistry, 1996; 35 (15); 4820-7	Barnes, KM; Dickstein, B; Cutler, GB; Fojo, T; Bates, SE;
44	Small P-gp modulating molecules: SAR studies on tetrahydroisoquinoline derivatives.	Bioorganic & medicinal chemistry, 2008; 16 (1); 362-73	Colabufo, NA; Berardi, F; Cantore, M; Perrone, MG; Contino, M; Inglese, C; Niso, M; Perrone, R; Azzariti, A; Simone, GM; Porcelli, L; Paradiso, A;
45	The importance of a nitrogen atom in modulators of multidrug resistance.	Molecular pharmacology, 1999; 56 (4); 791-6	Ecker, G; Huber, M; Schmid, D; Chiba, P;
46	Rapid identification of P-glycoprotein substrates and inhibitors.	Drug metabolism and disposition: the biological fate of chemicals, 2006; 34 (12); 1976-84	Chang, C; Bahadduri, PM; Polli, JE; Swaan, PW; Ekins, S;
47	Characterisation of (R/S)-propafenone and its metabolites as substrates and inhibitors of P-glycoprotein.	Naunyn-Schmiedeberg's archives of pharmacology, 2005; 371 (3); 195-201	Bachmakov, I; Rekersbrink, S; Hofmann, U; Eichelbaum, M; Fromm, MF;
48	European journal of pharmaceutical sciences : official journal of the European Federation for Pharmaceutical Sciences, 2001; 14 (1); 81-6	Active efflux of the 5-HT(1A) receptor agonist flesinoxan via P-glycoprotein at the blood-brain barrier.	van der Sandt, IC; Smolders, R; Nabulsi, L; Zuideveld, KP; de Boer, AG; Breimer, DD;
49	Can the enhanced renal clearance of antibiotics in cystic fibrosis patients be explained by P-glycoprotein transport?	Pharmaceutical research, 2002; 19 (4); 457-62	Susanto, M; Benet, LZ;
50	P-glycoprotein-mediated active efflux of the anti-HIV1 nucleoside abacavir limits cellular accumulation and brain distribution.	Drug metabolism and disposition: the biological fate of chemicals, 2007; 35 (11); 2076-85	Shaik, N; Giri, N; Pan, G; Elmquist, WF;
51	Rational use of in vitro P-glycoprotein assays in drug discovery.	The Journal of pharmacology and experimental therapeutics, 2001; 299 (2); 620-8	Polli, JW; Wring, SA; Humphreys, JE; Huang, L; Morgan, JB; Webster, LO; Serabjit-Singh, CS;
52	Comparative studies to determine the selective inhibitors for P-glycoprotein and cytochrome P4503A4.	AAPS pharmSci, 1999; 1 (4); E18	Achira, M; Suzuki, H; Ito, K; Sugiyama, Y;
53	Flavonoids: a class of modulators with bifunctional interactions at vicinal ATP- and steroid-binding sites on mouse P-glycoprotein.	Proceedings of the National Academy of Sciences of the United States of America, 1998; 95 (17); 9831-6	Conseil, G; Baubichon-Cortay, H; Dayan, G; Jault, JM; Barron, D; Di Pietro, A;
54	Synthesis, activity, and pharmacophore development for isatin-beta-thiosemicarbazones with selective activity toward multidrug-resistant cells.	Journal of Medicinal Chemistry, 2009; 52 (10); 3191-204	Hall, MD; Salam, NK; Hellawell, JL; Fales, HM; Kensler, CB; Ludwig, JA; Szakács, G; Hibbs, DE; Gottesman, MM;
55	Role of drug efflux transporters in the brain for drug disposition and treatment of brain diseases.	Progress in neurobiology, 2005; 76 (1); 22-76	Löscher, W; Potschka, H;
56	A computational ensemble pharmacophore model for identifying substrates of P-glycoprotein.	Journal of Medicinal Chemistry, 2002; 45 (9); 1737-40	Penzotti, JE; Lamb, ML; Evensen, E; Grootenhuis, PD;
57	Inhibition of P-glycoprotein-mediated transport by terpenoids contained in herbal medicines and natural products.	Food and chemical toxicology : an international journal published for the British Industrial Biological Research Association, 2006; 44 (12); 2033-9	Yoshida, N; Koizumi, M; Adachi, I; Kawakami, J;
58	Ranking of P-glycoprotein substrates and inhibitors by a calcein-AM fluorometry screening assay.	Anti-cancer drugs, 1996; 7 (5); 568-78	Tiberghien, F; Loor, F;
59	Annotating Human P-Glycoprotein Bioassay Data	Molecular informatics, 2012, 31, 599-609	Barbara Zdrazil,Marta Pinto,Poongavanam Vasanthanathan,Antony J. Williams,Linda Zander Balderud,Ola Engkvist,Christine Chichester,Anne Hersey,John P. Overington,and Gerhard F. Ecker
60	A Novel Approach for Predicting P-glycoprotein (ABCB1) Inhibition Using Molecular Interaction Fields	Journal of medicinal chemistry, 2011; 54(6): 1740–1751. doi:10.1021/jm101421d	Fabio Broccatellia, Emanuele Carosatia, Annalisa Nerib, Maria Frosinib, Laura Goraccic, Tudor I. Opread, and Gabriele Cruciania

61	ADME Evaluation in Drug Discovery. 10. Predictions of P-Glycoprotein Inhibitors Using Recursive Partitioning and Naive Bayesian Classification Techniques	Molecular pharmaceutics, 2011, 8, 889–900	Lei Chen,Youyong Li,Qing Zhao,Hui Peng,and Tingjun Hou
62	DrugBank 4.0: shedding new light on drug metabolism	Nucleic Acids Research,2014,42:D1091-7	Vivian Law, Craig Knox, Yannick Djoumbou, Tim Jewison1, An Chi Guo, Yifeng Liu, Adam Maciejewski, David Arndt, Michael Wilson, Vanessa Neveu, Alexandra Tang, Geraldine Gabriel, Carol Ly, Sakina Adamjee, Zerihun T. Dame, Beomsoo Han, You Zhou and David S. Wishart

Table S2. Descriptors calculated in the present work

Descriptor type	Number	Descriptor	Class	Reference
Acidic group	1	nAcid	2D	
ALOGP	3	ALogP, ALogp2, AMR	2D	Ghose, A.K. and Crippen, G.M. , Atomic physicochemical parameters for three-dimensional structure-directed quantitative structure-activity relationships. I. Partition coefficients as a measure of hydrophobicity, Journal of Computational
APol	1	apol	2D	
Aromatic atoms	1	naAromAtom	2D	
Aromatic bonds	1	nAromBond	2D	
Atom	14	nAtom, nHeavyAtom, nH, nB, nC, nN, nO, nS, nP, nF, nCl, nBr, nI, nX	2D	
Autocorrelation	346	ATS0m, ATS1m, ATS2m, ATS3m, ATS4m, ATS5m, ATS6m, ATS7m, ATS8m, ATS0v, ATS1v, ATS2v, ATS3v, ATS4v, ATS5v, ATS6v, ATS7v, ATS8v, ATS0e, ATS1e, ATS2e, ATS3e, ATS4e, ATS5e, ATS6e, ATS7e, ATS8e, ATS0p, ATS1p, ATS2p, ATS3p, ATS4p, ATS5p, ATS6p, ATS7p, ATS8p, ATS0i, ATS1i, ATS2i, ATS3i, ATS4i, ATS5i, ATS6i, ATS7i, ATS8i, ATS0s, ATS1s, ATS2s, ATS3s, ATS4s, ATS5s, ATS6s, ATS7s, ATS8s, AATS0m, AATS1m, AATS2m, AATS3m, AATS4m, AATS5m, AATS6m, AATS7m, AATS8m, AATS0v, AATS1v, AATS2v, AATS3v, AATS4v, AATS5v, AATS6v, AATS7v, AATS8v, AATS0e, AATS1e, AATS2e, AATS3e, AATS4e, AATS5e, AATS6e, AATS7e, AATS8e, AATS0p, AATS1p, AATS2p, AATS3p, AATS4p, AATS5p, AATS6p, AATS7p, AATS8p, AATS0i, AATS1i, AATS2i, AATS3i, AATS4i, AATS5i, AATS6i, AATS7i, AATS8i, AATS0s, AATS1s, AATS2s, AATS3s, AATS4s, AATS5s, AATS6s, AATS7s, AATS8s, ATSC0c, ATSC1c, ATSC2c, ATSC3c, ATSC4c, ATSC5c, ATSC6c, ATSC7c, ATSC8c, ATSC0m, ATSC1m, ATSC2m, ATSC3m, ATSC4m, ATSC5m, ATSC6m, ATSC7m, ATSC8m, ATSC0v, ATSC1v, ATSC2v, ATSC3v, ATSC4v, ATSC5v, ATSC6v, ATSC7v, ATSC8v, ATSC0e, ATSC1e, ATSC2e, ATSC3e, ATSC4e, ATSC5e, ATSC6e, ATSC7e, ATSC8e, ATSC0p, ATSC1p, ATSC2p, ATSC3p, ATSC4p, ATSC5p, ATSC6p, ATSC7p, ATSC8p, ATSC0i, ATSC1i, ATSC2i, ATSC3i, ATSC4i, ATSC5i, ATSC6i, ATSC7i, ATSC8i, ATSC0s, ATSC1s, ATSC2s, ATSC3s, ATSC4s, ATSC5s, ATSC6s, ATSC7s, ATSC8s, AATSC0c, AATSC1c, AATSC2c, AATSC3c, AATSC4c, AATSC5c, AATSC6c, AATSC7c, AATSC8c, AATSC0m, AATSC1m, AATSC2m, AATSC3m, AATSC4m, AATSC5m, AATSC6m, AATSC7m, AATSC8m, AATSC0v, AATSC1v, AATSC2v, AATSC3v, AATSC4v, AATSC5v, AATSC6v, AATSC7v, AATSC8v, AATSC0e, AATSC1e, AATSC2e, AATSC3e, AATSC4e, AATSC5e, AATSC6e, AATSC7e, AATSC8e, AATSC0p, AATSC1p, AATSC2p, AATSC3p, AATSC4p, AATSC5p, AATSC6p, AATSC7p, AATSC8p, AATSC0i, AATSC1i, AATSC2i, AATSC3i, AATSC4i, AATSC5i, AATSC6i, AATSC7i, AATSC8i, AATSC0s, AATSC1s, AATSC2s, AATSC3s, AATSC4s, AATSC5s, AATSC6s, AATSC7s, AATSC8s, MATS1c, MATS2c, MATS3c, MATS4c, MATS5c, MATS6c, MATS7c, MATS8c, MATS1m, MATS2m, MATS3m, MATS4m, MATS5m, MATS6m, MATS7m, MATS8m, MATS1v, MATS2v, MATS3v, MATS4v, MATS5v, MATS6v, MATS7v, MATS8v, MATS1e, MATS2e, MATS3e, MATS4e, MATS5e, MATS6e, MATS7e, MATS8e, MATS1p, MATS2p, MATS3p, MATS4p, MATS5p, MATS6p, MATS7p, MATS8p, MATS1i, MATS2i, MATS3i, MATS4i, MATS5i, MATS6i, MATS7i, MATS8i, MATS1s, MATS2s, MATS3s, MATS4s, MATS5s, MATS6s, MATS7s, MATS8s, GATS1c, GATS2c, GATS3c, GATS4c, GATS5c, GATS6c, GATS7c, GATS8c, GATS1m, GATS2m, GATS3m, GATS4m, GATS5m, GATS6m, GATS7m, GATS8m, GATS1v, GATS2v, GATS3v, GATS4v, GATS5v, GATS6v, GATS7v, GATS8v, GATS1e, GATS2e, GATS3e, GATS4e, GATS5e, GATS6e, GATS7e, GATS8e, GATS1p, GATS2p, GATS3p, GATS4p	2D	Todeschini, R. and Consonni, V. (2009). Molecular descriptors for chemoinformatics, (Weinheim: Wiley VCH) pg 27-37
Barysz matrix	91	SpAbs_DzZ, SpMax_DzZ, SpDiam_DzZ, SpAD_DzZ, SpMAD_DzZ, EE_DzZ, SM1_DzZ, VE1_DzZ, VE2_DzZ, VE3_DzZ, VR1_DzZ, VR2_DzZ, VR3_DzZ, SpAbs_Dzm, SpMax_Dzm, SpDiam_Dzm, SpAD_Dzm, SpMAD_Dzm, EE_Dzm, SM1_Dzm, VE1_Dzm, VE2_Dzm, VE3_Dzm, VR1_Dzm, VR2_Dzm, VR3_Dzm, SpAbs_Dzv, SpMax_Dzv, SpDiam_Dzv, SpAD_Dzv, SpMAD_Dzv, EE_Dzv, SM1_Dzv, VE1_Dzv, VE2_Dzv, VE3_Dzv, VR1_Dzv, VR2_Dzv, VR3_Dzv, SpAbs_Dze, SpMax_Dze, SpDiam_Dze, SpAD_Dze, SpMAD_Dze, EE_Dze, SM1_Dze, VE1_Dze, VE2_Dze, VE3_Dze, VR1_Dze, VR2_Dze, VR3_Dze, SpAbs_Dzp, SpMax_Dzp, SpDiam_Dzp, SpAD_Dzp, SpMAD_Dzp, EE_Dzp, SM1_Dzp, VE1_Dzp, VE2_Dzp, VE3_Dzp, VR1_Dzp, VR2_Dzp, VR3_Dzp, SpAbs_Dzi, SpMax_Dzi, SpDiam_Dzi, SpAD_Dzi, SpMAD_Dzi, EE_Dzi, SM1_Dzi, VE1_Dzi, VE2_Dzi, VE3_Dzi, VR1_Dzi, VR2_Dzi, VR3_Dzi, SpAbs_Dzs, SpMax_Dzs, SpDiam_Dzs, SpAD_Dzs, SpMAD_Dzs, EE_Dzs, SM1_Dzs, VE1_Dzs, VE2_Dzs, VE3_Dzs, VR1_Dzs, VR2_Dzs,	2D	Todeschini, R. and Consonni, V. (2009). Molecular descriptors for chemoinformatics, (Weinheim: Wiley VCH) pg 714-726
Basic group	1	nBase	2D	
BCUT	6	BCUTw-1l, BCUTw-1h, BCUTc-1l, BCUTc-1h, BCUTp-1l, BCUTp-1h	2D	Pearlman, R.S. and

Bond count	10	nBonds, nBonds2, nBondsS, nBondsS2, nBondsS3, nBondsD, nBondsD2, nBondsT, nBondsQ, nBondsM	2D	
BPol	1	bpol	2D	
Burden modified eigenvalues	96	SpMax1_Bhm, SpMax2_Bhm, SpMax3_Bhm, SpMax4_Bhm, SpMax5_Bhm, SpMax6_Bhm, SpMax7_Bhm, SpMax8_Bhm, SpMin1_Bhm, SpMin2_Bhm, SpMin3_Bhm, SpMin4_Bhm, SpMin5_Bhm, SpMin6_Bhm, SpMin7_Bhm, SpMin8_Bhm, SpMax1_Bhv, SpMax2_Bhv, SpMax3_Bhv, SpMax4_Bhv, SpMax5_Bhv, SpMax6_Bhv, SpMax7_Bhv, SpMax8_Bhv, SpMin1_Bhv, SpMin2_Bhv, SpMin3_Bhv, SpMin4_Bhv, SpMin5_Bhv, SpMin6_Bhv, SpMin7_Bhv, SpMin8_Bhv, SpMax1_Bhe, SpMax2_Bhe, SpMax3_Bhe, SpMax4_Bhe, SpMax5_Bhe, SpMax6_Bhe, SpMax7_Bhe, SpMax8_Bhe, SpMin1_Bhe, SpMin2_Bhe, SpMin3_Bhe, SpMin4_Bhe, SpMin5_Bhe, SpMin6_Bhe, SpMin7_Bhe, SpMin8_Bhe, SpMax1_Bhp, SpMax2_Bhp, SpMax3_Bhp, SpMax4_Bhp, SpMax5_Bhp, SpMax6_Bhp, SpMax7_Bhp, SpMax8_Bhp, SpMin1_Bhp, SpMin2_Bhp, SpMin3_Bhp, SpMin4_Bhp, SpMin5_Bhp, SpMin6_Bhp, SpMin7_Bhp, SpMin8_Bhp, SpMax1_Bhi, SpMax2_Bhi, SpMax3_Bhi, SpMax4_Bhi, SpMax5_Bhi, SpMax6_Bhi, SpMax7_Bhi, SpMax8_Bhi, SpMin1_Bhi, SpMin2_Bhi, SpMin3_Bhi, SpMin4_Bhi, SpMin5_Bhi, SpMin6_Bhi, SpMin7_Bhi, SpMin8_Bhi, SpMax1_Bhs, SpMax2_Bhs, SpMax3_Bhs, SpMax4_Bhs, SpMax5_Bhs, SpMax6_Bhs, SpMax7_Bhs, SpMax8_Bhs, SpMin1_Bhs, SpMin2_Bhs, SpMin3_Bhs, SpMin4_Bhs,	2D	Todeschini, R. and Consonni, V. (2009). Molecular descriptors for chemoinformatics, (Weinheim: Wiley VCH) pg 714-726
Carbon	9	C1SP1, C2SP1, C1SP2, C2SP2, C3SP2, C1SP3, C2SP3, C3SP3, C4SP3	2D	
Chi chain	10	SCH-3, SCH-4, SCH-5, SCH-6, SCH-7, VCH-3, VCH-4, VCH-5, VCH-6, VCH-7	2D	Kier, L. B., and Hall, L. H. (1976). Molecular
Chi cluster	8	SC-3, SC-4, SC-5, SC-6, VC-3, VC-4, VC-5, VC-6	2D	Kier, L. B., and Hall, L. H. (1976). Molecular
Chi path cluster	6	SPC-4, SPC-5, SPC-6, VPC-4, VPC-5, VPC-6	2D	Kier, L. B., and Hall, L. H. (1976). Molecular
Chi path	32	SP-0, SP-1, SP-2, SP-3, SP-4, SP-5, SP-6, SP-7, ASP-0, ASP-1, ASP-2, ASP-3, ASP-4, ASP-5, ASP-6, ASP-7, VP-0, VP-1, VP-2, VP-3, VP-4, VP-5, VP-6, VP-7, AVP-0, AVP-1, AVP-2, AVP-3, AVP-4, AVP-5, AVP-6, AVP-7	2D	Kier, L. B., and Hall, L. H. (1976). Molecular connectivity in chemistry
Constituti	12	Sv, Sse, Spe, Sare, Sp, Si, Mv, Mse, Mpe, Mare, Mp, Mi	2D	
Crippen logP and MR	2	CrippenLogP, CrippenMR	2D	Wildman, S. A., and Crippen, G. M. (1999). Prediction of
Detour matrix	11	SpMax_Dt, SpDiam_Dt, SpAD_Dt, SpMAD_Dt, EE_Dt, VE1_Dt, VE2_Dt, VE3_Dt, VR1_Dt, VR2_Dt, VR3_Dt	2D	Todeschini, R. and Consonni, V. (2009).
Eccentric connectivity index	1	ECCEN	2D	Sharma, V. and Goswami, R. and Madan, A.K. , Eccentric Connectivity Index: A Novel Highly Discriminating Topological
Atom type electrotopological state	489	nHBd, nwHBd, nHBa, nwHBa, nHBint2, nHBint3, nHBint4, nHBint5, nHBint6, nHBint7, nHBint8, nHBint9, nHBint10, nHsOH, nHdNH, nHssH, nHsNH2, nHssNH, nHaaNH, nHsNH3p, nHssNH2p, nHsssNHp, nHtCH, nHdCH2, nHdsCH, nHaaCH, nHCHnX, nHCsats, nHCsatu, nHAvin, nHother, nHmisc, nsLi, nssBe, nssssBem, nsBH2, nssBH, nsssB, nssssBm, nsCH3, ndCH2, nssCH2, ntCH, ndsCH, naaCH, nsssCH, nddC, ntsC, ndssC, naasC, naaaC, nssssC, nsNH3p, nsNH2, nssNH2p, ndNH, nssNH, naaNH, ntN, nsssNHp, ndsN, naaN, nsssN, nddsN, naasN, nssssNp, nsOH, ndO, nssO, naaO, naOm, nsOm, nsF, nsSiH3, nssSiH2, nsssSiH, nssssSi, nsPH2, nssPH, nsssP, ndsssP, nddsP, nssssssP, nsSH, ndS, nssS, naaS, ndssS, nddssS, nsssssssS, nSm, nsCl, nsGeH3, nssGeH2, nsssGeH, nssssGe, nsAsH2, nssAsH, nsssAs, ndsssAs, nddsAs, nsssssAs, nsSeH, ndSe, nssSe, naaSe, ndssSe, nsssssssSe, nddssSe, nsBr, nsSnH3, nssSnH2, nsssSnH, nssssSn, nsI, nsPbH3, nssPbH2, nsssPbH, nssssPb, SHBd, SwHBd, SHBa, SwHBa, SHBint2, SHBint3, SHBint4, SHBint5, SHBint6, SHBint7, SHBint8, SHBint9, SHBint10, SHsOH, SHdNH, SHsSH, SHsNH2, SHssNH, SHaaNH, SHsNH3p, SHssNH2p, SHsssNHp, SHtCH, SHdCH2, SHdsCH, SHaaCH, SHCHnX, SHCsats, SHCsatu, SHAvin, SHother, SHmisc, SsLi, SssBe, SssssBem, SsBH2, SssBH, SssssB, SssssBm, SsCH3, SdCH2, SssCH2, StCH, SdsCH, SaaCH, SsssCH, SddC, StsC, SdssC, SaasC, SaaaC, SssssC, SsNH3p, SsNH2, SssNH2p, SdNH, SssNH, SaaNH, StN, SsssNHp, SdsN, SaaN, SsssN, SddsN, SaasN, SssssNp, SsOH, SdO, SssO, SaaO, SaOm, SsOm, SsF, SsSiH3, SssSiH2, SsssSiH, SssssSi, SsPH2, SssPH, SsssP, SdsssP, SddsP, SssssssP, SsSH, SdS, SssS, SaaS, SdssS, SdddsS, SssssssS, SSm, SsCl, SsGeH3, SssGeH2, SsssGeH, SssssGe, SsAsH2, SssAsH, SsssAs, SdsssAs, SdddsAs, SssssssAs, SsSeH, SdSe, SssSe, SaaSe, SdssSe, SssssssSe, SdddsSe, SsBr, SsSnH3, SssSnH2, SssssSnH, SssssSn, SsI, SsPbH3, SssPbH2, SsssPbH, SssssPb, minHBd, minwHBd, minHBa, minwHBa, minHBint2, minHBint3, minHBint4, minHBint5, minHBint6, minHBint7, minHBint8, minHBint9, minHBint10, minHsOH, minHdNH, minHsSH, minHsNH2, minHssNH, minHaaNH, minHsNH3p, minHssNH2p, minHsssNHp, minHtCH, minHdCH2, minHdsCH, minHaaCH, minHCHnX, minHCsats, minHCsatu, minHAvin, minHother, minHmisc, minsLi, minssBe, minssssBem, minsBH2, minssBH, minsssB, minssssBm, minsCH3, mindCH2, minssCH2, mintCH, mindsCH, minaaCH, minsssCH, minddC, mintsC, mindssC, minaasC, minaaaC, minssssC, minsNH3p, minsNH2, minssNH2p, mindNH, minssNH, minaaNH, mintN, minsssNHp, mindsN, minaaN, minsssN, minddsN, minaasN, minssssNp, minsOH, mindO, minssO, minaaO, minaOm, minsOm, minsF, minsSiH3, minssSiH2, minsssSiH, minssssSi, minsPH2, minssPH, minsssP, mindsssP, minddsP, minsssssP, minsSH, mindS, minssS, minaaS, mindssS, minddssS, minsssssssS, minSm, minsCl, minsGeH3, minssGeH2, minsssGeH, minssssGe, minsAsH2, minssAsH, minsssAs, mindsssAs, minddsAs, minssssAs, minsSeH, mindSe, minssSe, minaaSe, mindssSe, minsssssssSe, minddsSe, minsBr, minsSnH3, minssSnH2, minsssSnH, minssssSn, minsI, minsPbH3, minssPbH2, minsssPbH, minssssPb, maxHBd, maxwHBd, maxHBa, maxwHBa, maxHBint2, maxHBint3, maxHBint4, maxHBint5, maxHBint6, maxHBint7, maxHBint8, maxHBint9, maxHBint10, maxHsOH, maxHdNH, maxHsSH, maxHsNH2, maxHssNH, maxHaaNH, maxHsNH3p, maxHssNH2p, maxHsssNHp, maxHtCH, maxHdCH2, maxHdsCH, maxHaaCH, maxHCHnX, maxHCsats, maxHCsatu, maxHAvin, maxHother, maxHmisc, maxsLi, maxssBe, maxssssBem, maxsBH2, maxssBH, maxsssB, maxssssBm, maxsCH3, maxdCH2, maxssCH2, maxtCH, maxdsCH, maxaaCH, maxsssCH, maxddC, maxtsC, maxdssC, maxaasC, maxaaaC, maxssssC, maxsNH3p, maxsNH2, maxssNH2p, maxdNH, maxssNH, maxaaNH, maxtN, maxsssNHp, maxdsN, maxaaN, maxsssN, maxddsN, maxaasN, maxssssNp, maxsOH, maxdO, maxssO, maxaaO, maxaOm, maxsOm, maxsF, maxsSiH3, maxssSiH2, maxsssSiH, maxssssSi, maxsPH2, maxssPH, maxsssP, maxdsssP, maxddsP, maxssssssP, maxsSH, maxdS, maxsssS, maxaaS, maxdssS, maxddssS, maxsssssssS, maxSm, maxsCl, maxsGeH3, maxssGeH2, maxsssGeH, maxssssGe, maxsAsH2, maxssAsH, maxsssAs, maxdsssAs, maxddsAs, maxssssssAs, maxsSeH, maxdSe, maxssSe, maxaaSe, maxdssSe, maxsssssssSe, maxddssSe, maxsBr, maxsSnH3, maxssSnH2, maxsssSnH, maxssssSn, maxsI, maxsPbH3, maxssPbH2, maxsssPbH, maxssssPb, sumI, meanI, hmax, gmax, hmin, gmin, LipoaffinityIndex, MAXDN, MAXDP, DELS, MAXDN2, MAXDP2, DELS2	2D	Hall, L. H., and Kier, L. B. (1995). Electrotopological state indices for atom types: A novel combination of electronic, topological, and valence state information. J Chem Inf Comput Sci 35, 1039-1045; Liu, R., Sun, H., and So, S. S. (2001). Development of quantitative structure-property relationship models for early ADME evaluation in drug discovery. 2. Blood-brain barrier penetration. J Chem Inf Comput Sci 41, 1623-1632.; Gramatica, P., Corradi, M., and Consonni, V. (2000). Modelling and prediction of soil sorption coefficients of non-ionic organic pesticides by molecular descriptors. Chemosphere 41, 763-777.

Extended topochemical atom	43	ETA_Alpha, ETA_AlphaP, ETA_dAlpha_A, ETA_dAlpha_B, ETA_Epsilon_1, ETA_Epsilon_2, ETA_Epsilon_3, ETA_Epsilon_4, ETA_Epsilon_5, ETA_dEpsilon_A, ETA_dEpsilon_B, ETA_dEpsilon_C, ETA_dEpsilon_D, ETA_Psi_1, ETA_dPsi_A, ETA_dPsi_B, ETA_Shape_P, ETA_Shape_Y, ETA_Shape_X, ETA_Beta, ETA_BetaP, ETA_Beta_s, ETA_BetaP_s, ETA_Beta_ns, ETA_BetaP_ns, ETA_dBeta, ETA_dBetaP, ETA_Beta_ns_d, ETA_BetaP_ns_d, ETA_Eta, ETA_EtaP, ETA_Eta_R, ETA_Eta_F, ETA_EtaP_F, ETA_Eta_L, ETA_EtaP_L, ETA_Eta_R_L, ETA_Eta_F_L, ETA_EtaP_F_L, ETA_Eta_B, ETA_EtaP_B, ETA_Eta_B_RC, ETA_EtaP_B_RC	2D	Roy K & Ghosh G, QSTR with Extended Topochemical Atom Indices. 2. Fish Toxicity of Substituted Benzenes. J. Chem. Inf. Comput. Sci., 44, 2004, 559-567. http://dx.doi.org/10.1021/ci0342066;
FMFDescriptor	1	FMF	2D	Roy K, Das R N, On some Yang, Y. and Chen, H. and Nilsson, I. and Muresan, S. and Engkvist, O., Investigation of the Relationship between
Fragment complexity	1	fragC	2D	Nilakantan, R. and Nunn, D.S. and Greenblatt, L. and Walker, G. and Haraki, K. and Mobilio, D., A family of ring system-based structural
Hbond acceptor count	4	nHBAcc, nHBAcc2, nHBAcc3, nHBAcc_Lipinski	2D	
Hbond donor	2	nHBDon, nHBDon_Lipinski	2D	
Hybridization ratio	1	HybRatio	2D	
Information content	42	IC0, IC1, IC2, IC3, IC4, IC5, TIC0, TIC1, TIC2, TIC3, TIC4, TIC5, SIC0, SIC1, SIC2, SIC3, SIC4, SIC5, CIC0, CIC1, CIC2, CIC3, CIC4, CIC5, BIC0, BIC1, BIC2, BIC3, BIC4, BIC5, MIC0, MIC1, MIC2, MIC3, MIC4, MIC5, ZMIC0, ZMIC1, ZMIC2, ZMIC3, ZMIC4, ZMIC5	2D	Todeschini, R. and Consonni, V. (2009). Molecular descriptors for
Kappa shape indices	3	Kier1, Kier2, Kier3	2D	Hall, L. H., and Kier, L. B. (1991). The molecular connectivity chi indices and kappa shape indices in structure-property
Largest	1	nAtomLC	2D	
Largest Pi system	1	nAtomP	2D	
Longest aliphatic	1	nAtomLAC	2D	
Mannhold LogP	1	MLogP	2D	Mannhold, R. and Poda, G.I. and Ostermann, C. and Tetko, I.V., Calculation of molecular lipophilicity: State of the
McGowan volume	1	McGowan_Volume	2D	Abraham MH, McGowan JC. The use of characteristic volumes to
Molecular distance edge	19	MDEC-11, MDEC-12, MDEC-13, MDEC-14, MDEC-22, MDEC-23, MDEC-24, MDEC-33, MDEC-34, MDEC-44, MDEO-11, MDEO-12, MDEO-22, MDEN-11, MDEN-12, MDEN-13, MDEN-22, MDEN-23, MDEN-33	2D	Liu, S. and Cao, C. and Li, Z. , Approach to Estimation and Prediction for Normal Boiling Point (NBP) of Alkanes Based
Molecular linear free energy relation	6	MLFER_A, MLFER_BH, MLFER_BO, MLFER_S, MLFER_E, MLFER_L	2D	Platts JA, Butina D, Abraham MH, Hersey A. Estimation of molecular free energy relation descriptors using a group
Path counts	22	MPC2, MPC3, MPC4, MPC5, MPC6, MPC7, MPC8, MPC9, MPC10, TPC, piPC1, piPC2, piPC3, piPC4, piPC5, piPC6, piPC7, piPC8, piPC9, piPC10, TpiPC, R_TpiPCTPC	2D	Todeschini, R. and Consonni, V. (2009). Molecular descriptors for
Petitjean number	1	PetitjeanNumber	2D	

Ring count	68	nRing, n3Ring, n4Ring, n5Ring, n6Ring, n7Ring, n8Ring, n9Ring, n10Ring, n11Ring, n12Ring, nG12Ring, nFRing, nF4Ring, nF5Ring, nF6Ring, nF7Ring, nF8Ring, nF9Ring, nF10Ring, nF11Ring, nF12Ring, nFG12Ring, nHeteroRing, n3HeteroRing, n4HeteroRing, n5HeteroRing, n6HeteroRing, n7HeteroRing, n8HeteroRing, n9HeteroRing, n10HeteroRing, n11HeteroRing, n12HeteroRing, nG12HeteroRing, nFHeteroRing, nF4HeteroRing, nF5HeteroRing, nF6HeteroRing, nF7HeteroRing, nF8HeteroRing, nF9HeteroRing, nF10HeteroRing, nF11HeteroRing, nF12HeteroRing, nFG12HeteroRing, nTHeteroRing, nT4HeteroRing, nT5HeteroRing, nT6HeteroRing, nT7HeteroRing, nT8HeteroRing, nT9HeteroRing, nT10HeteroRing, nT11HeteroRing, nT12HeteroRing, nTG12HeteroRing	2D	
Rotatable bonds	4	nRotB, RotBFrac, nRotBt, RotBtFrac	2D	
Rule of	1	LipinskiFailures	2D	
Topologic	3	topoRadius, topoDiameter, topoShape	2D	
Topological charge	21	GGI1, GGI2, GGI3, GGI4, GGI5, GGI6, GGI7, GGI8, GGI9, GGI10, JGI1, JGI2, JGI3, JGI4, JGI5, JGI6, JGI7, JGI8, JGI9, JGI10, JGT	2D	Todeschini, R. and Consonni, V. (2009). Molecular descriptors for
Topological distance	11	SpMax_D, SpDiam_D, SpAD_D, SpMAD_D, EE_D, VE1_D, VE2_D, VE3_D, VR1_D, VR2_D, VR3_D	2D	Todeschini, R. and Consonni, V. (2009). Molecular descriptors for
Topological polar surface area	1	TopoPSA	2D	Ertl, P. and Rohde, B. and Selzer, P., Fast Calculation of Molecular Polar Surface Area as a
Van der Waals	1	VABC	2D	
Vertex adjacency information	1	vAdjMat	2D	
Walk counts	20	MWC2, MWC3, MWC4, MWC5, MWC6, MWC7, MWC8, MWC9, MWC10, TWC, SRW2, SRW3, SRW4, SRW5, SRW6, SRW7, SRW8, SRW9, SRW10, TSRW	2D	Todeschini, R. and Consonni, V. (2009). Molecular descriptors for
Weight	2	MW, AMW	2D	
Weighted path	5	WTPT-1, WTPT-2, WTPT-3, WTPT-4, WTPT-5	2D	Randic, M. , On molecular identification numbers ,
Wiener numbers	2	WPATH, WPOL	2D	Wiener, Harry, Structural Determination of Paraffin
XLogP	1	XLogP	2D	Wang, R., Fu, Y., and Lai, L., A New Atom-Additive Method for Calculating Partition Coefficients, Journal of Chemical Information and Computer Sciences, 1997, 37:615-
Zagreb	1	Zagreb	2D	
Estate fingerprint	79	E-State fragments	Fingerprint	Hall LH, Kier LB. Electrotopological state indices for atom types: A
MACCS fingerprint	166	MACCS keys	Fingerprint	
Pubchem fingerprint	881	Pubchem fingerprint	Fingerprint	ftp://ftp.ncbi.nlm.nih.gov/pubchem/specifications/pu
Substructure	307	Presence of SMARTS Patterns for Functional Group Classification by Christian Laggner	Fingerprint	Openbabel's SMARTS_InteLigand.txt
Klekota-Roth	4860	Presence of chemical substructures	Fingerprint	Klekota J, Roth FP. Chemical substructures
2D atom pairs	780	Presence of atom pairs at various topological distances	Fingerprint	
Checkmol fingerprint	204	Functionality Pattern Matching	Fingerprint	Vienna.Functionality Pattern Matching as an Efficient Complementary Structure/Reaction Search

Table S3. Skewness of Box-Cox transformation for 28 continuous descriptors

Descriptors	Skewness of Box-Cox transformation		
	Original	Transformed	λ
AATS2m	4.35	-0.27	-0.9
AATS3m	19.50	-0.40	-0.3
AATS4m	14.36	-0.25	0
AATS4p	3.37	0.10	0
AATS2s	4.43	-0.08	-1.2
ATSC0m	11.53	0.69	-0.2
AATSC0c	34.01	-0.51	-0.3
AATSC0m	18.79	1.13	-2
AATSC0i	5.39	-0.30	-2
VR1_Dzp	18.59	-0.27	-0.3
VR1_Dzs	14.26	-0.85	-0.3
BCUTw.1l	-2.19	-2.01	2
SpMax1_Bhm	8.22	3.64	-2
SpMax2_Bhm	13.19	-1.66	-1.7
SpMax3_Bhm	10.10	0.43	-0.1
SpMax4_Bhm	2.21	2.21	1
SpMax2_Bhp	-2.67	-2.18	2
SpMin3_Bhs	-2.16	-1.39	2
AVP.0	3.18	0.10	-2
VR1_Dt	18.32	0.14	-0.3
VR2_Dt	7.63	0.33	-0.6
ETA_AlphaP	5.03	1.15	-2
BIC0	2.07	0.14	-2
MIC0	3.77	-0.09	-1.2
R_TpiPCTPC	2.52	0.00	0
VR1_D	9.88	-0.72	-0.4
VR3_D	2.39	-0.30	0.1
WPATH	5.03	-0.49	0.1

Table S4. Statistics of continuous descriptors for both data sets

Descriptors	Mean±SD	
	Training	Test
ALogp2	3.074±8.054	2.991±6.684
AATS2m	77.827±21.182	76.542±17.809
AATS3m	67.148±29.482	64.871±17.845
AATS4m	58.924±37.025	56.658±20.666
AATS5m	55.464±40.257	52.739±17.843
AATS6m	53.576±45.8	50.531±18.757
AATS7m	48.95±35.889	47.64±33.545
AATS8m	45.866±53.353	43.779±19.128
AATS2v	218.084±24.544	216.766±22.172
AATS2e	7.74±0.251	7.725±0.226
AATS5e	7.624±0.433	7.607±0.302
AATS6e	7.589±0.6	7.588±0.399
AATS4p	1.288±0.187	1.28±0.147
AATS5p	1.238±0.197	1.227±0.155
AATS6p	1.226±0.227	1.212±0.18
AATS7p	1.173±0.24	1.171±0.209
AATS8p	1.135±0.302	1.129±0.231
AATS0i	162.41±3.513	162.401±3.2
AATS2i	154.649±4.488	154.632±4.319
AATS3i	156.949±4.391	157.118±4.253
AATS4i	159.775±4.324	159.69±4.206
AATS5i	161.243±6.748	161.384±4.245
AATS6i	160.821±11.163	161.435±7.013
AATS7i	160.894±17.454	161.462±14.202
AATS8i	160.995±21.077	160.881±20.171
AATS1s	2.985±0.434	2.97±0.408
AATS2s	2.937±0.84	2.908±0.721
AATS4s	2.812±0.804	2.791±0.764
AATS5s	2.805±0.853	2.789±0.822
AATS6s	2.812±1.047	2.803±1.197
AATS7s	2.705±1.093	2.662±0.85
AATS8s	2.629±1.081	2.588±0.895
ATSC1c	-0.507±3.434	-0.571±3.905
ATSC4c	-0.033±0.422	-0.049±0.444
ATSC5c	-0.03±0.258	-0.027±0.249
ATSC6c	0.059±0.346	0.069±0.385
ATSC7c	-0.033±0.336	-0.039±0.372
ATSC8c	-0.004±0.243	0±0.259
ATSC0m	2371.169±1286.565	2383.539±1700.752
ATSC2m	201.086±453.099	196.995±470.097
ATSC3m	-197.288±508.252	-195.597±490.71

ATSC4m	-164.631±603.903	-180.185±678.45
ATSC5m	-135.605±633.519	-126.608±761.835
ATSC6m	-314.174±778.761	-349.181±918.349
ATSC7m	-174.041±765.331	-180.776±850.705
ATSC8m	-307.393±734.316	-306.123±781.185
ATSC1v	4.121±144.253	2.435±148.465
ATSC5v	-100.062±679.301	-98.711±695.885
ATSC7v	-219.286±904.917	-218.648±901.336
ATSC1e	-0.153±0.39	-0.153±0.377
ATSC3e	-0.029±1.158	-0.044±1.176
ATSC4e	-0.222±1.537	-0.283±1.549
ATSC5e	-0.377±1.264	-0.351±1.219
ATSC6e	-0.228±1.366	-0.24±1.294
ATSC8e	-0.313±1.365	-0.244±1.284
ATSC0p	14.197±5.691	14.291±5.981
ATSC3p	-1.431±3.087	-1.385±3.008
ATSC4p	-2.362±3.835	-2.434±3.906
ATSC5p	-0.17±3.457	-0.189±3.444
ATSC6p	-1.375±3.982	-1.456±4.133
ATSC8p	-0.747±3.681	-0.954±3.596
ATSC1i	-12.016±14.61	-12.382±14.951
ATSC4i	-14.646±26.472	-15.048±26.104
ATSC5i	-1.651±24.301	-1.638±23.738
ATSC6i	-6.386±25.083	-6.188±24.034
ATSC7i	-6.671±23.943	-6.384±23.498
ATSC8i	-0.416±20.687	-1.936±19.448
ATSC1s	-5.533±9.302	-5.491±9.772
ATSC2s	9.809±25.363	9.696±24.904
ATSC3s	-1.788±17.847	-2.561±17.689
ATSC5s	-3.991±28.181	-2.933±29.755
ATSC6s	-6.031±29.56	-6.719±28.959
ATSC7s	-4.456±28.649	-5.049±34.565
ATSC8s	-2.689±33.128	-1.986±32.919
AATSC0c	0.018±0.099	0.019±0.099
AATSC3c	0±0.003	0±0.002
AATSC4c	0±0.002	0±0.002
AATSC5c	0±0.002	0±0.002
AATSC6c	0±0.003	0±0.003
AATSC7c	0±0.002	0±0.002
AATSC8c	0±0.003	0±0.003
AATSC0m	42.535±32.732	41.841±38.581
AATSC1m	1.964±2.665	2.023±2.693
AATSC2m	1.636±4.574	1.535±4.433
AATSC3m	-1.736±4.752	-1.719±4.34

AATSC4m	-1.422±6.826	-1.489±6.318
AATSC5m	-0.7±6.418	-0.677±8.014
AATSC6m	-2.444±13.06	-2.361±10.474
AATSC7m	-1.853±14.671	-1.314±11.633
AATSC8m	-2.123±14.571	-1.648±10.622
AATSC0v	50.554±3.389	50.679±2.726
AATSC3e	-0.001±0.009	-0.001±0.009
AATSC5e	-0.003±0.011	-0.003±0.009
AATSC6e	-0.001±0.015	-0.001±0.017
AATSC7e	-0.002±0.019	-0.002±0.016
AATSC8e	-0.003±0.019	-0.002±0.014
AATSC1p	-0.008±0.021	-0.009±0.021
AATSC2p	0.015±0.028	0.013±0.029
AATSC3p	-0.011±0.025	-0.01±0.024
AATSC4p	-0.016±0.028	-0.017±0.028
AATSC6p	-0.01±0.037	-0.009±0.033
AATSC7p	-0.008±0.042	-0.006±0.034
AATSC8p	-0.003±0.044	-0.005±0.041
AATSC0i	1.484±0.306	1.473±0.229
AATSC1i	-0.182±0.207	-0.189±0.207
AATSC2i	0.1±0.218	0.087±0.194
AATSC3i	-0.044±0.176	-0.035±0.166
AATSC4i	-0.095±0.159	-0.095±0.156
AATSC5i	-0.014±0.165	-0.016±0.154
AATSC6i	-0.044±0.197	-0.04±0.175
AATSC7i	-0.033±0.196	-0.028±0.173
AATSC8i	0.001±0.197	-0.015±0.195
AATSC1s	-0.102±0.184	-0.101±0.182
AATSC2s	0.103±0.313	0.097±0.272
AATSC3s	-0.013±0.138	-0.023±0.152
AATSC4s	-0.024±0.224	-0.026±0.198
AATSC5s	-0.056±0.229	-0.045±0.213
AATSC6s	-0.026±0.305	-0.022±0.429
AATSC7s	-0.04±0.332	-0.043±0.355
MATS2c	-0.072±0.152	-0.069±0.149
MATS3c	0.022±0.113	0.024±0.111
MATS4c	0.007±0.109	0.004±0.108
MATS5c	-0.016±0.109	-0.015±0.102
MATS6c	0.016±0.12	0.019±0.137
MATS7c	-0.001±0.123	-0.004±0.126
MATS8c	-0.006±0.121	-0.002±0.109
MATS2m	0.039±0.089	0.034±0.086
MATS3m	-0.04±0.093	-0.039±0.085
MATS4m	-0.034±0.099	-0.04±0.098

MATS5m	-0.018±0.106	-0.016±0.105
MATS6m	-0.053±0.152	-0.052±0.137
MATS7m	-0.035±0.168	-0.034±0.172
MATS8m	-0.04±0.187	-0.038±0.186
MATS7v	-0.03±0.151	-0.027±0.148
MATS1e	-0.02±0.075	-0.02±0.072
MATS4e	-0.01±0.11	-0.014±0.104
MATS5e	-0.037±0.113	-0.035±0.103
MATS1s	-0.051±0.089	-0.049±0.086
MATS2s	0.043±0.118	0.04±0.112
MATS3s	-0.005±0.084	-0.005±0.083
MATS4s	-0.007±0.108	-0.011±0.099
MATS5s	-0.035±0.111	-0.031±0.102
MATS6s	-0.033±0.139	-0.031±0.144
MATS7s	-0.032±0.139	-0.032±0.144
MATS8s	-0.041±0.158	-0.041±0.147
GATS1c	1.423±0.168	1.427±0.161
GATS2c	1.239±0.337	1.237±0.34
GATS3c	1.088±0.212	1.085±0.191
GATS4c	1.03±0.216	1.037±0.219
GATS5c	1.064±0.254	1.062±0.253
GATS6c	1.013±0.281	1.021±0.279
GATS7c	0.984±0.281	0.991±0.281
GATS1m	0.823±0.131	0.832±0.128
GATS2m	0.892±0.144	0.903±0.139
GATS3m	1.002±0.127	1.005±0.116
GATS4m	1.004±0.129	1.015±0.127
GATS5m	0.994±0.161	0.997±0.149
GATS6m	1.04±0.238	1.044±0.201
GATS7m	1.025±0.25	1.028±0.247
GATS8m	1.042±0.343	1.029±0.266
GATS2v	0.925±0.126	0.935±0.122
GATS5v	0.979±0.136	0.98±0.11
GATS7v	0.997±0.188	0.999±0.172
GATS1e	0.818±0.14	0.821±0.14
GATS3e	1.018±0.206	1.024±0.187
GATS4e	1.025±0.236	1.034±0.23
GATS5e	1.091±0.309	1.091±0.308
GATS6e	1.061±0.346	1.07±0.329
GATS7e	1.017±0.349	1.023±0.352
GATS8e	1.023±0.395	1.007±0.399
GATS1p	1.133±0.183	1.141±0.184
GATS3p	1.054±0.141	1.051±0.131
GATS4p	1.05±0.131	1.058±0.133

GATS8p	0.965±0.282	0.973±0.228
GATS1i	1.32±0.214	1.331±0.22
GATS3i	1.083±0.129	1.078±0.128
GATS5i	0.974±0.14	0.981±0.125
GATS6i	0.995±0.176	0.992±0.17
GATS7i	0.968±0.192	0.967±0.181
GATS1s	0.764±0.195	0.759±0.191
GATS2s	0.721±0.229	0.72±0.23
GATS3s	0.904±0.176	0.906±0.163
GATS4s	1.017±0.252	1.022±0.236
GATS5s	1.13±0.334	1.122±0.326
GATS6s	1.103±0.367	1.11±0.346
GATS7s	1.054±0.457	1.054±0.376
GATS8s	1.065±0.452	1.061±0.429
SM1_Dzm	1.54±0.998	1.505±0.984
VE1_Dzp	0.276±0.208	0.27±0.203
VE2_Dzp	0.01±0.009	0.01±0.009
VE3_Dzp	-8.297±20.371	-8.433±18.691
VR1_Dzp	80891.66±1118705.856	97080.162±1012069.846
VE1_Dzi	0.175±0.155	0.177±0.15
SpMAD_Dzs	11.482±4.054	11.549±4.04
SM1_Dzs	2.075±2.471	2.069±2.511
VE1_Dzs	0.237±0.204	0.246±0.203
VR1_Dzs	71746.962±801018.7	48199.779±604104.11
nBase	0.762±0.737	0.784±0.716
BCUTw.1l	11.941±0.063	11.94±0.063
BCUTp.1l	4.983±0.742	4.97±0.688
BCUTp.1h	11.222±1.415	11.208±1.371
nBondsM	12.339±5.646	12.347±5.82
SpMax1_Bhm	4.034±0.491	4.031±0.464
SpMax2_Bhm	3.781±0.16	3.788±0.279
SpMax3_Bhm	3.598±0.215	3.597±0.308
SpMax4_Bhm	3.393±0.28	3.388±0.273
SpMax1_Bhp	3.9±0.101	3.9±0.097
SpMax2_Bhp	3.718±0.161	3.721±0.151
SpMin1_Bhi	1.894±0.081	1.894±0.078
SpMin8_Bhi	0.849±0.287	0.848±0.277
SpMax1_Bhs	4.6±0.399	4.605±0.394
SpMax2_Bhs	4.278±0.442	4.288±0.439
SpMax3_Bhs	3.993±0.437	4.004±0.445
SpMin3_Bhs	1.647±0.222	1.653±0.208
C1SP2	1.321±1.949	1.347±1.972
C3SP2	2.304±1.544	2.243±1.576
C1SP3	4.365±3.255	4.455±3.265

C2SP3	3.331±3.595	3.476±3.771
C3SP3	0.814±1.577	0.822±1.553
C4SP3	0.155±0.504	0.163±0.532
SCH.6	0.322±0.231	0.312±0.185
VCH.5	0.025±0.067	0.023±0.053
VCH.7	0.225±0.495	0.203±0.226
VC.6	0.024±0.132	0.02±0.065
ASP.3	0.183±0.017	0.183±0.016
ASP.5	0.075±0.011	0.076±0.011
ASP.7	0.032±0.007	0.032±0.007
AVP.0	0.597±0.039	0.596±0.036
AVP.4	0.056±0.013	0.056±0.013
AVP.6	0.018±0.007	0.018±0.006
AVP.7	0.01±0.004	0.01±0.004
CrippenLogP	3.935±2.044	3.877±1.998
SpMAD_Dt	22.307±8.633	22.425±9.173
VE1_Dt	0.14±0.126	0.139±0.125
VE2_Dt	0.005±0.005	0.005±0.005
VE3_Dt	-13.263±25.925	-13.873±27.219
VR1_Dt	276597.542±2448989.208	269156.483±2456122.615
VR2_Dt	9768.085±63790.063	9242.157±60396.549
nHBint6	1.06±2.303	1.191±2.749
nHsNH2	0.103±0.428	0.104±0.379
nHCsatu	1.559±2.453	1.546±2.399
nHother	7.713±4.257	7.679±4.326
nssCH2	5.018±3.453	5.192±3.428
nsssCH	1.819±3.092	1.869±3.213
naasC	2.859±2.795	2.85±2.761
naaaC	0.233±0.71	0.261±0.774
ndO	1.333±1.84	1.377±1.96
nssS	0.078±0.305	0.077±0.294
SHBd	0.508±0.667	0.51±0.646
SHBint2	2.4±5.208	2.465±5.693
SHBint3	2.26±5.985	2.247±5.8
SHBint4	2.587±6.397	2.303±5.933
SHBint5	1.864±6.26	1.803±5.675
SHBint6	2.564±6.175	2.861±7.543
SHBint7	1.854±5.293	1.957±7.643
SHBint8	1.972±7.035	1.911±6.275
SHBint9	1.709±6.568	1.701±5.833
SHBint10	1.254±5.428	1.203±4.946
SHsOH	0.25±0.506	0.249±0.49
SHaaCH	2.248±2.181	2.311±2.205
SsCH3	4.622±5.263	4.633±5.601

SssCH2	3.945±3.509	4.085±3.548
SsssCH	-0.882±3.258	-0.938±3.353
SdssC	0.864±2.864	0.715±2.818
SaasC	2.379±2.745	2.374±2.631
SaaN	1.467±3.763	1.501±3.864
SsssN	2.343±2.2	2.381±2.205
minHBa	2.403±2.083	2.434±2.153
minwHBa	0.048±0.714	0.048±0.688
minHBint2	1.107±2.16	1.086±2.109
minHBint3	0.471±1.048	0.433±0.965
minHBint4	0.441±1.001	0.447±1.047
minHBint5	0.422±1.195	0.381±1.143
minHBint6	0.749±1.59	0.682±1.517
minHBint7	0.646±1.415	0.644±1.407
minHBint8	0.519±1.348	0.525±1.387
minHBint9	0.378±1.002	0.384±1.092
minHBint10	0.293±1.039	0.297±1.008
minHssNH	0.112±0.168	0.111±0.167
minHCsats	0.408±0.179	0.405±0.177
minHCsatu	0.325±0.32	0.339±0.326
minHother	0.431±0.125	0.431±0.123
minsCH3	1.326±0.792	1.353±0.781
minssCH2	0.401±0.462	0.405±0.464
mindsCH	0.747±0.874	0.736±0.874
minsssCH	-0.237±0.547	-0.25±0.553
mindssC	-0.147±0.513	-0.152±0.497
minaasC	0.386±0.532	0.403±0.509
minssssC	-0.262±0.767	-0.252±0.704
minssNH	1.076±1.47	1.072±1.464
mindsN	0.498±1.403	0.431±1.33
minsssN	1.401±1.057	1.42±1.053
maxHBd	0.276±0.23	0.279±0.23
maxHBa	10.573±3.681	10.57±3.698
maxwHBa	2.084±0.67	2.055±0.649
maxHBint3	1.009±1.667	1.01±1.651
maxHBint4	1.12±2.06	1.061±1.977
maxHBint5	0.818±1.833	0.795±1.782
maxHBint6	1.247±2.1	1.287±2.158
maxHBint7	1.013±1.887	1.021±1.868
maxHBint8	0.879±1.849	0.905±1.856
maxHBint9	0.672±1.524	0.68±1.587
maxHBint10	0.525±1.535	0.536±1.5
maxHsOH	0.154±0.226	0.154±0.228
maxHaaCH	0.345±0.273	0.351±0.271

maxHCsats	0.628±0.266	0.632±0.263
maxssCH2	0.808±0.421	0.821±0.409
maxsssCH	0.115±0.222	0.115±0.217
maxdssC	0.463±0.565	0.435±0.552
hmax	0.771±0.218	0.768±0.205
hmin	-0.138±0.192	-0.142±0.196
gmin	-0.718±1.275	-0.718±1.263
LipoaffinityIndex	8.51±3.764	8.505±3.782
ETA_AlphaP	0.477±0.019	0.477±0.016
ETA_Epsilon_3	0.441±0.004	0.441±0.004
ETA_Epsilon_5	0.806±0.054	0.803±0.049
ETA_dEpsilon_D	0.026±0.032	0.026±0.031
ETA_Shape_Y	0.305±0.075	0.302±0.077
ETA_Shape_X	0.017±0.035	0.016±0.035
ETA_BetaP_s	0.63±0.035	0.63±0.035
ETA_Beta_ns_d	0.512±0.682	0.504±0.664
ETA_EtaP_F	0.889±0.205	0.885±0.202
ETA_EtaP_L	0.258±0.044	0.259±0.045
FMF	0.374±0.105	0.374±0.11
IC0	1.469±0.169	1.464±0.165
IC1	3.206±0.364	3.196±0.36
IC2	4.225±0.489	4.229±0.477
BIC0	0.247±0.044	0.246±0.044
BIC3	0.792±0.065	0.792±0.064
MIC0	14.399±3.92	14.229±3.771
MIC1	30.423±5.23	30.185±5.153
ZMIC5	29.729±8.124	29.683±7.377
Kier3	6.38±3.572	6.455±3.711
nAtomLC	6.302±7.502	6.518±8.457
nAtomP	11.884±6.476	11.602±6.422
nAtomLAC	2.508±2.559	2.536±2.374
MLogP	3.363±0.829	3.373±0.821
MDEC.11	0.6±1.362	0.563±1.337
MDEC.12	3.956±3.946	3.958±3.928
MDEC.13	3.691±5.202	3.509±4.994
MDEC.14	0.454±1.31	0.444±1.338
MDEC.22	13.625±9.321	13.712±9.253
MDEC.23	21.069±10.041	20.733±9.566
MDEC.24	0.966±2.305	1.031±2.435
MDEC.33	7.785±6.488	7.509±6.495
MDEO.11	0.486±1.125	0.492±1.101
MDEO.22	0.336±0.8	0.315±0.769
MDEN.22	0.292±0.781	0.282±0.778
MDEN.33	0.167±0.363	0.179±0.39

MLFER_A	0.276±0.429	0.287±0.454
MLFER_S	2.763±1.291	2.758±1.3
MLFER_E	2.383±0.967	2.371±0.969
MPC10	171.497±201.066	165.925±186.133
piPC9	6.35±1.419	6.32±1.409
R_TpiPCTPC	4.694±3.086	4.63±3.037
nRing	3.432±1.423	3.417±1.404
nF10Ring	0.617±0.921	0.623±1.005
nT6Ring	2.947±1.371	2.931±1.395
nT12Ring	0.065±0.294	0.075±0.317
nHeteroRing	1.297±1.123	1.313±1.105
nF9HeteroRing	0.189±0.606	0.216±0.634
nF10HeteroRing	0.464±0.773	0.445±0.812
nFG12HeteroRing	0.475±1.803	0.554±2.746
nT6HeteroRing	0.912±0.946	0.916±0.948
nRotB	7.38±4.411	7.416±4.361
RotBFrac	0.223±0.107	0.225±0.113
RotBtFrac	0.339±0.136	0.336±0.146
LipinskiFailures	0.65±0.773	0.669±0.797
topoDiameter	14.706±5.089	14.728±4.997
topoShape	0.909±0.115	0.911±0.106
JGI1	0.189±0.057	0.187±0.057
JGI2	0.081±0.02	0.08±0.019
JGI3	0.047±0.015	0.047±0.015
JGI4	0.041±0.011	0.04±0.011
JGI5	0.025±0.008	0.025±0.008
JGI6	0.018±0.006	0.018±0.006
JGI7	0.013±0.005	0.013±0.005
JGI8	0.01±0.004	0.01±0.004
JGI9	0.008±0.004	0.008±0.004
JGI10	0.006±0.004	0.006±0.003
VE2_D	0.005±0.004	0.005±0.004
VE3_D	-12.703±25.677	-13.422±27.239
VR1_D	238005.389±1846387.19	200689.337±1533878.387
VR3_D	19.266±10.671	19.428±11.397
TopoPSA	75.64±57.299	76.473±57.455
WPATH	3765.965±5647.722	3839.9±6109.874
XLogP	3.918±2.61	3.887±2.587
APC2D2_N_O	0.715±1.583	0.743±1.681
APC2D2_O_O	0.584±1.179	0.586±1.231
APC2D3_C_N	6.308±6.254	6.198±6.195
APC2D3_C_Cl	0.495±2.324	0.314±1.083
APC2D3_C_X	0.78±2.568	0.596±1.603
APC2D3_N_N	0.638±1.479	0.702±1.589

APC2D3_N_O	0.894±1.91	0.904±1.875
APC2D3_N_S	0.072±0.328	0.07±0.316
APC2D3_O_O	0.833±1.522	0.788±1.465
APC2D4_N_N	0.529±1.295	0.521±1.267
APC2D4_N_O	0.73±1.171	0.671±1.064
APC2D4_O_O	0.853±1.854	0.808±1.764
APC2D5_C_X	0.502±1.604	0.445±1.387
APC2D5_N_N	0.324±1.161	0.335±1.159
APC2D5_N_O	0.877±1.898	0.862±1.926
APC2D6_C_X	0.554±1.498	0.469±1.383
APC2D6_N_N	0.448±1.324	0.46±1.403
APC2D6_N_O	0.961±1.907	0.968±1.949
APC2D6_O_O	0.977±2.192	0.987±2.233
APC2D7_N_N	0.248±0.606	0.231±0.547
APC2D7_N_O	0.627±1.37	0.641±1.3
APC2D7_O_O	0.775±2.127	0.798±2.512
APC2D8_N_N	0.18±0.59	0.168±0.543
APC2D8_N_O	0.779±2.142	0.807±2.107
APC2D8_O_O	0.975±2.792	1.009±2.921
APC2D9_N_O	0.675±1.95	0.65±1.888
APC2D9_O_O	0.541±1.673	0.553±1.753
APC2D10_N_O	0.327±0.941	0.31±0.891
APC2D10_O_O	0.478±1.375	0.519±1.535
AlogP	3.679±2.152	3.603±2.114

Table S4. Statistics of binary descriptors for both data sets

Descriptors	The ratio of the presence to the non-presence	
	Training	Test
EStateFP8	0.055	0.049
EStateFP9	9.612	10.674
EStateFP11	0.281	0.296
EStateFP12	8.811	8.62
EStateFP13	1.316	1.45
EStateFP16	2.086	1.986
EStateFP18	0.225	0.228
EStateFP19	0.297	0.281
EStateFP25	0.062	0.061
EStateFP28	0.072	0.062
EStateFP29	0.294	0.273
EStateFP35	1.759	1.734
EStateFP36	1.803	1.734
EStateFP38	0.077	0.065
MACCSFP16	0.112	0.103
MACCSFP19	0.081	0.062
MACCSFP25	0.066	0.068
MACCSFP26	0.053	0.061
MACCSFP36	0.069	0.07
MACCSFP38	0.15	0.156
MACCSFP50	0.191	0.185
MACCSFP53	0.166	0.153
MACCSFP54	0.124	0.132
MACCSFP57	0.284	0.262
MACCSFP62	0.486	0.443
MACCSFP64	0.059	0.06
MACCSFP66	0.368	0.369
MACCSFP73	0.046	0.049
MACCSFP74	0.31	0.27
MACCSFP75	1.176	1.215
MACCSFP79	0.62	0.66
MACCSFP82	0.302	0.3
MACCSFP83	0.368	0.38
MACCSFP86	1.62	1.657
MACCSFP87	0.216	0.181
MACCSFP89	0.475	0.482
MACCSFP90	0.347	0.404
MACCSFP91	0.605	0.586
MACCSFP93	0.881	0.879
MACCSFP94	0.122	0.105
MACCSFP95	0.736	0.782

MACCSFP97	0.733	0.7
MACCSFP98	1.674	1.644
MACCSFP99	0.39	0.387
MACCSFP100	2.377	2.558
MACCSFP102	0.078	0.074
MACCSFP104	0.633	0.641
MACCSFP105	1.199	1.125
MACCSFP106	0.214	0.217
MACCSFP108	0.503	0.528
MACCSFP109	0.643	0.621
MACCSFP111	2.161	2.352
MACCSFP112	0.871	0.791
MACCSFP114	0.229	0.25
MACCSFP115	0.501	0.497
MACCSFP116	0.656	0.647
MACCSFP117	0.494	0.484
MACCSFP120	1.063	1.082
MACCSFP121	1.946	1.994
MACCSFP125	2.838	2.646
MACCSFP126	1.543	1.433
MACCSFP127	1.93	1.902
MACCSFP128	1.574	1.727
MACCSFP129	1.905	2.003
MACCSFP130	0.074	0.069
MACCSFP131	0.564	0.594
MACCSFP132	1.055	1.074
MACCSFP133	0.667	0.608
MACCSFP135	0.683	0.636
MACCSFP136	0.477	0.491
MACCSFP138	2.142	2.309
MACCSFP140	0.633	0.695
MACCSFP141	0.625	0.579
MACCSFP142	1.62	1.617
MACCSFP144	2.095	2.029
MACCSFP145	5.42	5.66
MACCSFP146	1.337	1.279
MACCSFP147	2.562	2.764
MACCSFP148	2.881	2.981
MACCSFP149	1.441	1.33
MACCSFP150	2.366	2.168
MACCSFP152	2.22	2.074
MACCSFP153	4.561	4.709
MACCSFP155	4	4.247
MACCSFP156	3.094	3.107

MACCSFP157	3.351	3.258
MACCSFP159	2.969	2.921
MACCSFP164	7.387	7.117
PubchemFP2	7.062	7.312
PubchemFP3	0.55	0.572
PubchemFP12	5.228	5.374
PubchemFP13	0.2	0.179
PubchemFP16	0.253	0.244
PubchemFP21	0.11	0.104
PubchemFP145	0.189	0.204
PubchemFP148	0.06	0.059
PubchemFP150	0.058	0.054
PubchemFP179	2.086	2.158
PubchemFP181	1.012	1.095
PubchemFP182	0.423	0.417
PubchemFP183	0.159	0.136
PubchemFP184	0.229	0.197
PubchemFP186	0.821	0.882
PubchemFP188	0.159	0.179
PubchemFP189	0.311	0.275
PubchemFP192	1.715	1.572
PubchemFP193	0.17	0.174
PubchemFP196	0.161	0.134
PubchemFP199	0.496	0.504
PubchemFP206	0.147	0.138
PubchemFP257	1.019	1.033
PubchemFP259	0.241	0.259
PubchemFP261	0.06	0.069
PubchemFP333	10.304	9.602
PubchemFP335	0.392	0.437
PubchemFP337	0.104	0.101
PubchemFP338	0.328	0.335
PubchemFP339	0.453	0.465
PubchemFP340	1.687	1.565
PubchemFP345	3.815	4.527
PubchemFP346	1.076	1.116
PubchemFP349	0.052	0.054
PubchemFP353	0.127	0.129
PubchemFP356	4.746	4.468
PubchemFP364	0.056	0.046
PubchemFP366	2.2	2.083
PubchemFP372	0.108	0.109
PubchemFP378	0.098	0.105
PubchemFP385	0.158	0.153

PubchemFP386	0.163	0.158
PubchemFP397	0.049	0.059
PubchemFP430	7.062	6.696
PubchemFP432	0.381	0.362
PubchemFP446	16.931	16.317
PubchemFP452	0.311	0.324
PubchemFP462	0.124	0.123
PubchemFP485	0.104	0.108
PubchemFP493	0.514	0.453
PubchemFP498	0.977	0.928
PubchemFP500	0.071	0.069
PubchemFP502	0.739	0.647
PubchemFP504	0.147	0.148
PubchemFP516	6.82	7.658
PubchemFP524	17.909	18.604
PubchemFP528	0.349	0.351
PubchemFP530	0.265	0.255
PubchemFP536	0.101	0.118
PubchemFP539	0.256	0.262
PubchemFP544	0.252	0.244
PubchemFP553	0.745	0.652
PubchemFP567	0.61	0.565
PubchemFP571	0.323	0.346
PubchemFP576	0.234	0.222
PubchemFP577	0.278	0.27
PubchemFP580	0.204	0.186
PubchemFP581	0.234	0.225
PubchemFP593	0.354	0.348
PubchemFP601	0.074	0.082
PubchemFP605	0.09	0.086
PubchemFP607	1.881	1.671
PubchemFP610	0.055	0.051
PubchemFP612	0.045	0.046
PubchemFP613	3.643	3.68
PubchemFP614	0.844	0.836
PubchemFP615	0.267	0.258
PubchemFP617	0.327	0.329
PubchemFP620	0.349	0.329
PubchemFP624	0.116	0.096
PubchemFP633	1.185	1.078
PubchemFP636	0.201	0.205
PubchemFP638	0.328	0.317
PubchemFP639	0.231	0.241
PubchemFP646	0.209	0.218

PubchemFP656	3.28	3.81
PubchemFP658	0.081	0.081
PubchemFP663	0.241	0.225
PubchemFP664	8.72	8.802
PubchemFP667	0.172	0.163
PubchemFP672	0.465	0.425
PubchemFP673	0.165	0.138
PubchemFP674	0.159	0.165
PubchemFP679	22.111	18.981
PubchemFP681	0.185	0.183
PubchemFP682	0.268	0.259
PubchemFP683	3.111	2.806
PubchemFP685	0.087	0.088
PubchemFP686	0.139	0.136
PubchemFP688	7.32	6.754
PubchemFP689	1.93	1.862
PubchemFP691	0.287	0.278
PubchemFP694	0.044	0.048
PubchemFP695	0.105	0.087
PubchemFP696	3.815	3.638
PubchemFP697	1.607	1.604
PubchemFP698	1.306	1.34
PubchemFP699	0.646	0.574
PubchemFP701	0.194	0.201
PubchemFP703	0.104	0.091
PubchemFP704	0.973	0.938
PubchemFP705	0.14	0.147
PubchemFP707	0.047	0.042
PubchemFP711	0.118	0.124
PubchemFP712	0.68	0.681
PubchemFP713	0.078	0.087
PubchemFP716	0.106	0.096
PubchemFP734	0.087	0.085
PubchemFP735	0.392	0.369
PubchemFP776	0.157	0.167
PubchemFP797	0.186	0.183
PubchemFP800	0.069	0.073
PubchemFP821	0.24	0.231
PubchemFP860	0.056	0.051
SubFP1	0.966	1.002
SubFP2	2.22	2.418
SubFP5	0.225	0.244
SubFP13	0.069	0.067
SubFP15	0.061	0.067

SubFP16	0.113	0.123
SubFP26	0.912	0.921
SubFP33	0.154	0.138
SubFP40	0.183	0.183
SubFP84	0.053	0.055
SubFP85	0.144	0.152
SubFP88	0.754	0.791
SubFP96	0.073	0.078
SubFP100	0.147	0.142
SubFP135	0.383	0.329
SubFP143	0.066	0.077
SubFP169	0.105	0.102
SubFP275	3.407	3.459
SubFP287	1.176	1.029
SubFP303	0.172	0.167
KRFP2	0.256	0.256
KRFP14	0.235	0.237
KRFP16	0.053	0.058
KRFP18	0.133	0.133
KRFP20	0.175	0.205
KRFP33	0.074	0.076
KRFP67	0.073	0.08
KRFP72	0.101	0.101
KRFP92	0.106	0.102
KRFP98	0.052	0.057
KRFP126	0.096	0.112
KRFP298	0.787	0.889
KRFP299	0.087	0.104
KRFP300	0.187	0.201
KRFP302	0.073	0.093
KRFP326	0.129	0.126
KRFP331	0.09	0.083
KRFP344	0.385	0.4
KRFP346	0.158	0.167
KRFP382	0.063	0.059
KRFP383	0.099	0.095
KRFP401	0.113	0.121
KRFP413	0.082	0.089
KRFP444	0.167	0.17
KRFP467	0.198	0.194
KRFP504	0.25	0.264
KRFP566	0.162	0.163
KRFP582	0.084	0.082
KRFP605	0.929	0.964

KRFP608	0.167	0.175
KRFP610	0.078	0.091
KRFP620	0.409	0.425
KRFP654	0.077	0.088
KRFP678	0.142	0.141
KRFP758	0.056	0.065
KRFP839	0.218	0.221
KRFP1156	0.137	0.122
KRFP1160	0.081	0.067
KRFP1263	0.078	0.083
KRFP1427	0.123	0.112
KRFP1564	0.481	0.495
KRFP1566	0.446	0.412
KRFP1591	0.056	0.057
KRFP1592	0.095	0.091
KRFP1642	0.352	0.332
KRFP1645	0.27	0.255
KRFP1816	0.062	0.06
KRFP1931	0.086	0.077
KRFP1999	0.061	0.054
KRFP2264	0.279	0.28
KRFP2265	0.154	0.165
KRFP2306	0.079	0.063
KRFP2548	0.202	0.201
KRFP2564	0.128	0.126
KRFP2667	0.467	0.465
KRFP2695	0.116	0.117
KRFP2711	0.082	0.085
KRFP2712	0.11	0.096
KRFP2855	0.108	0.115
KRFP2979	0.185	0.196
KRFP2981	0.072	0.063
KRFP3058	0.29	0.294
KRFP3081	0.073	0.061
KRFP3150	0.109	0.11
KRFP3163	0.061	0.053
KRFP3179	0.187	0.198
KRFP3268	0.082	0.089
KRFP3281	0.054	0.053
KRFP3283	0.172	0.163
KRFP3285	0.121	0.112
KRFP3293	0.044	0.047
KRFP3295	0.174	0.197
KRFP3336	0.079	0.077

KRFP3369	0.342	0.356
KRFP3375	0.122	0.128
KRFP3382	0.132	0.146
KRFP3389	0.087	0.085
KRFP3390	0.104	0.117
KRFP3393	0.091	0.087
KRFP3394	0.079	0.073
KRFP3396	0.103	0.111
KRFP3399	0.149	0.151
KRFP3400	0.056	0.059
KRFP3402	0.265	0.281
KRFP3404	0.081	0.086
KRFP3408	0.438	0.437
KRFP3430	0.078	0.081
KRFP3455	0.799	0.859
KRFP3550	0.067	0.056
KRFP3560	0.349	0.358
KRFP3561	0.083	0.077
KRFP3574	0.062	0.054
KRFP3596	0.179	0.156
KRFP3602	0.142	0.133
KRFP3606	0.247	0.228
KRFP3640	2.662	2.834
KRFP3645	0.106	0.103
KRFP3646	0.045	0.048
KRFP3647	0.112	0.126
KRFP3654	0.139	0.151
KRFP3660	0.216	0.224
KRFP3661	0.169	0.192
KRFP3668	0.053	0.052
KRFP3671	0.477	0.51
KRFP3680	0.15	0.142
KRFP3681	0.229	0.246
KRFP3682	1.311	1.324
KRFP3692	0.926	1.033
KRFP3693	0.072	0.078
KRFP3697	0.099	0.109
KRFP3701	0.262	0.28
KRFP3703	0.094	0.117
KRFP3704	0.494	0.537
KRFP3706	0.59	0.634
KRFP3708	0.069	0.065
KRFP3710	0.178	0.178
KRFP3712	0.305	0.309

KRFP3718	0.135	0.147
KRFP3719	0.171	0.174
KRFP3725	0.083	0.085
KRFP3727	0.176	0.17
KRFP3728	0.062	0.066
KRFP3729	0.321	0.362
KRFP3733	0.481	0.519
KRFP3735	0.066	0.073
KRFP3740	1.059	1.183
KRFP3741	0.571	0.618
KRFP3742	0.097	0.115
KRFP3744	0.686	0.709
KRFP3746	0.11	0.115
KRFP3750	3.315	3.597
KRFP3756	0.069	0.079
KRFP3757	0.45	0.474
KRFP3759	0.112	0.108
KRFP3763	0.198	0.219
KRFP3782	1.518	1.778
KRFP3786	0.374	0.427
KRFP3788	1.316	1.34
KRFP3795	0.088	0.097
KRFP3869	0.112	0.098
KRFP3884	1.281	1.34
KRFP3889	0.104	0.121
KRFP3892	0.128	0.115
KRFP3894	0.052	0.058
KRFP3899	0.058	0.069
KRFP3915	0.138	0.144
KRFP3926	3.015	3.224
KRFP3928	0.115	0.136
KRFP3940	0.045	0.044
KRFP3943	0.372	0.332
KRFP3946	0.206	0.21
KRFP3947	0.111	0.11
KRFP3957	0.383	0.414
KRFP3998	0.067	0.066
KRFP4015	0.086	0.08
KRFP4019	0.054	0.066
KRFP4080	5.46	5.836
KRFP4285	0.094	0.096
KRFP4287	0.289	0.259
KRFP4291	0.063	0.063
KRFP4293	0.215	0.215

KRFP4294	0.332	0.369
KRFP4516	0.058	0.067
KRFP4521	0.149	0.16
KRFP4531	0.051	0.061
KRFP4610	0.049	0.045
KRFP4717	0.078	0.074
KRFP4747	0.07	0.066
KRFP4752	0.087	0.09
KRFP4810	0.102	0.096
KRFP4813	0.205	0.197
KRFP4820	0.064	0.08
KRFP4821	0.052	0.054
KRFP4826	0.066	0.077
KRFP4829	0.247	0.235
KRFP4830	0.045	0.045
KRFP4853	0.07	0.069
C2O1C000	0.228	0.225
C3ONAZ00	0.137	0.117
C3ONC300	0.086	0.101
C3ONCZ00	0.063	0.079
N1C2CC00	0.111	0.116
N1C3AC00	0.24	0.222

Table S5. The corrected p-values for each comparison between classifiers by a Wilcoxon signed rank test

	C5T	CART	CSIMCA	ELM	FDA	J48	JRIP	KNN	LDA	MLHD	NB	NC	NNET	PLSDA	RanFerns	RanForest	SOM	SVM
C5T	1.000	1.000	0.000	0.000	0.000	1.000	1.000	0.000	0.000	0.050	0.000	0.680	0.004	0.000	1.000	0.000	1.000	0.000
CART	1.000	1.000	0.000	0.000	0.000	1.000	1.000	0.000	0.000	0.077	0.000	1.000	0.007	0.000	1.000	0.000	1.000	0.000
CSIMCA	0.000	0.000	1.000	0.000	0.000	0.000	0.000	1.000	0.000	0.000	0.000	0.000	0.000	0.070	0.000	0.000	0.000	0.000
ELM	0.000	0.000	0.000	1.000	0.000	0.000	0.000	0.001	1.000	0.000	1.000	0.000	0.000	0.666	0.000	0.000	0.000	0.000
FDA	0.000	0.000	0.000	0.000	1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.892	0.000	1.000
J48	1.000	1.000	0.000	0.000	0.000	1.000	0.921	0.000	0.000	0.775	0.000	1.000	0.138	0.000	1.000	0.000	1.000	0.000
JRIP	1.000	1.000	0.000	0.000	0.000	0.921	1.000	0.000	0.000	0.001	0.000	0.032	0.000	0.000	1.000	0.000	0.047	0.000
KNN	0.000	0.000	1.000	0.001	0.000	0.000	0.000	1.000	0.006	0.000	0.002	0.000	0.000	1.000	0.000	0.000	0.000	0.000
LDA	0.000	0.000	0.000	1.000	0.000	0.000	0.000	0.006	1.000	0.000	1.000	0.000	0.000	1.000	0.000	0.000	0.000	0.000
MLHD	0.050	0.077	0.000	0.000	0.000	0.775	0.001	0.000	0.000	1.000	0.000	1.000	1.000	0.000	0.122	0.001	1.000	0.000
NB	0.000	0.000	0.000	1.000	0.000	0.000	0.000	0.002	1.000	0.000	1.000	0.000	0.000	1.000	0.000	0.000	0.000	0.000
NC	0.680	1.000	0.000	0.000	0.000	1.000	0.032	0.000	0.000	1.000	0.000	1.000	1.000	0.000	1.000	0.000	1.000	0.000
NNET	0.004	0.007	0.000	0.000	0.000	0.138	0.000	0.000	0.000	1.000	0.000	1.000	1.000	0.000	0.006	0.021	1.000	0.000
PLSDA	0.000	0.000	0.070	0.666	0.000	0.000	0.000	1.000	1.000	0.000	1.000	0.000	0.000	1.000	0.000	0.000	0.000	0.000
RanFerns	1.000	1.000	0.000	0.000	0.000	1.000	1.000	0.000	0.000	0.122	0.000	1.000	0.006	0.000	1.000	0.000	1.000	0.000
RanForest	0.000	0.000	0.000	0.000	0.892	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.021	0.000	0.000	1.000	0.000	0.297
SOM	1.000	1.000	0.000	0.000	0.000	1.000	0.047	0.000	0.000	1.000	0.000	1.000	1.000	0.000	1.000	0.000	1.000	0.000
SVM	0.000	0.000	0.000	0.000	1.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.297	0.000	1.000

Table S6. Ranking information of our optimal descriptors by the rank-based feature selection methods

Final Optimal Descriptors	UTS	ReliefF	mRMR
MLogP	1	211	21
SpMAD_Dt	28	137	81
ATSC1i	88	347	122
LipoaffinityIndex	4	333	43
SpMax4_Bhm	11	560	66
SpMax1_Bhp	459	504	377
SubFP84	78	280	756
SHBint8	315	645	69
PubchemFP607	339	132	503
ATSC0p	13	204	42
ASP.3	417	650	407
SHBint3	200	614	104
MACCSFP142	261	160	477
AATS5i	161	618	113

UST, univariate statistical test.

Table S7. Classification performance with different Cutoff values of AD probability

Cutoff	Data Set	NC[a]	Model	MCC	SP	SE	OA	Kappa
0.5	Test	1002	FDA	0.642	0.746	0.886	0.829	0.641
			SVM	0.689	0.783	0.898	0.851	0.688
			RanForest	0.668	0.756	0.899	0.841	0.665
			EM	0.712	0.783	0.916	0.862	0.710
	External Validation	320	FDA	0.509	0.779	0.802	0.797	0.489
			SVM	0.562	0.853	0.798	0.809	0.533
			RanForest	0.511	0.794	0.794	0.794	0.488
			EM	0.571	0.853	0.806	0.816	0.544
0.6	Test	947	FDA	0.661	0.761	0.891	0.841	0.660
			SVM	0.707	0.796	0.903	0.862	0.706
			RanForest	0.672	0.758	0.902	0.846	0.670
			EM	0.724	0.791	0.921	0.870	0.722
	External Validation	301	FDA	0.498	0.774	0.799	0.794	0.477
			SVM	0.565	0.855	0.803	0.814	0.536
			RanForest	0.510	0.790	0.799	0.797	0.488
			EM	0.575	0.855	0.812	0.821	0.549
0.7	Test	808	FDA	0.689	0.779	0.902	0.856	0.689
			SVM	0.733	0.813	0.914	0.876	0.732
			RanForest	0.689	0.779	0.902	0.856	0.689
			EM	0.743	0.809	0.923	0.881	0.742
	External Validation	248	FDA	0.552	0.863	0.787	0.802	0.518
			SVM	0.609	0.922	0.797	0.823	0.570
			RanForest	0.536	0.843	0.787	0.798	0.505
			EM	0.614	0.922	0.802	0.827	0.577
0.8	Test	583	FDA	0.730	0.811	0.916	0.882	0.730
			SVM	0.760	0.821	0.931	0.895	0.760
			RanForest	0.710	0.800	0.908	0.873	0.710
			EM	0.759	0.816	0.934	0.895	0.759
	External Validation	167	FDA	0.571	0.865	0.792	0.808	0.542
			SVM	0.592	0.892	0.792	0.814	0.560
			RanForest	0.502	0.811	0.769	0.778	0.475
			EM	0.592	0.892	0.792	0.814	0.560

a: NC-Number of Inside-AD compounds.

Table S8. Predictions by the developed models for Inside-AD compounds in TCMSP database

id	Pro_EM_no	Pro_EM_yes	Pro_inAD	Herb	Molecule	PubChem_id	Duplicates in modeling data	SMILES
MOL000003	0.9456	0.0544	0.9689	Pollen Typhae	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Ailanthi Altissimae Fructus	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Acoritataninowii Rhizoma	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Eupatorium Fortunei Turcz	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Sargassum	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Trichosanthes Kirilowii Maxim	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Ilicis Cornutae Folium Immayuri	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Herba Clematidis Aethusaefoliae	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Polyporus Umbellatus(Pers)Fr.	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Rosae Laevigatae Fructus	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Coriolus	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Peucedani Radix	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Quisqualis Indica	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Thalluslaminariae	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Momordicae Fructus	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Gnaphalii Affinis Herba	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Picrorhizae Rhizoma	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Isatdis Radix	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Bamusaeconcretiosilicea	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Arisaematis Rhizoma	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Ganoderma	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Rehmanniae Radix Praeparata	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Granati Pericarpium	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Dolichos Lablab L	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Fructus Ligustri Lucidi	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Capsellae Herba	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Cistanches Herba	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Corayceps	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Saposhnikoviae Radix	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Peucedanidecursivi Radix	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Maydis Seigma	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O
MOL000003	0.9456	0.0544	0.9689	Veronicae Peregrinae Herba	MTL	6251	TRUE	C(C(C(CO)O)O)(C(CO)O)O

MOL000004	0.7022	0.2978	0.7572	Phaseoli Semen	Procyanidin B1	11250133	FALSE	C1(c2c3c(CC(C(O3)c3cc(c(cc3)O)O)O)c(cc2O)O)c2c(OC(C1O)c1cc(c(cc1)O)O)cc(cc2O)O
MOL000004	0.7022	0.2978	0.7572	Dolichos Lablab L	Procyanidin B1	11250133	FALSE	C1(c2c3c(CC(C(O3)c3cc(c(cc3)O)O)O)c(cc2O)O)c2c(OC(C1O)c1cc(c(cc1)O)O)cc(cc2O)O
MOL000004	0.7022	0.2978	0.7572	Arecae Semen	Procyanidin B1	11250133	FALSE	C1(c2c3c(CC(C(O3)c3cc(c(cc3)O)O)O)c(cc2O)O)c2c(OC(C1O)c1cc(c(cc1)O)O)cc(cc2O)O
MOL000004	0.7022	0.2978	0.7572	Apocyniveneti Folium	Procyanidin B1	11250133	FALSE	C1(c2c3c(CC(C(O3)c3cc(c(cc3)O)O)O)c(cc2O)O)c2c(OC(C1O)c1cc(c(cc1)O)O)cc(cc2O)O
MOL000004	0.7022	0.2978	0.7572	Rhizoma Fagopyri Cymosi	Procyanidin B1	11250133	FALSE	C1(c2c3c(CC(C(O3)c3cc(c(cc3)O)O)O)c(cc2O)O)c2c(OC(C1O)c1cc(c(cc1)O)O)cc(cc2O)O
MOL000004	0.7022	0.2978	0.7572	Areca Catechu L.	Procyanidin B1	11250133	FALSE	C1(c2c3c(CC(C(O3)c3cc(c(cc3)O)O)O)c(cc2O)O)c2c(OC(C1O)c1cc(c(cc1)O)O)cc(cc2O)O
MOL000005	0.6018	0.3982	0.7524	Dolichos Lablab L	(2R,3R,4R)-4-[(2R,3R)-2-(3,5-dihydroxy-4-methoxyphenyl)-3,5,7-trihydroxychroman-8-yl]-2-(4-hydroxyphenyl)chroman-3,5,7-triol	9808627	FALSE	C1(C(Cc2c(cc(c(c2O1)C1C(C(Oc2cc(cc(c12)O)O)c1ccc(cc1)O)O)O)O)O)c1cc(c(c(c1)O)OC)O
MOL000006	0.9183	0.0817	0.8942	Perillae Fructus	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Geranium Wilfordii Maxim.	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Agrimonia Eupatoria	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Chrysanthemi Indici Flos	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Calyx Seu Fructus Physalis	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Perilla Frutescens	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Schizonepetae Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Cayratiae Japonicae Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Trachelospermumjasminoides	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Anisi Stellati Fructus	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Herbahypericiperforati	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Verbenae Herb	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Celosia Cristata L.	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Sophorae Flavescentis Radix	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Epimrdii Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Cichorii Radix	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O

MOL000006	0.9183	0.0817	0.8942	Prunellae Spica	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Bidentis Bipinnatae Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Spirodelae Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Platycodon Grandiforus	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Phyllanthi Fructus	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Siphonostegiae Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Veronicae Peregrinae Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Flos Genkwa	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Malvae Fructus	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Fructus Carotae	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Belamcandae Rhizome	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Apocyniveneti Folium	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Aurantii Fructus Immaturus	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Dolichos Lablab L	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Euphorbiae Helioscopiae Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Commelinae Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Cannabis Sativa L.	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Fructus Ligustri Lucidi	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Codonopsis Radix	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Saussureae Involucratae Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Forsythiae Fructus	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Ginkgo Folium	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Santalum Album L.	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Buddlejae Flos	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Inulae Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Alpinia Katsumadai Hayat	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Ajugae Decumbentis Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Nelumbinis Stamen	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Viticis Fructus	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Humulus Scandens (Lour.) Merr.	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Pseudostellariae Radix	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Schizonepetae Spica	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Cymbopon Citratus(D C.) Stapf	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Portulacae Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Ecliptae Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Cyperi Rhizoma	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Maydis Seigma	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O

MOL000006	0.9183	0.0817	0.8942	Broussonetiae Fructus	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Chrysanthemi Flos	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Glechomae Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Bruceae Fructus	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Carthami Flos	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Trigonellae Semen	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Spatholobus Suberectus Dunn	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Eupatorium Fortunei Turcz	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Nelumbinis Plumula	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Peanut Skin	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Radix Salviae	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Drynariae Rhizoma	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Plantaginis Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Hordei Fructus Germinatus	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Rhizoma Fagopyri Cymosi	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Artemisia Annua L.	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Lobeliae Chinensis Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Asteris Radix Et Rhizoma	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Junci Medulla	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Dictamni Cortex	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Echinopsis Radix	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Polygoni Avicularis Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Abrus Precatorius L.	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Pteridis Multifidae Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Gnaphalii Affinis Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Herba Patriniae	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Polygoni Cuspidati Rhizoma Et Radix	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Inulae Flos	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Granati Pericarpium	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Sedi Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Menthae Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Hydnocarpi Anthelminticae Semen	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Moslae Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Gossampiniflos	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Equiseti Hiemalis Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Scutellariae Barbatae Herba	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000006	0.9183	0.0817	0.8942	Lonicerae Japonicae Flos	luteolin	5280445	TRUE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL000007	0.8782	0.1218	0.8620	Fructus Ligustri Lucidi	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1

MOL000007	0.8782	0.1218	0.8620	Buddlejae Flos	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL000007	0.8782	0.1218	0.8620	Ecliptae Herba	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL000007	0.8782	0.1218	0.8620	Saussureae Involucratae Herba	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL000007	0.8782	0.1218	0.8620	Trachelospermumjasminoides	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL000007	0.8782	0.1218	0.8620	Glechomae Herba	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL000007	0.8782	0.1218	0.8620	Lysimachiae Herba	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL000007	0.8782	0.1218	0.8620	Asteris Radix Et Rhizoma	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL000007	0.8782	0.1218	0.8620	Humulus Scandens (Lour.) Merr.	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL000007	0.8782	0.1218	0.8620	Schizonepetae Herba	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL000007	0.8782	0.1218	0.8620	Gnaphalii Affinis Herba	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL000007	0.8782	0.1218	0.8620	Dolichos Lablab L	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL000007	0.8782	0.1218	0.8620	Lobeliae Chinensis Herba	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL000007	0.8782	0.1218	0.8620	Chrysanthemi Flos	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL000007	0.8782	0.1218	0.8620	Verbenae Herb	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL000007	0.8782	0.1218	0.8620	Spirodelae Herba	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL000007	0.8782	0.1218	0.8620	Perilla Frutescens	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL000007	0.8782	0.1218	0.8620	Lunulatae Herba	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL000007	0.8782	0.1218	0.8620	Ginkgo Folium	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL000007	0.8782	0.1218	0.8620	Scutellariae Radix	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL000007	0.8782	0.1218	0.8620	Lonicerae Japonicae Flos	Cosmetin	5280704	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Platycladi Cacumen	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Selaginella Doederleinii Hieron	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1

MOL000008	0.9391	0.0609	0.8194	Centipedae Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Scutellariae Barbatae Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Glechomae Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Hoveniae Dulcis Semen	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Oroxyli Semen	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Verbenae Herb	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Codonopsis Radix	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Fructus Ligustri Lucidi	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Pteridis Multifidae Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Scutellariae Radix	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Citri Exocarpium Rubrum	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Lysimachiae Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Ginkgo Folium	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Epimrdii Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Ephedrae Radix Et Rhizoma	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Peanut Skin	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Buddlejae Flos	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Belamcandae Rhizome	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Moslae Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Herba Selaginellae Moellendorfii	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Campsis Flos	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Santalum Album L.	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Lonicerae Japonicae Flos	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Carthami Flos	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Herba Clinopodii Polycephali.	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Ilicis Purpureae Folium	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Trachelospermumjasminoides	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Perilla Frutescens	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Lycii Cortex	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Menthae Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Acoritataninowii Rhizoma	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Lygodii Spora	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Herba Patriniae	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Schizonepetae Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Lunulatae Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Leonuri Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Sophorae Flavescentis Radix	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Rosae Laevigatae Fructus	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1

MOL000008	0.9391	0.0609	0.8194	Siphonostegiae Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Flos Genkwa	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Portulacae Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Dolichos Lablab L	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Cayratiae Japonicae Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Equiseti Hiemalis Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Ephedra Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Lobeliae Chinensis Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Rose Rugosae Flos	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Agrimonia Eupatoria	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Radix Salviae	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Aurantii Fructus Immaturus	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Polygonati Rhizoma	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Chrysanthemi Flos	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Apocyniveneti Folium	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Isatdis Radix	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Humulus Scandens (Lour.) Merr.	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Herba Clematidis Aethusaefoliae	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Broussonetiae Fructus	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Saussureae Involucratae Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Gossampiniflos	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Artemisia Annua L.	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Asteris Radix Et Rhizoma	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Gnaphalii Affinis Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Alpiniae Officinarum Rhizome	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Lysimachiae Foenigraeci Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Perillae Fructus	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Pogostemon Cablin (Blanco) Benth.	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Dichroae Radix	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Cannabis Sativa L.	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Microctis Folium	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Spirodelae Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Schizonepetae Spica	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1

MOL000008	0.9391	0.0609	0.8194	Citri Grandis Exocarpium	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Ecliptae Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Polygoni Cuspidati Rhizoma Et Radix	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Plantaginis Semen	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000008	0.9391	0.0609	0.8194	Potentillae Chinensis Herba	apigenin	5280443	TRUE	c1(cc(=O)c2c(O)cc(cc2o1)O)c1ccc(O)cc1
MOL000009	0.9085	0.0915	0.8281	Perilla Frutescens	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Hordei Fructus Germinatus	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Menthae Herba	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Gnaphalii Affinis Herba	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Dolichos Lablab L	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Plantaginis Herba	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Humulus Scandens (Lour.) Merr.	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Drynariae Rhizoma	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Agrimonia Eupatoria	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Cichorii Radix	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Sophorae Flavescentis Radix	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Cayratiae Japonicae Herba	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Echinopsis Radix	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Codonopsis Radix	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Junci Medulla	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Sedi Herba	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Euphorbiae Helioscopiae Herba	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Buddlejae Flos	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1

MOL000009	0.9085	0.0915	0.8281	Glechomae Herba	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Saussureae Involucratae Herba	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Bruceae Fructus	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Flos Genkwa	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Gossampiniflos	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Viticis Fructus	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Polygoni Cuspidati Rhizoma Et Radix	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Radix Salviae	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Ecliptae Herba	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Chrysanthemi Flos	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Commelinae Herba	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Prunellae Spica	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Verbenae Herb	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Fructus Ligustri Lucidi	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000009	0.9085	0.0915	0.8281	Lonicerae Japonicae Flos	luteolin-7-o-glucoside	5280637	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000010	0.8687	0.1313	0.8896	Aurantii Fructus Immaturus	Rhoifolin	5282150	FALSE	c12c(c(=O)cc(o1)c1ccc(cc1)O)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL000010	0.8687	0.1313	0.8896	Acoritataninowii Rhizoma	Rhoifolin	5282150	FALSE	c12c(c(=O)cc(o1)c1ccc(cc1)O)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL000010	0.8687	0.1313	0.8896	Dolichos Lablab L	Rhoifolin	5282150	FALSE	c12c(c(=O)cc(o1)c1ccc(cc1)O)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL000010	0.8687	0.1313	0.8896	Citri Exocarpium Rubrum	Rhoifolin	5282150	FALSE	c12c(c(=O)cc(o1)c1ccc(cc1)O)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL000010	0.8687	0.1313	0.8896	Chrysanthemi Flos	Rhoifolin	5282150	FALSE	c12c(c(=O)cc(o1)c1ccc(cc1)O)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL000010	0.8687	0.1313	0.8896	Citri Grandis Exocarpium	Rhoifolin	5282150	FALSE	c12c(c(=O)cc(o1)c1ccc(cc1)O)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O

MOL000010	0.8687	0.1313	0.8896	Lonicerae Japonicae Flos	Rhoifolin	5282150	FALSE	c12c(c(=O)cc(o1)c1ccc(cc1)O)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL000011	0.5340	0.4660	0.7090	Semen Cleomis	(2R,3R)-3-(4-hydroxy-3-methoxy-phenyl)-5-methoxy-2-methylol-2,3-dihydropyrano[5,6-h][1,4]benzodioxin-9-one	442510	FALSE	c1(c(ccc(c1)C1C(CO)Oc2c(O1)c(cc1c2oc(=O)cc1)OC)O)OC
MOL000011	0.5340	0.4660	0.7090	Saposhnikoviae Radix	(2R,3R)-3-(4-hydroxy-3-methoxy-phenyl)-5-methoxy-2-methylol-2,3-dihydropyrano[5,6-h][1,4]benzodioxin-9-one	442510	FALSE	c1(c(ccc(c1)C1C(CO)Oc2c(O1)c(cc1c2oc(=O)cc1)OC)O)OC
MOL000013	0.8240	0.1760	0.7308	Semen Cleomis	glucocapparin	Not Available	FALSE	C1(C(C(C(OC1S/C(=C/OS(=O)(=O)O)/C)CO)O)O)O
MOL000014	0.8581	0.1419	0.6551	Semen Cleomis	glucobrassicin	Not Available	FALSE	c1ccc2c(c1)c(c[nH]2)C/C(=N\OS(=O)(=O)O)/CC1C(O)C(C(C(O1)CO)O)O
MOL000016	0.8113	0.1887	0.6689	Semen Cleomis	glucoiberin(e)_qt	Not Available	FALSE	S(=O)(=O)(O/N=C(/S)\CCCS(=O)C)O
MOL000018	0.9521	0.0479	0.8063	Cnidii Fructus	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Borneolum Syntheticum	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Codonopsis Radix	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Lignum Pini Nodi	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Chrysanthemi Flos	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Impatientis Semen	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Artemisia Annua L.	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Kaempferiae Rhizoma	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C

MOL000018	0.9521	0.0479	0.8063	Zingiberis Rhizoma	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Magnolia Officinalis Rehd Et Wils.	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Piperis Longi Fructus	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Asari Radix Et Rhizoma	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Paederiae Scandentis Herba	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Illicium Difengpi K. L. B. Et K. I. M.	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Curcumae Rhizoma	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Coriandri Sativi Herba	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Magnoliae Flos	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Toosendan Fructus	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Scutellariae Radix	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Alpiniae Officinarum Rhizome	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Linderae Radix	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Curcumae Radix	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Atractylodes Macrocephala Koidz.	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Homalomena Occulta (Lour.) Schott	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Moslae Herba	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Radix Bupleuri	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000018	0.9521	0.0479	0.8063	Folium Artemisiae Argyi	(+/-)-Isoborneol	6321405	FALSE	C12(C(CC(CC1)C2(C)C)O)C
MOL000019	0.9479	0.0521	0.7669	Cyperi Rhizoma	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Lignum Pini Nodi	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Viticis Fructus	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C

MOL000019	0.9479	0.0521	0.7669	Curcumae Rhizoma	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Cinnanmomi Cortex	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Ligustici Rhizoma Et Radix	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Leonuri Fructus	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Rhizome Of Whiteback Greenbrier	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Atractylodes Macrocephala Koidz.	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Canarii Fructus	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Rhizoma Seu Herba Aristolochiae Mollissimae	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Achyranthis Asperae Herba	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Chuanxiong Rhizoma	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Bidentis Bipinnatae Herba	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Houttuyniae Herba	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Lonicerae Japonicae Flos	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Illicium Difengpi K. L. B. Et K. I. M.	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Peucedanidecursivi Radix	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Coriandri Sativi Herba	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Radix Bupleuri	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Olibanun	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Folium Artemisiae Argyi	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Foeniculi Fructus	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Radix Salviae	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Linderae Radix	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Herba Clinopodii Polycephali.	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Peucedani Radix	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Asari Radix Et Rhizoma	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Cnidii Fructus	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Homalomena Occulta (Lour.) Schott	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Aurantii Fructus Immaturus	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Notopterygii Rhizoma Et Radix	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Gynostemmae Pentaphylli Herba	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C

MOL000019	0.9479	0.0521	0.7669	Viticis Negundo Folium	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Forsythiae Fructus	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Kaempferiae Rhizoma	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Agrimonia Eupatoria	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Artemisia Annua L.	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Citri Reticulatae Folium	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Cinnamomi Ramulus	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Semen Euphorbiae	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Evodiae Fructus	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Mume Flos	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Fructus Carotae	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Magnoliae Flos	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Alpinia Katsumadai Hayat	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Curcumae Radix	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Borneolum Syntheticum	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Citrus Aurantium	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Citri Fructus Retinervus	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Aristolochiae Fructus	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Myrrha	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Stephaniae Tetrandrae Radix	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Aucklandiae Radix	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Styrax	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Menthae Herba	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Magnolia Officinalis Rehd Et Wils.	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Moslae Herba	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Acoritataninowii Rhizoma	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Zingiberis Rhizoma	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000019	0.9479	0.0521	0.7669	Kadsurae Coccineae Radix Et Caulis	D-Camphene	92221	FALSE	C12C(C(=C)C(CC1)C2)(C)C
MOL000020	0.6112	0.3888	0.6331	Atractylodes Macrocephala Koidz.	12-senecioyl-2E,8E,10E-atractylentriol	Not Available	FALSE	C(=C(C)C)C(=O)OC(/C=C/C=C/C#CC#C/C=C\CO)CCO
MOL000023	0.9512	0.0488	0.9585	Moslae Herba	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Atractylodes Macrocephala Koidz.	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Perillae Fructus	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Capsici Fructus	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Rhododendri Daurici Folium	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Houttuyniae Herba	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Ginseng Folium	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C

MOL000023	0.9512	0.0488	0.9585	Herba Taxilli	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Violsse Herba	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Evodiae Fructus	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Echinopsis Radix	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Rose Rugosae Flos	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Eriobotryae Folium	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Lilii Bulbus	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Campsis Flos	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Ligustici Rhizoma Et Radix	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Santalum Album L.	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Asari Radix Et Rhizoma	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Siphonostegiae Herba	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Curcumae Rhizoma	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Myrrha	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Angelicae Sinensis Radix	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Zingiberis Rhizoma	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Forsythiae Fructus	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Cnidii Fructus	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Schizonepetae Spica	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Notopterygii Rhizoma Et Radix	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Viticis Cannabifoliae Fructus	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Spatholobus Suberectus Dunn	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Magnoliae Flos	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Anisi Stellati Fructus	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Schisandrae Chinensis Fructus	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Verbenae Herb	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Radix Angelicae Biseratae	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Magnolia Officinalis Rehd Et Wils.	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Lignum Pini Nodi	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Radix Bupleuri	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Homalomena Occulta (Lour.) Schott	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Ilicis Cornutae Folium Immayuri	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Curcumaelongae Rhizoma	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Eupatorium Fortunei Turcz	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C

MOL000023	0.9512	0.0488	0.9585	Citrus Aurantium	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Xanthii Fructus	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Borneolum Syntheticum	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Canarii Fructus	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Olibanun	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Morindae Officinalis Radix	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000023	0.9512	0.0488	0.9585	Citri Sarcodactylis Fructus	Hemo-sol	440917	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000024	0.8318	0.1682	0.7018	Litchi Semen	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Sinapis Semen	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Cuscutae Semen	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Aristolochiae Fructus	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Curcumae Rhizoma	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Herbahypericiperforati	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Acoritataninowii Rhizoma	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Flemingia Prostrata Roxb	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Arisaematis Rhizoma	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Atractylodes Macrocephala Koidz.	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Ardisiae Japonicae Herba	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Ephedra Herba	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Coriandri Sativi Herba	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Campsis Flos	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Verbenae Herb	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Dalbergiae Odoriferae Lignum	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Humulus Scandens (Lour.) Merr.	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Carthami Flos	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C

MOL000024	0.8318	0.1682	0.7018	Atractylodes Lancea (Thunb.)Dc.	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Lysimachiae Herba	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Perillae Fructus	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Schizonepetae Spica	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Folium Artemisiae Argyi	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Polygoni Orientalis Fructus	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Chuanxiong Rhizoma	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Viticis Fructus	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Herba Clinopodii Polycephali.	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Kadsurae Coccineae Radix Et Caulis	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Herba Patriniae	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Phragmitis Rhizoma	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Caryophylliflos	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Forsythiae Fructus	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Bidentis Bipinnatae Herba	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Radix Angelicae Biseratae	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Zanthoxyli Pericarpium	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Schizonepetae Herba	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Viticis Negundo Folium	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Gossampiniflos	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C

MOL000024	0.8318	0.1682	0.7018	Magnolia Officinalis Rehd Et Wils.	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Gnaphalii Affinis Herba	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Scutellariae Radix	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Echinopsis Radix	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Moslae Herba	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Flos Genkwa	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Piperis Fructus	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Cyperi Rhizoma	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Et Radix Patriniae Rhizoma	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Alpinia Katsumadai Hayat	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Cistanches Herba	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Citri Sarcodactylis Fructus	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Aucklandiae Radix	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Viticis Cannabifoliae Fructus	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Radix Cirsii Japonici	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Anisi Stellati Fructus	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Cinnanmomi Cortex	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Curcumae Radix	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Dichroae Radix	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Pogostemon Cablin (Blanco) Benth.	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Folium Nelumbinis	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C

MOL000024	0.8318	0.1682	0.7018	Piperis Longi Fructus	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Evodiae Fructus	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Anemarrhenae Rhizoma	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Cannabis Sativa L.	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Fructus Ligustri Lucidi	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Myrrha	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Schisandrae Chinensis Fructus	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Citrus Aurantium	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Fritillariaeussuriensis Bulbus	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Rubi Fructus	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Solidaginis Herba	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Eupatorium Fortunei Turcz	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	A. Dahurica (Fisch.) Benth. Et Hook	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Ligustici Rhizoma Et Radix	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000024	0.8318	0.1682	0.7018	Leonuri Herba	alpha-humulene	5281520	FALSE	C\1=C(/C/C=C/C(C/C=C(/CC1)\C)(C)C)\C
MOL000025	0.8318	0.1682	0.6026	Atractylodes Macrocephala Koidz.	α-Longipinene	Not Available	FALSE	C12C3(CCCC(C1C3C(=CC2)C)(C)C)C
MOL000025	0.8318	0.1682	0.6026	Sedi Herba	α-Longipinene	Not Available	FALSE	C12C3(CCCC(C1C3C(=CC2)C)(C)C)C
MOL000027	0.8816	0.1184	0.7446	Curcumae Rhizoma	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Aucklandiae Radix	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Codonopsis Radix	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Morindae Officinalis Radix	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C

MOL000027	0.8816	0.1184	0.7446	Cinnamomi Ramulus	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Radix Bupleuri	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Chuanxiong Rhizoma	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Mahoniae Caulis	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Atractylodes Macrocephala Koidz.	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Benzoinum	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Fructus Carotae	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Myrrha	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Lysimachiae Herba	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Curcumaelongae Rhizoma	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Platycladi Cacumen	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Radix Angelicae Biseratae	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Arisaematis Rhizoma	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Zingiberis Rhizoma	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Santalum Album L.	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Cnidii Fructus	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Folium Artemisiae Argyi	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Cornus Officinalis Sieb. Et Zucc.	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Ligustici Rhizoma Et Radix	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000027	0.8816	0.1184	0.7446	Panacis Quinquefolii Radix	alpha-Curcumene	442360	FALSE	c1(ccc(cc1)C)C(CCC=C(C)C)C
MOL000028	0.4015	0.5985	0.6981	Atractylodes Macrocephala Koidz.	α-Amyrin	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C)C(C)C4C3=CCC21)C)O

MOL000029	0.8219	0.1781	0.6920	Radix Bupleuri	beta-Humulene	5318102	FALSE	C\1(=C/CC(/C=C/CC(=C)CCC1)(C)C)/C
MOL000029	0.8219	0.1781	0.6920	Caryophylliflos	beta-Humulene	5318102	FALSE	C\1(=C/CC(/C=C/CC(=C)CCC1)(C)C)/C
MOL000029	0.8219	0.1781	0.6920	Acoritataninowii Rhizoma	beta-Humulene	5318102	FALSE	C\1(=C/CC(/C=C/CC(=C)CCC1)(C)C)/C
MOL000029	0.8219	0.1781	0.6920	Atractylodes Macrocephala Koidz.	beta-Humulene	5318102	FALSE	C\1(=C/CC(/C=C/CC(=C)CCC1)(C)C)/C
MOL000029	0.8219	0.1781	0.6920	Borneolum Syntheticum	beta-Humulene	5318102	FALSE	C\1(=C/CC(/C=C/CC(=C)CCC1)(C)C)/C
MOL000029	0.8219	0.1781	0.6920	Panax Ginseng C. A. Mey.	beta-Humulene	5318102	FALSE	C\1(=C/CC(/C=C/CC(=C)CCC1)(C)C)/C
MOL000030	0.9516	0.0484	0.9248	Atractylodes Macrocephala Koidz.	(1R)-2-methyl-1-phenylprop-2-en-1-ol	7015153	FALSE	C(C(=C)C)(O)c1ccccc1
MOL000031	0.8711	0.1289	0.7791	Fritillariaeussuriensis Bulbus	(3S)-3-[(1R)-1,5-dimethylhex-4-enyl]-6-methylenecyclohexene	11106487	FALSE	CC(=CCCC(C)C1C=CC(=C)CC1)C
MOL000031	0.8711	0.1289	0.7791	Atractylodes Macrocephala Koidz.	(3S)-3-[(1R)-1,5-dimethylhex-4-enyl]-6-methylenecyclohexene	11106487	FALSE	CC(=CCCC(C)C1C=CC(=C)CC1)C
MOL000032	0.8378	0.1622	0.7084	Rhododendri Daurici Folium	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Siphonostegiae Herba	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Illicium Difengpi K. L. B. Et K. I. M.	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Saposhnikoviae Radix	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Curcumae Rhizoma	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Atractylodes Macrocephala Koidz.	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Smilacis Glabrae Rhixoma	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Zingiberis Rhizoma	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Linderae Radix	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Linderae Radix	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Ardisiae Japonicae Herba	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O

MOL000032	0.8378	0.1622	0.7084	Magnolia Officinalis Rehd Et Wils.	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Nardostachyos Radix Et Rhizoma	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Ginkgo Folium	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Atractylodes Lancea (Thunb.)Dc.	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Flemingia Prostrata Roxb	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Aucklandiae Radix	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Ephedra Herba	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Campsis Flos	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Viticis Negundo Folium	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Radix Bupleuri	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Curcumae Radix	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000032	0.8378	0.1622	0.7084	Mahoniae Folum	beta-Eudesmol	91457	FALSE	C1C(CCC2(CCCC(=C)C12)C)C(C)(C)O
MOL000033	0.2503	0.7497	0.6061	Spatholobus Suberectus Dunn	(3S,8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-[(2R,5S)-5-propan-2-yloctan-2-yl]-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol	15976101	FALSE	C1(CCC2(C(=CCC3C4CCC(C(CCC(C(C)C)CCC)C)C4(C)CCC23)C1)C)O

MOL000033	0.2503	0.7497	0.6061	Atractylodes Macrocephala Koidz.	(3S,8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-[(2R,5S)-5-propan-2-yloctan-2-yl]-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol	15976101	FALSE	C1(CCC2(C(=CCC3C4CCC(C(CCC(C(C)C)CCC)C)C4(C)CCC23)C1)C)O
MOL000033	0.2503	0.7497	0.6061	Hedysarum Multijugum Maxim.	(3S,8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-[(2R,5S)-5-propan-2-yloctan-2-yl]-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol	15976101	FALSE	C1(CCC2(C(=CCC3C4CCC(C(CCC(C(C)C)CCC)C)C4(C)CCC23)C1)C)O
MOL000034	0.8624	0.1376	0.7025	Platycladi Cacumen	2-[(1R,3S,4S)-3-isopropenyl-4-methyl-4-vinylcyclohexyl]propan-2-ol	92138	FALSE	CC(C)(O)C1CC(C(CC1)(C)C=C)C(=C)C

MOL000034	0.8624	0.1376	0.7025	Folium Nelumbinis	2-[(1R,3S,4S)-3-isopropenyl-4-methyl-4-vinylcyclohexyl]propan-2-ol	92138	FALSE	CC(C)(O)C1CC(C(CC1)(C)C=C)C(=C)C
MOL000034	0.8624	0.1376	0.7025	Citrus Aurantium	2-[(1R,3S,4S)-3-isopropenyl-4-methyl-4-vinylcyclohexyl]propan-2-ol	92138	FALSE	CC(C)(O)C1CC(C(CC1)(C)C=C)C(=C)C
MOL000034	0.8624	0.1376	0.7025	Asari Radix Et Rhizoma	2-[(1R,3S,4S)-3-isopropenyl-4-methyl-4-vinylcyclohexyl]propan-2-ol	92138	FALSE	CC(C)(O)C1CC(C(CC1)(C)C=C)C(=C)C
MOL000034	0.8624	0.1376	0.7025	Evodiae Fructus	2-[(1R,3S,4S)-3-isopropenyl-4-methyl-4-vinylcyclohexyl]propan-2-ol	92138	FALSE	CC(C)(O)C1CC(C(CC1)(C)C=C)C(=C)C
MOL000034	0.8624	0.1376	0.7025	Aucklandiae Radix	2-[(1R,3S,4S)-3-isopropenyl-4-methyl-4-vinylcyclohexyl]propan-2-ol	92138	FALSE	CC(C)(O)C1CC(C(CC1)(C)C=C)C(=C)C
MOL000034	0.8624	0.1376	0.7025	Gnaphalii Affinis Herba	2-[(1R,3S,4S)-3-isopropenyl-4-methyl-4-vinylcyclohexyl]propan-2-ol	92138	FALSE	CC(C)(O)C1CC(C(CC1)(C)C=C)C(=C)C

MOL000034	0.8624	0.1376	0.7025	Magnolia Officinalis Rehd Et Wils.	2-[(1R,3S,4S)-3-isopropenyl-4-methyl-4-vinylcyclohexyl]propan-2-ol	92138	FALSE	CC(C)(O)C1CC(C(CC1)(C)C=C)C(=C)C
MOL000034	0.8624	0.1376	0.7025	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	2-[(1R,3S,4S)-3-isopropenyl-4-methyl-4-vinylcyclohexyl]propan-2-ol	92138	FALSE	CC(C)(O)C1CC(C(CC1)(C)C=C)C(=C)C
MOL000034	0.8624	0.1376	0.7025	Anisi Stellati Fructus	2-[(1R,3S,4S)-3-isopropenyl-4-methyl-4-vinylcyclohexyl]propan-2-ol	92138	FALSE	CC(C)(O)C1CC(C(CC1)(C)C=C)C(=C)C
MOL000034	0.8624	0.1376	0.7025	Atractylodes Lancea (Thunb.)Dc.	2-[(1R,3S,4S)-3-isopropenyl-4-methyl-4-vinylcyclohexyl]propan-2-ol	92138	FALSE	CC(C)(O)C1CC(C(CC1)(C)C=C)C(=C)C
MOL000034	0.8624	0.1376	0.7025	Zingiberis Rhizoma	2-[(1R,3S,4S)-3-isopropenyl-4-methyl-4-vinylcyclohexyl]propan-2-ol	92138	FALSE	CC(C)(O)C1CC(C(CC1)(C)C=C)C(=C)C
MOL000034	0.8624	0.1376	0.7025	Atractylodes Macrocephala Koidz.	2-[(1R,3S,4S)-3-isopropenyl-4-methyl-4-vinylcyclohexyl]propan-2-ol	92138	FALSE	CC(C)(O)C1CC(C(CC1)(C)C=C)C(=C)C

MOL000034	0.8624	0.1376	0.7025	Myrrha	2-[(1R,3S,4S)-3-isopropenyl-4-methyl-4-vinylcyclohexyl]propan-2-ol	92138	FALSE	CC(C)(O)C1CC(C(CC1)(C)C=C)C(=C)C
MOL000034	0.8624	0.1376	0.7025	Nardostachyos Radix Et Rhizoma	2-[(1R,3S,4S)-3-isopropenyl-4-methyl-4-vinylcyclohexyl]propan-2-ol	92138	FALSE	CC(C)(O)C1CC(C(CC1)(C)C=C)C(=C)C
MOL000034	0.8624	0.1376	0.7025	Lonicerae Japonicae Flos	2-[(1R,3S,4S)-3-isopropenyl-4-methyl-4-vinylcyclohexyl]propan-2-ol	92138	FALSE	CC(C)(O)C1CC(C(CC1)(C)C=C)C(=C)C
MOL000034	0.8624	0.1376	0.7025	Curcumae Radix	2-[(1R,3S,4S)-3-isopropenyl-4-methyl-4-vinylcyclohexyl]propan-2-ol	92138	FALSE	CC(C)(O)C1CC(C(CC1)(C)C=C)C(=C)C
MOL000034	0.8624	0.1376	0.7025	Chuanxiong Rhizoma	2-[(1R,3S,4S)-3-isopropenyl-4-methyl-4-vinylcyclohexyl]propan-2-ol	92138	FALSE	CC(C)(O)C1CC(C(CC1)(C)C=C)C(=C)C
MOL000034	0.8624	0.1376	0.7025	Cornus Officinalis Sieb. Et Zucc.	2-[(1R,3S,4S)-3-isopropenyl-4-methyl-4-vinylcyclohexyl]propan-2-ol	92138	FALSE	CC(C)(O)C1CC(C(CC1)(C)C=C)C(=C)C

MOL000034	0.8624	0.1376	0.7025	Folium Artemisiae Argyi	2-[(1R,3S,4S)-3-isopropenyl-4-methyl-4-vinylcyclohexyl]propan-2-ol	92138	FALSE	CC(C)(O)C1CC(C(CC1)(C)C=C)C(=C)C
MOL000035	0.8129	0.1871	0.6579	Cinnanmomi Cortex	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Chuanxiong Rhizoma	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Pogostemon Cablin (Blanco) Benth.	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Curcumae Rhizoma	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Sedi Herba	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Lysimachiae Herba	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Rhododendri Daurici Folium	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Humulus Scandens (Lour.) Merr.	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Magnolia Officinalis Rehd Et Wils.	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Zanthoxyli Pericarpium	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Panax Ginseng C. A. Mey.	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Xanthii Fructus	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Anisi Stellati Fructus	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Curcumae Radix	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Rubi Fructus	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Cnidii Fructus	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Peucedanidecursivi Radix	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Arisaematis Rhizoma	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Angelicae Sinensis Radix	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Peucedani Radix	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Campsis Flos	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Atractylodes Macrocephala Koidz.	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Acoritataninowii Rhizoma	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Ailanthi Cortex	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Gnaphalii Affinis Herba	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Notopterygii Rhizoma Et Radix	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	A. Dahurica (Fisch.) Benth. Et Hook	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Cyperi Rhizoma	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000035	0.8129	0.1871	0.6579	Solidaginis Herba	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C

MOL000035	0.8129	0.1871	0.6579	Herba Clinopodii Polycephali.	beta-Selinene	442393	FALSE	C1(=C)CCCC2(CCC(CC12)C(=C)C)C
MOL000036	0.8418	0.1582	0.6717	Echinopsis Radix	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Rhapontici Radix	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Ginsen Radix Et Rhizoma Rubra	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Campsis Flos	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Schisandrae Chinensis Fructus	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Curcumae Rhizoma	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Perillae Fructus	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Schizonepetae Herba	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Sedi Herba	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Carthami Flos	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Borneolum Syntheticum	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Radix Salviae	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Citri Fructus	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Panax Ginseng C. A. Mey.	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Artemisiae Scopariae Herba	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Olibanun	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Radix Bupleuri	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Atractylodes Macrocephala Koidz.	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Coriandri Sativi Herba	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Zanthoxyli Pericarpium	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C

MOL000036	0.8418	0.1582	0.6717	Panacis Quinquefolii Radix	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Lonicerae Japonicae Flos	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Houttuyniae Herba	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Ligustici Rhizoma Et Radix	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Leonuri Fructus	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Eriobotryae Folium	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Viticis Cannabifoliae Fructus	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Leonuri Herba	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Notoginseng Flos	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Xanthii Fructus	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Ginseng Folium	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Curcumaelongae Rhizoma	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Rubi Fructus	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000036	0.8418	0.1582	0.6717	Canarii Fructus	beta-caryophyllene	5281515	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL000037	0.8647	0.1353	0.6853	Curcumaelongae Rhizoma	γ-elemene	12309452	FALSE	C1(C(CC(=C(C)C)CC1)C(=C)C)(C)C=C
MOL000037	0.8647	0.1353	0.6853	Atractylodes Macrocephala Koidz.	γ-elemene	12309452	FALSE	C1(C(CC(=C(C)C)CC1)C(=C)C)(C)C=C
MOL000037	0.8647	0.1353	0.6853	Curcumae Rhizoma	γ-elemene	12309452	FALSE	C1(C(CC(=C(C)C)CC1)C(=C)C)(C)C=C
MOL000037	0.8647	0.1353	0.6853	Farfarae Flos	γ-elemene	12309452	FALSE	C1(C(CC(=C(C)C)CC1)C(=C)C)(C)C=C
MOL000037	0.8647	0.1353	0.6853	Leonuri Herba	γ-elemene	12309452	FALSE	C1(C(CC(=C(C)C)CC1)C(=C)C)(C)C=C
MOL000038	0.7966	0.2034	0.6606	Atractylodes Macrocephala Koidz.	Akridin	9215	TRUE	c1cccc2nc3ccccc3cc12
MOL000039	0.9570	0.0430	0.9744	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(1S,2R,4R)-Neoiso-dihydrocarveol	443166	FALSE	C1(C(CCC(C1)C(=C)C)C)O

MOL000039	0.9570	0.0430	0.9744	Atractylodes Macrocephala Koidz.	(1S,2R,4R)-Neoiso-dihydrocarveol	443166	FALSE	C1(C(CCC(C1)C(=C)C)C)O
MOL000040	0.9417	0.0583	0.8282	Prunellae Spica	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Trigonellae Semen	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Angelicae Sinensis Radix	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Glehniae Radix	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Herba Sarcandrae	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Apocyniveneti Folium	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Radix Bupleuri	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Herbahypericiperforati	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Euphorbiae Humifusae Herba	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Cortex Periplocae Radicis	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Folium Artemisiae Argyi	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Portulacae Herba	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Saposhnikoviae Radix	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Kansui Radix	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Erycibe Obtusifolia Benth	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Inulae Flos	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Herba Clematidis Aethusaefoliae	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Anisodus Acutangulus C. Y. Wu Et C .Chen Ex C. Che	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Citri Sarcodactylis Fructus	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Rubia Cordifolia	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Uncariae Ramulus Cumuncis	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Mori Cortex	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Atractylodes Macrocephala Koidz.	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Calendula Officinalis	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Radix Angelicae Biseratae	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Rhododendri Daurici Folium	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Fraxini Cortex	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Inulae Herba	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Artemisiae Scopariae Herba	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Canarii Fructus	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Peucedanidecursivi Radix	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O

MOL000040	0.9417	0.0583	0.8282	Lycii Cortex	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Bombyx Mori L.	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Lycii Fructus	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Peucedani Radix	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Physochlainae Radix	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Morindae Officinalis Radix	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Coriandri Sativi Herba	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	licorice	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	A. Dahurica (Fisch.) Benth. Et Hook	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Saussureae Involucratae Herba	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Hedyotis Diffusae Herba	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Solanum Nigrum Linn.	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Lunulatae Herba	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Dictamni Cortex	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Ailanthi Cortex	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Humulus Scandens (Lour.) Merr.	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Broussonetiae Fructus	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Artemisia Annua L.	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Violsse Herba	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000040	0.9417	0.0583	0.8282	Mori Follum	Scopoletol	5280460	FALSE	c1(=O)ccc2c(o1)cc(c(c2)OC)O
MOL000041	0.9201	0.0799	0.9504	Cornus Officinalis Sieb. Et Zucc.	PHA	6925665	FALSE	C(=O)(C(N)Cc1ccccc1)O
MOL000041	0.9201	0.0799	0.9504	Radix Salviae	PHA	6925665	FALSE	C(=O)(C(N)Cc1ccccc1)O
MOL000041	0.9201	0.0799	0.9504	Bamusaeconcretiosilicea	PHA	6925665	FALSE	C(=O)(C(N)Cc1ccccc1)O
MOL000041	0.9201	0.0799	0.9504	Santalum Album L.	PHA	6925665	FALSE	C(=O)(C(N)Cc1ccccc1)O
MOL000041	0.9201	0.0799	0.9504	Arecae Semen	PHA	6925665	FALSE	C(=O)(C(N)Cc1ccccc1)O
MOL000041	0.9201	0.0799	0.9504	Trichosanthes Kirilowii Maxim	PHA	6925665	FALSE	C(=O)(C(N)Cc1ccccc1)O
MOL000041	0.9201	0.0799	0.9504	Atractylodes Macrocephala Koidz.	PHA	6925665	FALSE	C(=O)(C(N)Cc1ccccc1)O
MOL000041	0.9201	0.0799	0.9504	Rhizoma Dioscoreae	PHA	6925665	FALSE	C(=O)(C(N)Cc1ccccc1)O
MOL000042	0.8955	0.1045	0.9646	Cornus Officinalis Sieb. Et Zucc.	LPG	7311724	FALSE	C(=O)(C(N)C)O
MOL000042	0.8955	0.1045	0.9646	Bamusaeconcretiosilicea	LPG	7311724	FALSE	C(=O)(C(N)C)O
MOL000042	0.8955	0.1045	0.9646	Jujubae Fructus	LPG	7311724	FALSE	C(=O)(C(N)C)O
MOL000042	0.8955	0.1045	0.9646	Rhizoma Dioscoreae	LPG	7311724	FALSE	C(=O)(C(N)C)O
MOL000042	0.8955	0.1045	0.9646	Atractylodes Macrocephala Koidz.	LPG	7311724	FALSE	C(=O)(C(N)C)O
MOL000042	0.8955	0.1045	0.9646	Radix Salviae	LPG	7311724	FALSE	C(=O)(C(N)C)O

MOL000043	0.7806	0.2194	0.8216	Atractylodes Macrocephala Koidz.	atractylenolide i	5321018	FALSE	C1CC(=C)C2C(C1)(C=C1C(=C(C(=O)O1)C)C2)C
MOL000043	0.7806	0.2194	0.8216	Atractylodes Lancea (Thunb.)Dc.	atractylenolide i	5321018	FALSE	C1CC(=C)C2C(C1)(C=C1C(=C(C(=O)O1)C)C2)C
MOL000044	0.7901	0.2099	0.7798	Herba Sarcandrae	atractylenolideII	14448070	FALSE	O1C2C(=C(C1=O)C)CC1C(=C)CCCC1(C2)C
MOL000044	0.7901	0.2099	0.7798	Atractylodes Lancea (Thunb.)Dc.	atractylenolideII	14448070	FALSE	O1C2C(=C(C1=O)C)CC1C(=C)CCCC1(C2)C
MOL000044	0.7901	0.2099	0.7798	Atractylodes Macrocephala Koidz.	atractylenolideII	14448070	FALSE	O1C2C(=C(C1=O)C)CC1C(=C)CCCC1(C2)C
MOL000044	0.7901	0.2099	0.7798	Codonopsis Radix	atractylenolideII	14448070	FALSE	O1C2C(=C(C1=O)C)CC1C(=C)CCCC1(C2)C
MOL000045	0.8582	0.1418	0.7918	Papaveris Pericarpium	atractylenolide iii	155948	FALSE	C1CC(=C)C2C(C1)(CC1(C(=C(C(=O)O1)C)C2)O)C
MOL000045	0.8582	0.1418	0.7918	Atractylodes Macrocephala Koidz.	atractylenolide iii	155948	FALSE	C1CC(=C)C2C(C1)(CC1(C(=C(C(=O)O1)C)C2)O)C
MOL000045	0.8582	0.1418	0.7918	Codonopsis Radix	atractylenolide iii	155948	FALSE	C1CC(=C)C2C(C1)(CC1(C(=C(C(=O)O1)C)C2)O)C
MOL000046	0.7220	0.2780	0.6881	Atractylodes Macrocephala Koidz.	atractylone	12299876	FALSE	C1CC(=C)C2C(C1)(Cc1c(C2)c(co1)C)C
MOL000047	0.8487	0.1513	0.7300	Atractylodes Macrocephala Koidz.	juniper camphor	7466421	FALSE	C1CC(C2C(C1)(CCC(=C(C)C)C2)C)(C)O
MOL000048	0.8073	0.1927	0.6924	Curcumae Rhizoma	(5E,9Z)-3,6,10-trimethyl-4,7,8,11-tetrahydrocyclodeca[b]furan	9601230	FALSE	o1c2c(c(c1)C)C/C=C(/CC/C=C(\C2)/C)\C
MOL000048	0.8073	0.1927	0.6924	Myrrha	(5E,9Z)-3,6,10-trimethyl-4,7,8,11-tetrahydrocyclodeca[b]furan	9601230	FALSE	o1c2c(c(c1)C)C/C=C(/CC/C=C(\C2)/C)\C
MOL000048	0.8073	0.1927	0.6924	Atractylodes Macrocephala Koidz.	(5E,9Z)-3,6,10-trimethyl-4,7,8,11-tetrahydrocyclodeca[b]furan	9601230	FALSE	o1c2c(c(c1)C)C/C=C(/CC/C=C(\C2)/C)\C
MOL000049	0.5203	0.4797	0.7870	Atractylodes Macrocephala Koidz.	3β-acetoxyatractylone	Not Available	FALSE	C1C(C(=C)C2C(C1)(Cc1c(C2)c(co1)C)C)OC(=O)C

MOL000050	0.8902	0.1098	0.9578	Bamusaeconcretiosilicea	GLY	5257127	FALSE	C(=O)(CN)O
MOL000050	0.8902	0.1098	0.9578	Cornus Officinalis Sieb. Et Zucc.	GLY	5257127	FALSE	C(=O)(CN)O
MOL000050	0.8902	0.1098	0.9578	Jujubae Fructus	GLY	5257127	FALSE	C(=O)(CN)O
MOL000050	0.8902	0.1098	0.9578	Santalum Album L.	GLY	5257127	FALSE	C(=O)(CN)O
MOL000050	0.8902	0.1098	0.9578	Euryales Semen	GLY	5257127	FALSE	C(=O)(CN)O
MOL000050	0.8902	0.1098	0.9578	Arum Ternatum Thunb.	GLY	5257127	FALSE	C(=O)(CN)O
MOL000050	0.8902	0.1098	0.9578	Radix Salviae	GLY	5257127	FALSE	C(=O)(CN)O
MOL000050	0.8902	0.1098	0.9578	Vigna Radiata	GLY	5257127	FALSE	C(=O)(CN)O
MOL000050	0.8902	0.1098	0.9578	Trichosanthes Kirilowii Maxim	GLY	5257127	FALSE	C(=O)(CN)O
MOL000050	0.8902	0.1098	0.9578	Rhizoma Dioscoreae	GLY	5257127	FALSE	C(=O)(CN)O
MOL000050	0.8902	0.1098	0.9578	Silybum Marianum	GLY	5257127	FALSE	C(=O)(CN)O
MOL000050	0.8902	0.1098	0.9578	Atractylodes Macrocephala Koidz.	GLY	5257127	FALSE	C(=O)(CN)O
MOL000051	0.9461	0.0539	0.9688	Atractylodes Macrocephala Koidz.	Polymannose	161658	FALSE	O=CC(O)C(O)C(O)C(O)CO
MOL000052	0.9126	0.0874	0.9760	Bombyx Mori L.	Gulutamine	44272391	FALSE	C(=O)(C(N)CCC(=O)O)O
MOL000052	0.9126	0.0874	0.9760	Gynostemmae Pentaphylli Herba	Gulutamine	44272391	FALSE	C(=O)(C(N)CCC(=O)O)O
MOL000052	0.9126	0.0874	0.9760	Humulus Scandens (Lour.) Merr.	Gulutamine	44272391	FALSE	C(=O)(C(N)CCC(=O)O)O
MOL000052	0.9126	0.0874	0.9760	Santalum Album L.	Gulutamine	44272391	FALSE	C(=O)(C(N)CCC(=O)O)O
MOL000052	0.9126	0.0874	0.9760	Radix Salviae	Gulutamine	44272391	FALSE	C(=O)(C(N)CCC(=O)O)O
MOL000052	0.9126	0.0874	0.9760	Vigna Radiata	Gulutamine	44272391	FALSE	C(=O)(C(N)CCC(=O)O)O
MOL000052	0.9126	0.0874	0.9760	Euryales Semen	Gulutamine	44272391	FALSE	C(=O)(C(N)CCC(=O)O)O
MOL000052	0.9126	0.0874	0.9760	Rhizoma Dioscoreae	Gulutamine	44272391	FALSE	C(=O)(C(N)CCC(=O)O)O
MOL000052	0.9126	0.0874	0.9760	Trichosanthes Kirilowii Maxim	Gulutamine	44272391	FALSE	C(=O)(C(N)CCC(=O)O)O
MOL000052	0.9126	0.0874	0.9760	Hordei Fructus Germinatus	Gulutamine	44272391	FALSE	C(=O)(C(N)CCC(=O)O)O
MOL000052	0.9126	0.0874	0.9760	Silybum Marianum	Gulutamine	44272391	FALSE	C(=O)(C(N)CCC(=O)O)O
MOL000052	0.9126	0.0874	0.9760	Arum Ternatum Thunb.	Gulutamine	44272391	FALSE	C(=O)(C(N)CCC(=O)O)O
MOL000052	0.9126	0.0874	0.9760	Cornus Officinalis Sieb. Et Zucc.	Gulutamine	44272391	FALSE	C(=O)(C(N)CCC(=O)O)O
MOL000052	0.9126	0.0874	0.9760	Atractylodes Macrocephala Koidz.	Gulutamine	44272391	FALSE	C(=O)(C(N)CCC(=O)O)O
MOL000053	0.9462	0.0538	0.9703	Benincasae Exocarpium	Methose	5984	FALSE	OCC(=O)C(O)C(O)C(O)CO
MOL000053	0.9462	0.0538	0.9703	Hippophae Fructus	Methose	5984	FALSE	OCC(=O)C(O)C(O)C(O)CO
MOL000053	0.9462	0.0538	0.9703	Semiaquilegiae Radix	Methose	5984	FALSE	OCC(=O)C(O)C(O)C(O)CO
MOL000053	0.9462	0.0538	0.9703	Atractylodes Macrocephala Koidz.	Methose	5984	FALSE	OCC(=O)C(O)C(O)C(O)CO
MOL000053	0.9462	0.0538	0.9703	Jujubae Fructus	Methose	5984	FALSE	OCC(=O)C(O)C(O)C(O)CO
MOL000053	0.9462	0.0538	0.9703	Ramulus Mori	Methose	5984	FALSE	OCC(=O)C(O)C(O)C(O)CO

MOL000053	0.9462	0.0538	0.9703	Cymbopon Citratus(D C.) Stapf	Methose	5984	FALSE	OCC(=O)C(O)C(O)C(O)CO
MOL000053	0.9462	0.0538	0.9703	Rhizoma Dioscoreae	Methose	5984	FALSE	OCC(=O)C(O)C(O)C(O)CO
MOL000053	0.9462	0.0538	0.9703	Panacis Quinquefolii Radix	Methose	5984	FALSE	OCC(=O)C(O)C(O)C(O)CO
MOL000054	0.9018	0.0982	0.9382	Euryales Semen	L-	28782	FALSE	C(=O)(C(N)CCCNC(=N)N)O
MOL000054	0.9018	0.0982	0.9382	Atractylodes Macrocephala Koidz.	L-	28782	FALSE	C(=O)(C(N)CCCNC(=N)N)O
MOL000054	0.9018	0.0982	0.9382	Arum Ternatum Thunb.	L-	28782	FALSE	C(=O)(C(N)CCCNC(=N)N)O
MOL000054	0.9018	0.0982	0.9382	Radix Salviae	L-	28782	FALSE	C(=O)(C(N)CCCNC(=N)N)O
MOL000054	0.9018	0.0982	0.9382	Hedysarum Multijugum Maxim.	L-	28782	FALSE	C(=O)(C(N)CCCNC(=N)N)O
MOL000054	0.9018	0.0982	0.9382	Bomboo Juice	L-	28782	FALSE	C(=O)(C(N)CCCNC(=N)N)O
MOL000054	0.9018	0.0982	0.9382	Vigna Radiata	L-	28782	FALSE	C(=O)(C(N)CCCNC(=N)N)O
MOL000054	0.9018	0.0982	0.9382	Rhizoma Dioscoreae	L-	28782	FALSE	C(=O)(C(N)CCCNC(=N)N)O
MOL000054	0.9018	0.0982	0.9382	Bamusaeconcretiosilicea	L-	28782	FALSE	C(=O)(C(N)CCCNC(=N)N)O
MOL000054	0.9018	0.0982	0.9382	Santalum Album L.	L-	28782	FALSE	C(=O)(C(N)CCCNC(=N)N)O
MOL000054	0.9018	0.0982	0.9382	Trichosanthes Kirilowii Maxim	L-	28782	FALSE	C(=O)(C(N)CCCNC(=N)N)O
MOL000055	0.9196	0.0804	0.9716	Radix Salviae	L-Lysin	5962	FALSE	C(=O)(C(N)CCCCN)O
MOL000055	0.9196	0.0804	0.9716	Rhizoma Dioscoreae	L-Lysin	5962	FALSE	C(=O)(C(N)CCCCN)O
MOL000055	0.9196	0.0804	0.9716	Arum Ternatum Thunb.	L-Lysin	5962	FALSE	C(=O)(C(N)CCCCN)O
MOL000055	0.9196	0.0804	0.9716	Carthami Flos	L-Lysin	5962	FALSE	C(=O)(C(N)CCCCN)O
MOL000055	0.9196	0.0804	0.9716	Euryales Semen	L-Lysin	5962	FALSE	C(=O)(C(N)CCCCN)O
MOL000055	0.9196	0.0804	0.9716	Atractylodes Macrocephala Koidz.	L-Lysin	5962	FALSE	C(=O)(C(N)CCCCN)O
MOL000055	0.9196	0.0804	0.9716	Vigna Radiata	L-Lysin	5962	FALSE	C(=O)(C(N)CCCCN)O
MOL000055	0.9196	0.0804	0.9716	Santalum Album L.	L-Lysin	5962	FALSE	C(=O)(C(N)CCCCN)O
MOL000055	0.9196	0.0804	0.9716	Bamusaeconcretiosilicea	L-Lysin	5962	FALSE	C(=O)(C(N)CCCCN)O
MOL000055	0.9196	0.0804	0.9716	Trichosanthes Kirilowii Maxim	L-Lysin	5962	FALSE	C(=O)(C(N)CCCCN)O
MOL000056	0.9138	0.0862	0.9210	Bamusaeconcretiosilicea	DTY	6942100	FALSE	C(=O)(C(N)Cc1ccc(O)cc1)O
MOL000056	0.9138	0.0862	0.9210	Arum Ternatum Thunb.	DTY	6942100	FALSE	C(=O)(C(N)Cc1ccc(O)cc1)O
MOL000056	0.9138	0.0862	0.9210	Trichosanthes Kirilowii Maxim	DTY	6942100	FALSE	C(=O)(C(N)Cc1ccc(O)cc1)O
MOL000056	0.9138	0.0862	0.9210	Radix Salviae	DTY	6942100	FALSE	C(=O)(C(N)Cc1ccc(O)cc1)O
MOL000056	0.9138	0.0862	0.9210	Rhizoma Dioscoreae	DTY	6942100	FALSE	C(=O)(C(N)Cc1ccc(O)cc1)O
MOL000056	0.9138	0.0862	0.9210	Atractylodes Macrocephala Koidz.	DTY	6942100	FALSE	C(=O)(C(N)Cc1ccc(O)cc1)O
MOL000056	0.9138	0.0862	0.9210	Santalum Album L.	DTY	6942100	FALSE	C(=O)(C(N)Cc1ccc(O)cc1)O
MOL000057	0.7987	0.2013	0.8105	Sargassum	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	licorice	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Allii Fistulost Bulbus	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Celastri Orbiculati Fructus	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C

MOL000057	0.7987	0.2013	0.8105	Eriobotryae Folium	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Radix Cirsii Japonici	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Ranunculi Ternati Radix	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Citrus Reticulata	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Amygdalus Communis Vas	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Humulus Scandens (Lour.) Merr.	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Oroxyli Semen	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Perillae Fructus	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Et Radix Patriniae Rhizoma	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Alpiniae Officinarum Rhizome	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Flemingia Prostrata Roxb	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Radix Bupleuri	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Paederiae Scandentis Herba	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Momordicae Fructus	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Cornus Officinalis Sieb. Et Zucc.	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Achyranthis Bidentatae Radix	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Litchi Semen	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Ginkgo Folium	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Isatdis Radix	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Cinnanmomi Cortex	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Uncariae Ramulus Cumuncis	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Pogostemon Cablin (Blanco) Benth.	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Gossampiniflos	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Caryophylliflos	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Achyranthis Asperae Herba	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Ephedra Herba	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Atractylodes Macrocephala Koidz.	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Folium Ilicis Cornutae	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C
MOL000057	0.7987	0.2013	0.8105	Pseudostellariae Radix	DIBP	6782	FALSE	c1(c(cccc1)C(=O)OCC(C)C)C(=O)OCC(C)C

MOL000058	0.8323	0.1677	0.7140	Atractylodes Macrocephala Koidz.	2-[(2R,5S,6S)-6,10-dimethylspiro[4.5]dec-9-en-2-yl]propan-2-ol	10878761	FALSE	C1C(CCC21C(=CCCC2C)C)C(O)(C)C
MOL000059	0.9341	0.0659	0.8962	Corayceps	uridine	6029	FALSE	OCC1C(O)C(O)C(O1)n1c(=O)[nH]c(=O)cc1
MOL000059	0.9341	0.0659	0.8962	Atractylodes Macrocephala Koidz.	uridine	6029	FALSE	OCC1C(O)C(O)C(O1)n1c(=O)[nH]c(=O)cc1
MOL000059	0.9341	0.0659	0.8962	Semiaquilegiae Radix	uridine	6029	FALSE	OCC1C(O)C(O)C(O1)n1c(=O)[nH]c(=O)cc1
MOL000059	0.9341	0.0659	0.8962	Ranunculi Ternati Radix	uridine	6029	FALSE	OCC1C(O)C(O)C(O1)n1c(=O)[nH]c(=O)cc1
MOL000060	0.8710	0.1290	0.7795	Atractylodes Macrocephala Koidz.	selina-4(14),7(11)-dien-8-one	13986099	FALSE	C1C(=O)C(=C(C)C)CC2C(=C)CCCC12C
MOL000060	0.8710	0.1290	0.7795	Atractylodes Lancea (Thunb.)Dc.	selina-4(14),7(11)-dien-8-one	13986099	FALSE	C1C(=O)C(=C(C)C)CC2C(=C)CCCC12C
MOL000061	0.9081	0.0919	0.9705	Vigna Radiata	Prolinum	6971047	FALSE	C(=O)(C1NCCC1)O
MOL000061	0.9081	0.0919	0.9705	Hippophae Fructus	Prolinum	6971047	FALSE	C(=O)(C1NCCC1)O
MOL000061	0.9081	0.0919	0.9705	Jujubae Fructus	Prolinum	6971047	FALSE	C(=O)(C1NCCC1)O
MOL000061	0.9081	0.0919	0.9705	Santalum Album L.	Prolinum	6971047	FALSE	C(=O)(C1NCCC1)O
MOL000061	0.9081	0.0919	0.9705	Hedysarum Multijugum Maxim.	Prolinum	6971047	FALSE	C(=O)(C1NCCC1)O
MOL000061	0.9081	0.0919	0.9705	Euryales Semen	Prolinum	6971047	FALSE	C(=O)(C1NCCC1)O
MOL000061	0.9081	0.0919	0.9705	Bamusaeconcretiosilicea	Prolinum	6971047	FALSE	C(=O)(C1NCCC1)O
MOL000061	0.9081	0.0919	0.9705	Rhizoma Dioscoreae	Prolinum	6971047	FALSE	C(=O)(C1NCCC1)O
MOL000061	0.9081	0.0919	0.9705	Atractylodes Macrocephala Koidz.	Prolinum	6971047	FALSE	C(=O)(C1NCCC1)O
MOL000061	0.9081	0.0919	0.9705	Radix Salviae	Prolinum	6971047	FALSE	C(=O)(C1NCCC1)O
MOL000061	0.9081	0.0919	0.9705	Cornus Officinalis Sieb. Et Zucc.	Prolinum	6971047	FALSE	C(=O)(C1NCCC1)O
MOL000061	0.9081	0.0919	0.9705	Trichosanthes Kirilowii Maxim	Prolinum	6971047	FALSE	C(=O)(C1NCCC1)O
MOL000062	0.1407	0.8593	0.7723	Atractylodes Macrocephala Koidz.	biatractylolide	Not Available	FALSE	C1CCC2(C(C1=C)CC1=C(C(=O)OC1(C2)C12CC3(C(CC1=C(C(=O)O2)C)C(=C)CCC3)C)C)C
MOL000063	0.1407	0.8593	0.7723	Atractylodes Macrocephala Koidz.	ATRACTYLODES MACROCEPHALA	Not Available	FALSE	C1CC(=C)C2C(C1)(CC1(C(=C(C(=O)O1)C)C2)C12C(=C(C(=O)O2)C)CC2C(C1)(CCCC2=C)C)C
MOL000064	0.8929	0.1071	0.9599	Euryales Semen	D-Serin	6857549	FALSE	C(=O)(C(N)CO)O
MOL000064	0.8929	0.1071	0.9599	Atractylodes Macrocephala Koidz.	D-Serin	6857549	FALSE	C(=O)(C(N)CO)O
MOL000064	0.8929	0.1071	0.9599	Vigna Radiata	D-Serin	6857549	FALSE	C(=O)(C(N)CO)O

MOL000065	0.9027	0.0973	0.9693	Radix Salviae	ASI	44367445	FALSE	C(=O)(C(N)CC(=O)O)O
MOL000065	0.9027	0.0973	0.9693	Arum Ternatum Thunb.	ASI	44367445	FALSE	C(=O)(C(N)CC(=O)O)O
MOL000065	0.9027	0.0973	0.9693	Cornus Officinalis Sieb. Et Zucc.	ASI	44367445	FALSE	C(=O)(C(N)CC(=O)O)O
MOL000065	0.9027	0.0973	0.9693	Santalum Album L.	ASI	44367445	FALSE	C(=O)(C(N)CC(=O)O)O
MOL000065	0.9027	0.0973	0.9693	Gynostemmae Pentaphylli Herba	ASI	44367445	FALSE	C(=O)(C(N)CC(=O)O)O
MOL000065	0.9027	0.0973	0.9693	Humulus Scandens (Lour.) Merr.	ASI	44367445	FALSE	C(=O)(C(N)CC(=O)O)O
MOL000065	0.9027	0.0973	0.9693	Rhizoma Dioscoreae	ASI	44367445	FALSE	C(=O)(C(N)CC(=O)O)O
MOL000065	0.9027	0.0973	0.9693	Vigna Radiata	ASI	44367445	FALSE	C(=O)(C(N)CC(=O)O)O
MOL000065	0.9027	0.0973	0.9693	Jujubae Fructus	ASI	44367445	FALSE	C(=O)(C(N)CC(=O)O)O
MOL000065	0.9027	0.0973	0.9693	Trichosanthes Kirilowii Maxim	ASI	44367445	FALSE	C(=O)(C(N)CC(=O)O)O
MOL000065	0.9027	0.0973	0.9693	Euryales Semen	ASI	44367445	FALSE	C(=O)(C(N)CC(=O)O)O
MOL000065	0.9027	0.0973	0.9693	Atractylodes Macrocephala Koidz.	ASI	44367445	FALSE	C(=O)(C(N)CC(=O)O)O
MOL000067	0.9093	0.0907	0.9722	Platycodon Grandiforus	L-Valin	6971018	FALSE	C(=O)(C(N)C(C)C)O
MOL000067	0.9093	0.0907	0.9722	Radix Salviae	L-Valin	6971018	FALSE	C(=O)(C(N)C(C)C)O
MOL000067	0.9093	0.0907	0.9722	Bamusaeconcretiosilicea	L-Valin	6971018	FALSE	C(=O)(C(N)C(C)C)O
MOL000067	0.9093	0.0907	0.9722	Euryales Semen	L-Valin	6971018	FALSE	C(=O)(C(N)C(C)C)O
MOL000067	0.9093	0.0907	0.9722	Trichosanthes Kirilowii Maxim	L-Valin	6971018	FALSE	C(=O)(C(N)C(C)C)O
MOL000067	0.9093	0.0907	0.9722	Jujubae Fructus	L-Valin	6971018	FALSE	C(=O)(C(N)C(C)C)O
MOL000067	0.9093	0.0907	0.9722	Santalum Album L.	L-Valin	6971018	FALSE	C(=O)(C(N)C(C)C)O
MOL000067	0.9093	0.0907	0.9722	Arum Ternatum Thunb.	L-Valin	6971018	FALSE	C(=O)(C(N)C(C)C)O
MOL000067	0.9093	0.0907	0.9722	Atractylodes Macrocephala Koidz.	L-Valin	6971018	FALSE	C(=O)(C(N)C(C)C)O
MOL000067	0.9093	0.0907	0.9722	Vigna Radiata	L-Valin	6971018	FALSE	C(=O)(C(N)C(C)C)O
MOL000067	0.9093	0.0907	0.9722	Rhizoma Dioscoreae	L-Valin	6971018	FALSE	C(=O)(C(N)C(C)C)O
MOL000068	0.9185	0.0815	0.9712	Euryales Semen	L-Ile	7043901	FALSE	C(=O)(C(N)C(CC)C)O
MOL000068	0.9185	0.0815	0.9712	Atractylodes Macrocephala Koidz.	L-Ile	7043901	FALSE	C(=O)(C(N)C(CC)C)O
MOL000068	0.9185	0.0815	0.9712	Radix Salviae	L-Ile	7043901	FALSE	C(=O)(C(N)C(CC)C)O
MOL000068	0.9185	0.0815	0.9712	Cornus Officinalis Sieb. Et Zucc.	L-Ile	7043901	FALSE	C(=O)(C(N)C(CC)C)O
MOL000068	0.9185	0.0815	0.9712	Platycodon Grandiforus	L-Ile	7043901	FALSE	C(=O)(C(N)C(CC)C)O
MOL000068	0.9185	0.0815	0.9712	Vigna Radiata	L-Ile	7043901	FALSE	C(=O)(C(N)C(CC)C)O
MOL000068	0.9185	0.0815	0.9712	Bamusaeconcretiosilicea	L-Ile	7043901	FALSE	C(=O)(C(N)C(CC)C)O
MOL000068	0.9185	0.0815	0.9712	Arum Ternatum Thunb.	L-Ile	7043901	FALSE	C(=O)(C(N)C(CC)C)O
MOL000068	0.9185	0.0815	0.9712	Trichosanthes Kirilowii Maxim	L-Ile	7043901	FALSE	C(=O)(C(N)C(CC)C)O
MOL000068	0.9185	0.0815	0.9712	Santalum Album L.	L-Ile	7043901	FALSE	C(=O)(C(N)C(CC)C)O

MOL000068	0.9185	0.0815	0.9712	Rhizoma Dioscoreae	L-Ile	7043901	FALSE	C(=O)(C(N)C(CC)C)O
MOL000068	0.9185	0.0815	0.9712	Bombyx Mori L.	L-Ile	7043901	FALSE	C(=O)(C(N)C(CC)C)O
MOL000068	0.9185	0.0815	0.9712	Olibanun	L-Ile	7043901	FALSE	C(=O)(C(N)C(CC)C)O
MOL000069	0.8587	0.1413	0.6576	Allii Tuberosi Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Corayceps	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Mahoniae Folum	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Mori Cortex	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Santalum Album L.	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Croci Stigma	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Sterculiae Lychnophorae Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Celosia Cristata L.	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Coriolus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Angelicae Sinensis Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Eriobotryae Folium	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Forsythiae Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Capsellae Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Raphani Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Bolbostemae Paniculati Bulbus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Imperatae Rhizoma	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Allium Azureum Ledeb.	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Rhizoma Fagopyri Cymosi	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Prunellae Spica	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Hippophae Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Polygonati Odorati Rhizoma	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Leonuri Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Phyllanthi Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Lasiosphaera Seu Calvatia	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Radix Paeoniae Rubra	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Puerariae Flos	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Herba Sarcandrae	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Phytolaccae Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Smilacis Glabrae Rhixoma	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Citrus Aurantium	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Chebulae Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Dalbergiae Odoriferae Lignum	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Malvae Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O

MOL000069	0.8587	0.1413	0.6576	Astragali Cpmplanatisemen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Cayratiae Japonicae Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Lonicerae Japonicae Flos	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Cimicifugae Rhizoma	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Cinnamomi Ramulus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Lysimachiae Foenigraeci Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Melo Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Silybum Marianum	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Polygoni Orientalis Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Aconiti Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Peucedani Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Achyranthis Bidentatae Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Alpiniae Oxyphyliae Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Platycladi Cacumen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Spirodelae Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Radix Angelicae Biseratae	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Verbenae Herb	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Canarii Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Cyathulae Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Fritillariaeussuriensis Bulbus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Cornus Officinalis Sieb. Et Zucc.	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Sedi Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Olibanun	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Lycii Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Perillae Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Gleditsiae Spina	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Coicis Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Piperis Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Mori Cortex	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Piperis Longi Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Toosendan Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Zingiberis Rhizoma	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Cynanchistauntonii Rhizoma Et Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Evodiae Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Cannabis Sativa L.	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O

MOL000069	0.8587	0.1413	0.6576	Pogostemon Cablin (Blanco) Benth.	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Atractylodes Macrocephala Koidz.	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Arum Ternatum Thunb.	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Aloe	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Dioscoreaebulbiferae	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Radix Cynanchi	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Gypsophila Licentiana Hand.-Mazz.	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Xanthii Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Ginseng Folium	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Mahoniae Caulis	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Platycladi Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Hyperici Japonici Herber	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Viscum Angulatum Heyne	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Hyoscyami Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Millettiae Speciosae Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Lycii Cortex	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Ilicis Purpureae Folium	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Ranunculi Ternati Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Eriocauli Flos	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Foeniculi Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Schizonepetae Spica	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Nardostachyos Radix Et Rhizoma	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Tamaricis Cacumen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Humulus Scandens (Lour.) Merr.	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Saxifraga Stolonifera	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Choerospondiatis Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Ephedra Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Semen Pharbitidis	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Radix Salviae	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Bidentis Bipinnatae Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Chuanxiong Rhizoma	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Ginkgo Folium	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Vaccariae Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Euphorbiae Helioscopiae Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Mylabris	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O

MOL000069	0.8587	0.1413	0.6576	Lepidii Semen Descurainiae Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Trollius Chinensis	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Broussonetiae Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Lablab Semen Album	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Cinnanmomi Cortex	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Linderae Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Semen Firmianae	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Platycodon Grandiforus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Curcumae Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Semiaquilegiae Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Citri Grandis Exocarpium	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Dichroae Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Lobeliae Chinensis Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Cortex Hibisci	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Euryales Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Cnidii Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Achyranthis Asperae Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Quisqualis Indica	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Citri Sarcodactylis Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Arisaematis Rhizoma	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Folium Nelumbinis	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Semen Lini	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Panax Ginseng C. A. Mey.	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Kansui Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Panacis Quinquefolii Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Sparganii Rhizoma	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Cucurbitae Moschatae Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Trichosanthes Kirilowii Maxim	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Asparagi Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Ginsen Radix Et Rhizoma Rubra	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Semen Aesculi	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Asteris Radix Et Rhizoma	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Glechomae Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Oroxyli Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Curculiginis Rhizome	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Herba Patriniae	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Caryophylliflos	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Flos Genkwa	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O

MOL000069	0.8587	0.1413	0.6576	Arecae Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Fritiliariae Irrhosae Bulbus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Gnaphalii Affinis Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Flemingia Prostrata Roxb	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Celastri Orbiculati Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Clematidis Armandii Caulis	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Pteridis Multifidae Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Linderae Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Litseae Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Maydis Seigma	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Viticis Cannabifoliae Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Isatdis Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Euphorbiae Humifusae Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Abutili Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Radix Bupleuri	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Acoritataninowii Rhizoma	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Momordicae Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Magnolia Officinalis Rehd Et Wils.	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Alpiniae Officinarum Rhizome	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Pseudostellariae Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Rosae Laevigatae Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Radix Clematidis	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Echinopsis Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Semen Euphorbiae	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Ginkgo Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Eucommiae Folium	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Aconitum Kusnezoffii Reichb	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Homalomena Occulta (Lour.) Schott	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Celosiae Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Capsici Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Smilax Scodinicaulis C.H. Wrisht?	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Morindae Officinalis Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Cortex Periplocae Radicis	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Typhonii Rhizoma	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Paederiae Scandentis Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Portulacae Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O

MOL000069	0.8587	0.1413	0.6576	Poria Cocos(Schw.) Wolf.	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Crotonis Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Codonopsis Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Radix Cynanchi Paniculati	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Aauropi Folium	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Zanthoxyli Pericarpium	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Momordicae Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Citri Reticulatae Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Kochiae Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Rhapontici Radix	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Gynostemmae Pentaphylli Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Rhizome Of Whiteback Greenbrier	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Amygdalus Communis Vas	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Gossampiniflos	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Saururi Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Sinapis Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Lithospermum Erythrorhizon	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Meliae Azedarach Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Litchi Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Mori Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Farfarae Flos	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Radix Cirsii Japonici	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Ampelopsis Japonica	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Dianthi Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Violsse Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Gleditsiae Sinensis Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Sojae Semen Nigrum	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Sapindi Mukorossi Semen	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Carthami Flos	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Mume Fructus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Thalluslaminariae	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Hedysarum Multijugum Maxim.	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Rhododendri Daurici Folium	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Smilax China	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Microctis Folium	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O

MOL000069	0.8587	0.1413	0.6576	Isatidis Folium	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Scutellariae Barbatae Herba	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000069	0.8587	0.1413	0.6576	Akebiae Frucyus	palmitic acid	985	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL000070	0.9379	0.0621	0.9652	Atractylodes Macrocephala Koidz.	Ethyl pivaloylacetate	86950	FALSE	C(=O)(CC(=O)C(C)(C)C)OCC
MOL000071	0.8911	0.1089	0.9267	Radix Salviae	Istidina	6971009	FALSE	C(=O)(C(N)Cc1c[nH]cn1)O
MOL000071	0.8911	0.1089	0.9267	Cornus Officinalis Sieb. Et Zucc.	Istidina	6971009	FALSE	C(=O)(C(N)Cc1c[nH]cn1)O
MOL000071	0.8911	0.1089	0.9267	Euryales Semen	Istidina	6971009	FALSE	C(=O)(C(N)Cc1c[nH]cn1)O
MOL000071	0.8911	0.1089	0.9267	Arum Ternatum Thunb.	Istidina	6971009	FALSE	C(=O)(C(N)Cc1c[nH]cn1)O
MOL000071	0.8911	0.1089	0.9267	Trichosanthes Kirilowii Maxim	Istidina	6971009	FALSE	C(=O)(C(N)Cc1c[nH]cn1)O
MOL000071	0.8911	0.1089	0.9267	Atractylodes Macrocephala Koidz.	Istidina	6971009	FALSE	C(=O)(C(N)Cc1c[nH]cn1)O
MOL000071	0.8911	0.1089	0.9267	Rhizoma Dioscoreae	Istidina	6971009	FALSE	C(=O)(C(N)Cc1c[nH]cn1)O
MOL000071	0.8911	0.1089	0.9267	Santalum Album L.	Istidina	6971009	FALSE	C(=O)(C(N)Cc1c[nH]cn1)O
MOL000071	0.8911	0.1089	0.9267	Bamusaeconcretiosilicea	Istidina	6971009	FALSE	C(=O)(C(N)Cc1c[nH]cn1)O
MOL000071	0.8911	0.1089	0.9267	Smilacis Glabrae Rhixoma	Istidina	6971009	FALSE	C(=O)(C(N)Cc1c[nH]cn1)O
MOL000072	0.6048	0.3952	0.7556	Atractylodes Macrocephala Koidz.	8β-ethoxy atractylenolide III	14448075	FALSE	O1C2(C(=C(C1=O)C)CC1C(=C)CCCC1(C2)C)OCC
MOL000073	0.9402	0.0598	0.8161	Areca Catechu L.	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Uncariae Ramulus Cumuncis	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Dioscoreaebulbiferae	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Gleditsiae Spina	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Apocyniveneti Folium	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Rhizoma Fagopyri Cymosi	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Chaenomeles Sinensis (Thouin) Koehne	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Crataegi Folium	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Arecae Semen	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Celastri Orbiculati Fructus	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O

MOL000073	0.9402	0.0598	0.8161	Litchi Semen	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Cinnamomi Ramulus	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Actinidia Chinensis Planch	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Amomum Tsao-Ko Crevostet	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Lysimachiae Herba	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Herba Pyrolae	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Phaseoli Semen	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Eucommiae Cortex	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Hippophae Fructus	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Hordei Fructus Germinatus	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Ampelopsis Japonica	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Semen Aesculi	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Folium Nelumbinis	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Herbahypericiperforati	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Gleditsiae Fructus	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000073	0.9402	0.0598	0.8161	Catechu	ent-Epicatechin	182232	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O
MOL000074	0.5923	0.4077	0.6097	Amomum Tsao-Ko Crevostet	(4E,6E)-1,7-bis(4-hydroxyphenyl)hepta-4,6-dien-3-one	10613719	FALSE	c1c(ccc(c1)CCC(=O)/C=C/C=C/c1ccc(cc1)O)O
MOL000075	0.4486	0.5514	0.7304	Amomum Tsao-Ko Crevostet	(4E,6E)-7-(4-hydroxy-3-methoxyphenyl)-1-(4-hydroxyphenyl)-4	24901215	FALSE	c1c(ccc(c1)CCC(=O)/C=C/C=C/c1ccc(c(c1)OC)O)O

MOL000076	0.3919	0.6081	0.8135	Amomum Tsao-Ko Crevostet	1,7-bis(4-hydroxy-3-methoxyphenyl)-4,6-heptadien-3one	46881044	FALSE	C(CC(=O)/C=C/C=C/c1cc(c(cc1)O)OC)c1cc(c(cc1)O)OC
MOL000077	0.9277	0.0723	0.9640	Amomum Tsao-Ko Crevostet	Aldrich	7041	FALSE	c1(cccc(c1O)OC)OC
MOL000077	0.9277	0.0723	0.9640	Calyx Seu Fructus Physalis	Aldrich	7041	FALSE	c1(cccc(c1O)OC)OC
MOL000077	0.9277	0.0723	0.9640	Linderae Radix	Aldrich	7041	FALSE	c1(cccc(c1O)OC)OC
MOL000077	0.9277	0.0723	0.9640	Herba Patriniae	Aldrich	7041	FALSE	c1(cccc(c1O)OC)OC
MOL000077	0.9277	0.0723	0.9640	Spatholobus Suberectus Dunn	Aldrich	7041	FALSE	c1(cccc(c1O)OC)OC
MOL000077	0.9277	0.0723	0.9640	Bomboo Juice	Aldrich	7041	FALSE	c1(cccc(c1O)OC)OC
MOL000078	0.9345	0.0655	0.9471	Amomum Tsao-Ko Crevostet	6,7-dihydroxy-3,7-dimethyloct-2-enoic acid	Not Available	FALSE	C(=O)(/C=C(/CCC(C(C)(C)O)O)\C)O
MOL000079	0.9500	0.0500	0.8481	Amomum Tsao-Ko Crevostet	6,7-dihydroxy-indan-4-carbaldehyde	24901150	FALSE	C1CCc2c(cc(c(c12)O)O)C=O
MOL000080	0.9511	0.0489	0.8780	Amomum Tsao-Ko Crevostet	6-(4-hydroxyphenyl)-4-hydroxyhexan-2-one	Not Available	FALSE	c1c(ccc(c1)CCC(CC(=O)C)O)O
MOL000081	0.9535	0.0465	0.8173	Amomum Tsao-Ko Crevostet	6-hydroxy-indan-4-carbaldehyde	24901151	FALSE	C1CCc2c(cc(cc12)O)C=O
MOL000082	0.7899	0.2101	0.6165	Amomum Tsao-Ko Crevostet	(3R,5R)-1,7-bis(4-hydroxyphenyl)heptane-3,5-diol	11034432	FALSE	c1c(ccc(c1)CCC(CC(CCc1ccc(cc1)O)O)O)O
MOL000083	0.9404	0.0596	0.9523	Amomum Tsao-Ko Crevostet	(2E,6E)-8-hydroxy-2,6-dimethylocta-2,6-dienal	11412603	FALSE	C(/C=C(\C)/CC/C=C(\C)/C=O)O
MOL000089	0.8738	0.1262	0.9622	Sesami Nigrum Semen	catechol	289	FALSE	c1(O)c(O)cccc1
MOL000089	0.8738	0.1262	0.9622	Amomum Tsao-Ko Crevostet	catechol	289	FALSE	c1(O)c(O)cccc1

MOL000089	0.8738	0.1262	0.9622	Arum Ternatum Thunb.	catechol	289	FALSE	c1(O)c(O)cccc1
MOL000089	0.8738	0.1262	0.9622	Carthami Flos	catechol	289	FALSE	c1(O)c(O)cccc1
MOL000089	0.8738	0.1262	0.9622	Jujubae Fructus	catechol	289	FALSE	c1(O)c(O)cccc1
MOL000089	0.8738	0.1262	0.9622	Cyperi Rhizoma	catechol	289	FALSE	c1(O)c(O)cccc1
MOL000089	0.8738	0.1262	0.9622	Croci Stigma	catechol	289	FALSE	c1(O)c(O)cccc1
MOL000089	0.8738	0.1262	0.9622	Mori Cortex	catechol	289	FALSE	c1(O)c(O)cccc1
MOL000089	0.8738	0.1262	0.9622	Eucommiae Cortex	catechol	289	FALSE	c1(O)c(O)cccc1
MOL000089	0.8738	0.1262	0.9622	Citri Grandis Exocarpium	catechol	289	FALSE	c1(O)c(O)cccc1
MOL000089	0.8738	0.1262	0.9622	Folium Nelumbinis	catechol	289	FALSE	c1(O)c(O)cccc1
MOL000089	0.8738	0.1262	0.9622	Ginkgo Semen	catechol	289	FALSE	c1(O)c(O)cccc1
MOL000090	0.5271	0.4729	0.7282	Amomum Tsao-Ko Crevostet	Curcumin	5281767	FALSE	c1c(c(cc(c1)/C=C/C(=O)/C=C(\O)/C=C/c1cc(c(cc1)O)OC)OC)O
MOL000096	0.9402	0.0598	0.8161	Dioscoreaebulbiferae	(-)-catechin	73160	FALSE	C1(C(O)Cc2c(O)cc(O)cc2O1)c1cc(O)c(O)cc1
MOL000096	0.9402	0.0598	0.8161	Jujubae Fructus	(-)-catechin	73160	FALSE	C1(C(O)Cc2c(O)cc(O)cc2O1)c1cc(O)c(O)cc1
MOL000096	0.9402	0.0598	0.8161	Phaseoli Semen	(-)-catechin	73160	FALSE	C1(C(O)Cc2c(O)cc(O)cc2O1)c1cc(O)c(O)cc1
MOL000096	0.9402	0.0598	0.8161	Sargentodoxae Caulis	(-)-catechin	73160	FALSE	C1(C(O)Cc2c(O)cc(O)cc2O1)c1cc(O)c(O)cc1
MOL000096	0.9402	0.0598	0.8161	Amomum Tsao-Ko Crevostet	(-)-catechin	73160	FALSE	C1(C(O)Cc2c(O)cc(O)cc2O1)c1cc(O)c(O)cc1
MOL000096	0.9402	0.0598	0.8161	Ginkgo Folium	(-)-catechin	73160	FALSE	C1(C(O)Cc2c(O)cc(O)cc2O1)c1cc(O)c(O)cc1
MOL000096	0.9402	0.0598	0.8161	Microctis Folium	(-)-catechin	73160	FALSE	C1(C(O)Cc2c(O)cc(O)cc2O1)c1cc(O)c(O)cc1
MOL000096	0.9402	0.0598	0.8161	Choerospondiatis Fructus	(-)-catechin	73160	FALSE	C1(C(O)Cc2c(O)cc(O)cc2O1)c1cc(O)c(O)cc1
MOL000096	0.9402	0.0598	0.8161	Rhizoma Fagopyri Cymosi	(-)-catechin	73160	FALSE	C1(C(O)Cc2c(O)cc(O)cc2O1)c1cc(O)c(O)cc1
MOL000096	0.9402	0.0598	0.8161	Radix Rhei Et Rhizome	(-)-catechin	73160	FALSE	C1(C(O)Cc2c(O)cc(O)cc2O1)c1cc(O)c(O)cc1
MOL000096	0.9402	0.0598	0.8161	Folium Nelumbinis	(-)-catechin	73160	FALSE	C1(C(O)Cc2c(O)cc(O)cc2O1)c1cc(O)c(O)cc1
MOL000098	0.9305	0.0695	0.9063	Allium Azureum Ledeb.	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Oroxyli Semen	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Saussureae Involucratae Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Silybum Marianum	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Lepidii Semen Descurainiae Semen	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Asparagi Radix	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Et Radix Patriniae Rhizoma	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Geranium Wilfordii Maxim.	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Ginseng Folium	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Verbenae Herb	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Anisi Stellati Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Granati Pericarpium	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O

MOL000098	0.9305	0.0695	0.9063	Ilicis Purpureae Folium	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Euphorbiae Humifusae Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Toosendan Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Caryophylliflos	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Cortex Moutan	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Plantaginis Semen	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Lycii Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Dictamni Cortex	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Dioscoreaebulbiferae	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Potentillae Chinensis Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Hedysari Radix	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Litseae Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Ailanthi Cortex	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Inulae Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Ephedra Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Epimrdii Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Saxifraga Stolonifera	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Pogostemon Cablin (Blanco) Benth.	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Aloe	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Chaenomeles Sinensis (Thouin) Koehne	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Gleditsiae Spina	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Ailanthi Altissimae Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Tamaricis Cacumen	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Herba Pyrolae	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Flos Genkwa	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Polygoni Orientalis Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Lobeliae Chinensis Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Crataegi Folium	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Salviae Chinensis Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Eriocauli Flos	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Eucommiae Cortex	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Polygoni Cuspidati Rhizoma Et Radix	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Litchi Semen	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Ecliptae Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Carthami Flos	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Artemisia Annua L.	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O

MOL000098	0.9305	0.0695	0.9063	Euphorbiae Helioscopiae Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Leonuri Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Saururi Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Astragali Cpmplanatisemen	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Forsythiae Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Hedyotis Diffusae Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Gossampiniflos	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Corydalis Rhizoma	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Viticis Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Sedi Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Impatientis Semen	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Inulae Flos	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Gynostemmae Pentaphylli Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Artemisiae Scopariae Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Folium Nelumbinis	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Euonymi Alati Ramulus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Herba Clematidis Aethusaefoliae	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Ephedrae Radix Et Rhizoma	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Folium Artemisiae Argyi	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Amomum Tsao-Ko Crevostet	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Bistortae Rhizoma	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Celastri Orbiculati Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Choerospondiatis Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Semen Pruni	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Hyperici Japonici Herber	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Platycladi Cacumen	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Chrysanthemi Flos	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Calendula Officinalis	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Solanum Nigrum Linn.	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Kaki Calyx	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Bidentis Bipinnatae Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Herbahypericiperforati	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Evodiae Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O

MOL000098	0.9305	0.0695	0.9063	Cyperi Rhizoma	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Rubi Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Echinopsis Radix	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Ilicis Cornutae Folium Immayuri	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Gleditsiae Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Gnaphalii Affinis Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Cuscutae Semen	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Phellodendri Amurensis Cortex	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Nelumbinis Stamen	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Peucedani Radix	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Gardeniae Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Hedysarum Multijugum Maxim.	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Boehmeriae Rhizoma Et Radix	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Alpiniae Officinarum Rhizome	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Croci Stigma	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Alpinia Katsumadai Hayat	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Folium Ilicis Cornutae	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Puerariae Flos	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Hoveniae Dulcis Semen	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Mori Cortex	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Vaccariae Semen	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Canarii Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Solidaginis Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Rhododendri Daurici Folium	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Potentillae Discoloris Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Herba Taxilli	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Radix Bupleuri	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Eriobotryae Folium	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Agrimonia Eupatoria	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Ampelopsis Japonica	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Dysosmae Verspiellis Rhixoma Et Radix	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Jujubae Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Pollen Typhae	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Semen Aesculi	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Chrysanthemi Indici Flos	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O

MOL000098	0.9305	0.0695	0.9063	Lysimachiae Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Linderae Radix	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Lunulatae Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Phyllanthi Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Glehniae Radix	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Sargassum	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Nelumbinis Plumula	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Actinidia Chinensis Planch	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	licorice	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Uncariae Ramulus Cumuncis	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Mori Cortex	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Catechu	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Mume Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Smilacis Glabrae Rhixoma	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Farfarae Flos	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Myrrha	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Pyrrosiae Folium	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Receptaculum Nelumbinis	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Daturae Flos	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Eucommiae Folium	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Stachyurimedulla Helwingiaemedulla	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Ardisiae Japonicae Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Portulacae Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Ginkgo Folium	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Fructussophorae	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Impatiens Balsamina	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Rosae Laevigatae Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Malvae Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Glechomae Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Pteridis Multifidae Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Prinsepiae Nux	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Herba Sarcandrae	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Sophorae Flavescentis Radix	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Herba Cirsii	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Ginkgo Semen	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Radix Sanguisorbae	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Trigonellae Semen	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Achyranthis Bidentatae Radix	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Herba Patriniae	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O

MOL000098	0.9305	0.0695	0.9063	Lonicerae Japonicae Flos	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Equiseti Hiemalis Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Hippophae Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Schizonepetae Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Rhizoma Fagopyri Cymosi	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Sophora Japonica L.	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Zanthoxyli Pericarpium	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Cyathulae Radix	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Asteris Radix Et Rhizoma	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Sapindi Mukorossiperic Arpium	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Prunellae Spica	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Paederiae Scandentis Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Mori Fructus	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Polygoni Avicularis Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Mori Follum	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Houttuyniae Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Rhododendronmolle	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Scutellariae Barbatae Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Moslae Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Sophorae Tonkinensis Radix Et Rhizome	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Rose Rugosae Flos	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Cotyledon Fimbriata Turcz.	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Coriandri Sativi Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Cistanches Herba	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Microctis Folium	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Fructus Ligustri Lucidi	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000098	0.9305	0.0695	0.9063	Trollius Chinensis	quercetin	5280343	TRUE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)O)O)O
MOL000101	0.9562	0.0438	0.8936	Amomum Tsao-Ko Crevostet	(3aS,7R,7aR)-7-hydroxy-2,3,3a,6,7,7a-hexahydro-1H-indene-4-carbaldehyde	10397152	FALSE	C1=C(C2C(C(C1)O)CCC2)C=O
MOL000102	0.7899	0.2101	0.6165	Amomum Tsao-Ko Crevostet	meso-hannokinol	25763835	FALSE	c1c(ccc(c1)O)CCC(CC(CCc1ccc(cc1)O)O)O
MOL000103	0.9357	0.0643	0.9629	Chaenomeles Sinensis (Thouin) Koehne	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Cortex Moutan	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Trollius Chinensis	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Belamcandae Rhizome	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O

MOL000103	0.9357	0.0643	0.9629	Cyperi Rhizoma	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Rubi Fructus	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Zanthoxylum Nitidum	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Ranunculi Ternati Radix	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Lobeliae Chinensis Herba	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Sophorae Tonkinensis Radix Et Rhizome	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Catechu	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Rhododendri Daurici Folium	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Chuanxiong Rhizoma	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Lysimachiae Herba	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Herba Clematidis Aethusaefoliae	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Stemonae Radix	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Ginkgo Folium	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Cinnamomi Ramulus	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Celastri Orbiculati Fructus	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Herba Sarcandrae	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Folium Nelumbinis	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Amomum Tsao-Ko Crevostet	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Cyathulae Radix	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Lepidii Semen Descurainiae Semen	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Semen Euphorbiae	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Solanum Nigrum Linn.	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Sargassum	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Allii Fistulost Bulbus	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Lasiosphaera Seu Calvatia	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Inulae Herba	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Allium Azureum Ledeb.	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Corydalis Rhizoma	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Semiaquilegiae Radix	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Asteris Radix Et Rhizoma	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Lonicerae Japonicae Flos	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Calendula Officinalis	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Cotyledon Fimbriata Turcz.	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Plantaginis Herba	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Ephedra Herba	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O

MOL000103	0.9357	0.0643	0.9629	Viticis Fructus	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Pine Pollen	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Equiseti Hiemalis Herba	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Coriolus	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Ecliptae Herba	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000103	0.9357	0.0643	0.9629	Ginseng Folium	PHB	3702506	FALSE	c1c(ccc(c1)C(=O)O)O
MOL000104	0.9474	0.0526	0.9684	Amomum Tsao-Ko Crevostet	p-menth-1-ene-5,6-diol	Not Available	FALSE	C1C(C(C(C(=C1)C)O)O)C(C)C
MOL000105	0.9384	0.0616	0.9667	Citri Sarcodactylis Fructus	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Rhododendri Daurici Folium	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Amomum Tsao-Ko Crevostet	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Spatholobus Suberectus Dunn	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Herba Sarcandrae	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Pine Pollen	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Ephedrae Radix Et Rhizoma	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Ginseng Folium	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Cotyledon Fimbriata Turcz.	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Polygoni Cuspidati Rhizoma Et Radix	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Sargentodoxae Caulis	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Smilax China	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Pollen Typhae	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Cornus Officinalis Sieb. Et Zucc.	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	licorice	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Choerospondiatis Fructus	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Geranium Wilfordii Maxim.	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O

MOL000105	0.9384	0.0616	0.9667	Inulae Herba	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Saussureae Involucratae Herba	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Abri Herba	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Drynariae Rhizoma	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Prinsepiae Nux	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Alpinia Katsumadai Hayat	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Ephedra Herba	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Arum Ternatum Thunb.	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Acoritataninowii Rhizoma	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Lygodii Spora	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Maydis Seigma	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Radix Salviae	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Dioscoreaebulbiferae	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Radix Euphorbiae Pekinensis	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Mori Cortex	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Myristicae Semen	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Chaenomeles Sinensis (Thouin) Koehne	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Bidentis Bipinnatae Herba	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Eucommiae Cortex	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Houttuyniae Herba	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Actinidia Chinensis Planch	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O

MOL000105	0.9384	0.0616	0.9667	Schisandrae Chinensis Fructus	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Potentillae Discoloris Herba	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Canarii Fructus	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Ecliptae Herba	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Herba Cirsii	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Pseudobulbus Cremastrae Seu Pleiones	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Cyperi Rhizoma	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Viscum Angulatum Heyne	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Ampelopsis Japonica	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Eucommiae Folium	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Herba Pyrolae	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Calendula Officinalis	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Solanum Nigrum Linn.	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Viticis Fructus	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Trollius Chinensis	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Pyrrosiae Folium	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Alpiniae Officinarum Rhizome	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Cicadae Periostracum	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Rhizoma Fagopyri Cymosi	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Rosae Laevigatae Fructus	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Lonicerae Japonicae Flos	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O

MOL000105	0.9384	0.0616	0.9667	Hyperici Japonici Herber	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Impatiens Balsamina	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Lycopi Herba	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Ginkgo Folium	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Picrorhizae Rhizoma	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Veronicae Peregrinae Herba	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Semen Pruni	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Saxifraga Stolonifera	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Hordei Fructus Germinatus	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Scutellariae Barbatae Herba	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Cinnamomi Ramulus	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Bistortae Rhizoma	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Ilicis Purpureae Folium	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000105	0.9384	0.0616	0.9667	Herba Clematidis Aethusaefoliae	protocatechuic acid	72	FALSE	C(=O)(c1cc(O)c(O)cc1)O
MOL000106	0.8689	0.1311	0.9577	Canarii Fructus	PYG	1057	FALSE	c1cc(c(c(c1)O)O)O
MOL000106	0.8689	0.1311	0.9577	Eucommiae Cortex	PYG	1057	FALSE	c1cc(c(c(c1)O)O)O
MOL000106	0.8689	0.1311	0.9577	Semen Euphorbiae	PYG	1057	FALSE	c1cc(c(c(c1)O)O)O
MOL000106	0.8689	0.1311	0.9577	Radix Paeoniae Rubra	PYG	1057	FALSE	c1cc(c(c(c1)O)O)O
MOL000106	0.8689	0.1311	0.9577	Euphorbiae Helioscopiae Herba	PYG	1057	FALSE	c1cc(c(c(c1)O)O)O
MOL000106	0.8689	0.1311	0.9577	Paeoniae Radix Alba	PYG	1057	FALSE	c1cc(c(c(c1)O)O)O
MOL000106	0.8689	0.1311	0.9577	Saxifraga Stolonifera	PYG	1057	FALSE	c1cc(c(c(c1)O)O)O
MOL000106	0.8689	0.1311	0.9577	Amomum Tsao-Ko Crevostet	PYG	1057	FALSE	c1cc(c(c(c1)O)O)O

MOL000107	0.9265	0.0735	0.8040	Amomum Tsao-Ko Crevostet	quercertin,3-o-beta-d-glucopyranoside	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)c1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1
MOL000107	0.9265	0.0735	0.8040	Folium Nelumbinis	quercertin,3-o-beta-d-glucopyranoside	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)c1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1
MOL000107	0.9265	0.0735	0.8040	Artemisia Annua L.	quercertin,3-o-beta-d-glucopyranoside	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)c1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1
MOL000108	0.8865	0.1135	0.8282	Folium Nelumbinis	quercetin 3-o-rhamnopyranosyl	Not Available	FALSE	C1(C(C(OC(C1O)C)OCC1C(C(C(C(O1)Oc1c(oc2c(c1=O)c(cc(c2)O)O)c1ccc(c(c1)O)O)O)O)O)O)O
MOL000108	0.8865	0.1135	0.8282	Ardisiae Japonicae Herba	quercetin 3-o-rhamnopyranosyl	Not Available	FALSE	C1(C(C(OC(C1O)C)OCC1C(C(C(C(O1)Oc1c(oc2c(c1=O)c(cc(c2)O)O)c1ccc(c(c1)O)O)O)O)O)O)O
MOL000108	0.8865	0.1135	0.8282	Amomum Tsao-Ko Crevostet	quercetin 3-o-rhamnopyranosyl	Not Available	FALSE	C1(C(C(OC(C1O)C)OCC1C(C(C(C(O1)Oc1c(oc2c(c1=O)c(cc(c2)O)O)c1ccc(c(c1)O)O)O)O)O)O)O
MOL000108	0.8865	0.1135	0.8282	Rhizoma Fagopyri Cymosi	quercetin 3-o-rhamnopyranosyl	Not Available	FALSE	C1(C(C(OC(C1O)C)OCC1C(C(C(C(O1)Oc1c(oc2c(c1=O)c(cc(c2)O)O)c1ccc(c(c1)O)O)O)O)O)O)O
MOL000108	0.8865	0.1135	0.8282	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	quercetin 3-o-rhamnopyranosyl	Not Available	FALSE	C1(C(C(OC(C1O)C)OCC1C(C(C(C(O1)Oc1c(oc2c(c1=O)c(cc(c2)O)O)c1ccc(c(c1)O)O)O)O)O)O)O
MOL000108	0.8865	0.1135	0.8282	Leonuri Herba	quercetin 3-o-rhamnopyranosyl	Not Available	FALSE	C1(C(C(OC(C1O)C)OCC1C(C(C(C(O1)Oc1c(oc2c(c1=O)c(cc(c2)O)O)c1ccc(c(c1)O)O)O)O)O)O)O
MOL000109	0.9265	0.0735	0.8040	Folium Nelumbinis	quercetin,3-o-glucoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000109	0.9265	0.0735	0.8040	Artemisia Annua L.	quercetin,3-o-glucoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000109	0.9265	0.0735	0.8040	Amomum Tsao-Ko Crevostet	quercetin,3-o-glucoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000111	0.8866	0.1134	0.8314	Rhizoma Fagopyri Cymosi	quercetin,3-o-rutinoside	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1C(C(C(C(O1)COC1C(C(C(C(O1)C)O)O)O)O)O)O)c1ccc(c(c1)O)O)O)O
MOL000111	0.8866	0.1134	0.8314	Ardisiae Japonicae Herba	quercetin,3-o-rutinoside	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1C(C(C(C(O1)COC1C(C(C(C(O1)C)O)O)O)O)O)O)c1ccc(c(c1)O)O)O)O
MOL000111	0.8866	0.1134	0.8314	Leonuri Herba	quercetin,3-o-rutinoside	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1C(C(C(C(O1)COC1C(C(C(C(O1)C)O)O)O)O)O)O)c1ccc(c(c1)O)O)O)O

MOL000111	0.8866	0.1134	0.8314	Amomum Tsao-Ko Crevostet	quercetin,3-o-rutinoside	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1C(C(C(C(O1)COC1C(C(C(C(O1)C)O)O)O)O)O)O)c1ccc(c(c1)O)O)O)O
MOL000111	0.8866	0.1134	0.8314	Folium Nelumbinis	quercetin,3-o-rutinoside	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1C(C(C(C(O1)COC1C(C(C(C(O1)C)O)O)O)O)O)O)c1ccc(c(c1)O)O)O)O
MOL000111	0.8866	0.1134	0.8314	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	quercetin,3-o-rutinoside	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1C(C(C(C(O1)COC1C(C(C(C(O1)C)O)O)O)O)O)O)c1ccc(c(c1)O)O)O)O
MOL000112	0.9265	0.0735	0.8040	Artemisia Annua L.	quercetin-3-o-galactopyranoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000112	0.9265	0.0735	0.8040	Amomum Tsao-Ko Crevostet	quercetin-3-o-galactopyranoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000112	0.9265	0.0735	0.8040	Leonuri Herba	quercetin-3-o-galactopyranoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000112	0.9265	0.0735	0.8040	Folium Nelumbinis	quercetin-3-o-galactopyranoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL000113	0.9562	0.0438	0.8936	Amomum Tsao-Ko Crevostet	(3aR,7R,7aS)-7-hydroxy-2,3,3a,6,7,7a-hexahydro-1H-indene-4-carbaldehyde	11389600	FALSE	C1=C(C2C(C(C1)O)CCC2)C=O
MOL000114	0.9411	0.0589	0.9574	Corydalis Rhizoma	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Phragmitis Rhizoma	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Equiseti Hiemalis Herba	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Radix Clematidis	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Plantaginis Herba	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Sophorae Tonkinensis Radix Et Rhizome	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Aristolochiae Fructus	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Lygodii Spora	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Polygoni Orientalis Fructus	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Imperatae Rhizoma	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Hemerocallis Radix	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Herba Selaginellae Moellendorfii	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Curcumae Radix	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Buddlejae Flos	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Coriolus	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O

MOL000114	0.9411	0.0589	0.9574	Viticis Cannabifoliae Fructus	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Cortex Moutan	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Viticis Fructus	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Actinidia Chinensis Planch	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Peanut Skin	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Figwort Root	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Pyrrosiae Folium	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Benzoinum	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Chuanxiong Rhizoma	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Peucedani Radix	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Mori Cortex	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Sargentodoxae Caulis	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Radix Paeoniae Rubra	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Stemonae Radix	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Semiaquilegiae Radix	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Rhizoma Seu Herba Aristolochiae Mollissimae	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Ginkgo Folium	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Dioscoreaebulbiferae	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Saposhnikoviae Radix	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Hyperici Japonici Herber	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Impatiens Balsamina	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Gypsophila Licentiana Hand.-Mazz.	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Picrorhizae Rhizoma	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Eucommiae Cortex	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Forsythiae Fructus	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Citri Sarcodactylis Fructus	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Amomum Tsao-Ko Crevostet	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Tribulifructus	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Maydis Seigma	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Ephedra Herba	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Hedysari Radix	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Arum Ternatum Thunb.	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Meliae Azedarach Fructus	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Pseudolaricis Cortex	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Inulae Herba	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Allii Fistulost Bulbus	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Acoritataninowii Rhizoma	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Mahoniae Caulis	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Cyperi Rhizoma	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O

MOL000114	0.9411	0.0589	0.9574	Trichosanthes Kirilowii Maxim	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Prinsepiae Nux	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Capsici Fructus	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Herba Sarcandrae	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Hedysarum Multijugum Maxim.	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Solanum Nigrum Linn.	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Rhododendri Daurici Folium	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Momordicae Fructus	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Glehniae Radix	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Smilax China	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Notopterygii Rhizoma Et Radix	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Scutellariae Barbatae Herba	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Herba Solani Lyrati	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Celastri Orbiculati Fructus	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Atractylodes Lancea (Thunb.)Dc.	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Herbahypericiperforati	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Mori Cortex	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Dysosmae Verspiellis Rhixoma Et Radix	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Trollius Chinensis	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Hoveniae Dulcis Semen	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Ephedrae Radix Et Rhizoma	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Choerospondiatis Fructus	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Semen Pruni	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Hordei Fructus Germinatus	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Caulis Akebiae	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000114	0.9411	0.0589	0.9574	Rubi Fructus	vanillic acid	8468	FALSE	c1(cc(c(cc1)O)OC)C(=O)O
MOL000115	0.9026	0.0974	0.8939	Amomum Tsao-Ko Crevostet	Undecenal	5283356	FALSE	C(CC/C=C/C=O)CCCCC
MOL000115	0.9026	0.0974	0.8939	Adenophprae Ae Radix	Undecenal	5283356	FALSE	C(CC/C=C/C=O)CCCCC
MOL000115	0.9026	0.0974	0.8939	Chaenomeles Sinensis (Thouin) Koehne	Undecenal	5283356	FALSE	C(CC/C=C/C=O)CCCCC
MOL000115	0.9026	0.0974	0.8939	Hippophae Fructus	Undecenal	5283356	FALSE	C(CC/C=C/C=O)CCCCC
MOL000115	0.9026	0.0974	0.8939	Polygoni Orientalis Fructus	Undecenal	5283356	FALSE	C(CC/C=C/C=O)CCCCC

MOL000115	0.9026	0.0974	0.8939	Morindae Officinalis Radix	Undecenal	5283356	FALSE	C(CC/C=C/C=O)CCCCC
MOL000116	0.9336	0.0664	0.9361	Campsis Flos	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Lonicerae Japonicae Flos	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Leonuri Fructus	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Sinapis Semen	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Peucedanidecursivi Radix	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Semen Euphorbiae	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Coriandri Sativi Herba	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Radix Angelicae Biseratae	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Citrus Aurantium	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Amomum Tsao-Ko Crevostet	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Mume Flos	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Farfarae Flos	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Ganoderma	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Morindae Officinalis Radix	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Cnidii Fructus	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Polygonati Odorati Rhizoma	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Ginkgo Folium	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Lysimachiae Herba	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Radix Cynanchi	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Momordicae Fructus	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Saposhnikoviae Radix	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Cynanchistauntonii Rhizoma Et Radix	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Rhizome Of Whiteback Greenbrier	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Adenophprae Ae Radix	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Carthami Flos	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Herba Taxilli	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Capsellae Herba	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Maydis Seigma	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Dianthi Herba	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Raphani Semen	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Curcumae Radix	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Rhododendri Daurici Folium	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Xanthii Fructus	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Meliae Azedarach Fructus	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Allii Tuberosi Semen	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Angelicae Sinensis Radix	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Apocyniveneti Folium	Nonanal	31289	FALSE	C(CCCC=O)CCCC

MOL000116	0.9336	0.0664	0.9361	Rhizoma Fagopyri Cymosi	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Celastri Orbiculati Fructus	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Croci Stigma	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	A. Dahurica (Fisch.) Benth. Et Hook	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Capsici Fructus	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Eriobotryae Folium	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Peucedani Radix	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Humulus Scandens (Lour.) Merr.	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Dysosmae Verspiellis Rhixoma Et Radix	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Perillae Fructus	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Radix Cynanchi Paniculati	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Chuanxiong Rhizoma	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Ephedra Herba	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Hippophae Fructus	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000116	0.9336	0.0664	0.9361	Eucommiae Folium	Nonanal	31289	FALSE	C(CCCC=O)CCCC
MOL000117	0.9568	0.0432	0.9206	Piperis Longi Fructus	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Rhizome Of Whiteback Greenbrier	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Ginkgo Folium	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Kaempferiae Rhizoma	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Zanthoxyli Pericarpium	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Zingiber Officinale Roscoe	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Angelicae Sinensis Radix	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Acoritataninowii Rhizoma	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Viticis Negundo Folium	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Morindae Officinalis Radix	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Glechomae Herba	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Moslae Herba	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Foeniculi Fructus	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Arisaematis Rhizoma	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Schisandrae Chinensis Fructus	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Aucklandiae Radix	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Rubi Fructus	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Alpinia Katsumadai Hayat	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Forsythiae Fructus	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Farfarae Flos	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Cnidii Fructus	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Linderae Radix	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Magnoliae Flos	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C

MOL000117	0.9568	0.0432	0.9206	Asari Radix Et Rhizoma	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Zingiberis Rhizoma	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Radix Bupleuri	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Viticis Fructus	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Campsis Flos	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Ligustici Rhizoma Et Radix	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Hippophae Fructus	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Nardostachyos Radix Et Rhizoma	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Styrax	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Alpiniae Officinarum Rhizome	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Ephedra Herba	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Myrrha	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Citri Exocarpium Rubrum	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Notopterygii Rhizoma Et Radix	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Mahoniae Caulis	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Cyperi Rhizoma	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Kadsurae Coccineae Radix Et Caulis	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Curcumae Radix	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Chuanxiong Rhizoma	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Viticis Cannabifoliae Fructus	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Cinnanmomi Cortex	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Alpiniae Oxyphyliae Fructus	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Magnolia Officinalis Rehd Et Wils.	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Curcumae Rhizoma	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Aurantii Fructus Immaturus	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Amomum Tsao-Ko Crevostet	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Chrysanthemi Flos	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Eupatorium Fortunei Turcz	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Cinnamomi Ramulus	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C

MOL000117	0.9568	0.0432	0.9206	Borneolum Syntheticum	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Sesami Nigrum Semen	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Citri Reticulatae Pericarpium Viride	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Piperis Fructus	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Menthae Herba	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Eriobotryae Folium	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Radix Salviae	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Radix Angelicae Biseratae	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Schizonepetae Herba	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Gnaphalii Affinis Herba	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000117	0.9568	0.0432	0.9206	Citri Fructus	Cymol	7463	FALSE	c1(ccc(cc1)C(C)C)C
MOL000118	0.9322	0.0678	0.9688	Rose Rugosae Flos	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Viticis Negundo Folium	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Calyx Seu Fructus Physalis	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Eriobotryae Folium	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Curcumae Rhizoma	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Ilicis Cornutae Folium Immayuri	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Mori Cortex	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Styrax	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Ginkgo Folium	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Menthae Herba	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Zingiber Officinale Roscoe	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Rhizome Of Whiteback Greenbrier	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Viticis Fructus	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Ephedra Herba	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C

MOL000118	0.9322	0.0678	0.9688	Aucklandiae Radix	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Cinnamomi Ramulus	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Campsis Flos	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Nardostachyos Radix Et Rhizoma	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Glechomae Herba	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Gnaphalii Affinis Herba	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Flemingia Prostrata Roxb	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Zingiberis Rhizoma	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Citrus Aurantium	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Morindae Officinalis Radix	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Perilla Frutescens	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Platycladi Cacumen	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Alpiniae Officinarum Rhizome	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Cayratiae Japonicae Herba	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Cnidii Fructus	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Chuanxiong Rhizoma	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Piperis Fructus	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Agrimonia Eupatoria	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Citrus Reticulata	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Cuscutae Semen	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Artemisia Annua L.	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C

MOL000118	0.9322	0.0678	0.9688	Kaempferiae Rhizoma	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Amygdalus Communis Vas	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Curcumae Radix	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Violsse Herba	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Artemisiae Scopariae Herba	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Lysimachiae Herba	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Rubi Fructus	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Amomum Tsao-Ko Crevostet	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Anemarrhenae Rhizoma	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Citri Reticulatae Pericarpium Viride	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Magnolia Officinalis Rehd Et Wils.	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Epimrdii Herba	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Linderae Radix	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Zanthoxyli Pericarpium	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	licorice	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Cornus Officinalis Sieb. Et Zucc.	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Smilacis Glabrae Rhixoma	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Folium Artemisiae Argyi	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Hippophae Fructus	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Alpinia Katsumadai Hayat	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C

MOL000118	0.9322	0.0678	0.9688	Illicium Difengpi K. L. B. Et K. I. M.	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Kadsurae Coccineae Radix Et Caulis	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Dianthi Herba	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Citri Sarcodactylis Fructus	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Schisandrae Chinensis Fructus	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Fructus Carotae	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Radix Bupleuri	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Citri Fructus	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Lilii Bulbus	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Arisaematis Rhizoma	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Cinnanmomi Cortex	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Perillae Fructus	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000118	0.9322	0.0678	0.9688	Homalomena Occulta (Lour.) Schott	(L)-alpha-Terpineol	443162	FALSE	CC(C)(O)C1CC=C(CC1)C
MOL000119	0.8642	0.1358	0.7920	Folium Artemisiae Argyi	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Evodiae Fructus	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Cinnanmomi Cortex	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Acoritataninowii Rhizoma	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Citrus Aurantium	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Celastri Orbiculati Fructus	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Eupatorium Fortunei Turcz	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Ginkgo Folium	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O

MOL000119	0.8642	0.1358	0.7920	Zanthoxyli Pericarpium	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Alpinia Katsumadai Hayat	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Anisi Stellati Fructus	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Pogostemon Cablin (Blanco) Benth.	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Santalum Album L.	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Schisandrae Chinensis Fructus	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Amomum Tsao-Ko Crevostet	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Radix Angelicae Biseratae	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Tamaricis Cacumen	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Zingiberis Rhizoma	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Illicium Difengpi K. L. B. Et K. I. M.	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Dianthi Herba	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Herba Taxilli	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Mahoniae Folum	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Capsici Fructus	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Zingiber Officinale Roscoe	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Chrysanthemi Flos	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000119	0.8642	0.1358	0.7920	Benzoinum	ZINC02040970	11241545	FALSE	C(CC/C=C(/CCC=C(C)C)\C)(C=C)(C)O
MOL000120	0.9212	0.0788	0.9178	Herba Taxilli	dec-2-enal	5283345	FALSE	C(CCCCC)C/C=C/C=O
MOL000120	0.9212	0.0788	0.9178	Amygdalus Communis Vas	dec-2-enal	5283345	FALSE	C(CCCCC)C/C=C/C=O
MOL000120	0.9212	0.0788	0.9178	Meliae Azedarach Fructus	dec-2-enal	5283345	FALSE	C(CCCCC)C/C=C/C=O
MOL000120	0.9212	0.0788	0.9178	Lignum Pini Nodi	dec-2-enal	5283345	FALSE	C(CCCCC)C/C=C/C=O
MOL000120	0.9212	0.0788	0.9178	Radix Bupleuri	dec-2-enal	5283345	FALSE	C(CCCCC)C/C=C/C=O

MOL000120	0.9212	0.0788	0.9178	Hippophae Fructus	dec-2-enal	5283345	FALSE	C(CCCCC)C/C=C/C=O
MOL000120	0.9212	0.0788	0.9178	Ganoderma	dec-2-enal	5283345	FALSE	C(CCCCC)C/C=C/C=O
MOL000120	0.9212	0.0788	0.9178	Amomum Tsao-Ko Crevostet	dec-2-enal	5283345	FALSE	C(CCCCC)C/C=C/C=O
MOL000120	0.9212	0.0788	0.9178	Broussonetiae Fructus	dec-2-enal	5283345	FALSE	C(CCCCC)C/C=C/C=O
MOL000120	0.9212	0.0788	0.9178	Ginkgo Folium	dec-2-enal	5283345	FALSE	C(CCCCC)C/C=C/C=O
MOL000120	0.9212	0.0788	0.9178	Allii Sativi Bulbus	dec-2-enal	5283345	FALSE	C(CCCCC)C/C=C/C=O
MOL000120	0.9212	0.0788	0.9178	Cucurbitae Moschatae Semen	dec-2-enal	5283345	FALSE	C(CCCCC)C/C=C/C=O
MOL000120	0.9212	0.0788	0.9178	Epimrdii Herba	dec-2-enal	5283345	FALSE	C(CCCCC)C/C=C/C=O
MOL000121	0.9201	0.0799	0.9210	Coriandri Sativi Herba	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000121	0.9201	0.0799	0.9210	Ganoderma	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000121	0.9201	0.0799	0.9210	Lilii Bulbus	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000121	0.9201	0.0799	0.9210	Citri Fructus	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000121	0.9201	0.0799	0.9210	Mume Flos	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000121	0.9201	0.0799	0.9210	Capsici Fructus	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000121	0.9201	0.0799	0.9210	Amomum Tsao-Ko Crevostet	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000121	0.9201	0.0799	0.9210	Hippophae Fructus	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000121	0.9201	0.0799	0.9210	Carthami Flos	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000121	0.9201	0.0799	0.9210	Citrus Aurantium	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000121	0.9201	0.0799	0.9210	Siphonostegiae Herba	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000121	0.9201	0.0799	0.9210	Houttuyniae Herba	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000121	0.9201	0.0799	0.9210	Angelicae Sinensis Radix	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000121	0.9201	0.0799	0.9210	Lysimachiae Foenigraeci Herba	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000121	0.9201	0.0799	0.9210	Citrus Reticulata	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000121	0.9201	0.0799	0.9210	Dianthi Herba	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000121	0.9201	0.0799	0.9210	Adenophprae Ae Radix	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000121	0.9201	0.0799	0.9210	Campsis Flos	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000121	0.9201	0.0799	0.9210	Herba Taxilli	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000121	0.9201	0.0799	0.9210	Zingiberis Rhizoma	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000121	0.9201	0.0799	0.9210	Dichroae Radix	Decanal	8175	FALSE	C(CCCCC)CCCC=O
MOL000122	0.9678	0.0322	0.8618	Borneolum Syntheticum	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Zingiberis Rhizoma	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Herba Patriniae	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Benzoinum	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Magnolia Officinalis Rehd Et Wils.	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Perillae Fructus	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Zanthoxyli Pericarpium	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C

MOL000122	0.9678	0.0322	0.8618	Piperis Longi Fructus	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Styrax	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Celastri Orbiculati Fructus	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Dalbergiae Odoriferae Lignum	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Alpinia Katsumadai Hayat	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Cyperi Rhizoma	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Prunellae Spica	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Eupatorium Fortunei Turcz	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Violsse Herba	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Caryophylliflos	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Siphonostegiae Herba	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Ephedra Herba	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Viticis Negundo Folium	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Agrimonia Eupatoria	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Herba Clinopodii Polycephali.	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Chrysanthemi Flos	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Verbenae Herb	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Cinnanmomi Cortex	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Aristolochiae Fructus	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Illicium Difengpi K. L. B. Et K. I. M.	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Viticis Fructus	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Glechomae Herba	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Foeniculi Fructus	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Centipedae Herba	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Kadsurae Coccineae Radix Et Caulis	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Rhizome Of Whiteback Greenbrier	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Magnoliae Flos	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Anisi Stellati Fructus	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Zingiber Officinale Roscoe	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Gossampiniflos	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Menthae Herba	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Radix Bupleuri	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Rubi Fructus	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Herba Taxilli	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Chuanxiong Rhizoma	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Amomum Tsao-Ko Crevostet	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C

MOL000122	0.9678	0.0322	0.8618	Artemisia Annua L.	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Schizonepetae Herba	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Viticis Cannabifoliae Fructus	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Arisaematis Rhizoma	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Kaempferiae Rhizoma	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Alpiniae Officinarum Rhizome	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Curcumae Radix	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Rhododendri Daurici Folium	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Nardostachyos Radix Et Rhizoma	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Mori Fructus	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Scutellariae Radix	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Piperis Fructus	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Campsis Flos	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Flemingia Prostrata Roxb	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Asari Radix Et Rhizoma	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Schisandrae Chinensis Fructus	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Paederiae Scandentis Herba	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000122	0.9678	0.0322	0.8618	Ginkgo Folium	1,8-cineole	2758	FALSE	C12(OC(C(CC1)CC2)(C)C)C
MOL000123	0.9319	0.0681	0.9465	Hippophae Fructus	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Mori Fructus	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Illicium Difengpi K. L. B. Et K. I. M.	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Eriobotryae Folium	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Mori Cortex	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Zingiberis Rhizoma	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Lonicerae Japonicae Flos	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Citri Grandis Exocarpium	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Geranium Wilfordii Maxim.	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Dysosmae Verspiellis Rhixoma Et Radix	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Homalomena Occulta (Lour.) Schott	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Radix Bupleuri	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Citrus Aurantium	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C

MOL000123	0.9319	0.0681	0.9465	Eucommiae Folium	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Ligustici Rhizoma Et Radix	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Cymbopon Citratus(D C.) Stapf	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Semen Pharbitidis	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Zingiber Officinale Roscoe	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Morindae Officinalis Radix	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Citri Fructus	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Citri Exocarpium Rubrum	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Ephedra Herba	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Myrrha	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Fructus Ligustri Lucidi	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Zanthoxyli Pericarpium	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Siphonostegiae Herba	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Amomum Tsao-Ko Crevostet	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Amygdalus Communis Vas	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Rose Rugosae Flos	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000123	0.9319	0.0681	0.9465	Lysimachiae Foenigraeci Herba	geraniol	637566	FALSE	C(=C\CO)(/CCC=C(C)C)\C
MOL000124	0.9352	0.0648	0.9452	Coriandri Sativi Herba	citral	638011	FALSE	C(=O)/C=C(/CCC=C(C)C)\C
MOL000124	0.9352	0.0648	0.9452	Citri Fructus	citral	638011	FALSE	C(=O)/C=C(/CCC=C(C)C)\C
MOL000124	0.9352	0.0648	0.9452	Zingiber Officinale Roscoe	citral	638011	FALSE	C(=O)/C=C(/CCC=C(C)C)\C
MOL000124	0.9352	0.0648	0.9452	Ganoderma	citral	638011	FALSE	C(=O)/C=C(/CCC=C(C)C)\C
MOL000124	0.9352	0.0648	0.9452	Amomum Tsao-Ko Crevostet	citral	638011	FALSE	C(=O)/C=C(/CCC=C(C)C)\C
MOL000124	0.9352	0.0648	0.9452	Verbenae Herb	citral	638011	FALSE	C(=O)/C=C(/CCC=C(C)C)\C
MOL000124	0.9352	0.0648	0.9452	Campsis Flos	citral	638011	FALSE	C(=O)/C=C(/CCC=C(C)C)\C
MOL000124	0.9352	0.0648	0.9452	Homalomena Occulta (Lour.) Schott	citral	638011	FALSE	C(=O)/C=C(/CCC=C(C)C)\C
MOL000124	0.9352	0.0648	0.9452	Zingiberis Rhizoma	citral	638011	FALSE	C(=O)/C=C(/CCC=C(C)C)\C
MOL000124	0.9352	0.0648	0.9452	Forsythiae Fructus	citral	638011	FALSE	C(=O)/C=C(/CCC=C(C)C)\C
MOL000125	0.9512	0.0488	0.7730	Peucedanidecursivi Radix	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Glechomae Herba	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Ganoderma	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Notopterygii Rhizoma Et Radix	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C

MOL000125	0.9512	0.0488	0.7730	Herba Taxilli	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Angelicae Sinensis Radix	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Viticis Fructus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Gossampiniflos	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Menthae Herba	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Bidentis Bipinnatae Herba	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Cnidii Fructus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Et Radix Patriniae Rhizoma	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Eriobotryae Folium	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Solidaginis Herba	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Citri Reticulatae Pericarpium Viride	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Lysimachiae Foenigraeci Herba	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Mume Flos	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Evodiae Fructus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Herbahypericiperforati	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Citri Exocarpium Rubrum	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Aucklandiae Radix	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Citri Reticulatae Folium	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Citri Fructus Retinervus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Mori Fructus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Aristolochiae Fructus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C

MOL000125	0.9512	0.0488	0.7730	Asari Radix Et Rhizoma	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Coriandri Sativi Herba	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Litseae Fructus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Olibanun	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Kadsurae Coccineae Radix Et Caulis	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Campsis Flos	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Alpinia Katsumadai Hayat	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Piperis Fructus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Magnolia Officinalis Rehd Et Wils.	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Sesami Nigrum Semen	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Illicium Difengpi K. L. B. Et K. I. M.	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Isatidis Folium	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Rubi Fructus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Citrus Reticulata	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Eupatorium Fortunei Turcz	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Dichroae Radix	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Agrimonia Eupatoria	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Folium Artemisiae Argyi	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Styrax	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Peucedani Radix	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C

MOL000125	0.9512	0.0488	0.7730	Lignum Pini Nodi	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Caryophylliflos	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Cinnanmomi Cortex	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Amomum Tsao-Ko Crevostet	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Ligustici Rhizoma Et Radix	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Morindae Officinalis Radix	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Zanthoxyli Pericarpium	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Nardostachyos Radix Et Rhizoma	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Rhododendri Daurici Folium	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Magnoliae Flos	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Cinnamomi Ramulus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Viticis Cannabifoliae Fructus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Linderae Radix	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Fructus Carotae	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Schisandrae Chinensis Fructus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Lonicerae Japonicae Flos	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Paederiae Scandentis Herba	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Polygoni Orientalis Fructus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Myrrha	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Forsythiae Fructus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Pollen Typhae	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C

MOL000125	0.9512	0.0488	0.7730	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Myristicae Semen	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Citri Sarcodactylis Fructus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Artemisia Annua L.	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Curcumae Radix	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Lysimachiae Herba	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Foeniculi Fructus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Viticis Negundo Folium	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Fructus Ligustri Lucidi	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Citri Fructus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Chuanxiong Rhizoma	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Anisi Stellati Fructus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Lilii Bulbus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Citrus Aurantium	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Maydis Seigma	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Dalbergiae Odoriferae Lignum	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Cyperi Rhizoma	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Piperis Longi Fructus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Kaempferiae Rhizoma	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Ephedra Herba	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Homalomena Occulta (Lour.) Schott	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C

MOL000125	0.9512	0.0488	0.7730	Herba Clinopodii Polycephali.	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Zingiberis Rhizoma	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Capsici Fructus	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000125	0.9512	0.0488	0.7730	Codonopsis Radix	(-)-alpha-Pinene	440968	FALSE	C12C(=CCC(C1)C2(C)C)C
MOL000126	0.9548	0.0452	0.7808	Kaempferiae Rhizoma	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Notopterygii Rhizoma Et Radix	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Amomum Tsao-Ko Crevostet	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Eriobotryae Folium	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Viticis Fructus	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Folium Artemisiae Argyi	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Moslae Herba	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Zanthoxyli Pericarpium	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Artemisiae Scopariae Herba	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Glechomae Herba	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Pogostemon Cablin (Blanco) Benth.	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Aristolochiae Fructus	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Alpiniae Officinarum Rhizome	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Citri Fructus	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Styrax	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Litseae Fructus	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Magnoliae Flos	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Zingiberis Rhizoma	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Alpinia Katsumadai Hayat	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Homalomena Occulta (Lour.) Schott	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Citri Sarcodactylis Fructus	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Curcumae Radix	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Agrimonia Eupatoria	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Cornus Officinalis Sieb. Et Zucc.	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Lysimachiae Herba	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Forsythiae Fructus	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Solidaginis Herba	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C

MOL000126	0.9548	0.0452	0.7808	Alpiniae Oxyphyliae Fructus	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Rubi Fructus	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Illicium Difengpi K. L. B. Et K. I. M.	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Chuanxiong Rhizoma	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Coriandri Sativi Herba	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Nardostachyos Radix Et Rhizoma	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Ephedra Herba	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Radix Bupleuri	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Prunellae Spica	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Olibanun	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Foeniculi Fructus	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Schisandrae Chinensis Fructus	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Lignum Pini Nodi	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Eupatorium Fortunei Turcz	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Perillae Fructus	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Cinnamomi Ramulus	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Viticis Negundo Folium	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Aurantii Fructus	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Myristicae Semen	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Xanthii Fructus	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Fructus Ligustri Lucidi	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Kadsurae Coccineae Radix Et Caulis	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Cnidii Fructus	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Caryophylliflos	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Et Radix Patriniae Rhizoma	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Myrrha	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Piperis Longi Fructus	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Artemisia Annua L.	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Cyperi Rhizoma	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Menthae Herba	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Rhododendri Daurici Folium	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Piperis Fructus	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C

MOL000126	0.9548	0.0452	0.7808	Lilii Bulbus	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Linderae Radix	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Paederiae Scandentis Herba	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Magnolia Officinalis Rehd Et Wils.	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000126	0.9548	0.0452	0.7808	Cinnanmomi Cortex	(-)-nopinene	440967	FALSE	C12C(C(C1)CCC2=C)(C)C
MOL000127	0.9352	0.0648	0.9452	Ligustici Rhizoma Et Radix	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000127	0.9352	0.0648	0.9452	Cistanches Herba	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000127	0.9352	0.0648	0.9452	Campsis Flos	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000127	0.9352	0.0648	0.9452	Perilla Frutescens	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000127	0.9352	0.0648	0.9452	Rose Rugosae Flos	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000127	0.9352	0.0648	0.9452	Radix Bupleuri	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000127	0.9352	0.0648	0.9452	Curculiginis Rhizome	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000127	0.9352	0.0648	0.9452	Litseae Fructus	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000127	0.9352	0.0648	0.9452	Homalomena Occulta (Lour.) Schott	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000127	0.9352	0.0648	0.9452	Citri Reticulatae Pericarpium Viride	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000127	0.9352	0.0648	0.9452	Citrus Reticulata	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000127	0.9352	0.0648	0.9452	Citri Exocarpium Rubrum	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000127	0.9352	0.0648	0.9452	Zingiberis Rhizoma	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000127	0.9352	0.0648	0.9452	Citri Sarcodactylis Fructus	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000127	0.9352	0.0648	0.9452	Cymbopon Citratus(D C.) Stapf	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000127	0.9352	0.0648	0.9452	Arum Ternatum Thunb.	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000127	0.9352	0.0648	0.9452	Herba Taxilli	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000127	0.9352	0.0648	0.9452	Amomum Tsao-Ko Crevostet	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000127	0.9352	0.0648	0.9452	Mori Cortex	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000127	0.9352	0.0648	0.9452	Zingiber Officinale Roscoe	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000127	0.9352	0.0648	0.9452	Citri Grandis Exocarpium	Neral	643779	FALSE	C(=C\C=O)(\CCC=C(C)C)/C
MOL000128	0.9283	0.0717	0.9287	Schisandrae Chinensis Fructus	NERYLACETATE	1549026	FALSE	C(=C\COC(=O)C)(/CCC=C(C)C)\C
MOL000128	0.9283	0.0717	0.9287	Fructus Carotae	NERYLACETATE	1549026	FALSE	C(=C\COC(=O)C)(/CCC=C(C)C)\C
MOL000128	0.9283	0.0717	0.9287	Ephedra Herba	NERYLACETATE	1549026	FALSE	C(=C\COC(=O)C)(/CCC=C(C)C)\C
MOL000128	0.9283	0.0717	0.9287	Olibanun	NERYLACETATE	1549026	FALSE	C(=C\COC(=O)C)(/CCC=C(C)C)\C

MOL000128	0.9283	0.0717	0.9287	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	NERYLACETATE	1549026	FALSE	C(=C\COC(=O)C)(/CCC=C(C)C)\C
MOL000128	0.9283	0.0717	0.9287	Rose Rugosae Flos	NERYLACETATE	1549026	FALSE	C(=C\COC(=O)C)(/CCC=C(C)C)\C
MOL000128	0.9283	0.0717	0.9287	Amomum Tsao-Ko Crevostet	NERYLACETATE	1549026	FALSE	C(=C\COC(=O)C)(/CCC=C(C)C)\C
MOL000128	0.9283	0.0717	0.9287	Magnolia Officinalis Rehd Et Wils.	NERYLACETATE	1549026	FALSE	C(=C\COC(=O)C)(/CCC=C(C)C)\C
MOL000128	0.9283	0.0717	0.9287	Citri Fructus	NERYLACETATE	1549026	FALSE	C(=C\COC(=O)C)(/CCC=C(C)C)\C
MOL000128	0.9283	0.0717	0.9287	Cinnanmomi Cortex	NERYLACETATE	1549026	FALSE	C(=C\COC(=O)C)(/CCC=C(C)C)\C
MOL000128	0.9283	0.0717	0.9287	Alpinia Katsumadai Hayat	NERYLACETATE	1549026	FALSE	C(=C\COC(=O)C)(/CCC=C(C)C)\C
MOL000128	0.9283	0.0717	0.9287	Folium Artemisiae Argyi	NERYLACETATE	1549026	FALSE	C(=C\COC(=O)C)(/CCC=C(C)C)\C
MOL000128	0.9283	0.0717	0.9287	Cymbopon Citratus(D C.) Stapf	NERYLACETATE	1549026	FALSE	C(=C\COC(=O)C)(/CCC=C(C)C)\C
MOL000128	0.9283	0.0717	0.9287	Zanthoxyli Pericarpium	NERYLACETATE	1549026	FALSE	C(=C\COC(=O)C)(/CCC=C(C)C)\C
MOL000128	0.9283	0.0717	0.9287	Cnidii Fructus	NERYLACETATE	1549026	FALSE	C(=C\COC(=O)C)(/CCC=C(C)C)\C
MOL000128	0.9283	0.0717	0.9287	Radix Bupleuri	NERYLACETATE	1549026	FALSE	C(=C\COC(=O)C)(/CCC=C(C)C)\C
MOL000128	0.9283	0.0717	0.9287	Zingiberis Rhizoma	NERYLACETATE	1549026	FALSE	C(=C\COC(=O)C)(/CCC=C(C)C)\C
MOL000128	0.9283	0.0717	0.9287	Radix Salviae	NERYLACETATE	1549026	FALSE	C(=C\COC(=O)C)(/CCC=C(C)C)\C
MOL000128	0.9283	0.0717	0.9287	Lilii Bulbus	NERYLACETATE	1549026	FALSE	C(=C\COC(=O)C)(/CCC=C(C)C)\C
MOL000129	0.9282	0.0718	0.9307	Notopterygii Rhizoma Et Radix	Acetate C-8	8164	FALSE	C(CCCCCC)COC(=O)C
MOL000129	0.9282	0.0718	0.9307	Mume Flos	Acetate C-8	8164	FALSE	C(CCCCCC)COC(=O)C
MOL000129	0.9282	0.0718	0.9307	Amomum Tsao-Ko Crevostet	Acetate C-8	8164	FALSE	C(CCCCCC)COC(=O)C
MOL000129	0.9282	0.0718	0.9307	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Acetate C-8	8164	FALSE	C(CCCCCC)COC(=O)C
MOL000129	0.9282	0.0718	0.9307	Olibanun	Acetate C-8	8164	FALSE	C(CCCCCC)COC(=O)C
MOL000130	0.9388	0.0612	0.8042	Curcumae Rhizoma	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Folium Nelumbinis	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Illicium Difengpi K. L. B. Et K. I. M.	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Prunellae Spica	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C

MOL000130	0.9388	0.0612	0.8042	Phragmitis Rhizoma	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Sennae Folium	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Rhizoma Seu Herba Aristolochiae Mollissimae	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Alpiniae Officinarum Rhizome	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Paederiae Scandentis Herba	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Herba Patriniae	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Rhododendri Daurici Folium	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Linderae Radix	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Folium Artemisiae Argyi	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Piperis Fructus	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Benzoinum	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Mahoniae Caulis	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Mahoniae Folum	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Malvae Fructus	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Ligustici Rhizoma Et Radix	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Campsis Flos	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Magnoliae Flos	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Foeniculi Fructus	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Mume Flos	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Notoginseng Flos	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Magnolia Officinalis Rehd Et Wils.	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Rhizoma Fagopyri Cymosi	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Lonicerae Japonicae Flos	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Epimrdii Herba	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Cinnanmomi Cortex	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Ginkgo Folium	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Amomum Tsao-Ko Crevostet	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Forsythiae Fructus	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Aristolochiae Fructus	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Eupatorium Fortunei Turcz	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Coriandri Sativi Herba	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Eriobotryae Folium	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Cayratiae Japonicae Herba	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Gossampiniflos	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C

MOL000130	0.9388	0.0612	0.8042	Gypsophila Licentiana Hand.-Mazz.	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Piperis Longi Fructus	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Ailanthi Cortex	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Cinnamomi Ramulus	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Ephedra Herba	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Peucedanidecursivi Radix	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Apocyniveneti Folium	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Curcumae Radix	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Acoritataninowii Rhizoma	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Mori Fructus	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Cnidii Fructus	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Asari Radix Et Rhizoma	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Ardisiae Japonicae Herba	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Peucedani Radix	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Cannabis Sativa L.	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Centipedae Herba	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Alpinia Katsumadai Hayat	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Herba Taxilli	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Lysimachiae Herba	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Myristicae Semen	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Chrysanthemi Flos	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Semen Euphorbiae	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Agrimonia Eupatoria	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Xanthii Fructus	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000130	0.9388	0.0612	0.8042	Celastri Orbiculati Fructus	CAM	159055	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000131	0.7705	0.2295	0.6325	Viticis Cannabifoliae Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Thalictri Glandulosissimi Et	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Curcumae Radix	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Ligustici Rhizoma Et Radix	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Semen Aesculi	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Portulacae Herba	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Semen Lini	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Arisaematis Rhizoma	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Citri Sarcodactylis Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Cannabis Sativa L.	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Aurantii Fructus Immaturus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Millettiae Speciosae Radix	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Radix Cynanchi Paniculati	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O

MOL000131	0.7705	0.2295	0.6325	Typhonii Rhizoma	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Mori Cortex	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Momordicae Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Choerospondiatis Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Sojae Semen Nigrum	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Hippophae Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Prunellae Spica	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Melo Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Lysimachiae Foenigraeci Herba	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Smilax Scodinicaulis C.H. Wrisht?	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Rhizoma Anemones Raddeanae	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Litseae Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Eucommiae Cortex	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Mahoniae Folum	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Cortex Periplocae Radicis	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Sinapis Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Arecae Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Mahoniae Caulis	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Coicis Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Allium Azureum Ledeb.	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Ganoderma	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Raphani Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Moslae Herba	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Ephedra Herba	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Morindae Officinalis Radix	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Sapindi Mukorossiperic Arpium	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Semen Pharbitidis	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Linderae Radix	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Carpesiumabrotanoidesl.	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Styrax	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Hedysarum Multijugum Maxim.	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Thalluslaminariae	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Cinnanmomi Cortex	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Perillae Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Trollius Chinensis	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Sesami Nigrum Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Ginkgo Folium	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Mori Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O

MOL000131	0.7705	0.2295	0.6325	Chuanxiong Rhizoma	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Eucommiae Folium	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Arum Ternatum Thunb.	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Pseudostellariae Radix	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Codonopsis Radix	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Lablab Semen Album	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Junci Medulla	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Foeniculi Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Croci Stigma	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Semiaquilegiae Radix	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Aloe	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Rhapontici Radix	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Gossampiniflos	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Gnaphalii Affinis Herba	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Corayceps	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Smilacis Glabrae Rhixoma	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Gleditsiae Sinensis Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Radix Paeoniae Rubra	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Ranunculi Ternati Radix	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Semen Firmianae	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Benincasae Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Aconiti Lateralis Radix Praeparata	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Hyoscyami Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Isatdis Radix	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Canavaliae Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Nardostachyos Radix Et Rhizoma	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Fructus Carotae	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Allii Fistulost Bulbus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Corydalis Rhizoma	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Magnolia Officinalis Rehd Et Wils.	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Cucurbitae Moschatae Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Amygdalus Communis Vas	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Silybum Marianum	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Linderae Radix	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Amomum Tsao-Ko Crevostet	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Lycii Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Chaenomeles Sinensis (Thouin) Koehne	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O

MOL000131	0.7705	0.2295	0.6325	Momordicae Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Polygoni Orientalis Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Capsici Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Abutili Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Citri Reticulatae Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Chebulae Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Semen Euphorbiae	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Puerariae Flos	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Cimicifugae Rhizoma	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Sterculiae Lychnophorae Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Cassiae Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Glehniae Radix	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Fructussophorae	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Cornus Officinalis Sieb. Et Zucc.	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Crotonis Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Mume Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Humulus Scandens (Lour.) Merr.	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Persicae Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Gynostemmae Pentaphylli Herba	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Oroxyli Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Zingiberis Rhizoma	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Ricini Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Cnidii Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Malvae Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Rehmanniae Radix Praeparata	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Flos Genkwa	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Tamaricis Cacumen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Viticis Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Euryales Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Litchi Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Carthami Flos	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Vaccariae Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Platycladi Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Maydis Seigma	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Meliae Azedarach Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Folium Artemisiae Argyi	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O

MOL000131	0.7705	0.2295	0.6325	Lepidii Semen Descurainiae Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Phyllanthi Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Sophora Japonica L.	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Mylabris	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Quisqualis Indica	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Lithospermum Erythrorhizon	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Radix Bupleuri	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Allii Tuberosi Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Broussonetiae Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Sapindi Mukorossi Semen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Xanthii Fructus	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Aucklandiae Radix	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Radix Salviae	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Euphorbiae Helioscopiae Herba	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Celosia Cristata L.	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000131	0.7705	0.2295	0.6325	Astragali Cpmplanatisemen	EIC	5280450	FALSE	C(C/C=C\C/C=C\CCCCC)CCCCCC(=O)O
MOL000132	0.7090	0.2910	0.8644	Rhizoma Dioscoreae Nipponicae	(5beta,25S)-Spirostan-3beta,15alpha,23alpha-diol-3-O-D-glucopyranosyl-(1-2)-beta-D-galactopyranoside	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2O)C)C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL000133	0.5753	0.4247	0.9038	Rhizoma Dioscoreae Nipponicae	7-Epitaxol	Not Available	FALSE	C12=C(C(CC(C1(C)C)(C(C1C(C(=O)C2OC(=O)C)(C(CC2C1(CO2)OC(=O)C)O)C)OC(=O)c1ccccc1)O)OC(=O)C(C(c1ccccc1)NC(=O)c1ccccc1)O)C
MOL000134	0.2726	0.7274	0.7674	Rhizoma Dioscoreae Nipponicae	Delta3,5-Deoxytigogenin	Not Available	FALSE	C1C(=CC2=CCC3C(C2(C1)C)CCC1(C3CC2C1C(C1(O2)OCC(CC1)C)C)C)O
MOL000135	0.9352	0.0648	0.7040	Isatdis Radix	Deoxyvasicinone	68261	FALSE	c1ccc2c(c1)c(=O)n1c(n2)CCC1
MOL000135	0.9352	0.0648	0.7040	Dioscoreae Septemlo Bae Rhizoma	Deoxyvasicinone	68261	FALSE	c1ccc2c(c1)c(=O)n1c(n2)CCC1

MOL000135	0.9352	0.0648	0.7040	Rhizoma Dioscoreae Nipponicae	Deoxyvasicinone	68261	FALSE	c1ccc2c(c1)c(=O)n1c(n2)CCC1
MOL000136	0.7131	0.2869	0.8084	Rhizoma Dioscoreae Nipponicae	Dioscoreside C	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC2C1C(=C(O2)C(CC(COC1OC(C(C(C1O)O)O)CO)C)OC)C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)OC1C(C(C(C(O1)C)O)O)O)CO
MOL000136	0.7131	0.2869	0.8084	Rhizoma Dioscoreae	Dioscoreside C	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC2C1C(=C(O2)C(CC(COC1OC(C(C(C1O)O)O)CO)C)OC)C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)OC1C(C(C(C(O1)C)O)O)O)CO
MOL000137	0.2056	0.7944	0.7254	Rhizoma Dioscoreae Nipponicae	Diosgenin acetate	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC2C1C(C1(O2)OCC(CC1)C)C)C)OC(=O)C
MOL000139	0.9026	0.0974	0.8377	Rhizoma Dioscoreae Nipponicae	Smitilbin	6325418	FALSE	c1(cc(c2c(c1)OC(C(C2=O)OC1C(C(C(C(O1)C)O)O)O)O)c1cc(cc(c1)O)O)O
MOL000140	0.2587	0.7413	0.7024	Dioscoreae Septemlo Bae Rhizoma	DIOSGENIN, DEHYDRO	Not Available	FALSE	C1=CC2=CCC3C4CC5OC6(C(C5C4(C)CCC3C2(CC1)C)C)OCC(CC6)C
MOL000140	0.2587	0.7413	0.7024	Dioscoreae Hypoglaucae Rhizoma	DIOSGENIN, DEHYDRO	Not Available	FALSE	C1=CC2=CCC3C4CC5OC6(C(C5C4(C)CCC3C2(CC1)C)C)OCC(CC6)C
MOL000140	0.2587	0.7413	0.7024	Rhizoma Dioscoreae Nipponicae	DIOSGENIN, DEHYDRO	Not Available	FALSE	C1=CC2=CCC3C4CC5OC6(C(C5C4(C)CCC3C2(CC1)C)C)OCC(CC6)C
MOL000141	0.9424	0.0576	0.9712	Figwort Root	hydroxytyrosol	82755	FALSE	c1(ccc(cc1O)CCO)O
MOL000141	0.9424	0.0576	0.9712	Cimicifugae Rhizoma	hydroxytyrosol	82755	FALSE	c1(ccc(cc1O)CCO)O
MOL000141	0.9424	0.0576	0.9712	Pseudobulbus Cremastrae Seu Pleiones	hydroxytyrosol	82755	FALSE	c1(ccc(cc1O)CCO)O
MOL000141	0.9424	0.0576	0.9712	Sargentodoxae Caulis	hydroxytyrosol	82755	FALSE	c1(ccc(cc1O)CCO)O
MOL000141	0.9424	0.0576	0.9712	Trollius Chinensis	hydroxytyrosol	82755	FALSE	c1(ccc(cc1O)CCO)O
MOL000141	0.9424	0.0576	0.9712	Semiaquilegiae Radix	hydroxytyrosol	82755	FALSE	c1(ccc(cc1O)CCO)O
MOL000141	0.9424	0.0576	0.9712	Fructus Ligustri Lucidi	hydroxytyrosol	82755	FALSE	c1(ccc(cc1O)CCO)O
MOL000141	0.9424	0.0576	0.9712	Clerodendrum Trichotomum Thunb	hydroxytyrosol	82755	FALSE	c1(ccc(cc1O)CCO)O
MOL000141	0.9424	0.0576	0.9712	Leonuri Herba	hydroxytyrosol	82755	FALSE	c1(ccc(cc1O)CCO)O
MOL000141	0.9424	0.0576	0.9712	Forsythiae Fructus	hydroxytyrosol	82755	FALSE	c1(ccc(cc1O)CCO)O
MOL000142	0.7854	0.2146	0.7148	Plantaginis Semen	Calceolarioside B	5273567	FALSE	O(C1C(O)C(O)C(O)C(O1)COC(=O)/C=C/c1cc(O)c(O)cc1)CCc1cc(c(cc1)O)O

MOL000142	0.7854	0.2146	0.7148	Clerodendrum Trichotomum Thunb	Calceolarioside B	5273567	FALSE	O(C1C(O)C(O)C(O)C(O1)COC(=O)/C=C/c1cc(O)c(O)cc1)CCc1cc(c(cc1)O)O
MOL000142	0.7854	0.2146	0.7148	Caulis Akebiae	Calceolarioside B	5273567	FALSE	O(C1C(O)C(O)C(O)C(O1)COC(=O)/C=C/c1cc(O)c(O)cc1)CCc1cc(c(cc1)O)O
MOL000142	0.7854	0.2146	0.7148	Plantaginis Herba	Calceolarioside B	5273567	FALSE	O(C1C(O)C(O)C(O)C(O1)COC(=O)/C=C/c1cc(O)c(O)cc1)CCc1cc(c(cc1)O)O
MOL000144	0.3502	0.6498	0.6744	Clerodendrum Trichotomum Thunb	Kirenol	Not Available	FALSE	C1(CC(C2C(C1)(C1C(=CC(CC1)(C)C(O)CCO)CC2)C)(C)CO)O
MOL000145	0.6629	0.3371	0.7044	Clerodendrum Trichotomum Thunb	leucosceptoside A	Not Available	FALSE	c1(/C=C/C(=O)OC2C(C(C(OC2CO)OCCc2cc(c(cc2)O)O)O)OC2C(C(C(C(O2)C)O)O)O)ccc(c(c1)OC)O
MOL000148	0.3360	0.6640	0.6862	Clerodendrum Trichotomum Thunb	trichotomoside	Not Available	FALSE	c1(ccc(cc1OC)/C=C/C(=O)OCC1C(C(C(C(O1)OCCc1cc(c(cc1)OC)O)O)OC1OC(C(C(C1OC(=O)C)OC(=O)C)O)C)OC(=O)/C=C/c1cc(c(cc1)O)OC)O
MOL000149	0.9247	0.0753	0.9448	Radix Aconiti Kusnezoffii	inositol	892	FALSE	OC1C(O)C(O)C(O)C(O)C1O
MOL000149	0.9247	0.0753	0.9448	Lonicerae Japonicae Flos	inositol	892	FALSE	OC1C(O)C(O)C(O)C(O)C1O
MOL000149	0.9247	0.0753	0.9448	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	inositol	892	FALSE	OC1C(O)C(O)C(O)C(O)C1O
MOL000149	0.9247	0.0753	0.9448	Litchi Semen	inositol	892	FALSE	OC1C(O)C(O)C(O)C(O)C1O
MOL000149	0.9247	0.0753	0.9448	Clerodendrum Trichotomum Thunb	inositol	892	FALSE	OC1C(O)C(O)C(O)C(O)C1O
MOL000149	0.9247	0.0753	0.9448	Arisaematis Rhizoma	inositol	892	FALSE	OC1C(O)C(O)C(O)C(O)C1O
MOL000149	0.9247	0.0753	0.9448	Viscum Angulatum Heyne	inositol	892	FALSE	OC1C(O)C(O)C(O)C(O)C1O
MOL000150	0.8685	0.1315	0.7711	Clerodendrum Trichotomum Thunb	acacetin-7-glucurono-(1→2)-glucuronide	Not Available	FALSE	c1(cc(=O)c2c(o1)cc(cc2O)OC1(C(O)C(O)C(O)C(O1)CO)C(=O)C(OO)C(O)C(O)C(O)C)c1ccc(cc1)O
MOL000152	0.8439	0.1561	0.8062	Clerodendrum Trichotomum Thunb	Acacetin-7-glucurono-(1-2)-glucuronide	Not Available	FALSE	c12c(cc(cc1O)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C(=O)O)O)O)C(=O)O)oc(cc2=O)c1ccc(cc1)OC
MOL000155	0.7832	0.2168	0.7292	Clerodendrum Trichotomum Thunb	acteoside isomer	Not Available	FALSE	c1(/C=C/C(=O)OCC2C(C(C(C(O2)OCCc2cc(c(cc2)O)O)O)OC2C(C(C(C(O2)C)O)O)O)O)ccc(c(c1)O)O
MOL000155	0.7832	0.2168	0.7292	Plantaginis Semen	acteoside isomer	Not Available	FALSE	c1(/C=C/C(=O)OCC2C(C(C(C(O2)OCCc2cc(c(cc2)O)O)O)OC2C(C(C(C(O2)C)O)O)O)O)ccc(c(c1)O)O
MOL000156	0.9113	0.0887	0.8073	Figwort Root	decaffeoylacteoside	Not Available	FALSE	C1(C(C(C(OC1CO)OCCc1ccc(c(c1)O)O)O)OC1C(C(C(C(O1)C)O)O)O)O
MOL000156	0.9113	0.0887	0.8073	Cistanches Herba	decaffeoylacteoside	Not Available	FALSE	C1(C(C(C(OC1CO)OCCc1ccc(c(c1)O)O)O)OC1C(C(C(C(O1)C)O)O)O)O
MOL000156	0.9113	0.0887	0.8073	Clerodendrum Trichotomum Thunb	decaffeoylacteoside	Not Available	FALSE	C1(C(C(C(OC1CO)OCCc1ccc(c(c1)O)O)O)OC1C(C(C(C(O1)C)O)O)O)O

MOL000157	0.7728	0.2272	0.7308	Clerodendrum Trichotomum Thunb	[(2R,3S,4S,5R,6R)-6-[2-(3,4-dihydroxyphenyl)ethoxy]-4,5-dihydroxy-2-(hydroxymethyl)oxan-3-yl] (E)-3-(3,4-dihydroxyphenyl)prop-2-enoate	10457774	FALSE	c1(cc(ccc1O)CCOC1OC(C(C(C1O)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)CO)O
MOL000157	0.7728	0.2272	0.7308	Plantaginis Herba	[(2R,3S,4S,5R,6R)-6-[2-(3,4-dihydroxyphenyl)ethoxy]-4,5-dihydroxy-2-(hydroxymethyl)oxan-3-yl] (E)-3-(3,4-dihydroxyphenyl)prop-2-enoate	10457774	FALSE	c1(cc(ccc1O)CCOC1OC(C(C(C1O)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)CO)O
MOL000158	0.7854	0.2146	0.7148	Plantaginis Semen	desrhamnosyl isoacteoside	Not Available	FALSE	c1(cc(ccc1O)CCOC1OC(C(C(C1O)O)O)O)COC(=O)/C=C/c1cc(c(cc1)O)O)O
MOL000158	0.7854	0.2146	0.7148	Clerodendrum Trichotomum Thunb	desrhamnosyl isoacteoside	Not Available	FALSE	c1(cc(ccc1O)CCOC1OC(C(C(C1O)O)O)O)COC(=O)/C=C/c1cc(c(cc1)O)O)O

MOL000159	0.7832	0.2168	0.7292	Clerodendrum Trichotomum Thunb	[(2R,3R,4S,5R,6R)-6-[2-(3,4-dihydroxyphenyl)ethoxy]-3,5-dihydroxy-4-[(2R,3S,4S,5S,6R)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-tetrahydropyran-2-yl]methyl (E)-3-(3,4-dihydroxyphenyl)prop-2-enoate	16755425	FALSE	c1(c(cc(cc1)/C=C/C(=O)OCC1OC(C(C(C1O)OC1C(C(C(C(O1)C)O)O)O)O)OCCc1cc(c(cc1)O)O)O)O
MOL000159	0.7832	0.2168	0.7292	Plantaginis Semen	[(2R,3R,4S,5R,6R)-6-[2-(3,4-dihydroxyphenyl)ethoxy]-3,5-dihydroxy-4-[(2R,3S,4S,5S,6R)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-tetrahydropyran-2-yl]methyl (E)-3-(3,4-dihydroxyphenyl)prop-2-enoate	16755425	FALSE	c1(c(cc(cc1)/C=C/C(=O)OCC1OC(C(C(C1O)OC1C(C(C(C(O1)C)O)O)O)O)OCCc1cc(c(cc1)O)O)O)O
MOL000161	0.1300	0.8700	0.6466	Clerodendrum Trichotomum Thunb	Isopropylidenkirenol	Not Available	FALSE	C1(CC(C2C(C1)(C1C(=CC(CC1)(C1COC(O1)(C)C)C)CC2)C)(C)CO)O

MOL000162	0.8364	0.1636	0.6372	Magnolia Officinalis Rehd Et Wils.	beta-Chamigrene	442353	FALSE	C12(C(CCCC1=C)(C)C)CC=C(CC2)C
MOL000162	0.8364	0.1636	0.6372	Angelicae Sinensis Radix	beta-Chamigrene	442353	FALSE	C12(C(CCCC1=C)(C)C)CC=C(CC2)C
MOL000162	0.8364	0.1636	0.6372	Cnidii Fructus	beta-Chamigrene	442353	FALSE	C12(C(CCCC1=C)(C)C)CC=C(CC2)C
MOL000162	0.8364	0.1636	0.6372	Radix Salviae	beta-Chamigrene	442353	FALSE	C12(C(CCCC1=C)(C)C)CC=C(CC2)C
MOL000162	0.8364	0.1636	0.6372	Atractylodes Lancea (Thunb.)Dc.	beta-Chamigrene	442353	FALSE	C12(C(CCCC1=C)(C)C)CC=C(CC2)C
MOL000162	0.8364	0.1636	0.6372	Schisandrae Chinensis Fructus	beta-Chamigrene	442353	FALSE	C12(C(CCCC1=C)(C)C)CC=C(CC2)C
MOL000163	0.8680	0.1320	0.7895	Atractylodes Lancea (Thunb.)Dc.	Atractylodin	5321047	FALSE	c1(ccco1)/C=C/C#CC#C/C=C/C
MOL000163	0.8680	0.1320	0.7895	Lonicerae Japonicae Flos	Atractylodin	5321047	FALSE	c1(ccco1)/C=C/C#CC#C/C=C/C
MOL000164	0.7220	0.2780	0.6881	Atractylodes Lancea (Thunb.)Dc.	atractylone	12138536	FALSE	o1c2c(c(c1)C)CC1C(=C)CCCC1(C2)C
MOL000165	0.8323	0.1677	0.7140	Gypsophila Licentiana Hand.-Mazz.	2-[(2S,5S,6S)-6,10-dimethylspiro[4.5]dec-9-en-2-yl]propan-2-ol	10353528	FALSE	CC(C)(O)C1CC2(CC1)C(=CCCC2C)C
MOL000165	0.8323	0.1677	0.7140	Linderae Radix	2-[(2S,5S,6S)-6,10-dimethylspiro[4.5]dec-9-en-2-yl]propan-2-ol	10353528	FALSE	CC(C)(O)C1CC2(CC1)C(=CCCC2C)C
MOL000165	0.8323	0.1677	0.7140	Curcumae Radix	2-[(2S,5S,6S)-6,10-dimethylspiro[4.5]dec-9-en-2-yl]propan-2-ol	10353528	FALSE	CC(C)(O)C1CC2(CC1)C(=CCCC2C)C
MOL000165	0.8323	0.1677	0.7140	Chuanxiong Rhizoma	2-[(2S,5S,6S)-6,10-dimethylspiro[4.5]dec-9-en-2-yl]propan-2-ol	10353528	FALSE	CC(C)(O)C1CC2(CC1)C(=CCCC2C)C

MOL000165	0.8323	0.1677	0.7140	Atractylodes Lancea (Thunb.)Dc.	2-[(2S,5S,6S)-6,10-dimethylspiro[4.5]dec-9-en-2-yl]propan-2-ol	10353528	FALSE	CC(C)(O)C1CC2(CC1)C(=CCCC2C)C
MOL000165	0.8323	0.1677	0.7140	Magnolia Officinalis Rehd Et Wils.	2-[(2S,5S,6S)-6,10-dimethylspiro[4.5]dec-9-en-2-yl]propan-2-ol	10353528	FALSE	CC(C)(O)C1CC2(CC1)C(=CCCC2C)C
MOL000166	0.8905	0.1095	0.8395	Acoritataninowii Rhizoma	ZINC01609418	1549992	FALSE	C1(C(CCC=C(C)C)(C)O)CCC(=CC1)C
MOL000166	0.8905	0.1095	0.8395	Curcumaelongae Rhizoma	ZINC01609418	1549992	FALSE	C1(C(CCC=C(C)C)(C)O)CCC(=CC1)C
MOL000166	0.8905	0.1095	0.8395	Cinnanmomi Cortex	ZINC01609418	1549992	FALSE	C1(C(CCC=C(C)C)(C)O)CCC(=CC1)C
MOL000166	0.8905	0.1095	0.8395	Atractylodes Lancea (Thunb.)Dc.	ZINC01609418	1549992	FALSE	C1(C(CCC=C(C)C)(C)O)CCC(=CC1)C
MOL000166	0.8905	0.1095	0.8395	Alpiniae Officinarum Rhizome	ZINC01609418	1549992	FALSE	C1(C(CCC=C(C)C)(C)O)CCC(=CC1)C
MOL000166	0.8905	0.1095	0.8395	Cinnamomi Ramulus	ZINC01609418	1549992	FALSE	C1(C(CCC=C(C)C)(C)O)CCC(=CC1)C
MOL000166	0.8905	0.1095	0.8395	Dalbergiae Odoriferae Lignum	ZINC01609418	1549992	FALSE	C1(C(CCC=C(C)C)(C)O)CCC(=CC1)C
MOL000166	0.8905	0.1095	0.8395	Zingiber Officinale Roscoe	ZINC01609418	1549992	FALSE	C1(C(CCC=C(C)C)(C)O)CCC(=CC1)C
MOL000166	0.8905	0.1095	0.8395	Calyx Seu Fructus Physalis	ZINC01609418	1549992	FALSE	C1(C(CCC=C(C)C)(C)O)CCC(=CC1)C
MOL000166	0.8905	0.1095	0.8395	Lignum Pini Nodi	ZINC01609418	1549992	FALSE	C1(C(CCC=C(C)C)(C)O)CCC(=CC1)C
MOL000166	0.8905	0.1095	0.8395	Radix Angelicae Biseratae	ZINC01609418	1549992	FALSE	C1(C(CCC=C(C)C)(C)O)CCC(=CC1)C
MOL000166	0.8905	0.1095	0.8395	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	ZINC01609418	1549992	FALSE	C1(C(CCC=C(C)C)(C)O)CCC(=CC1)C
MOL000166	0.8905	0.1095	0.8395	Spatholobus Suberectus Dunn	ZINC01609418	1549992	FALSE	C1(C(CCC=C(C)C)(C)O)CCC(=CC1)C
MOL000166	0.8905	0.1095	0.8395	Hyperici Japonici Herber	ZINC01609418	1549992	FALSE	C1(C(CCC=C(C)C)(C)O)CCC(=CC1)C
MOL000166	0.8905	0.1095	0.8395	Herba Taxilli	ZINC01609418	1549992	FALSE	C1(C(CCC=C(C)C)(C)O)CCC(=CC1)C

MOL000166	0.8905	0.1095	0.8395	Litchi Semen	ZINC01609418	1549992	FALSE	C1(C(CCC=C(C)C)(C)O)CCC(=CC1)C
MOL000167	0.8140	0.1860	0.7632	Atractylodes Lancea (Thunb.)Dc.	3β-hydroxyatractylone	71448961	FALSE	o1c2c(c(c1)C)CC1C(=C)C(CCC1(C2)C)O
MOL000168	0.9483	0.0517	0.7603	Homalomena Occulta (Lour.) Schott	()-2-Carene	78249	FALSE	C12C(C1(C)C)C=C(CC2)C
MOL000168	0.9483	0.0517	0.7603	Herba Clinopodii Polycephali.	()-2-Carene	78249	FALSE	C12C(C1(C)C)C=C(CC2)C
MOL000168	0.9483	0.0517	0.7603	Rubi Fructus	()-2-Carene	78249	FALSE	C12C(C1(C)C)C=C(CC2)C
MOL000168	0.9483	0.0517	0.7603	Rhizome Of Whiteback Greenbrier	()-2-Carene	78249	FALSE	C12C(C1(C)C)C=C(CC2)C
MOL000168	0.9483	0.0517	0.7603	Magnolia Officinalis Rehd Et Wils.	()-2-Carene	78249	FALSE	C12C(C1(C)C)C=C(CC2)C
MOL000168	0.9483	0.0517	0.7603	Atractylodes Lancea (Thunb.)Dc.	()-2-Carene	78249	FALSE	C12C(C1(C)C)C=C(CC2)C
MOL000168	0.9483	0.0517	0.7603	Notopterygii Rhizoma Et Radix	()-2-Carene	78249	FALSE	C12C(C1(C)C)C=C(CC2)C
MOL000168	0.9483	0.0517	0.7603	Lignum Pini Nodi	()-2-Carene	78249	FALSE	C12C(C1(C)C)C=C(CC2)C
MOL000168	0.9483	0.0517	0.7603	Citrus Reticulata	()-2-Carene	78249	FALSE	C12C(C1(C)C)C=C(CC2)C
MOL000168	0.9483	0.0517	0.7603	Myrrha	()-2-Carene	78249	FALSE	C12C(C1(C)C)C=C(CC2)C
MOL000168	0.9483	0.0517	0.7603	Piperis Fructus	()-2-Carene	78249	FALSE	C12C(C1(C)C)C=C(CC2)C
MOL000169	0.8514	0.1486	0.7005	Lysimachiae Herba	alpha-Guaiene	5317844	FALSE	C1(CCC2=C1CC(CCC2C)C(=C)C)C
MOL000169	0.8514	0.1486	0.7005	Ginsen Radix Et Rhizoma Rubra	alpha-Guaiene	5317844	FALSE	C1(CCC2=C1CC(CCC2C)C(=C)C)C
MOL000169	0.8514	0.1486	0.7005	Ginseng Folium	alpha-Guaiene	5317844	FALSE	C1(CCC2=C1CC(CCC2C)C(=C)C)C
MOL000169	0.8514	0.1486	0.7005	Atractylodes Lancea (Thunb.)Dc.	alpha-Guaiene	5317844	FALSE	C1(CCC2=C1CC(CCC2C)C(=C)C)C
MOL000169	0.8514	0.1486	0.7005	Myrrha	alpha-Guaiene	5317844	FALSE	C1(CCC2=C1CC(CCC2C)C(=C)C)C
MOL000169	0.8514	0.1486	0.7005	Radix Bupleuri	alpha-Guaiene	5317844	FALSE	C1(CCC2=C1CC(CCC2C)C(=C)C)C
MOL000169	0.8514	0.1486	0.7005	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	alpha-Guaiene	5317844	FALSE	C1(CCC2=C1CC(CCC2C)C(=C)C)C
MOL000169	0.8514	0.1486	0.7005	Pogostemon Cablin (Blanco) Benth.	alpha-Guaiene	5317844	FALSE	C1(CCC2=C1CC(CCC2C)C(=C)C)C
MOL000169	0.8514	0.1486	0.7005	Scutellariae Radix	alpha-Guaiene	5317844	FALSE	C1(CCC2=C1CC(CCC2C)C(=C)C)C
MOL000169	0.8514	0.1486	0.7005	Cannabis Sativa L.	alpha-Guaiene	5317844	FALSE	C1(CCC2=C1CC(CCC2C)C(=C)C)C
MOL000169	0.8514	0.1486	0.7005	Achyranthis Asperae Herba	alpha-Guaiene	5317844	FALSE	C1(CCC2=C1CC(CCC2C)C(=C)C)C
MOL000170	0.8597	0.1403	0.6921	Anisi Stellati Fructus	guaiene	Not Available	FALSE	C12=C(C(CCC(=C(C)C)C1)C)CCC2C
MOL000170	0.8597	0.1403	0.6921	Stephaniae Tetrandrae Radix	guaiene	Not Available	FALSE	C12=C(C(CCC(=C(C)C)C1)C)CCC2C
MOL000170	0.8597	0.1403	0.6921	Viticis Negundo Folium	guaiene	Not Available	FALSE	C12=C(C(CCC(=C(C)C)C1)C)CCC2C

MOL000170	0.8597	0.1403	0.6921	Piperis Fructus	guaiene	Not Available	FALSE	C12=C(C(CCC(=C(C)C)C1)C)CCC2C
MOL000170	0.8597	0.1403	0.6921	Lysimachiae Herba	guaiene	Not Available	FALSE	C12=C(C(CCC(=C(C)C)C1)C)CCC2C
MOL000170	0.8597	0.1403	0.6921	Alpiniae Officinarum Rhizome	guaiene	Not Available	FALSE	C12=C(C(CCC(=C(C)C)C1)C)CCC2C
MOL000170	0.8597	0.1403	0.6921	Flemingia Prostrata Roxb	guaiene	Not Available	FALSE	C12=C(C(CCC(=C(C)C)C1)C)CCC2C
MOL000170	0.8597	0.1403	0.6921	Cinnanmomi Cortex	guaiene	Not Available	FALSE	C12=C(C(CCC(=C(C)C)C1)C)CCC2C
MOL000170	0.8597	0.1403	0.6921	Atractylodes Lancea (Thunb.)Dc.	guaiene	Not Available	FALSE	C12=C(C(CCC(=C(C)C)C1)C)CCC2C
MOL000170	0.8597	0.1403	0.6921	Curcumae Radix	guaiene	Not Available	FALSE	C12=C(C(CCC(=C(C)C)C1)C)CCC2C
MOL000170	0.8597	0.1403	0.6921	Cyperi Rhizoma	guaiene	Not Available	FALSE	C12=C(C(CCC(=C(C)C)C1)C)CCC2C
MOL000170	0.8597	0.1403	0.6921	Pogostemon Cablin (Blanco) Benth.	guaiene	Not Available	FALSE	C12=C(C(CCC(=C(C)C)C1)C)CCC2C
MOL000170	0.8597	0.1403	0.6921	Zingiberis Rhizoma	guaiene	Not Available	FALSE	C12=C(C(CCC(=C(C)C)C1)C)CCC2C
MOL000171	0.8500	0.1500	0.7275	Magnolia Officinalis Rehd Et Wils.	Guaiol	227829	FALSE	C(C1CC2=C(C(CC1)C)CCC2C)(C)(C)O
MOL000171	0.8500	0.1500	0.7275	Atractylodes Lancea (Thunb.)Dc.	Guaiol	227829	FALSE	C(C1CC2=C(C(CC1)C)CCC2C)(C)(C)O
MOL000171	0.8500	0.1500	0.7275	Curcumae Radix	Guaiol	227829	FALSE	C(C1CC2=C(C(CC1)C)CCC2C)(C)(C)O
MOL000171	0.8500	0.1500	0.7275	Radix Angelicae Biseratae	Guaiol	227829	FALSE	C(C1CC2=C(C(CC1)C)CCC2C)(C)(C)O
MOL000171	0.8500	0.1500	0.7275	Siphonostegiae Herba	Guaiol	227829	FALSE	C(C1CC2=C(C(CC1)C)CCC2C)(C)(C)O
MOL000171	0.8500	0.1500	0.7275	Lonicerae Japonicae Flos	Guaiol	227829	FALSE	C(C1CC2=C(C(CC1)C)CCC2C)(C)(C)O
MOL000171	0.8500	0.1500	0.7275	Linderae Radix	Guaiol	227829	FALSE	C(C1CC2=C(C(CC1)C)CCC2C)(C)(C)O
MOL000171	0.8500	0.1500	0.7275	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Guaiol	227829	FALSE	C(C1CC2=C(C(CC1)C)CCC2C)(C)(C)O
MOL000171	0.8500	0.1500	0.7275	Acoritataninowii Rhizoma	Guaiol	227829	FALSE	C(C1CC2=C(C(CC1)C)CCC2C)(C)(C)O
MOL000171	0.8500	0.1500	0.7275	Notopterygii Rhizoma Et Radix	Guaiol	227829	FALSE	C(C1CC2=C(C(CC1)C)CCC2C)(C)(C)O
MOL000171	0.8500	0.1500	0.7275	Kadsurae Coccineae Radix Et Caulis	Guaiol	227829	FALSE	C(C1CC2=C(C(CC1)C)CCC2C)(C)(C)O
MOL000172	0.8725	0.1275	0.9684	Magnolia Officinalis Rehd Et Wils.	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Citri Reticulatae Folium	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Chuanxiong Rhizoma	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Mume Fructus	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Cuscutae Semen	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Momordicae Fructus	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Citri Fructus Retinervus	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Citri Grandis Exocarpium	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Cinnanmomi Cortex	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Caryophylliflos	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Pseudostellariae Radix	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Achyranthis Bidentatae Radix	Furol	7362	FALSE	C(=O)c1ccco1

MOL000172	0.8725	0.1275	0.9684	Campsis Flos	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Artemisiae Scopariae Herba	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Sinapis Semen	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Eriobotryae Folium	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Capsici Fructus	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Anemarrhenae Rhizoma	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Notoginseng Flos	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Arum Ternatum Thunb.	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Phragmitis Rhizoma	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Flos Genkwa	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Scutellariae Barbatae Herba	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Bomboo Juice	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Ginkgo Folium	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Cornus Officinalis Sieb. Et Zucc.	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Atractylodes Lancea (Thunb.)Dc.	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Ephedra Herba	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Hippophae Fructus	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Rhododendri Daurici Folium	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Paederiae Scandentis Herba	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Lonicerae Japonicae Flos	Furol	7362	FALSE	C(=O)c1ccco1
MOL000172	0.8725	0.1275	0.9684	Semen Pharbitidis	Furol	7362	FALSE	C(=O)c1ccco1
MOL000173	0.7400	0.2600	0.9547	Phellodendri Amurensis Cortex	wogonin	5281703	FALSE	c12c(c(c(cc2O)O)OC)oc(cc1=O)c1ccccc1
MOL000173	0.7400	0.2600	0.9547	Achyranthis Bidentatae Radix	wogonin	5281703	FALSE	c12c(c(c(cc2O)O)OC)oc(cc1=O)c1ccccc1
MOL000173	0.7400	0.2600	0.9547	Andrographis Herba	wogonin	5281703	FALSE	c12c(c(c(cc2O)O)OC)oc(cc1=O)c1ccccc1
MOL000173	0.7400	0.2600	0.9547	Scutellariae Radix	wogonin	5281703	FALSE	c12c(c(c(cc2O)O)OC)oc(cc1=O)c1ccccc1
MOL000173	0.7400	0.2600	0.9547	Oroxyli Semen	wogonin	5281703	FALSE	c12c(c(c(cc2O)O)OC)oc(cc1=O)c1ccccc1
MOL000173	0.7400	0.2600	0.9547	Forsythiae Fructus	wogonin	5281703	FALSE	c12c(c(c(cc2O)O)OC)oc(cc1=O)c1ccccc1
MOL000173	0.7400	0.2600	0.9547	Dictamni Cortex	wogonin	5281703	FALSE	c12c(c(c(cc2O)O)OC)oc(cc1=O)c1ccccc1
MOL000173	0.7400	0.2600	0.9547	Scutellariae Barbatae Herba	wogonin	5281703	FALSE	c12c(c(c(cc2O)O)OC)oc(cc1=O)c1ccccc1
MOL000173	0.7400	0.2600	0.9547	Atractylodes Lancea (Thunb.)Dc.	wogonin	5281703	FALSE	c12c(c(c(cc2O)O)OC)oc(cc1=O)c1ccccc1
MOL000174	0.8776	0.1224	0.8027	Atractylodes Lancea (Thunb.)Dc.	(2E,8E)-9-(2-furyl)nona-2,8-dien-4,6-diyn-1-ol	10012964	FALSE	C(#C/C=C/c1occc1)C#C/C=C/CO
MOL000175	0.8254	0.1746	0.6165	Aucklandiae Radix	cyperene	Not Available	FALSE	C1(=C2C3(CC1)C(CCC(C2)C3(C)C)C)C

MOL000175	0.8254	0.1746	0.6165	Atractylodes Lancea (Thunb.)Dc.	cyperene	Not Available	FALSE	C1(=C2C3(CC1)C(CCC(C2)C3(C)C)C)C
MOL000175	0.8254	0.1746	0.6165	Campsis Flos	cyperene	Not Available	FALSE	C1(=C2C3(CC1)C(CCC(C2)C3(C)C)C)C
MOL000178	0.8582	0.1418	0.7918	Atractylodes Lancea (Thunb.)Dc.	atractylenolide iii	14420566	FALSE	C12(C(=C(C(=O)O2)C)CC2C(C1)(CCCC2=C)C)O
MOL000178	0.8582	0.1418	0.7918	Herba Sarcandrae	atractylenolide iii	14420566	FALSE	C12(C(=C(C(=O)O2)C)CC2C(C1)(CCCC2=C)C)O
MOL000179	0.8756	0.1244	0.8330	Atractylodes Lancea (Thunb.)Dc.	2-Hydroxyisoxypropyl-3-hydroxy-7-isopentene-2,3-dihydrobenzofuran-5-carboxylic	70697841	FALSE	c1(cc(c2c(c1)C(C(O2)C(C)(C)O)O)CC=C(C)C)C(=O)O
MOL000180	0.7703	0.2297	0.8177	Atractylodes Lancea (Thunb.)Dc.	Aractylenolide II	Not Available	FALSE	C1CC(=C)C2C(C1)(C=C1C(C2)C(C(=O)O1)C)C
MOL000181	0.8582	0.1418	0.7918	Atractylodes Lancea (Thunb.)Dc.	atractylenolide III	Not Available	FALSE	O1C(=O)C(=C2C1(CC1(C(C2)C(=C)CCC1)C)O)C
MOL000182	0.4632	0.5368	0.6165	Atractylodes Lancea (Thunb.)Dc.	Atractyloyne	Not Available	FALSE	CC(CC(=C)OCCC(O)/C=C/C=C/C#CC#C/C=C/CO)C
MOL000183	0.8378	0.1622	0.7084	Atractylodes Lancea (Thunb.)Dc.	Beta-Eudesmol	12309818	FALSE	C1CC(=C)C2C(C1)(CCC(C2)C(C)(O)C)C
MOL000187	0.8872	0.1128	0.8129	Atractylodes Lancea (Thunb.)Dc.	butenolide B	Not Available	FALSE	O1C2(C(=CC1=O)CC1C(=C)CCCC1(C2)C)O
MOL000188	0.5203	0.4797	0.7870	Atractylodes Lancea (Thunb.)Dc.	3β-acetoxyatractylone	Not Available	FALSE	o1c2c(c(c1)C)CC1C(=C)C(CCC1(C2)C)OC(=O)C
MOL000189	0.7917	0.2083	0.7287	Atractylodes Lancea (Thunb.)Dc.	acetyl atractylodinol	Not Available	FALSE	C(/C=C/C#CC#C/C=C\c1occc1)OC(=O)C
MOL000190	0.9311	0.0689	0.8305	Atractylodes Lancea (Thunb.)Dc.	3,5-dimethoxy-4-glucosyloxyphenylallylalcohol	Not Available	FALSE	C(C=C)(O)c1cc(c(c(c1)OC)OC1C(O)C(O)C(O)C(O1)CO)OC
MOL000191	0.9416	0.0584	0.9623	Atractylodes Lancea (Thunb.)Dc.	3,5-dimethoxy-4-glucosyloxyphenylallylalcohol_qt	Not Available	FALSE	C(C=C)(O)c1cc(c(c(c1)OC)O)OC

MOL000192	0.7825	0.2175	0.7370	Atractylodes Lancea (Thunb.)Dc.	2-(1,4a-dimethyl-2,3-dihydroxydecahydronaphthalen-7-yl)isopropyl glucoside	Not Available	FALSE	O(C1C(O)(C(O)C(O)C(O1)CO)C1CCC2(CC(C(C(C2C1)C)O)O)C)C(C)C
MOL000193	0.8418	0.1582	0.6717	Cinnanmomi Cortex	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Dictamni Cortex	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Herbahypericiperforati	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Piperis Longi Fructus	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Lysimachiae Herba	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Cynanchistauntonii Rhizoma Et Radix	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Ephedra Herba	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Herba Taxilli	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Menthae Herba	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Ardisiae Japonicae Herba	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Chrysanthemi Flos	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Herba Clinopodii Polycephali.	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Acoritataninowii Rhizoma	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Folium Nelumbinis	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Rhizome Of Whiteback Greenbrier	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Apocyniveneti Folium	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Aucklandiae Radix	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Violsse Herba	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C

MOL000193	0.8418	0.1582	0.6717	Radix Cynanchi Paniculati	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Artemisia Annua L.	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Viticis Negundo Folium	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Caryophylliflos	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Pogostemon Cablin (Blanco) Benth.	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Atractylodes Lancea (Thunb.)Dc.	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Curcumae Radix	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Myrrha	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Et Radix Patriniae Rhizoma	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Flemingia Prostrata Roxb	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Citri Grandis Exocarpium	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Broussonetiae Fructus	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Evodiae Fructus	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Piperis Fructus	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Alpinia Katsumadai Hayat	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Humulus Scandens (Lour.) Merr.	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Litchi Semen	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Kadsurae Coccineae Radix Et Caulis	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Phragmitis Rhizoma	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Paederiae Scandentis Herba	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C

MOL000193	0.8418	0.1582	0.6717	Peucedani Radix	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Bidentis Bipinnatae Herba	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Aurantii Fructus Immaturus	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Verbenae Herb	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Viticis Fructus	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Calyx Seu Fructus Physalis	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Herba Patriniae	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Gnaphalii Affinis Herba	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Fructus Carotae	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Eupatorium Fortunei Turcz	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Illicium Difengpi K. L. B. Et K. I. M.	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Magnolia Officinalis Rehd Et Wils.	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Alpiniae Officinarum Rhizome	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Fritillariaeussuriensis Bulbus	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Siphonostegiae Herba	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Panacis Quinquefolii Radix	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Radix Bupleuri	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Hyperici Japonici Herber	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Cnidii Fructus	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Rhizoma Seu Herba Aristolochiae Mollissimae	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Peucedanidecursivi Radix	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C

MOL000193	0.8418	0.1582	0.6717	Celastri Orbiculati Fructus	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Anisi Stellati Fructus	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Radix Cirsii Japonici	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000193	0.8418	0.1582	0.6717	Arisaematis Rhizoma	(Z)-caryophyllene	6429301	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(/CC2)\C
MOL000195	0.3247	0.6753	0.6589	Illicium Difengpi K. L. B. Et K. I. M.	Mangostin	5281650	FALSE	c1(c(c(c2c(c1)oc1c(c2=O)c(c(c(c1)O)OC)CC=C(C)C)O)CC=C(C)C)O
MOL000196	0.9586	0.0414	0.7752	Morindae Officinalis Radix	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Notopterygii Rhizoma Et Radix	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Kadsurae Coccineae Radix Et Caulis	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Ephedra Herba	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Zanthoxyli Pericarpium	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Lysimachiae Foenigraeci Herba	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Alpiniae Officinarum Rhizome	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Gypsophila Licentiana Hand.-Mazz.	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Lonicerae Japonicae Flos	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Zingiberis Rhizoma	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Smilacis Glabrae Rhixoma	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Fructus Carotae	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Kaempferiae Rhizoma	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Alpinia Katsumadai Hayat	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Curcumae Radix	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Schisandrae Chinensis Fructus	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C

MOL000196	0.9586	0.0414	0.7752	Rhododendri Daurici Folium	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Viticis Negundo Folium	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Cayratiae Japonicae Herba	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Olibanun	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Radix Bupleuri	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Artemisia Annua L.	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Linderae Radix	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Chrysanthemi Flos	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Houttuyniae Herba	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Fructus Ligustri Lucidi	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Cnidii Fructus	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Chuanxiong Rhizoma	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Illicium Difengpi K. L. B. Et K. I. M.	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Aristolochiae Fructus	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Paederiae Scandentis Herba	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Magnolia Officinalis Rehd Et Wils.	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000196	0.9586	0.0414	0.7752	Ligustici Rhizoma Et Radix	L-Bornyl acetate	93009	FALSE	C(=O)(C)OC1CC2CCC1(C2(C)C)C
MOL000197	0.9159	0.0841	0.9177	Angelicae Sinensis Radix	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Notopterygii Rhizoma Et Radix	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Schisandrae Chinensis Fructus	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Herbahypericiperforati	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Houttuyniae Herba	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Menthae Herba	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Piperis Longi Fructus	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C

MOL000197	0.9159	0.0841	0.9177	Ligustici Rhizoma Et Radix	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Aucklandiae Radix	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Litseae Fructus	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Asari Radix Et Rhizoma	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Kadsurae Coccineae Radix Et Caulis	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Xanthii Fructus	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Eriobotryae Folium	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Aurantii Fructus Immaturus	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Rubi Fructus	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Alpiniae Officinarum Rhizome	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Foeniculi Fructus	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Prunellae Spica	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Magnolia Officinalis Rehd Et Wils.	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Eupatorium Fortunei Turcz	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Zingiberis Rhizoma	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Citri Reticulatae Pericarpium Viride	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Citri Fructus Retinervus	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Perilla Frutescens	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Schizonepetae Herba	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Evodiae Fructus	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Aristolochiae Fructus	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Rhododendri Daurici Folium	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Cinnamomi Ramulus	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Aurantii Fructus	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Schizonepetae Spica	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Zingiber Officinale Roscoe	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Arecae Semen	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Campsis Flos	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Forsythiae Fructus	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Folium Artemisiae Argyi	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Fructus Carotae	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Magnoliae Flos	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C

MOL000197	0.9159	0.0841	0.9177	Illicium Difengpi K. L. B. Et K. I. M.	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Borneolum Syntheticum	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Anisi Stellati Fructus	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Linderae Radix	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Viticis Negundo Folium	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Cymbopon Citratus(D C.) Stapf	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Alpinia Katsumadai Hayat	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Dichroae Radix	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Acoritataninowii Rhizoma	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Zanthoxyli Pericarpium	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Curcumae Rhizoma	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Herba Clinopodii Polycephali.	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Chuanxiong Rhizoma	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Sesami Nigrum Semen	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Mume Flos	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Bidentis Bipinnatae Herba	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Citri Fructus	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Cnidii Fructus	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Citri Exocarpium Rubrum	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Solidaginis Herba	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Artemisia Annua L.	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Citrus Aurantium	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Platycladi Cacumen	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Citri Reticulatae Folium	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Radix Angelicae Biseratae	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Piperis Fructus	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Cinnanmomi Cortex	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Curcumae Radix	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Myrrha	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Styrax	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Radix Bupleuri	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000197	0.9159	0.0841	0.9177	Homalomena Occulta (Lour.) Schott	Myrcene	31253	FALSE	C(=C)(CCC=C(C)C)C=C
MOL000198	0.9299	0.0701	0.9389	Fructus Carotae	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Rhizoma Fagopyri Cymosi	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Piperis Fructus	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Citri Exocarpium Rubrum	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Citri Fructus	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Cnidii Fructus	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O

MOL000198	0.9299	0.0701	0.9389	Citri Reticulatae Pericarpium Viride	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Paederiae Scandentis Herba	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Piperis Longi Fructus	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Olibanun	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Chuanxiong Rhizoma	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Lilii Bulbus	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Zanthoxyli Pericarpium	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Anisi Stellati Fructus	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Cinnanmomi Cortex	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Junci Medulla	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Mume Fructus	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Scutellariae Radix	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Hippophae Fructus	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Viticis Negundo Folium	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Gynostemmae Pentaphylli Herba	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Rhizome Of Whiteback Greenbrier	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Perilla Frutescens	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Myristicae Semen	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Mahoniae Folum	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Rhododendri Daurici Folium	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Radix Salviae	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Schizonepetae Herba	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Magnolia Officinalis Rehd Et Wils.	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Radix Bupleuri	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Morindae Officinalis Radix	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Chaenomeles Sinensis (Thouin) Koehne	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Citri Grandis Exocarpium	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Glechomae Herba	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Illicium Difengpi K. L. B. Et K. I. M.	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Fructus Ligustri Lucidi	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Verbenae Herb	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Celastri Orbiculati Fructus	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Zingiberis Rhizoma	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Eriobotryae Folium	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O

MOL000198	0.9299	0.0701	0.9389	Eupatorium Fortunei Turcz	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Aucklandiae Radix	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Citrus Reticulata	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Nardostachyos Radix Et Rhizoma	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Ginkgo Folium	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Ardisiae Japonicae Herba	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Cuscutae Semen	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Smilacis Glabrae Rhixoma	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Mori Cortex	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Rose Rugosae Flos	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Dysosmae Verspiellis Rhixoma Et Radix	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Viticis Fructus	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Menthae Herba	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Houttuyniae Herba	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Alpiniae Officinarum Rhizome	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Chrysanthemi Flos	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Citrus Aurantium	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Ailanthi Cortex	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Lysimachiae Foenigraeci Herba	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Puerariae Flos	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Arisaematis Rhizoma	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Amygdalus Communis Vas	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Evodiae Fructus	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Linderae Radix	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Cymbopon Citratus(D C.) Stapf	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Geranium Wilfordii Maxim.	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Caryophylliflos	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Alpinia Katsumadai Hayat	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Rubi Fructus	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Maydis Seigma	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Mahoniae Caulis	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Homalomena Occulta (Lour.) Schott	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Agrimonia Eupatoria	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Phragmitis Rhizoma	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Semen Pharbitidis	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O

MOL000198	0.9299	0.0701	0.9389	Gnaphalii Affinis Herba	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Litseae Fructus	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Lysimachiae Herba	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Mori Fructus	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Artemisia Annua L.	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Styrax	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Coriandri Sativi Herba	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Forsythiae Fructus	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Ephedra Herba	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Curcumae Radix	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Acoritataninowii Rhizoma	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Capsici Fructus	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Epimrdii Herba	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Arecae Semen	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Ganoderma	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Schisandrae Chinensis Fructus	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Ilicis Cornutae Folium Immayuri	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000198	0.9299	0.0701	0.9389	Perillae Fructus	(R)-linalool	443158	FALSE	C(CCC=C(C)C)(C=C)(C)O
MOL000199	0.9590	0.0410	0.8511	Asari Radix Et Rhizoma	Safrol	5144	FALSE	c12c(ccc(c1)CC=C)OCO2
MOL000199	0.9590	0.0410	0.8511	Magnoliae Flos	Safrol	5144	FALSE	c12c(ccc(c1)CC=C)OCO2
MOL000199	0.9590	0.0410	0.8511	Magnolia Officinalis Rehd Et Wils.	Safrol	5144	FALSE	c12c(ccc(c1)CC=C)OCO2
MOL000199	0.9590	0.0410	0.8511	Platycladi Cacumen	Safrol	5144	FALSE	c12c(ccc(c1)CC=C)OCO2
MOL000199	0.9590	0.0410	0.8511	Campsis Flos	Safrol	5144	FALSE	c12c(ccc(c1)CC=C)OCO2
MOL000199	0.9590	0.0410	0.8511	Lycii Fructus	Safrol	5144	FALSE	c12c(ccc(c1)CC=C)OCO2
MOL000199	0.9590	0.0410	0.8511	Gypsophila Licentiana Hand.-Mazz.	Safrol	5144	FALSE	c12c(ccc(c1)CC=C)OCO2
MOL000199	0.9590	0.0410	0.8511	Alpinia Katsumadai Hayat	Safrol	5144	FALSE	c12c(ccc(c1)CC=C)OCO2
MOL000199	0.9590	0.0410	0.8511	Forsythiae Fructus	Safrol	5144	FALSE	c12c(ccc(c1)CC=C)OCO2
MOL000199	0.9590	0.0410	0.8511	Cornus Officinalis Sieb. Et Zucc.	Safrol	5144	FALSE	c12c(ccc(c1)CC=C)OCO2
MOL000199	0.9590	0.0410	0.8511	Myristicae Semen	Safrol	5144	FALSE	c12c(ccc(c1)CC=C)OCO2
MOL000199	0.9590	0.0410	0.8511	Illicium Difengpi K. L. B. Et K. I. M.	Safrol	5144	FALSE	c12c(ccc(c1)CC=C)OCO2
MOL000199	0.9590	0.0410	0.8511	Aristolochiae Fructus	Safrol	5144	FALSE	c12c(ccc(c1)CC=C)OCO2
MOL000199	0.9590	0.0410	0.8511	Angelicae Sinensis Radix	Safrol	5144	FALSE	c12c(ccc(c1)CC=C)OCO2
MOL000200	0.9582	0.0418	0.9560	Radix Angelicae Biseratae	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C

MOL000200	0.9582	0.0418	0.9560	Chuanxiong Rhizoma	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Foeniculi Fructus	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Zingiber Officinale Roscoe	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Borneolum Syntheticum	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Curcumae Radix	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Ligustici Rhizoma Et Radix	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Alpinia Katsumadai Hayat	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Kaempferiae Rhizoma	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Myrrha	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Viticis Negundo Folium	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Moslae Herba	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Eupatorium Fortunei Turcz	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Olibanun	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Magnolia Officinalis Rehd Et Wils.	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Phellodendri Chinrnsis Cortex	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Peucedanidecursivi Radix	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Myristicae Semen	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Anisi Stellati Fructus	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Folium Artemisiae Argyi	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Platycladi Cacumen	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C

MOL000200	0.9582	0.0418	0.9560	Aucklandiae Radix	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Zingiberis Rhizoma	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Evodiae Fructus	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Farfarae Flos	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Linderae Radix	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Notopterygii Rhizoma Et Radix	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Illicium Difengpi K. L. B. Et K. I. M.	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000200	0.9582	0.0418	0.9560	Peucedani Radix	(S)-(+)-alpha-Phellandrene	443160	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000201	0.9237	0.0763	0.9230	Illicium Difengpi K. L. B. Et K. I. M.	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Curcumae Radix	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Caryophylliflos	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Aristolochiae Fructus	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Aurantii Fructus	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Campsis Flos	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Sesami Nigrum Semen	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Homalomena Occulta (Lour.) Schott	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Menthae Herba	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Radix Angelicae Biseratae	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Mahoniae Folum	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Borneolum Syntheticum	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Chuanxiong Rhizoma	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Myrrha	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Solidaginis Herba	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Olibanun	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Cinnanmomi Cortex	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Zanthoxyli Pericarpium	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Zingiberis Rhizoma	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Alpiniae Officinarum Rhizome	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Piperis Longi Fructus	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Hippophae Fructus	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C

MOL000201	0.9237	0.0763	0.9230	Bidentis Bipinnatae Herba	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Zingiber Officinale Roscoe	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Evodiae Fructus	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Citrus Reticulata	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Rubi Fructus	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Rhododendri Daurici Folium	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Ephedra Herba	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Forsythiae Fructus	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Radix Bupleuri	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Herba Clinopodii Polycephali.	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Rhizoma Seu Herba Aristolochiae Mollissimae	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Citri Fructus	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Citrus Aurantium	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Notopterygii Rhizoma Et Radix	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Linderae Radix	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000201	0.9237	0.0763	0.9230	Angelicae Sinensis Radix	p-Ocimene	5281553	FALSE	C(=C\CC=C(C)C)(/C=C)\C
MOL000202	0.9509	0.0491	0.9548	Radix Angelicae Biseratae	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Curcumae Radix	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Aucklandiae Radix	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Alpinia Katsumadai Hayat	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Menthae Herba	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Viticis Fructus	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Cinnanmomi Cortex	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Rhizome Of Whiteback Greenbrier	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Radix Salviae	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Canarii Fructus	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Illicium Difengpi K. L. B. Et K. I. M.	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Kadsurae Coccineae Radix Et Caulis	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Asari Radix Et Rhizoma	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Cnidii Fructus	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Zingiberis Rhizoma	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Gypsophila Licentiana Hand.-Mazz.	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Citri Fructus	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C

MOL000202	0.9509	0.0491	0.9548	Zanthoxyli Pericarpium	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Campsis Flos	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Piperis Fructus	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Evodiae Fructus	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Magnolia Officinalis Rehd Et Wils.	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Homalomena Occulta (Lour.) Schott	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Notopterygii Rhizoma Et Radix	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Moslae Herba	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Magnoliae Flos	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Foeniculi Fructus	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Lysimachiae Herba	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Chrysanthemi Flos	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Aurantii Fructus Immaturus	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Platycladi Cacumen	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Angelicae Sinensis Radix	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Chuanxiong Rhizoma	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Nardostachyos Radix Et Rhizoma	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Schisandrae Chinensis Fructus	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Rubi Fructus	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Lilii Bulbus	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Ephedra Herba	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Ligustici Rhizoma Et Radix	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Zingiber Officinale Roscoe	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	A. Dahurica (Fisch.) Benth. Et Hook	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Piperis Longi Fructus	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Viticis Negundo Folium	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Rhododendri Daurici Folium	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000202	0.9509	0.0491	0.9548	Alpiniae Officinarum Rhizome	Moslene	7461	FALSE	C1(=CCC(=CC1)C)C(C)C
MOL000203	0.9591	0.0409	0.8313	Illicium Difengpi K. L. B. Et K. I. M.	Izosafrol	1549044	FALSE	c12c(ccc(c1)/C=C\C)OCO2
MOL000203	0.9591	0.0409	0.8313	Linderae Radix	Izosafrol	1549044	FALSE	c12c(ccc(c1)/C=C\C)OCO2
MOL000203	0.9591	0.0409	0.8313	Epimrdii Herba	Izosafrol	1549044	FALSE	c12c(ccc(c1)/C=C\C)OCO2

MOL000204	0.8619	0.1381	0.6520	Viticis Negundo Folium	-cis-.beta.-Elemene diastereomer	6431152	FALSE	C1(C(CCC(C1)C(=C)C)(C=C)C)C(=C)C
MOL000204	0.8619	0.1381	0.6520	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	-cis-.beta.-Elemene diastereomer	6431152	FALSE	C1(C(CCC(C1)C(=C)C)(C=C)C)C(=C)C
MOL000204	0.8619	0.1381	0.6520	Solidaginis Herba	-cis-.beta.-Elemene diastereomer	6431152	FALSE	C1(C(CCC(C1)C(=C)C)(C=C)C)C(=C)C
MOL000204	0.8619	0.1381	0.6520	Eupatorium Fortunei Turcz	-cis-.beta.-Elemene diastereomer	6431152	FALSE	C1(C(CCC(C1)C(=C)C)(C=C)C)C(=C)C
MOL000204	0.8619	0.1381	0.6520	Piperis Longi Fructus	-cis-.beta.-Elemene diastereomer	6431152	FALSE	C1(C(CCC(C1)C(=C)C)(C=C)C)C(=C)C
MOL000204	0.8619	0.1381	0.6520	Chrysanthemi Flos	-cis-.beta.-Elemene diastereomer	6431152	FALSE	C1(C(CCC(C1)C(=C)C)(C=C)C)C(=C)C
MOL000204	0.8619	0.1381	0.6520	Illicium Difengpi K. L. B. Et K. I. M.	-cis-.beta.-Elemene diastereomer	6431152	FALSE	C1(C(CCC(C1)C(=C)C)(C=C)C)C(=C)C
MOL000204	0.8619	0.1381	0.6520	Zingiberis Rhizoma	-cis-.beta.-Elemene diastereomer	6431152	FALSE	C1(C(CCC(C1)C(=C)C)(C=C)C)C(=C)C
MOL000204	0.8619	0.1381	0.6520	Chuanxiong Rhizoma	-cis-.beta.-Elemene diastereomer	6431152	FALSE	C1(C(CCC(C1)C(=C)C)(C=C)C)C(=C)C
MOL000204	0.8619	0.1381	0.6520	Artemisia Annua L.	-cis-.beta.-Elemene diastereomer	6431152	FALSE	C1(C(CCC(C1)C(=C)C)(C=C)C)C(=C)C
MOL000204	0.8619	0.1381	0.6520	Pogostemon Cablin (Blanco) Benth.	-cis-.beta.-Elemene diastereomer	6431152	FALSE	C1(C(CCC(C1)C(=C)C)(C=C)C)C(=C)C
MOL000204	0.8619	0.1381	0.6520	Flemingia Prostrata Roxb	-cis-.beta.-Elemene diastereomer	6431152	FALSE	C1(C(CCC(C1)C(=C)C)(C=C)C)C(=C)C
MOL000204	0.8619	0.1381	0.6520	Viticis Fructus	-cis-.beta.-Elemene diastereomer	6431152	FALSE	C1(C(CCC(C1)C(=C)C)(C=C)C)C(=C)C
MOL000204	0.8619	0.1381	0.6520	Perilla Frutescens	-cis-.beta.-Elemene diastereomer	6431152	FALSE	C1(C(CCC(C1)C(=C)C)(C=C)C)C(=C)C

MOL000204	0.8619	0.1381	0.6520	Piperis Fructus	-cis-.beta.-Elemene diastereomer	6431152	FALSE	C1(C(CCC(C1)C(=C)C)(C=C)C)C(=C)C
MOL000204	0.8619	0.1381	0.6520	Magnolia Officinalis Rehd Et Wils.	-cis-.beta.-Elemene diastereomer	6431152	FALSE	C1(C(CCC(C1)C(=C)C)(C=C)C)C(=C)C
MOL000204	0.8619	0.1381	0.6520	Ligustici Rhizoma Et Radix	-cis-.beta.-Elemene diastereomer	6431152	FALSE	C1(C(CCC(C1)C(=C)C)(C=C)C)C(=C)C
MOL000204	0.8619	0.1381	0.6520	Aucklandiae Radix	-cis-.beta.-Elemene diastereomer	6431152	FALSE	C1(C(CCC(C1)C(=C)C)(C=C)C)C(=C)C
MOL000204	0.8619	0.1381	0.6520	Evodiae Fructus	-cis-.beta.-Elemene diastereomer	6431152	FALSE	C1(C(CCC(C1)C(=C)C)(C=C)C)C(=C)C
MOL000205	0.9615	0.0385	0.9600	Zanthoxyli Pericarpium	(6R)-6-isopropyl-3-methyl-1-cyclohex-2-enone	107561	FALSE	C1(C(=O)C=C(CC1)C)C(C)C
MOL000205	0.9615	0.0385	0.9600	Linderae Radix	(6R)-6-isopropyl-3-methyl-1-cyclohex-2-enone	107561	FALSE	C1(C(=O)C=C(CC1)C)C(C)C
MOL000205	0.9615	0.0385	0.9600	Menthae Herba	(6R)-6-isopropyl-3-methyl-1-cyclohex-2-enone	107561	FALSE	C1(C(=O)C=C(CC1)C)C(C)C
MOL000205	0.9615	0.0385	0.9600	Rubi Fructus	(6R)-6-isopropyl-3-methyl-1-cyclohex-2-enone	107561	FALSE	C1(C(=O)C=C(CC1)C)C(C)C
MOL000205	0.9615	0.0385	0.9600	Cayratiae Japonicae Herba	(6R)-6-isopropyl-3-methyl-1-cyclohex-2-enone	107561	FALSE	C1(C(=O)C=C(CC1)C)C(C)C

MOL000205	0.9615	0.0385	0.9600	Olibanun	(6R)-6-isopropyl-3-methyl-1-cyclohex-2-enone	107561	FALSE	C1(C(=O)C=C(CC1)C)C(C)C
MOL000205	0.9615	0.0385	0.9600	Epimrdii Herba	(6R)-6-isopropyl-3-methyl-1-cyclohex-2-enone	107561	FALSE	C1(C(=O)C=C(CC1)C)C(C)C
MOL000205	0.9615	0.0385	0.9600	Piperis Fructus	(6R)-6-isopropyl-3-methyl-1-cyclohex-2-enone	107561	FALSE	C1(C(=O)C=C(CC1)C)C(C)C
MOL000205	0.9615	0.0385	0.9600	Magnolia Officinalis Rehd Et Wils.	(6R)-6-isopropyl-3-methyl-1-cyclohex-2-enone	107561	FALSE	C1(C(=O)C=C(CC1)C)C(C)C
MOL000205	0.9615	0.0385	0.9600	Ephedra Herba	(6R)-6-isopropyl-3-methyl-1-cyclohex-2-enone	107561	FALSE	C1(C(=O)C=C(CC1)C)C(C)C
MOL000205	0.9615	0.0385	0.9600	Illicium Difengpi K. L. B. Et K. I. M.	(6R)-6-isopropyl-3-methyl-1-cyclohex-2-enone	107561	FALSE	C1(C(=O)C=C(CC1)C)C(C)C
MOL000206	0.9506	0.0494	0.9462	Caryophylliflos	isoeugenol	853433	FALSE	c1(cc(ccc1O)/C=C/C)OC
MOL000206	0.9506	0.0494	0.9462	Zingiber Officinale Roscoe	isoeugenol	853433	FALSE	c1(cc(ccc1O)/C=C/C)OC
MOL000206	0.9506	0.0494	0.9462	Illicium Difengpi K. L. B. Et K. I. M.	isoeugenol	853433	FALSE	c1(cc(ccc1O)/C=C/C)OC
MOL000206	0.9506	0.0494	0.9462	Cornus Officinalis Sieb. Et Zucc.	isoeugenol	853433	FALSE	c1(cc(ccc1O)/C=C/C)OC
MOL000206	0.9506	0.0494	0.9462	Ardisiae Japonicae Herba	isoeugenol	853433	FALSE	c1(cc(ccc1O)/C=C/C)OC
MOL000206	0.9506	0.0494	0.9462	Myristicae Semen	isoeugenol	853433	FALSE	c1(cc(ccc1O)/C=C/C)OC
MOL000206	0.9506	0.0494	0.9462	Phytolaccae Radix	isoeugenol	853433	FALSE	c1(cc(ccc1O)/C=C/C)OC
MOL000206	0.9506	0.0494	0.9462	Angelicae Sinensis Radix	isoeugenol	853433	FALSE	c1(cc(ccc1O)/C=C/C)OC
MOL000206	0.9506	0.0494	0.9462	Pseudostellariae Radix	isoeugenol	853433	FALSE	c1(cc(ccc1O)/C=C/C)OC
MOL000206	0.9506	0.0494	0.9462	Panacis Quinquefolii Radix	isoeugenol	853433	FALSE	c1(cc(ccc1O)/C=C/C)OC
MOL000206	0.9506	0.0494	0.9462	Rose Rugosae Flos	isoeugenol	853433	FALSE	c1(cc(ccc1O)/C=C/C)OC

MOL000206	0.9506	0.0494	0.9462	Piperis Longi Fructus	isoeugenol	853433	FALSE	c1(cc(ccc1O)/C=C/C)OC
MOL000206	0.9506	0.0494	0.9462	Mume Flos	isoeugenol	853433	FALSE	c1(cc(ccc1O)/C=C/C)OC
MOL000207	0.9644	0.0356	0.9290	Folium Artemisiae Argyi	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Evodiae Fructus	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Chaenomeles Sinensis (Thouin) Koehne	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Caryophylliflos	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Acoritataninowii Rhizoma	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Radix Bupleuri	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Scutellariae Barbatae Herba	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Rhododendri Daurici Folium	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Campsis Flos	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Chuanxiong Rhizoma	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Myristicae Semen	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Illicium Difengpi K. L. B. Et K. I. M.	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Mori Follum	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Alpiniae Officinarum Rhizome	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Alpinia Katsumadai Hayat	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Radix Angelicae Biseratae	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Magnoliae Flos	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Zanthoxyli Pericarpium	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Cornus Officinalis Sieb. Et Zucc.	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Rose Rugosae Flos	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC

MOL000207	0.9644	0.0356	0.9290	Ginkgo Folium	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Epimrdii Herba	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Asari Radix Et Rhizoma	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Artemisiae Scopariae Herba	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Sinapis Semen	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Magnolia Officinalis Rehd Et Wils.	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Herba Taxilli	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Arisaematis Rhizoma	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Adenophprae Ae Radix	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000207	0.9644	0.0356	0.9290	Mume Flos	Methyleugenol	7127	FALSE	c1(c(ccc(c1)CC=C)OC)OC
MOL000209	0.8517	0.1483	0.6995	Cyperi Rhizoma	(1R,3aR,4R,7R)-7-isopropenyl-1,4-dimethyl-1,2,3,3a,4,5,6,7-octahydroazulene	15560285	FALSE	C12=CC(CCC(C1CCC2C)C)C(=C)C
MOL000209	0.8517	0.1483	0.6995	Illicium Difengpi K. L. B. Et K. I. M.	(1R,3aR,4R,7R)-7-isopropenyl-1,4-dimethyl-1,2,3,3a,4,5,6,7-octahydroazulene	15560285	FALSE	C12=CC(CCC(C1CCC2C)C)C(=C)C
MOL000210	0.6835	0.3165	0.7444	Momordicae Fructus	Magnolol	72300	FALSE	c1(c2cc(ccc2O)CC=C)cc(ccc1O)CC=C
MOL000210	0.6835	0.3165	0.7444	Illicium Difengpi K. L. B. Et K. I. M.	Magnolol	72300	FALSE	c1(c2cc(ccc2O)CC=C)cc(ccc1O)CC=C
MOL000210	0.6835	0.3165	0.7444	Magnolia Officinalis Rehd Et Wils.	Magnolol	72300	FALSE	c1(c2cc(ccc2O)CC=C)cc(ccc1O)CC=C
MOL000211	0.7391	0.2609	0.9223	Boehmeriae Rhizoma Et Radix	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O

MOL000211	0.7391	0.2609	0.9223	Trigonellae Semen	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Eucommiae Cortex	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Ilicis Cornutae Folium Immayuri	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Anisi Stellati Fructus	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Cortex Moutan	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Glechomae Herba	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Tamaricis Cacumen	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Jujubae Fructus	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Forsythiae Fructus	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Kaki Calyx	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Pulsatilliae Radix	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Radix Sanguisorbae	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	licorice	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Paeoniae Radix Alba	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Hyperici Japonici Herber	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Mori Cortex	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Illicium Difengpi K. L. B. Et K. I. M.	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Pseudolaricis Cortex	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Aucklandiae Radix	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Quisqualis Indica	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Chaenomeles Sinensis (Thouin) Koehne	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O

MOL000211	0.7391	0.2609	0.9223	Ziziphi Spinosae Semen	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Potentillae Chinensis Herba	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Viscum Angulatum Heyne	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000211	0.7391	0.2609	0.9223	Hedysarum Multijugum Maxim.	Mairin	64971	FALSE	C12C(CCC3(C1CCC1C3(CCC3C1(CCC(C3(C)C)O)C)C)C)(CCC2C(=C)C)C(=O)O
MOL000212	0.6186	0.3814	0.7317	Illicium Difengpi K. L. B. Et K. I. M.	3beta-O-Acetyl-mangiferolic acid	Not Available	FALSE	C1/C(=C/OC(=O)C)/C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C(CC2)C(CC/C=C(/C)\C(=O)O)C)C)C)C3)(C)C
MOL000213	0.8603	0.1397	0.6393	Illicium Difengpi K. L. B. Et K. I. M.	Dirhizomic acid	94870	FALSE	c1(cc(c(c(c1C(=O)Oc1c(c(c(c(c1)C)C(=O)O)O)C)OC)C)OC)C
MOL000214	0.6593	0.3407	0.7576	Illicium Difengpi K. L. B. Et K. I. M.	Mangiferonic acid	Not Available	FALSE	C1C(=O)C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C(CC2)C(CC/C=C(/C(=O)O)\C)C)C)C)C3)(C)C
MOL000215	0.8989	0.1011	0.8998	Erycibe Obtusifolia Benth	(1S,2S,5R,7R)-8-azabicyclo[3.2.1]octane-2,7-diol	21121210	FALSE	C12C(CCC(CC1O)N2)O
MOL000216	0.9190	0.0810	0.8272	Trigonellae Semen	Scopolin	Not Available	FALSE	[illegible]
MOL000216	0.9190	0.0810	0.8272	Erycibe Obtusifolia Benth	Scopolin	Not Available	FALSE	[illegible]
MOL000216	0.9190	0.0810	0.8272	Inulae Flos	Scopolin	Not Available	FALSE	[illegible]
MOL000216	0.9190	0.0810	0.8272	Lycii Fructus	Scopolin	Not Available	FALSE	[illegible]
MOL000217	0.5352	0.4648	0.8848	Chelidonii Herba	(S)-Scoulerine	439654	TRUE	c12c(cc(c(c1)O)OC)CCN1C2Cc2c(C1)c(c(cc2)OC)O
MOL000217	0.5352	0.4648	0.8848	Corydalis Bungeanae Herba	(S)-Scoulerine	439654	TRUE	c12c(cc(c(c1)O)OC)CCN1C2Cc2c(C1)c(c(cc2)OC)O
MOL000217	0.5352	0.4648	0.8848	Corydalis Rhizoma	(S)-Scoulerine	439654	TRUE	c12c(cc(c(c1)O)OC)CCN1C2Cc2c(C1)c(c(cc2)OC)O
MOL000217	0.5352	0.4648	0.8848	Erycibe Obtusifolia Benth	(S)-Scoulerine	439654	TRUE	c12c(cc(c(c1)O)OC)CCN1C2Cc2c(C1)c(c(cc2)OC)O
MOL000218	0.9048	0.0952	0.9094	Erycibe Obtusifolia Benth	baogongtengC	Not Available	FALSE	C12C(CCC(C(C1)O)N2)O
MOL000219	0.9344	0.0656	0.9629	Chebulae Fructus	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Arisaematis Rhizoma	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Isatidis Folium	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Benzoinum	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Radix Cynanchi Paniculati	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Oroxyli Semen	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Meliae Azedarach Fructus	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Bomboo Juice	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Trollius Chinensis	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Plantaginis Herba	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Menthae Herba	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Mume Fructus	BOX	20144841	FALSE	c1(ccccc1)C(=O)O

MOL000219	0.9344	0.0656	0.9629	Erycibe Obtusifolia Benth	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Semen Euphorbiae	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Flos Genkwa	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Celastri Orbiculati Fructus	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Campsis Flos	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Potentillae Chinensis Herba	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Euonymi Alati Ramulus	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Uncariae Ramulus Cumuncis	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Lygodii Spora	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Styrax	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Quisqualis Indica	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Tribulifructus	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Zanthoxyli Pericarpium	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Lasiosphaera Seu Calvatia	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Bombyx Mori L.	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Cinnamomi Ramulus	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Stemonae Radix	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Isatdis Radix	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Sparganii Rhizoma	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Gnaphalii Affinis Herba	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Gossampiniflos	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Scutellariae Radix	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Citrus Aurantium	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Curcumae Radix	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Salviae Chinensis Herba	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Cassiae Semen	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Cortex Moutan	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Ephedra Herba	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Meliae Cortex	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Folium Nelumbinis	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Paeoniae Radix Alba	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Mume Flos	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Asteris Radix Et Rhizoma	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Radix Paeoniae Rubra	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Scutellariae Barbatae Herba	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Chaenomeles Sinensis (Thouin) Koehne	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Radix Cynanchi	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Radix Clematidis	BOX	20144841	FALSE	c1(ccccc1)C(=O)O
MOL000219	0.9344	0.0656	0.9629	Cinnanmomi Cortex	BOX	20144841	FALSE	c1(ccccc1)C(=O)O

MOL000220	0.9480	0.0520	0.9084	Erycibe Obtusifolia Benth	baogongtengA	Not Available	FALSE	C12C(CCC([NH2+]1)C(C2)O)OC(=O)C
MOL000222	0.9497	0.0503	0.9440	Erycibe Obtusifolia Benth	terephthaldehyde	7067335	FALSE	C1C(C(C(CC1(O)C(=O)O)OC(=O)/C=C/c1ccc(c(c1)O)O)O)O
MOL000222	0.9497	0.0503	0.9440	Pyrrosiae Folium	terephthaldehyde	7067335	FALSE	C1C(C(C(CC1(O)C(=O)O)OC(=O)/C=C/c1ccc(c(c1)O)O)O)O
MOL000222	0.9497	0.0503	0.9440	Amygdalus Communis Vas	terephthaldehyde	7067335	FALSE	C1C(C(C(CC1(O)C(=O)O)OC(=O)/C=C/c1ccc(c(c1)O)O)O)O
MOL000222	0.9497	0.0503	0.9440	Cymbopon Citratus(D C.) Stapf	terephthaldehyde	7067335	FALSE	C1C(C(C(CC1(O)C(=O)O)OC(=O)/C=C/c1ccc(c(c1)O)O)O)O
MOL000222	0.9497	0.0503	0.9440	Lignum Pini Nodi	terephthaldehyde	7067335	FALSE	C1C(C(C(CC1(O)C(=O)O)OC(=O)/C=C/c1ccc(c(c1)O)O)O)O
MOL000222	0.9497	0.0503	0.9440	Saxifraga Stolonifera	terephthaldehyde	7067335	FALSE	C1C(C(C(CC1(O)C(=O)O)OC(=O)/C=C/c1ccc(c(c1)O)O)O)O
MOL000222	0.9497	0.0503	0.9440	Anisi Stellati Fructus	terephthaldehyde	7067335	FALSE	C1C(C(C(CC1(O)C(=O)O)OC(=O)/C=C/c1ccc(c(c1)O)O)O)O
MOL000222	0.9497	0.0503	0.9440	Plantaginis Herba	terephthaldehyde	7067335	FALSE	C1C(C(C(CC1(O)C(=O)O)OC(=O)/C=C/c1ccc(c(c1)O)O)O)O
MOL000222	0.9497	0.0503	0.9440	Calendula Officinalis	terephthaldehyde	7067335	FALSE	C1C(C(C(CC1(O)C(=O)O)OC(=O)/C=C/c1ccc(c(c1)O)O)O)O
MOL000222	0.9497	0.0503	0.9440	Carthami Flos	terephthaldehyde	7067335	FALSE	C1C(C(C(CC1(O)C(=O)O)OC(=O)/C=C/c1ccc(c(c1)O)O)O)O
MOL000222	0.9497	0.0503	0.9440	Inulae Herba	terephthaldehyde	7067335	FALSE	C1C(C(C(CC1(O)C(=O)O)OC(=O)/C=C/c1ccc(c(c1)O)O)O)O
MOL000222	0.9497	0.0503	0.9440	Herba Cirsii	terephthaldehyde	7067335	FALSE	C1C(C(C(CC1(O)C(=O)O)OC(=O)/C=C/c1ccc(c(c1)O)O)O)O
MOL000223	0.9416	0.0584	0.9275	Solidaginis Herba	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Andrographis Herba	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Herba Selaginellae Moellendorfii	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Polygoni Avicularis Herba	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Lithospermum Erythrorhizon	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Prunellae Spica	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Figwort Root	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Salviae Chinensis Herba	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Ginkgo Folium	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Viscum Angulatum Heyne	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Folium Artemisiae Argyi	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Xanthii Fructus	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Inulae Flos	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Morindae Officinalis Radix	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Smilax China	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O

MOL000223	0.9416	0.0584	0.9275	Cimicifugae Rhizoma	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Plantaginis Herba	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Saussureae Involucratae Herba	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Herba Solani Lyrati	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Fritiliariae Irrhosae Bulbus	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Cyperi Rhizoma	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Arum Ternatum Thunb.	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Glehniae Radix	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Menthae Herba	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Phragmitis Rhizoma	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Eucommiae Cortex	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Fructus Ligustri Lucidi	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Ginseng Folium	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Semen Lini	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Herba Sarcandrae	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Cymbopon Citratus(D C.) Stapf	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Farfarae Flos	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Asteris Radix Et Rhizoma	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Equiseti Hiemalis Herba	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Semen Pharbitidis	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Bistortae Rhizoma	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Acoritataninowii Rhizoma	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Saxifraga Stolonifera	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Chaenomeles Sinensis (Thouin) Koehne	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Herba Cirsii	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Sophorae Tonkinensis Radix Et Rhizome	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Cornus Officinalis Sieb. Et Zucc.	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Carthami Flos	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Herba Clematidis Aethusaefoliae	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Maydis Seigma	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Gleditsiae Spina	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Portulacae Herba	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Glechomae Herba	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Crataegi Folium	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O

MOL000223	0.9416	0.0584	0.9275	Potentillae Discoloris Herba	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Paederiae Scandentis Herba	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Moslae Herba	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Chuanxiong Rhizoma	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Cortex Moutan	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Agrimonia Eupatoria	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Radix Salviae	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Erycibe Obtusifolia Benth	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Schizonepetae Herba	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Gleditsiae Fructus	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Hippophae Fructus	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Ilicis Purpureae Folium	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Calendula Officinalis	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Herbahypericiperforati	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Inulae Herba	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Perilla Frutescens	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Fraxini Cortex	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000223	0.9416	0.0584	0.9275	Boschniakia Rossica Herba	caffeic acid	689043	TRUE	c1(cc(c(cc1)O)O)/C=C/C(=O)O
MOL000224	0.6992	0.3008	0.7283	Alpinia Katsumadai Hayat	(4E,6E)-1,7-bis(3,4-dihydroxyphenyl)hepta-4,6-dien-3-one	10426520	FALSE	C(CC(=O)/C=C/C=C/c1cc(c(cc1)O)O)c1cc(c(cc1)O)O
MOL000226	0.5091	0.4909	0.7443	Alpinia Katsumadai Hayat	1,7-diphenyl-5-hydroxy-4,6-heptadien-3-one	Not Available	FALSE	C(CC(=O)/C=C(/C=C/c1ccccc1)\O)c1ccccc1
MOL000227	0.5240	0.4760	0.6844	Alpinia Katsumadai Hayat	Alnusone	5317598	FALSE	c1cccc(c1)/C=C/C=C/C(=O)CCc1ccccc1
MOL000227	0.5240	0.4760	0.6844	Curcumae Radix	Alnusone	5317598	FALSE	c1cccc(c1)/C=C/C=C/C(=O)CCc1ccccc1
MOL000228	0.8630	0.1370	0.9272	Scutellariae Radix	(2R)-7-hydroxy-5-methoxy-2-phenylchroman-4-one	821279	FALSE	c1c(cc2c(c1OC)C(=O)CC(O2)c1ccccc1)O
MOL000228	0.8630	0.1370	0.9272	Alpinia Katsumadai Hayat	(2R)-7-hydroxy-5-methoxy-2-phenylchroman-4-one	821279	FALSE	c1c(cc2c(c1OC)C(=O)CC(O2)c1ccccc1)O

MOL000228	0.8630	0.1370	0.9272	Dalbergiae Odoriferae Lignum	(2R)-7-hydroxy-5-methoxy-2-phenylchroman-4-one	821279	FALSE	c1c(cc2c(c1OC)C(=O)CC(O2)c1ccccc1)O
MOL000229	0.9148	0.0852	0.8974	Alpinia Katsumadai Hayat	cardamomin	641785	FALSE	c1(c(cc(cc1OC)O)O)C(=O)/C=C/c1ccccc1
MOL000230	0.8999	0.1001	0.9210	Alpinia Katsumadai Hayat	Pinocembrin	Not Available	FALSE	c1ccc(cc1)C1CC(=O)c2c(O1)cc(cc2O)CO
MOL000231	0.5151	0.4849	0.7055	Alpinia Katsumadai Hayat	trans-1,7-Diphenyl-1hepten-5-ol	Not Available	FALSE	c1cccc(c1)/C=C/CCC(CCc1ccccc1)O
MOL000232	0.9322	0.0678	0.9688	Forsythiae Fructus	()-alpha-Terpineol	442501	FALSE	CC1=CCC(CC1)C(C)(C)O
MOL000232	0.9322	0.0678	0.9688	Alpinia Katsumadai Hayat	()-alpha-Terpineol	442501	FALSE	CC1=CCC(CC1)C(C)(C)O
MOL000232	0.9322	0.0678	0.9688	Magnoliae Flos	()-alpha-Terpineol	442501	FALSE	CC1=CCC(CC1)C(C)(C)O
MOL000232	0.9322	0.0678	0.9688	Myrrha	()-alpha-Terpineol	442501	FALSE	CC1=CCC(CC1)C(C)(C)O
MOL000232	0.9322	0.0678	0.9688	Capsici Fructus	()-alpha-Terpineol	442501	FALSE	CC1=CCC(CC1)C(C)(C)O
MOL000232	0.9322	0.0678	0.9688	Leonuri Fructus	()-alpha-Terpineol	442501	FALSE	CC1=CCC(CC1)C(C)(C)O
MOL000232	0.9322	0.0678	0.9688	Borneolum Syntheticum	()-alpha-Terpineol	442501	FALSE	CC1=CCC(CC1)C(C)(C)O
MOL000232	0.9322	0.0678	0.9688	Morindae Officinalis Radix	()-alpha-Terpineol	442501	FALSE	CC1=CCC(CC1)C(C)(C)O
MOL000232	0.9322	0.0678	0.9688	Rhododendri Daurici Folium	()-alpha-Terpineol	442501	FALSE	CC1=CCC(CC1)C(C)(C)O
MOL000232	0.9322	0.0678	0.9688	Viticis Fructus	()-alpha-Terpineol	442501	FALSE	CC1=CCC(CC1)C(C)(C)O
MOL000232	0.9322	0.0678	0.9688	Siphonostegiae Herba	()-alpha-Terpineol	442501	FALSE	CC1=CCC(CC1)C(C)(C)O
MOL000232	0.9322	0.0678	0.9688	Asari Radix Et Rhizoma	()-alpha-Terpineol	442501	FALSE	CC1=CCC(CC1)C(C)(C)O
MOL000232	0.9322	0.0678	0.9688	Notopterygii Rhizoma Et Radix	()-alpha-Terpineol	442501	FALSE	CC1=CCC(CC1)C(C)(C)O
MOL000232	0.9322	0.0678	0.9688	Thalluslaminariae	()-alpha-Terpineol	442501	FALSE	CC1=CCC(CC1)C(C)(C)O
MOL000232	0.9322	0.0678	0.9688	Ligustici Rhizoma Et Radix	()-alpha-Terpineol	442501	FALSE	CC1=CCC(CC1)C(C)(C)O
MOL000232	0.9322	0.0678	0.9688	Lonicerae Japonicae Flos	()-alpha-Terpineol	442501	FALSE	CC1=CCC(CC1)C(C)(C)O

MOL000232	0.9322	0.0678	0.9688	Radix Angelicae Biseratae	()-alpha-Terpineol	442501	FALSE	CC1=CCC(CC1)C(C)(C)O
MOL000232	0.9322	0.0678	0.9688	Angelicae Sinensis Radix	()-alpha-Terpineol	442501	FALSE	CC1=CCC(CC1)C(C)(C)O
MOL000232	0.9322	0.0678	0.9688	Herba Patriniae	()-alpha-Terpineol	442501	FALSE	CC1=CCC(CC1)C(C)(C)O
MOL000232	0.9322	0.0678	0.9688	Platycladi Cacumen	()-alpha-Terpineol	442501	FALSE	CC1=CCC(CC1)C(C)(C)O
MOL000233	0.9363	0.0637	0.9677	Schisandrae Chinensis Fructus	delta-Terpineol	81722	FALSE	C=C1CCC(CC1)C(C)(C)O
MOL000233	0.9363	0.0637	0.9677	Alpinia Katsumadai Hayat	delta-Terpineol	81722	FALSE	C=C1CCC(CC1)C(C)(C)O
MOL000233	0.9363	0.0637	0.9677	Radix Bupleuri	delta-Terpineol	81722	FALSE	C=C1CCC(CC1)C(C)(C)O
MOL000233	0.9363	0.0637	0.9677	Forsythiae Fructus	delta-Terpineol	81722	FALSE	C=C1CCC(CC1)C(C)(C)O
MOL000233	0.9363	0.0637	0.9677	Asari Radix Et Rhizoma	delta-Terpineol	81722	FALSE	C=C1CCC(CC1)C(C)(C)O
MOL000234	0.9512	0.0488	0.9585	Zingiber Officinale Roscoe	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Olibanun	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Myristicae Semen	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Citri Fructus Retinervus	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Styrax	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Citri Sarcodactylis Fructus	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Coriandri Sativi Herba	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Schizonepetae Herba	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Aristolochiae Fructus	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Dichroae Radix	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Linderae Radix	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Folium Artemisiae Argyi	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Piperis Fructus	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Litseae Fructus	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Rhapontici Radix	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Foeniculi Fructus	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Chuanxiong Rhizoma	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Kaempferiae Rhizoma	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Viticis Negundo Folium	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Glechomae Herba	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Arecae Semen	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Sinapis Semen	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C

MOL000234	0.9512	0.0488	0.9585	Viticis Fructus	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Aurantii Fructus Immaturus	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Cinnanmomi Cortex	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Celastri Orbiculati Fructus	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Cymbopon Citratus(D C.) Stapf	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Cinnamomi Ramulus	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Santalum Album L.	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Fructus Ligustri Lucidi	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Aurantii Fructus	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Herbahypericiperforati	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Citri Exocarpium Rubrum	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Pogostemon Cablin (Blanco) Benth.	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Cyperi Rhizoma	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Agrimonia Eupatoria	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Houttuyniae Herba	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Artemisia Annua L.	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Citri Fructus	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Menthae Herba	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Et Radix Patriniae Rhizoma	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Zanthoxyli Pericarpium	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Phellodendri Chinrnsis Cortex	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Sesami Nigrum Semen	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Semen Euphorbiae	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Citri Reticulatae Pericarpium Viride	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Citri Reticulatae Folium	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Mume Flos	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Alpiniae Officinarum Rhizome	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Nardostachyos Radix Et Rhizoma	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Solidaginis Herba	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Citrus Aurantium	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Ephedra Herba	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Homalomena Occulta (Lour.) Schott	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C

MOL000234	0.9512	0.0488	0.9585	Kadsurae Coccineae Radix Et Caulis	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Alpinia Katsumadai Hayat	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Citri Grandis Exocarpium	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Radix Bupleuri	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000234	0.9512	0.0488	0.9585	Curcumae Radix	L-Limonen	439250	FALSE	C1(=CCC(CC1)C(=C)C)C
MOL000235	0.5838	0.4162	0.7357	Alpinia Katsumadai Hayat	1,7-diphenyl-3,5-dihydroxy-1-heptene	Not Available	FALSE	C(=C\C(CC(CCc1ccccc1)O)O)\c1ccccc1
MOL000236	0.5240	0.4760	0.6844	Alpinia Katsumadai Hayat	1,7-diphenyl-4,6-heptadien-3-one	Not Available	FALSE	C(CC(=O)/C=C/C=C\c1ccccc1)c1ccccc1
MOL000237	0.5151	0.4849	0.7055	Alpinia Katsumadai Hayat	Trans-1,7-diphenyl-1-hepten-5-ol	44560846	FALSE	C(=C\CCC(CCc1ccccc1)O)/c1ccccc1
MOL000237	0.5151	0.4849	0.7055	Curcumae Radix	Trans-1,7-diphenyl-1-hepten-5-ol	44560846	FALSE	C(=C\CCC(CCc1ccccc1)O)/c1ccccc1
MOL000238	0.5123	0.4877	0.7386	Alpinia Katsumadai Hayat	1,7-diphenyl-5-hydroxy-6-hepten-3-one	57520989	FALSE	C(CC(=O)CC(/C=C/c1ccccc1)O)c1ccccc1
MOL000239	0.8866	0.1134	0.8210	Alpinia Katsumadai Hayat	Jaranol	5318869	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC)OC)c1ccc(cc1)O
MOL000239	0.8866	0.1134	0.8210	Hedysarum Multijugum Maxim.	Jaranol	5318869	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC)OC)c1ccc(cc1)O
MOL000239	0.8866	0.1134	0.8210	Dioscoreaebulbiferae	Jaranol	5318869	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC)OC)c1ccc(cc1)O
MOL000239	0.8866	0.1134	0.8210	licorice	Jaranol	5318869	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC)OC)c1ccc(cc1)O
MOL000239	0.8866	0.1134	0.8210	Moslae Herba	Jaranol	5318869	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC)OC)c1ccc(cc1)O
MOL000240	0.6166	0.3834	0.7592	Alpinia Katsumadai Hayat	(3R,5S)-1,7-di(phenyl)heptane-3,5-diol	21637670	FALSE	C(CC(CC(CCc1ccccc1)O)O)c1ccccc1
MOL000241	0.9148	0.0852	0.8974	Alpinia Katsumadai Hayat	2',4'-dihydroxy-6'-methhoxychalcone	Not Available	FALSE	C(=O)(/C=C\c1ccccc1)c1c(cc(cc1OC)O)O
MOL000242	0.9068	0.0932	0.9025	Alpinia Katsumadai Hayat	7-O-Methyleriodictyol	1268276	FALSE	C1(CC(=O)c2c(O1)cc(cc2O)OC)c1cc(c(cc1)O)O
MOL000242	0.9068	0.0932	0.9025	Ranunculi Ternati Radix	7-O-Methyleriodictyol	1268276	FALSE	C1(CC(=O)c2c(O1)cc(cc2O)OC)c1cc(c(cc1)O)O

MOL000243	0.8611	0.1389	0.7417	Alpinia Katsumadai Hayat	alpinolide peroxide	Not Available	FALSE	O1OC2(C3C(C1(C)O)CCC3C)OC(=O)C=C2C(C)C
MOL000244	0.9521	0.0479	0.8063	Viticis Fructus	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Fructus Ligustri Lucidi	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Herba Patriniae	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Kadsurae Coccineae Radix Et Caulis	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Moslae Herba	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Linderae Radix	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Kaempferiae Rhizoma	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Alpinia Katsumadai Hayat	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Curcumaelongae Rhizoma	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Zingiberis Rhizoma	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Cinnamomi Ramulus	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Stephaniae Tetrandrae Radix	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Cuscutae Semen	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Notoginseng Flos	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Magnoliae Flos	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Chrysanthemi Flos	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Cannabis Sativa L.	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Mahoniae Folum	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Aucklandiae Radix	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Epimrdii Herba	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Borneolum Syntheticum	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Morindae Officinalis Radix	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Rhizome Of Whiteback Greenbrier	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Hippophae Fructus	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Anemarrhenae Rhizoma	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Lysimachiae Foenigraeci Herba	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Coriandri Sativi Herba	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Mahoniae Caulis	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Et Radix Patriniae Rhizoma	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Menthae Herba	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Toosendan Fructus	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Ardisiae Japonicae Herba	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Radix Bupleuri	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Asari Radix Et Rhizoma	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Curcumae Rhizoma	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Gossampiniflos	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C

MOL000244	0.9521	0.0479	0.8063	Magnolia Officinalis Rehd Et Wils.	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000244	0.9521	0.0479	0.8063	Leonuri Fructus	()-Borneol	6552009	FALSE	C12(C(C(CC1O)CC2)(C)C)C
MOL000245	0.7725	0.2275	0.9681	Alpinia Katsumadai Hayat	Demethoxyyangonin	5273621	TRUE	c1(=O)cc(cc(o1)/C=C/c1ccccc1)OC
MOL000246	0.9121	0.0879	0.9154	Gypsophila Licentiana Hand.-Mazz.	(2R)-5,7-dihydroxy-2-phenylchroman-4-one	667544	FALSE	C1(CC(=O)c2c(O)cc(O)cc2O1)c1ccccc1
MOL000246	0.9121	0.0879	0.9154	Dalbergiae Odoriferae Lignum	(2R)-5,7-dihydroxy-2-phenylchroman-4-one	667544	FALSE	C1(CC(=O)c2c(O)cc(O)cc2O1)c1ccccc1
MOL000246	0.9121	0.0879	0.9154	Alpinia Katsumadai Hayat	(2R)-5,7-dihydroxy-2-phenylchroman-4-one	667544	FALSE	C1(CC(=O)c2c(O)cc(O)cc2O1)c1ccccc1
MOL000246	0.9121	0.0879	0.9154	Alpiniae Officinarum Rhizome	(2R)-5,7-dihydroxy-2-phenylchroman-4-one	667544	FALSE	C1(CC(=O)c2c(O)cc(O)cc2O1)c1ccccc1
MOL000247	0.8635	0.1365	0.8063	Momordicae Fructus	(Z,Z)-farnesol	1549107	FALSE	C(/C=C(/C)\CC/C=C(/C)\CCC=C(C)C)O
MOL000247	0.8635	0.1365	0.8063	Magnolia Officinalis Rehd Et Wils.	(Z,Z)-farnesol	1549107	FALSE	C(/C=C(/C)\CC/C=C(/C)\CCC=C(C)C)O
MOL000247	0.8635	0.1365	0.8063	Alpiniae Officinarum Rhizome	(Z,Z)-farnesol	1549107	FALSE	C(/C=C(/C)\CC/C=C(/C)\CCC=C(C)C)O
MOL000247	0.8635	0.1365	0.8063	Ephedra Herba	(Z,Z)-farnesol	1549107	FALSE	C(/C=C(/C)\CC/C=C(/C)\CCC=C(C)C)O
MOL000247	0.8635	0.1365	0.8063	Kadsurae Coccineae Radix Et Caulis	(Z,Z)-farnesol	1549107	FALSE	C(/C=C(/C)\CC/C=C(/C)\CCC=C(C)C)O
MOL000247	0.8635	0.1365	0.8063	Alpinia Katsumadai Hayat	(Z,Z)-farnesol	1549107	FALSE	C(/C=C(/C)\CC/C=C(/C)\CCC=C(C)C)O
MOL000247	0.8635	0.1365	0.8063	Perilla Frutescens	(Z,Z)-farnesol	1549107	FALSE	C(/C=C(/C)\CC/C=C(/C)\CCC=C(C)C)O
MOL000247	0.8635	0.1365	0.8063	Cinnanmomi Cortex	(Z,Z)-farnesol	1549107	FALSE	C(/C=C(/C)\CC/C=C(/C)\CCC=C(C)C)O
MOL000247	0.8635	0.1365	0.8063	Gossampiniflos	(Z,Z)-farnesol	1549107	FALSE	C(/C=C(/C)\CC/C=C(/C)\CCC=C(C)C)O
MOL000247	0.8635	0.1365	0.8063	Cinnamomi Ramulus	(Z,Z)-farnesol	1549107	FALSE	C(/C=C(/C)\CC/C=C(/C)\CCC=C(C)C)O
MOL000247	0.8635	0.1365	0.8063	Radix Bupleuri	(Z,Z)-farnesol	1549107	FALSE	C(/C=C(/C)\CC/C=C(/C)\CCC=C(C)C)O
MOL000247	0.8635	0.1365	0.8063	Citrus Aurantium	(Z,Z)-farnesol	1549107	FALSE	C(/C=C(/C)\CC/C=C(/C)\CCC=C(C)C)O
MOL000247	0.8635	0.1365	0.8063	Zingiberis Rhizoma	(Z,Z)-farnesol	1549107	FALSE	C(/C=C(/C)\CC/C=C(/C)\CCC=C(C)C)O
MOL000247	0.8635	0.1365	0.8063	Celastri Orbiculati Fructus	(Z,Z)-farnesol	1549107	FALSE	C(/C=C(/C)\CC/C=C(/C)\CCC=C(C)C)O
MOL000247	0.8635	0.1365	0.8063	Litchi Semen	(Z,Z)-farnesol	1549107	FALSE	C(/C=C(/C)\CC/C=C(/C)\CCC=C(C)C)O

MOL000248	0.9597	0.0403	0.9791	Alpinia Katsumadai Hayat	(5S)-5-isopropyl-2-methyl-1-cyclohex-2-enone	6432475	FALSE	C1(=O)C(=CCC(C1)C(C)C)C
MOL000249	0.9315	0.0685	0.9122	Styrax	Methylcinnamate	637520	FALSE	c1(/C=C/C(=O)OC)ccccc1
MOL000249	0.9315	0.0685	0.9122	Fructus Ligustri Lucidi	Methylcinnamate	637520	FALSE	c1(/C=C/C(=O)OC)ccccc1
MOL000249	0.9315	0.0685	0.9122	Alpinia Katsumadai Hayat	Methylcinnamate	637520	FALSE	c1(/C=C/C(=O)OC)ccccc1
MOL000249	0.9315	0.0685	0.9122	Carthami Flos	Methylcinnamate	637520	FALSE	c1(/C=C/C(=O)OC)ccccc1
MOL000249	0.9315	0.0685	0.9122	Alpiniae Officinarum Rhizome	Methylcinnamate	637520	FALSE	c1(/C=C/C(=O)OC)ccccc1
MOL000249	0.9315	0.0685	0.9122	Cinnanmomi Cortex	Methylcinnamate	637520	FALSE	c1(/C=C/C(=O)OC)ccccc1
MOL000249	0.9315	0.0685	0.9122	Trollius Chinensis	Methylcinnamate	637520	FALSE	c1(/C=C/C(=O)OC)ccccc1
MOL000249	0.9315	0.0685	0.9122	Benzoinum	Methylcinnamate	637520	FALSE	c1(/C=C/C(=O)OC)ccccc1
MOL000250	0.9278	0.0722	0.9097	Herba Taxilli	cis-Cinnamaldehyde	6428995	FALSE	c1(ccccc1)/C=C\C=O
MOL000250	0.9278	0.0722	0.9097	Cinnamomi Ramulus	cis-Cinnamaldehyde	6428995	FALSE	c1(ccccc1)/C=C\C=O
MOL000250	0.9278	0.0722	0.9097	Cinnanmomi Cortex	cis-Cinnamaldehyde	6428995	FALSE	c1(ccccc1)/C=C\C=O
MOL000250	0.9278	0.0722	0.9097	Alpinia Katsumadai Hayat	cis-Cinnamaldehyde	6428995	FALSE	c1(ccccc1)/C=C\C=O
MOL000250	0.9278	0.0722	0.9097	Pogostemon Cablin (Blanco) Benth.	cis-Cinnamaldehyde	6428995	FALSE	c1(ccccc1)/C=C\C=O
MOL000251	0.9214	0.0786	0.7918	Lysimachiae Herba	Rhamnocitrin	5320946	FALSE	c1(c(c(=O)c2c(cc(cc2o1)OC)O)O)c1ccc(cc1)O
MOL000251	0.9214	0.0786	0.7918	Astragali Cpmplanatisemen	Rhamnocitrin	5320946	FALSE	c1(c(c(=O)c2c(cc(cc2o1)OC)O)O)c1ccc(cc1)O
MOL000251	0.9214	0.0786	0.7918	Caryophylliflos	Rhamnocitrin	5320946	FALSE	c1(c(c(=O)c2c(cc(cc2o1)OC)O)O)c1ccc(cc1)O
MOL000251	0.9214	0.0786	0.7918	Belamcandae Rhizome	Rhamnocitrin	5320946	FALSE	c1(c(c(=O)c2c(cc(cc2o1)OC)O)O)c1ccc(cc1)O
MOL000251	0.9214	0.0786	0.7918	Eriobotryae Folium	Rhamnocitrin	5320946	FALSE	c1(c(c(=O)c2c(cc(cc2o1)OC)O)O)c1ccc(cc1)O
MOL000251	0.9214	0.0786	0.7918	Mume Fructus	Rhamnocitrin	5320946	FALSE	c1(c(c(=O)c2c(cc(cc2o1)OC)O)O)c1ccc(cc1)O

MOL000251	0.9214	0.0786	0.7918	Alpiniae Officinarum Rhizome	Rhamnocitrin	5320946	FALSE	c1(c(c(=O)c2c(cc(cc2o1)OC)O)O)c1ccc(cc1)O
MOL000251	0.9214	0.0786	0.7918	Artemisia Annua L.	Rhamnocitrin	5320946	FALSE	c1(c(c(=O)c2c(cc(cc2o1)OC)O)O)c1ccc(cc1)O
MOL000251	0.9214	0.0786	0.7918	Hedysarum Multijugum Maxim.	Rhamnocitrin	5320946	FALSE	c1(c(c(=O)c2c(cc(cc2o1)OC)O)O)c1ccc(cc1)O
MOL000251	0.9214	0.0786	0.7918	Alpinia Katsumadai Hayat	Rhamnocitrin	5320946	FALSE	c1(c(c(=O)c2c(cc(cc2o1)OC)O)O)c1ccc(cc1)O
MOL000251	0.9214	0.0786	0.7918	Iridis Tectori Rhizoma	Rhamnocitrin	5320946	FALSE	c1(c(c(=O)c2c(cc(cc2o1)OC)O)O)c1ccc(cc1)O
MOL000251	0.9214	0.0786	0.7918	Tamaricis Cacumen	Rhamnocitrin	5320946	FALSE	c1(c(c(=O)c2c(cc(cc2o1)OC)O)O)c1ccc(cc1)O
MOL000251	0.9214	0.0786	0.7918	Artemisiae Scopariae Herba	Rhamnocitrin	5320946	FALSE	c1(c(c(=O)c2c(cc(cc2o1)OC)O)O)c1ccc(cc1)O
MOL000252	0.8635	0.1365	0.8063	Ephedra Herba	farnesol	445070	FALSE	C(=C\CC/C(=C/CO)/C)(/CCC=C(C)C)\C
MOL000252	0.8635	0.1365	0.8063	Curcumae Radix	farnesol	445070	FALSE	C(=C\CC/C(=C/CO)/C)(/CCC=C(C)C)\C
MOL000252	0.8635	0.1365	0.8063	Ginkgo Folium	farnesol	445070	FALSE	C(=C\CC/C(=C/CO)/C)(/CCC=C(C)C)\C
MOL000252	0.8635	0.1365	0.8063	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	farnesol	445070	FALSE	C(=C\CC/C(=C/CO)/C)(/CCC=C(C)C)\C
MOL000252	0.8635	0.1365	0.8063	Lonicerae Japonicae Flos	farnesol	445070	FALSE	C(=C\CC/C(=C/CO)/C)(/CCC=C(C)C)\C
MOL000252	0.8635	0.1365	0.8063	Ardisiae Japonicae Herba	farnesol	445070	FALSE	C(=C\CC/C(=C/CO)/C)(/CCC=C(C)C)\C
MOL000252	0.8635	0.1365	0.8063	Eriobotryae Folium	farnesol	445070	FALSE	C(=C\CC/C(=C/CO)/C)(/CCC=C(C)C)\C
MOL000252	0.8635	0.1365	0.8063	Alpinia Katsumadai Hayat	farnesol	445070	FALSE	C(=C\CC/C(=C/CO)/C)(/CCC=C(C)C)\C
MOL000252	0.8635	0.1365	0.8063	Caryophylliflos	farnesol	445070	FALSE	C(=C\CC/C(=C/CO)/C)(/CCC=C(C)C)\C
MOL000252	0.8635	0.1365	0.8063	Folium Artemisiae Argyi	farnesol	445070	FALSE	C(=C\CC/C(=C/CO)/C)(/CCC=C(C)C)\C
MOL000252	0.8635	0.1365	0.8063	Flemingia Prostrata Roxb	farnesol	445070	FALSE	C(=C\CC/C(=C/CO)/C)(/CCC=C(C)C)\C
MOL000252	0.8635	0.1365	0.8063	Cinnamomi Ramulus	farnesol	445070	FALSE	C(=C\CC/C(=C/CO)/C)(/CCC=C(C)C)\C
MOL000253	0.9671	0.0329	0.8940	Alpiniae Officinarum Rhizome	Styrene, 3,4-dimethyl-	33937	FALSE	c1(c(cc(cc1)C=C)C)C
MOL000253	0.9671	0.0329	0.8940	Alpinia Katsumadai Hayat	Styrene, 3,4-dimethyl-	33937	FALSE	c1(c(cc(cc1)C=C)C)C
MOL000254	0.9585	0.0415	0.9546	Dianthi Herba	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Aurantii Fructus Immaturus	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Phragmitis Rhizoma	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Cistanches Herba	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Alpiniae Officinarum Rhizome	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Caryophylliflos	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Mume Fructus	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Magnolia Officinalis Rehd Et Wils.	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Cortex Moutan	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Perillae Fructus	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Magnoliae Flos	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Bombyx Mori L.	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC

MOL000254	0.9585	0.0415	0.9546	Citri Grandis Exocarpium	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Viticis Fructus	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Cinnanmomi Cortex	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Ginkgo Folium	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Lonicerae Japonicae Flos	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Rhizome Of Whiteback Greenbrier	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Myrrha	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Evodiae Fructus	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Zanthoxyli Pericarpium	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Scutellariae Radix	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Paederiae Scandentis Herba	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Bidentis Bipinnatae Herba	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Alpinia Katsumadai Hayat	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Chaenomeles Sinensis (Thouin) Koehne	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Junci Medulla	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Radix Bupleuri	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Siphonostegiae Herba	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Curcumae Radix	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Andrographis Herba	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Mori Follum	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Forsythiae Fructus	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Fructus Ligustri Lucidi	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Sennae Folium	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Gnaphalii Affinis Herba	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Mume Flos	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Puerariae Flos	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Artemisiae Scopariae Herba	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Perilla Frutescens	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Cinnamomi Ramulus	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Pogostemon Cablin (Blanco) Benth.	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000254	0.9585	0.0415	0.9546	Campsis Flos	eugenol	3314	FALSE	c1(cc(ccc1O)CC=C)OC
MOL000255	0.5565	0.4435	0.6146	Alpinia Katsumadai Hayat	Myristin	11148	FALSE	C(COC(=O)CCCCCCCCCCCCC)(COC(=O)CCCCCCCCCCCCC)OC(=O)CCCCCCCCCCCCC
MOL000257	0.9620	0.0380	0.9523	Aristolochiae Fructus	(-)-beta-Phellandrene	443161	FALSE	C1=CC(=C)CCC1C(C)C
MOL000257	0.9620	0.0380	0.9523	Olibanun	(-)-beta-Phellandrene	443161	FALSE	C1=CC(=C)CCC1C(C)C

MOL000257	0.9620	0.0380	0.9523	Alpinia Katsumadai Hayat	(-)-beta-Phellandrene	443161	FALSE	C1=CC(=C)CCC1C(C)C
MOL000257	0.9620	0.0380	0.9523	Piperis Fructus	(-)-beta-Phellandrene	443161	FALSE	C1=CC(=C)CCC1C(C)C
MOL000257	0.9620	0.0380	0.9523	Zanthoxyli Pericarpium	(-)-beta-Phellandrene	443161	FALSE	C1=CC(=C)CCC1C(C)C
MOL000257	0.9620	0.0380	0.9523	Canarii Fructus	(-)-beta-Phellandrene	443161	FALSE	C1=CC(=C)CCC1C(C)C
MOL000257	0.9620	0.0380	0.9523	Magnoliae Flos	(-)-beta-Phellandrene	443161	FALSE	C1=CC(=C)CCC1C(C)C
MOL000257	0.9620	0.0380	0.9523	Radix Salviae	(-)-beta-Phellandrene	443161	FALSE	C1=CC(=C)CCC1C(C)C
MOL000257	0.9620	0.0380	0.9523	Acoritataninowii Rhizoma	(-)-beta-Phellandrene	443161	FALSE	C1=CC(=C)CCC1C(C)C
MOL000257	0.9620	0.0380	0.9523	Ligustici Rhizoma Et Radix	(-)-beta-Phellandrene	443161	FALSE	C1=CC(=C)CCC1C(C)C
MOL000257	0.9620	0.0380	0.9523	Asari Radix Et Rhizoma	(-)-beta-Phellandrene	443161	FALSE	C1=CC(=C)CCC1C(C)C
MOL000257	0.9620	0.0380	0.9523	Curcumae Radix	(-)-beta-Phellandrene	443161	FALSE	C1=CC(=C)CCC1C(C)C
MOL000257	0.9620	0.0380	0.9523	Schizonepetae Herba	(-)-beta-Phellandrene	443161	FALSE	C1=CC(=C)CCC1C(C)C
MOL000258	0.4564	0.5436	0.8814	Alpinia Katsumadai Hayat	dehydrodiisoeugenol	Not Available	FALSE	C(=C\c1cc(c2c(c1)CC(O2)c1cc(c(cc1)O)OC)OC)/C
MOL000259	0.9718	0.0282	0.9453	Aucklandiae Radix	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Citrus Reticulata	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Lonicerae Japonicae Flos	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Campsis Flos	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Coriandri Sativi Herba	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Ardisiae Japonicae Herba	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Maydis Seigma	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Caryophylliflos	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Homalomena Occulta (Lour.) Schott	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Magnolia Officinalis Rehd Et Wils.	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Perilla Frutescens	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Rhizome Of Whiteback Greenbrier	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Radix Bupleuri	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Flemingia Prostrata Roxb	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Ligustici Rhizoma Et Radix	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O

MOL000259	0.9718	0.0282	0.9453	Angelicae Sinensis Radix	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Farfarae Flos	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Ephedra Herba	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Menthae Herba	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Andrographis Herba	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Lilii Bulbus	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Gynostemmae Pentaphylli Herba	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Alpinia Katsumadai Hayat	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Humulus Scandens (Lour.) Merr.	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Centipedae Herba	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Folium Artemisiae Argyi	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Curcumae Radix	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Radix Angelicae Biseratae	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000259	0.9718	0.0282	0.9453	Moslae Herba	o-Thymol	10364	FALSE	c1(c(ccc(c1)C(C)C)C)O
MOL000260	0.2693	0.7307	0.8993	Alpinia Katsumadai Hayat	5-[(2R,3R)-7-methoxy-3-methyl-5-[(E)-prop-1-enyl]-2,3-dihydrobenzofuran-2-yl]-1,3-benzodioxole	6441061	FALSE	c1(cc(c2c(c1)C(C(O2)c1cc2c(cc1)OCO2)C)OC)/C=C/C
MOL000261	0.9749	0.0251	0.8477	Crotonis Fructus	Myristicin	4276	FALSE	c12c(cc(cc1OC)CC=C)OCO2
MOL000261	0.9749	0.0251	0.8477	Jujubae Fructus	Myristicin	4276	FALSE	c12c(cc(cc1OC)CC=C)OCO2
MOL000261	0.9749	0.0251	0.8477	Cornus Officinalis Sieb. Et Zucc.	Myristicin	4276	FALSE	c12c(cc(cc1OC)CC=C)OCO2
MOL000261	0.9749	0.0251	0.8477	Codonopsis Radix	Myristicin	4276	FALSE	c12c(cc(cc1OC)CC=C)OCO2
MOL000261	0.9749	0.0251	0.8477	Benzoinum	Myristicin	4276	FALSE	c12c(cc(cc1OC)CC=C)OCO2
MOL000261	0.9749	0.0251	0.8477	Perilla Frutescens	Myristicin	4276	FALSE	c12c(cc(cc1OC)CC=C)OCO2
MOL000261	0.9749	0.0251	0.8477	Alpinia Katsumadai Hayat	Myristicin	4276	FALSE	c12c(cc(cc1OC)CC=C)OCO2
MOL000261	0.9749	0.0251	0.8477	Myristicae Semen	Myristicin	4276	FALSE	c12c(cc(cc1OC)CC=C)OCO2
MOL000261	0.9749	0.0251	0.8477	Magnoliae Flos	Myristicin	4276	FALSE	c12c(cc(cc1OC)CC=C)OCO2
MOL000261	0.9749	0.0251	0.8477	Croci Stigma	Myristicin	4276	FALSE	c12c(cc(cc1OC)CC=C)OCO2
MOL000261	0.9749	0.0251	0.8477	Asari Radix Et Rhizoma	Myristicin	4276	FALSE	c12c(cc(cc1OC)CC=C)OCO2
MOL000261	0.9749	0.0251	0.8477	Radix Cynanchi Paniculati	Myristicin	4276	FALSE	c12c(cc(cc1OC)CC=C)OCO2
MOL000261	0.9749	0.0251	0.8477	Ligustici Rhizoma Et Radix	Myristicin	4276	FALSE	c12c(cc(cc1OC)CC=C)OCO2

MOL000262	0.9480	0.0520	0.7421	Folium Artemisiae Argyi	(1R,4S)-1,7,7-trimethylbicyclo[2.2.1]hept-2-ene	20055133	FALSE	C1=CC2CCC1(C2(C)C)C
MOL000262	0.9480	0.0520	0.7421	Alpinia Katsumadai Hayat	(1R,4S)-1,7,7-trimethylbicyclo[2.2.1]hept-2-ene	20055133	FALSE	C1=CC2CCC1(C2(C)C)C
MOL000262	0.9480	0.0520	0.7421	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(1R,4S)-1,7,7-trimethylbicyclo[2.2.1]hept-2-ene	20055133	FALSE	C1=CC2CCC1(C2(C)C)C
MOL000263	0.7553	0.2447	0.9079	Potentillae Discoloris Herba	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Potentillae Chinensis Herba	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Humulus Scandens (Lour.) Merr.	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Smilax China	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Canarii Fructus	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Achyranthis Asperae Herba	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Paeoniae Radix Alba	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Cortex Periplocae Radicis	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Cornus Officinalis Sieb. Et Zucc.	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Cortex Moutan	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Aucklandiae Radix	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Eriobotryae Folium	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Mori Cortex	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Panacis Quinquefolii Radix	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Plantaginis Herba	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C

MOL000263	0.7553	0.2447	0.9079	Styrax	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Euonymi Alati Ramulus	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Rosae Laevigatae Fructus	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Omphalia	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Alpinia Katsumadai Hayat	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Epimrdii Herba	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Pogostemon Cablin (Blanco) Benth.	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Et Radix Patriniae Rhizoma	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Sedum Aizoon L.	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Radix Clematidis	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Verbenae Herb	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Akebiae Frucyus	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Cotyledon Fimbriata Turcz.	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Caryophylliflos	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Uncariae Ramulus Cumuncis	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Foeniculi Fructus	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Gentianae Radix Et Rhozima	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Rubia Cordifolia	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Paederiae Scandentis Herba	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Chaenomeles Sinensis (Thouin) Koehne	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Kochiae Fructus	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C

MOL000263	0.7553	0.2447	0.9079	Fructus Ligustri Lucidi	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Nardostachyos Radix Et Rhizoma	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Asteris Radix Et Rhizoma	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Gentiana Macrophylla Pall	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Radix Salviae	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Bovis Calculus	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	licorice	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Salviae Chinensis Herba	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Cyperi Rhizoma	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Pulsatilliae Radix	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Achyranthis Bidentatae Radix	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Fructuslipuidambaris	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Viscum Angulatum Heyne	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Benzoinum	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Hydnocarpi Anthelminticae Semen	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Lonicerae Japonicae Flos	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Lysimachiae Foenigraeci Herba	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Momordicae Semen	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Folium Ilicis Cornutae	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Ardisiae Japonicae Herba	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Menthae Herba	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C

MOL000263	0.7553	0.2447	0.9079	Plantaginis Semen	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Hippophae Fructus	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Granati Pericarpium	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Borneolum Syntheticum	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Celosiae Semen	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Lithospermum Erythrorhizon	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Schizonepetae Herba	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Gossampiniflos	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Glechomae Herba	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Kaki Calyx	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Herba Pyrolae	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Herba Patriniae	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Abri Herba	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Prunellae Spica	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Clematidis Armandii Caulis	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Rubi Fructus	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Polygoni Cuspidati Rhizoma Et Radix	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Herba Taxilli	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Mori Cortex	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Campsis Flos	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Mume Fructus	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C

MOL000263	0.7553	0.2447	0.9079	Ampelopsis Japonica	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Evodiae Fructus	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Cyathulae Radix	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Phragmitis Rhizoma	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Swertiae Mileensis Herba	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Phytolaccae Radix	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Forsythiae Fructus	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Jujubae Fructus	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000263	0.7553	0.2447	0.9079	Ilicis Cornutae Folium Immayuri	oleanolic acid	10494	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL000264	0.9488	0.0512	0.9594	Viticis Fructus	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Alpinia Katsumadai Hayat	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Cnidii Fructus	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Lilii Bulbus	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Citri Sarcodactylis Fructus	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Zingiberis Rhizoma	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Radix Angelicae Biseratae	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Curcumae Radix	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Schisandrae Chinensis Fructus	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Styrax	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Flemingia Prostrata Roxb	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Zingiber Officinale Roscoe	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Kadsurae Coccineae Radix Et Caulis	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Asari Radix Et Rhizoma	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Alpiniae Officinarum Rhizome	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Magnoliae Flos	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Chuanxiong Rhizoma	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Campsis Flos	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Citri Fructus	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C

MOL000264	0.9488	0.0512	0.9594	Viticis Negundo Folium	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Myrrha	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Schizonepetae Herba	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Piperis Fructus	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Magnolia Officinalis Rehd Et Wils.	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Platycladi Cacumen	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Peucedani Radix	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Rhizome Of Whiteback Greenbrier	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Folium Artemisiae Argyi	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Aucklandiae Radix	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Ligustici Rhizoma Et Radix	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Citrus Aurantium	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000264	0.9488	0.0512	0.9594	Olibanun	Tereben	11463	FALSE	C1(=C(C)C)CCC(=CC1)C
MOL000265	0.9594	0.0406	0.8527	Acoritataninowii Rhizoma	ISOELEMICIN	5318557	FALSE	c1(c(cc(cc1OC)/C=C/C)OC)OC
MOL000265	0.9594	0.0406	0.8527	Alpinia Katsumadai Hayat	ISOELEMICIN	5318557	FALSE	c1(c(cc(cc1OC)/C=C/C)OC)OC
MOL000267	0.9310	0.0690	0.9422	Rose Rugosae Flos	beta-Citronellol	101977	FALSE	C(CCC=C(C)C)(CCO)C
MOL000267	0.9310	0.0690	0.9422	Alpinia Katsumadai Hayat	beta-Citronellol	101977	FALSE	C(CCC=C(C)C)(CCO)C
MOL000267	0.9310	0.0690	0.9422	Lonicerae Japonicae Flos	beta-Citronellol	101977	FALSE	C(CCC=C(C)C)(CCO)C
MOL000267	0.9310	0.0690	0.9422	Cymbopon Citratus(D C.) Stapf	beta-Citronellol	101977	FALSE	C(CCC=C(C)C)(CCO)C
MOL000267	0.9310	0.0690	0.9422	Zingiberis Rhizoma	beta-Citronellol	101977	FALSE	C(CCC=C(C)C)(CCO)C
MOL000267	0.9310	0.0690	0.9422	Coriandri Sativi Herba	beta-Citronellol	101977	FALSE	C(CCC=C(C)C)(CCO)C
MOL000267	0.9310	0.0690	0.9422	Citrus Aurantium	beta-Citronellol	101977	FALSE	C(CCC=C(C)C)(CCO)C
MOL000267	0.9310	0.0690	0.9422	Zingiber Officinale Roscoe	beta-Citronellol	101977	FALSE	C(CCC=C(C)C)(CCO)C
MOL000267	0.9310	0.0690	0.9422	Ephedra Herba	beta-Citronellol	101977	FALSE	C(CCC=C(C)C)(CCO)C
MOL000267	0.9310	0.0690	0.9422	Folium Artemisiae Argyi	beta-Citronellol	101977	FALSE	C(CCC=C(C)C)(CCO)C

MOL000267	0.9310	0.0690	0.9422	Schisandrae Chinensis Fructus	beta-Citronellol	101977	FALSE	C(CCC=C(C)C)(CCO)C
MOL000267	0.9310	0.0690	0.9422	Capsici Fructus	beta-Citronellol	101977	FALSE	C(CCC=C(C)C)(CCO)C
MOL000267	0.9310	0.0690	0.9422	Aucklandiae Radix	beta-Citronellol	101977	FALSE	C(CCC=C(C)C)(CCO)C
MOL000267	0.9310	0.0690	0.9422	Perillae Fructus	beta-Citronellol	101977	FALSE	C(CCC=C(C)C)(CCO)C
MOL000268	0.9619	0.0381	0.7610	Gossampiniflos	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Alpinia Katsumadai Hayat	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Citrus Reticulata	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Zingiber Officinale Roscoe	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Anisi Stellati Fructus	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Platycladi Cacumen	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Rhododendri Daurici Folium	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C

MOL000268	0.9619	0.0381	0.7610	Magnoliae Flos	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Viticis Fructus	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Piperis Fructus	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Fructus Carotae	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Notopterygii Rhizoma Et Radix	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Bidentis Bipinnatae Herba	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Myrrha	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Chuanxiong Rhizoma	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C

MOL000268	0.9619	0.0381	0.7610	Zanthoxyli Pericarpium	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Aurantii Fructus Immaturus	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Zingiberis Rhizoma	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Cayratiae Japonicae Herba	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Acoritataninowii Rhizoma	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Asari Radix Et Rhizoma	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Homalomena Occulta (Lour.) Schott	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Ligustici Rhizoma Et Radix	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C

MOL000268	0.9619	0.0381	0.7610	Viticis Cannabifoliae Fructus	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Evodiae Fructus	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Forsythiae Fructus	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Schizonepetae Herba	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Foeniculi Fructus	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Ephedra Herba	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Alpiniae Officinarum Rhizome	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Viticis Negundo Folium	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C

MOL000268	0.9619	0.0381	0.7610	Rubi Fructus	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Dichroae Radix	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Kaempferiae Rhizoma	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Curcumae Rhizoma	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Folium Artemisiae Argyi	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Sesami Nigrum Semen	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000268	0.9619	0.0381	0.7610	Piperis Longi Fructus	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C

MOL000268	0.9619	0.0381	0.7610	Semen Pharbitidis	(1S,5S)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	11051711	FALSE	C12(C(C1)C(=C)CC2)C(C)C
MOL000269	0.9565	0.0435	0.8564	Fructus Carotae	Elemicin	10248	FALSE	c1(c(cc(cc1OC)CC=C)OC)OC
MOL000269	0.9565	0.0435	0.8564	Acoritataninowii Rhizoma	Elemicin	10248	FALSE	c1(c(cc(cc1OC)CC=C)OC)OC
MOL000269	0.9565	0.0435	0.8564	Caryophylliflos	Elemicin	10248	FALSE	c1(c(cc(cc1OC)CC=C)OC)OC
MOL000269	0.9565	0.0435	0.8564	Magnoliae Flos	Elemicin	10248	FALSE	c1(c(cc(cc1OC)CC=C)OC)OC
MOL000269	0.9565	0.0435	0.8564	Schisandrae Chinensis Fructus	Elemicin	10248	FALSE	c1(c(cc(cc1OC)CC=C)OC)OC
MOL000269	0.9565	0.0435	0.8564	Myristicae Semen	Elemicin	10248	FALSE	c1(c(cc(cc1OC)CC=C)OC)OC
MOL000269	0.9565	0.0435	0.8564	Campsis Flos	Elemicin	10248	FALSE	c1(c(cc(cc1OC)CC=C)OC)OC
MOL000269	0.9565	0.0435	0.8564	Asari Radix Et Rhizoma	Elemicin	10248	FALSE	c1(c(cc(cc1OC)CC=C)OC)OC
MOL000269	0.9565	0.0435	0.8564	Eriobotryae Folium	Elemicin	10248	FALSE	c1(c(cc(cc1OC)CC=C)OC)OC
MOL000269	0.9565	0.0435	0.8564	Alpinia Katsumadai Hayat	Elemicin	10248	FALSE	c1(c(cc(cc1OC)CC=C)OC)OC
MOL000269	0.9565	0.0435	0.8564	Panax Ginseng C. A. Mey.	Elemicin	10248	FALSE	c1(c(cc(cc1OC)CC=C)OC)OC
MOL000269	0.9565	0.0435	0.8564	Ligustici Rhizoma Et Radix	Elemicin	10248	FALSE	c1(c(cc(cc1OC)CC=C)OC)OC
MOL000269	0.9565	0.0435	0.8564	Citri Grandis Exocarpium	Elemicin	10248	FALSE	c1(c(cc(cc1OC)CC=C)OC)OC
MOL000269	0.9565	0.0435	0.8564	Perilla Frutescens	Elemicin	10248	FALSE	c1(c(cc(cc1OC)CC=C)OC)OC
MOL000269	0.9565	0.0435	0.8564	Cornus Officinalis Sieb. Et Zucc.	Elemicin	10248	FALSE	c1(c(cc(cc1OC)CC=C)OC)OC
MOL000269	0.9565	0.0435	0.8564	Schizonepetae Herba	Elemicin	10248	FALSE	c1(c(cc(cc1OC)CC=C)OC)OC
MOL000270	0.9541	0.0459	0.7681	Bidentis Bipinnatae Herba	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Forsythiae Fructus	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Homalomena Occulta (Lour.) Schott	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Alpiniae Officinarum Rhizome	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Calyx Seu Fructus Physalis	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Citrus Aurantium	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Angelicae Sinensis Radix	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Magnolia Officinalis Rehd Et Wils.	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Kaempferiae Rhizoma	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Chuanxiong Rhizoma	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Borneolum Syntheticum	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Anisi Stellati Fructus	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Lignum Pini Nodi	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Ligustici Rhizoma Et Radix	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Piperis Longi Fructus	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C

MOL000270	0.9541	0.0459	0.7681	Evodiae Fructus	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Alpinia Katsumadai Hayat	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Curcumae Radix	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Piperis Fructus	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Artemisia Annua L.	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Notopterygii Rhizoma Et Radix	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Myrrha	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Nardostachyos Radix Et Rhizoma	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Radix Bupleuri	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Olibanun	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Coriandri Sativi Herba	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Litseae Fructus	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000270	0.9541	0.0459	0.7681	Dichroae Radix	CHEBI:7	443156	FALSE	C12C(C1(C)C)CC(=CC2)C
MOL000271	0.9587	0.0413	0.9777	Magnolia Officinalis Rehd Et Wils.	l-carvone	439570	FALSE	C1(CC(=O)C(=CC1)C)C(=C)C
MOL000271	0.9587	0.0413	0.9777	Piperis Fructus	l-carvone	439570	FALSE	C1(CC(=O)C(=CC1)C)C(=C)C
MOL000271	0.9587	0.0413	0.9777	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	l-carvone	439570	FALSE	C1(CC(=O)C(=CC1)C)C(=C)C
MOL000271	0.9587	0.0413	0.9777	Evodiae Fructus	l-carvone	439570	FALSE	C1(CC(=O)C(=CC1)C)C(=C)C
MOL000271	0.9587	0.0413	0.9777	Folium Artemisiae Argyi	l-carvone	439570	FALSE	C1(CC(=O)C(=CC1)C)C(=C)C
MOL000271	0.9587	0.0413	0.9777	Ganoderma	l-carvone	439570	FALSE	C1(CC(=O)C(=CC1)C)C(=C)C
MOL000271	0.9587	0.0413	0.9777	Alpinia Katsumadai Hayat	l-carvone	439570	FALSE	C1(CC(=O)C(=CC1)C)C(=C)C
MOL000271	0.9587	0.0413	0.9777	Olibanun	l-carvone	439570	FALSE	C1(CC(=O)C(=CC1)C)C(=C)C
MOL000271	0.9587	0.0413	0.9777	Radix Bupleuri	l-carvone	439570	FALSE	C1(CC(=O)C(=CC1)C)C(=C)C

MOL000273	0.6210	0.3790	0.7634	Poria Cocos(Schw.) Wolf.	(2R)-2-[(3S,5R,10S,13R,14R,16R,17R)-3,16-dihydroxy-4,4,10,13,14-pentamethyl-2,3,5,6,12,15,16,17-octahydro-1H-cyclopenta[a]phenanthren-17-yl]-6-methylhept-5-enoic acid	10743008	FALSE	C1(CCC2(C(C1(C)C)CC=C1C3(C)CC(C(C(CCC=C(C)C)C(=O)O)C3(C)CC=C21)O)C)O
MOL000274	0.5895	0.4105	0.7779	Poria Cocos(Schw.) Wolf.	3β-hydroxylanosta-7,9(11),24-trien-21-oic acid	15391340	FALSE	C1(CCC2(C(C1(C)C)CC=C1C3(C)CCC(C(CCC=C(C)C)C(=O)O)C3(C)CC=C21)C)O
MOL000275	0.5904	0.4096	0.7867	Poria Cocos(Schw.) Wolf.	trametenolic acid	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1=C2CCC2(C1(C)CCC2C(CCC=C(C)C)C(=O)O)C)C)O
MOL000276	0.5365	0.4635	0.7530	Poria Cocos(Schw.) Wolf.	7,9(11)-dehydropachymic acid	15226717	FALSE	C1(CCC2(C(C1(C)C)CC=C1C3(C)CC(C(C(CCC(=C)C(C)C)C(=O)O)C3(C)CC=C21)O)C)OC(=O)C
MOL000277	0.5711	0.4289	0.7507	Poria Cocos(Schw.) Wolf.	tumulosic acid	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1=C2CCC2(C1(C)CC(C2C(CCC(=C)C(C)C)C(=O)O)O)C)C)O
MOL000278	0.8756	0.1244	0.7506	Poria Cocos(Schw.) Wolf.	Beta-Glucan	Not Available	FALSE	C1(C(C(OC2C(C(OC(C2O)C)CO)O)OC(C1O)CO)O)OC1C(C(C(C(O1)CO)O)OC)O
MOL000279	0.2521	0.7479	0.6554	Polyporus Umbellatus(Pers)Fr.	Cerevisterol	10181133	FALSE	C1(CCC2(C(C1)(C(C=C1C3CCC(C(/C=C/C(C)C(C)C)C)C3(C)CCC21)O)O)C)O
MOL000279	0.2521	0.7479	0.6554	Ganoderma	Cerevisterol	10181133	FALSE	C1(CCC2(C(C1)(C(C=C1C3CCC(C(/C=C/C(C)C(C)C)C)C3(C)CCC21)O)O)C)O
MOL000279	0.2521	0.7479	0.6554	Poria Cocos(Schw.) Wolf.	Cerevisterol	10181133	FALSE	C1(CCC2(C(C1)(C(C=C1C3CCC(C(/C=C/C(C)C(C)C)C)C3(C)CCC21)O)O)C)O

MOL000280	0.5958	0.4042	0.7582	Poria Cocos(Schw.) Wolf.	(2R)-2-[(3S,5R,10S,13R,14R,16R,17R)-3,16-dihydroxy-4,4,10,13,14-pentamethyl-2,3,5,6,12,15,16,17-octahydro-1H-cyclopenta[a]phenanthren-17-yl]-5-isopropyl-hex-5-enoic acid	15225964	FALSE	C1=C2C(=CCC3C2(CCC(C3(C)C)O)C)C2(C(C1)(C(C(C2)O)C(C(=O)O)CCC(=C)C(C)C)C)C
MOL000281	0.9366	0.0634	0.9594	Poria Cocos(Schw.) Wolf.	Dimethyl L-malate	10285815	FALSE	C(=O)(C(O)CC(=O)OC)OC
MOL000283	0.2803	0.7197	0.7153	Poria Cocos(Schw.) Wolf.	Ergosterol peroxide	Not Available	FALSE	C1CC2C3(CC1O)C=CC1(C2(CCC2(C1CCC2C(CCC(C)C(C)C)C)C)C)OO3
MOL000284	0.9341	0.0659	0.8962	Poria Cocos(Schw.) Wolf.	L-uridine	40428662	FALSE	c1(=O)[nH]c(=O)ccn1C1C(O)C(O)C(O1)CO
MOL000285	0.5865	0.4135	0.7682	Poria Cocos(Schw.) Wolf.	(2R)-2-[(5R,10S,13R,14R,16R,17R)-16-hydroxy-3-keto-4,4,10,13,14-pentamethyl-1,2,5,6,12,15,16,17-octahydrocyclopenta[a]phenanthren-17-yl]-5-isopropyl-hex-5-enoic acid	9805290	FALSE	C1(=O)CCC2(C(C1(C)C)CC=C1C3(C)CC(C(C(CCC(=C)C(C)C)C(=O)O)C3(C)CC=C21)O)C
MOL000286	0.3289	0.6711	0.7461	Carthami Flos	β-amyrin acetate	51398127	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C)(C)CC4C3=CCC21)C)OC(=O)C
MOL000286	0.3289	0.6711	0.7461	Forsythiae Fructus	β-amyrin acetate	51398127	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C)(C)CC4C3=CCC21)C)OC(=O)C

MOL000286	0.3289	0.6711	0.7461	Cortex Periplocae Radicis	β-amyrin acetate	51398127	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C)(C)CC4C3=CCC21)C)OC(=O)C
MOL000286	0.3289	0.6711	0.7461	Myrrha	β-amyrin acetate	51398127	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C)(C)CC4C3=CCC21)C)OC(=O)C
MOL000286	0.3289	0.6711	0.7461	Poria Cocos(Schw.) Wolf.	β-amyrin acetate	51398127	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C)(C)CC4C3=CCC21)C)OC(=O)C
MOL000287	0.5389	0.4611	0.7422	Poria Cocos(Schw.) Wolf.	3beta-Hydroxy-24-methylene-8-lanostene-21-oic acid	73402	FALSE	C12(C3=C(C4(C(CC3)C(C(CC4)O)(C)C)C)CCC1(C(CC2)C(CCC(=C)C(C)C)C(=O)O)C)C
MOL000288	0.8989	0.1011	0.7769	Poria Cocos(Schw.) Wolf.	pachyman	Not Available	FALSE	C1(C(C(OC2C(C(OC(C2O)C)CO)O)OC(C1O)CO)O)OC1OC(C(C(C1O)C)O)CO
MOL000289	0.5744	0.4256	0.7594	Poria Cocos(Schw.) Wolf.	pachymic acid	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1=C2CCC2(C1(C)CC(C2C(CCC(=C)C(C)C)C(=O)O)O)C)C)OC(=O)C
MOL000290	0.4848	0.5152	0.6236	Poria Cocos(Schw.) Wolf.	Poricoic acid A	5471851	FALSE	C1(C(CC2(C3=CCC(C(C3=CCC12C)(CCC(=O)O)C)C(=C)C)C)O)C(CCC(=C)C(C)C)C(=O)O
MOL000291	0.5009	0.4991	0.6052	Poria Cocos(Schw.) Wolf.	Poricoic acid B	5471852	FALSE	C1=C2C(=CCC3(C2(CC(C3C(C(=O)O)CCC=C(C)C)O)C)C)C(C(C1)C(=C)C)(CCC(=O)O)C
MOL000292	0.4752	0.5248	0.6196	Poria Cocos(Schw.) Wolf.	poricoic acid C	56668247	FALSE	C1(CCC2(C3=CCC(C(C3=CCC12C)(CCC(=O)O)C)C(=C)C)C)C(CCC(=C)C(C)C)C(=O)O
MOL000297	0.5711	0.4289	0.7507	Poria Cocos(Schw.) Wolf.	Tumulosic acid	12314446	FALSE	C12(C(C(C(C2)O)C(CCC(=C)C(C)C)C(=O)O)(CCC2=C1CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000298	0.2032	0.7968	0.6108	Omphalia	ergosterol	444679	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC23)C1)C)O
MOL000298	0.2032	0.7968	0.6108	Bombyx Mori L.	ergosterol	444679	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC23)C1)C)O
MOL000298	0.2032	0.7968	0.6108	Coriolus	ergosterol	444679	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC23)C1)C)O
MOL000298	0.2032	0.7968	0.6108	Coicis Semen	ergosterol	444679	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC23)C1)C)O
MOL000298	0.2032	0.7968	0.6108	Rhizoma Dioscoreae	ergosterol	444679	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC23)C1)C)O
MOL000298	0.2032	0.7968	0.6108	Ganoderma	ergosterol	444679	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC23)C1)C)O
MOL000298	0.2032	0.7968	0.6108	Clematidis Armandii Caulis	ergosterol	444679	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC23)C1)C)O
MOL000298	0.2032	0.7968	0.6108	Polyporus Umbellatus(Pers)Fr.	ergosterol	444679	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC23)C1)C)O
MOL000298	0.2032	0.7968	0.6108	Corayceps	ergosterol	444679	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC23)C1)C)O
MOL000298	0.2032	0.7968	0.6108	Bovis Calculus	ergosterol	444679	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC23)C1)C)O

MOL000298	0.2032	0.7968	0.6108	Pulsatilliae Radix	ergosterol	444679	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC23)C1)C)O
MOL000298	0.2032	0.7968	0.6108	Smilax China	ergosterol	444679	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC23)C1)C)O
MOL000298	0.2032	0.7968	0.6108	Choerospondiatis Fructus	ergosterol	444679	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC23)C1)C)O
MOL000298	0.2032	0.7968	0.6108	Semen Aesculi	ergosterol	444679	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC23)C1)C)O
MOL000298	0.2032	0.7968	0.6108	Poria Cocos(Schw.) Wolf.	ergosterol	444679	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC23)C1)C)O
MOL000298	0.2032	0.7968	0.6108	Cannabis Sativa L.	ergosterol	444679	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC23)C1)C)O
MOL000299	0.9346	0.0654	0.9261	Mume Fructus	Trimethyl citrate	74112	FALSE	C(C(CC(=O)OC)(C(=O)OC)O)C(=O)OC
MOL000299	0.9346	0.0654	0.9261	Poria Cocos(Schw.) Wolf.	Trimethyl citrate	74112	FALSE	C(C(CC(=O)OC)(C(=O)OC)O)C(=O)OC
MOL000300	0.5766	0.4234	0.7545	Poria Cocos(Schw.) Wolf.	dehydroeburicoic acid	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC=C1C2=CCC2(C1CCC2C(C(=O)O)CCC(=C)C(C)C)C)C)O
MOL000301	0.9062	0.0938	0.8710	Abutili Semen	2-lauroleic acid	5282729	FALSE	C(=O)(/C=C/CCCCCCCCC)O
MOL000301	0.9062	0.0938	0.8710	Sophora Japonica L.	2-lauroleic acid	5282729	FALSE	C(=O)(/C=C/CCCCCCCCC)O
MOL000301	0.9062	0.0938	0.8710	Poria Cocos(Schw.) Wolf.	2-lauroleic acid	5282729	FALSE	C(=O)(/C=C/CCCCCCCCC)O
MOL000301	0.9062	0.0938	0.8710	Arecae Semen	2-lauroleic acid	5282729	FALSE	C(=O)(/C=C/CCCCCCCCC)O
MOL000301	0.9062	0.0938	0.8710	Linderae Radix	2-lauroleic acid	5282729	FALSE	C(=O)(/C=C/CCCCCCCCC)O
MOL000302	0.9124	0.0876	0.9045	Poria Cocos(Schw.) Wolf.	Undekansaeure	8180	FALSE	C(=O)(CCCCCCCCCC)O
MOL000302	0.9124	0.0876	0.9045	Chuanxiong Rhizoma	Undekansaeure	8180	FALSE	C(=O)(CCCCCCCCCC)O
MOL000302	0.9124	0.0876	0.9045	Portulacae Herba	Undekansaeure	8180	FALSE	C(=O)(CCCCCCCCCC)O
MOL000302	0.9124	0.0876	0.9045	Radix Bupleuri	Undekansaeure	8180	FALSE	C(=O)(CCCCCCCCCC)O
MOL000302	0.9124	0.0876	0.9045	Momordicae Fructus	Undekansaeure	8180	FALSE	C(=O)(CCCCCCCCCC)O
MOL000302	0.9124	0.0876	0.9045	Santalum Album L.	Undekansaeure	8180	FALSE	C(=O)(CCCCCCCCCC)O
MOL000302	0.9124	0.0876	0.9045	Actinidia Chinensis Planch	Undekansaeure	8180	FALSE	C(=O)(CCCCCCCCCC)O

MOL000302	0.9124	0.0876	0.9045	Tamaricis Cacumen	Undekansaeure	8180	FALSE	C(=O)(CCCCCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Hippophae Fructus	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Arisaematis Rhizoma	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Oroxyli Semen	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Citrus Aurantium	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Panacis Japonici Rhizoma	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Malvae Fructus	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Gynostemmae Pentaphylli Herba	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Campsis Flos	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Semen Euphorbiae	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Ganoderma	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Croci Stigma	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Panacis Quinquefolii Radix	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Rubi Fructus	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Crotonis Fructus	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Radix Bupleuri	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Poria Cocos(Schw.) Wolf.	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Typhonii Rhizoma	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Coicis Semen	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Magnolia Officinalis Rehd Et Wils.	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Eriobotryae Folium	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Mori Fructus	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Ephedra Herba	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Ginkgo Semen	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Capsici Fructus	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Calyx Seu Fructus Physalis	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Radix Cynanchi Paniculati	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Achyranthis Bidentatae Radix	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Codonopsis Radix	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Tamaricis Cacumen	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Canarii Fructus	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Semiaquilegiae Radix	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Phyllanthi Fructus	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Portulacae Herba	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Lonicerae Japonicae Flos	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Ilicis Purpureae Folium	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O

MOL000303	0.9240	0.0760	0.9549	Ginkgo Folium	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Radix Clematidis	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Meliae Azedarach Fructus	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000303	0.9240	0.0760	0.9549	Morindae Officinalis Radix	caprylic acid	379	FALSE	C(=O)(CCCCCCC)O
MOL000304	0.9292	0.0708	0.9347	Poria Cocos(Schw.) Wolf.	Ethyl glucoside	121667	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)CC
MOL000305	0.9050	0.0950	0.8730	Lysimachiae Foenigraeci Herba	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Poria Cocos(Schw.) Wolf.	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Campsis Flos	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Ganoderma	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Leonuri Herba	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Crotonis Fructus	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Trollius Chinensis	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Croci Stigma	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Rehmanniae Radix Praeparata	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Lycii Fructus	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Agrimonia Eupatoria	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Arecae Semen	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Quisqualis Indica	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Lonicerae Japonicae Flos	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Epimrdii Herba	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Mahoniae Caulis	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Junci Medulla	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Platycladi Semen	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Citri Sarcodactylis Fructus	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Platycladi Cacumen	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Paederiae Scandentis Herba	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Tamaricis Cacumen	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Scutellariae Barbatae Herba	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Codonopsis Radix	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Portulacae Herba	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Oroxyli Semen	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Amygdalus Communis Vas	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Polygonati Odorati Rhizoma	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Ginkgo Folium	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Allium Azureum Ledeb.	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Gossampiniflos	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Herbahypericiperforati	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Rhododendri Daurici Folium	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O

MOL000305	0.9050	0.0950	0.8730	Radix Bupleuri	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Cornus Officinalis Sieb. Et Zucc.	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Zingiber Officinale Roscoe	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Glechomae Herba	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Mori Cortex	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Broussonetiae Fructus	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Trichosanthes Kirilowii Maxim	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Morindae Officinalis Radix	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Aloe	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Folium Ilicis Cornutae	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Mume Fructus	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Carthami Flos	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Cortex Hibisci	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Millettiae Speciosae Radix	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Ephedra Herba	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Linderae Radix	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Prunellae Spica	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Momordicae Fructus	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Olibanun	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Hippophae Fructus	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Ardisiae Japonicae Herba	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000305	0.9050	0.0950	0.8730	Citrus Reticulata	lauric acid	3893	FALSE	C(=O)(CCCCCCCCCCC)O
MOL000307	0.7991	0.2009	0.7212	Caulis Piperis Kadsurae	aristololactam A IIIa	Not Available	FALSE	COc1c(cc2c3c(cc4ccc(cc4c13)O)[nH]c2=O)O
MOL000308	0.3893	0.6107	0.8281	Caulis Piperis Kadsurae	(2R,3R,3aS)-3a-allyl-2-(1,3-benzodioxol-5-yl)-5-methoxy-3-methyl-2,3-dihydrobenzofuran-6-one	21722980	FALSE	CC1C(OC2=CC(=O)C(=CC12CC=C)OC)c1cc2c(cc1)OCO2
MOL000309	0.3664	0.6336	0.8548	Magnoliae Flos	denudatin,a	13336517	FALSE	c12c(ccc(c1)C1OC3=CC(=O)C(=CC3(C1C)OC)CC=C)OCO2
MOL000309	0.3664	0.6336	0.8548	Rhizoma Dioscoreae	denudatin,a	13336517	FALSE	c12c(ccc(c1)C1OC3=CC(=O)C(=CC3(C1C)OC)CC=C)OCO2

MOL000309	0.3664	0.6336	0.8548	Caulis Piperis Kadsurae	denudatin,a	13336517	FALSE	c12c(ccc(c1)C1OC3=CC(=O)C(=CC3(C1C)OC)CC=C)OCO2
MOL000310	0.3320	0.6680	0.8592	Magnoliae Flos	Denudatin B	442834	FALSE	c1c(c(ccc1C1OC2=CC(=O)C(=CC2(C1C)OC)CC=C)OC)OC
MOL000310	0.3320	0.6680	0.8592	Caulis Piperis Kadsurae	Denudatin B	442834	FALSE	c1c(c(ccc1C1OC2=CC(=O)C(=CC2(C1C)OC)CC=C)OC)OC
MOL000310	0.3320	0.6680	0.8592	Rhizoma Dioscoreae	Denudatin B	442834	FALSE	c1c(c(ccc1C1OC2=CC(=O)C(=CC2(C1C)OC)CC=C)OC)OC
MOL000311	0.4860	0.5140	0.8160	Caulis Piperis Kadsurae	futoenone	Not Available	FALSE	CC1C(CC2CC31C=C(C(=O)C=C3O2)OC)c1cc2c(cc1)OCO2
MOL000312	0.3275	0.6725	0.8217	Caulis Piperis Kadsurae	futokadsurin C	46228348	FALSE	O1COC2c1ccc(c2)C1OC(C(C1C)C)c1c(c(ccc1)OC)OC
MOL000315	0.3664	0.6336	0.8548	Caulis Piperis Kadsurae	hancinone	Not Available	FALSE	c12c(ccc(c1)C1OC3=CC(=O)C(=CC3(C1C)OC)CC=C)OCO2
MOL000315	0.3664	0.6336	0.8548	Magnoliae Flos	hancinone	Not Available	FALSE	c12c(ccc(c1)C1OC3=CC(=O)C(=CC3(C1C)OC)CC=C)OCO2
MOL000316	0.4826	0.5174	0.7217	Caulis Piperis Kadsurae	isofutoquinol A	Not Available	FALSE	O(C12C3(C1C(C3c1cc3OCOc3cc1)(C(=O)C=C2OC)CC=C)C)C
MOL000317	0.5619	0.4381	0.7158	Caulis Piperis Kadsurae	Kadsurenin B	Not Available	FALSE	C1(C(C2C(=O)C(=CC1(OC)C2O)CC=C)c1cc2c(cc1)OCO2)C
MOL000318	0.5132	0.4868	0.6588	Caulis Piperis Kadsurae	(1R,5S,6R,7R,8R)-3-allyl-6-(3,4-dimethoxyphenyl)-8-hydroxy-1-methoxy-7-methyl-4-bicyclo[3.2.1]oct-2-enone	11439770	FALSE	C1(C(C2C(=O)C(=CC1(OC)C2O)CC=C)c1cc(c(cc1)OC)OC)C
MOL000319	0.6948	0.3052	0.6389	Caulis Piperis Kadsurae	Bicyclo(3.2.1)oct-3-ene-2,8-dione, 7-(4-hydroxy-3-methoxyphenyl)-5-methoxy-6-methyl-3-(2-propenyl)-, (1R-(6-endo,7-exo))-	3083438	FALSE	C1(C(C2C(=O)C(=CC1(OC)C2=O)CC=C)c1cc(c(cc1)O)OC)C

MOL000320	0.2096	0.7904	0.6301	Caulis Piperis Kadsurae	acetic acid [(1R,5S,6R,7R,8R)-3-allyl-6-(3,4-dimethoxyphenyl)-1-methoxy-7-methyl-4-oxo-8-bicyclo[3.2.1]oct-2-enyl] ester	11429497	FALSE	C1(C(C2C(=O)C(=CC1(OC)C2OC(=O)C)CC=C)c1cc(c(cc1)OC)OC)C
MOL000321	0.5882	0.4118	0.9164	Caulis Piperis Kadsurae	(2S,3S)-2-(3,4-dimethoxyphenyl)-7-methoxy-3-methyl-2,3-dihydrobenzofuran-5-carbaldehyde	208856	FALSE	C1(C(Oc2c1cc(cc2OC)C=O)c1cc(c(cc1)OC)OC)C
MOL000322	0.3320	0.6680	0.8592	Caulis Piperis Kadsurae	Kadsurenone	122159	FALSE	C12=CC(=O)C(=CC1(C(C(O2)c1cc(c(cc1)OC)OC)C)OC)CC=C
MOL000322	0.3320	0.6680	0.8592	Rhizoma Dioscoreae	Kadsurenone	122159	FALSE	C12=CC(=O)C(=CC1(C(C(O2)c1cc(c(cc1)OC)OC)C)OC)CC=C
MOL000323	0.4095	0.5905	0.6825	Caulis Piperis Kadsurae	Kadsurin A	442885	FALSE	C12(C(C=C(C(=O)C1)CC=C)(C(C(O2)c1cc2c(cc1)OCO2)C)OC)OC
MOL000324	0.2826	0.7174	0.6525	Caulis Piperis Kadsurae	kadsurin B	Not Available	FALSE	O1C2(OC)C(OC)(C(C1c1cc3OCOc3cc1)C)C=C(CC2)CC=C
MOL000325	0.2336	0.7664	0.8647	Caulis Piperis Kadsurae	(2R,3R)-2-(3,4-dimethoxyphenyl)-7-methoxy-3-methyl-5-[(E)-prop-1-enyl]-2,3-dihydrobenzofuran	6441048	FALSE	c1c(cc2c(c1OC)OC(C2C)c1ccc(c(c1)OC)OC)/C=C/C

MOL000325	0.2336	0.7664	0.8647	Epimrdii Herba	(2R,3R)-2-(3,4-dimethoxyphenyl)-7-methoxy-3-methyl-5-[(E)-prop-1-enyl]-2,3-dihydrobenzofuran	6441048	FALSE	c1c(cc2c(c1OC)OC(C2C)c1ccc(c(c1)OC)OC)/C=C/C
MOL000326	0.4809	0.5191	0.6047	Caulis Piperis Kadsurae	liliflone	Not Available	FALSE	c1(c(ccc(c1)C1OC2(C(C1C)(CC(C(=O)C2)CC=C)OC)OC)O)OC
MOL000327	0.3618	0.6382	0.7214	Caulis Piperis Kadsurae	(4R)-2-allyl-4-[(E)-2-(4-hydroxy-3-methoxyphenyl)-1-methylvinyl]-4,5-dimethoxy-1-cyclohexa-2,5-dienone	11717379	FALSE	C(=C(\C)/C1(C(=CC(=O)C(=C1)CC=C)OC)OC)\c1cc(c(O)cc1)OC
MOL000329	0.5892	0.4108	0.7682	Caulis Piperis Kadsurae	piperkadsin C	46228396	FALSE	C1(C(O)c2cc3OCOc3cc2)(C)C2C(=C1C=C(C2=O)CC=C)OC
MOL000330	0.7511	0.2489	0.7617	Caulis Piperis Kadsurae	piperlactam S	Not Available	FALSE	c1c2c(ccc1)cc1c3c2c(c(cc3c(=O)n1OC)O)OC
MOL000332	0.9030	0.0970	0.6858	Polygonati Odorati Rhizoma	n-coumaroyltyramine	5372945	FALSE	c1c(ccc(c1)/C=C/C(=O)NCCc1ccc(cc1)O)O
MOL000332	0.9030	0.0970	0.6858	Caulis Piperis Kadsurae	n-coumaroyltyramine	5372945	FALSE	c1c(ccc(c1)/C=C/C(=O)NCCc1ccc(cc1)O)O
MOL000332	0.9030	0.0970	0.6858	Polygoni Orientalis Fructus	n-coumaroyltyramine	5372945	FALSE	c1c(ccc(c1)/C=C/C(=O)NCCc1ccc(cc1)O)O
MOL000332	0.9030	0.0970	0.6858	Allium Azureum Ledeb.	n-coumaroyltyramine	5372945	FALSE	c1c(ccc(c1)/C=C/C(=O)NCCc1ccc(cc1)O)O
MOL000334	0.3091	0.6909	0.7837	Caulis Piperis Kadsurae	wallichinine	Not Available	FALSE	C1(=O)C(=CC(C(=C1)OC)(OC)/C(=C/c1cc(c(cc1)OC)OC)/C)CC=C
MOL000335	0.5356	0.4644	0.8562	Caulis Piperis Kadsurae	futoamide	Not Available	FALSE	C(=O)(/C=C/CC/C=C\c1cc2OCOc2cc1)NCC(C)C
MOL000336	0.2825	0.7175	0.8722	Caulis Piperis Kadsurae	futoquinol	Not Available	FALSE	C1(=O)C(=CC(C(=C1)OC)(OC)/C(=C\c1cc2OCOc2cc1)/C)CC=C

MOL000337	0.8520	0.1480	0.8271	Viscum Angulatum Heyne	3'-Methyl eriodictyol-7-O-beta-D-glucoside	Not Available	FALSE	C1(C(C(C(C(O1)Oc1cc(c2c(c1)OC(CC2=O)c1ccc(c(c1)OC)O)O)O)O)O)CO
MOL000338	0.9019	0.0981	0.8954	Gynostemmae Pentaphylli Herba	3'-methyleriodictyol	12310452	FALSE	Oc1cc(c2c(c1)OC(CC2=O)c1ccc(c(c1)OC)O)O
MOL000338	0.9019	0.0981	0.8954	Viscum Angulatum Heyne	3'-methyleriodictyol	12310452	FALSE	Oc1cc(c2c(c1)OC(CC2=O)c1ccc(c(c1)OC)O)O
MOL000339	0.9402	0.0598	0.8181	Paederiae Scandentis Herba	Isoscopoletin	69894	FALSE	COc1c(O)cc2c(c1)oc(=O)cc2
MOL000339	0.9402	0.0598	0.8181	Actinidia Chinensis Planch	Isoscopoletin	69894	FALSE	COc1c(O)cc2c(c1)oc(=O)cc2
MOL000339	0.9402	0.0598	0.8181	Violsse Herba	Isoscopoletin	69894	FALSE	COc1c(O)cc2c(c1)oc(=O)cc2
MOL000339	0.9402	0.0598	0.8181	Euphorbiae Humifusae Herba	Isoscopoletin	69894	FALSE	COc1c(O)cc2c(c1)oc(=O)cc2
MOL000339	0.9402	0.0598	0.8181	Solanum Melongena L	Isoscopoletin	69894	FALSE	COc1c(O)cc2c(c1)oc(=O)cc2
MOL000339	0.9402	0.0598	0.8181	Lobeliae Chinensis Herba	Isoscopoletin	69894	FALSE	COc1c(O)cc2c(c1)oc(=O)cc2
MOL000339	0.9402	0.0598	0.8181	Artemisiae Scopariae Herba	Isoscopoletin	69894	FALSE	COc1c(O)cc2c(c1)oc(=O)cc2
MOL000339	0.9402	0.0598	0.8181	Kansui Radix	Isoscopoletin	69894	FALSE	COc1c(O)cc2c(c1)oc(=O)cc2
MOL000339	0.9402	0.0598	0.8181	Viscum Angulatum Heyne	Isoscopoletin	69894	FALSE	COc1c(O)cc2c(c1)oc(=O)cc2
MOL000340	0.9289	0.0711	0.9514	Eriobotryae Folium	HCl	107	FALSE	c1cccc(c1)CCC(=O)O
MOL000340	0.9289	0.0711	0.9514	Carthami Flos	HCl	107	FALSE	c1cccc(c1)CCC(=O)O
MOL000340	0.9289	0.0711	0.9514	Cinnamomi Ramulus	HCl	107	FALSE	c1cccc(c1)CCC(=O)O
MOL000340	0.9289	0.0711	0.9514	Viscum Angulatum Heyne	HCl	107	FALSE	c1cccc(c1)CCC(=O)O
MOL000340	0.9289	0.0711	0.9514	Anisi Stellati Fructus	HCl	107	FALSE	c1cccc(c1)CCC(=O)O
MOL000340	0.9289	0.0711	0.9514	Piperis Longi Fructus	HCl	107	FALSE	c1cccc(c1)CCC(=O)O
MOL000340	0.9289	0.0711	0.9514	Linderae Radix	HCl	107	FALSE	c1cccc(c1)CCC(=O)O
MOL000341	0.8462	0.1538	0.8525	Viscum Angulatum Heyne	Viscumneoside III+B11772	Not Available	FALSE	c12c(cc(cc1O)OC1OC(C(C(C1OC1OCC(C1O)(CO)O)O)O)CO)OC(CC2=O)c1ccc(c(c1)OC)O
MOL000342	0.7831	0.2169	0.7657	Viscum Angulatum Heyne	Viscumneoside IV	Not Available	FALSE	o1c2c(c(=O)c(c1c1ccc(c(c1)OC)O)OC1OC(C(C(C1O)O)O)COC(=O)CC(O)(CC(=O)O)C)c(cc(c2)OC)O
MOL000343	0.8411	0.1589	0.7723	Viscum Angulatum Heyne	Viscumneoside V	Not Available	FALSE	c12c(cc(cc1O)OC1OC(C(C(C1OC1OCC(C1O)(O)COC1OCC(C1O)(CO)O)O)O)CO)OC(CC2=O)c1ccc(c(c1)OC)O
MOL000344	0.7826	0.2174	0.7388	Viscum Angulatum Heyne	Viscumneoside VI	Not Available	FALSE	c12c(cc(cc1O)OC1OC(C(C(C1O)O)O)O)COC(=O)C)OC(CC2=O)c1ccc(c(c1)OC)O
MOL000346	0.9009	0.0991	0.9600	Mori Fructus	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Hedysari Radix	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Pseudobulbus Cremastrae Seu Pleiones	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Geranium Wilfordii Maxim.	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Isatidis Folium	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O

MOL000346	0.9009	0.0991	0.9600	Xanthii Fructus	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Pine Pollen	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Dioscoreaebulbiferae	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Apocyniveneti Folium	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Arum Ternatum Thunb.	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Stemonae Radix	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Farfarae Flos	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Spatholobus Suberectus Dunn	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Arisaematis Rhizoma	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Sparganii Rhizoma	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Hippophae Fructus	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Forsythiae Fructus	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Radix Cynanchi	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Isatdis Radix	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Rhizoma Fagopyri Cymosi	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Pollen Typhae	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Allium Azureum Ledeb.	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Ranunculi Ternati Radix	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Lonicerae Japonicae Flos	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Cistanches Herba	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Mori Cortex	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Prinsepiae Nux	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Viscum Angulatum Heyne	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Saussureae Involucratae Herba	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Folium Nelumbinis	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Tripterygii Radix	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Lygodii Spora	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Euphorbiae Helioscopiae Herba	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Maydis Seigma	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Hedyotis Diffusae Herba	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Kaki Calyx	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Herba Sarcandrae	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Momordicae Fructus	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Glechomae Herba	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Smilacis Glabrae Rhixoma	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Chelidonii Herba	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Typhonii Rhizoma	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Achyranthis Bidentatae Radix	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O

MOL000346	0.9009	0.0991	0.9600	Fritillariaeussuriensis Bulbus	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Saxifraga Stolonifera	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Plantaginis Semen	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Tribulifructus	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Angelicae Sinensis Radix	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Equiseti Hiemalis Herba	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Bistortae Rhizoma	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Citri Fructus	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Carthami Flos	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Cyathulae Radix	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Eupatorium Fortunei Turcz	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Portulacae Herba	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Radix Rhei Et Rhizome	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Siegesbeckiae Herba	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Polygonati Rhizoma	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Schizonepetae Herba	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Quisqualis Indica	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Lobeliae Chinensis Herba	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Rehmanniae Radix Praeparata	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Aloe	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Radix Salviae	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Choerospondiatis Fructus	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Meliae Cortex	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Morindae Officinalis Radix	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000346	0.9009	0.0991	0.9600	Figwort Root	succinic acid	21952380	FALSE	C(=O)(O)CCC(=O)O
MOL000347	0.9214	0.0786	0.8194	Isatdis Radix	Syrigin	5316860	FALSE	c1(c(cc(cc1OC)/C=C/CO)OC)OC1OC(C(C(C1O)O)O)CO
MOL000347	0.9214	0.0786	0.8194	Radix Cirsii Japonici	Syrigin	5316860	FALSE	c1(c(cc(cc1OC)/C=C/CO)OC)OC1OC(C(C(C1O)O)O)CO
MOL000347	0.9214	0.0786	0.8194	Aucklandiae Radix	Syrigin	5316860	FALSE	c1(c(cc(cc1OC)/C=C/CO)OC)OC1OC(C(C(C1O)O)O)CO
MOL000347	0.9214	0.0786	0.8194	Viscum Angulatum Heyne	Syrigin	5316860	FALSE	c1(c(cc(cc1OC)/C=C/CO)OC)OC1OC(C(C(C1O)O)O)CO
MOL000347	0.9214	0.0786	0.8194	Ilicis Purpureae Folium	Syrigin	5316860	FALSE	c1(c(cc(cc1OC)/C=C/CO)OC)OC1OC(C(C(C1O)O)O)CO
MOL000347	0.9214	0.0786	0.8194	Phellodendri Chinrnsis Cortex	Syrigin	5316860	FALSE	c1(c(cc(cc1OC)/C=C/CO)OC)OC1OC(C(C(C1O)O)O)CO
MOL000347	0.9214	0.0786	0.8194	Bistortae Rhizoma	Syrigin	5316860	FALSE	c1(c(cc(cc1OC)/C=C/CO)OC)OC1OC(C(C(C1O)O)O)CO
MOL000347	0.9214	0.0786	0.8194	Saussureae Involucratae Herba	Syrigin	5316860	FALSE	c1(c(cc(cc1OC)/C=C/CO)OC)OC1OC(C(C(C1O)O)O)CO
MOL000347	0.9214	0.0786	0.8194	Aurantii Fructus Immaturus	Syrigin	5316860	FALSE	c1(c(cc(cc1OC)/C=C/CO)OC)OC1OC(C(C(C1O)O)O)CO

MOL000347	0.9214	0.0786	0.8194	Bidentis Bipinnatae Herba	Syrigin	5316860	FALSE	c1(c(cc(cc1OC)/C=C/CO)OC)OC1OC(C(C(C1O)O)O)CO
MOL000347	0.9214	0.0786	0.8194	Tinosporae Radix	Syrigin	5316860	FALSE	c1(c(cc(cc1OC)/C=C/CO)OC)OC1OC(C(C(C1O)O)O)CO
MOL000347	0.9214	0.0786	0.8194	Carthami Flos	Syrigin	5316860	FALSE	c1(c(cc(cc1OC)/C=C/CO)OC)OC1OC(C(C(C1O)O)O)CO
MOL000347	0.9214	0.0786	0.8194	Fraxini Cortex	Syrigin	5316860	FALSE	c1(c(cc(cc1OC)/C=C/CO)OC)OC1OC(C(C(C1O)O)O)CO
MOL000347	0.9214	0.0786	0.8194	Eucommiae Cortex	Syrigin	5316860	FALSE	c1(c(cc(cc1OC)/C=C/CO)OC)OC1OC(C(C(C1O)O)O)CO
MOL000347	0.9214	0.0786	0.8194	Codonopsis Radix	Syrigin	5316860	FALSE	c1(c(cc(cc1OC)/C=C/CO)OC)OC1OC(C(C(C1O)O)O)CO
MOL000347	0.9214	0.0786	0.8194	Allium Azureum Ledeb.	Syrigin	5316860	FALSE	c1(c(cc(cc1OC)/C=C/CO)OC)OC1OC(C(C(C1O)O)O)CO
MOL000347	0.9214	0.0786	0.8194	Isatidis Folium	Syrigin	5316860	FALSE	c1(c(cc(cc1OC)/C=C/CO)OC)OC1OC(C(C(C1O)O)O)CO
MOL000347	0.9214	0.0786	0.8194	Glehniae Radix	Syrigin	5316860	FALSE	c1(c(cc(cc1OC)/C=C/CO)OC)OC1OC(C(C(C1O)O)O)CO
MOL000348	0.9154	0.0846	0.9154	Carthami Flos	4-[(Z)-3-hydroxyprop-1-enyl]-2,6-dimethoxyphenol	10130521	FALSE	c1(c(cc(cc1OC)/C=C\CO)OC)O
MOL000348	0.9154	0.0846	0.9154	Viscum Angulatum Heyne	4-[(Z)-3-hydroxyprop-1-enyl]-2,6-dimethoxyphenol	10130521	FALSE	c1(c(cc(cc1OC)/C=C\CO)OC)O
MOL000348	0.9154	0.0846	0.9154	Bidentis Bipinnatae Herba	4-[(Z)-3-hydroxyprop-1-enyl]-2,6-dimethoxyphenol	10130521	FALSE	c1(c(cc(cc1OC)/C=C\CO)OC)O
MOL000348	0.9154	0.0846	0.9154	Isatdis Radix	4-[(Z)-3-hydroxyprop-1-enyl]-2,6-dimethoxyphenol	10130521	FALSE	c1(c(cc(cc1OC)/C=C\CO)OC)O
MOL000348	0.9154	0.0846	0.9154	Phellodendri Chinrnsis Cortex	4-[(Z)-3-hydroxyprop-1-enyl]-2,6-dimethoxyphenol	10130521	FALSE	c1(c(cc(cc1OC)/C=C\CO)OC)O
MOL000348	0.9154	0.0846	0.9154	Radix Cirsii Japonici	4-[(Z)-3-hydroxyprop-1-enyl]-2,6-dimethoxyphenol	10130521	FALSE	c1(c(cc(cc1OC)/C=C\CO)OC)O

MOL000348	0.9154	0.0846	0.9154	Aucklandiae Radix	4-[(Z)-3-hydroxyprop-1-enyl]-2,6-dimethoxyphenol	10130521	FALSE	c1(c(cc(cc1OC)/C=C\CO)OC)O
MOL000348	0.9154	0.0846	0.9154	Allium Azureum Ledeb.	4-[(Z)-3-hydroxyprop-1-enyl]-2,6-dimethoxyphenol	10130521	FALSE	c1(c(cc(cc1OC)/C=C\CO)OC)O
MOL000348	0.9154	0.0846	0.9154	Aurantii Fructus Immaturus	4-[(Z)-3-hydroxyprop-1-enyl]-2,6-dimethoxyphenol	10130521	FALSE	c1(c(cc(cc1OC)/C=C\CO)OC)O
MOL000349	0.8520	0.1480	0.8271	Viscum Angulatum Heyne	(2S)-5-hydroxy-2-(4-hydroxy-3-methoxyphenyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychroman-4-one	21629877	FALSE	C1(CC(=O)c2c(O1)cc(cc2O)OC1C(O)C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)OC
MOL000350	0.9019	0.0981	0.8954	Viscum Angulatum Heyne	Homoeriodictyol	73635	FALSE	C1(CC(=O)c2c(O1)cc(cc2O)O)c1cc(c(cc1)O)OC
MOL000351	0.8887	0.1113	0.8494	Scutellariae Barbatae Herba	Rhamnazin	5320945	FALSE	c12c(c(=O)c(c(o1)c1cc(c(cc1)O)OC)O)c(cc(c2)OC)O
MOL000351	0.8887	0.1113	0.8494	Viscum Angulatum Heyne	Rhamnazin	5320945	FALSE	c12c(c(=O)c(c(o1)c1cc(c(cc1)O)OC)O)c(cc(c2)OC)O
MOL000351	0.8887	0.1113	0.8494	Belamcandae Rhizome	Rhamnazin	5320945	FALSE	c12c(c(=O)c(c(o1)c1cc(c(cc1)O)OC)O)c(cc(c2)OC)O
MOL000351	0.8887	0.1113	0.8494	Iridis Tectori Rhizoma	Rhamnazin	5320945	FALSE	c12c(c(=O)c(c(o1)c1cc(c(cc1)O)OC)O)c(cc(c2)OC)O
MOL000351	0.8887	0.1113	0.8494	Gynostemmae Pentaphylli Herba	Rhamnazin	5320945	FALSE	c12c(c(=O)c(c(o1)c1cc(c(cc1)O)OC)O)c(cc(c2)OC)O
MOL000352	0.8495	0.1505	0.7704	Viscum Angulatum Heyne	rhamnazin-3-glucoside	Not Available	FALSE	c1(c(c(=O)c2c(cc(cc2o1)OC)O)OC1C(C(C(C(O1)CO)O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Rhizoma Fagopyri Cymosi	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Viscum Angulatum Heyne	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Asteris Radix Et Rhizoma	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Sapindi Mukorossiperic Arpium	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Microctis Folium	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC

MOL000354	0.9035	0.0965	0.8755	Potentillae Chinensis Herba	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Cuscutae Semen	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Ginkgo Semen	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Lepidii Semen Descurainiae Semen	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Sedi Herba	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Sophora Japonica L.	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Evodiae Fructus	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Radix Bupleuri	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Rhododendronmolle	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Lysimachiae Herba	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Tamaricis Cacumen	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Santalum Album L.	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Tribulifructus	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Calendula Officinalis	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Hedysarum Multijugum Maxim.	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Leonuri Herba	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Cyperi Rhizoma	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Pulsatilliae Radix	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Chrysanthemi Flos	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Artemisiae Scopariae Herba	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Alpiniae Officinarum Rhizome	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Eriobotryae Folium	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Folium Ilicis Cornutae	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Artemisia Annua L.	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Inulae Flos	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Crataegi Folium	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Hippophae Fructus	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Belamcandae Rhizome	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Ginkgo Folium	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Folium Nelumbinis	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Croci Stigma	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Celosia Cristata L.	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Pollen Typhae	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	Sophorae Tonkinensis Radix Et Rhizome	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC
MOL000354	0.9035	0.0965	0.8755	licorice	isorhamnetin	5281654	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1cc(c(cc1)O)OC

MOL000355	0.8743	0.1257	0.7948	Viscum Angulatum Heyne	isorhamnetin-7-O-β-D-glucopyranoside	Not Available	FALSE	c1(c(c(=O)c2c(cc(cc2o1)OC1OC(C(C(C1O)O)O)CO)O)O)c1cc(c(cc1)O)OC
MOL000356	0.3812	0.6188	0.7418	Jujubae Fructus	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Herba Sarcandrae	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Canavaliae Semen	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Gossampiniflos	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Abri Herba	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Apocyniveneti Folium	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Portulacae Herba	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Euphorbiae Helioscopiae Herba	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Cayratiae Japonicae Herba	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Aloe	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Isatdis Radix	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Figwort Root	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Tamaricis Cacumen	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Oroxyli Semen	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Calendula Officinalis	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Sophorae Tonkinensis Radix Et Rhizome	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Flemingia Prostrata Roxb	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Glehniae Radix	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Euonymi Alati Ramulus	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C

MOL000356	0.3812	0.6188	0.7418	Hippophae Fructus	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Trachelospermumjasminoides	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Lycii Fructus	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Hedysarum Multijugum Maxim.	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Herba Taxilli	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Folium Ilicis Cornutae	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Chrysanthemi Indici Flos	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Carthami Flos	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Lysimachiae Foenigraeci Herba	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Bombyx Mori L.	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Cichorii Radix	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Meliae Cortex	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Meliae Azedarach Fructus	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Viscum Angulatum Heyne	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Gentianae Radix Et Rhozima	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Trigonellae Semen	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Acoritataninowii Rhizoma	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Centipedae Herba	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Ilicis Cornutae Folium Immayuri	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000356	0.3812	0.6188	0.7418	Ampelopsis Japonica	lupeol	259846	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C
MOL000358	0.2481	0.7519	0.6027	Trollius Chinensis	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C

MOL000358	0.2481	0.7519	0.6027	Cyperi Rhizoma	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Portulacae Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Sterculiae Lychnophorae Semen	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Bistortae Rhizoma	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Figwort Root	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Lonicerae Japonicae Flos	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Radix Paeoniae Rubra	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Peucedanidecursivi Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Echinopsis Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Rosae Laevigatae Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Folium Artemisiae Argyi	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Celosiae Semen	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Citri Exocarpium Rubrum	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Myrrha	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Ilicis Purpureae Folium	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Phyllanthi Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Citri Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Radix Clematidis	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Wikstroemiae Indicae Rasix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Ampelopsis Japonica	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Adenophprae Ae Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C

MOL000358	0.2481	0.7519	0.6027	Coriolus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Evodiae Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Cichorii Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Caryophylliflos	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Boehmeriae Rhizoma Et Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Arisaematis Rhizoma	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Meliae Azedarach Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Myristicae Semen	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Peanut Skin	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Sedi Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Thalictri Glandulosissimi Et	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Cuscutae Semen	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Platycladi Cacumen	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Cayratiae Japonicae Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Saussureae Involucratae Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Zanthoxyli Pericarpium	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Caulis Akebiae	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Campsis Flos	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Cotyledon Fimbriata Turcz.	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Asparagi Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C

MOL000358	0.2481	0.7519	0.6027	Ailanthi Cortex	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Glehniae Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Typhonii Rhizoma	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Viticis Cannabifoliae Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Sargentodoxae Caulis	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Pollen Typhae	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Morindae Officinalis Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Peucedani Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Asteris Radix Et Rhizoma	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Rhapontici Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Actinidia Chinensis Planch	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Pseudobulbus Cremastrae Seu Pleiones	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Hyperici Japonici Herber	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Siphonostegiae Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Paeoniae Radix Alba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Pyrrosiae Folium	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Canarii Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Rose Rugosae Flos	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Akebiae Frucyus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Angelicae Sinensis Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Curcumae Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C

MOL000358	0.2481	0.7519	0.6027	Smilax China	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Isatdis Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Artemisiae Scopariae Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Bruceae Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Cortex Periplocae Radicis	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Potentillae Discoloris Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Boschniakia Rossica Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Impatientis Semen	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Oroxyli Semen	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Eriobotryae Folium	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Trigonellae Semen	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Viscum Angulatum Heyne	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Picrorhizae Rhizoma	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Sojae Semen Nigrum	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Folium Ilicis Cornutae	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Foeniculi Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Corayceps	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Verbenae Herb	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Ginkgo Folium	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Humulus Scandens (Lour.) Merr.	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C

MOL000358	0.2481	0.7519	0.6027	Radix Sanguisorbae	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Radix Cynanchi	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Dipsaci Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Spatholobus Suberectus Dunn	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Microctis Folium	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Salviae Chinensis Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Paederiae Scandentis Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Polygonati Rhizoma	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Ajugae Decumbentis Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Gnaphalii Affinis Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Zanthoxylum Nitidum	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Allium Azureum Ledeb.	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Citri Grandis Exocarpium	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Forsythiae Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Broussonetiae Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Iridis Tectori Rhizoma	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Curculiginis Rhizome	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Inulae Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Litseae Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Pulsatilliae Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Abri Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C

MOL000358	0.2481	0.7519	0.6027	Lycopi Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Choerospondiatis Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Commelinae Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Isatidis Folium	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Semen Euphorbiae	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Crotonis Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Ginkgo Semen	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Fructuslipuidambaris	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Moslae Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Polygoni Orientalis Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Mahoniae Caulis	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Panacis Quinquefolii Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Lycii Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Herba Patriniae	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Malvae Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Gentiana Macrophylla Pall	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Rubia Cordifolia	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Panax Ginseng C. A. Mey.	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Farfarae Flos	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Drynariae Rhizoma	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Arum Ternatum Thunb.	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C

MOL000358	0.2481	0.7519	0.6027	Chrysanthemi Indici Flos	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Gleditsiae Spina	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Radix Angelicae Biseratae	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Scutellariae Barbatae Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Rubi Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Perillae Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Ephedrae Radix Et Rhizoma	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Hippophae Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Glechomae Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Gossampiniflos	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Momordicae Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Hedysari Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Sparganii Rhizoma	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Radix Rhei Et Rhizome	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Litchi Semen	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Siegesbeckiae Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Herba Sarcandrae	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Prunellae Spica	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Homalomena Occulta (Lour.) Schott	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Tripterygii Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Indigo Naturalis	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C

MOL000358	0.2481	0.7519	0.6027	Ailanthi Altissimae Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Lycii Cortex	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Dalbergiae Odoriferae Lignum	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Dysosmae Verspiellis Rhixoma Et Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Cornus Officinalis Sieb. Et Zucc.	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Jujubae Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Hoveniae Dulcis Semen	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Zingiberis Rhizoma	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Lasiosphaera Seu Calvatia	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Aurantii Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Fructus Ligustri Lucidi	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Ginsen Radix Et Rhizoma Rubra	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Momordicae Semen	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Impatiens Balsamina	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Ganoderma	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Ilicis Cornutae Folium Immayuri	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Inulae Flos	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Calyx Seu Fructus Physalis	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Lilii Bulbus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Fritillariae Thunbrgii Bulbus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Pseudostellariae Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C

MOL000358	0.2481	0.7519	0.6027	Cyathulae Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Caulis Sinomenii	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Sophora Japonica L.	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Granati Pericarpium	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Mume Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Allii Tuberosi Semen	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Semen Pharbitidis	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Cistanches Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Zingiber Officinale Roscoe	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Uncariae Ramulus Cumuncis	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Cnidii Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Euonymi Alati Ramulus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Notoginseng Flos	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Rhizoma Seu Herba Aristolochiae Mollissimae	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Stemonae Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Scutellariae Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Kaki Calyx	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Cinnamomi Ramulus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Herba Pyrolae	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Linderae Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Aristolochiae Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C

MOL000358	0.2481	0.7519	0.6027	Spirodelae Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Cynanchistauntonii Rhizoma Et Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Lygodii Spora	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Euphorbiae Helioscopiae Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Sedum Aizoon L.	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Phellodendri Amurensis Cortex	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Astragali Cpmplanatisemen	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Rhizoma Fagopyri Cymosi	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Hedyotis Diffusae Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Imperatae Rhizoma	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Fraxini Cortex	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Phellodendri Chinrnsis Cortex	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Eucommiae Cortex	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Ranunculi Ternati Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Semen Lini	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Alpiniae Officinarum Rhizome	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Rhododendri Daurici Folium	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Meliae Cortex	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Fritiliariae Irrhosae Bulbus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Dioscoreaebulbiferae	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Hordei Fructus Germinatus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C

MOL000358	0.2481	0.7519	0.6027	Carthami Flos	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Achyranthis Bidentatae Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Bolbostemae Paniculati Bulbus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Stephaniae Tetrandrae Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Celastri Orbiculati Fructus	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Clematidis Armandii Caulis	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Dictamni Cortex	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Potentillae Chinensis Herba	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Radix Puerariae	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Polygoni Tinctorii Foliu	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Polygoni Cuspidati Rhizoma Et Radix	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Persicae Semen	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Lepidii Semen Descurainiae Semen	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Mori Cortex	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Smilacis Glabrae Rhixoma	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000358	0.2481	0.7519	0.6027	Pseudolaricis Cortex	beta-sitosterol	222284	FALSE	C12C3C(C4(C(=CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC(C(C)C)CC)C)C
MOL000360	0.9414	0.0586	0.9460	Ligustici Rhizoma Et Radix	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Cyathulae Radix	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Glechomae Herba	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Herba Clematidis Aethusaefoliae	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Figwort Root	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Asparagi Radix	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Cimicifugae Rhizoma	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	A. Dahurica (Fisch.) Benth. Et Hook	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O

MOL000360	0.9414	0.0586	0.9460	Meliae Cortex	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Carthami Flos	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Herbahypericiperforati	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Menthae Herba	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Semen Pharbitidis	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Herba Patriniae	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Hedyotis Diffusae Herba	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Corydalis Decumbens(Thunb.)Pers.	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Caulis Akebiae	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Solanum Melongena L	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Angelicae Sinensis Radix	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Semiaquilegiae Radix	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Notopterygii Rhizoma Et Radix	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Ginkgo Folium	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Fritiliariae Irrhosae Bulbus	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Malvae Fructus	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Microctis Folium	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Equiseti Hiemalis Herba	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Portulacae Herba	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Picrorhizae Rhizoma	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Rehmanniae Radix Praeparata	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Peucedani Radix	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Perilla Frutescens	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Hordei Fructus Germinatus	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Coptidis Rhizoma	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Rhizoma Fagopyri Cymosi	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Siegesbeckiae Herba	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Phragmitis Rhizoma	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Ziziphi Spinosae Semen	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Semen Lini	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Smilacis Glabrae Rhixoma	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Gentianae Radix Et Rhozima	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Ephedrae Radix Et Rhizoma	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Plantaginis Herba	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Glehniae Radix	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O

MOL000360	0.9414	0.0586	0.9460	Viscum Angulatum Heyne	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Radix Angelicae Biseratae	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Herba Selaginellae Moellendorfii	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000360	0.9414	0.0586	0.9460	Inulae Herba	FER	445858	TRUE	c1(cc(c(cc1)O)OC)/C=C/C(=O)O
MOL000361	0.3982	0.6018	0.7218	Tamaricis Cacumen	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Ailanthi Cortex	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Celastri Orbiculati Fructus	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Radix Paeoniae Rubra	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Gnaphalii Affinis Herba	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Campsis Flos	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Phyllanthi Fructus	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Viscum Angulatum Heyne	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Potentillae Chinensis Herba	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Zanthoxylum Nitidum	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Canarii Fructus	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Gentianae Radix Et Rhozima	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Cortex Periplocae Radicis	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Abrus Precatorius L.	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Asteris Radix Et Rhizoma	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Ecliptae Herba	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Prunellae Spica	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Ailanthi Altissimae Fructus	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Folium Artemisiae Argyi	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C 1C(CC3)(CCC(C1)(C)C)C)C)C

MOL000361	0.3982	0.6018	0.7218	Tinosporae Radix	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Myrrha	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Trachelospermumjasminoides	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Lycii Fructus	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Hippophae Fructus	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Clematidis Armandii Caulis	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Lobeliae Chinensis Herba	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Ilicis Cornutae Folium Immayuri	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Cuscutae Semen	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Impatientis Semen	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000361	0.3982	0.6018	0.7218	Portulacae Herba	Amyrin	73145	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C)C)C
MOL000362	0.3289	0.6711	0.7461	Solidaginis Herba	O-Acetyl-beta-amyrin	92156	FALSE	C12C(C3(C(=CC2)C2C(CC3)(CCC(C2)(C)C)C)C)(CCC2C1(CCC(C2(C)C)OC(=O)C)C)C
MOL000362	0.3289	0.6711	0.7461	Viscum Angulatum Heyne	O-Acetyl-beta-amyrin	92156	FALSE	C12C(C3(C(=CC2)C2C(CC3)(CCC(C2)(C)C)C)C)(CCC2C1(CCC(C2(C)C)OC(=O)C)C)C
MOL000362	0.3289	0.6711	0.7461	Eupatorium Fortunei Turcz	O-Acetyl-beta-amyrin	92156	FALSE	C12C(C3(C(=CC2)C2C(CC3)(CCC(C2)(C)C)C)C)(CCC2C1(CCC(C2(C)C)OC(=O)C)C)C
MOL000362	0.3289	0.6711	0.7461	Radix Cynanchi	O-Acetyl-beta-amyrin	92156	FALSE	C12C(C3(C(=CC2)C2C(CC3)(CCC(C2)(C)C)C)C)(CCC2C1(CCC(C2(C)C)OC(=O)C)C)C
MOL000362	0.3289	0.6711	0.7461	Euphorbiae Humifusae Herba	O-Acetyl-beta-amyrin	92156	FALSE	C12C(C3(C(=CC2)C2C(CC3)(CCC(C2)(C)C)C)C)(CCC2C1(CCC(C2(C)C)OC(=O)C)C)C
MOL000362	0.3289	0.6711	0.7461	Trachelospermumjasminoides	O-Acetyl-beta-amyrin	92156	FALSE	C12C(C3(C(=CC2)C2C(CC3)(CCC(C2)(C)C)C)C)(CCC2C1(CCC(C2(C)C)OC(=O)C)C)C
MOL000363	0.5908	0.4092	0.6244	Eupatorium Fortunei Turcz	amyrin Palmitate	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C)(C)CC4C3=CCC21)C)OC(=O)CCCCCCCCCCCCCC
MOL000363	0.5908	0.4092	0.6244	Inulae Flos	amyrin Palmitate	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C)(C)CC4C3=CCC21)C)OC(=O)CCCCCCCCCCCCCC
MOL000363	0.5908	0.4092	0.6244	Viscum Angulatum Heyne	amyrin Palmitate	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C)(C)CC4C3=CCC21)C)OC(=O)CCCCCCCCCCCCCC
MOL000363	0.5908	0.4092	0.6244	Ilicis Cornutae Folium Immayuri	amyrin Palmitate	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C)(C)CC4C3=CCC21)C)OC(=O)CCCCCCCCCCCCCC

MOL000364	0.5932	0.4068	0.6751	Eucommiae Folium	liriodendrin	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)c1c(cc(cc1OC)C1OCC2C1COC2c1cc(c(c(c1)OC)OC1C(O)C(O)C(O)C(O1)CO)OC)OC
MOL000364	0.5932	0.4068	0.6751	Viscum Angulatum Heyne	liriodendrin	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)c1c(cc(cc1OC)C1OCC2C1COC2c1cc(c(c(c1)OC)OC1C(O)C(O)C(O)C(O1)CO)OC)OC
MOL000365	0.5284	0.4716	0.6200	Codonopsis Radix	syringaresinol	12309694	FALSE	Oc1c(cc(cc1OC)C1OCC2C1COC2c1cc(c(c(c1)OC)O)OC)OC
MOL000365	0.5284	0.4716	0.6200	Fritillariae Thunbrgii Bulbus	syringaresinol	12309694	FALSE	Oc1c(cc(cc1OC)C1OCC2C1COC2c1cc(c(c(c1)OC)O)OC)OC
MOL000365	0.5284	0.4716	0.6200	Tripterygii Radix	syringaresinol	12309694	FALSE	Oc1c(cc(cc1OC)C1OCC2C1COC2c1cc(c(c(c1)OC)O)OC)OC
MOL000365	0.5284	0.4716	0.6200	Eucommiae Folium	syringaresinol	12309694	FALSE	Oc1c(cc(cc1OC)C1OCC2C1COC2c1cc(c(c(c1)OC)O)OC)OC
MOL000365	0.5284	0.4716	0.6200	Hedysari Radix	syringaresinol	12309694	FALSE	Oc1c(cc(cc1OC)C1OCC2C1COC2c1cc(c(c(c1)OC)O)OC)OC
MOL000365	0.5284	0.4716	0.6200	Caulis Sinomenii	syringaresinol	12309694	FALSE	Oc1c(cc(cc1OC)C1OCC2C1COC2c1cc(c(c(c1)OC)O)OC)OC
MOL000365	0.5284	0.4716	0.6200	Viscum Angulatum Heyne	syringaresinol	12309694	FALSE	Oc1c(cc(cc1OC)C1OCC2C1COC2c1cc(c(c(c1)OC)O)OC)OC
MOL000366	0.7764	0.2236	0.7192	Viscum Angulatum Heyne	viscumneosideII	Not Available	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC)OC1C(O)C(O)C(O)C(O1)COC(=O)C)c1cc(c(cc1)O)OC
MOL000367	0.8462	0.1538	0.8525	Viscum Angulatum Heyne	viscumneosideIII	Not Available	FALSE	C1(C(C(C(OC1CO)Oc1cc(c2c(c1)OC(CC2=O)c1cc(cc(cc1)O)OC)O)OC1OCC(C1O)(CO)O)O)O
MOL000368	0.7831	0.2169	0.7635	Viscum Angulatum Heyne	viscumneosideIV	Not Available	FALSE	C(=O)(CC(CC(=O)OCC1C(C(C(C(O1)Oc1c(oc2c(c1=O)c(cc(c2)OC)O)c1cc(c(cc1)O)OC)O)O)O)(C)O)O
MOL000369	0.8676	0.1324	0.7924	Viscum Angulatum Heyne	viscumneosideV	Not Available	FALSE	C1(C(C(OC(C1OC1OCC(C1O)(COC1C(C(C(O1)CO)O)O)O)Oc1cc(c2c(c1)OC(CC2=O)c1cc(c(cc1)O)O)O)CO)O)O
MOL000370	0.7826	0.2174	0.7388	Viscum Angulatum Heyne	Homoeriodictyol-7-O-(6'-O-acetyl)glucopyranoside	3082946	FALSE	C1(CC(=O)c2c(O1)cc(cc2O)OC1C(O)C(O)C(O)C(O1)COC(=O)C)c1cc(c(cc1)O)OC
MOL000371	0.7278	0.2722	0.7232	Hedysarum Multijugum Maxim.	3,9-di-O-methylnissolin	15689655	FALSE	C1C2C(c3ccc(cc3O1)OC)Oc1c2ccc(c1OC)OC
MOL000372	0.9001	0.0999	0.9431	Arisaematis Rhizoma	3-Hydroxy-2-picoline	70719	FALSE	c1(c(cccn1)O)C
MOL000372	0.9001	0.0999	0.9431	Hedysarum Multijugum Maxim.	3-Hydroxy-2-picoline	70719	FALSE	c1(c(cccn1)O)C

MOL000373	0.7136	0.2864	0.7139	Saposhnikoviae Radix	(2S)-4-methoxy-7-methyl-2-[1-methyl-1-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]oxy-ethyl]-2,3-dihydrofuro[3,2-g]chromen-5-one	21670038	FALSE	c1(cc(=O)c2c(o1)cc1c(c2OC)CC(O1)C(C)(C)OC1C(O)C(O)C(O)C(O1)CO)C
MOL000373	0.7136	0.2864	0.7139	Hedysarum Multijugum Maxim.	(2S)-4-methoxy-7-methyl-2-[1-methyl-1-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]oxy-ethyl]-2,3-dihydrofuro[3,2-g]chromen-5-one	21670038	FALSE	c1(cc(=O)c2c(o1)cc1c(c2OC)CC(O1)C(C)(C)OC1C(O)C(O)C(O)C(O1)CO)C
MOL000374	0.7909	0.2091	0.7186	Hedysarum Multijugum Maxim.	5'-hydroxyiso-muronulatol-2',5'-di-O-glucoside	Not Available	FALSE	c1(ccc2c(c1)OCC(C2)c1c(OC2OC(C(C(C2O)O)O)CO)c(OC)c(c(c1)OC1OC(C(C(C1O)O)O)CO)OC)O
MOL000375	0.7890	0.2110	0.7700	Hedysarum Multijugum Maxim.	5'-hydroxyiso-muronulatol-2',5'-di-O-glucoside_qt	Not Available	FALSE	c1(ccc2c(c1)OCC(C2)c1c(OC2OC(C(C(C2O)O)O)CO)c(OC)c(c(c1)O)OC)O

MOL000376	0.7032	0.2968	0.6258	Hedysarum Multijugum Maxim.	7,2'-dihydroxy-3',4'-dimethoxyisoflavone-7-O-β-D-glucoside	46899140	FALSE	c1c(c(=O)c2c(o1)cc(cc2)OC1C(O)C(O)C(O)C(O1)CO)c1c(c(cc1)OC)OC)O
MOL000377	0.8666	0.1334	0.9163	Hedysarum Multijugum Maxim.	7-hydroxy-3-(2-hydroxy-3,4-dimethoxy-phenyl)chromone	5359024	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1c(c(c(cc1)OC)OC)O
MOL000378	0.6607	0.3393	0.8306	Hedysarum Multijugum Maxim.	7-O-methylisomucronulatol	15689652	FALSE	c1(c(c(ccc1C1COc2c(C1)ccc(c2)OC)OC)OC)O
MOL000380	0.8306	0.1694	0.7594	Hedysarum Multijugum Maxim.	(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	14077830	FALSE	Oc1cc2c(C3C(CO2)c2c(O3)c(c(cc2)OC)OC)cc1
MOL000380	0.8306	0.1694	0.7594	Dalbergiae Odoriferae Lignum	(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	14077830	FALSE	Oc1cc2c(C3C(CO2)c2c(O3)c(c(cc2)OC)OC)cc1
MOL000381	0.8404	0.1596	0.6849	Hedysarum Multijugum Maxim.	13-hydroxy-9,11-octadecadienoic acid	21159006	FALSE	C(=O)(CCCCCCC/C=C/C=C/C(CCCCC)O)O
MOL000382	0.9429	0.0571	0.9672	Carthami Flos	Arabinose,d	66308	FALSE	O=CC(O)C(O)C(O)CO
MOL000382	0.9429	0.0571	0.9672	Hedysarum Multijugum Maxim.	Arabinose,d	66308	FALSE	O=CC(O)C(O)C(O)CO
MOL000382	0.9429	0.0571	0.9672	Radix Bupleuri	Arabinose,d	66308	FALSE	O=CC(O)C(O)C(O)CO
MOL000383	0.9137	0.0863	0.9617	Phellodendri Amurensis Cortex	D-Galacturonic acid, homopolymer	84740	FALSE	O=CC(O)C(O)C(O)C(O)C(=O)O

MOL000383	0.9137	0.0863	0.9617	Hedysarum Multijugum Maxim.	D-Galacturonic acid, homopolymer	84740	FALSE	O=CC(O)C(O)C(O)C(O)C(=O)O
MOL000383	0.9137	0.0863	0.9617	Hippophae Fructus	D-Galacturonic acid, homopolymer	84740	FALSE	O=CC(O)C(O)C(O)C(O)C(=O)O
MOL000383	0.9137	0.0863	0.9617	Angelicae Sinensis Radix	D-Galacturonic acid, homopolymer	84740	FALSE	O=CC(O)C(O)C(O)C(O)C(=O)O
MOL000383	0.9137	0.0863	0.9617	Achyranthis Bidentatae Radix	D-Galacturonic acid, homopolymer	84740	FALSE	O=CC(O)C(O)C(O)C(O)C(=O)O
MOL000383	0.9137	0.0863	0.9617	Pollen Typhae	D-Galacturonic acid, homopolymer	84740	FALSE	O=CC(O)C(O)C(O)C(O)C(=O)O
MOL000384	0.9137	0.0863	0.9617	Arum Ternatum Thunb.	DL-Glucuronic acid	65041	FALSE	O=CC(O)C(O)C(O)C(O)C(=O)O
MOL000384	0.9137	0.0863	0.9617	Choerospondiatis Fructus	DL-Glucuronic acid	65041	FALSE	O=CC(O)C(O)C(O)C(O)C(=O)O
MOL000384	0.9137	0.0863	0.9617	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	DL-Glucuronic acid	65041	FALSE	O=CC(O)C(O)C(O)C(O)C(=O)O
MOL000384	0.9137	0.0863	0.9617	Hedysarum Multijugum Maxim.	DL-Glucuronic acid	65041	FALSE	O=CC(O)C(O)C(O)C(O)C(=O)O
MOL000386	0.9464	0.0536	0.9717	Hedysarum Multijugum Maxim.	Fucopyranose, L-	3034656	FALSE	O=CC(O)C(O)C(O)C(O)C
MOL000388	0.9038	0.0962	0.9668	Aucklandiae Radix	gamma-aminobutyric acid	6992099	FALSE	C(=O)(CCCN)O
MOL000388	0.9038	0.0962	0.9668	Farfarae Flos	gamma-aminobutyric acid	6992099	FALSE	C(=O)(CCCN)O
MOL000388	0.9038	0.0962	0.9668	Bamusaeconcretiosilicea	gamma-aminobutyric acid	6992099	FALSE	C(=O)(CCCN)O

MOL000388	0.9038	0.0962	0.9668	Hedysari Radix	gamma-aminobutyric acid	6992099	FALSE	C(=O)(CCCN)O
MOL000388	0.9038	0.0962	0.9668	Rhizoma Dioscoreae	gamma-aminobutyric acid	6992099	FALSE	C(=O)(CCCN)O
MOL000388	0.9038	0.0962	0.9668	Trichosanthis Radix	gamma-aminobutyric acid	6992099	FALSE	C(=O)(CCCN)O
MOL000388	0.9038	0.0962	0.9668	Momordicae Fructus	gamma-aminobutyric acid	6992099	FALSE	C(=O)(CCCN)O
MOL000388	0.9038	0.0962	0.9668	Isatdis Radix	gamma-aminobutyric acid	6992099	FALSE	C(=O)(CCCN)O
MOL000388	0.9038	0.0962	0.9668	Lycii Fructus	gamma-aminobutyric acid	6992099	FALSE	C(=O)(CCCN)O
MOL000388	0.9038	0.0962	0.9668	Hedysarum Multijugum Maxim.	gamma-aminobutyric acid	6992099	FALSE	C(=O)(CCCN)O
MOL000388	0.9038	0.0962	0.9668	Arum Ternatum Thunb.	gamma-aminobutyric acid	6992099	FALSE	C(=O)(CCCN)O
MOL000388	0.9038	0.0962	0.9668	Phytolaccae Radix	gamma-aminobutyric acid	6992099	FALSE	C(=O)(CCCN)O
MOL000388	0.9038	0.0962	0.9668	Ganoderma	gamma-aminobutyric acid	6992099	FALSE	C(=O)(CCCN)O
MOL000389	0.9414	0.0586	0.9460	Angelicae Sinensis Radix	FERULIC ACID (CIS)	1548883	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)OC)O
MOL000389	0.9414	0.0586	0.9460	Toosendan Fructus	FERULIC ACID (CIS)	1548883	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)OC)O
MOL000389	0.9414	0.0586	0.9460	Arum Ternatum Thunb.	FERULIC ACID (CIS)	1548883	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)OC)O
MOL000389	0.9414	0.0586	0.9460	Hedysarum Multijugum Maxim.	FERULIC ACID (CIS)	1548883	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)OC)O
MOL000389	0.9414	0.0586	0.9460	Figwort Root	FERULIC ACID (CIS)	1548883	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)OC)O
MOL000389	0.9414	0.0586	0.9460	Rubi Fructus	FERULIC ACID (CIS)	1548883	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)OC)O

MOL000389	0.9414	0.0586	0.9460	Hedysari Radix	FERULIC ACID (CIS)	1548883	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)OC)O
MOL000390	0.9266	0.0734	0.8734	Radix Puerariae	daidzein	5281708	TRUE	c1c(c(=O)c2ccc(O)cc2o1)c1ccc(O)cc1
MOL000390	0.9266	0.0734	0.8734	Olibanun	daidzein	5281708	TRUE	c1c(c(=O)c2ccc(O)cc2o1)c1ccc(O)cc1
MOL000390	0.9266	0.0734	0.8734	Spatholobus Suberectus Dunn	daidzein	5281708	TRUE	c1c(c(=O)c2ccc(O)cc2o1)c1ccc(O)cc1
MOL000390	0.9266	0.0734	0.8734	Puerariae Flos	daidzein	5281708	TRUE	c1c(c(=O)c2ccc(O)cc2o1)c1ccc(O)cc1
MOL000390	0.9266	0.0734	0.8734	Cyathulae Radix	daidzein	5281708	TRUE	c1c(c(=O)c2ccc(O)cc2o1)c1ccc(O)cc1
MOL000390	0.9266	0.0734	0.8734	Sojae Semen Praeparatum	daidzein	5281708	TRUE	c1c(c(=O)c2ccc(O)cc2o1)c1ccc(O)cc1
MOL000390	0.9266	0.0734	0.8734	Trigonellae Semen	daidzein	5281708	TRUE	c1c(c(=O)c2ccc(O)cc2o1)c1ccc(O)cc1
MOL000390	0.9266	0.0734	0.8734	Hedysarum Multijugum Maxim.	daidzein	5281708	TRUE	c1c(c(=O)c2ccc(O)cc2o1)c1ccc(O)cc1
MOL000390	0.9266	0.0734	0.8734	Sojae Semen Nigrum	daidzein	5281708	TRUE	c1c(c(=O)c2ccc(O)cc2o1)c1ccc(O)cc1
MOL000390	0.9266	0.0734	0.8734	Sophorae Tonkinensis Radix Et Rhizome	daidzein	5281708	TRUE	c1c(c(=O)c2ccc(O)cc2o1)c1ccc(O)cc1
MOL000390	0.9266	0.0734	0.8734	Paederiae Scandentis Herba	daidzein	5281708	TRUE	c1c(c(=O)c2ccc(O)cc2o1)c1ccc(O)cc1
MOL000390	0.9266	0.0734	0.8734	Fructus Ligustri Lucidi	daidzein	5281708	TRUE	c1c(c(=O)c2ccc(O)cc2o1)c1ccc(O)cc1
MOL000391	0.6169	0.3831	0.6128	Pseudolaricis Cortex	Ononin	442813	FALSE	c1c(c(=O)c2c(o1)cc(cc2)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)OC
MOL000391	0.6169	0.3831	0.6128	Rhizome Of Whiteback Greenbrier	Ononin	442813	FALSE	c1c(c(=O)c2c(o1)cc(cc2)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)OC
MOL000391	0.6169	0.3831	0.6128	licorice	Ononin	442813	FALSE	c1c(c(=O)c2c(o1)cc(cc2)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)OC
MOL000391	0.6169	0.3831	0.6128	Spatholobus Suberectus Dunn	Ononin	442813	FALSE	c1c(c(=O)c2c(o1)cc(cc2)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)OC
MOL000391	0.6169	0.3831	0.6128	Radix Puerariae	Ononin	442813	FALSE	c1c(c(=O)c2c(o1)cc(cc2)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)OC
MOL000391	0.6169	0.3831	0.6128	Puerariae Flos	Ononin	442813	FALSE	c1c(c(=O)c2c(o1)cc(cc2)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)OC
MOL000391	0.6169	0.3831	0.6128	Hedysari Radix	Ononin	442813	FALSE	c1c(c(=O)c2c(o1)cc(cc2)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)OC
MOL000391	0.6169	0.3831	0.6128	Hedysarum Multijugum Maxim.	Ononin	442813	FALSE	c1c(c(=O)c2c(o1)cc(cc2)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)OC
MOL000392	0.9019	0.0981	0.9336	Folium Ilicis Cornutae	formononetin	5280378	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1ccc(cc1)OC
MOL000392	0.9019	0.0981	0.9336	Puerariae Flos	formononetin	5280378	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1ccc(cc1)OC
MOL000392	0.9019	0.0981	0.9336	Pseudolaricis Cortex	formononetin	5280378	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1ccc(cc1)OC
MOL000392	0.9019	0.0981	0.9336	Astragali Cpmplanatisemen	formononetin	5280378	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1ccc(cc1)OC
MOL000392	0.9019	0.0981	0.9336	Sophorae Tonkinensis Radix Et Rhizome	formononetin	5280378	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1ccc(cc1)OC
MOL000392	0.9019	0.0981	0.9336	Hedysarum Multijugum Maxim.	formononetin	5280378	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1ccc(cc1)OC
MOL000392	0.9019	0.0981	0.9336	Sparganii Rhizoma	formononetin	5280378	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1ccc(cc1)OC

MOL000392	0.9019	0.0981	0.9336	Radix Puerariae	formononetin	5280378	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1ccc(cc1)OC
MOL000392	0.9019	0.0981	0.9336	Dalbergiae Odoriferae Lignum	formononetin	5280378	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1ccc(cc1)OC
MOL000392	0.9019	0.0981	0.9336	licorice	formononetin	5280378	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1ccc(cc1)OC
MOL000392	0.9019	0.0981	0.9336	Trigonellae Semen	formononetin	5280378	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1ccc(cc1)OC
MOL000392	0.9019	0.0981	0.9336	Ginkgo Semen	formononetin	5280378	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1ccc(cc1)OC
MOL000392	0.9019	0.0981	0.9336	Hedysari Radix	formononetin	5280378	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1ccc(cc1)OC
MOL000392	0.9019	0.0981	0.9336	Stemonae Radix	formononetin	5280378	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1ccc(cc1)OC
MOL000392	0.9019	0.0981	0.9336	Spatholobus Suberectus Dunn	formononetin	5280378	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1ccc(cc1)OC
MOL000392	0.9019	0.0981	0.9336	Rhizome Of Whiteback Greenbrier	formononetin	5280378	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1ccc(cc1)OC
MOL000392	0.9019	0.0981	0.9336	Sophorae Flavescentis Radix	formononetin	5280378	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1ccc(cc1)OC
MOL000393	0.7746	0.2254	0.8365	Trigonellae Semen	Soyasaponin I	122097	FALSE	C12C(C3(C(=CC2)C2C(CC3)(C(CC(C2)(C)C)O)C)C)(CCC2C1(CCC(C2(CO)C)OC1C(OC2C(OC3C(C(C(C(O3)C)O)O)O)C(C(C(O2)CO)O)O)C(C(C(O1)C(=O)O)O)O)C)C
MOL000393	0.7746	0.2254	0.8365	Abri Herba	Soyasaponin I	122097	FALSE	C12C(C3(C(=CC2)C2C(CC3)(C(CC(C2)(C)C)O)C)C)(CCC2C1(CCC(C2(CO)C)OC1C(OC2C(OC3C(C(C(C(O3)C)O)O)O)C(C(C(O2)CO)O)O)C(C(C(O1)C(=O)O)O)O)C)C
MOL000393	0.7746	0.2254	0.8365	Sophorae Flavescentis Radix	Soyasaponin I	122097	FALSE	C12C(C3(C(=CC2)C2C(CC3)(C(CC(C2)(C)C)O)C)C)(CCC2C1(CCC(C2(CO)C)OC1C(OC2C(OC3C(C(C(C(O3)C)O)O)O)C(C(C(O2)CO)O)O)C(C(C(O1)C(=O)O)O)O)C)C
MOL000393	0.7746	0.2254	0.8365	Puerariae Flos	Soyasaponin I	122097	FALSE	C12C(C3(C(=CC2)C2C(CC3)(C(CC(C2)(C)C)O)C)C)(CCC2C1(CCC(C2(CO)C)OC1C(OC2C(OC3C(C(C(C(O3)C)O)O)O)C(C(C(O2)CO)O)O)C(C(C(O1)C(=O)O)O)O)C)C
MOL000393	0.7746	0.2254	0.8365	Peanut Skin	Soyasaponin I	122097	FALSE	C12C(C3(C(=CC2)C2C(CC3)(C(CC(C2)(C)C)O)C)C)(CCC2C1(CCC(C2(CO)C)OC1C(OC2C(OC3C(C(C(C(O3)C)O)O)O)C(C(C(O2)CO)O)O)C(C(C(O1)C(=O)O)O)O)C)C
MOL000393	0.7746	0.2254	0.8365	Hedysarum Multijugum Maxim.	Soyasaponin I	122097	FALSE	C12C(C3(C(=CC2)C2C(CC3)(C(CC(C2)(C)C)O)C)C)(CCC2C1(CCC(C2(CO)C)OC1C(OC2C(OC3C(C(C(C(O3)C)O)O)O)C(C(C(O2)CO)O)O)C(C(C(O1)C(=O)O)O)O)C)C
MOL000393	0.7746	0.2254	0.8365	Sophora Japonica L.	Soyasaponin I	122097	FALSE	C12C(C3(C(=CC2)C2C(CC3)(C(CC(C2)(C)C)O)C)C)(CCC2C1(CCC(C2(CO)C)OC1C(OC2C(OC3C(C(C(C(O3)C)O)O)O)C(C(C(O2)CO)O)O)C(C(C(O1)C(=O)O)O)O)C)C
MOL000393	0.7746	0.2254	0.8365	Sophorae Tonkinensis Radix Et Rhizome	Soyasaponin I	122097	FALSE	C12C(C3(C(=CC2)C2C(CC3)(C(CC(C2)(C)C)O)C)C)(CCC2C1(CCC(C2(CO)C)OC1C(OC2C(OC3C(C(C(C(O3)C)O)O)O)C(C(C(O2)CO)O)O)C(C(C(O1)C(=O)O)O)O)C)C
MOL000393	0.7746	0.2254	0.8365	Sojae Semen Nigrum	Soyasaponin I	122097	FALSE	C12C(C3(C(=CC2)C2C(CC3)(C(CC(C2)(C)C)O)C)C)(CCC2C1(CCC(C2(CO)C)OC1C(OC2C(OC3C(C(C(C(O3)C)O)O)O)C(C(C(O2)CO)O)O)C(C(C(O1)C(=O)O)O)O)C)C
MOL000394	0.9289	0.0711	0.9465	Bamusaeconcretiosilicea	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Chelidonii Herba	choline	305	FALSE	C(CO)[N+](C)(C)C

MOL000394	0.9289	0.0711	0.9465	Sojae Semen Nigrum	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Herbahypericiperforati	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Hordei Fructus Germinatus	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Glechomae Herba	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Trigonellae Semen	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Humulus Scandens (Lour.) Merr.	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Codonopsis Radix	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Typhonii Rhizoma	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Arum Ternatum Thunb.	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Hedysarum Multijugum Maxim.	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Arisaematis Rhizoma	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Dictamni Cortex	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Mori Follum	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Plantaginis Semen	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Rhizoma Dioscoreae	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Alisma Orientale (Sam.) Juz.	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Abri Herba	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Capsellae Herba	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Abrus Precatorius L.	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Ganoderma	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000394	0.9289	0.0711	0.9465	Farfarae Flos	choline	305	FALSE	C(CO)[N+](C)(C)C
MOL000395	0.8860	0.1140	0.9365	Canavaliae Semen	GGB	46224610	FALSE	C(=O)(C(N)CCONC(=N)N)O
MOL000395	0.8860	0.1140	0.9365	Hedysarum Multijugum Maxim.	GGB	46224610	FALSE	C(=O)(C(N)CCONC(=N)N)O
MOL000396	0.5284	0.4716	0.6200	Polygonati Rhizoma	(+)-Syringaresinol	443023	FALSE	O1C(C2C(C1)C(OC2)c1cc(c(c(c1)OC)O)OC)c1cc(c(c(c1)OC)O)OC
MOL000396	0.5284	0.4716	0.6200	Scutellariae Radix	(+)-Syringaresinol	443023	FALSE	O1C(C2C(C1)C(OC2)c1cc(c(c(c1)OC)O)OC)c1cc(c(c(c1)OC)O)OC
MOL000396	0.5284	0.4716	0.6200	Eucommiae Cortex	(+)-Syringaresinol	443023	FALSE	O1C(C2C(C1)C(OC2)c1cc(c(c(c1)OC)O)OC)c1cc(c(c(c1)OC)O)OC
MOL000396	0.5284	0.4716	0.6200	Zanthoxylum Nitidum	(+)-Syringaresinol	443023	FALSE	O1C(C2C(C1)C(OC2)c1cc(c(c(c1)OC)O)OC)c1cc(c(c(c1)OC)O)OC
MOL000396	0.5284	0.4716	0.6200	Saussureae Involucratae Herba	(+)-Syringaresinol	443023	FALSE	O1C(C2C(C1)C(OC2)c1cc(c(c(c1)OC)O)OC)c1cc(c(c(c1)OC)O)OC
MOL000396	0.5284	0.4716	0.6200	Semiaquilegiae Radix	(+)-Syringaresinol	443023	FALSE	O1C(C2C(C1)C(OC2)c1cc(c(c(c1)OC)O)OC)c1cc(c(c(c1)OC)O)OC
MOL000396	0.5284	0.4716	0.6200	Hedysarum Multijugum Maxim.	(+)-Syringaresinol	443023	FALSE	O1C(C2C(C1)C(OC2)c1cc(c(c(c1)OC)O)OC)c1cc(c(c(c1)OC)O)OC
MOL000396	0.5284	0.4716	0.6200	Curculiginis Rhizome	(+)-Syringaresinol	443023	FALSE	O1C(C2C(C1)C(OC2)c1cc(c(c(c1)OC)O)OC)c1cc(c(c(c1)OC)O)OC

MOL000396	0.5284	0.4716	0.6200	Magnoliae Flos	(+)-Syringaresinol	443023	FALSE	O1C(C2C(C1)C(OC2)c1cc(c(c(c1)OC)O)OC)c1cc(c(c(c1)OC)O)OC
MOL000396	0.5284	0.4716	0.6200	Polygoni Avicularis Herba	(+)-Syringaresinol	443023	FALSE	O1C(C2C(C1)C(OC2)c1cc(c(c(c1)OC)O)OC)c1cc(c(c(c1)OC)O)OC
MOL000396	0.5284	0.4716	0.6200	Carthami Flos	(+)-Syringaresinol	443023	FALSE	O1C(C2C(C1)C(OC2)c1cc(c(c(c1)OC)O)OC)c1cc(c(c(c1)OC)O)OC
MOL000396	0.5284	0.4716	0.6200	Solanum Nigrum Linn.	(+)-Syringaresinol	443023	FALSE	O1C(C2C(C1)C(OC2)c1cc(c(c(c1)OC)O)OC)c1cc(c(c(c1)OC)O)OC
MOL000397	0.9297	0.0703	0.8613	Notopterygii Rhizoma Et Radix	cis-p-Coumarate	1549106	FALSE	C(=O)(/C=C\c1ccc(cc1)O)O
MOL000397	0.9297	0.0703	0.8613	Persicae Semen	cis-p-Coumarate	1549106	FALSE	C(=O)(/C=C\c1ccc(cc1)O)O
MOL000397	0.9297	0.0703	0.8613	Eucommiae Cortex	cis-p-Coumarate	1549106	FALSE	C(=O)(/C=C\c1ccc(cc1)O)O
MOL000397	0.9297	0.0703	0.8613	Arum Ternatum Thunb.	cis-p-Coumarate	1549106	FALSE	C(=O)(/C=C\c1ccc(cc1)O)O
MOL000397	0.9297	0.0703	0.8613	Broussonetiae Fructus	cis-p-Coumarate	1549106	FALSE	C(=O)(/C=C\c1ccc(cc1)O)O
MOL000397	0.9297	0.0703	0.8613	Hedysarum Multijugum Maxim.	cis-p-Coumarate	1549106	FALSE	C(=O)(/C=C\c1ccc(cc1)O)O
MOL000397	0.9297	0.0703	0.8613	Flos Genkwa	cis-p-Coumarate	1549106	FALSE	C(=O)(/C=C\c1ccc(cc1)O)O
MOL000397	0.9297	0.0703	0.8613	Lycii Fructus	cis-p-Coumarate	1549106	FALSE	C(=O)(/C=C\c1ccc(cc1)O)O
MOL000397	0.9297	0.0703	0.8613	Curcumae Radix	cis-p-Coumarate	1549106	FALSE	C(=O)(/C=C\c1ccc(cc1)O)O
MOL000397	0.9297	0.0703	0.8613	Rhizoma Fagopyri Cymosi	cis-p-Coumarate	1549106	FALSE	C(=O)(/C=C\c1ccc(cc1)O)O
MOL000397	0.9297	0.0703	0.8613	Selaginella Doederleinii Hieron	cis-p-Coumarate	1549106	FALSE	C(=O)(/C=C\c1ccc(cc1)O)O
MOL000398	0.8863	0.1137	0.8258	Hedysarum Multijugum Maxim.	isoflavanone	Not Available	FALSE	C1C(C(=O)c2c(O1)ccc(c2OC)OC)c1ccc(O)cc1O
MOL000400	0.8784	0.1216	0.6346	Thalluslaminariae	Flavaxin	6759	FALSE	Cc1cc2c(nc3c(=O)[nH]c(=O)nc3n2CC(O)C(O)C(O)CO)cc1C
MOL000400	0.8784	0.1216	0.6346	Hedysarum Multijugum Maxim.	Flavaxin	6759	FALSE	Cc1cc2c(nc3c(=O)[nH]c(=O)nc3n2CC(O)C(O)C(O)CO)cc1C
MOL000401	0.5159	0.4841	0.7217	Hedysarum Multijugum Maxim.	astragalosideI	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)C1C2C(C(CCC32C2(C(C1)C1(C)CC(C(C4(CCC(C(C)(C)O)O4)C)C1(C)CC2)O)C3)OC1C(OC(=O)C)C(OC(=O)C)C(O)CO1)(C)C
MOL000402	0.3616	0.6384	0.7356	Hedysarum Multijugum Maxim.	astragalosideI_qt	Not Available	FALSE	OC1C2C(C(CCC32C2(C(C1)C1(C)CC(C(C4(CCC(C(C)(C)O)O4)C)C1(C)CC2)O)C3)OC1C(OC(=O)C)C(OC(=O)C)C(O)CO1)(C)C

MOL000403	0.5884	0.4116	0.7211	Hedysarum Multijugum Maxim.	astragalosideII	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)C1C2C(C(CCC32C2(C(C1)C1(C)CC(C(C4(CCC(C(C)(C)O)O4)C)C1(C)CC2)O)C3)OC1C(OC(=O)C)C(O)C(O)C(O)CO1)(C)C
MOL000404	0.4398	0.5602	0.7206	Hedysarum Multijugum Maxim.	astragalosideII_qt	Not Available	FALSE	OC1C2C(C(CCC32C2(C(C1)C1(C)CC(C(C4(CCC(C(C)(C)O)O4)C)C1(C)CC2)O)C3)OC1C(OC(=O)C)C(O)C(O)C(O)CO1)(C)C
MOL000405	0.6925	0.3075	0.8226	Hedysarum Multijugum Maxim.	astragaloside III	Not Available	FALSE	O(C1C(OC2C(O)C(O)C(O)C(O2)CO)C(O)C(O)CO1)C1CCC23C(C1(C)C)C(CC1C4(C)CC(C(C5(CCC(C(C)(C)O)O5)C)C4(C)CCC21C3)O)O
MOL000406	0.5001	0.4999	0.7029	Hedysarum Multijugum Maxim.	astragaloside III_qt	Not Available	FALSE	O(C1C(O)C(O)C(O)CO1)C1CCC23C(C1(C)C)C(CC1C4(C)CC(C(C5(CCC(C(C)(C)O)O5)C)C4(C)CCC21C3)O)O
MOL000407	0.7100	0.2900	0.7434	Hedysarum Multijugum Maxim.	astragaloside IV	Not Available	FALSE	C123C4(C2)C(C(CC1C1(C(CC3)(C(C(C1)O)C1(OC(CC1)C(C)(C)O)C)C)C)OC1OC(C(C(C1O)O)O)CO)C(C(CC4)OC1C(C(C(CO1)O)O)O)(C)C
MOL000408	0.5001	0.4999	0.7029	Hedysarum Multijugum Maxim.	astragaloside IV_qt	Not Available	FALSE	C123C4(C2)C(C(CC1C1(C(CC3)(C(C(C1)O)C1(OC(CC1)C(C)(C)O)C)C)C)O)C(C(CC4)OC1C(C(C(CO1)O)O)O)(C)C
MOL000409	0.7100	0.2900	0.7434	Hedysarum Multijugum Maxim.	AstragalosideIV	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)C1C2C(C(CCC32C2(C(C1)C1(C)CC(C(C4(CCC(C(C)(C)O)O4)C)C1(C)CC2)O)C3)OC1C(O)C(O)C(O)CO1)(C)C
MOL000410	0.5001	0.4999	0.7029	Hedysarum Multijugum Maxim.	AstragalosideIV_qt	Not Available	FALSE	OC1C2C(C(CCC32C2(C(C1)C1(C)CC(C(C4(CCC(C(C)(C)O)O4)C)C1(C)CC2)O)C3)OC1C(O)C(O)C(O)CO1)(C)C
MOL000412	0.7453	0.2547	0.9110	Hedysarum Multijugum Maxim.	Mucronulatol	442811	FALSE	Oc1cc2c(CC(CO2)c2c(c(c(cc2)OC)O)OC)cc1
MOL000412	0.7453	0.2547	0.9110	Dalbergiae Odoriferae Lignum	Mucronulatol	442811	FALSE	Oc1cc2c(CC(CO2)c2c(c(c(cc2)OC)O)OC)cc1
MOL000413	0.6593	0.3407	0.8152	Hedysarum Multijugum Maxim.	astrachrysoside A	Not Available	FALSE	O(C1C(OC2C(O)C(O)C(O)C(O2)C)C(O)C(O)CO1)C1CCC23C(C1(C)C)C(CC1C4(C)CC(C(C5(CCC(C(C)(C)O)O5)C)C4(C)CCC21C3)O)O
MOL000414	0.9416	0.0584	0.9275	Lycopi Herba	Caffeate	1549111	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)O)O
MOL000414	0.9416	0.0584	0.9275	Croci Stigma	Caffeate	1549111	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)O)O
MOL000414	0.9416	0.0584	0.9275	Boehmeriae Rhizoma Et Radix	Caffeate	1549111	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)O)O
MOL000414	0.9416	0.0584	0.9275	Rehmanniae Radix Praeparata	Caffeate	1549111	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)O)O
MOL000414	0.9416	0.0584	0.9275	Imperatae Rhizoma	Caffeate	1549111	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)O)O
MOL000414	0.9416	0.0584	0.9275	Forsythiae Fructus	Caffeate	1549111	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)O)O
MOL000414	0.9416	0.0584	0.9275	Crataegi Folium	Caffeate	1549111	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)O)O
MOL000414	0.9416	0.0584	0.9275	Plantaginis Herba	Caffeate	1549111	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)O)O
MOL000414	0.9416	0.0584	0.9275	Hyperici Japonici Herber	Caffeate	1549111	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)O)O
MOL000414	0.9416	0.0584	0.9275	Lonicerae Japonicae Flos	Caffeate	1549111	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)O)O
MOL000414	0.9416	0.0584	0.9275	Curcumae Radix	Caffeate	1549111	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)O)O

MOL000414	0.9416	0.0584	0.9275	Hedysarum Multijugum Maxim.	Caffeate	1549111	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)O)O
MOL000414	0.9416	0.0584	0.9275	Lygodii Spora	Caffeate	1549111	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)O)O
MOL000415	0.8866	0.1134	0.8314	Lonicerae Japonicae Flos	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Folium Artemisiae Argyi	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Forsythiae Fructus	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Paederiae Scandentis Herba	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Boehmeriae Rhizoma Et Radix	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Houttuyniae Herba	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Asteris Radix Et Rhizoma	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Hedysarum Multijugum Maxim.	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Echinopsis Radix	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Euphorbiae Helioscopiae Herba	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Calendula Officinalis	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Saussureae Involucratae Herba	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Rubi Fructus	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Radix Bupleuri	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Dysosmae Verspiellis Rhixoma Et Radix	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Herba Sarcandrae	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Mori Cortex	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Linderae Radix	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Litchi Semen	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Malvae Fructus	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O

MOL000415	0.8866	0.1134	0.8314	Bistortae Rhizoma	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Euonymi Alati Ramulus	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Aloe	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Toosendan Fructus	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Impatiens Balsamina	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Puerariae Flos	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Nelumbinis Plumula	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Herba Patriniae	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Microctis Folium	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Eucommiae Cortex	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Ailanthi Cortex	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Ginkgo Semen	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Solidaginis Herba	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Canarii Fructus	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Lycii Fructus	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Daturae Flos	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Ilicis Cornutae Folium Immayuri	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Artemisiae Scopariae Herba	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Mori Fructus	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Carthami Flos	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Herbahypericiperforati	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O

MOL000415	0.8866	0.1134	0.8314	Saururi Herba	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Gynostemmae Pentaphylli Herba	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	licorice	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Uncariae Ramulus Cumuncis	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Evodiae Fructus	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Herba Cirsii	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Geranium Wilfordii Maxim.	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Coriandri Sativi Herba	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Lysimachiae Herba	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Pteridis Multifidae Herba	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Sophorae Tonkinensis Radix Et Rhizome	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Crataegi Folium	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Prunellae Spica	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Gardeniae Fructus	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Gnaphalii Affinis Herba	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Ephedra Herba	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Litseae Fructus	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Hedyotis Diffusae Herba	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Eucommiae Folium	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Rhizoma Fagopyri Cymosi	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Eriobotryae Folium	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O

MOL000415	0.8866	0.1134	0.8314	Ginkgo Folium	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Glechomae Herba	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Achyranthis Bidentatae Radix	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Glehniae Radix	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Fructussophorae	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Jujubae Fructus	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Apocyniveneti Folium	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Herba Clematidis Aethusaefoliae	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Fructus Ligustri Lucidi	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Sapindi Mukorossiperic Arpium	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Farfarae Flos	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Mori Follum	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000415	0.8866	0.1134	0.8314	Hippophae Fructus	rutin	5280805	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1cc(c(cc1)O)O
MOL000416	0.6977	0.3023	0.6636	Paederiae Scandentis Herba	Lariciresinol	332427	FALSE	O1C(C(C(C1)Cc1cc(c(cc1)O)OC)CO)c1cc(c(cc1)O)OC
MOL000416	0.6977	0.3023	0.6636	Forsythiae Fructus	Lariciresinol	332427	FALSE	O1C(C(C(C1)Cc1cc(c(cc1)O)OC)CO)c1cc(c(cc1)O)OC
MOL000416	0.6977	0.3023	0.6636	Indigo Naturalis	Lariciresinol	332427	FALSE	O1C(C(C(C1)Cc1cc(c(cc1)O)OC)CO)c1cc(c(cc1)O)OC
MOL000416	0.6977	0.3023	0.6636	Capsici Fructus	Lariciresinol	332427	FALSE	O1C(C(C(C1)Cc1cc(c(cc1)O)OC)CO)c1cc(c(cc1)O)OC
MOL000416	0.6977	0.3023	0.6636	Hedysarum Multijugum Maxim.	Lariciresinol	332427	FALSE	O1C(C(C(C1)Cc1cc(c(cc1)O)OC)CO)c1cc(c(cc1)O)OC
MOL000416	0.6977	0.3023	0.6636	Isatdis Radix	Lariciresinol	332427	FALSE	O1C(C(C(C1)Cc1cc(c(cc1)O)OC)CO)c1cc(c(cc1)O)OC
MOL000417	0.8404	0.1596	0.9236	Hedysari Radix	Calycosin	5280448	FALSE	c1(c2cc(c(cc2)OC)O)c(=O)c2c(oc1)cc(cc2)O
MOL000417	0.8404	0.1596	0.9236	Trigonellae Semen	Calycosin	5280448	FALSE	c1(c2cc(c(cc2)OC)O)c(=O)c2c(oc1)cc(cc2)O
MOL000417	0.8404	0.1596	0.9236	Pseudolaricis Cortex	Calycosin	5280448	FALSE	c1(c2cc(c(cc2)OC)O)c(=O)c2c(oc1)cc(cc2)O
MOL000417	0.8404	0.1596	0.9236	Hedysarum Multijugum Maxim.	Calycosin	5280448	FALSE	c1(c2cc(c(cc2)OC)O)c(=O)c2c(oc1)cc(cc2)O
MOL000417	0.8404	0.1596	0.9236	Astragali Cpmplanatisemen	Calycosin	5280448	FALSE	c1(c2cc(c(cc2)OC)O)c(=O)c2c(oc1)cc(cc2)O
MOL000417	0.8404	0.1596	0.9236	licorice	Calycosin	5280448	FALSE	c1(c2cc(c(cc2)OC)O)c(=O)c2c(oc1)cc(cc2)O
MOL000417	0.8404	0.1596	0.9236	Spatholobus Suberectus Dunn	Calycosin	5280448	FALSE	c1(c2cc(c(cc2)OC)O)c(=O)c2c(oc1)cc(cc2)O

MOL000418	0.7297	0.2703	0.6712	Hedysarum Multijugum Maxim.	3'-Hydroxy-4'-methoxyisoflavone-7-O-beta-D-glucoside	5318267	FALSE	C1(C(C(OC(C1O)Oc1ccc2c(c1)occ(c2=O)c1cc(c(cc1)OC)O)CO)O)O
MOL000418	0.7297	0.2703	0.6712	Pseudolaricis Cortex	3'-Hydroxy-4'-methoxyisoflavone-7-O-beta-D-glucoside	5318267	FALSE	C1(C(C(OC(C1O)Oc1ccc2c(c1)occ(c2=O)c1cc(c(cc1)OC)O)CO)O)O
MOL000419	0.7107	0.2893	0.8115	Hedysarum Multijugum Maxim.	astrasieversianin XV	Not Available	FALSE	C123C4(C2)C(C(CC1C1(C(C(C2(OC(C(O)(C)C)CC2)C)C(C1)O)(CC3)C)C)OC1C(C(C(CO1)O)O)O)C(C(OC1C(OC2C(C(C(C(O2)C)O)O)O)O)C(C(CO1)O)O)CC4)(C)C
MOL000420	0.9429	0.0571	0.9672	Tetrapanacis Medulla	XLS	644160	FALSE	O=CC(O)C(O)C(O)CO
MOL000420	0.9429	0.0571	0.9672	Hippophae Fructus	XLS	644160	FALSE	O=CC(O)C(O)C(O)CO
MOL000420	0.9429	0.0571	0.9672	Stachyurimedulla Helwingiaemedulla	XLS	644160	FALSE	O=CC(O)C(O)C(O)CO
MOL000420	0.9429	0.0571	0.9672	Gossampiniflos	XLS	644160	FALSE	O=CC(O)C(O)C(O)CO
MOL000420	0.9429	0.0571	0.9672	Hedysarum Multijugum Maxim.	XLS	644160	FALSE	O=CC(O)C(O)C(O)CO
MOL000420	0.9429	0.0571	0.9672	Radix Bupleuri	XLS	644160	FALSE	O=CC(O)C(O)C(O)CO
MOL000420	0.9429	0.0571	0.9672	Phragmitis Rhizoma	XLS	644160	FALSE	O=CC(O)C(O)C(O)CO
MOL000421	0.9097	0.0903	0.9387	Citri Grandis Exocarpium	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Isatdis Radix	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Isatidis Folium	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Capsici Fructus	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Lepidii Semen Descurainiae Semen	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Angelicae Sinensis Radix	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Lablab Semen Album	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Hordei Fructus Germinatus	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Corayceps	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Coriolus	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Crataegi Folium	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Portulacae Herba	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Ecliptae Herba	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Anemarrhenae Rhizoma	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Platycodon Grandiforus	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Sojae Semen Nigrum	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Vigna Radiata	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Herbahypericiperforati	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O

MOL000421	0.9097	0.0903	0.9387	Codonopsis Radix	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Lycii Fructus	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Typhonii Rhizoma	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Jujubae Fructus	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000421	0.9097	0.0903	0.9387	Hedysarum Multijugum Maxim.	nicotinic acid	938	FALSE	C(=O)(c1cccnc1)O
MOL000422	0.9434	0.0566	0.8071	Prunellae Spica	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Rhododendri Daurici Folium	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Lonicerae Japonicae Flos	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Apocyniveneti Folium	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Agrimonia Eupatoria	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Mume Fructus	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Nelumbinis Stamen	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Ephedra Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Ilicis Cornutae Folium Immayuri	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Hyperici Japonici Herber	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Potentillae Chinensis Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Rhododendronmolle	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Prinsepiae Nux	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Mori Cortex	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Hemerocallis Radix	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Paeoniae Radix Alba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Fructussophorae	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Granati Pericarpium	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Asari Radix Et Rhizoma	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Pine Pollen	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Lunulatae Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Folium Nelumbinis	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Oryzae Glutinosae Radix	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Acoritataninowii Rhizoma	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Fortunes Bossfern Rhizome	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Impatiens Balsamina	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Sennae Folium	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Ilicis Purpureae Folium	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Radix Sanguisorbae	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Cyperi Rhizoma	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Polygoni Orientalis Fructus	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Folium Ilicis Cornutae	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O

MOL000422	0.9434	0.0566	0.8071	Microctis Folium	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Rubi Fructus	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Gnaphalii Affinis Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Inulae Flos	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Sophora Japonica L.	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Ailanthi Cortex	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Farfarae Flos	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Solidaginis Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Herba Patriniae	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Momordicae Fructus	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Dioscoreaebulbiferae	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Trigonellae Semen	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Sophorae Tonkinensis Radix Et Rhizome	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Hoveniae Dulcis Semen	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Phyllanthi Fructus	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Euonymi Alati Ramulus	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Tamaricis Cacumen	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Pollen Typhae	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Choerospondiatis Fructus	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Gleditsiae Spina	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Glechomae Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Euphorbiae Helioscopiae Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Equiseti Hiemalis Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Geranium Wilfordii Maxim.	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Alpiniae Officinarum Rhizome	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Lygodii Spora	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Carthami Flos	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Ginkgo Semen	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Platycladi Cacumen	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Puerariae Flos	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Kaki Calyx	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Crataegi Folium	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Celastri Orbiculati Fructus	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Herbahypericiperforati	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Radix Bupleuri	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Lysimachiae Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Cortex Moutan	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Euphorbiae Humifusae Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O

MOL000422	0.9434	0.0566	0.8071	Hippophae Fructus	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Pyrrosiae Folium	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Ginkgo Folium	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Chrysanthemi Flos	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Cuscutae Semen	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Croci Stigma	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	licorice	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Ephedrae Radix Et Rhizoma	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Moslae Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Eriobotryae Folium	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Lobeliae Chinensis Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Ginseng Folium	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Ardisiae Japonicae Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Anemarrhenae Rhizoma	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Allii Fistulost Bulbus	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Ailanthi Altissimae Fructus	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Eucommiae Cortex	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Gentianae Radix Et Rhozima	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Lepidii Semen Descurainiae Semen	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Houttuyniae Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Kaempferiae Rhizoma	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Hedysarum Multijugum Maxim.	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Impatientis Semen	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Rosae Laevigatae Fructus	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Daturae Flos	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Flos Genkwa	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Dysosmae Verspiellis Rhixoma Et Radix	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Forsythiae Fructus	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Uncariae Ramulus Cumuncis	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Lysimachiae Foenigraeci Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Catechu	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Asteris Radix Et Rhizoma	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Astragali Cpmplanatisemen	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Tribulifructus	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Polygoni Tinctorii Foliu	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O

MOL000422	0.9434	0.0566	0.8071	Leonuri Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Viticis Fructus	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Ramulus Mori	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Paederiae Scandentis Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Achyranthis Bidentatae Radix	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Drynariae Rhizoma	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Semen Aesculi	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Potentillae Discoloris Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Artemisia Annua L.	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Portulacae Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Anisi Stellati Fructus	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Caryophylliflos	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Cotyledon Fimbriata Turcz.	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Semen Pruni	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Eucommiae Folium	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Saussureae Involucratae Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Polygoni Avicularis Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Verbenae Herb	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Herba Pyrolae	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Panax Ginseng C. A. Mey.	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Epimrdii Herba	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Herba Clematidis Aethusaefoliae	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000422	0.9434	0.0566	0.8071	Fructus Ligustri Lucidi	kaempferol	5280863	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL000423	0.8652	0.1348	0.8161	Hedysarum Multijugum Maxim.	rhamnocitrin-3-O-glucoside	14704550	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)O
MOL000424	0.9392	0.0608	0.9678	Fructus Ligustri Lucidi	RAM	439710	FALSE	OC1C(O)C(O)C(O)C(O1)C
MOL000424	0.9392	0.0608	0.9678	Sterculiae Lychnophorae Semen	RAM	439710	FALSE	OC1C(O)C(O)C(O)C(O)C(O1)C
MOL000424	0.9392	0.0608	0.9678	Hedysarum Multijugum Maxim.	RAM	439710	FALSE	OC1C(O)C(O)C(O)C(O)C(O1)C
MOL000424	0.9392	0.0608	0.9678	Rosae Laevigatae Fructus	RAM	439710	FALSE	OC1C(O)C(O)C(O)C(O1)C
MOL000425	0.7437	0.2563	0.8105	Hedysarum Multijugum Maxim.	asernestioside A	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)C(C1CCC(C2C(CC3(C4CC(C5C(C(CCC65C4(CCC23C)C6)OC2C(OC3C(O)C(O)C(O)C(O3)C)C(O)C(O)CO2)(C)C)O)C)O)(C)O1)(C)C
MOL000426	0.6593	0.3407	0.8152	Hedysarum Multijugum Maxim.	asernestioside A_qt	Not Available	FALSE	OC(C1CCC(C2C(CC3(C4CC(C5C(C(CCC65C4(CCC23C)C6)OC2C(OC3C(O)C(O)C(O)C(O3)C)C(O)C(O)CO2)(C)C)O)C)O)(C)O1)(C)C

MOL000427	0.6949	0.3051	0.8026	Hedysarum Multijugum Maxim.	asernestioside B	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)C(C1CCC(C2C(CC3(C4CC(C5C(C(CCC65C4(CCC23C)C6)OC2C(OC3C(O)C(O)C(O)C(O3)C)C(OC(=O)C)C(O)CO2)(C)C)O)C)O)(C)O1)(C)C
MOL000428	0.5851	0.4149	0.8082	Hedysarum Multijugum Maxim.	asernestioside B_qt	Not Available	FALSE	OC(C1CCC(C2C(CC3(C4CC(C5C(C(CCC65C4(CCC23C)C6)OC2C(OC3C(O)C(O)C(O)C(O3)C)C(OC(=O)C)C(O)CO2)(C)C)O)C)O)(C)O1)(C)C
MOL000429	0.8972	0.1028	0.9610	Humulus Scandens (Lour.) Merr.	Crystal VI	6992089	FALSE	C(=O)(C(N)CC(=O)N)O
MOL000429	0.8972	0.1028	0.9610	Jujubae Fructus	Crystal VI	6992089	FALSE	C(=O)(C(N)CC(=O)N)O
MOL000429	0.8972	0.1028	0.9610	Hemerocallis Radix	Crystal VI	6992089	FALSE	C(=O)(C(N)CC(=O)N)O
MOL000429	0.8972	0.1028	0.9610	Xanthii Fructus	Crystal VI	6992089	FALSE	C(=O)(C(N)CC(=O)N)O
MOL000429	0.8972	0.1028	0.9610	Figwort Root	Crystal VI	6992089	FALSE	C(=O)(C(N)CC(=O)N)O
MOL000429	0.8972	0.1028	0.9610	Phragmitis Rhizoma	Crystal VI	6992089	FALSE	C(=O)(C(N)CC(=O)N)O
MOL000429	0.8972	0.1028	0.9610	Nodus Nelumbinis Rhizomatis	Crystal VI	6992089	FALSE	C(=O)(C(N)CC(=O)N)O
MOL000429	0.8972	0.1028	0.9610	Hedysarum Multijugum Maxim.	Crystal VI	6992089	FALSE	C(=O)(C(N)CC(=O)N)O
MOL000429	0.8972	0.1028	0.9610	Ginkgo Semen	Crystal VI	6992089	FALSE	C(=O)(C(N)CC(=O)N)O
MOL000429	0.8972	0.1028	0.9610	Lycii Fructus	Crystal VI	6992089	FALSE	C(=O)(C(N)CC(=O)N)O
MOL000430	0.8762	0.1238	0.9280	Lycii Cortex	betaine	248	FALSE	OC(=O)C[N+](C)(C)C
MOL000430	0.8762	0.1238	0.9280	Ganoderma	betaine	248	FALSE	OC(=O)C[N+](C)(C)C
MOL000430	0.8762	0.1238	0.9280	Hedysarum Multijugum Maxim.	betaine	248	FALSE	OC(=O)C[N+](C)(C)C
MOL000430	0.8762	0.1238	0.9280	Silybum Marianum	betaine	248	FALSE	OC(=O)C[N+](C)(C)C
MOL000430	0.8762	0.1238	0.9280	Hordei Fructus Germinatus	betaine	248	FALSE	OC(=O)C[N+](C)(C)C
MOL000430	0.8762	0.1238	0.9280	Achyranthis Bidentatae Radix	betaine	248	FALSE	OC(=O)C[N+](C)(C)C
MOL000430	0.8762	0.1238	0.9280	Bombyx Mori L.	betaine	248	FALSE	OC(=O)C[N+](C)(C)C
MOL000430	0.8762	0.1238	0.9280	Lycii Fructus	betaine	248	FALSE	OC(=O)C[N+](C)(C)C
MOL000431	0.9509	0.0491	0.8161	Hedysarum Multijugum Maxim.	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Boehmeriae Rhizoma Et Radix	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Saxifraga Stolonifera	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Peucedanidecursivi Radix	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Cinnamomi Ramulus	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Choerospondiatis Fructus	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Cinnanmomi Cortex	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Hydnocarpi Anthelminticae Semen	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Artemisia Annua L.	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Folium Artemisiae Argyi	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Rubi Fructus	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2

MOL000431	0.9509	0.0491	0.8161	Glehniae Radix	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Sophorae Tonkinensis Radix Et Rhizome	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Gleditsiae Spina	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Polygoni Cuspidati Rhizoma Et Radix	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Trollius Chinensis	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Hippophae Fructus	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Momordicae Fructus	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Magnolia Officinalis Rehd Et Wils.	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Radix Bupleuri	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Agrimonia Eupatoria	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Smilax China	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000431	0.9509	0.0491	0.8161	Cornus Officinalis Sieb. Et Zucc.	coumarin	323	FALSE	c1(=O)ccc2c(o1)cccc2
MOL000432	0.7659	0.2341	0.6499	Capsici Fructus	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Euphorbiae Humifusae Herba	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Cortex Periplocae Radicis	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Amygdalus Communis Vas	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Tamaricis Cacumen	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Cucurbitae Moschatae Semen	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Hippophae Fructus	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Thalictri Glandulosissimi Et	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Cannabis Sativa L.	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Sojae Semen Nigrum	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Rosae Laevigatae Fructus	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Semen Aesculi	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Ephedra Herba	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Semen Lini	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Silybum Marianum	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Lycii Cortex	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Malvae Fructus	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Alpiniae Oxyphyliae Fructus	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Arum Ternatum Thunb.	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Hedysarum Multijugum Maxim.	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Potentillae Discoloris Herba	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O

MOL000432	0.7659	0.2341	0.6499	Toosendan Fructus	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Mori Fructus	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Lysimachiae Foenigraeci Herba	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Benincasae Semen	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Portulacae Herba	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Thalluslaminariae	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Sinapis Semen	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Sapindi Mukorossi Semen	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Allii Tuberosi Semen	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Semen Pharbitidis	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Spirodelae Herba	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Platycladi Semen	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Phyllanthi Fructus	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Isatdis Radix	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Schizonepetae Spica	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Ginkgo Folium	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Coicis Semen	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Trichosanthes Kirilowii Maxim	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Raphani Semen	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Ranunculi Ternati Radix	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Litseae Fructus	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Carthami Flos	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Astragali Cpmplanatisemen	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Fructussophorae	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Semen Pini Koraiensis	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Sophora Japonica L.	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Perilla Frutescens	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Broussonetiae Fructus	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Lepidii Semen Descurainiae Semen	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Sennae Folium	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Semen Euphorbiae	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Arisaematis Rhizoma	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Perillae Fructus	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Panacis Quinquefolii Radix	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000432	0.7659	0.2341	0.6499	Vaccariae Semen	linolenic acid	5280934	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL000433	0.8875	0.1125	0.6000	Sesami Nigrum Semen	FA	6037	TRUE	C(=O)(CCC(C(=O)O)NC(=O)c1ccc(cc1)NCc1nc2c(=O)[nH]c(N)nc2nc1)O
MOL000433	0.8875	0.1125	0.6000	Sojae Semen Nigrum	FA	6037	TRUE	C(=O)(CCC(C(=O)O)NC(=O)c1ccc(cc1)NCc1nc2c(=O)[nH]c(N)nc2nc1)O

MOL000433	0.8875	0.1125	0.6000	Hordei Fructus Germinatus	FA	6037	TRUE	C(=O)(CCC(C(=O)O)NC(=O)c1ccc(cc1)NCc1nc2c(=O)[nH]c(N)nc2nc1)O
MOL000433	0.8875	0.1125	0.6000	Mori Follum	FA	6037	TRUE	C(=O)(CCC(C(=O)O)NC(=O)c1ccc(cc1)NCc1nc2c(=O)[nH]c(N)nc2nc1)O
MOL000433	0.8875	0.1125	0.6000	Bombyx Mori L.	FA	6037	TRUE	C(=O)(CCC(C(=O)O)NC(=O)c1ccc(cc1)NCc1nc2c(=O)[nH]c(N)nc2nc1)O
MOL000433	0.8875	0.1125	0.6000	Chuanxiong Rhizoma	FA	6037	TRUE	C(=O)(CCC(C(=O)O)NC(=O)c1ccc(cc1)NCc1nc2c(=O)[nH]c(N)nc2nc1)O
MOL000433	0.8875	0.1125	0.6000	Capsici Fructus	FA	6037	TRUE	C(=O)(CCC(C(=O)O)NC(=O)c1ccc(cc1)NCc1nc2c(=O)[nH]c(N)nc2nc1)O
MOL000433	0.8875	0.1125	0.6000	Hedysarum Multijugum Maxim.	FA	6037	TRUE	C(=O)(CCC(C(=O)O)NC(=O)c1ccc(cc1)NCc1nc2c(=O)[nH]c(N)nc2nc1)O
MOL000433	0.8875	0.1125	0.6000	Hippophae Fructus	FA	6037	TRUE	C(=O)(CCC(C(=O)O)NC(=O)c1ccc(cc1)NCc1nc2c(=O)[nH]c(N)nc2nc1)O
MOL000434	0.4475	0.5525	0.6960	Hedysarum Multijugum Maxim.	acetylastragaloside I	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)C1C2C(C(CCC32C2(C(C1)C1(C)CC(C(C4(CCC(C(C)(C)O)O)O4)C)C1(C)CC2)O)C3)OC1C(OC(=O)C)C(OC(=O)C)C(OC(=O)C)CO1)(C)C
MOL000435	0.3048	0.6952	0.7054	Hedysarum Multijugum Maxim.	acetylastragaloside I_qt	Not Available	FALSE	OC1C2C(C(CCC32C2(C(C1)C1(C)CC(C(C4(CCC(C(C)(C)O)O4)C)C1(C)CC2)O)C3)OC1C(OC(=O)C)C(OC(=O)C)C(OC(=O)C)CO1)(C)C
MOL000436	0.9030	0.0970	0.8088	Polygonati Rhizoma	(Z)-1-(2,4-dihydroxyphenyl)-3-(4-hydroxyphenyl)prop-2-en-1-one	6603886	FALSE	C(=O)(/C=C\c1ccc(cc1)O)c1c(cc(cc1)O)O
MOL000436	0.9030	0.0970	0.8088	Hedysari Radix	(Z)-1-(2,4-dihydroxyphenyl)-3-(4-hydroxyphenyl)prop-2-en-1-one	6603886	FALSE	C(=O)(/C=C\c1ccc(cc1)O)c1c(cc(cc1)O)O
MOL000436	0.9030	0.0970	0.8088	Boehmeriae Rhizoma Et Radix	(Z)-1-(2,4-dihydroxyphenyl)-3-(4-hydroxyphenyl)prop-2-en-1-one	6603886	FALSE	C(=O)(/C=C\c1ccc(cc1)O)c1c(cc(cc1)O)O

MOL000436	0.9030	0.0970	0.8088	Dalbergiae Odoriferae Lignum	(Z)-1-(2,4-dihydroxyphenyl)-3-(4-hydroxyphenyl)prop-2-en-1-one	6603886	FALSE	C(=O)(/C=C\c1ccc(cc1)O)c1c(cc(cc1)O)O
MOL000436	0.9030	0.0970	0.8088	Hedysarum Multijugum Maxim.	(Z)-1-(2,4-dihydroxyphenyl)-3-(4-hydroxyphenyl)prop-2-en-1-one	6603886	FALSE	C(=O)(/C=C\c1ccc(cc1)O)c1c(cc(cc1)O)O
MOL000436	0.9030	0.0970	0.8088	Spatholobus Suberectus Dunn	(Z)-1-(2,4-dihydroxyphenyl)-3-(4-hydroxyphenyl)prop-2-en-1-one	6603886	FALSE	C(=O)(/C=C\c1ccc(cc1)O)c1c(cc(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Impatientis Semen	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Artemisiae Scopariae Herba	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Solanum Nigrum Linn.	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Euphorbiae Humifusae Herba	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Chrysanthemi Indici Flos	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Astragali Cpmplanatisemen	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	licorice	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Nelumbinis Stamen	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Folium Nelumbinis	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Dictamni Cortex	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Granati Pericarpium	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Inulae Flos	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O

MOL000437	0.9265	0.0735	0.8040	Epimrdii Herba	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Impatiens Balsamina	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Saururi Herba	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Herbahypericiperforati	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Polygoni Cuspidati Rhizoma Et Radix	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Artemisia Annua L.	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Rubi Fructus	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Plantaginis Semen	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Cotyledon Fimbriata Turcz.	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Leonuri Herba	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Anisi Stellati Fructus	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Eriobotryae Folium	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Herba Patriniae	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Schizonepetae Herba	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Flos Genkwa	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Paederiae Scandentis Herba	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Herba Pyrolae	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Geranium Wilfordii Maxim.	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Gardeniae Fructus	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Mori Follum	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O

MOL000437	0.9265	0.0735	0.8040	Lysimachiae Herba	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Uncariae Ramulus Cumuncis	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Houttuyniae Herba	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Eucommiae Cortex	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Sedi Herba	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Radix Bupleuri	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Hedysarum Multijugum Maxim.	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Hyperici Japonici Herber	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Glehniae Radix	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Amomum Tsao-Ko Crevostet	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Celastri Orbiculati Fructus	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Inulae Herba	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Farfarae Flos	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Coriandri Sativi Herba	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Pyrrosiae Folium	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Dysosmae Verspiellis Rhixoma Et Radix	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Rose Rugosae Flos	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Forsythiae Fructus	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000437	0.9265	0.0735	0.8040	Saussureae Involucratae Herba	Hirsutrin	5280804	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000438	0.8324	0.1676	0.8738	Hedysarum Multijugum Maxim.	(3R)-3-(2-hydroxy-3,4-dimethoxyphenyl)chroman-7-ol	10380176	FALSE	C1C(Cc2c(O1)cc(cc2)O)c1c(c(c(cc1)OC)OC)O

MOL000439	0.7352	0.2648	0.7003	Hedysarum Multijugum Maxim.	isomucronulatol-7,2'-di-O-glucosiole	15689653	FALSE	C1(C(C(C(C(O1)CO)O)O)O)Oc1ccc2CC(COc2c1)c1c(c(cc1)OC)OC)OC1C(C(C(C(O1)CO)O)O)O
MOL000440	0.6650	0.3350	0.7218	Hedysarum Multijugum Maxim.	isomucronulatol-7,2'-di-O-glucosiole_qt	Not Available	FALSE	Oc1ccc2CC(COc2c1)c1c(c(cc1)OC)OC)OC1C(C(C(C(O1)CO)O)O)O
MOL000441	0.3399	0.6601	0.7428	Isatdis Radix	LUPENONE	92158	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C(=C)C)C4C3CCC21)C
MOL000441	0.3399	0.6601	0.7428	Gossampiniflos	LUPENONE	92158	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C(=C)C)C4C3CCC21)C
MOL000441	0.3399	0.6601	0.7428	Radix Puerariae	LUPENONE	92158	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C(=C)C)C4C3CCC21)C
MOL000441	0.3399	0.6601	0.7428	Millettiae Speciosae Radix	LUPENONE	92158	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C(=C)C)C4C3CCC21)C
MOL000441	0.3399	0.6601	0.7428	Hedysarum Multijugum Maxim.	LUPENONE	92158	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C(=C)C)C4C3CCC21)C
MOL000441	0.3399	0.6601	0.7428	Folium Artemisiae Argyi	LUPENONE	92158	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C(=C)C)C4C3CCC21)C
MOL000441	0.3399	0.6601	0.7428	Adenophprae Ae Radix	LUPENONE	92158	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C(=C)C)C4C3CCC21)C
MOL000442	0.8937	0.1063	0.6998	Hedysarum Multijugum Maxim.	1,7-Dihydroxy-3,9-dimethoxy pterocarpene	5316760	FALSE	o1c2c(c3c1cc(cc3O)OC)COc1c2c(cc(c1)OC)O
MOL000443	0.7441	0.2559	0.8338	Eucommiae Cortex	Erythraline	Not Available	FALSE	c12c(cc3c(c1)CCN1C43C(=CC1)C=CC(C4)OC)OC
MOL000443	0.7441	0.2559	0.8338	Cortex Erythrinae	Erythraline	Not Available	FALSE	c12c(cc3c(c1)CCN1C43C(=CC1)C=CC(C4)OC)OC
MOL000444	0.9039	0.0961	0.8000	Cortex Erythrinae	methyl (2S)-2-dimethylamino-3-(1H-indol-3-yl)propanoate	21140335	FALSE	C(=O)(C(N(C)C)Cc1c[nH]c2ccccc12)OC
MOL000446	0.9365	0.0635	0.7697	Hedysari Radix	hypaphorine	442107	FALSE	c1cc2c(cc1)[nH]cc2CC(C(=O)O)[N+](C)(C)C
MOL000446	0.9365	0.0635	0.7697	Cortex Erythrinae	hypaphorine	442107	FALSE	c1cc2c(cc1)[nH]cc2CC(C(=O)O)[N+](C)(C)C
MOL000447	0.9159	0.0841	0.8780	Leonuri Herba	stachydrine	448301	FALSE	C(=O)(C1[N+](CCC1)(C)C)O
MOL000447	0.9159	0.0841	0.8780	Citri Grandis Exocarpium	stachydrine	448301	FALSE	C(=O)(C1[N+](CCC1)(C)C)O
MOL000447	0.9159	0.0841	0.8780	Citrus Aurantium	stachydrine	448301	FALSE	C(=O)(C1[N+](CCC1)(C)C)O
MOL000447	0.9159	0.0841	0.8780	Cortex Erythrinae	stachydrine	448301	FALSE	C(=O)(C1[N+](CCC1)(C)C)O
MOL000448	0.3814	0.6186	0.6314	Cortex Erythrinae	isobavachin	Not Available	FALSE	C1(CC(=O)c2c(O1)cc(cc2O)CC=C(C)C)c1ccc(cc1)O

MOL000450	0.1270	0.8730	0.7063	Cortex Erythrinae	(6aR,11aR)-2,10-bis(3-methylbut-2-enyl)-6a,11a-dihydro-6H-benzofurano[3,2-c]chromene-3,9-diol	10408212	FALSE	C1C2C(c3c(O1)cc(c(c3)CC=C(C)C)O)Oc1c2ccc(c1CC=C(C)C)O
MOL000451	0.6962	0.3038	0.7420	Cortex Erythrinae	erysodienone	Not Available	FALSE	C123N(CCc4cc([cH]cc14)OC)O)CCC2=CC(=O)C(=C3)OC
MOL000452	0.4610	0.5390	0.7724	Cortex Erythrinae	eryvariestyrene	Not Available	FALSE	c1(cc(c(cc1C/C=C\c1ccccc1)CC=C(C)C)O)O
MOL000453	0.6250	0.3750	0.7577	Cortex Erythrinae	1,2,6,7-Tetradehydro-3,15-dimethoxyerythrinan-16-ol	169017	FALSE	C123c4c(CCN1CC=C2C=CC(C3)OC)cc(c(c4)OC)O
MOL000454	0.7117	0.2883	0.7841	Cortex Erythrinae	erysotine	Not Available	FALSE	C1([cH]cc2c(c1)C13N(CC2)CCC1=CC(C(C3)OC)O)O
MOL000455	0.5781	0.4219	0.8636	Cortex Erythrinae	Erysotrine	442219	FALSE	C1([cH]cc2c(c1)C13N(CC2)CC=C1C=CC(C3)OC)OC
MOL000456	0.6519	0.3481	0.8499	Sophorae Flavescentis Radix	Phaseolin	Not Available	FALSE	c12c(C3C(O2)c2c(OC3)cc(cc2)O)ccc2c1C=CC(O2)(C)C
MOL000456	0.6519	0.3481	0.8499	Cortex Erythrinae	Phaseolin	Not Available	FALSE	C12C(C3C(O2)c2c(OC3)cc(cc2)O)ccc2c1C=CC(O2)(
MOL000457	0.4989	0.5011	0.8433	Cortex Erythrinae	Phaseollidin	119268	FALSE	C12C(C3C(O2)c([cH]cc3)O)CC=C(C)C)COc2c1ccc(c2)
MOL000457	0.4989	0.5011	0.8433	Semen Pharbitidis	Phaseollidin	119268	FALSE	C12C(C3C(O2)c([cH]cc3)O)CC=C(C)C)COc2c1ccc(c2)
MOL000459	0.9332	0.0668	0.9488	Radix Bupleuri	CHEBI:39932	6992244	FALSE	C=CC(CCCCC)O
MOL000459	0.9332	0.0668	0.9488	Campsis Flos	CHEBI:39932	6992244	FALSE	C=CC(CCCCC)O
MOL000459	0.9332	0.0668	0.9488	Polygonati Odorati Rhizoma	CHEBI:39932	6992244	FALSE	C=CC(CCCCC)O
MOL000459	0.9332	0.0668	0.9488	Verbenae Herb	CHEBI:39932	6992244	FALSE	C=CC(CCCCC)O
MOL000459	0.9332	0.0668	0.9488	Spatholobus Suberectus Dunn	CHEBI:39932	6992244	FALSE	C=CC(CCCCC)O
MOL000459	0.9332	0.0668	0.9488	Thalluslaminariae	CHEBI:39932	6992244	FALSE	C=CC(CCCCC)O
MOL000459	0.9332	0.0668	0.9488	Aauropi Folium	CHEBI:39932	6992244	FALSE	C=CC(CCCCC)O
MOL000459	0.9332	0.0668	0.9488	Folium Artemisiae Argyi	CHEBI:39932	6992244	FALSE	C=CC(CCCCC)O
MOL000459	0.9332	0.0668	0.9488	Violsse Herba	CHEBI:39932	6992244	FALSE	C=CC(CCCCC)O
MOL000459	0.9332	0.0668	0.9488	Dianthi Herba	CHEBI:39932	6992244	FALSE	C=CC(CCCCC)O
MOL000459	0.9332	0.0668	0.9488	Adenophprae Ae Radix	CHEBI:39932	6992244	FALSE	C=CC(CCCCC)O
MOL000459	0.9332	0.0668	0.9488	Coriolus	CHEBI:39932	6992244	FALSE	C=CC(CCCCC)O
MOL000459	0.9332	0.0668	0.9488	Scutellariae Barbatae Herba	CHEBI:39932	6992244	FALSE	C=CC(CCCCC)O

MOL000460	0.9253	0.0747	0.8705	Spatholobus Suberectus Dunn	(Z)-1-(2,4-dihydroxyphenyl)-3-(3,4-dihydroxyphenyl)prop-2-en-1-one	5315562	FALSE	C(=C\c1cc(c(cc1)O)O)\C(=O)c1c(cc(cc1)O)O
MOL000460	0.9253	0.0747	0.8705	Ecliptae Herba	(Z)-1-(2,4-dihydroxyphenyl)-3-(3,4-dihydroxyphenyl)prop-2-en-1-one	5315562	FALSE	C(=C\c1cc(c(cc1)O)O)\C(=O)c1c(cc(cc1)O)O
MOL000461	0.8996	0.1004	0.8412	Spatholobus Suberectus Dunn	3,7-dihydroxy-6-methoxy-dihydroflavonol	Not Available	FALSE	C1(C(C(=O)c2cc(c(cc2O1)O)OC)(O)O)c1ccccc1
MOL000462	0.5188	0.4812	0.8066	Spatholobus Suberectus Dunn	3-O-(6-O-methyl-β-D-glucuronopyranosyl)methyl asiatate	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)C(=O)OC)C1C(CC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C(=O)OC)CCC(C)C(C)C4C3=CCC21)C)O
MOL000463	0.4429	0.5571	0.7028	Euonymi Alati Ramulus	16844-71-6	119242	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(C1C)O)C)C)C)C
MOL000463	0.4429	0.5571	0.7028	Omphalia	16844-71-6	119242	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(C1C)O)C)C)C)C
MOL000463	0.4429	0.5571	0.7028	Radix Paeoniae Rubra	16844-71-6	119242	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(C1C)O)C)C)C)C
MOL000463	0.4429	0.5571	0.7028	Artemisia Annua L.	16844-71-6	119242	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(C1C)O)C)C)C)C
MOL000463	0.4429	0.5571	0.7028	Paederiae Scandentis Herba	16844-71-6	119242	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(C1C)O)C)C)C)C
MOL000463	0.4429	0.5571	0.7028	Humulus Scandens (Lour.) Merr.	16844-71-6	119242	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(C1C)O)C)C)C)C
MOL000463	0.4429	0.5571	0.7028	Spatholobus Suberectus Dunn	16844-71-6	119242	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(C1C)O)C)C)C)C
MOL000463	0.4429	0.5571	0.7028	Ardisiae Japonicae Herba	16844-71-6	119242	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(C1C)O)C)C)C)C
MOL000463	0.4429	0.5571	0.7028	Pogostemon Cablin (Blanco) Benth.	16844-71-6	119242	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(C1C)O)C)C)C)C
MOL000463	0.4429	0.5571	0.7028	Inulae Herba	16844-71-6	119242	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(C1C)O)C)C)C)C

MOL000464	0.8960	0.1040	0.9662	Spatholobus Suberectus Dunn	4-Pipecoline	69381	FALSE	N1CCC(CC1)C
MOL000465	0.2366	0.7634	0.6622	Maydis Seigma	Hydroxysitosterol	161816	FALSE	C1(CCC2(C(=CC(C3C4CCC(C(CCC(CC)C(C)C)C)C4(C)CCC23)O)C1)C)O
MOL000465	0.2366	0.7634	0.6622	Commelinae Herba	Hydroxysitosterol	161816	FALSE	C1(CCC2(C(=CC(C3C4CCC(C(CCC(CC)C(C)C)C)C4(C)CCC23)O)C1)C)O
MOL000465	0.2366	0.7634	0.6622	Spatholobus Suberectus Dunn	Hydroxysitosterol	161816	FALSE	C1(CCC2(C(=CC(C3C4CCC(C(CCC(CC)C(C)C)C)C4(C)CCC23)O)C1)C)O
MOL000465	0.2366	0.7634	0.6622	Ailanthi Altissimae Fructus	Hydroxysitosterol	161816	FALSE	C1(CCC2(C(=CC(C3C4CCC(C(CCC(CC)C(C)C)C)C4(C)CCC23)O)C1)C)O
MOL000466	0.8595	0.1405	0.7658	Spatholobus Suberectus Dunn	6,8-di-C-α-L-arabinosylapigenin	21576179	FALSE	c1(cc(=O)c2c(o1)c(c(c(c2O)C1C(O)C(O)C(O)CO1)O)C1C(O)C(O)C(O)CO1)c1ccc(cc1)O
MOL000467	0.7499	0.2501	0.9053	licorice	Castanin	5281704	FALSE	c1c(c(=O)c2c(o1)cc(c(c2)OC)O)c1ccc(cc1)OC
MOL000467	0.7499	0.2501	0.9053	Spatholobus Suberectus Dunn	Castanin	5281704	FALSE	c1c(c(=O)c2c(o1)cc(c(c2)OC)O)c1ccc(cc1)OC
MOL000467	0.7499	0.2501	0.9053	Hedysari Radix	Castanin	5281704	FALSE	c1c(c(=O)c2c(o1)cc(c(c2)OC)O)c1ccc(cc1)OC
MOL000468	0.7275	0.2725	0.9249	Spatholobus Suberectus Dunn	8-o-Methylreyusi	5319771	FALSE	c1c(c(=O)c2c(o1)c(c(cc2)O)OC)c1ccc(cc1)OC
MOL000469	0.2127	0.7873	0.6657	Spatholobus Suberectus Dunn	3-Hydroxystigmast-5-en-7-one	160608	FALSE	C1(CCC2(C(=CC(=O)C3C4CCC(C(CCC(CC)C(C)C)C)C4(C)CCC23)C1)C)O
MOL000469	0.2127	0.7873	0.6657	Wikstroemiae Indicae Rasix	3-Hydroxystigmast-5-en-7-one	160608	FALSE	C1(CCC2(C(=CC(=O)C3C4CCC(C(CCC(CC)C(C)C)C)C4(C)CCC23)C1)C)O
MOL000470	0.8990	0.1010	0.8251	Spatholobus Suberectus Dunn	8-C-α-L-arabinosylluteolin	14018803	FALSE	c1(cc(=O)c2c(o1)c(c(cc2O)O)C1C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL000471	0.9108	0.0892	0.7847	Spatholobus Suberectus Dunn	aloe-emodin	10207	FALSE	c1(cc(cc2C(=O)c3cccc(c3C(=O)c12)O)CO)O
MOL000471	0.9108	0.0892	0.7847	Xanthii Fructus	aloe-emodin	10207	FALSE	c1(cc(cc2C(=O)c3cccc(c3C(=O)c12)O)CO)O
MOL000471	0.9108	0.0892	0.7847	Hemerocallis Radix	aloe-emodin	10207	FALSE	c1(cc(cc2C(=O)c3cccc(c3C(=O)c12)O)CO)O
MOL000471	0.9108	0.0892	0.7847	Menthae Herba	aloe-emodin	10207	FALSE	c1(cc(cc2C(=O)c3cccc(c3C(=O)c12)O)CO)O
MOL000471	0.9108	0.0892	0.7847	Actinidia Chinensis Planch	aloe-emodin	10207	FALSE	c1(cc(cc2C(=O)c3cccc(c3C(=O)c12)O)CO)O
MOL000471	0.9108	0.0892	0.7847	Cassiae Semen	aloe-emodin	10207	FALSE	c1(cc(cc2C(=O)c3cccc(c3C(=O)c12)O)CO)O
MOL000471	0.9108	0.0892	0.7847	Oroxyli Semen	aloe-emodin	10207	FALSE	c1(cc(cc2C(=O)c3cccc(c3C(=O)c12)O)CO)O
MOL000471	0.9108	0.0892	0.7847	Radix Rhei Et Rhizome	aloe-emodin	10207	FALSE	c1(cc(cc2C(=O)c3cccc(c3C(=O)c12)O)CO)O
MOL000471	0.9108	0.0892	0.7847	Aloe	aloe-emodin	10207	FALSE	c1(cc(cc2C(=O)c3cccc(c3C(=O)c12)O)CO)O
MOL000472	0.9145	0.0855	0.7393	Rhizoma Fagopyri Cymosi	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Radix Rhei Et Rhizome	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Ampelopsis Japonica	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O

MOL000472	0.9145	0.0855	0.7393	Sennae Folium	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Gnaphalii Affinis Herba	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Xanthii Fructus	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Alpiniae Officinarum Rhizome	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Polygoni Cuspidati Rhizoma Et Radix	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Actinidia Chinensis Planch	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Asteris Radix Et Rhizoma	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Semen Pharbitidis	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Corydalis Rhizoma	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Lilii Bulbus	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Dioscoreaebulbiferae	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Acoritataninowii Rhizoma	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Tribulifructus	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Hoveniae Dulcis Semen	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Alisma Orientale (Sam.) Juz.	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Menthae Herba	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Isatdis Radix	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Cassiae Semen	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Sargentodoxae Caulis	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Dianthi Herba	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Abri Herba	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Bolbostemae Paniculati Bulbus	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Boehmeriae Rhizoma Et Radix	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Spatholobus Suberectus Dunn	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Epimrdii Herba	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Sophorae Tonkinensis Radix Et Rhizome	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000472	0.9145	0.0855	0.7393	Lycii Cortex	emodin	3220	FALSE	c1(cc(cc2C(=O)c3cc(cc(c3C(=O)c12)O)C)O)O
MOL000473	0.9566	0.0434	0.9769	Acoritataninowii Rhizoma	(-)-trans-Carveol	94221	FALSE	C1(C(=CCC(C1)C(=C)C)C)O
MOL000473	0.9566	0.0434	0.9769	Artemisia Annua L.	(-)-trans-Carveol	94221	FALSE	C1(C(=CCC(C1)C(=C)C)C)O
MOL000473	0.9566	0.0434	0.9769	Spatholobus Suberectus Dunn	(-)-trans-Carveol	94221	FALSE	C1(C(=CCC(C1)C(=C)C)C)O
MOL000473	0.9566	0.0434	0.9769	Campsis Flos	(-)-trans-Carveol	94221	FALSE	C1(C(=CCC(C1)C(=C)C)C)O

MOL000474	0.8035	0.1965	0.6474	Borneolum Syntheticum	(-)-Epoxycaryophyllene	Not Available	FALSE	C12CCC3(OC3CCC(=C)C1CC2(C)C)C
MOL000474	0.8035	0.1965	0.6474	Schizonepetae Spica	(-)-Epoxycaryophyllene	Not Available	FALSE	C12CCC3(OC3CCC(=C)C1CC2(C)C)C
MOL000474	0.8035	0.1965	0.6474	Violsse Herba	(-)-Epoxycaryophyllene	Not Available	FALSE	C12CCC3(OC3CCC(=C)C1CC2(C)C)C
MOL000474	0.8035	0.1965	0.6474	Leonuri Herba	(-)-Epoxycaryophyllene	Not Available	FALSE	C12CCC3(OC3CCC(=C)C1CC2(C)C)C
MOL000474	0.8035	0.1965	0.6474	Spatholobus Suberectus Dunn	(-)-Epoxycaryophyllene	Not Available	FALSE	C12CCC3(OC3CCC(=C)C1CC2(C)C)C
MOL000474	0.8035	0.1965	0.6474	Curcumae Rhizoma	(-)-Epoxycaryophyllene	Not Available	FALSE	C12CCC3(OC3CCC(=C)C1CC2(C)C)C
MOL000474	0.8035	0.1965	0.6474	Cnidii Fructus	(-)-Epoxycaryophyllene	Not Available	FALSE	C12CCC3(OC3CCC(=C)C1CC2(C)C)C
MOL000474	0.8035	0.1965	0.6474	Olibanun	(-)-Epoxycaryophyllene	Not Available	FALSE	C12CCC3(OC3CCC(=C)C1CC2(C)C)C
MOL000474	0.8035	0.1965	0.6474	Ardisiae Japonicae Herba	(-)-Epoxycaryophyllene	Not Available	FALSE	C12CCC3(OC3CCC(=C)C1CC2(C)C)C
MOL000475	0.9568	0.0432	0.9300	Dianthi Herba	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Foeniculi Fructus	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Eupatorium Fortunei Turcz	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Zanthoxyli Pericarpium	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Phragmitis Rhizoma	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Citri Grandis Exocarpium	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	licorice	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Spatholobus Suberectus Dunn	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Ganoderma	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Asteris Radix Et Rhizoma	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Coriandri Sativi Herba	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Cornus Officinalis Sieb. Et Zucc.	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Rubi Fructus	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC

MOL000475	0.9568	0.0432	0.9300	Piperis Longi Fructus	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Anisi Stellati Fructus	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Curcumaelongae Rhizoma	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Flemingia Prostrata Roxb	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Piperis Fructus	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Crotonis Fructus	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Rhizome Of Whiteback Greenbrier	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Arum Ternatum Thunb.	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Aucklandiae Radix	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Pogostemon Cablin (Blanco) Benth.	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Cinnanmomi Cortex	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Cinnamomi Ramulus	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Ginkgo Folium	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000475	0.9568	0.0432	0.9300	Platycladi Cacumen	anethole	637563	FALSE	c1(ccc(cc1)/C=C/C)OC
MOL000476	0.8420	0.1580	0.7734	Radix Salviae	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Areca Catechu L.	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Viticis Fructus	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Sennae Folium	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Menthae Herba	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Rubia Cordifolia	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Cassiae Semen	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Morindae Officinalis Radix	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Tribulifructus	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Boehmeriae Rhizoma Et Radix	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Evodiae Fructus	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Lycii Fructus	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Sargentodoxae Caulis	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Radix Rhei Et Rhizome	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Dianthi Herba	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Gnaphalii Affinis Herba	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Glechomae Herba	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Corydalis Rhizoma	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Sophorae Tonkinensis Radix Et Rhizome	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Abri Herba	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Asteris Radix Et Rhizoma	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Lycii Cortex	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O

MOL000476	0.8420	0.1580	0.7734	Spatholobus Suberectus Dunn	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Folium Ilicis Cornutae	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Ampelopsis Japonica	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Dysosmae Verspiellis Rhixoma Et Radix	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Polygoni Cuspidati Rhizoma Et Radix	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000476	0.8420	0.1580	0.7734	Semen Pharbitidis	Physcion	10639	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C)c(cc(c2)OC)O
MOL000477	0.8460	0.1540	0.8083	Gossampiniflos	Ethyllaurate	7800	FALSE	C(=O)(CCCCCCCCCCC)OCC
MOL000477	0.8460	0.1540	0.8083	Spatholobus Suberectus Dunn	Ethyllaurate	7800	FALSE	C(=O)(CCCCCCCCCCC)OCC
MOL000477	0.8460	0.1540	0.8083	Saussureae Involucratae Herba	Ethyllaurate	7800	FALSE	C(=O)(CCCCCCCCCCC)OCC
MOL000477	0.8460	0.1540	0.8083	Radix Angelicae Biseratae	Ethyllaurate	7800	FALSE	C(=O)(CCCCCCCCCCC)OCC
MOL000478	0.9517	0.0483	0.9706	Piperis Fructus	Eucarvone	136330	FALSE	C1(=O)C(=CC=CC(C1)(C)C)C
MOL000478	0.9517	0.0483	0.9706	Ginkgo Folium	Eucarvone	136330	FALSE	C1(=O)C(=CC=CC(C1)(C)C)C
MOL000478	0.9517	0.0483	0.9706	Spatholobus Suberectus Dunn	Eucarvone	136330	FALSE	C1(=O)C(=CC=CC(C1)(C)C)C
MOL000478	0.9517	0.0483	0.9706	Chrysanthemi Flos	Eucarvone	136330	FALSE	C1(=O)C(=CC=CC(C1)(C)C)C
MOL000478	0.9517	0.0483	0.9706	Asari Radix Et Rhizoma	Eucarvone	136330	FALSE	C1(=O)C(=CC=CC(C1)(C)C)C
MOL000478	0.9517	0.0483	0.9706	Kaempferiae Rhizoma	Eucarvone	136330	FALSE	C1(=O)C(=CC=CC(C1)(C)C)C
MOL000478	0.9517	0.0483	0.9706	Folium Artemisiae Argyi	Eucarvone	136330	FALSE	C1(=O)C(=CC=CC(C1)(C)C)C
MOL000478	0.9517	0.0483	0.9706	Olibanun	Eucarvone	136330	FALSE	C1(=O)C(=CC=CC(C1)(C)C)C
MOL000478	0.9517	0.0483	0.9706	Angelicae Sinensis Radix	Eucarvone	136330	FALSE	C1(=O)C(=CC=CC(C1)(C)C)C
MOL000478	0.9517	0.0483	0.9706	Myrrha	Eucarvone	136330	FALSE	C1(=O)C(=CC=CC(C1)(C)C)C
MOL000478	0.9517	0.0483	0.9706	Epimrdii Herba	Eucarvone	136330	FALSE	C1(=O)C(=CC=CC(C1)(C)C)C
MOL000478	0.9517	0.0483	0.9706	Magnoliae Flos	Eucarvone	136330	FALSE	C1(=O)C(=CC=CC(C1)(C)C)C
MOL000478	0.9517	0.0483	0.9706	Citrus Aurantium	Eucarvone	136330	FALSE	C1(=O)C(=CC=CC(C1)(C)C)C
MOL000479	0.8298	0.1702	0.7447	Myrrha	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Zingiberis Rhizoma	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Magnolia Officinalis Rehd Et Wils.	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Angelicae Sinensis Radix	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Ligustici Rhizoma Et Radix	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Herba Clinopodii Polycephali.	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Schisandrae Chinensis Fructus	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Panacis Japonici Rhizoma	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Notopterygii Rhizoma Et Radix	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C

MOL000479	0.8298	0.1702	0.7447	Panacis Quinquefolii Radix	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Dalbergiae Odoriferae Lignum	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Cinnanmomi Cortex	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Rhizome Of Whiteback Greenbrier	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Broussonetiae Fructus	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Verbenae Herb	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Farfarae Flos	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Ginkgo Folium	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Radix Bupleuri	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Eupatorium Fortunei Turcz	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Lonicerae Japonicae Flos	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Perilla Frutescens	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Cnidii Fructus	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Carthami Flos	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Ginseng Folium	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Bidentis Bipinnatae Herba	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Spatholobus Suberectus Dunn	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Aucklandiae Radix	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Curcumae Radix	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Folium Artemisiae Argyi	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Solidaginis Herba	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Artemisia Annua L.	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Piperis Fructus	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Eriobotryae Folium	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Citrus Aurantium	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Platycladi Cacumen	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Piperis Longi Fructus	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Ailanthi Cortex	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Herba Taxilli	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Viticis Negundo Folium	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Ginsen Radix Et Rhizoma Rubra	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Rubi Fructus	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000479	0.8298	0.1702	0.7447	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Farnesene	5281517	FALSE	C=CC(=C)CC/C=C(/CCC=C(C)C)\C
MOL000480	0.8640	0.1360	0.8555	Sojae Semen Nigrum	genistin	5281377	FALSE	c1c(c(=O)c2c(o1)cc(cc2O)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)O
MOL000480	0.8640	0.1360	0.8555	Belamcandae Rhizome	genistin	5281377	FALSE	c1c(c(=O)c2c(o1)cc(cc2O)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)O

MOL000480	0.8640	0.1360	0.8555	Sojae Semen Praeparatum	genistin	5281377	FALSE	c1c(c(=O)c2c(o1)cc(cc2O)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)O
MOL000480	0.8640	0.1360	0.8555	Spatholobus Suberectus Dunn	genistin	5281377	FALSE	c1c(c(=O)c2c(o1)cc(cc2O)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)O
MOL000480	0.8640	0.1360	0.8555	Fructussophorae	genistin	5281377	FALSE	c1c(c(=O)c2c(o1)cc(cc2O)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)O
MOL000481	0.9496	0.0504	0.9465	Puerariae Flos	genistein	5280961	TRUE	c1c(c(=O)c2c(o1)cc(cc2O)O)c1ccc(cc1)O
MOL000481	0.9496	0.0504	0.9465	Flos Genkwa	genistein	5280961	TRUE	c1c(c(=O)c2c(o1)cc(cc2O)O)c1ccc(cc1)O
MOL000481	0.9496	0.0504	0.9465	Radix Puerariae	genistein	5280961	TRUE	c1c(c(=O)c2c(o1)cc(cc2O)O)c1ccc(cc1)O
MOL000481	0.9496	0.0504	0.9465	Cistanches Herba	genistein	5280961	TRUE	c1c(c(=O)c2c(o1)cc(cc2O)O)c1ccc(cc1)O
MOL000481	0.9496	0.0504	0.9465	Sojae Semen Nigrum	genistein	5280961	TRUE	c1c(c(=O)c2c(o1)cc(cc2O)O)c1ccc(cc1)O
MOL000481	0.9496	0.0504	0.9465	Semiaquilegiae Radix	genistein	5280961	TRUE	c1c(c(=O)c2c(o1)cc(cc2O)O)c1ccc(cc1)O
MOL000481	0.9496	0.0504	0.9465	Spatholobus Suberectus Dunn	genistein	5280961	TRUE	c1c(c(=O)c2c(o1)cc(cc2O)O)c1ccc(cc1)O
MOL000481	0.9496	0.0504	0.9465	Fructussophorae	genistein	5280961	TRUE	c1c(c(=O)c2c(o1)cc(cc2O)O)c1ccc(cc1)O
MOL000481	0.9496	0.0504	0.9465	Eucommiae Cortex	genistein	5280961	TRUE	c1c(c(=O)c2c(o1)cc(cc2O)O)c1ccc(cc1)O
MOL000481	0.9496	0.0504	0.9465	Sojae Semen Praeparatum	genistein	5280961	TRUE	c1c(c(=O)c2c(o1)cc(cc2O)O)c1ccc(cc1)O
MOL000481	0.9496	0.0504	0.9465	Sophorae Tonkinensis Radix Et Rhizome	genistein	5280961	TRUE	c1c(c(=O)c2c(o1)cc(cc2O)O)c1ccc(cc1)O
MOL000481	0.9496	0.0504	0.9465	Iridis Tectori Rhizoma	genistein	5280961	TRUE	c1c(c(=O)c2c(o1)cc(cc2O)O)c1ccc(cc1)O
MOL000481	0.9496	0.0504	0.9465	Belamcandae Rhizome	genistein	5280961	TRUE	c1c(c(=O)c2c(o1)cc(cc2O)O)c1ccc(cc1)O
MOL000482	0.9229	0.0771	0.9169	Spatholobus Suberectus Dunn	levodopa	6971033	TRUE	C(=O)(C(Cc1cc(c(cc1)O)O)N)O
MOL000483	0.8309	0.1691	0.7609	Tribulifructus	(Z)-3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	6440659	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)OC)NCCc1ccc(cc1)O
MOL000483	0.8309	0.1691	0.7609	Solanum Melongena L	(Z)-3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	6440659	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)OC)NCCc1ccc(cc1)O

MOL000483	0.8309	0.1691	0.7609	Piperis Fructus	(Z)-3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	6440659	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)OC)NCCc1ccc(cc1)O
MOL000483	0.8309	0.1691	0.7609	Cannabis Sativa L.	(Z)-3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	6440659	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)OC)NCCc1ccc(cc1)O
MOL000483	0.8309	0.1691	0.7609	Anemarrhenae Rhizoma	(Z)-3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	6440659	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)OC)NCCc1ccc(cc1)O
MOL000483	0.8309	0.1691	0.7609	Allium Azureum Ledeb.	(Z)-3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	6440659	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)OC)NCCc1ccc(cc1)O
MOL000483	0.8309	0.1691	0.7609	Polygonati Odorati Rhizoma	(Z)-3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	6440659	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)OC)NCCc1ccc(cc1)O

MOL000483	0.8309	0.1691	0.7609	Cimicifugae Rhizoma	(Z)-3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	6440659	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)OC)NCCc1ccc(cc1)O
MOL000483	0.8309	0.1691	0.7609	Spatholobus Suberectus Dunn	(Z)-3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	6440659	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)OC)NCCc1ccc(cc1)O
MOL000484	0.8757	0.1243	0.9536	Spatholobus Suberectus Dunn	Dilospan S	359	FALSE	c1(cc(cc(c1)O)O)O
MOL000485	0.9512	0.0488	0.7730	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	TMH	82227	FALSE	C12C(=CCC(C1(C)C)C2)C
MOL000485	0.9512	0.0488	0.7730	Leonuri Fructus	TMH	82227	FALSE	C12C(=CCC(C1(C)C)C2)C
MOL000485	0.9512	0.0488	0.7730	Coriandri Sativi Herba	TMH	82227	FALSE	C12C(=CCC(C1(C)C)C2)C
MOL000485	0.9512	0.0488	0.7730	Radix Salviae	TMH	82227	FALSE	C12C(=CCC(C1(C)C)C2)C
MOL000485	0.9512	0.0488	0.7730	Moslae Herba	TMH	82227	FALSE	C12C(=CCC(C1(C)C)C2)C
MOL000485	0.9512	0.0488	0.7730	Pogostemon Cablin (Blanco) Benth.	TMH	82227	FALSE	C12C(=CCC(C1(C)C)C2)C
MOL000485	0.9512	0.0488	0.7730	Curcumae Rhizoma	TMH	82227	FALSE	C12C(=CCC(C1(C)C)C2)C
MOL000485	0.9512	0.0488	0.7730	Houttuyniae Herba	TMH	82227	FALSE	C12C(=CCC(C1(C)C)C2)C
MOL000485	0.9512	0.0488	0.7730	Olibanun	TMH	82227	FALSE	C12C(=CCC(C1(C)C)C2)C
MOL000485	0.9512	0.0488	0.7730	Myristicae Semen	TMH	82227	FALSE	C12C(=CCC(C1(C)C)C2)C
MOL000485	0.9512	0.0488	0.7730	Spatholobus Suberectus Dunn	TMH	82227	FALSE	C12C(=CCC(C1(C)C)C2)C
MOL000485	0.9512	0.0488	0.7730	Curcumaelongae Rhizoma	TMH	82227	FALSE	C12C(=CCC(C1(C)C)C2)C
MOL000486	0.9208	0.0792	0.9346	licorice	Prunetin	5281804	FALSE	c1c(c(=O)c2c(o1)cc(cc2O)OC)c1ccc(cc1)O
MOL000486	0.9208	0.0792	0.9346	Spatholobus Suberectus Dunn	Prunetin	5281804	FALSE	c1c(c(=O)c2c(o1)cc(cc2O)OC)c1ccc(cc1)O
MOL000486	0.9208	0.0792	0.9346	Dalbergiae Odoriferae Lignum	Prunetin	5281804	FALSE	c1c(c(=O)c2c(o1)cc(cc2O)OC)c1ccc(cc1)O
MOL000486	0.9208	0.0792	0.9346	Oroxyli Semen	Prunetin	5281804	FALSE	c1c(c(=O)c2c(o1)cc(cc2O)OC)c1ccc(cc1)O
MOL000487	0.3400	0.6600	0.6971	Spatholobus Suberectus Dunn	Schisandrin	Not Available	FALSE	c12c3c(c(c(cc3CCCCc2cc(c(c1OC)OC)OC)OC)OC)OC

MOL000487	0.3400	0.6600	0.6971	Kadsurae Coccineae Radix Et Caulis	Schisandrin	Not Available	FALSE	c12c3c(c(c(cc3CCCCc2cc(c(c1OC)OC)OC)OC)OC)OC
MOL000488	0.4523	0.5477	0.7301	Spatholobus Suberectus Dunn	Schizandrol	Not Available	FALSE	c12c3c(cc(c(c3OC)OC)OC)CC(C(Cc1cc1c(c2OC)OCO1)C)(C)O
MOL000489	0.8550	0.1450	0.6445	Gnaphalii Affinis Herba	(1S,4aR,8aR)-1-isopropyl-7-methyl-4-methylene-2,3,4a,5,6,8a-hexahydro-1H-naphthalene	6432404	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C
MOL000489	0.8550	0.1450	0.6445	Zingiberis Rhizoma	(1S,4aR,8aR)-1-isopropyl-7-methyl-4-methylene-2,3,4a,5,6,8a-hexahydro-1H-naphthalene	6432404	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C
MOL000489	0.8550	0.1450	0.6445	Cinnanmomi Cortex	(1S,4aR,8aR)-1-isopropyl-7-methyl-4-methylene-2,3,4a,5,6,8a-hexahydro-1H-naphthalene	6432404	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C
MOL000489	0.8550	0.1450	0.6445	Cayratiae Japonicae Herba	(1S,4aR,8aR)-1-isopropyl-7-methyl-4-methylene-2,3,4a,5,6,8a-hexahydro-1H-naphthalene	6432404	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C

MOL000489	0.8550	0.1450	0.6445	Spatholobus Suberectus Dunn	(1S,4aR,8aR)-1-isopropyl-7-methyl-4-methylene-2,3,4a,5,6,8a-hexahydro-1H-naphthalene	6432404	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C
MOL000489	0.8550	0.1450	0.6445	Angelicae Sinensis Radix	(1S,4aR,8aR)-1-isopropyl-7-methyl-4-methylene-2,3,4a,5,6,8a-hexahydro-1H-naphthalene	6432404	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C
MOL000489	0.8550	0.1450	0.6445	Myrrha	(1S,4aR,8aR)-1-isopropyl-7-methyl-4-methylene-2,3,4a,5,6,8a-hexahydro-1H-naphthalene	6432404	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C
MOL000489	0.8550	0.1450	0.6445	Bidentis Bipinnatae Herba	(1S,4aR,8aR)-1-isopropyl-7-methyl-4-methylene-2,3,4a,5,6,8a-hexahydro-1H-naphthalene	6432404	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C
MOL000489	0.8550	0.1450	0.6445	Solidaginis Herba	(1S,4aR,8aR)-1-isopropyl-7-methyl-4-methylene-2,3,4a,5,6,8a-hexahydro-1H-naphthalene	6432404	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C

MOL000489	0.8550	0.1450	0.6445	Sedi Herba	(1S,4aR,8aR)-1-isopropyl-7-methyl-4-methylene-2,3,4a,5,6,8a-hexahydro-1H-naphthalene	6432404	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C
MOL000492	0.9402	0.0598	0.8161	Polygoni Cuspidati Rhizoma Et Radix	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Bistortae Rhizoma	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Sesami Nigrum Semen	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Eucommiae Folium	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Cinnamomi Ramulus	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Hordei Fructus Germinatus	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Spatholobus Suberectus Dunn	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Boehmeriae Rhizoma Et Radix	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Apocyniveneti Folium	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Hippophae Fructus	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Potentillae Discoloris Herba	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Rhizoma Fagopyri Cymosi	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Radix Paeoniae Rubra	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Allii Fistulost Bulbus	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Ginkgo Folium	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Drynariae Rhizoma	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Saxifraga Stolonifera	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Ilicis Cornutae Folium Immayuri	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Paeoniae Radix Alba	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Herbahypericiperforati	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Ampelopsis Japonica	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Moslae Herba	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Granati Pericarpium	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Phaseoli Semen	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Actinidia Chinensis Planch	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Phyllanthi Fructus	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Celastri Orbiculati Fructus	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Ephedrae Radix Et Rhizoma	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Jujubae Fructus	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O

MOL000492	0.9402	0.0598	0.8161	Cortex Moutan	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Polygoni Avicularis Herba	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Agrimonia Eupatoria	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Ginkgo Semen	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Anisi Stellati Fructus	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Catechu	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000492	0.9402	0.0598	0.8161	Polygoni Orientalis Fructus	(+)-catechin	9064	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)O)c1cc(c(cc1)O)O
MOL000494	0.8905	0.1095	0.8567	Spatholobus Suberectus Dunn	5-[(3R)-7-hydroxychroman-3-yl]-2,3-dimethoxy-p-benzoquinone	10403457	FALSE	C1(=O)C(=C(C(=O)C(=C1)C1COc2c(C1)ccc(c2)O)OC)OC
MOL000495	0.7663	0.2337	0.8726	Spatholobus Suberectus Dunn	odoratin	Not Available	FALSE	C(=O)(/C=C\c1ccc(cc1)OC)c1c(c(cc1O)OC)OC)OC
MOL000497	0.4669	0.5331	0.6477	Spatholobus Suberectus Dunn	licochalcone a	5318998	FALSE	C(=O)(/C=C/c1c(cc(c(c1)C(C)(C=C)C)O)OC)c1ccc(cc1)O
MOL000497	0.4669	0.5331	0.6477	licorice	licochalcone a	5318998	FALSE	C(=O)(/C=C/c1c(cc(c(c1)C(C)(C=C)C)O)OC)c1ccc(cc1)O
MOL000498	0.9101	0.0899	0.8220	Herba Patriniae	isoorientin	114776	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)C1C(O)C(O)C(O)C(O1)CO)O)c1cc(c(cc1)O)O
MOL000498	0.9101	0.0899	0.8220	Spatholobus Suberectus Dunn	isoorientin	114776	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)C1C(O)C(O)C(O)C(O1)CO)O)c1cc(c(cc1)O)O
MOL000498	0.9101	0.0899	0.8220	Prunellae Spica	isoorientin	114776	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)C1C(O)C(O)C(O)C(O1)CO)O)c1cc(c(cc1)O)O
MOL000498	0.9101	0.0899	0.8220	Trigonellae Semen	isoorientin	114776	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)C1C(O)C(O)C(O)C(O1)CO)O)c1cc(c(cc1)O)O
MOL000498	0.9101	0.0899	0.8220	Polygoni Orientalis Fructus	isoorientin	114776	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)C1C(O)C(O)C(O)C(O1)CO)O)c1cc(c(cc1)O)O
MOL000498	0.9101	0.0899	0.8220	Commelinae Herba	isoorientin	114776	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)C1C(O)C(O)C(O)C(O1)CO)O)c1cc(c(cc1)O)O
MOL000498	0.9101	0.0899	0.8220	Cymbopon Citratus(D C.) Stapf	isoorientin	114776	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)C1C(O)C(O)C(O)C(O1)CO)O)c1cc(c(cc1)O)O
MOL000498	0.9101	0.0899	0.8220	Abrus Precatorius L.	isoorientin	114776	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)C1C(O)C(O)C(O)C(O1)CO)O)c1cc(c(cc1)O)O
MOL000498	0.9101	0.0899	0.8220	Gentianae Radix Et Rhozima	isoorientin	114776	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)C1C(O)C(O)C(O)C(O1)CO)O)c1cc(c(cc1)O)O
MOL000498	0.9101	0.0899	0.8220	Santalum Album L.	isoorientin	114776	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)C1C(O)C(O)C(O)C(O1)CO)O)c1cc(c(cc1)O)O
MOL000498	0.9101	0.0899	0.8220	Hordei Fructus Germinatus	isoorientin	114776	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)C1C(O)C(O)C(O)C(O1)CO)O)c1cc(c(cc1)O)O
MOL000498	0.9101	0.0899	0.8220	Crataegi Folium	isoorientin	114776	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)C1C(O)C(O)C(O)C(O1)CO)O)c1cc(c(cc1)O)O

MOL000498	0.9101	0.0899	0.8220	Viticis Fructus	isoorientin	114776	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)C1C(O)C(O)C(O)C(O1)CO)O)c1cc(c(cc1)O)O
MOL000500	0.9005	0.0995	0.8992	Hedysari Radix	Vestitol	177149	FALSE	C1C(Cc2c(O1)cc(cc2)O)c1c(cc(cc1)OC)O
MOL000500	0.9005	0.0995	0.8992	Spatholobus Suberectus Dunn	Vestitol	177149	FALSE	C1C(Cc2c(O1)cc(cc2)O)c1c(cc(cc1)OC)O
MOL000500	0.9005	0.0995	0.8992	licorice	Vestitol	177149	FALSE	C1C(Cc2c(O1)cc(cc2)O)c1c(cc(cc1)OC)O
MOL000501	0.9021	0.0979	0.8673	Spatholobus Suberectus Dunn	Consume close grain	Not Available	FALSE	c1(c(cc2c(c1)OC(CC2=O)c1cc(c(O)cc1)O)OC)O
MOL000502	0.9354	0.0646	0.9056	Spatholobus Suberectus Dunn	Cajinin	5281706	FALSE	c1c(c(=O)c2c(cc(cc2o1)OC)O)c1c(cc(cc1)O)O
MOL000503	0.9394	0.0606	0.6960	Spatholobus Suberectus Dunn	Medicagol	Not Available	FALSE	c1(=O)c2c(c3c(o1)cc(cc3)O)oc1c2cc2c(c1)OCO2
MOL000504	0.1841	0.8159	0.6119	Spatholobus Suberectus Dunn	kadsurin	Not Available	FALSE	c1(c(c(c2c(c1)CC(C(C(c1c2c(c2c(c1)OCO2)OC)OC(=C)C)C)C)OC)OC)OC
MOL000505	0.2621	0.7379	0.6572	Spatholobus Suberectus Dunn	interiorin	Not Available	FALSE	O1COc2c1cc1c3C4(COc23)C(C(C(=O)CC4CC(C(C1OC(=O)/C(=C/C)/C)C)C)OC)OC
MOL000507	0.8057	0.1943	0.8979	Spatholobus Suberectus Dunn	Psi-Baptigenin	5281805	FALSE	c1(c2c(=O)c3c(oc2)cc(cc3)O)cc2c(cc1)OCO2
MOL000508	0.3879	0.6121	0.7207	Lygodii Spora	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Gleditsiae Spina	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Omphalia	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Paederiae Scandentis Herba	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Clematidis Armandii Caulis	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Euonymi Alati Ramulus	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Radix Clematidis	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Asteris Radix Et Rhizoma	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Humulus Scandens (Lour.) Merr.	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Codonopsis Radix	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Pogostemon Cablin (Blanco) Benth.	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Portulacae Herba	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C

MOL000508	0.3879	0.6121	0.7207	Citri Exocarpium Rubrum	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Bistortae Rhizoma	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Maydis Seigma	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Radix Paeoniae Rubra	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Imperatae Rhizoma	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Ardisiae Japonicae Herba	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Commelinae Herba	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Phellodendri Amurensis Cortex	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Artemisia Annua L.	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Spatholobus Suberectus Dunn	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Microctis Folium	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Folium Artemisiae Argyi	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Glechomae Herba	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Kaki Calyx	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Caulis Akebiae	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000508	0.3879	0.6121	0.7207	Coicis Semen	Friedelin	91472	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(=O)C1C)C)C)C)C
MOL000509	0.8185	0.1815	0.8955	Spatholobus Suberectus Dunn	isosativan	14058036	FALSE	c1(c(ccc(c1)OC)C1COc2c(C1)ccc(c2)OC)O
MOL000510	0.9253	0.0747	0.9373	Puerariae Flos	olmelin	5280373	TRUE	c1c(c(=O)c2c(o1)cc(cc2O)O)c1ccc(cc1)OC
MOL000510	0.9253	0.0747	0.9373	Trigonellae Semen	olmelin	5280373	TRUE	c1c(c(=O)c2c(o1)cc(cc2O)O)c1ccc(cc1)OC
MOL000510	0.9253	0.0747	0.9373	Sojae Semen Praeparatum	olmelin	5280373	TRUE	c1c(c(=O)c2c(o1)cc(cc2O)O)c1ccc(cc1)OC
MOL000510	0.9253	0.0747	0.9373	Spatholobus Suberectus Dunn	olmelin	5280373	TRUE	c1c(c(=O)c2c(o1)cc(cc2O)O)c1ccc(cc1)OC
MOL000511	0.7574	0.2426	0.9071	Gardeniae Fructus	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Glechomae Herba	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O

MOL000511	0.7574	0.2426	0.9071	Herba Patriniae	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Herba Clinopodii Polycephali.	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Chrysanthemi Indici Flos	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Strychni Semen	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Abri Herba	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Lithospermum Erythrorhizon	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Hippophae Fructus	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Maydis Seigma	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Ilicis Purpureae Folium	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Peucedani Radix	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Rhododendri Daurici Folium	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Tripterygii Radix	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Uncariae Ramulus Cumuncis	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Ailanthi Cortex	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Trollius Chinensis	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Semen Pruni	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Eucommiae Cortex	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Bovis Calculus	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Folium Ilicis Cornutae	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Tamaricis Cacumen	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Mori Cortex	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O

MOL000511	0.7574	0.2426	0.9071	Pseudostellariae Radix	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Herba Pyrolae	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Jujubae Fructus	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Hedysari Radix	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Dipsaci Radix	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Crataegi Folium	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Lysimachiae Foenigraeci Herba	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Salviae Chinensis Herba	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Ilicis Cornutae Folium Immayuri	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Nardostachyos Radix Et Rhizoma	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Sedum Aizoon L.	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Plantaginis Herba	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Forsythiae Fructus	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Rubi Fructus	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Actinidia Chinensis Planch	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Hedyotis Diffusae Herba	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Schizonepetae Spica	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Figwort Root	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Lignum Pini Nodi	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Rosae Laevigatae Fructus	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Achyranthis Asperae Herba	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O

MOL000511	0.7574	0.2426	0.9071	Eriobotryae Folium	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Kaki Calyx	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Momordicae Semen	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Prinsepiae Nux	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Schizonepetae Herba	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Lonicerae Japonicae Flos	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Campsis Flos	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Cornus Officinalis Sieb. Et Zucc.	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Granati Pericarpium	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Verbenae Herb	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Pulsatilliae Radix	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Potentillae Chinensis Herba	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Paederiae Scandentis Herba	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Cortex Periplocae Radicis	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Scutellariae Barbatae Herba	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Ailanthi Altissimae Fructus	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Fructuslipuidambaris	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	licorice	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Radix Salviae	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Mume Fructus	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Mori Cortex	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O

MOL000511	0.7574	0.2426	0.9071	Chaenomeles Sinensis (Thouin) Koehne	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Agrimonia Eupatoria	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Moslae Herba	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Rhapontici Radix	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Fructus Ligustri Lucidi	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Prunellae Spica	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Potentillae Discoloris Herba	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Perilla Frutescens	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Gentianae Radix Et Rhozima	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Menthae Herba	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Fraxini Cortex	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000511	0.7574	0.2426	0.9071	Lycopi Herba	ursolic acid	64945	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)O
MOL000513	0.9372	0.0628	0.9580	Chaenomeles Sinensis (Thouin) Koehne	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Apocyniveneti Folium	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Saxifraga Stolonifera	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Potentillae Discoloris Herba	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Folium Nelumbinis	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O

MOL000513	0.9372	0.0628	0.9580	Mori Cortex	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Cotyledon Fimbriata Turcz.	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Rhododendri Daurici Folium	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Canarii Fructus	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Paeoniae Radix Alba	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Canavaliae Semen	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Areca Catechu L.	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Euphorbiae Helioscopiae Herba	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Choerospondiatis Fructus	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Phyllanthi Fructus	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Polygoni Orientalis Fructus	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Chebulae Fructus	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Abrus Precatorius L.	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Sesami Nigrum Semen	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O

MOL000513	0.9372	0.0628	0.9580	Galla Chinensis	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Tamaricis Cacumen	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Kaki Calyx	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Polygoni Avicularis Herba	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Rubi Fructus	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Agrimonia Eupatoria	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Fructussophorae	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Hoveniae Dulcis Semen	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Cornus Officinalis Sieb. Et Zucc.	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Rose Rugosae Flos	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Ampelopsis Japonica	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Euphorbiae Humifusae Herba	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Radix Paeoniae Rubra	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Arisaematis Rhizoma	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O

MOL000513	0.9372	0.0628	0.9580	Zanthoxyli Pericarpium	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Smilax China	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Peucedani Radix	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Bistortae Rhizoma	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Cortex Moutan	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Arum Ternatum Thunb.	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Prinsepiae Nux	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Polygoni Cuspidati Rhizoma Et Radix	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Farfarae Flos	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Granati Pericarpium	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Quisqualis Indica	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Fructuslipuidambaris	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Radix Rhei Et Rhizome	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Potentillae Chinensis Herba	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O

MOL000513	0.9372	0.0628	0.9580	Ailanthi Altissimae Fructus	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Geranium Wilfordii Maxim.	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Sedum Aizoon L.	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000513	0.9372	0.0628	0.9580	Boschniakia Rossica Herba	3,4,5-trihydroxybenzoic acid	370	FALSE	C(=O)(c1cc(O)c(O)c(O)c1)O
MOL000517	0.6030	0.3970	0.7199	Fructuslipuidambaris	isostyracin epoxide	Not Available	FALSE	c1cc(ccc1)/C=C\C(=O)OCC1OC1c1ccccc1
MOL000519	0.5872	0.4128	0.7888	Fructuslipuidambaris	coniferin	389888	FALSE	C1(=O)C(=C(C(=O)c2c3cccc(c3ccc12)C)C)O)C(
MOL000519	0.5872	0.4128	0.7888	Arum Ternatum Thunb.	coniferin	389888	FALSE	C1(=O)C(=C(C(=O)c2c3cccc(c3ccc12)C)C)O)C(
MOL000520	0.4015	0.5985	0.6981	Campsis Flos	alpha-amyrin	73170	FALSE	C12C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)C)(CCC(C1(C)C)O)C
MOL000520	0.4015	0.5985	0.6981	Fructuslipuidambaris	alpha-amyrin	73170	FALSE	C12C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)C)(CCC(C1(C)C)O)C
MOL000520	0.4015	0.5985	0.6981	Folium Artemisiae Argyi	alpha-amyrin	73170	FALSE	C12C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)C)(CCC(C1(C)C)O)C
MOL000520	0.4015	0.5985	0.6981	Hippophae Fructus	alpha-amyrin	73170	FALSE	C12C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)C)(CCC(C1(C)C)O)C
MOL000520	0.4015	0.5985	0.6981	Sedi Herba	alpha-amyrin	73170	FALSE	C12C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)C)(CCC(C1(C)C)O)C
MOL000520	0.4015	0.5985	0.6981	Gentianae Radix Et Rhozima	alpha-amyrin	73170	FALSE	C12C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)C)(CCC(C1(C)C)O)C
MOL000520	0.4015	0.5985	0.6981	Canarii Fructus	alpha-amyrin	73170	FALSE	C12C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)C)(CCC(C1(C)C)O)C
MOL000520	0.4015	0.5985	0.6981	Phyllanthi Fructus	alpha-amyrin	73170	FALSE	C12C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)C)(CCC(C1(C)C)O)C
MOL000520	0.4015	0.5985	0.6981	Mori Cortex	alpha-amyrin	73170	FALSE	C12C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)C)(CCC(C1(C)C)O)C
MOL000520	0.4015	0.5985	0.6981	Cortex Periplocae Radicis	alpha-amyrin	73170	FALSE	C12C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)C)(CCC(C1(C)C)O)C
MOL000520	0.4015	0.5985	0.6981	Gentiana Macrophylla Pall	alpha-amyrin	73170	FALSE	C12C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)C)(CCC(C1(C)C)O)C
MOL000520	0.4015	0.5985	0.6981	Ilicis Cornutae Folium Immayuri	alpha-amyrin	73170	FALSE	C12C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)C)(CCC(C1(C)C)O)C
MOL000520	0.4015	0.5985	0.6981	Foeniculi Fructus	alpha-amyrin	73170	FALSE	C12C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)C)(CCC(C1(C)C)O)C

MOL000520	0.4015	0.5985	0.6981	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	alpha-amyrin	73170	FALSE	C12C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)C)(CCC(C1(C)C)O)C
MOL000520	0.4015	0.5985	0.6981	Strychni Semen	alpha-amyrin	73170	FALSE	C12C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)C)(CCC(C1(C)C)O)C
MOL000520	0.4015	0.5985	0.6981	Portulacae Herba	alpha-amyrin	73170	FALSE	C12C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)C)(CCC(C1(C)C)O)C
MOL000520	0.4015	0.5985	0.6981	Cornus Officinalis Sieb. Et Zucc.	alpha-amyrin	73170	FALSE	C12C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)C)(CCC(C1(C)C)O)C
MOL000520	0.4015	0.5985	0.6981	Cichorii Radix	alpha-amyrin	73170	FALSE	C12C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)C)(CCC(C1(C)C)O)C
MOL000520	0.4015	0.5985	0.6981	Myrrha	alpha-amyrin	73170	FALSE	C12C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)C)(CCC(C1(C)C)O)C
MOL000520	0.4015	0.5985	0.6981	Potentillae Chinensis Herba	alpha-amyrin	73170	FALSE	C12C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)C)(CCC(C1(C)C)O)C
MOL000521	0.4015	0.5985	0.6981	Fructuslipuidambaris	alpha-amyrin acetate	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1C)C)C)C)C)C)(C)C)O
MOL000523	0.4603	0.5397	0.6382	Wikstroemiae Indicae Rasix	arctigenin	64981	FALSE	Oc1ccc(cc1OC)CC1C(Cc2cc(c(cc2)OC)OC)COC1=O
MOL000523	0.4603	0.5397	0.6382	Forsythiae Fructus	arctigenin	64981	FALSE	Oc1ccc(cc1OC)CC1C(Cc2cc(c(cc2)OC)OC)COC1=O
MOL000523	0.4603	0.5397	0.6382	Trachelospermumjasminoides	arctigenin	64981	FALSE	Oc1ccc(cc1OC)CC1C(Cc2cc(c(cc2)OC)OC)COC1=O
MOL000523	0.4603	0.5397	0.6382	Fructus Arctii	arctigenin	64981	FALSE	Oc1ccc(cc1OC)CC1C(Cc2cc(c(cc2)OC)OC)COC1=O
MOL000524	0.2220	0.7780	0.7171	Trachelospermumjasminoides	Dammara-20,24-dien-3beta-ol	Not Available	FALSE	C1(C(C2C(CC1)(C1C(CC2)(C2(C(CC1)C(CC2)C(=C)CCC=C(C)C)C)C)C)(C)C)O
MOL000525	0.9014	0.0986	0.8611	Scutellariae Radix	Norwogonin	5281674	FALSE	c1(cc(c2c(c1O)oc(cc2=O)c1ccccc1)O)O
MOL000525	0.9014	0.0986	0.8611	Trachelospermumjasminoides	Norwogonin	5281674	FALSE	c1(cc(c2c(c1O)oc(cc2=O)c1ccccc1)O)O
MOL000526	0.8958	0.1042	0.8683	Trachelospermumjasminoides	TRE	7427	FALSE	C1(C(C(C(OC1CO)OC1OC(C(C(C1O)O)O)CO)O)O)O
MOL000526	0.8958	0.1042	0.8683	Corayceps	TRE	7427	FALSE	C1(C(C(C(OC1CO)OC1OC(C(C(C1O)O)O)CO)O)O)O
MOL000527	0.9096	0.0904	0.8497	Trachelospermumjasminoides	luteolin-4'-O-β-D-glucoside	67128659	FALSE	c12c(oc(cc1=O)c1cc(c(cc1)OC1OC(C(C(C1O)O)O)CO)O)cc(cc2O)O
MOL000528	0.3301	0.6699	0.8139	Trachelospermumjasminoides	voacangine	Not Available	FALSE	C12(C3N(CC(C2)CC3CC)CCc2c1[nH]c1c2cc(cc1)OC)C(=O)OC
MOL000529	0.3724	0.6276	0.6876	Trachelospermumjasminoides	Ibogain	Not Available	FALSE	C12c3c(c4c([nH]3)ccc(c4)OC)CCN3C1C(CC(C2)C3)CC
MOL000530	0.3048	0.6952	0.7437	Centipedae Herba	Lupeol acetate	92157	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)OC(=O)C)C)C)C
MOL000530	0.3048	0.6952	0.7437	Euphorbiae Helioscopiae Herba	Lupeol acetate	92157	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)OC(=O)C)C)C)C
MOL000530	0.3048	0.6952	0.7437	Euphorbiae Humifusae Herba	Lupeol acetate	92157	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)OC(=O)C)C)C)C

MOL000530	0.3048	0.6952	0.7437	Cortex Periplocae Radicis	Lupeol acetate	92157	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)OC(=O)C)C)C)C
MOL000530	0.3048	0.6952	0.7437	Sophorae Tonkinensis Radix Et Rhizome	Lupeol acetate	92157	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)OC(=O)C)C)C)C
MOL000530	0.3048	0.6952	0.7437	Trachelospermumjasminoides	Lupeol acetate	92157	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)OC(=O)C)C)C)C
MOL000530	0.3048	0.6952	0.7437	Mori Follum	Lupeol acetate	92157	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)OC(=O)C)C)C)C
MOL000530	0.3048	0.6952	0.7437	Lycii Fructus	Lupeol acetate	92157	FALSE	C12(C(C3C(CC2)(CCC3C(=C)C)C)CCC2C1(CCC1C2(CCC(C1(C)C)OC(=O)C)C)C)C
MOL000531	0.8760	0.1240	0.8338	Trachelospermumjasminoides	5-hydroxy-2-(4-hydroxyphenyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]oxymethyl]tetrahydropyran-2-yl]oxy-chromone	10841200	FALSE	c1(cc(=O)c2c(o1)cc(cc2O)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)O
MOL000532	0.7705	0.2295	0.6931	Selaginella Doederleinii Hieron	Nortrachelogenin	394846	FALSE	C1(C(Cc2cc(c(cc2)O)OC)(C(=O)OC1)O)Cc1cc(c(cc1)O)OC
MOL000532	0.7705	0.2295	0.6931	Trachelospermumjasminoides	Nortrachelogenin	394846	FALSE	C1(C(Cc2cc(c(cc2)O)OC)(C(=O)OC1)O)Cc1cc(c(cc1)O)OC
MOL000532	0.7705	0.2295	0.6931	Wikstroemiae Indicae Rasix	Nortrachelogenin	394846	FALSE	C1(C(Cc2cc(c(cc2)O)OC)(C(=O)OC1)O)Cc1cc(c(cc1)O)OC
MOL000534	0.6296	0.3704	0.6706	Trachelospermumjasminoides	(-)-Trachelogenin	452855	FALSE	C1(C(Cc2cc(c(cc2)O)OC)(C(=O)OC1)O)Cc1cc(c(cc1)OC)OC
MOL000535	0.9275	0.0725	0.9142	Trachelospermumjasminoides	dambonitol	21627888	FALSE	O(C1C(O)C(OC)C(O)C(O)C1O)C
MOL000537	0.6568	0.3432	0.6761	Trachelospermumjasminoides	MAX	119205	FALSE	O1C(=O)C(C(C1)Cc1cc(c(cc1)O)OC)Cc1cc(c(cc1)O)OC
MOL000537	0.6568	0.3432	0.6761	Selaginella Doederleinii Hieron	MAX	119205	FALSE	O1C(=O)C(C(C1)Cc1cc(c(cc1)O)OC)Cc1cc(c(cc1)O)OC
MOL000537	0.6568	0.3432	0.6761	Forsythiae Fructus	MAX	119205	FALSE	O1C(=O)C(C(C1)Cc1cc(c(cc1)O)OC)Cc1cc(c(cc1)O)OC

MOL000537	0.6568	0.3432	0.6761	Wikstroemiae Indicae Rasix	MAX	119205	FALSE	O1C(=O)C(C(C1)Cc1cc(c(cc1)O)OC)Cc1cc(c(cc1)O)OC
MOL000537	0.6568	0.3432	0.6761	Fructus Arctii	MAX	119205	FALSE	O1C(=O)C(C(C1)Cc1cc(c(cc1)O)OC)Cc1cc(c(cc1)O)OC
MOL000538	0.2991	0.7009	0.7372	Rhizoma Anemones Raddeanae	hypaconitine	Not Available	FALSE	C1CC2(C3C4(C1OC)C1CC5C(C(C3OC)C4N(C2)C)(C(C(C5OC(=O)c2ccccc2)(C1)O)OC)O)OC(=O)C
MOL000538	0.2991	0.7009	0.7372	Aconitum Kusnezoffii Reichb	hypaconitine	Not Available	FALSE	C1CC2(C3C4(C1OC)C1CC5C(C(C3OC)C4N(C2)C)(C(C(C5OC(=O)c2ccccc2)(C1)O)OC)O)OC(=O)C
MOL000538	0.2991	0.7009	0.7372	Aconiti Lateralis Radix Praeparata	hypaconitine	Not Available	FALSE	C1CC2(C3C4(C1OC)C1CC5C(C(C3OC)C4N(C2)C)(C(C(C5OC(=O)c2ccccc2)(C1)O)OC)O)OC(=O)C
MOL000538	0.2991	0.7009	0.7372	Aconiti Radix	hypaconitine	Not Available	FALSE	C1CC2(C3C4(C1OC)C1CC5C(C(C3OC)C4N(C2)C)(C(C(C5OC(=O)c2ccccc2)(C1)O)OC)O)OC(=O)C
MOL000538	0.2991	0.7009	0.7372	Radix Aconiti Kusnezoffii	hypaconitine	Not Available	FALSE	C1CC2(C3C4(C1OC)C1CC5C(C(C3OC)C4N(C2)C)(C(C(C5OC(=O)c2ccccc2)(C1)O)OC)O)OC(=O)C
MOL000539	0.7003	0.2997	0.7864	Rhizoma Anemones Raddeanae	guanfu base A	Not Available	FALSE	C123C4C56C(C1N1C(C2C(C1)(CC(C3)OC(=O)C)C)C5)(C(C(C4OC(=O)C)C(=C)C6)O)O
MOL000540	0.9060	0.0940	0.9205	Rhizoma Anemones Raddeanae	Ranunculin	441581	FALSE	O1C(=O)C=CC1COC1C(O)C(O)C(O)C(O1)CO
MOL000541	0.9080	0.0920	0.9651	Rhizoma Anemones Raddeanae	55675_FLUKA	10176122	FALSE	O1C(=O)C=CC1CO
MOL000542	0.9183	0.0817	0.8870	Rhizoma Anemones Raddeanae	anemonin	Not Available	FALSE	[n+]1(c(cn(c1)C)CC(=O)O)C
MOL000543	0.7570	0.2430	0.8456	Rhizoma Anemones Raddeanae	raddeanin A	Not Available	FALSE	C1(C2C(CCC1OC1OCC(C(C1OC1C(C(C(O1)CO)O)O)OC1OC(C(C(C1O)O)O)C)O)O)(C1C(CC2)(C)C2(C)C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)(C)C
MOL000544	0.6773	0.3227	0.6888	Rhizoma Anemones Raddeanae	(4aS,6aR,6aS,6bR,8aR,10S,12aR,14bS)-2,2,6a,6b,9,9,12a-heptamethyl-10-[(2S,3R,4S,5S)-3,4,5-trihydroxyoxan-2-yl]oxy-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	13878127	FALSE	C1(C2C(CCC1OC1OCC(C(C1O)O)O)(C1C(CC2)(C)C2(C)C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)(C)C

MOL000545	0.7042	0.2958	0.7758	Rhizoma Anemones Raddeanae	raddeanoside R8	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(OC2C(O)C(O)C(O)C(O2)C)C(O1)CO)C(=O)C12CCC3(C4(CCC5C(C(CCC5(C4CC=C3C2CC(CC1)(C)C)C)OC1C(OC2C(OC3C(O)C(O)C(O)C(O3)C)C(O)C(O)C(O2)CO)C(O)C(O)CO1)(C)C)C)C
MOL000546	0.2872	0.7128	0.7586	Dioscoreae Septemlo Bae Rhizoma	diosgenin	Not Available	FALSE	C12(C(C3C(O1)CC1C3(CCC3C1CC=C1C3(CCC(C1)O)C)C)C)CCC(CO2)C
MOL000546	0.2872	0.7128	0.7586	Broussonetiae Fructus	diosgenin	Not Available	FALSE	C12(C(C3C(O1)CC1C3(CCC3C1CC=C1C3(CCC(C1)O)C)C)C)CCC(CO2)C
MOL000546	0.2872	0.7128	0.7586	Anemarrhenae Rhizoma	diosgenin	Not Available	FALSE	C12(C(C3C(O1)CC1C3(CCC3C1CC=C1C3(CCC(C1)O)C)C)C)CCC(CO2)C
MOL000546	0.2872	0.7128	0.7586	Smilax China	diosgenin	Not Available	FALSE	C12(C(C3C(O1)CC1C3(CCC3C1CC=C1C3(CCC(C1)O)C)C)C)CCC(CO2)C
MOL000546	0.2872	0.7128	0.7586	Solanum Melongena L	diosgenin	Not Available	FALSE	C12(C(C3C(O1)CC1C3(CCC3C1CC=C1C3(CCC(C1)O)C)C)C)CCC(CO2)C
MOL000546	0.2872	0.7128	0.7586	Rhizoma Anemones Raddeanae	diosgenin	Not Available	FALSE	C12(C(C3C(O1)CC1C3(CCC3C1CC=C1C3(CCC(C1)O)C)C)C)CCC(CO2)C
MOL000546	0.2872	0.7128	0.7586	Asparagi Radix	diosgenin	Not Available	FALSE	C12(C(C3C(O1)CC1C3(CCC3C1CC=C1C3(CCC(C1)O)C)C)C)CCC(CO2)C
MOL000546	0.2872	0.7128	0.7586	Calyx Cucumis	diosgenin	Not Available	FALSE	C12(C(C3C(O1)CC1C3(CCC3C1CC=C1C3(CCC(C1)O)C)C)C)CCC(CO2)C
MOL000546	0.2872	0.7128	0.7586	Dioscoreae Hypoglaucae Rhizoma	diosgenin	Not Available	FALSE	C12(C(C3C(O1)CC1C3(CCC3C1CC=C1C3(CCC(C1)O)C)C)C)CCC(CO2)C
MOL000546	0.2872	0.7128	0.7586	Smilacis Glabrae Rhixoma	diosgenin	Not Available	FALSE	C12(C(C3C(O1)CC1C3(CCC3C1CC=C1C3(CCC(C1)O)C)C)C)CCC(CO2)C
MOL000546	0.2872	0.7128	0.7586	Solanum Nigrum Linn.	diosgenin	Not Available	FALSE	C12(C(C3C(O1)CC1C3(CCC3C1CC=C1C3(CCC(C1)O)C)C)C)CCC(CO2)C
MOL000546	0.2872	0.7128	0.7586	Trigonellae Semen	diosgenin	Not Available	FALSE	C12(C(C3C(O1)CC1C3(CCC3C1CC=C1C3(CCC(C1)O)C)C)C)CCC(CO2)C
MOL000546	0.2872	0.7128	0.7586	Polygonati Rhizoma	diosgenin	Not Available	FALSE	C12(C(C3C(O1)CC1C3(CCC3C1CC=C1C3(CCC(C1)O)C)C)C)CCC(CO2)C
MOL000546	0.2872	0.7128	0.7586	Dioscoreaebulbiferae	diosgenin	Not Available	FALSE	C12(C(C3C(O1)CC1C3(CCC3C1CC=C1C3(CCC(C1)O)C)C)C)CCC(CO2)C
MOL000546	0.2872	0.7128	0.7586	Rhizoma Dioscoreae	diosgenin	Not Available	FALSE	C12(C(C3C(O1)CC1C3(CCC3C1CC=C1C3(CCC(C1)O)C)C)C)CCC(CO2)C
MOL000547	0.2872	0.7128	0.7586	Solanum Melongena L	BB_NC-0149	Not Available	FALSE	C1(CCC2(C(=CCC3C4CC5OC6(C(C5C4(C)CCC23)C)OCC(CC6)C)C1)C)O
MOL000547	0.2872	0.7128	0.7586	Rhizoma Anemones Raddeanae	BB_NC-0149	Not Available	FALSE	C1(CCC2(C(=CCC3C4CC5OC6(C(C5C4(C)CCC23)C)OCC(CC6)C)C1)C)O
MOL000547	0.2872	0.7128	0.7586	Asparagi Radix	BB_NC-0149	Not Available	FALSE	C1(CCC2(C(=CCC3C4CC5OC6(C(C5C4(C)CCC23)C)OCC(CC6)C)C1)C)O
MOL000548	0.5313	0.4687	0.8230	Rhizoma Anemones Raddeanae	raddeanin C	Not Available	FALSE	C1CCC23C(C1(C)C)C(C(C14C2CCC(C(=C)C1OC(=O)C)C4O)(OC3)O)OC(=O)C

MOL000549	0.8221	0.1779	0.8307	Rhizoma Anemones Raddeanae	raddeanin E	Not Available	FALSE	C1CC(C23C(C1(C)C)C(C(C14C2CCC(C(=C)C1=O)C4O)(O)OC3OC)O)O
MOL000550	0.9456	0.0544	0.9689	Homalomena Occulta (Lour.) Schott	meso-galactitol	11850	FALSE	C(C(C(CO)O)O)(C(CO)O)O
MOL000550	0.9456	0.0544	0.9689	Peucedani Radix	meso-galactitol	11850	FALSE	C(C(C(CO)O)O)(C(CO)O)O
MOL000550	0.9456	0.0544	0.9689	Litchi Semen	meso-galactitol	11850	FALSE	C(C(C(CO)O)O)(C(CO)O)O
MOL000550	0.9456	0.0544	0.9689	Ampelopsis Japonica	meso-galactitol	11850	FALSE	C(C(C(CO)O)O)(C(CO)O)O
MOL000550	0.9456	0.0544	0.9689	Capsellae Herba	meso-galactitol	11850	FALSE	C(C(C(CO)O)O)(C(CO)O)O
MOL000550	0.9456	0.0544	0.9689	Fritillariaeussuriensis Bulbus	meso-galactitol	11850	FALSE	C(C(C(CO)O)O)(C(CO)O)O
MOL000550	0.9456	0.0544	0.9689	Rhizoma Anemones Raddeanae	meso-galactitol	11850	FALSE	C(C(C(CO)O)O)(C(CO)O)O
MOL000550	0.9456	0.0544	0.9689	Celastri Orbiculati Fructus	meso-galactitol	11850	FALSE	C(C(C(CO)O)O)(C(CO)O)O
MOL000550	0.9456	0.0544	0.9689	Alisma Orientale (Sam.) Juz.	meso-galactitol	11850	FALSE	C(C(C(CO)O)O)(C(CO)O)O
MOL000551	0.7613	0.2387	0.8412	Campsis Flos	Hederagenol	73299	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(CO)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C
MOL000551	0.7613	0.2387	0.8412	Akebiae Frucyus	Hederagenol	73299	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(CO)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C
MOL000551	0.7613	0.2387	0.8412	Clematidis Armandii Caulis	Hederagenol	73299	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(CO)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C
MOL000551	0.7613	0.2387	0.8412	Et Radix Patriniae Rhizoma	Hederagenol	73299	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(CO)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C
MOL000551	0.7613	0.2387	0.8412	Boehmeriae Rhizoma Et Radix	Hederagenol	73299	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(CO)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C
MOL000551	0.7613	0.2387	0.8412	Radix Clematidis	Hederagenol	73299	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(CO)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C
MOL000551	0.7613	0.2387	0.8412	Rosae Laevigatae Fructus	Hederagenol	73299	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(CO)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C
MOL000551	0.7613	0.2387	0.8412	Paeoniae Radix Alba	Hederagenol	73299	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(CO)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C
MOL000551	0.7613	0.2387	0.8412	Rhizoma Anemones Raddeanae	Hederagenol	73299	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(CO)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C
MOL000551	0.7613	0.2387	0.8412	Caulis Akebiae	Hederagenol	73299	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(CO)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C
MOL000551	0.7613	0.2387	0.8412	Cortex Periplocae Radicis	Hederagenol	73299	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(CO)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C

MOL000551	0.7613	0.2387	0.8412	Dipsaci Radix	Hederagenol	73299	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(CO)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C
MOL000551	0.7613	0.2387	0.8412	Pulsatilliae Radix	Hederagenol	73299	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(CO)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C
MOL000551	0.7613	0.2387	0.8412	Sapindi Mukorossiperic Arpium	Hederagenol	73299	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(CO)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C
MOL000551	0.7613	0.2387	0.8412	Gardeniae Fructus	Hederagenol	73299	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(CO)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C
MOL000551	0.7613	0.2387	0.8412	Sapindi Mukorossi Semen	Hederagenol	73299	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(CO)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C
MOL000551	0.7613	0.2387	0.8412	Asteris Radix Et Rhizoma	Hederagenol	73299	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(CO)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C
MOL000551	0.7613	0.2387	0.8412	Lonicerae Japonicae Flos	Hederagenol	73299	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(CO)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C
MOL000552	0.7789	0.2211	0.7913	Scutellariae Radix	5,2'-Dihydroxy-6,7,8-trimethoxyflavone	159029	FALSE	COc1c(OC)c(OC)c2c(c1O)c(=O)cc(o2)c1c(O)cccc1
MOL000552	0.7789	0.2211	0.7913	Herba Pyrolae	5,2'-Dihydroxy-6,7,8-trimethoxyflavone	159029	FALSE	COc1c(OC)c(OC)c2c(c1O)c(=O)cc(o2)c1c(O)cccc1
MOL000553	0.2638	0.7362	0.6591	Herba Pyrolae	(-)-Chimonanthine	442058	FALSE	C1CC2(C(N1C)Nc1c2cccc1)C12CCN(C1Nc1c2cccc1)C
MOL000554	0.9067	0.0933	0.7973	Herba Pyrolae	gallic acid-3-O-(6'-O-galloyl)-glucoside	Not Available	FALSE	c1(cc(c(c(c1)O)O)O)C(=O)OCC1C(C(C(C(O1)Oc1c(c(cc(c1)C(=O)O)O)O)O)O)O
MOL000554	0.9067	0.0933	0.7973	Mori Cortex	gallic acid-3-O-(6'-O-galloyl)-glucoside	Not Available	FALSE	c1(cc(c(c(c1)O)O)O)C(=O)OCC1C(C(C(C(O1)Oc1c(c(cc(c1)C(=O)O)O)O)O)O)O
MOL000554	0.9067	0.0933	0.7973	Radix Rhei Et Rhizome	gallic acid-3-O-(6'-O-galloyl)-glucoside	Not Available	FALSE	c1(cc(c(c(c1)O)O)O)C(=O)OCC1C(C(C(C(O1)Oc1c(c(cc(c1)C(=O)O)O)O)O)O)O
MOL000554	0.9067	0.0933	0.7973	Semen Pharbitidis	gallic acid-3-O-(6'-O-galloyl)-glucoside	Not Available	FALSE	c1(cc(c(c(c1)O)O)O)C(=O)OCC1C(C(C(C(O1)Oc1c(c(cc(c1)C(=O)O)O)O)O)O)O

MOL000554	0.9067	0.0933	0.7973	Cornus Officinalis Sieb. Et Zucc.	gallic acid-3-O-(6'-O-galloyl)-glucoside	Not Available	FALSE	c1(cc(c(c(c1)O)O)O)C(=O)OCC1C(C(C(C(O1)Oc1c(c(cc(c1)C(=O)O)O)O)O)O)O
MOL000554	0.9067	0.0933	0.7973	Farfarae Flos	gallic acid-3-O-(6'-O-galloyl)-glucoside	Not Available	FALSE	c1(cc(c(c(c1)O)O)O)C(=O)OCC1C(C(C(C(O1)Oc1c(c(cc(c1)C(=O)O)O)O)O)O)O
MOL000554	0.9067	0.0933	0.7973	Polygoni Avicularis Herba	gallic acid-3-O-(6'-O-galloyl)-glucoside	Not Available	FALSE	c1(cc(c(c(c1)O)O)O)C(=O)OCC1C(C(C(C(O1)Oc1c(c(cc(c1)C(=O)O)O)O)O)O)O
MOL000554	0.9067	0.0933	0.7973	Trigonellae Semen	gallic acid-3-O-(6'-O-galloyl)-glucoside	Not Available	FALSE	c1(cc(c(c(c1)O)O)O)C(=O)OCC1C(C(C(C(O1)Oc1c(c(cc(c1)C(=O)O)O)O)O)O)O
MOL000555	0.9591	0.0409	0.9277	Arecae Semen	Homoarecoline	34167	FALSE	C1(=CCCN(C1)C)C(=O)OCC
MOL000555	0.9591	0.0409	0.9277	Herba Pyrolae	Homoarecoline	34167	FALSE	C1(=CCCN(C1)C)C(=O)OCC
MOL000557	0.9037	0.0963	0.9040	Picrorhizae Rhizoma	Protocatechuic acid-3-glucoside	11972438	FALSE	c1c(cc(c(c1)O)OC1OC(C(C(C1O)O)O)CO)C(=O)O
MOL000557	0.9037	0.0963	0.9040	Inulae Flos	Protocatechuic acid-3-glucoside	11972438	FALSE	c1c(cc(c(c1)O)OC1OC(C(C(C1O)O)O)CO)C(=O)O
MOL000557	0.9037	0.0963	0.9040	Herba Pyrolae	Protocatechuic acid-3-glucoside	11972438	FALSE	c1c(cc(c(c1)O)OC1OC(C(C(C1O)O)O)CO)C(=O)O
MOL000557	0.9037	0.0963	0.9040	Polygoni Cuspidati Rhizoma Et Radix	Protocatechuic acid-3-glucoside	11972438	FALSE	c1c(cc(c(c1)O)OC1OC(C(C(C1O)O)O)CO)C(=O)O
MOL000558	0.8955	0.1045	0.7550	Polygoni Cuspidati Rhizoma Et Radix	quercetin-3-L-arabinon-7-D-glucoside	Not Available	FALSE	c1c(cc2c(c1O)c(=O)c(c(o2)c1ccc(c(c1)O)O)OC1C(C(C(C(O1)O)O)O)O)OC1OC(C(C(C1O)O)O)CO
MOL000558	0.8955	0.1045	0.7550	Houttuyniae Herba	quercetin-3-L-arabinon-7-D-glucoside	Not Available	FALSE	c1c(cc2c(c1O)c(=O)c(c(o2)c1ccc(c(c1)O)O)OC1C(C(C(C(O1)O)O)O)O)OC1OC(C(C(C1O)O)O)CO
MOL000558	0.8955	0.1045	0.7550	Herba Pyrolae	quercetin-3-L-arabinon-7-D-glucoside	Not Available	FALSE	c1c(cc2c(c1O)c(=O)c(c(o2)c1ccc(c(c1)O)O)OC1C(C(C(C(O1)O)O)O)O)OC1OC(C(C(C1O)O)O)CO

MOL000558	0.8955	0.1045	0.7550	Ginkgo Semen	quercetin-3-L-arabinon-7-D-glucoside	Not Available	FALSE	c1c(cc2c(c1O)c(=O)c(c(o2)c1ccc(c(c1)O)O)OC1C(C(C(C(O1)O)O)O)O)OC1OC(C(C(C1O)O)O)CO
MOL000558	0.8955	0.1045	0.7550	Inulae Flos	quercetin-3-L-arabinon-7-D-glucoside	Not Available	FALSE	c1c(cc2c(c1O)c(=O)c(c(o2)c1ccc(c(c1)O)O)OC1C(C(C(C(O1)O)O)O)O)OC1OC(C(C(C1O)O)O)CO
MOL000558	0.8955	0.1045	0.7550	Pyrrosiae Folium	quercetin-3-L-arabinon-7-D-glucoside	Not Available	FALSE	c1c(cc2c(c1O)c(=O)c(c(o2)c1ccc(c(c1)O)O)OC1C(C(C(C(O1)O)O)O)O)OC1OC(C(C(C1O)O)O)CO
MOL000558	0.8955	0.1045	0.7550	Asteris Radix Et Rhizoma	quercetin-3-L-arabinon-7-D-glucoside	Not Available	FALSE	c1c(cc2c(c1O)c(=O)c(c(o2)c1ccc(c(c1)O)O)OC1C(C(C(C(O1)O)O)O)O)OC1OC(C(C(C1O)O)O)CO
MOL000559	0.8559	0.1441	0.7557	Herba Pyrolae	Repandusinic acid A	Not Available	FALSE	C1(cc2c(c(c1O)O)c1c(cc(c(c1O)O)O)C(=O)OC1C(C(COC2=O)OC(C1O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)/C(=C\C(=O)O)/C1c2c(C(=O)OC1C(=O)O)cc(c(c2O)O)O)O
MOL000560	0.8884	0.1116	0.9594	Herba Pyrolae	Pyrolin	7253	FALSE	c1(c(ccc(c1)O)O)C
MOL000561	0.9140	0.0860	0.8280	Paeoniae Radix Alba	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Hippophae Fructus	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Polygoni Tinctorii Foliu	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Drynariae Rhizoma	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Asari Radix Et Rhizoma	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	licorice	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Rubi Fructus	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Eriobotryae Folium	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Astragali Cpmplanatisemen	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Allii Fistulost Bulbus	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Impatientis Semen	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Polygoni Avicularis Herba	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Epimrdii Herba	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O

MOL000561	0.9140	0.0860	0.8280	Euphorbiae Humifusae Herba	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Lonicerae Japonicae Flos	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Moslae Herba	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Acoritataninowii Rhizoma	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Eucommiae Cortex	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Folium Ilicis Cornutae	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Forsythiae Fructus	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Carthami Flos	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Geranium Wilfordii Maxim.	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Apocyniveneti Folium	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Dysosmae Verspiellis Rhixoma Et Radix	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Lysimachiae Herba	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Impatiens Balsamina	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Potentillae Chinensis Herba	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Herba Pyrolae	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Eucommiae Folium	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Anisi Stellati Fructus	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Farfarae Flos	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Viticis Fructus	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Achyranthis Bidentatae Radix	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Paederiae Scandentis Herba	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O

MOL000561	0.9140	0.0860	0.8280	Prunellae Spica	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000561	0.9140	0.0860	0.8280	Granati Pericarpium	Astragalin	5282102	FALSE	c12c(oc(c(c1=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)cc(cc2O)O
MOL000562	0.9315	0.0685	0.8791	Herba Pyrolae	Methylarbutin	80131	FALSE	C1(C(C(C(C(O1)CO)O)O)O)Oc1ccc(cc1)OC
MOL000563	0.9468	0.0532	0.8070	Herba Pyrolae	Chimaphylin	101211	FALSE	c12c(C(=O)C=C(C1=O)C)ccc(c2)C
MOL000564	0.9342	0.0658	0.9184	Herba Pyrolae	Isohomoarbutin	5318573	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)c1c(cc(cc1)O)C
MOL000566	0.8683	0.1317	0.7577	Rubi Fructus	galloylhyperin	Not Available	FALSE	c1(c(oc2c(c1=O)c(cc(c2)O)O)c1cc(c(cc1)O)O)OC1C(C(C(C(O1)CO)O)O)OC(=O)c1cc(c(c(c1)O)O)O
MOL000566	0.8683	0.1317	0.7577	Herba Pyrolae	galloylhyperin	Not Available	FALSE	c1(c(oc2c(c1=O)c(cc(c2)O)O)c1cc(c(cc1)O)O)OC1C(C(C(C(O1)CO)O)O)OC(=O)c1cc(c(c(c1)O)O)O
MOL000567	0.9181	0.0819	0.8078	Herba Pyrolae	6-O-galloylhomoarbutin	Not Available	FALSE	C(=O)(c1cc(c(c(c1)O)O)O)OCC1C(C(C(C(O1)Oc1cc(c(cc1)O)C)O)O)O
MOL000569	0.9278	0.0722	0.8760	Humulus Scandens (Lour.) Merr.	digallate	341	FALSE	OC(=O)c1cc(c(c(c1)O)O)OC(=O)c1cc(c(c(c1)O)O)O
MOL000569	0.9278	0.0722	0.8760	Radix Aconiti Kusnezoffii	digallate	341	FALSE	OC(=O)c1cc(c(c(c1)O)O)OC(=O)c1cc(c(c(c1)O)O)O
MOL000569	0.9278	0.0722	0.8760	Citrus Aurantium	digallate	341	FALSE	OC(=O)c1cc(c(c(c1)O)O)OC(=O)c1cc(c(c(c1)O)O)O
MOL000569	0.9278	0.0722	0.8760	Cortex Hibisci	digallate	341	FALSE	OC(=O)c1cc(c(c(c1)O)O)OC(=O)c1cc(c(c(c1)O)O)O
MOL000569	0.9278	0.0722	0.8760	Radix Salviae	digallate	341	FALSE	OC(=O)c1cc(c(c(c1)O)O)OC(=O)c1cc(c(c(c1)O)O)O
MOL000569	0.9278	0.0722	0.8760	Hordei Fructus Germinatus	digallate	341	FALSE	OC(=O)c1cc(c(c(c1)O)O)OC(=O)c1cc(c(c(c1)O)O)O
MOL000569	0.9278	0.0722	0.8760	Ampelopsis Japonica	digallate	341	FALSE	OC(=O)c1cc(c(c(c1)O)O)OC(=O)c1cc(c(c(c1)O)O)O
MOL000569	0.9278	0.0722	0.8760	Phyllanthi Fructus	digallate	341	FALSE	OC(=O)c1cc(c(c(c1)O)O)OC(=O)c1cc(c(c(c1)O)O)O
MOL000569	0.9278	0.0722	0.8760	Drynariae Rhizoma	digallate	341	FALSE	OC(=O)c1cc(c(c(c1)O)O)OC(=O)c1cc(c(c(c1)O)O)O
MOL000569	0.9278	0.0722	0.8760	Galla Chinensis	digallate	341	FALSE	OC(=O)c1cc(c(c(c1)O)O)OC(=O)c1cc(c(c(c1)O)O)O
MOL000569	0.9278	0.0722	0.8760	Rhizoma Fagopyri Cymosi	digallate	341	FALSE	OC(=O)c1cc(c(c(c1)O)O)OC(=O)c1cc(c(c(c1)O)O)O
MOL000569	0.9278	0.0722	0.8760	Herba Pyrolae	digallate	341	FALSE	OC(=O)c1cc(c(c(c1)O)O)OC(=O)c1cc(c(c(c1)O)O)O
MOL000570	0.8397	0.1603	0.8450	Polygoni Tinctorii Foliu	Nonox D	8679	TRUE	c12c(ccc(c1)Nc1ccccc1)cccc2
MOL000570	0.8397	0.1603	0.8450	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Nonox D	8679	TRUE	c12c(ccc(c1)Nc1ccccc1)cccc2
MOL000570	0.8397	0.1603	0.8450	Cornus Officinalis Sieb. Et Zucc.	Nonox D	8679	TRUE	c12c(ccc(c1)Nc1ccccc1)cccc2
MOL000570	0.8397	0.1603	0.8450	Momordicae Fructus	Nonox D	8679	TRUE	c12c(ccc(c1)Nc1ccccc1)cccc2
MOL000570	0.8397	0.1603	0.8450	Fraxini Cortex	Nonox D	8679	TRUE	c12c(ccc(c1)Nc1ccccc1)cccc2
MOL000570	0.8397	0.1603	0.8450	Indigo Naturalis	Nonox D	8679	TRUE	c12c(ccc(c1)Nc1ccccc1)cccc2
MOL000570	0.8397	0.1603	0.8450	Herba Pyrolae	Nonox D	8679	TRUE	c12c(ccc(c1)Nc1ccccc1)cccc2
MOL000570	0.8397	0.1603	0.8450	Sargassum	Nonox D	8679	TRUE	c12c(ccc(c1)Nc1ccccc1)cccc2
MOL000571	0.9049	0.0951	0.8471	Herba Pyrolae	renifolin	Not Available	FALSE	C1(=CCc2c(C1)c(c(cc2O)C)OC1OC(C(C(C1O)O)O)CO)C
MOL000572	0.9501	0.0499	0.8615	Herba Pyrolae	renifolin_qt	Not Available	FALSE	C1(=CCc2c(C1)c(c(cc2O)C)O)C
MOL000573	0.7022	0.2978	0.7572	Herba Pyrolae	Catechin-(4.alpha.-->8)catechin	146798	FALSE	c1c(cc2c(c1O)C(C(C(O2)c1cc(c(cc1)O)O)O)c1c(cc(c2c1OC(C(C2)O)c1ccc(c(c1)O)O)O)O)O

MOL000573	0.7022	0.2978	0.7572	Phaseoli Semen	Catechin-(4.alpha.-->8)catechin	146798	FALSE	c1c(cc2c(c1O)C(C(C(O2)c1cc(c(cc1)O)O)O)c1c(cc(c2c1OC(C(C2)O)c1ccc(c(c1)O)O)O)O)O
MOL000574	0.7166	0.2834	0.7752	Herba Pyrolae	3,3'-digalloylprocyanidin	Not Available	FALSE	C(=O)(c1cc(c(c(c1)O)O)O)OC1C(Oc2c(C1c1c(cc(c3CC(C(Oc13)c1cc(c(cc1)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O)c(cc(c2)O)O)c1cc(c(cc1)O)O
MOL000575	0.9310	0.0690	0.9395	Herba Pyrolae	(2S,3R,4S,5S,6R)-2-(4-hydroxy-3-methyl-phenoxy)-6-methylol-tetrahydropyran-3,4,5-triol	5318079	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)C
MOL000576	0.5251	0.4749	0.6441	Herba Pyrolae	pirolatin	Not Available	FALSE	C1(C(C(C(C(O1)Oc1c(cc(c(c1)C)O)C/C=C(/C)\CC/C=C(/C)\CO)O)O)O)CO
MOL000577	0.8762	0.1238	0.7872	Herba Pyrolae	pirolatin_qt	Not Available	FALSE	Oc1c(cc(c(c1)C)O)C/C=C(/C)\CC/C=C(/C)\CO
MOL000578	0.9336	0.0664	0.9400	Herba Pyrolae	arbutin	40467854	FALSE	C1(OC(C(C(C1O)O)O)CO)Oc1ccc(cc1)O
MOL000578	0.9336	0.0664	0.9400	Radix Paeoniae Rubra	arbutin	40467854	FALSE	C1(OC(C(C(C1O)O)O)CO)Oc1ccc(cc1)O
MOL000578	0.9336	0.0664	0.9400	Rhododendronmolle	arbutin	40467854	FALSE	C1(OC(C(C(C1O)O)O)CO)Oc1ccc(cc1)O
MOL000578	0.9336	0.0664	0.9400	Paederiae Scandentis Herba	arbutin	40467854	FALSE	C1(OC(C(C(C1O)O)O)CO)Oc1ccc(cc1)O
MOL000578	0.9336	0.0664	0.9400	Saxifraga Stolonifera	arbutin	40467854	FALSE	C1(OC(C(C(C1O)O)O)CO)Oc1ccc(cc1)O
MOL000578	0.9336	0.0664	0.9400	Sedum Aizoon L.	arbutin	40467854	FALSE	C1(OC(C(C(C1O)O)O)CO)Oc1ccc(cc1)O
MOL000579	0.8792	0.1208	0.9631	Rhododendri Daurici Folium	hydroquinone	785	FALSE	Oc1ccc(cc1)O
MOL000579	0.8792	0.1208	0.9631	Sparganii Rhizoma	hydroquinone	785	FALSE	Oc1ccc(cc1)O
MOL000579	0.8792	0.1208	0.9631	Chaenomeles Sinensis (Thouin) Koehne	hydroquinone	785	FALSE	Oc1ccc(cc1)O
MOL000579	0.8792	0.1208	0.9631	Folium Ilicis Cornutae	hydroquinone	785	FALSE	Oc1ccc(cc1)O
MOL000579	0.8792	0.1208	0.9631	Herba Pyrolae	hydroquinone	785	FALSE	Oc1ccc(cc1)O
MOL000579	0.8792	0.1208	0.9631	Rhododendronmolle	hydroquinone	785	FALSE	Oc1ccc(cc1)O
MOL000579	0.8792	0.1208	0.9631	Herba Selaginellae Moellendorfii	hydroquinone	785	FALSE	Oc1ccc(cc1)O
MOL000579	0.8792	0.1208	0.9631	Sesami Nigrum Semen	hydroquinone	785	FALSE	Oc1ccc(cc1)O
MOL000579	0.8792	0.1208	0.9631	Paederiae Scandentis Herba	hydroquinone	785	FALSE	Oc1ccc(cc1)O
MOL000579	0.8792	0.1208	0.9631	Radix Paeoniae Rubra	hydroquinone	785	FALSE	Oc1ccc(cc1)O
MOL000579	0.8792	0.1208	0.9631	Sedum Aizoon L.	hydroquinone	785	FALSE	Oc1ccc(cc1)O
MOL000579	0.8792	0.1208	0.9631	Xanthii Fructus	hydroquinone	785	FALSE	Oc1ccc(cc1)O
MOL000579	0.8792	0.1208	0.9631	Saxifraga Stolonifera	hydroquinone	785	FALSE	Oc1ccc(cc1)O
MOL000579	0.8792	0.1208	0.9631	Picrorhizae Rhizoma	hydroquinone	785	FALSE	Oc1ccc(cc1)O
MOL000579	0.8792	0.1208	0.9631	Choerospondiatis Fructus	hydroquinone	785	FALSE	Oc1ccc(cc1)O
MOL000579	0.8792	0.1208	0.9631	Lonicerae Japonicae Flos	hydroquinone	785	FALSE	Oc1ccc(cc1)O
MOL000579	0.8792	0.1208	0.9631	Arum Ternatum Thunb.	hydroquinone	785	FALSE	Oc1ccc(cc1)O

MOL000580	0.8964	0.1036	0.8985	Eupatorium Fortunei Turcz	2-methylbutyryl oxy moiety	Not Available	FALSE	c1cc(c(cc1C)O)C(COC(=O)C(CC)C)(C)OC
MOL000581	0.8605	0.1395	0.8642	Eupatorium Fortunei Turcz	3-O-(3-methyl-2-butenoyl) derivative	Not Available	FALSE	c1cc(c(cc1C)OC(=O)C=C(C)C)C(CO)(C)OC
MOL000582	0.9071	0.0929	0.8780	Eupatorium Fortunei Turcz	3-O-isobutyryl derivative	Not Available	FALSE	c1cc(c(cc1C)OC(=O)C(C)C)C(CO)(C)OC
MOL000583	0.8920	0.1080	0.8772	Eupatorium Fortunei Turcz	3-O-tiglate derivative	Not Available	FALSE	c1cc(c(cc1C)OC(=O)/C(=C/C)/C)C(CO)(C)OC
MOL000584	0.8595	0.1405	0.8140	Eupatorium Fortunei Turcz	7-acetoxy-8-hydroxy-9-isobutyryloxythymol	Not Available	FALSE	c1cc(c(cc1COC(=O)C)O)C(COC(=O)C(C)C)(C)O
MOL000585	0.8910	0.1090	0.8837	Eupatorium Fortunei Turcz	(2-isopropenyl-5-methyl-phenyl) (E)-2-methylbut-2-enoate	10977290	FALSE	c1cc(c(cc1C)OC(=O)/C(=C/C)/C)C(=C)C
MOL000586	0.9604	0.0396	0.9298	Eupatorium Fortunei Turcz	8-methoxy-9-hydroxythymol	Not Available	FALSE	c1cc(c(cc1C)O)C(CO)(C)OC
MOL000587	0.7922	0.2078	0.8851	Eupatorium Fortunei Turcz	[2-[1-(acetoxymethyl)vinyl]-5-methyl-phenyl] (E)-2-methylbut-2-enoate	10869933	FALSE	c1cc(c(cc1C)OC(=O)/C(=C/C)/C)C(=C)COC(=O)C
MOL000588	0.7843	0.2157	0.6774	Eupatorium Fortunei Turcz	9-acetoxy-8,10-epoxy-6-hydroxythymol 3-O-angelate	Not Available	FALSE	c1(cc(c(cc1C)OC(=O)/C(=C\C)/C)C1(COC(=O)C)CO1)O
MOL000589	0.7656	0.2344	0.8980	Eupatorium Fortunei Turcz	9-acetoxythymol 3-O-tiglate	Not Available	FALSE	c1cc(c(cc1C)OC(=O)/C(=C/C)/C)C(COC(=O)C)C
MOL000590	0.9104	0.0896	0.9022	Eupatorium Fortunei Turcz	9-O-angeloyl derivative	Not Available	FALSE	c1cc(c(cc1C)O)C(COC(=O)/C(=C\C)/C)(C)OC

MOL000591	0.9273	0.0727	0.9062	Eupatorium Fortunei Turcz	9-O-isobutyryl derivative	Not Available	FALSE	c1cc(c(cc1C)O)C(COC(=O)C(C)C)(C)OC
MOL000592	0.1843	0.8157	0.6926	Eupatorium Fortunei Turcz	Dammaradienyl acetate	14137680	FALSE	C1(C(C2C(CC1)(C1C(CC2)(C2(C(CC1)C(CC2)C(=C)CCC=C(C)C)C)C)(C)C)OC(=O)C
MOL000593	0.9490	0.0510	0.8706	Eupatorium Fortunei Turcz	Euparin	119039	FALSE	c1(c(cc2c(c1)cc(o2)C(=C)C)O)C(=O)C
MOL000594	0.8430	0.1570	0.7661	Eupatorium Fortunei Turcz	Eupatolin	Not Available	FALSE	c1(c(c(=O)c2c(o1)cc(c(c2O)OC)OC)OC1OC(C(C(C1O)O)O)C)c1cc(c(cc1)O)O
MOL000596	0.3451	0.6549	0.7434	Centipedae Herba	[(3S,4aR,6aR,6aR,6bR,8aR,12S,12aR,14aR,14bR)-4,4,6a,6b,8a,12,14b-heptamethyl-11-methylene-1,2,3,4a,5,6,6a,7,8,9,10,12,12a,13,14,14a-hexadecahydropicen-3-yl] acetate	13889352	FALSE	C12(C3(C(C4C(CC3)(CCC(=C)C4C)C)CCC1C1(C(CC2)C(C(CC1)OC(=O)C)(C)C)C)C
MOL000596	0.3451	0.6549	0.7434	Eupatorium Fortunei Turcz	[(3S,4aR,6aR,6aR,6bR,8aR,12S,12aR,14aR,14bR)-4,4,6a,6b,8a,12,14b-heptamethyl-11-methylene-1,2,3,4a,5,6,6a,7,8,9,10,12,12a,13,14,14a-hexadecahydropicen-3-yl] acetate	13889352	FALSE	C12(C3(C(C4C(CC3)(CCC(=C)C4C)C)CCC1C1(C(CC2)C(C(CC1)OC(=O)C)(C)C)C)C

MOL000596	0.3451	0.6549	0.7434	Inulae Flos	[(3S,4aR,6aR,6aR,6bR,8aR,12S,12aR,14aR,14bR)-4,4,6a,6b,8a,12,14b-heptamethyl-11-methylene-1,2,3,4a,5,6,6a,7,8,9,10,12,12a,13,14,14a-hexadecahydropicen-3-yl] acetate	13889352	FALSE	C12(C3(C(C4C(CC3)(CCC(=C)C4C)C)CCC1C1(C(CC2)C(C(CC1)OC(=O)C)(C)C)C)C)C
MOL000596	0.3451	0.6549	0.7434	Radix Cirsii Japonici	[(3S,4aR,6aR,6aR,6bR,8aR,12S,12aR,14aR,14bR)-4,4,6a,6b,8a,12,14b-heptamethyl-11-methylene-1,2,3,4a,5,6,6a,7,8,9,10,12,12a,13,14,14a-hexadecahydropicen-3-yl] acetate	13889352	FALSE	C12(C3(C(C4C(CC3)(CCC(=C)C4C)C)CCC1C1(C(CC2)C(C(CC1)OC(=O)C)(C)C)C)C)C

MOL000596	0.3451	0.6549	0.7434	Inulae Herba	[(3S,4aR,6aR,6aR,6bR,8aR,12S,12aR,14aR,14bR)-4,4,6a,6b,8a,12,14b-heptamethyl-11-methylene-1,2,3,4a,5,6,6a,7,8,9,10,12,12a,13,14,14a-hexadecahydropicen-3-yl] acetate	13889352	FALSE	C12(C3(C(C4C(CC3)(CCC(=C)C4C)C)CCC1C1(C(CC2)C(C(CC1)OC(=O)C)(C)C)C)C)C
MOL000597	0.9283	0.0717	0.9287	Citrus Reticulata	Neryl acetate	1549025	FALSE	C(=C\COC(=O)C)(\CCC=C(C)C)/C
MOL000597	0.9283	0.0717	0.9287	Evodiae Fructus	Neryl acetate	1549025	FALSE	C(=C\COC(=O)C)(\CCC=C(C)C)/C
MOL000597	0.9283	0.0717	0.9287	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Neryl acetate	1549025	FALSE	C(=C\COC(=O)C)(\CCC=C(C)C)/C
MOL000597	0.9283	0.0717	0.9287	Olibanun	Neryl acetate	1549025	FALSE	C(=C\COC(=O)C)(\CCC=C(C)C)/C
MOL000597	0.9283	0.0717	0.9287	Viticis Negundo Folium	Neryl acetate	1549025	FALSE	C(=C\COC(=O)C)(\CCC=C(C)C)/C
MOL000597	0.9283	0.0717	0.9287	Lonicerae Japonicae Flos	Neryl acetate	1549025	FALSE	C(=C\COC(=O)C)(\CCC=C(C)C)/C
MOL000597	0.9283	0.0717	0.9287	Eupatorium Fortunei Turcz	Neryl acetate	1549025	FALSE	C(=C\COC(=O)C)(\CCC=C(C)C)/C
MOL000597	0.9283	0.0717	0.9287	Zingiberis Rhizoma	Neryl acetate	1549025	FALSE	C(=C\COC(=O)C)(\CCC=C(C)C)/C
MOL000597	0.9283	0.0717	0.9287	Cnidii Fructus	Neryl acetate	1549025	FALSE	C(=C\COC(=O)C)(\CCC=C(C)C)/C
MOL000597	0.9283	0.0717	0.9287	Lilii Bulbus	Neryl acetate	1549025	FALSE	C(=C\COC(=O)C)(\CCC=C(C)C)/C
MOL000597	0.9283	0.0717	0.9287	Borneolum Syntheticum	Neryl acetate	1549025	FALSE	C(=C\COC(=O)C)(\CCC=C(C)C)/C
MOL000597	0.9283	0.0717	0.9287	Rose Rugosae Flos	Neryl acetate	1549025	FALSE	C(=C\COC(=O)C)(\CCC=C(C)C)/C
MOL000597	0.9283	0.0717	0.9287	Rubi Fructus	Neryl acetate	1549025	FALSE	C(=C\COC(=O)C)(\CCC=C(C)C)/C
MOL000597	0.9283	0.0717	0.9287	Coriandri Sativi Herba	Neryl acetate	1549025	FALSE	C(=C\COC(=O)C)(\CCC=C(C)C)/C
MOL000599	0.9473	0.0527	0.8073	Eupatorium Fortunei Turcz	(2S)-2-hydroxy-2-(1-hydroxyethyl)-3-methyl-butyric acid [(1R,8R)-pyrrolizidin-1-yl]methyl ester	164622	FALSE	C(=O)(C(C(C)O)(C(C)C)O)OCC1C2N(CCC2)CC1

MOL000601	0.9270	0.0730	0.8733	Rhizome Of Whiteback Greenbrier	O-Methylthymol	14104	FALSE	c1(c(ccc(c1)C)C(C)C)OC
MOL000601	0.9270	0.0730	0.8733	Lysimachiae Herba	O-Methylthymol	14104	FALSE	c1(c(ccc(c1)C)C(C)C)OC
MOL000601	0.9270	0.0730	0.8733	Sinapis Semen	O-Methylthymol	14104	FALSE	c1(c(ccc(c1)C)C(C)C)OC
MOL000601	0.9270	0.0730	0.8733	Rubi Fructus	O-Methylthymol	14104	FALSE	c1(c(ccc(c1)C)C(C)C)OC
MOL000601	0.9270	0.0730	0.8733	Lilii Bulbus	O-Methylthymol	14104	FALSE	c1(c(ccc(c1)C)C(C)C)OC
MOL000601	0.9270	0.0730	0.8733	Asari Radix Et Rhizoma	O-Methylthymol	14104	FALSE	c1(c(ccc(c1)C)C(C)C)OC
MOL000601	0.9270	0.0730	0.8733	Magnoliae Flos	O-Methylthymol	14104	FALSE	c1(c(ccc(c1)C)C(C)C)OC
MOL000601	0.9270	0.0730	0.8733	Linderae Radix	O-Methylthymol	14104	FALSE	c1(c(ccc(c1)C)C(C)C)OC
MOL000601	0.9270	0.0730	0.8733	Nardostachyos Radix Et Rhizoma	O-Methylthymol	14104	FALSE	c1(c(ccc(c1)C)C(C)C)OC
MOL000601	0.9270	0.0730	0.8733	Eupatorium Fortunei Turcz	O-Methylthymol	14104	FALSE	c1(c(ccc(c1)C)C(C)C)OC
MOL000602	0.9023	0.0977	0.9675	Semiaquilegiae Radix	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Gnaphalii Affinis Herba	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Leonuri Herba	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Pyrrosiae Folium	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Lobeliae Chinensis Herba	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Trichosanthes Kirilowii Maxim	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Capsellae Herba	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Semen Aesculi	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Isatidis Folium	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Chaenomeles Sinensis (Thouin) Koehne	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Equiseti Hiemalis Herba	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O

MOL000602	0.9023	0.0977	0.9675	Mori Fructus	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Xanthii Fructus	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Ganoderma	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Ampelopsis Japonica	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Eupatorium Fortunei Turcz	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Potentillae Discoloris Herba	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Portulacae Herba	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Plantaginis Herba	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Herba Sarcandrae	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Typhonii Rhizoma	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Apocyniveneti Folium	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000602	0.9023	0.0977	0.9675	Eucommiae Folium	FUM	21883788	FALSE	C(=O)(/C=C/C(=O)O)O
MOL000603	0.8338	0.1662	0.7094	Eupatorium Fortunei Turcz	(3aR,4R,6Z,10Z,11aR)-4-hydroxy-6,10-dimethyl-3-methylene-3a,4,5,8,9,11a-hexahydrocyclodeca[d]furan-2-one	10399772	FALSE	O1C2C(C(=C)C1=O)C(C/C(=C\CC/C(=C\2)/C)/C)O
MOL000605	0.5925	0.4075	0.6247	Eupatorium Fortunei Turcz	taraxasteryl palmitate	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(=C)C(C)C4C3CCC21C)OC(=O)CCCCCCCCCCCCCCCC
MOL000606	0.9085	0.0915	0.8555	Eupatorium Fortunei Turcz	Isooctane	10907	FALSE	CC(CC(C)C)(C)C
MOL000606	0.9085	0.0915	0.8555	Platycladi Cacumen	Isooctane	10907	FALSE	CC(CC(C)C)(C)C
MOL000607	0.9592	0.0408	0.9061	Cnidii Fructus	Dehydro-p-cymene	62385	FALSE	c1(C(=C)C)ccc(cc1)C
MOL000607	0.9592	0.0408	0.9061	Canarii Fructus	Dehydro-p-cymene	62385	FALSE	c1(C(=C)C)ccc(cc1)C
MOL000607	0.9592	0.0408	0.9061	Magnolia Officinalis Rehd Et Wils.	Dehydro-p-cymene	62385	FALSE	c1(C(=C)C)ccc(cc1)C
MOL000607	0.9592	0.0408	0.9061	Piperis Fructus	Dehydro-p-cymene	62385	FALSE	c1(C(=C)C)ccc(cc1)C
MOL000607	0.9592	0.0408	0.9061	Eupatorium Fortunei Turcz	Dehydro-p-cymene	62385	FALSE	c1(C(=C)C)ccc(cc1)C
MOL000608	0.9498	0.0502	0.9678	Curcumae Radix	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O

MOL000608	0.9498	0.0502	0.9678	Ephedra Herba	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Gossampiniflos	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Citrus Reticulata	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Schisandrae Chinensis Fructus	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Chuanxiong Rhizoma	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Evodiae Fructus	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Anisi Stellati Fructus	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Acoritataninowii Rhizoma	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Zingiber Officinale Roscoe	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Styrax	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Eupatorium Fortunei Turcz	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Flemingia Prostrata Roxb	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Morindae Officinalis Radix	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Folium Artemisiae Argyi	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Cnidii Fructus	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Herbahypericiperforati	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Herba Taxilli	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Citrus Aurantium	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Cinnamomi Ramulus	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Panacis Japonici Rhizoma	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Celastri Orbiculati Fructus	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O

MOL000608	0.9498	0.0502	0.9678	Mume Flos	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Smilacis Glabrae Rhixoma	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Cinnanmomi Cortex	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Carthami Flos	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Fructus Ligustri Lucidi	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Artemisia Annua L.	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Gypsophila Licentiana Hand.-Mazz.	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Kadsurae Coccineae Radix Et Caulis	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Ginkgo Folium	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Citri Reticulatae Folium	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Ligustici Rhizoma Et Radix	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Viticis Fructus	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Citri Fructus	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Piperis Longi Fructus	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Notopterygii Rhizoma Et Radix	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Semen Pharbitidis	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Kaempferiae Rhizoma	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Foeniculi Fructus	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Fructus Carotae	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Alpiniae Officinarum Rhizome	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Nardostachyos Radix Et Rhizoma	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O

MOL000608	0.9498	0.0502	0.9678	Eriobotryae Folium	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Magnolia Officinalis Rehd Et Wils.	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Citri Fructus Retinervus	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Rubi Fructus	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Zanthoxyli Pericarpium	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Rhizome Of Whiteback Greenbrier	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Viticis Negundo Folium	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000608	0.9498	0.0502	0.9678	Amygdalus Communis Vas	()-Terpinen-4-ol	2724161	FALSE	C1(C(C)C)(CCC(=CC1)C)O
MOL000609	0.9554	0.0446	0.8004	Cyperi Rhizoma	(1R,5S)-7,7-dimethyl-4-bicyclo[3.1.1]hept-3-enecarboxaldehyde	1201528	FALSE	C(=O)C1=CCC2CC1C2(C)C
MOL000609	0.9554	0.0446	0.8004	Alpiniae Oxyphyliae Fructus	(1R,5S)-7,7-dimethyl-4-bicyclo[3.1.1]hept-3-enecarboxaldehyde	1201528	FALSE	C(=O)C1=CCC2CC1C2(C)C
MOL000609	0.9554	0.0446	0.8004	Aristolochiae Fructus	(1R,5S)-7,7-dimethyl-4-bicyclo[3.1.1]hept-3-enecarboxaldehyde	1201528	FALSE	C(=O)C1=CCC2CC1C2(C)C
MOL000609	0.9554	0.0446	0.8004	Caryophylliflos	(1R,5S)-7,7-dimethyl-4-bicyclo[3.1.1]hept-3-enecarboxaldehyde	1201528	FALSE	C(=O)C1=CCC2CC1C2(C)C

MOL000609	0.9554	0.0446	0.8004	Eupatorium Fortunei Turcz	(1R,5S)-7,7-dimethyl-4-bicyclo[3.1.1]hept-3-enecarboxaldehyde	1201528	FALSE	C(=O)C1=CCC2CC1C2(C)C
MOL000609	0.9554	0.0446	0.8004	Rhododendri Daurici Folium	(1R,5S)-7,7-dimethyl-4-bicyclo[3.1.1]hept-3-enecarboxaldehyde	1201528	FALSE	C(=O)C1=CCC2CC1C2(C)C
MOL000609	0.9554	0.0446	0.8004	Radix Bupleuri	(1R,5S)-7,7-dimethyl-4-bicyclo[3.1.1]hept-3-enecarboxaldehyde	1201528	FALSE	C(=O)C1=CCC2CC1C2(C)C
MOL000610	0.8537	0.1463	0.7099	Capsici Fructus	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000610	0.8537	0.1463	0.7099	Meliae Cortex	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000610	0.8537	0.1463	0.7099	Arisaematis Rhizoma	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000610	0.8537	0.1463	0.7099	Hippophae Fructus	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000610	0.8537	0.1463	0.7099	Cornus Officinalis Sieb. Et Zucc.	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000610	0.8537	0.1463	0.7099	Typhonii Rhizoma	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000610	0.8537	0.1463	0.7099	Caryophylliflos	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000610	0.8537	0.1463	0.7099	Cynanchistauntonii Rhizoma Et Radix	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000610	0.8537	0.1463	0.7099	Piperis Longi Fructus	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000610	0.8537	0.1463	0.7099	Radix Angelicae Biseratae	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000610	0.8537	0.1463	0.7099	Semen Pharbitidis	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000610	0.8537	0.1463	0.7099	Lysimachiae Foenigraeci Herba	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000610	0.8537	0.1463	0.7099	Perillae Fructus	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000610	0.8537	0.1463	0.7099	Rubi Fructus	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000610	0.8537	0.1463	0.7099	Amygdalus Communis Vas	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000610	0.8537	0.1463	0.7099	Paeoniae Radix Alba	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000610	0.8537	0.1463	0.7099	Sesami Nigrum Semen	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000610	0.8537	0.1463	0.7099	Mahoniae Caulis	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000610	0.8537	0.1463	0.7099	Eupatorium Fortunei Turcz	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000610	0.8537	0.1463	0.7099	Rose Rugosae Flos	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000610	0.8537	0.1463	0.7099	Radix Bupleuri	TRD	12388	FALSE	C(CCCCCC)CCCCCC

MOL000610	0.8537	0.1463	0.7099	Campsis Flos	TRD	12388	FALSE	C(CCCCCC)CCCCCC
MOL000613	0.8616	0.1384	0.8179	Aurantii Fructus	8-isopropylidene-1,5-dimethylcyclodeca-1,5-diene	6370843	FALSE	C\1(=C\CC/C(=C\CC(=C(C)C)CC1)/C)/C
MOL000613	0.8616	0.1384	0.8179	Eupatorium Fortunei Turcz	8-isopropylidene-1,5-dimethylcyclodeca-1,5-diene	6370843	FALSE	C\1(=C\CC/C(=C\CC(=C(C)C)CC1)/C)/C
MOL000613	0.8616	0.1384	0.8179	Meliae Azedarach Fructus	8-isopropylidene-1,5-dimethylcyclodeca-1,5-diene	6370843	FALSE	C\1(=C\CC/C(=C\CC(=C(C)C)CC1)/C)/C
MOL000613	0.8616	0.1384	0.8179	Radix Salviae	8-isopropylidene-1,5-dimethylcyclodeca-1,5-diene	6370843	FALSE	C\1(=C\CC/C(=C\CC(=C(C)C)CC1)/C)/C
MOL000614	0.9094	0.0906	0.9418	Eupatorium Fortunei Turcz	osthol	10228	FALSE	c12c(c(ccc1ccc(=O)o2)OC)CC=C(C)C
MOL000614	0.9094	0.0906	0.9418	Agrimonia Eupatoria	osthol	10228	FALSE	c12c(c(ccc1ccc(=O)o2)OC)CC=C(C)C
MOL000614	0.9094	0.0906	0.9418	Cnidii Fructus	osthol	10228	FALSE	c12c(c(ccc1ccc(=O)o2)OC)CC=C(C)C
MOL000614	0.9094	0.0906	0.9418	Radix Angelicae Biseratae	osthol	10228	FALSE	c12c(c(ccc1ccc(=O)o2)OC)CC=C(C)C
MOL000614	0.9094	0.0906	0.9418	Peucedani Radix	osthol	10228	FALSE	c12c(c(ccc1ccc(=O)o2)OC)CC=C(C)C
MOL000614	0.9094	0.0906	0.9418	Saussureae Involucratae Herba	osthol	10228	FALSE	c12c(c(ccc1ccc(=O)o2)OC)CC=C(C)C
MOL000614	0.9094	0.0906	0.9418	A. Dahurica (Fisch.) Benth. Et Hook	osthol	10228	FALSE	c12c(c(ccc1ccc(=O)o2)OC)CC=C(C)C
MOL000615	0.8526	0.1474	0.6851	Lycii Fructus	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Viticis Negundo Folium	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Lonicerae Japonicae Flos	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Rubi Fructus	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Cinnanmomi Cortex	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Alpiniae Officinarum Rhizome	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C

MOL000615	0.8526	0.1474	0.6851	Folium Artemisiae Argyi	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Curcumae Rhizoma	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Smilacis Glabrae Rhixoma	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Stephaniae Tetrandrae Radix	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Rhododendri Daurici Folium	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Zanthoxyli Pericarpium	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Curcumae Radix	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Cayratiae Japonicae Herba	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Schisandrae Chinensis Fructus	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Eupatorium Fortunei Turcz	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Viticis Fructus	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Myrrha	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Caryophylliflos	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Moslae Herba	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Rhizome Of Whiteback Greenbrier	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Siegesbeckiae Herba	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Ephedra Herba	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Ailanthi Cortex	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Solidaginis Herba	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Piperis Fructus	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Ganoderma	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C

MOL000615	0.8526	0.1474	0.6851	Evodiae Fructus	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Citrus Reticulata	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Perillae Fructus	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000615	0.8526	0.1474	0.6851	Ginsen Radix Et Rhizoma Rubra	delta-amorphene	441005	FALSE	C12C(=C(CCC1C(C)C)C)CCC(=C2)C
MOL000616	0.5932	0.4068	0.6751	Caulis Sinomenii	(+)-Suyringaresinol-di-O-beta-D-glucoside	Not Available	FALSE	c1(cc(cc(c1OC1OC(C(C(C1O)O)O)CO)OC)C1OCC2C1COC2c1cc(c(c(c1)OC)OC1C(C(C(C(O1)CO)O)O)O)OC)OC
MOL000616	0.5932	0.4068	0.6751	Tripterygii Radix	(+)-Suyringaresinol-di-O-beta-D-glucoside	Not Available	FALSE	c1(cc(cc(c1OC1OC(C(C(C1O)O)O)CO)OC)C1OCC2C1COC2c1cc(c(c(c1)OC)OC1C(C(C(C(O1)CO)O)O)O)OC)OC
MOL000617	0.8020	0.1980	0.6032	Codonopsis Radix	(14S)-14-methylpalmitic acid	16039117	FALSE	CCC(CCCCCCCCCCCCC(=O)O)C
MOL000617	0.8020	0.1980	0.6032	Caulis Sinomenii	(14S)-14-methylpalmitic acid	16039117	FALSE	CCC(CCCCCCCCCCCCC(=O)O)C
MOL000620	0.3281	0.6719	0.7744	Caulis Sinomenii	Dispegatrine	Not Available	FALSE	c1cc(c(c2c1[nH]c1c2CC2N(C1CC(C2CO)/C(=C/C)/CC)C)c1c(ccc2c1c1c([nH]2)C2[N+]3(C(C1)C(C(/C(=C/C)/C3)C2)CO)C)O)O
MOL000621	0.4336	0.5664	0.8201	Caulis Sinomenii	16-epi-Isositsirikine	6436828	FALSE	c1ccc2c(c1)c1c([nH]2)C2N(CC1)C/C(=C/C)/C(C2)C(CO)C(=O)OC
MOL000622	0.9025	0.0975	0.7540	Epimrdii Herba	Magnograndiolide	5319198	FALSE	C12C(C3C(CCC1(C)O)C(=C)C(=O)O3)C(CC2)(O)C
MOL000622	0.9025	0.0975	0.7540	Coptidis Rhizoma	Magnograndiolide	5319198	FALSE	C12C(C3C(CCC1(C)O)C(=C)C(=O)O3)C(CC2)(O)C
MOL000622	0.9025	0.0975	0.7540	Phellodendri Chinrnsis Cortex	Magnograndiolide	5319198	FALSE	C12C(C3C(CCC1(C)O)C(=C)C(=O)O3)C(CC2)(O)C
MOL000622	0.9025	0.0975	0.7540	Caulis Sinomenii	Magnograndiolide	5319198	FALSE	C12C(C3C(CCC1(C)O)C(=C)C(=O)O3)C(CC2)(O)C
MOL000622	0.9025	0.0975	0.7540	Aristolochiae Fructus	Magnograndiolide	5319198	FALSE	C12C(C3C(CCC1(C)O)C(=C)C(=O)O3)C(CC2)(O)C
MOL000623	0.8163	0.1837	0.6882	Caulis Sinomenii	Michelenolide	Not Available	FALSE	C1CC2C(C3C(CCC4C1(O4)C)(O3)C)OC(=O)C2=C

MOL000624	0.8311	0.1689	0.6525	Caulis Sinomenii	[[2-(4-hydroxyphenyl)-1-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]sulfanylethylidene]amino] hydrogen sulfate	9601115	FALSE	C1(C(C(OC(C1O)CO)S/C(=N/OS(=O)(=O)O)/Cc1ccc(cc1)O)O)O
MOL000625	0.6953	0.3047	0.8098	Caulis Sinomenii	Sinomenine	Not Available	FALSE	C12C3(c4c(C5(C1C=C(C(=O)C5)OC)C3)c(c(cc4)OC)O)CN2C
MOL000626	0.8138	0.1862	0.6973	Caulis Sinomenii	Sinomontanine D	Not Available	FALSE	C1C(C2(C3C4(C1O)C1C5(C(C(C3)(O)C4N(C2)CC)(CC(C(C1)C5OC)OC)O)O)O)O
MOL000627	0.6130	0.3870	0.8073	Jujubae Fructus	Stepholidine	12442999	FALSE	c1(cc2c(cc1OC)CCN1C2Cc2c(C1)c(c(cc2)O)OC)O
MOL000627	0.6130	0.3870	0.8073	Caulis Sinomenii	Stepholidine	12442999	FALSE	c1(cc2c(cc1OC)CCN1C2Cc2c(C1)c(c(cc2)O)OC)O
MOL000629	0.9257	0.0743	0.8952	Caulis Sinomenii	Tufulingoside	Not Available	FALSE	c1(cc(c2c(c1)OCC(C2=O)OC1OC(C(C(C1O)O)O)C)O)O
MOL000630	0.8681	0.1319	0.8115	Solanum Melongena L	N-p-coumaroyloctopamine	Not Available	FALSE	C(=O)(/C=C\c1ccc(cc1)O)NCC(c1ccc(cc1)O)O
MOL000631	0.9030	0.0970	0.6858	Solanum Melongena L	coumaroyltyramine	13939145	FALSE	C(=O)(/C=C\c1ccc(cc1)O)NCCc1ccc(cc1)O
MOL000631	0.9030	0.0970	0.6858	Anemarrhenae Rhizoma	coumaroyltyramine	13939145	FALSE	C(=O)(/C=C\c1ccc(cc1)O)NCCc1ccc(cc1)O
MOL000631	0.9030	0.0970	0.6858	Rhizoma Fagopyri Cymosi	coumaroyltyramine	13939145	FALSE	C(=O)(/C=C\c1ccc(cc1)O)NCCc1ccc(cc1)O
MOL000631	0.9030	0.0970	0.6858	Allium Azureum Ledeb.	coumaroyltyramine	13939145	FALSE	C(=O)(/C=C\c1ccc(cc1)O)NCCc1ccc(cc1)O
MOL000631	0.9030	0.0970	0.6858	Daturae Flos	coumaroyltyramine	13939145	FALSE	C(=O)(/C=C\c1ccc(cc1)O)NCCc1ccc(cc1)O
MOL000632	0.9250	0.0750	0.9463	Solanum Melongena L	WLN: ZR DVH	11158	FALSE	c1(ccc(cc1)N)C=O
MOL000633	0.8997	0.1003	0.8223	Solanum Melongena L	N-feruloyloctopamine	Not Available	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)OC)NCC(c1ccc(cc1)O)O
MOL000635	0.9198	0.0802	0.9587	Benzoinum	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Asparagi Radix	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Chuanxiong Rhizoma	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Salviae Chinensis Herba	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Junci Medulla	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Ailanthi Cortex	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC

MOL000635	0.9198	0.0802	0.9587	Caryophylliflos	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Cortex Periplocae Radicis	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Euonymi Alati Ramulus	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Ailanthi Altissimae Fructus	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Toosendan Fructus	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Meliae Cortex	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Santalum Album L.	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Gypsophila Licentiana Hand.-Mazz.	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Trichosanthes Kirilowii Maxim	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Zingiber Officinale Roscoe	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Stemonae Radix	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Capsici Fructus	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Cornus Officinalis Sieb. Et Zucc.	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Isatidis Folium	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Citrus Reticulata	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Radix Bupleuri	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Isatdis Radix	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Equiseti Hiemalis Herba	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Momordicae Fructus	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Coicis Semen	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Radix Clematidis	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Cannabis Sativa L.	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Angelicae Sinensis Radix	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Styrax	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Hydnocarpi Anthelminticae Semen	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Olibanun	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Solanum Melongena L	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Alpiniae Officinarum Rhizome	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Mori Cortex	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Arecae Semen	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Artemisiae Scopariae Herba	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000635	0.9198	0.0802	0.9587	Meliae Azedarach Fructus	vanillin	1183	FALSE	C(=O)c1cc(c(cc1)O)OC
MOL000636	0.9119	0.0881	0.7693	Gentiana Macrophylla Pall	gentiopicroside	Not Available	FALSE	O1CC=C2C(=CC(=O)C(C2C=C)OC2C(C(C(C(O)O2)O)O)O)/C/1=C/O
MOL000637	0.9263	0.0737	0.8042	Gentiana Macrophylla Pall	loganic,acid	Not Available	FALSE	C12C(C(OC=C1C(=O)O)OC1OC(CCC1O)C)C(CC2)C

MOL000638	0.5190	0.4810	0.7074	Gentiana Macrophylla Pall	Macrophyllosi de A	Not Available	FALSE	C1CC2C(=COC(C2C=C)OC2OC(C(C(C2OC(=O)c2 c(c(ccc2)O)O)OC(=O)C)CC(=O)c2c(c(ccc2)OC2C(O)C(O)C(O)C(O2)CO)O)COC(=O)C)C(=O)O1
MOL000640	0.5455	0.4545	0.6996	Gentiana Macrophylla Pall	Macrophyllosi de B	Not Available	FALSE	C1CC2(C(=COC(C2C=C)OC2OC(C(C(C2OC(=O)c2 c(c(ccc2)O)O)OC(=O)C)CC(=O)c2c(c(ccc2)OC2C(O)C(O)C(O)C(O2)CO)O)COC(=O)C)C(=O)O1)O
MOL000641	0.3554	0.6446	0.6169	Gentiana Macrophylla Pall	Macrophyllosi de B_qt	Not Available	FALSE	C1CC2(C(=COC(C2C=C)OC2OC(C(C(C2OC(=O)c2 c(c(ccc2)O)O)OC(=O)C)CC(=O)c2c(c(ccc2)O)O)CO C(=O)C)C(=O)O1)O
MOL000642	0.4925	0.5075	0.6494	Gentiana Macrophylla Pall	Roburic acid	Not Available	FALSE	C1(C(CCC2(C1=CCC1C2(CCC(C1(C)CCC(=O)O)C (=C)C)C)C)(C)C)C(CC)C
MOL000644	0.9543	0.0457	0.8450	Gentiana Macrophylla Pall	swertiamarin_ qt	Not Available	FALSE	C1CC2(C(=COC(C2C=C)O)C(=O)O1)O
MOL000644	0.9543	0.0457	0.8450	Gentianae Radix Et Rhozima	swertiamarin_ qt	Not Available	FALSE	C1CC2(C(=COC(C2C=C)O)C(=O)O1)O
MOL000644	0.9543	0.0457	0.8450	Swertiae Mileensis Herba	swertiamarin_ qt	Not Available	FALSE	C1CC2(C(=COC(C2C=C)O)C(=O)O1)O
MOL000644	0.9543	0.0457	0.8450	Cornus Officinalis Sieb. Et Zucc.	swertiamarin_ qt	Not Available	FALSE	C1CC2(C(=COC(C2C=C)O)C(=O)O1)O
MOL000645	0.9231	0.0769	0.8706	Gentianae Radix Et Rhozima	Gentianidine	362908	FALSE	c12C(=O)OCCc1cc(nc2)C
MOL000645	0.9231	0.0769	0.8706	Gentiana Macrophylla Pall	Gentianidine	362908	FALSE	c12C(=O)OCCc1cc(nc2)C
MOL000646	0.9119	0.0881	0.7381	Verbenae Herb	Gentiopicrin	88708	FALSE	C12=CCOC(=O)C2=COC(C1C=C)OC1OC(C(C(C1 O)O)O)O)CO
MOL000646	0.9119	0.0881	0.7381	Gentianae Radix Et Rhozima	Gentiopicrin	88708	FALSE	C12=CCOC(=O)C2=COC(C1C=C)OC1OC(C(C(C1 O)O)O)O)CO
MOL000646	0.9119	0.0881	0.7381	Gentiana Macrophylla Pall	Gentiopicrin	88708	FALSE	C12=CCOC(=O)C2=COC(C1C=C)OC1OC(C(C(C1 O)O)O)O)CO
MOL000647	0.9546	0.0454	0.8169	Gentianae Radix Et Rhozima	scabrans G5_qt	Not Available	FALSE	C12=CCOC(=O)C2=COC(C1C=C)O
MOL000647	0.9546	0.0454	0.8169	Verbenae Herb	scabrans G5_qt	Not Available	FALSE	C12=CCOC(=O)C2=COC(C1C=C)O
MOL000647	0.9546	0.0454	0.8169	Gentiana Macrophylla Pall	scabrans G5_qt	Not Available	FALSE	C12=CCOC(=O)C2=COC(C1C=C)O
MOL000648	0.9415	0.0585	0.8513	Gentiana Macrophylla Pall	Gentianine	354616	FALSE	c12c(C(=O)OCC2)cncc1C=C
MOL000648	0.9415	0.0585	0.8513	Gentianae Radix Et Rhozima	Gentianine	354616	FALSE	c12c(C(=O)OCC2)cncc1C=C
MOL000649	0.9463	0.0537	0.8784	Gentianae Radix Et Rhozima	gentiatibetine	Not Available	FALSE	c1(c2c(ccn1)CCOC2O)C
MOL000649	0.9463	0.0537	0.8784	Gentiana Macrophylla Pall	gentiatibetine	Not Available	FALSE	c1(c2c(ccn1)CCOC2O)C

MOL000650	0.9112	0.0888	0.7353	Cornus Officinalis Sieb. Et Zucc.	1H,3H-Pyrano(3,4-c)pyran-1-one, 5-ethenyl-6-(beta-D-glucopyranosyloxy)-4,4a,5,6-tetrahydro-, (4aS-(4aalpha,5beta,6alpha))-	161036	FALSE	C12=COC(OC3C(C(C(C(O3)CO)O)O)O)C(C1CCOC2=O)C=C
MOL000650	0.9112	0.0888	0.7353	Gentianae Radix Et Rhozima	1H,3H-Pyrano(3,4-c)pyran-1-one, 5-ethenyl-6-(beta-D-glucopyranosyloxy)-4,4a,5,6-tetrahydro-, (4aS-(4aalpha,5beta,6alpha))-	161036	FALSE	C12=COC(OC3C(C(C(C(O3)CO)O)O)O)C(C1CCOC2=O)C=C
MOL000650	0.9112	0.0888	0.7353	Gentiana Macrophylla Pall	1H,3H-Pyrano(3,4-c)pyran-1-one, 5-ethenyl-6-(beta-D-glucopyranosyloxy)-4,4a,5,6-tetrahydro-, (4aS-(4aalpha,5beta,6alpha))-	161036	FALSE	C12=COC(OC3C(C(C(C(O3)CO)O)O)O)C(C1CCOC2=O)C=C

MOL000650	0.9112	0.0888	0.7353	Swertiae Mileensis Herba	1H,3H-Pyrano(3,4-c)pyran-1-one, 5-ethenyl-6-(beta-D-glucopyranosyloxy)-4,4a,5,6-tetrahydro-, (4aS-(4aalpha,5beta,6alpha))-	161036	FALSE	C12=COC(OC3C(C(C(C(O3)CO)O)O)O)C(C1CCOC2=O)C=C
MOL000650	0.9112	0.0888	0.7353	Dipsaci Radix	1H,3H-Pyrano(3,4-c)pyran-1-one, 5-ethenyl-6-(beta-D-glucopyranosyloxy)-4,4a,5,6-tetrahydro-, (4aS-(4aalpha,5beta,6alpha))-	161036	FALSE	C12=COC(OC3C(C(C(C(O3)CO)O)O)O)C(C1CCOC2=O)C=C
MOL000650	0.9112	0.0888	0.7353	Hemerocallis Radix	1H,3H-Pyrano(3,4-c)pyran-1-one, 5-ethenyl-6-(beta-D-glucopyranosyloxy)-4,4a,5,6-tetrahydro-, (4aS-(4aalpha,5beta,6alpha))-	161036	FALSE	C12=COC(OC3C(C(C(C(O3)CO)O)O)O)C(C1CCOC2=O)C=C

MOL000650	0.9112	0.0888	0.7353	Lonicerae Japonicae Flos	1H,3H-Pyrano(3,4-c)pyran-1-one, 5-ethenyl-6-(beta-D-glucopyranosyloxy)-4,4a,5,6-tetrahydro-, (4aS-(4aalpha,5beta,6alpha))-	161036	FALSE	C12=COC(OC3C(C(C(C(O3)CO)O)O)O)C(C1CCOC2=O)C=C
MOL000651	0.9196	0.0804	0.8612	Gentianae Radix Et Rhozima	Sweroside aglycone	203797	FALSE	C12=COC(O)C(C1CCOC2=O)C=C
MOL000651	0.9196	0.0804	0.8612	Lonicerae Japonicae Flos	Sweroside aglycone	203797	FALSE	C12=COC(O)C(C1CCOC2=O)C=C
MOL000651	0.9196	0.0804	0.8612	Swertiae Mileensis Herba	Sweroside aglycone	203797	FALSE	C12=COC(O)C(C1CCOC2=O)C=C
MOL000651	0.9196	0.0804	0.8612	Gentiana Macrophylla Pall	Sweroside aglycone	203797	FALSE	C12=COC(O)C(C1CCOC2=O)C=C
MOL000651	0.9196	0.0804	0.8612	Cornus Officinalis Sieb. Et Zucc.	Sweroside aglycone	203797	FALSE	C12=COC(O)C(C1CCOC2=O)C=C
MOL000651	0.9196	0.0804	0.8612	Dipsaci Radix	Sweroside aglycone	203797	FALSE	C12=COC(O)C(C1CCOC2=O)C=C
MOL000651	0.9196	0.0804	0.8612	Hemerocallis Radix	Sweroside aglycone	203797	FALSE	C12=COC(O)C(C1CCOC2=O)C=C
MOL000652	0.9324	0.0676	0.8658	Dipsaci Radix	Venoterpine	Not Available	FALSE	c1c2c(ccn1)CC(C2C)O
MOL000652	0.9324	0.0676	0.8658	Gentiana Macrophylla Pall	Venoterpine	Not Available	FALSE	c1c2c(ccn1)CC(C2C)O
MOL000653	0.9603	0.0397	0.8704	Gentiana Macrophylla Pall	gentianal	Not Available	FALSE	c1c2c(c(c(=O)[nH]1)C=O)CCOC2C
MOL000655	0.9352	0.0648	0.8855	Gentiana Macrophylla Pall	Loganic acid	89640	FALSE	C12C(C(=COC1OC1OC(C(C(C1O)O)O)O)CO)C(=O)O)CC(C2C)O
MOL000655	0.9352	0.0648	0.8855	Strychni Semen	Loganic acid	89640	FALSE	C12C(C(=COC1OC1OC(C(C(C1O)O)O)O)CO)C(=O)O)CC(C2C)O
MOL000655	0.9352	0.0648	0.8855	Gentianae Radix Et Rhozima	Loganic acid	89640	FALSE	C12C(C(=COC1OC1OC(C(C(C1O)O)O)O)CO)C(=O)O)CC(C2C)O
MOL000655	0.9352	0.0648	0.8855	Lonicerae Japonicae Flos	Loganic acid	89640	FALSE	C12C(C(=COC1OC1OC(C(C(C1O)O)O)O)CO)C(=O)O)CC(C2C)O
MOL000656	0.9508	0.0492	0.8563	Gentiana Macrophylla Pall	loganic acid_qt	25026155	FALSE	C12C(C(=COC1O)C(=O)O)CC(C2C)O
MOL000656	0.9508	0.0492	0.8563	Lonicerae Japonicae Flos	loganic acid_qt	25026155	FALSE	C12C(C(=COC1O)C(=O)O)CC(C2C)O

MOL000656	0.9508	0.0492	0.8563	Gentianae Radix Et Rhozima	loganic acid_qt	25026155	FALSE	C12C(C(=COC1O)C(=O)O)CC(C2C)O
MOL000656	0.9508	0.0492	0.8563	Strychni Semen	loganic acid_qt	25026155	FALSE	C12C(C(=COC1O)C(=O)O)CC(C2C)O
MOL000664	0.2359	0.7641	0.6507	Flemingia Prostrata Roxb	3-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6,8-bis(3-methylbut-2-enyl)chromone	21148065	FALSE	c1c(c(=O)c2c(o1)c(c(c(c2O)CC=C(C)C)O)CC=C(C)C)c1cc(c(cc1)O)O
MOL000665	0.1829	0.8171	0.7981	Flemingia Prostrata Roxb	flemiphilippin C	Not Available	FALSE	C1(C=Cc2c(O1)c(c1c(c2O)c(=O)c(co1)c1cc(c(cc1)O)OC)CC=C)(C)C
MOL000666	0.9341	0.0659	0.9601	Lonicerae Japonicae Flos	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Rubi Fructus	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Rhizome Of Whiteback Greenbrier	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Bombyx Mori L.	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Thalluslaminariae	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Flemingia Prostrata Roxb	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Cornus Officinalis Sieb. Et Zucc.	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Perillae Fructus	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Dichroae Radix	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Evodiae Fructus	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Aucklandiae Radix	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Lysimachiae Foenigraeci Herba	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Amygdalus Communis Vas	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Achyranthis Bidentatae Radix	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Paederiae Scandentis Herba	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Sesami Nigrum Semen	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Scutellariae Barbatae Herba	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Zingiberis Rhizoma	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Leonuri Fructus	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Chuanxiong Rhizoma	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Polygonati Odorati Rhizoma	hexanal	6184	FALSE	C(CCC)CC=O

MOL000666	0.9341	0.0659	0.9601	Radix Angelicae Biseratae	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Radix Cynanchi	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Capsici Fructus	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Coicis Semen	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Polygoni Orientalis Fructus	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Celastri Orbiculati Fructus	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Cinnamomi Ramulus	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Saposhnikoviae Radix	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Ephedra Herba	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Campsis Flos	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Eucommiae Folium	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Allii Tuberosi Semen	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Notopterygii Rhizoma Et Radix	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Radix Bupleuri	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Meliae Azedarach Fructus	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Adenophprae Ae Radix	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Cinnanmomi Cortex	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Piperis Fructus	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Benincasae Exocarpium	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Anemarrhenae Rhizoma	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Allii Sativi Bulbus	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Tamaricis Cacumen	hexanal	6184	FALSE	C(CCC)CC=O
MOL000666	0.9341	0.0659	0.9601	Mahoniae Folum	hexanal	6184	FALSE	C(CCC)CC=O
MOL000667	0.9335	0.0665	0.9607	Folium Nelumbinis	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Thalluslaminariae	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Codonopsis Radix	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Amygdalus Communis Vas	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Scutellariae Barbatae Herba	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Coriandri Sativi Herba	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Sesami Nigrum Semen	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Radix Bupleuri	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Momordicae Fructus	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Ephedra Herba	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Capsellae Herba	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Epimrdii Herba	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Siphonostegiae Herba	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Dianthi Herba	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Chaenomeles Sinensis (Thouin) Koehne	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Campsis Flos	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Flemingia Prostrata Roxb	1-hexanol	8103	FALSE	C(CCC)CCO

MOL000667	0.9335	0.0665	0.9607	Semen Pharbitidis	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Eriobotryae Folium	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Achyranthis Bidentatae Radix	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Mume Flos	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Morindae Officinalis Radix	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Rose Rugosae Flos	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Solidaginis Herba	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Capsici Fructus	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000667	0.9335	0.0665	0.9607	Ginkgo Folium	1-hexanol	8103	FALSE	C(CCC)CCO
MOL000668	0.9027	0.0973	0.9396	Cannabis Sativa L.	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Hippophae Fructus	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Capsici Fructus	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Bombyx Mori L.	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Pollen Typhae	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Adenophprae Ae Radix	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Morindae Officinalis Radix	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Magnolia Officinalis Rehd Et Wils.	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Scutellariae Barbatae Herba	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Meliae Azedarach Fructus	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Violsse Herba	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Arisaematis Rhizoma	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Leonuri Fructus	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Semen Pharbitidis	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Radix Cynanchi Paniculati	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Flemingia Prostrata Roxb	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC

MOL000668	0.9027	0.0973	0.9396	licorice	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Ginkgo Folium	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Allii Tuberosi Semen	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Chuanxiong Rhizoma	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Polygonati Odorati Rhizoma	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Radix Bupleuri	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Campsis Flos	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Ganoderma	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Cuscutae Semen	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Ephedra Herba	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Rhododendri Daurici Folium	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Aucklandiae Radix	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000668	0.9027	0.0973	0.9396	Herba Taxilli	PENTYLFURAN	19602	FALSE	c1(ccco1)CCCCC
MOL000669	0.9388	0.0612	0.8042	Myristicae Semen	(S)-camphor	444294	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000669	0.9388	0.0612	0.8042	Curcumae Rhizoma	(S)-camphor	444294	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000669	0.9388	0.0612	0.8042	Flemingia Prostrata Roxb	(S)-camphor	444294	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000669	0.9388	0.0612	0.8042	Polygonati Odorati Rhizoma	(S)-camphor	444294	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000669	0.9388	0.0612	0.8042	Coriandri Sativi Herba	(S)-camphor	444294	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000669	0.9388	0.0612	0.8042	Borneolum Syntheticum	(S)-camphor	444294	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000669	0.9388	0.0612	0.8042	Morindae Officinalis Radix	(S)-camphor	444294	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000669	0.9388	0.0612	0.8042	Scutellariae Barbatae Herba	(S)-camphor	444294	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000669	0.9388	0.0612	0.8042	Platycladi Cacumen	(S)-camphor	444294	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000669	0.9388	0.0612	0.8042	Artemisia Annua L.	(S)-camphor	444294	FALSE	C12(C(C(CC1=O)CC2)(C)C)C
MOL000670	0.9167	0.0833	0.9532	Flemingia Prostrata Roxb	m-Acetylphenol	8487	FALSE	c1(cc(ccc1)O)C(=O)C
MOL000671	0.9543	0.0457	0.9542	Cannabis Sativa L.	()-Menthol	165675	FALSE	C1(C(CC(CC1)C)O)C(C)C
MOL000671	0.9543	0.0457	0.9542	Menthae Herba	()-Menthol	165675	FALSE	C1(C(CC(CC1)C)O)C(C)C
MOL000671	0.9543	0.0457	0.9542	Cinnamomi Ramulus	()-Menthol	165675	FALSE	C1(C(CC(CC1)C)O)C(C)C
MOL000671	0.9543	0.0457	0.9542	Schizonepetae Spica	()-Menthol	165675	FALSE	C1(C(CC(CC1)C)O)C(C)C

MOL000671	0.9543	0.0457	0.9542	Lonicerae Japonicae Flos	()-Menthol	165675	FALSE	C1(C(CC(CC1)C)O)C(C)C
MOL000671	0.9543	0.0457	0.9542	Schizonepetae Herba	()-Menthol	165675	FALSE	C1(C(CC(CC1)C)O)C(C)C
MOL000671	0.9543	0.0457	0.9542	Rhododendri Daurici Folium	()-Menthol	165675	FALSE	C1(C(CC(CC1)C)O)C(C)C
MOL000671	0.9543	0.0457	0.9542	Herba Patriniae	()-Menthol	165675	FALSE	C1(C(CC(CC1)C)O)C(C)C
MOL000671	0.9543	0.0457	0.9542	Mori Cortex	()-Menthol	165675	FALSE	C1(C(CC(CC1)C)O)C(C)C
MOL000671	0.9543	0.0457	0.9542	Coriandri Sativi Herba	()-Menthol	165675	FALSE	C1(C(CC(CC1)C)O)C(C)C
MOL000671	0.9543	0.0457	0.9542	Stephaniae Tetrandrae Radix	()-Menthol	165675	FALSE	C1(C(CC(CC1)C)O)C(C)C
MOL000671	0.9543	0.0457	0.9542	Campsis Flos	()-Menthol	165675	FALSE	C1(C(CC(CC1)C)O)C(C)C
MOL000671	0.9543	0.0457	0.9542	Flemingia Prostrata Roxb	()-Menthol	165675	FALSE	C1(C(CC(CC1)C)O)C(C)C
MOL000671	0.9543	0.0457	0.9542	Herba Taxilli	()-Menthol	165675	FALSE	C1(C(CC(CC1)C)O)C(C)C
MOL000671	0.9543	0.0457	0.9542	licorice	()-Menthol	165675	FALSE	C1(C(CC(CC1)C)O)C(C)C
MOL000672	0.9033	0.0967	0.8251	Flemingia Prostrata Roxb	3-Isopropylcumene	7450	FALSE	c1(cc(ccc1)C(C)C)C(C)C
MOL000674	0.6845	0.3155	0.7103	Flemingia Prostrata Roxb	Farnesol acetate	638500	FALSE	C(=C\CC/C(=C/COC(=O)C)/C)(/CCC=C(C)C)\C
MOL000674	0.6845	0.3155	0.7103	Folium Artemisiae Argyi	Farnesol acetate	638500	FALSE	C(=C\CC/C(=C/COC(=O)C)/C)(/CCC=C(C)C)\C
MOL000674	0.6845	0.3155	0.7103	Lonicerae Japonicae Flos	Farnesol acetate	638500	FALSE	C(=C\CC/C(=C/COC(=O)C)/C)(/CCC=C(C)C)\C
MOL000674	0.6845	0.3155	0.7103	Ginkgo Folium	Farnesol acetate	638500	FALSE	C(=C\CC/C(=C/COC(=O)C)/C)(/CCC=C(C)C)\C
MOL000674	0.6845	0.3155	0.7103	Ardisiae Japonicae Herba	Farnesol acetate	638500	FALSE	C(=C\CC/C(=C/COC(=O)C)/C)(/CCC=C(C)C)\C
MOL000675	0.7657	0.2343	0.6074	Perillae Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Mori Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Cucurbitae Moschatae Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Lablab Semen Album	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Lycii Cortex	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Curculiginis Rhizome	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Radix Bupleuri	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Coicis Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Malvae Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Radix Salviae	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Scutellariae Barbatae Herba	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Momordicae Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Citri Reticulatae Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Junci Medulla	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O

MOL000675	0.7657	0.2343	0.6074	Semiaquilegiae Radix	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Maydis Seigma	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Gleditsiae Sinensis Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Vaccariae Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Typhonii Rhizoma	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Zingiberis Rhizoma	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Cannabis Sativa L.	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Ranunculi Ternati Radix	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Celastri Orbiculati Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Xanthii Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Linderae Radix	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Smilacis Glabrae Rhixoma	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Platycladi Cacumen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Corydalis Rhizoma	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Flemingia Prostrata Roxb	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Platycladi Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Cinnanmomi Cortex	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Linderae Radix	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Lasiosphaera Seu Calvatia	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Cortex Periplocae Radicis	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Gynostemmae Pentaphylli Herba	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Sojae Semen Nigrum	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Melo Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Broussonetiae Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Oroxyli Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Semen Firmianae	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Hippophae Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Crotonis Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Figwort Root	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Capsellae Herba	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Folium Ilicis Cornutae	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Sterculiae Lychnophorae Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Santalum Album L.	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Thalluslaminariae	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Trollius Chinensis	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Carthami Flos	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Trichosanthes Kirilowii Maxim	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Silybum Marianum	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Viticis Cannabifoliae Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O

MOL000675	0.7657	0.2343	0.6074	Cortex Moutan	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Phyllanthi Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Arum Ternatum Thunb.	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Sinapis Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Momordicae Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Choerospondiatis Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Sapindi Mukorossiperic Arpium	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Ricini Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Nardostachyos Radix Et Rhizoma	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Rosae Laevigatae Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Semen Pharbitidis	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Amygdalus Communis Vas	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Croci Stigma	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Allii Tuberosi Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Lithospermum Erythrorhizon	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Radix Cynanchi Paniculati	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Foeniculi Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Allium Azureum Ledeb.	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Cnidii Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Fructussophorae	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Meliae Azedarach Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Myristicae Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Piperis Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Semen Aesculi	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Semen Euphorbiae	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Quisqualis Indica	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Arecae Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Radix Cirsii Japonici	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Aloe	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Jujubae Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Euryales Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Kochiae Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Curcumae Radix	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Lepidii Semen Descurainiae Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Prunellae Spica	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Sapindi Mukorossi Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O

MOL000675	0.7657	0.2343	0.6074	Semen Lini	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Sesami Nigrum Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Litseae Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Hyoscyami Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Morindae Officinalis Radix	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Portulacae Herba	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Capsici Fructus	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Zanthoxyli Pericarpium	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Chuanxiong Rhizoma	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Litchi Semen	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Alpiniae Officinarum Rhizome	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Calyx Seu Fructus Physalis	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Gleditsiae Spina	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000675	0.7657	0.2343	0.6074	Ginkgo Folium	oleic acid	445639	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)O
MOL000676	0.8439	0.1561	0.9409	Lygodii Spora	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Sargassum	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Ranunculi Ternati Radix	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Alpiniae Officinarum Rhizome	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Millettiae Speciosae Radix	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Morindae Officinalis Radix	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Uncariae Ramulus Cumuncis	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Hyperici Japonici Herber	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Malvae Fructus	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Flemingia Prostrata Roxb	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Echinopsis Radix	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Tamaricis Cacumen	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Folium Artemisiae Argyi	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Pteridis Multifidae Herba	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	licorice	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Ephedra Herba	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Caryophylliflos	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Lycopi Herba	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Eriocauli Flos	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Raphani Semen	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Ginkgo Folium	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Lysimachiae Foenigraeci Herba	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Zingiberis Rhizoma	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Cornus Officinalis Sieb. Et Zucc.	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC

MOL000676	0.8439	0.1561	0.9409	Folium Ilicis Cornutae	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Curcumae Radix	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Radix Bupleuri	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Litchi Semen	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Fructus Ligustri Lucidi	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Tripterygii Radix	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Maydis Seigma	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Paeoniae Radix Alba	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Phytolaccae Radix	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Rhizome Of Whiteback Greenbrier	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Panax Ginseng C. A. Mey.	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Magnolia Officinalis Rehd Et Wils.	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Lepidii Semen Descurainiae Semen	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Violsse Herba	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Mahoniae Folum	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Oroxyli Semen	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Mori Fructus	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Isatdis Radix	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Et Radix Patriniae Rhizoma	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Achyranthis Bidentatae Radix	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Amygdalus Communis Vas	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Flos Genkwa	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Radix Cirsii Japonici	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Schisandrae Chinensis Fructus	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Momordicae Fructus	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Radix Cynanchi Paniculati	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Arecae Semen	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Cinnamomi Ramulus	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Radix Clematidis	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Farfarae Flos	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Pseudostellariae Radix	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Myristicae Semen	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Celastri Orbiculati Fructus	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000676	0.8439	0.1561	0.9409	Pogostemon Cablin (Blanco) Benth.	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC

MOL000676	0.8439	0.1561	0.9409	Lycii Fructus	DBP	3026	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCC
MOL000677	0.8644	0.1356	0.6151	Litchi Semen	(1R,4R)-4-isopropyl-1,6-dimethyltetralin	11298625	FALSE	C1(CCC(c2cc(ccc12)C)C(C)C)C
MOL000677	0.8644	0.1356	0.6151	Viticis Negundo Folium	(1R,4R)-4-isopropyl-1,6-dimethyltetralin	11298625	FALSE	C1(CCC(c2cc(ccc12)C)C(C)C)C
MOL000677	0.8644	0.1356	0.6151	Cinnanmomi Cortex	(1R,4R)-4-isopropyl-1,6-dimethyltetralin	11298625	FALSE	C1(CCC(c2cc(ccc12)C)C(C)C)C
MOL000677	0.8644	0.1356	0.6151	Flemingia Prostrata Roxb	(1R,4R)-4-isopropyl-1,6-dimethyltetralin	11298625	FALSE	C1(CCC(c2cc(ccc12)C)C(C)C)C
MOL000677	0.8644	0.1356	0.6151	Ephedra Herba	(1R,4R)-4-isopropyl-1,6-dimethyltetralin	11298625	FALSE	C1(CCC(c2cc(ccc12)C)C(C)C)C
MOL000677	0.8644	0.1356	0.6151	Menthae Herba	(1R,4R)-4-isopropyl-1,6-dimethyltetralin	11298625	FALSE	C1(CCC(c2cc(ccc12)C)C(C)C)C
MOL000677	0.8644	0.1356	0.6151	Cinnamomi Ramulus	(1R,4R)-4-isopropyl-1,6-dimethyltetralin	11298625	FALSE	C1(CCC(c2cc(ccc12)C)C(C)C)C
MOL000677	0.8644	0.1356	0.6151	Solidaginis Herba	(1R,4R)-4-isopropyl-1,6-dimethyltetralin	11298625	FALSE	C1(CCC(c2cc(ccc12)C)C(C)C)C
MOL000677	0.8644	0.1356	0.6151	Aucklandiae Radix	(1R,4R)-4-isopropyl-1,6-dimethyltetralin	11298625	FALSE	C1(CCC(c2cc(ccc12)C)C(C)C)C
MOL000677	0.8644	0.1356	0.6151	Alpiniae Officinarum Rhizome	(1R,4R)-4-isopropyl-1,6-dimethyltetralin	11298625	FALSE	C1(CCC(c2cc(ccc12)C)C(C)C)C

MOL000677	0.8644	0.1356	0.6151	Styrax	(1R,4R)-4-isopropyl-1,6-dimethyltetralin	11298625	FALSE	C1(CCC(c2cc(ccc12)C)C(C)C)C
MOL000678	0.8913	0.1087	0.7647	Homalomena Occulta (Lour.) Schott	1 beta,4 beta,6 beta,11-tetrahydroxyeudesmane	Not Available	FALSE	C1CC(C2C(C1O)(CCC(C2O)C(C)(O)C)C)(O)C
MOL000679	0.8850	0.1150	0.8059	Homalomena Occulta (Lour.) Schott	1 beta,4 beta,7 alpha-trihydroxyeudcsmane	Not Available	FALSE	C1CC(C2C(C1O)(CCC(C2)(C(C)C)O)C)(O)C
MOL000680	0.8850	0.1150	0.8059	Homalomena Occulta (Lour.) Schott	1 beta,4 beta,7 beta-trihydroxyeudcsmane	Not Available	FALSE	C1CC(C2C(C1O)(CCC(C2)(C(C)C)O)C)(O)C
MOL000681	0.8891	0.1109	0.7894	Homalomena Occulta (Lour.) Schott	1beta, 4beta, 7beta, 11-tetrahydroxyeudesmane	Not Available	FALSE	C1CC(C2C(C1O)(CCC(C2)(C(C)(C)O)O)C)(O)C
MOL000686	0.7264	0.2736	0.6990	Homalomena Occulta (Lour.) Schott	acetylbullatantriol	Not Available	FALSE	C1CC(C2C(C1OC(=O)C)(CCC2CC(O)(C)C)C)(C)O
MOL000687	0.7227	0.2773	0.6261	Homalomena Occulta (Lour.) Schott	asperpenoid	Not Available	FALSE	C(=O)(C)CCC1OC(C2C1(CCC2C(C)C)C)OCC
MOL000688	0.8360	0.1640	0.7859	Homalomena Occulta (Lour.) Schott	bullatantriol	Not Available	FALSE	C1CC(C2C(C1O)(CCC2CC(O)(C)C)C)(C)O
MOL000689	0.8358	0.1642	0.7982	Homalomena Occulta (Lour.) Schott	homalomenol	Not Available	FALSE	C1CC(C2C(C1O)(CCC2C=C(C)C)C)(O)C
MOL000690	0.8608	0.1392	0.8156	Homalomena Occulta (Lour.) Schott	Homalomentraol	Not Available	FALSE	C1(CC(C2C(C1O)(CCC2CC(O)(C)C)C)(C)O)O
MOL000691	0.5352	0.4648	0.7389	Homalomena Occulta (Lour.) Schott	maristeminol	Not Available	FALSE	C1C(C(C(C2C1(C13C(CC2)CC(C1)C(CC3)(C)O)C)(C)C)O)O
MOL000692	0.8719	0.1281	0.7743	Homalomena Occulta (Lour.) Schott	mucrolidin	Not Available	FALSE	C1CC(C2C(C1O)(CCC(C2O)C(C)C)C)(O)C
MOL000693	0.8658	0.1342	0.8133	Homalomena Occulta (Lour.) Schott	oplodiol	Not Available	FALSE	C1CC(C2C(C1O)(CC=C(C2)C(C)C)C)(O)C
MOL000694	0.8399	0.1601	0.7760	Homalomena Occulta (Lour.) Schott	oplopanone	Not Available	FALSE	CC(C)C1CCC(C2C1C(CC2)C(=O)C)(C)O
MOL000694	0.8399	0.1601	0.7760	Alpiniae Oxyphyliae Fructus	oplopanone	Not Available	FALSE	CC(C)C1CCC(C2C1C(CC2)C(=O)C)(C)O
MOL000695	0.8160	0.1840	0.6626	Cyperi Rhizoma	patchouli alcohol	Not Available	FALSE	C12(C3(C(C(CC1C(CC3)C)CC2)(C)C)O)C

MOL000695	0.8160	0.1840	0.6626	Radix Cynanchi Paniculati	patchouli alcohol	Not Available	FALSE	C12(C3(C(C(CC1C(CC3)C)CC2)(C)C)O)C
MOL000695	0.8160	0.1840	0.6626	Epimrdii Herba	patchouli alcohol	Not Available	FALSE	C12(C3(C(C(CC1C(CC3)C)CC2)(C)C)O)C
MOL000695	0.8160	0.1840	0.6626	Stephaniae Tetrandrae Radix	patchouli alcohol	Not Available	FALSE	C12(C3(C(C(CC1C(CC3)C)CC2)(C)C)O)C
MOL000695	0.8160	0.1840	0.6626	Homalomena Occulta (Lour.) Schott	patchouli alcohol	Not Available	FALSE	C12(C3(C(C(CC1C(CC3)C)CC2)(C)C)O)C
MOL000695	0.8160	0.1840	0.6626	Aauropi Folium	patchouli alcohol	Not Available	FALSE	C12(C3(C(C(CC1C(CC3)C)CC2)(C)C)O)C
MOL000695	0.8160	0.1840	0.6626	Oroxyli Semen	patchouli alcohol	Not Available	FALSE	C12(C3(C(C(CC1C(CC3)C)CC2)(C)C)O)C
MOL000695	0.8160	0.1840	0.6626	Lysimachiae Herba	patchouli alcohol	Not Available	FALSE	C12(C3(C(C(CC1C(CC3)C)CC2)(C)C)O)C
MOL000695	0.8160	0.1840	0.6626	Nardostachyos Radix Et Rhizoma	patchouli alcohol	Not Available	FALSE	C12(C3(C(C(CC1C(CC3)C)CC2)(C)C)O)C
MOL000695	0.8160	0.1840	0.6626	Pogostemon Cablin (Blanco) Benth.	patchouli alcohol	Not Available	FALSE	C12(C3(C(C(CC1C(CC3)C)CC2)(C)C)O)C
MOL000695	0.8160	0.1840	0.6626	Agrimonia Eupatoria	patchouli alcohol	Not Available	FALSE	C12(C3(C(C(CC1C(CC3)C)CC2)(C)C)O)C
MOL000696	0.9523	0.0477	0.9704	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	β-terpineol	8748	FALSE	C1(CCC(CC1)C(=C)C)(C)O
MOL000696	0.9523	0.0477	0.9704	Forsythiae Fructus	β-terpineol	8748	FALSE	C1(CCC(CC1)C(=C)C)(C)O
MOL000696	0.9523	0.0477	0.9704	Homalomena Occulta (Lour.) Schott	β-terpineol	8748	FALSE	C1(CCC(CC1)C(=C)C)(C)O
MOL000696	0.9523	0.0477	0.9704	Citrus Reticulata	β-terpineol	8748	FALSE	C1(CCC(CC1)C(=C)C)(C)O
MOL000696	0.9523	0.0477	0.9704	Asari Radix Et Rhizoma	β-terpineol	8748	FALSE	C1(CCC(CC1)C(=C)C)(C)O
MOL000696	0.9523	0.0477	0.9704	Alpiniae Officinarum Rhizome	β-terpineol	8748	FALSE	C1(CCC(CC1)C(=C)C)(C)O
MOL000696	0.9523	0.0477	0.9704	Linderae Radix	β-terpineol	8748	FALSE	C1(CCC(CC1)C(=C)C)(C)O
MOL000696	0.9523	0.0477	0.9704	Artemisia Annua L.	β-terpineol	8748	FALSE	C1(CCC(CC1)C(=C)C)(C)O
MOL000696	0.9523	0.0477	0.9704	Lilii Bulbus	β-terpineol	8748	FALSE	C1(CCC(CC1)C(=C)C)(C)O
MOL000696	0.9523	0.0477	0.9704	Schisandrae Chinensis Fructus	β-terpineol	8748	FALSE	C1(CCC(CC1)C(=C)C)(C)O
MOL000697	0.9416	0.0584	0.9625	Radix Cynanchi Paniculati	MRY	222285	FALSE	C(C(CO)O)(CO)O
MOL000697	0.9416	0.0584	0.9625	Homalomena Occulta (Lour.) Schott	MRY	222285	FALSE	C(C(CO)O)(CO)O
MOL000697	0.9416	0.0584	0.9625	Hippophae Fructus	MRY	222285	FALSE	C(C(CO)O)(CO)O
MOL000697	0.9416	0.0584	0.9625	Arum Ternatum Thunb.	MRY	222285	FALSE	C(C(CO)O)(CO)O
MOL000698	0.9582	0.0418	0.9560	Cayratiae Japonicae Herba	(R)-(-)-alpha-Phellandrene	442482	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000698	0.9582	0.0418	0.9560	Aurantii Fructus Immaturus	(R)-(-)-alpha-Phellandrene	442482	FALSE	C1(C(C)C)CC=C(C=C1)C

MOL000698	0.9582	0.0418	0.9560	Canarii Fructus	(R)-(-)-alpha-Phellandrene	442482	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000698	0.9582	0.0418	0.9560	Zanthoxyli Pericarpium	(R)-(-)-alpha-Phellandrene	442482	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000698	0.9582	0.0418	0.9560	Cinnanmomi Cortex	(R)-(-)-alpha-Phellandrene	442482	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000698	0.9582	0.0418	0.9560	Moslae Herba	(R)-(-)-alpha-Phellandrene	442482	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000698	0.9582	0.0418	0.9560	Citri Fructus	(R)-(-)-alpha-Phellandrene	442482	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000698	0.9582	0.0418	0.9560	Capsici Fructus	(R)-(-)-alpha-Phellandrene	442482	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000698	0.9582	0.0418	0.9560	Croci Stigma	(R)-(-)-alpha-Phellandrene	442482	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000698	0.9582	0.0418	0.9560	Prunellae Spica	(R)-(-)-alpha-Phellandrene	442482	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000698	0.9582	0.0418	0.9560	Homalomena Occulta (Lour.) Schott	(R)-(-)-alpha-Phellandrene	442482	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000698	0.9582	0.0418	0.9560	Chuanxiong Rhizoma	(R)-(-)-alpha-Phellandrene	442482	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000698	0.9582	0.0418	0.9560	Myristicae Semen	(R)-(-)-alpha-Phellandrene	442482	FALSE	C1(C(C)C)CC=C(C=C1)C
MOL000699	0.9362	0.0638	0.8926	Lysimachiae Herba	m-Cymol	10812	FALSE	c1(cc(ccc1)C)C(C)C
MOL000699	0.9362	0.0638	0.8926	Radix Angelicae Biseratae	m-Cymol	10812	FALSE	c1(cc(ccc1)C)C(C)C
MOL000699	0.9362	0.0638	0.8926	Piperis Fructus	m-Cymol	10812	FALSE	c1(cc(ccc1)C)C(C)C
MOL000699	0.9362	0.0638	0.8926	Magnolia Officinalis Rehd Et Wils.	m-Cymol	10812	FALSE	c1(cc(ccc1)C)C(C)C
MOL000699	0.9362	0.0638	0.8926	Homalomena Occulta (Lour.) Schott	m-Cymol	10812	FALSE	c1(cc(ccc1)C)C(C)C
MOL000699	0.9362	0.0638	0.8926	Foeniculi Fructus	m-Cymol	10812	FALSE	c1(cc(ccc1)C)C(C)C
MOL000699	0.9362	0.0638	0.8926	Cinnanmomi Cortex	m-Cymol	10812	FALSE	c1(cc(ccc1)C)C(C)C
MOL000699	0.9362	0.0638	0.8926	Gnaphalii Affinis Herba	m-Cymol	10812	FALSE	c1(cc(ccc1)C)C(C)C
MOL000699	0.9362	0.0638	0.8926	Radix Cynanchi Paniculati	m-Cymol	10812	FALSE	c1(cc(ccc1)C)C(C)C
MOL000700	0.9319	0.0681	0.9465	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Nerol	643820	FALSE	C(=C\CO)(\CCC=C(C)C)/C
MOL000700	0.9319	0.0681	0.9465	Homalomena Occulta (Lour.) Schott	Nerol	643820	FALSE	C(=C\CO)(\CCC=C(C)C)/C
MOL000700	0.9319	0.0681	0.9465	Magnolia Officinalis Rehd Et Wils.	Nerol	643820	FALSE	C(=C\CO)(\CCC=C(C)C)/C
MOL000700	0.9319	0.0681	0.9465	Curcumae Radix	Nerol	643820	FALSE	C(=C\CO)(\CCC=C(C)C)/C
MOL000700	0.9319	0.0681	0.9465	Lonicerae Japonicae Flos	Nerol	643820	FALSE	C(=C\CO)(\CCC=C(C)C)/C
MOL000700	0.9319	0.0681	0.9465	Alpiniae Officinarum Rhizome	Nerol	643820	FALSE	C(=C\CO)(\CCC=C(C)C)/C

MOL000700	0.9319	0.0681	0.9465	Citrus Aurantium	Nerol	643820	FALSE	C(=C\CO)(\CCC=C(C)C)/C
MOL000700	0.9319	0.0681	0.9465	Campsis Flos	Nerol	643820	FALSE	C(=C\CO)(\CCC=C(C)C)/C
MOL000700	0.9319	0.0681	0.9465	Citri Sarcodactylis Fructus	Nerol	643820	FALSE	C(=C\CO)(\CCC=C(C)C)/C
MOL000700	0.9319	0.0681	0.9465	Fructus Ligustri Lucidi	Nerol	643820	FALSE	C(=C\CO)(\CCC=C(C)C)/C
MOL000700	0.9319	0.0681	0.9465	Eriobotryae Folium	Nerol	643820	FALSE	C(=C\CO)(\CCC=C(C)C)/C
MOL000701	0.9133	0.0867	0.8176	Apocyniveneti Folium	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000701	0.9133	0.0867	0.8176	Polygoni Avicularis Herba	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000701	0.9133	0.0867	0.8176	Verbenae Herb	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000701	0.9133	0.0867	0.8176	Herbahypericiperforati	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000701	0.9133	0.0867	0.8176	Mori Cortex	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000701	0.9133	0.0867	0.8176	Herba Taxilli	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000701	0.9133	0.0867	0.8176	Chaenomeles Sinensis (Thouin) Koehne	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000701	0.9133	0.0867	0.8176	Platycladi Cacumen	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000701	0.9133	0.0867	0.8176	Saussureae Involucratae Herba	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000701	0.9133	0.0867	0.8176	Dysosmae Verspiellis Rhixoma Et Radix	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000701	0.9133	0.0867	0.8176	Geranium Wilfordii Maxim.	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000701	0.9133	0.0867	0.8176	Rhododendronmolle	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000701	0.9133	0.0867	0.8176	Ardisiae Japonicae Herba	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000701	0.9133	0.0867	0.8176	Ampelopsis Japonica	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000701	0.9133	0.0867	0.8176	Saururi Herba	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000701	0.9133	0.0867	0.8176	Semen Aesculi	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000701	0.9133	0.0867	0.8176	Microctis Folium	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000701	0.9133	0.0867	0.8176	Stachyurimedulla Helwingiaemedulla	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000701	0.9133	0.0867	0.8176	Hyperici Japonici Herber	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O

MOL000701	0.9133	0.0867	0.8176	Houttuyniae Herba	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000701	0.9133	0.0867	0.8176	Ginkgo Folium	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000701	0.9133	0.0867	0.8176	Saxifraga Stolonifera	quercitrin	5280459	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(C(O1)C)O)O)O)c1cc(c(cc1)O)O
MOL000702	0.9208	0.0792	0.7851	Astragali Cpmplanatisemen	Guajavarin	5481224	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(CO1)O)O)O)c1cc(c(cc1)O)O
MOL000702	0.9208	0.0792	0.7851	Forsythiae Fructus	Guajavarin	5481224	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(CO1)O)O)O)c1cc(c(cc1)O)O
MOL000702	0.9208	0.0792	0.7851	Farfarae Flos	Guajavarin	5481224	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(CO1)O)O)O)c1cc(c(cc1)O)O
MOL000702	0.9208	0.0792	0.7851	Herba Taxilli	Guajavarin	5481224	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(CO1)O)O)O)c1cc(c(cc1)O)O
MOL000703	0.9346	0.0654	0.9506	licorice	2-heptanone	8051	FALSE	C(CCCC)C(=O)C
MOL000703	0.9346	0.0654	0.9506	Herba Taxilli	2-heptanone	8051	FALSE	C(CCCC)C(=O)C
MOL000703	0.9346	0.0654	0.9506	Achyranthis Bidentatae Radix	2-heptanone	8051	FALSE	C(CCCC)C(=O)C
MOL000703	0.9346	0.0654	0.9506	Morindae Officinalis Radix	2-heptanone	8051	FALSE	C(CCCC)C(=O)C
MOL000703	0.9346	0.0654	0.9506	Sesami Nigrum Semen	2-heptanone	8051	FALSE	C(CCCC)C(=O)C
MOL000703	0.9346	0.0654	0.9506	Semen Pharbitidis	2-heptanone	8051	FALSE	C(CCCC)C(=O)C
MOL000703	0.9346	0.0654	0.9506	Caryophylliflos	2-heptanone	8051	FALSE	C(CCCC)C(=O)C
MOL000703	0.9346	0.0654	0.9506	Polygonati Odorati Rhizoma	2-heptanone	8051	FALSE	C(CCCC)C(=O)C
MOL000703	0.9346	0.0654	0.9506	Capsici Fructus	2-heptanone	8051	FALSE	C(CCCC)C(=O)C
MOL000703	0.9346	0.0654	0.9506	Momordicae Fructus	2-heptanone	8051	FALSE	C(CCCC)C(=O)C
MOL000703	0.9346	0.0654	0.9506	Lysimachiae Foenigraeci Herba	2-heptanone	8051	FALSE	C(CCCC)C(=O)C
MOL000704	0.9209	0.0791	0.9256	Cornus Officinalis Sieb. Et Zucc.	styrene	7501	FALSE	c1(ccccc1)C=C
MOL000704	0.9209	0.0791	0.9256	Benzoinum	styrene	7501	FALSE	c1(ccccc1)C=C
MOL000704	0.9209	0.0791	0.9256	Ephedra Herba	styrene	7501	FALSE	c1(ccccc1)C=C
MOL000704	0.9209	0.0791	0.9256	Cnidii Fructus	styrene	7501	FALSE	c1(ccccc1)C=C
MOL000704	0.9209	0.0791	0.9256	Cinnamomi Ramulus	styrene	7501	FALSE	c1(ccccc1)C=C
MOL000704	0.9209	0.0791	0.9256	Myrrha	styrene	7501	FALSE	c1(ccccc1)C=C
MOL000704	0.9209	0.0791	0.9256	Dalbergiae Odoriferae Lignum	styrene	7501	FALSE	c1(ccccc1)C=C
MOL000704	0.9209	0.0791	0.9256	Mori Fructus	styrene	7501	FALSE	c1(ccccc1)C=C
MOL000704	0.9209	0.0791	0.9256	Cinnanmomi Cortex	styrene	7501	FALSE	c1(ccccc1)C=C
MOL000704	0.9209	0.0791	0.9256	Mahoniae Caulis	styrene	7501	FALSE	c1(ccccc1)C=C
MOL000704	0.9209	0.0791	0.9256	Semen Pharbitidis	styrene	7501	FALSE	c1(ccccc1)C=C
MOL000704	0.9209	0.0791	0.9256	Herba Taxilli	styrene	7501	FALSE	c1(ccccc1)C=C
MOL000704	0.9209	0.0791	0.9256	Styrax	styrene	7501	FALSE	c1(ccccc1)C=C

MOL000704	0.9209	0.0791	0.9256	Arisaematis Rhizoma	styrene	7501	FALSE	c1(ccccc1)C=C
MOL000705	0.9368	0.0632	0.9501	Apocyniveneti Folium	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Chuanxiong Rhizoma	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Morindae Officinalis Radix	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Meliae Azedarach Fructus	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Angelicae Sinensis Radix	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Cuscutae Semen	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Herba Taxilli	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Ganoderma	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Peucedani Radix	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Lysimachiae Foenigraeci Herba	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Ligustici Rhizoma Et Radix	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Notopterygii Rhizoma Et Radix	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Magnolia Officinalis Rehd Et Wils.	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Maydis Seigma	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Adenophprae Ae Radix	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Peucedanidecursivi Radix	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Rose Rugosae Flos	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Campsis Flos	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	licorice	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Hippophae Fructus	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Arisaematis Rhizoma	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Evodiae Fructus	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Allii Tuberosi Semen	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Notoginseng Flos	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Radix Angelicae Biseratae	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Rhizome Of Whiteback Greenbrier	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Citri Fructus	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Coriandri Sativi Herba	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Radix Bupleuri	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Capsici Fructus	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Semen Pharbitidis	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Ginkgo Folium	WLN: VH6	8130	FALSE	C(CCC=O)CCC
MOL000705	0.9368	0.0632	0.9501	Zanthoxyli Pericarpium	WLN: VH6	8130	FALSE	C(CCC=O)CCC

MOL000706	0.9251	0.0749	0.9561	Herba Taxilli	3-methylheptan-2-one	Not Available	FALSE	C(C(=O)C)(CCCC)C
MOL000707	0.9321	0.0679	0.9460	Ilicis Cornutae Folium Immayuri	Heptenal	5283316	FALSE	C(=O)/C=C/CCCC
MOL000707	0.9321	0.0679	0.9460	Broussonetiae Fructus	Heptenal	5283316	FALSE	C(=O)/C=C/CCCC
MOL000707	0.9321	0.0679	0.9460	Mahoniae Folum	Heptenal	5283316	FALSE	C(=O)/C=C/CCCC
MOL000707	0.9321	0.0679	0.9460	Semen Pharbitidis	Heptenal	5283316	FALSE	C(=O)/C=C/CCCC
MOL000707	0.9321	0.0679	0.9460	Maydis Seigma	Heptenal	5283316	FALSE	C(=O)/C=C/CCCC
MOL000707	0.9321	0.0679	0.9460	Radix Bupleuri	Heptenal	5283316	FALSE	C(=O)/C=C/CCCC
MOL000707	0.9321	0.0679	0.9460	Lonicerae Japonicae Flos	Heptenal	5283316	FALSE	C(=O)/C=C/CCCC
MOL000707	0.9321	0.0679	0.9460	Herba Taxilli	Heptenal	5283316	FALSE	C(=O)/C=C/CCCC
MOL000707	0.9321	0.0679	0.9460	Eucommiae Folium	Heptenal	5283316	FALSE	C(=O)/C=C/CCCC
MOL000707	0.9321	0.0679	0.9460	Hippophae Fructus	Heptenal	5283316	FALSE	C(=O)/C=C/CCCC
MOL000707	0.9321	0.0679	0.9460	Ginkgo Folium	Heptenal	5283316	FALSE	C(=O)/C=C/CCCC
MOL000707	0.9321	0.0679	0.9460	Celastri Orbiculati Fructus	Heptenal	5283316	FALSE	C(=O)/C=C/CCCC
MOL000707	0.9321	0.0679	0.9460	Amygdalus Communis Vas	Heptenal	5283316	FALSE	C(=O)/C=C/CCCC
MOL000707	0.9321	0.0679	0.9460	Morindae Officinalis Radix	Heptenal	5283316	FALSE	C(=O)/C=C/CCCC
MOL000707	0.9321	0.0679	0.9460	Cnidii Fructus	Heptenal	5283316	FALSE	C(=O)/C=C/CCCC
MOL000707	0.9321	0.0679	0.9460	Adenophprae Ae Radix	Heptenal	5283316	FALSE	C(=O)/C=C/CCCC
MOL000708	0.9009	0.0991	0.9572	Pogostemon Cablin (Blanco) Benth.	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Apocyniveneti Folium	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Dalbergiae Odoriferae Lignum	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Scutellariae Barbatae Herba	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Caryophylliflos	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Semen Pharbitidis	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Dianthi Herba	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Radix Cynanchi Paniculati	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Evodiae Fructus	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Rhododendri Daurici Folium	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Capsici Fructus	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Benzoinum	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Piperis Fructus	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Kaempferiae Rhizoma	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Dichroae Radix	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Campsis Flos	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Lignum Pini Nodi	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Arum Ternatum Thunb.	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Lepidii Semen Descurainiae Semen	WLN: VHR	240	FALSE	c1(ccccc1)C=O

MOL000708	0.9009	0.0991	0.9572	Humulus Scandens (Lour.) Merr.	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Oroxyli Semen	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Rose Rugosae Flos	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Radix Bupleuri	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Amygdalus Communis Vas	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Schizonepetae Herba	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Meliae Azedarach Fructus	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Stephaniae Tetrandrae Radix	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Solidaginis Herba	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Lonicerae Japonicae Flos	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Platycladi Cacumen	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Flos Genkwa	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Mori Follum	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Schizonepetae Spica	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Cinnanmomi Cortex	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Herba Clinopodii Polycephali.	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Mume Flos	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Cistanches Herba	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Litchi Semen	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Ilicis Cornutae Folium Immayuri	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Acoritataninowii Rhizoma	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Herba Taxilli	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Eriobotryae Folium	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Siphonostegiae Herba	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Perillae Fructus	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Ardisiae Japonicae Herba	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Cannabis Sativa L.	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Morindae Officinalis Radix	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Lysimachiae Foenigraeci Herba	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Achyranthis Bidentatae Radix	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000708	0.9009	0.0991	0.9572	Cinnamomi Ramulus	WLN: VHR	240	FALSE	c1(ccccc1)C=O
MOL000709	0.9332	0.0668	0.9488	Allii Fistulost Bulbus	(S)-Matsutake alcohol	2724898	FALSE	C(CCCCC)(C=C)O
MOL000709	0.9332	0.0668	0.9488	Puerariae Flos	(S)-Matsutake alcohol	2724898	FALSE	C(CCCCC)(C=C)O
MOL000709	0.9332	0.0668	0.9488	Ephedra Herba	(S)-Matsutake alcohol	2724898	FALSE	C(CCCCC)(C=C)O

MOL000709	0.9332	0.0668	0.9488	Siphonostegiae Herba	(S)-Matsutake alcohol	2724898	FALSE	C(CCCCC)(C=C)O
MOL000709	0.9332	0.0668	0.9488	Capsici Fructus	(S)-Matsutake alcohol	2724898	FALSE	C(CCCCC)(C=C)O
MOL000709	0.9332	0.0668	0.9488	Celastri Orbiculati Fructus	(S)-Matsutake alcohol	2724898	FALSE	C(CCCCC)(C=C)O
MOL000709	0.9332	0.0668	0.9488	Flos Genkwa	(S)-Matsutake alcohol	2724898	FALSE	C(CCCCC)(C=C)O
MOL000709	0.9332	0.0668	0.9488	Schizonepetae Spica	(S)-Matsutake alcohol	2724898	FALSE	C(CCCCC)(C=C)O
MOL000709	0.9332	0.0668	0.9488	Maydis Seigma	(S)-Matsutake alcohol	2724898	FALSE	C(CCCCC)(C=C)O
MOL000709	0.9332	0.0668	0.9488	Violsse Herba	(S)-Matsutake alcohol	2724898	FALSE	C(CCCCC)(C=C)O
MOL000709	0.9332	0.0668	0.9488	Scutellariae Radix	(S)-Matsutake alcohol	2724898	FALSE	C(CCCCC)(C=C)O
MOL000709	0.9332	0.0668	0.9488	Paederiae Scandentis Herba	(S)-Matsutake alcohol	2724898	FALSE	C(CCCCC)(C=C)O
MOL000709	0.9332	0.0668	0.9488	Schizonepetae Herba	(S)-Matsutake alcohol	2724898	FALSE	C(CCCCC)(C=C)O
MOL000709	0.9332	0.0668	0.9488	Folium Artemisiae Argyi	(S)-Matsutake alcohol	2724898	FALSE	C(CCCCC)(C=C)O
MOL000709	0.9332	0.0668	0.9488	Herba Taxilli	(S)-Matsutake alcohol	2724898	FALSE	C(CCCCC)(C=C)O
MOL000710	0.9347	0.0653	0.9472	Notopterygii Rhizoma Et Radix	OYA	454	FALSE	C(CCCC)CCC=O
MOL000710	0.9347	0.0653	0.9472	Radix Bupleuri	OYA	454	FALSE	C(CCCC)CCC=O
MOL000710	0.9347	0.0653	0.9472	Hippophae Fructus	OYA	454	FALSE	C(CCCC)CCC=O
MOL000710	0.9347	0.0653	0.9472	Chuanxiong Rhizoma	OYA	454	FALSE	C(CCCC)CCC=O
MOL000710	0.9347	0.0653	0.9472	Morindae Officinalis Radix	OYA	454	FALSE	C(CCCC)CCC=O
MOL000710	0.9347	0.0653	0.9472	Zingiberis Rhizoma	OYA	454	FALSE	C(CCCC)CCC=O
MOL000710	0.9347	0.0653	0.9472	Saposhnikoviae Radix	OYA	454	FALSE	C(CCCC)CCC=O
MOL000710	0.9347	0.0653	0.9472	Notoginseng Flos	OYA	454	FALSE	C(CCCC)CCC=O
MOL000710	0.9347	0.0653	0.9472	Zingiber Officinale Roscoe	OYA	454	FALSE	C(CCCC)CCC=O
MOL000710	0.9347	0.0653	0.9472	Adenophprae Ae Radix	OYA	454	FALSE	C(CCCC)CCC=O
MOL000710	0.9347	0.0653	0.9472	Meliae Azedarach Fructus	OYA	454	FALSE	C(CCCC)CCC=O
MOL000710	0.9347	0.0653	0.9472	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	OYA	454	FALSE	C(CCCC)CCC=O
MOL000710	0.9347	0.0653	0.9472	Citri Fructus	OYA	454	FALSE	C(CCCC)CCC=O
MOL000710	0.9347	0.0653	0.9472	Capsici Fructus	OYA	454	FALSE	C(CCCC)CCC=O
MOL000710	0.9347	0.0653	0.9472	Coriandri Sativi Herba	OYA	454	FALSE	C(CCCC)CCC=O
MOL000710	0.9347	0.0653	0.9472	Celastri Orbiculati Fructus	OYA	454	FALSE	C(CCCC)CCC=O
MOL000710	0.9347	0.0653	0.9472	Lilii Bulbus	OYA	454	FALSE	C(CCCC)CCC=O

MOL000710	0.9347	0.0653	0.9472	Semen Euphorbiae	OYA	454	FALSE	C(CCCC)CCC=O
MOL000710	0.9347	0.0653	0.9472	Herba Taxilli	OYA	454	FALSE	C(CCCC)CCC=O
MOL000710	0.9347	0.0653	0.9472	Arisaematis Rhizoma	OYA	454	FALSE	C(CCCC)CCC=O
MOL000710	0.9347	0.0653	0.9472	Citrus Reticulata	OYA	454	FALSE	C(CCCC)CCC=O
MOL000710	0.9347	0.0653	0.9472	Rose Rugosae Flos	OYA	454	FALSE	C(CCCC)CCC=O
MOL000711	0.9079	0.0921	0.9178	Eucommiae Folium	2,4-Heptdienal	5283321	FALSE	C(=C\CC)/C=C/C=O
MOL000711	0.9079	0.0921	0.9178	Celastri Orbiculati Fructus	2,4-Heptdienal	5283321	FALSE	C(=C\CC)/C=C/C=O
MOL000711	0.9079	0.0921	0.9178	Croci Stigma	2,4-Heptdienal	5283321	FALSE	C(=C\CC)/C=C/C=O
MOL000711	0.9079	0.0921	0.9178	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	2,4-Heptdienal	5283321	FALSE	C(=C\CC)/C=C/C=O
MOL000711	0.9079	0.0921	0.9178	Thalluslaminariae	2,4-Heptdienal	5283321	FALSE	C(=C\CC)/C=C/C=O
MOL000711	0.9079	0.0921	0.9178	Ginkgo Folium	2,4-Heptdienal	5283321	FALSE	C(=C\CC)/C=C/C=O
MOL000711	0.9079	0.0921	0.9178	Lygodii Spora	2,4-Heptdienal	5283321	FALSE	C(=C\CC)/C=C/C=O
MOL000711	0.9079	0.0921	0.9178	Eriobotryae Folium	2,4-Heptdienal	5283321	FALSE	C(=C\CC)/C=C/C=O
MOL000711	0.9079	0.0921	0.9178	Lysimachiae Foenigraeci Herba	2,4-Heptdienal	5283321	FALSE	C(=C\CC)/C=C/C=O
MOL000711	0.9079	0.0921	0.9178	Herba Taxilli	2,4-Heptdienal	5283321	FALSE	C(=C\CC)/C=C/C=O
MOL000712	0.9304	0.0696	0.8868	Chuanxiong Rhizoma	o-Cymol	10703	FALSE	c1(c(cccc1)C)C(C)C
MOL000712	0.9304	0.0696	0.8868	Evodiae Fructus	o-Cymol	10703	FALSE	c1(c(cccc1)C)C(C)C
MOL000712	0.9304	0.0696	0.8868	Zanthoxyli Pericarpium	o-Cymol	10703	FALSE	c1(c(cccc1)C)C(C)C
MOL000712	0.9304	0.0696	0.8868	Sesami Nigrum Semen	o-Cymol	10703	FALSE	c1(c(cccc1)C)C(C)C
MOL000712	0.9304	0.0696	0.8868	Piperis Fructus	o-Cymol	10703	FALSE	c1(c(cccc1)C)C(C)C
MOL000712	0.9304	0.0696	0.8868	Zingiberis Rhizoma	o-Cymol	10703	FALSE	c1(c(cccc1)C)C(C)C
MOL000712	0.9304	0.0696	0.8868	Rhododendri Daurici Folium	o-Cymol	10703	FALSE	c1(c(cccc1)C)C(C)C
MOL000712	0.9304	0.0696	0.8868	Alpiniae Officinarum Rhizome	o-Cymol	10703	FALSE	c1(c(cccc1)C)C(C)C
MOL000712	0.9304	0.0696	0.8868	Ginkgo Folium	o-Cymol	10703	FALSE	c1(c(cccc1)C)C(C)C
MOL000712	0.9304	0.0696	0.8868	Adenophprae Ae Radix	o-Cymol	10703	FALSE	c1(c(cccc1)C)C(C)C
MOL000712	0.9304	0.0696	0.8868	Sinapis Semen	o-Cymol	10703	FALSE	c1(c(cccc1)C)C(C)C
MOL000712	0.9304	0.0696	0.8868	Radix Clematidis	o-Cymol	10703	FALSE	c1(c(cccc1)C)C(C)C
MOL000712	0.9304	0.0696	0.8868	Ganoderma	o-Cymol	10703	FALSE	c1(c(cccc1)C)C(C)C
MOL000712	0.9304	0.0696	0.8868	Herba Taxilli	o-Cymol	10703	FALSE	c1(c(cccc1)C)C(C)C

MOL000712	0.9304	0.0696	0.8868	Magnolia Officinalis Rehd Et Wils.	o-Cymol	10703	FALSE	c1(c(cccc1)C)C(C)C
MOL000713	0.9194	0.0806	0.9298	Herba Taxilli	(E)-oct-3-en-2-one	5363229	FALSE	C(=C\C(=O)C)/CCCC
MOL000713	0.9194	0.0806	0.9298	Achyranthis Bidentatae Radix	(E)-oct-3-en-2-one	5363229	FALSE	C(=C\C(=O)C)/CCCC
MOL000714	0.9481	0.0519	0.9596	Folium Artemisiae Argyi	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Dichroae Radix	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Bombyx Mori L.	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Lysimachiae Foenigraeci Herba	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Notoginseng Flos	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Humulus Scandens (Lour.) Merr.	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Carthami Flos	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Ganoderma	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Magnolia Officinalis Rehd Et Wils.	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Herba Taxilli	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Paederiae Scandentis Herba	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Campsis Flos	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Oroxyli Semen	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Ardisiae Japonicae Herba	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Violsse Herba	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Lepidii Semen Descurainiae Semen	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Celastri Orbiculati Fructus	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Eriobotryae Folium	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Ginkgo Folium	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Dysosmae Verspiellis Rhixoma Et Radix	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Nardostachyos Radix Et Rhizoma	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Sinapis Semen	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Hippophae Fructus	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Cannabis Sativa L.	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Gynostemmae Pentaphylli Herba	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Litchi Semen	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Scutellariae Barbatae Herba	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Morindae Officinalis Radix	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Radix Cynanchi Paniculati	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Momordicae Fructus	Hyacinthin	998	FALSE	c1(ccccc1)CC=O

MOL000714	0.9481	0.0519	0.9596	Dianthi Herba	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Lygodii Spora	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Typhonii Rhizoma	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Platycladi Cacumen	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Gnaphalii Affinis Herba	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Cistanches Herba	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Cinnamomi Ramulus	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Capsici Fructus	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Curculiginis Rhizome	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Lonicerae Japonicae Flos	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000714	0.9481	0.0519	0.9596	Benzoinum	Hyacinthin	998	FALSE	c1(ccccc1)CC=O
MOL000715	0.9586	0.0414	0.9571	Schizonepetae Spica	l-Menthone	26447	FALSE	C1(C(=O)CC(CC1)C)C(C)C
MOL000715	0.9586	0.0414	0.9571	Lysimachiae Herba	l-Menthone	26447	FALSE	C1(C(=O)CC(CC1)C)C(C)C
MOL000715	0.9586	0.0414	0.9571	Hippophae Fructus	l-Menthone	26447	FALSE	C1(C(=O)CC(CC1)C)C(C)C
MOL000715	0.9586	0.0414	0.9571	Radix Bupleuri	l-Menthone	26447	FALSE	C1(C(=O)CC(CC1)C)C(C)C
MOL000715	0.9586	0.0414	0.9571	Capsici Fructus	l-Menthone	26447	FALSE	C1(C(=O)CC(CC1)C)C(C)C
MOL000715	0.9586	0.0414	0.9571	Herba Taxilli	l-Menthone	26447	FALSE	C1(C(=O)CC(CC1)C)C(C)C
MOL000715	0.9586	0.0414	0.9571	Radix Cynanchi Paniculati	l-Menthone	26447	FALSE	C1(C(=O)CC(CC1)C)C(C)C
MOL000715	0.9586	0.0414	0.9571	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	l-Menthone	26447	FALSE	C1(C(=O)CC(CC1)C)C(C)C
MOL000715	0.9586	0.0414	0.9571	Violsse Herba	l-Menthone	26447	FALSE	C1(C(=O)CC(CC1)C)C(C)C
MOL000715	0.9586	0.0414	0.9571	Magnolia Officinalis Rehd Et Wils.	l-Menthone	26447	FALSE	C1(C(=O)CC(CC1)C)C(C)C
MOL000715	0.9586	0.0414	0.9571	Apocyniveneti Folium	l-Menthone	26447	FALSE	C1(C(=O)CC(CC1)C)C(C)C
MOL000715	0.9586	0.0414	0.9571	Schizonepetae Herba	l-Menthone	26447	FALSE	C1(C(=O)CC(CC1)C)C(C)C
MOL000715	0.9586	0.0414	0.9571	Sennae Folium	l-Menthone	26447	FALSE	C1(C(=O)CC(CC1)C)C(C)C
MOL000715	0.9586	0.0414	0.9571	Menthae Herba	l-Menthone	26447	FALSE	C1(C(=O)CC(CC1)C)C(C)C
MOL000715	0.9586	0.0414	0.9571	Scutellariae Radix	l-Menthone	26447	FALSE	C1(C(=O)CC(CC1)C)C(C)C
MOL000716	0.9279	0.0721	0.9326	Ginkgo Folium	trans-2-nonenal	5283335	FALSE	C(=O)/C=C/CCCCCC
MOL000716	0.9279	0.0721	0.9326	Xanthii Fructus	trans-2-nonenal	5283335	FALSE	C(=O)/C=C/CCCCCC
MOL000716	0.9279	0.0721	0.9326	Herba Taxilli	trans-2-nonenal	5283335	FALSE	C(=O)/C=C/CCCCCC
MOL000716	0.9279	0.0721	0.9326	Lysimachiae Foenigraeci Herba	trans-2-nonenal	5283335	FALSE	C(=O)/C=C/CCCCCC
MOL000716	0.9279	0.0721	0.9326	Campsis Flos	trans-2-nonenal	5283335	FALSE	C(=O)/C=C/CCCCCC
MOL000716	0.9279	0.0721	0.9326	Meliae Azedarach Fructus	trans-2-nonenal	5283335	FALSE	C(=O)/C=C/CCCCCC
MOL000716	0.9279	0.0721	0.9326	Semen Pharbitidis	trans-2-nonenal	5283335	FALSE	C(=O)/C=C/CCCCCC

MOL000716	0.9279	0.0721	0.9326	Adenophprae Ae Radix	trans-2-nonenal	5283335	FALSE	C(=O)/C=C/CCCCCC
MOL000716	0.9279	0.0721	0.9326	Eucommiae Folium	trans-2-nonenal	5283335	FALSE	C(=O)/C=C/CCCCCC
MOL000716	0.9279	0.0721	0.9326	Ephedra Herba	trans-2-nonenal	5283335	FALSE	C(=O)/C=C/CCCCCC
MOL000716	0.9279	0.0721	0.9326	Hippophae Fructus	trans-2-nonenal	5283335	FALSE	C(=O)/C=C/CCCCCC
MOL000716	0.9279	0.0721	0.9326	Aucklandiae Radix	trans-2-nonenal	5283335	FALSE	C(=O)/C=C/CCCCCC
MOL000716	0.9279	0.0721	0.9326	Thalluslaminariae	trans-2-nonenal	5283335	FALSE	C(=O)/C=C/CCCCCC
MOL000716	0.9279	0.0721	0.9326	Magnolia Officinalis Rehd Et Wils.	trans-2-nonenal	5283335	FALSE	C(=O)/C=C/CCCCCC
MOL000716	0.9279	0.0721	0.9326	Radix Bupleuri	trans-2-nonenal	5283335	FALSE	C(=O)/C=C/CCCCCC
MOL000717	0.9586	0.0414	0.9571	Menthae Herba	d-isomenthone	70962	FALSE	C1(=O)C(CCC(C1)C)C(C)C
MOL000717	0.9586	0.0414	0.9571	Siphonostegiae Herba	d-isomenthone	70962	FALSE	C1(=O)C(CCC(C1)C)C(C)C
MOL000717	0.9586	0.0414	0.9571	Herba Taxilli	d-isomenthone	70962	FALSE	C1(=O)C(CCC(C1)C)C(C)C
MOL000718	0.9311	0.0689	0.9629	Curculiginis Rhizome	3-Methoxyanisole	9025	FALSE	c1c(cccc1OC)OC
MOL000718	0.9311	0.0689	0.9629	Herba Taxilli	3-Methoxyanisole	9025	FALSE	c1c(cccc1OC)OC
MOL000719	0.9455	0.0545	0.9583	Herba Taxilli	methyl salicylate	4133	FALSE	c1(c(cccc1)O)C(=O)OC
MOL000719	0.9455	0.0545	0.9583	Cortex Moutan	methyl salicylate	4133	FALSE	c1(c(cccc1)O)C(=O)OC
MOL000719	0.9455	0.0545	0.9583	Radix Cynanchi Paniculati	methyl salicylate	4133	FALSE	c1(c(cccc1)O)C(=O)OC
MOL000719	0.9455	0.0545	0.9583	Capsici Fructus	methyl salicylate	4133	FALSE	c1(c(cccc1)O)C(=O)OC
MOL000719	0.9455	0.0545	0.9583	Mahoniae Folum	methyl salicylate	4133	FALSE	c1(c(cccc1)O)C(=O)OC
MOL000719	0.9455	0.0545	0.9583	Dianthi Herba	methyl salicylate	4133	FALSE	c1(c(cccc1)O)C(=O)OC
MOL000719	0.9455	0.0545	0.9583	Mume Flos	methyl salicylate	4133	FALSE	c1(c(cccc1)O)C(=O)OC

MOL000719	0.9455	0.0545	0.9583	Ardisiae Japonicae Herba	methyl salicylate	4133	FALSE	c1(c(cccc1)O)C(=O)OC
MOL000719	0.9455	0.0545	0.9583	Caryophylliflos	methyl salicylate	4133	FALSE	c1(c(cccc1)O)C(=O)OC
MOL000719	0.9455	0.0545	0.9583	Eriobotryae Folium	methyl salicylate	4133	FALSE	c1(c(cccc1)O)C(=O)OC
MOL000720	0.9641	0.0359	0.9228	Evodiae Fructus	Safranal	61041	FALSE	C1(=C(C=CCC1(C)C)C)C=O
MOL000720	0.9641	0.0359	0.9228	Rubi Fructus	Safranal	61041	FALSE	C1(=C(C=CCC1(C)C)C)C=O
MOL000720	0.9641	0.0359	0.9228	Ginkgo Folium	Safranal	61041	FALSE	C1(=C(C=CCC1(C)C)C)C=O
MOL000720	0.9641	0.0359	0.9228	Lycii Fructus	Safranal	61041	FALSE	C1(=C(C=CCC1(C)C)C)C=O
MOL000720	0.9641	0.0359	0.9228	Campsis Flos	Safranal	61041	FALSE	C1(=C(C=CCC1(C)C)C)C=O
MOL000720	0.9641	0.0359	0.9228	Capsici Fructus	Safranal	61041	FALSE	C1(=C(C=CCC1(C)C)C)C=O
MOL000720	0.9641	0.0359	0.9228	Ephedra Herba	Safranal	61041	FALSE	C1(=C(C=CCC1(C)C)C)C=O
MOL000720	0.9641	0.0359	0.9228	Croci Stigma	Safranal	61041	FALSE	C1(=C(C=CCC1(C)C)C)C=O
MOL000720	0.9641	0.0359	0.9228	Apocyniveneti Folium	Safranal	61041	FALSE	C1(=C(C=CCC1(C)C)C)C=O
MOL000720	0.9641	0.0359	0.9228	Lysimachiae Foenigraeci Herba	Safranal	61041	FALSE	C1(=C(C=CCC1(C)C)C)C=O
MOL000720	0.9641	0.0359	0.9228	Herba Taxilli	Safranal	61041	FALSE	C1(=C(C=CCC1(C)C)C)C=O
MOL000720	0.9641	0.0359	0.9228	Eriobotryae Folium	Safranal	61041	FALSE	C1(=C(C=CCC1(C)C)C)C=O
MOL000721	0.9231	0.0769	0.9209	Apocyniveneti Folium	Nonadienal	5283339	FALSE	C(=C\C=C\C=O)/CCCC
MOL000721	0.9231	0.0769	0.9209	Anemarrhenae Rhizoma	Nonadienal	5283339	FALSE	C(=C\C=C\C=O)/CCCC
MOL000721	0.9231	0.0769	0.9209	Codonopsis Radix	Nonadienal	5283339	FALSE	C(=C\C=C\C=O)/CCCC
MOL000721	0.9231	0.0769	0.9209	Herba Taxilli	Nonadienal	5283339	FALSE	C(=C\C=C\C=O)/CCCC
MOL000721	0.9231	0.0769	0.9209	Lignum Pini Nodi	Nonadienal	5283339	FALSE	C(=C\C=C\C=O)/CCCC
MOL000721	0.9231	0.0769	0.9209	Adenophprae Ae Radix	Nonadienal	5283339	FALSE	C(=C\C=C\C=O)/CCCC
MOL000722	0.9635	0.0365	0.9266	Thalluslaminariae	beta-Cyclocitral	9895	FALSE	C1(=C(CCCC1(C)C)C)C=O
MOL000722	0.9635	0.0365	0.9266	Canarii Fructus	beta-Cyclocitral	9895	FALSE	C1(=C(CCCC1(C)C)C)C=O
MOL000722	0.9635	0.0365	0.9266	Celastri Orbiculati Fructus	beta-Cyclocitral	9895	FALSE	C1(=C(CCCC1(C)C)C)C=O
MOL000722	0.9635	0.0365	0.9266	Herba Taxilli	beta-Cyclocitral	9895	FALSE	C1(=C(CCCC1(C)C)C)C=O
MOL000722	0.9635	0.0365	0.9266	Dianthi Herba	beta-Cyclocitral	9895	FALSE	C1(=C(CCCC1(C)C)C)C=O
MOL000722	0.9635	0.0365	0.9266	Ephedra Herba	beta-Cyclocitral	9895	FALSE	C1(=C(CCCC1(C)C)C)C=O
MOL000722	0.9635	0.0365	0.9266	Eucommiae Folium	beta-Cyclocitral	9895	FALSE	C1(=C(CCCC1(C)C)C)C=O
MOL000722	0.9635	0.0365	0.9266	Lysimachiae Foenigraeci Herba	beta-Cyclocitral	9895	FALSE	C1(=C(CCCC1(C)C)C)C=O
MOL000722	0.9635	0.0365	0.9266	Apocyniveneti Folium	beta-Cyclocitral	9895	FALSE	C1(=C(CCCC1(C)C)C)C=O

MOL000722	0.9635	0.0365	0.9266	Sennae Folium	beta-Cyclocitral	9895	FALSE	C1(=C(CCCC1(C)C)C)C=O
MOL000723	0.9246	0.0754	0.9092	Ganoderma	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Smilacis Glabrae Rhixoma	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Litchi Semen	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Hippophae Fructus	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Malvae Fructus	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Leonuri Fructus	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Amygdalus Communis Vas	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Adenophprae Ae Radix	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Cnidii Fructus	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Cucurbitae Moschatae Semen	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Sinapis Semen	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Ephedra Herba	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Lygodii Spora	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Tamaricis Cacumen	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Croci Stigma	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Allii Tuberosi Semen	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Magnolia Officinalis Rehd Et Wils.	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Carthami Flos	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Radix Bupleuri	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Herba Taxilli	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC

MOL000723	0.9246	0.0754	0.9092	Broussonetiae Fructus	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Capsici Fructus	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Thalluslaminariae	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Gossampiniflos	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000723	0.9246	0.0754	0.9092	Ginseng Folium	trans-2,4-decadienal	5283349	FALSE	C(=O)/C=C/C=C/CCCCC
MOL000724	0.9069	0.0931	0.8812	Mahoniae Folum	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Ilicis Purpureae Folium	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Dalbergiae Odoriferae Lignum	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Mume Flos	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Croci Stigma	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Rhododendri Daurici Folium	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Ephedra Herba	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Lygodii Spora	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Polygoni Orientalis Fructus	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Campsis Flos	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Hippophae Fructus	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Lysimachiae Foenigraeci Herba	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Eriobotryae Folium	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Celastri Orbiculati Fructus	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Leonuri Fructus	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Scutellariae Barbatae Herba	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C

MOL000724	0.9069	0.0931	0.8812	Ginkgo Folium	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Rose Rugosae Flos	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Aucklandiae Radix	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Eucommiae Folium	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Tamaricis Cacumen	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Aauropi Folium	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Herba Taxilli	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Radix Bupleuri	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000724	0.9069	0.0931	0.8812	Capsici Fructus	Geranylacetone	1549778	FALSE	C(=C\CCC(=O)C)(/CCC=C(C)C)\C
MOL000726	0.8827	0.1173	0.8216	Ramulus Mori	Morindin	5319896	FALSE	C1(C(C(C(OC1C)OCC1C(C(C(C(O1)Oc1c(c2c(cc1)C(=O)c1c(C2=O)ccc(c1O)C)O)O)O)O)O)O)O
MOL000726	0.8827	0.1173	0.8216	Mori Follum	Morindin	5319896	FALSE	C1(C(C(C(OC1C)OCC1C(C(C(C(O1)Oc1c(c2c(cc1)C(=O)c1c(C2=O)ccc(c1O)C)O)O)O)O)O)O)O
MOL000728	0.0920	0.9080	0.6940	Ramulus Mori	Mulberrofuran A	5281332	FALSE	CC(=CCC/C(=C/Cc1c(cc(cc1c1cc2c(o1)cc(cc2)O)O)OC)/C)C
MOL000728	0.0920	0.9080	0.6940	Mori Cortex	Mulberrofuran A	5281332	FALSE	CC(=CCC/C(=C/Cc1c(cc(cc1c1cc2c(o1)cc(cc2)O)O)OC)/C)C
MOL000729	0.8351	0.1649	0.7269	Chelidonii Herba	Oxysanguinarine	Not Available	FALSE	c12cc3c(cc1OCO2)c1c(cc3)c2c(c(=O)n1C)c1c(cc2)OCO1
MOL000729	0.8351	0.1649	0.7269	Corydalis Bungeanae Herba	Oxysanguinarine	Not Available	FALSE	c12cc3c(cc1OCO2)c1c(cc3)c2c(c(=O)n1C)c1c(cc2)OCO1
MOL000729	0.8351	0.1649	0.7269	Ramulus Mori	Oxysanguinarine	Not Available	FALSE	c12cc3c(cc1OCO2)c1c(cc3)c2c(c(=O)n1C)c1c(cc2)OCO1
MOL000729	0.8351	0.1649	0.7269	Mori Follum	Oxysanguinarine	Not Available	FALSE	c12cc3c(cc1OCO2)c1c(cc3)c2c(c(=O)n1C)c1c(cc2)OCO1
MOL000730	0.9230	0.0770	0.8944	Smilacis Glabrae Rhixoma	(2S,3R)-3,5,7-trihydroxy-2-(4-hydroxyphenyl)chroman-4-one	11449086	FALSE	C1(C(C(=O)c2c(cc(cc2O1)O)O)O)c1ccc(cc1)O

MOL000730	0.9230	0.0770	0.8944	Ramulus Mori	(2S,3R)-3,5,7-trihydroxy-2-(4-hydroxyphenyl)chroman-4-one	11449086	FALSE	C1(C(C(=O)c2c(cc(cc2O1)O)O)O)c1ccc(cc1)O
MOL000730	0.9230	0.0770	0.8944	Euonymi Alati Ramulus	(2S,3R)-3,5,7-trihydroxy-2-(4-hydroxyphenyl)chroman-4-one	11449086	FALSE	C1(C(C(=O)c2c(cc(cc2O1)O)O)O)c1ccc(cc1)O
MOL000730	0.9230	0.0770	0.8944	Catechu	(2S,3R)-3,5,7-trihydroxy-2-(4-hydroxyphenyl)chroman-4-one	11449086	FALSE	C1(C(C(=O)c2c(cc(cc2O1)O)O)O)c1ccc(cc1)O
MOL000730	0.9230	0.0770	0.8944	Smilax China	(2S,3R)-3,5,7-trihydroxy-2-(4-hydroxyphenyl)chroman-4-one	11449086	FALSE	C1(C(C(=O)c2c(cc(cc2O1)O)O)O)c1ccc(cc1)O
MOL000731	0.9346	0.0654	0.9639	Rosae Laevigatae Fructus	XYS	6027	FALSE	C1(C(C(OCC1O)O)O)O
MOL000731	0.9346	0.0654	0.9639	Abrus Precatorius L.	XYS	6027	FALSE	C1(C(C(OCC1O)O)O)O
MOL000731	0.9346	0.0654	0.9639	Sterculiae Lychnophorae Semen	XYS	6027	FALSE	C1(C(C(OCC1O)O)O)O
MOL000731	0.9346	0.0654	0.9639	Trichosanthes Kirilowii Maxim	XYS	6027	FALSE	C1(C(C(OCC1O)O)O)O
MOL000731	0.9346	0.0654	0.9639	Hippophae Fructus	XYS	6027	FALSE	C1(C(C(OCC1O)O)O)O
MOL000731	0.9346	0.0654	0.9639	Ramulus Mori	XYS	6027	FALSE	C1(C(C(OCC1O)O)O)O
MOL000732	0.8669	0.1331	0.7595	Rehmanniae Radix Praeparata	Stachyose	439531	FALSE	C1(OC2OC(COC3OC(COC4OC(C(C(C4O)O)O)O)CO)C(C(C3O)O)O)C(C(C2O)O)O)(OC(C(C1O)O)CO)CO
MOL000732	0.8669	0.1331	0.7595	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	Stachyose	439531	FALSE	C1(OC2OC(COC3OC(COC4OC(C(C(C4O)O)O)O)CO)C(C(C3O)O)O)C(C(C2O)O)O)(OC(C(C1O)O)CO)CO
MOL000732	0.8669	0.1331	0.7595	Plantaginis Herba	Stachyose	439531	FALSE	C1(OC2OC(COC3OC(COC4OC(C(C(C4O)O)O)O)CO)C(C(C3O)O)O)C(C(C2O)O)O)(OC(C(C1O)O)CO)CO
MOL000732	0.8669	0.1331	0.7595	Ramulus Mori	Stachyose	439531	FALSE	C1(OC2OC(COC3OC(COC4OC(C(C(C4O)O)O)O)CO)C(C(C3O)O)O)C(C(C2O)O)O)(OC(C(C1O)O)CO)CO
MOL000732	0.8669	0.1331	0.7595	Lablab Semen Album	Stachyose	439531	FALSE	C1(OC2OC(COC3OC(COC4OC(C(C(C4O)O)O)O)CO)C(C(C3O)O)O)C(C(C2O)O)O)(OC(C(C1O)O)CO)CO

MOL000733	0.9070	0.0930	0.8932	Vigna Radiata	37417-41-7	181526	FALSE	C1(OC(C(C(C=O)O)O)C(CO)O)OC(C(C(C1O)O)O)CO
MOL000733	0.9070	0.0930	0.8932	Ramulus Mori	37417-41-7	181526	FALSE	C1(OC(C(C(C=O)O)O)C(CO)O)OC(C(C(C1O)O)O)CO
MOL000733	0.9070	0.0930	0.8932	Bolbostemae Paniculati Bulbus	37417-41-7	181526	FALSE	C1(OC(C(C(C=O)O)O)C(CO)O)OC(C(C(C1O)O)O)CO
MOL000734	0.9461	0.0539	0.9688	Cyperi Rhizoma	GLO	107526	FALSE	C(C(O)C(CO)O)(C(C=O)O)O
MOL000734	0.9461	0.0539	0.9688	Trichosanthes Kirilowii Maxim	GLO	107526	FALSE	C(C(O)C(CO)O)(C(C=O)O)O
MOL000734	0.9461	0.0539	0.9688	Rosae Laevigatae Fructus	GLO	107526	FALSE	C(C(O)C(CO)O)(C(C=O)O)O
MOL000734	0.9461	0.0539	0.9688	Alisma Orientale (Sam.) Juz.	GLO	107526	FALSE	C(C(O)C(CO)O)(C(C=O)O)O
MOL000734	0.9461	0.0539	0.9688	Gynostemmae Pentaphylli Herba	GLO	107526	FALSE	C(C(O)C(CO)O)(C(C=O)O)O
MOL000734	0.9461	0.0539	0.9688	Bamusaeconcretiosilicea	GLO	107526	FALSE	C(C(O)C(CO)O)(C(C=O)O)O
MOL000734	0.9461	0.0539	0.9688	Tetrapanacis Medulla	GLO	107526	FALSE	C(C(O)C(CO)O)(C(C=O)O)O
MOL000734	0.9461	0.0539	0.9688	Ramulus Mori	GLO	107526	FALSE	C(C(O)C(CO)O)(C(C=O)O)O
MOL000734	0.9461	0.0539	0.9688	Vigna Radiata	GLO	107526	FALSE	C(C(O)C(CO)O)(C(C=O)O)O
MOL000734	0.9461	0.0539	0.9688	Bolbostemae Paniculati Bulbus	GLO	107526	FALSE	C(C(O)C(CO)O)(C(C=O)O)O
MOL000734	0.9461	0.0539	0.9688	Lonicerae Japonicae Flos	GLO	107526	FALSE	C(C(O)C(CO)O)(C(C=O)O)O
MOL000734	0.9461	0.0539	0.9688	Rhizoma Fagopyri Cymosi	GLO	107526	FALSE	C(C(O)C(CO)O)(C(C=O)O)O
MOL000734	0.9461	0.0539	0.9688	Stachyurimedulla Helwingiaemedulla	GLO	107526	FALSE	C(C(O)C(CO)O)(C(C=O)O)O
MOL000734	0.9461	0.0539	0.9688	Hippophae Fructus	GLO	107526	FALSE	C(C(O)C(CO)O)(C(C=O)O)O
MOL000735	0.3097	0.6903	0.6643	Mori Cortex	cyclomulberrin	Not Available	FALSE	c12c(c(=O)c3c(o1)c(c(cc3O)O)CC=C(C)C)C(Oc1c2ccc(c1)O)C=C(C)C
MOL000735	0.3097	0.6903	0.6643	Ramulus Mori	cyclomulberrin	Not Available	FALSE	c12c(c(=O)c3c(o1)c(c(cc3O)O)CC=C(C)C)C(Oc1c2ccc(c1)O)C=C(C)C
MOL000737	0.9298	0.0702	0.7445	Moslae Herba	morin	5281670	TRUE	c12c(oc(c(c1=O)O)c1c(cc(cc1)O)O)cc(cc2O)O
MOL000737	0.9298	0.0702	0.7445	Ramulus Mori	morin	5281670	TRUE	c12c(oc(c(c1=O)O)c1c(cc(cc1)O)O)cc(cc2O)O
MOL000737	0.9298	0.0702	0.7445	Mori Fructus	morin	5281670	TRUE	c12c(oc(c(c1=O)O)c1c(cc(cc1)O)O)cc(cc2O)O
MOL000737	0.9298	0.0702	0.7445	Prunellae Spica	morin	5281670	TRUE	c12c(oc(c(c1=O)O)c1c(cc(cc1)O)O)cc(cc2O)O
MOL000739	0.1822	0.8178	0.7493	Ramulus Mori	morusin	Not Available	FALSE	C1(C(=Cc2c3c(c(cc2O1)O)c(=O)c(co3)CC=C(C)C)c1c(cc(cc1)O)O)(C)C
MOL000740	0.7820	0.2180	0.7735	Ramulus Mori	(+)-Cycloolivil	5316262	FALSE	COc1c(O)cc2c(c1)CC(C(C2c1ccc(c(c1)OC)O)CO)(CO)O
MOL000740	0.7820	0.2180	0.7735	Eucommiae Cortex	(+)-Cycloolivil	5316262	FALSE	COc1c(O)cc2c(c1)CC(C(C2c1ccc(c(c1)OC)O)CO)(CO)O
MOL000740	0.7820	0.2180	0.7735	Mori Cortex	(+)-Cycloolivil	5316262	FALSE	COc1c(O)cc2c(c1)CC(C(C2c1ccc(c(c1)OC)O)CO)(CO)O
MOL000740	0.7820	0.2180	0.7735	Epimrdii Herba	(+)-Cycloolivil	5316262	FALSE	COc1c(O)cc2c(c1)CC(C(C2c1ccc(c(c1)OC)O)CO)(CO)O

MOL000741	0.9230	0.0770	0.8944	Polygoni Avicularis Herba	(2S,3S)-3,5,7-trihydroxy-2-(4-hydroxyphenyl)chroman-4-one	9838882	FALSE	c1cc(ccc1O)C1C(O)C(=O)c2c(O1)cc(cc2O)O
MOL000741	0.9230	0.0770	0.8944	Polygoni Orientalis Fructus	(2S,3S)-3,5,7-trihydroxy-2-(4-hydroxyphenyl)chroman-4-one	9838882	FALSE	c1cc(ccc1O)C1C(O)C(=O)c2c(O1)cc(cc2O)O
MOL000741	0.9230	0.0770	0.8944	Ramulus Mori	(2S,3S)-3,5,7-trihydroxy-2-(4-hydroxyphenyl)chroman-4-one	9838882	FALSE	c1cc(ccc1O)C1C(O)C(=O)c2c(O1)cc(cc2O)O
MOL000741	0.9230	0.0770	0.8944	Hippophae Fructus	(2S,3S)-3,5,7-trihydroxy-2-(4-hydroxyphenyl)chroman-4-one	9838882	FALSE	c1cc(ccc1O)C1C(O)C(=O)c2c(O1)cc(cc2O)O
MOL000741	0.9230	0.0770	0.8944	Silybum Marianum	(2S,3S)-3,5,7-trihydroxy-2-(4-hydroxyphenyl)chroman-4-one	9838882	FALSE	c1cc(ccc1O)C1C(O)C(=O)c2c(O1)cc(cc2O)O
MOL000741	0.9230	0.0770	0.8944	Phellodendri Chinrnsis Cortex	(2S,3S)-3,5,7-trihydroxy-2-(4-hydroxyphenyl)chroman-4-one	9838882	FALSE	c1cc(ccc1O)C1C(O)C(=O)c2c(O1)cc(cc2O)O
MOL000741	0.9230	0.0770	0.8944	Platycladi Cacumen	(2S,3S)-3,5,7-trihydroxy-2-(4-hydroxyphenyl)chroman-4-one	9838882	FALSE	c1cc(ccc1O)C1C(O)C(=O)c2c(O1)cc(cc2O)O
MOL000742	0.7648	0.2352	0.6760	Ramulus Mori	Cularicine	Not Available	FALSE	C12c3c(Oc4c(C1)cc1c(c4)OCO1)c(ccc3CCN2C)O

MOL000743	0.4118	0.5882	0.6748	Ramulus Mori	Cyclomulberrochromene	Not Available	FALSE	C1(C=Cc2c(O1)cc1c(c2O)c(=O)c2c(o1)c1c(OC2C=C(C)C)cc(cc1)O)(C)C
MOL000744	0.9672	0.0328	0.8932	Ramulus Mori	Dihydronepetalactone	58651660	FALSE	C1CC2C(C1C)C(=O)OCC2C
MOL000745	0.7843	0.2157	0.7848	Ramulus Mori	Macranthoidin A	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)CO)OC1OCC(C(C1OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)C)O)O)C)C)C)C(=O)OC1CC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO
MOL000745	0.7843	0.2157	0.7848	Mori Follum	Macranthoidin A	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)CO)OC1OCC(C(C1OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)C)O)O)C)C)C)C(=O)OC1CC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO
MOL000746	0.8090	0.1910	0.8344	Ramulus Mori	Macranthoidin A_qt	Not Available	FALSE	C12=CCC3C4(C(CCC3(C2(CCC2(C(=O)OC3CC(C(C(C3O)O)O)CO)C1CC(C)(CC2)C)C)C(C)(C(OC1OCC(C(O)C1OC1OC(C)C(C(C1O)O)O)O)CC4)CO)C
MOL000747	0.9056	0.0944	0.9668	Smilax Scodinicaulis C.H. Wrisht?	5-hydroxy-4-oxopentanoic acid	10080438	FALSE	C(=O)(CCC(=O)CO)O
MOL000748	0.8777	0.1223	0.9530	Gypsophila Licentiana Hand.-Mazz.	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Lobeliae Chinensis Herba	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Imperatae Rhizoma	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Acoritataninowii Rhizoma	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Kansui Radix	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Bolbostemae Paniculati Bulbus	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Polygonati Rhizoma	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Lepidii Semen Descurainiae Semen	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Sparganii Rhizoma	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Chaenomeles Sinensis (Thouin) Koehne	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Semiaquilegiae Radix	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Arum Ternatum Thunb.	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Caulis Akebiae	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Toosendan Fructus	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Meliae Cortex	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Alisma Orientale (Sam.) Juz.	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Asparagi Radix	HMF	237332	FALSE	o1c(ccc1CO)C=O

MOL000748	0.8777	0.1223	0.9530	Polygonati Odorati Rhizoma	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Smilacis Glabrae Rhixoma	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Lasiosphaera Seu Calvatia	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Schisandrae Chinensis Fructus	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Cichorii Radix	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Trichosanthes Kirilowii Maxim	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Hordei Fructus Germinatus	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Ranunculi Ternati Radix	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Rehmanniae Radix Praeparata	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Carthami Flos	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Isatdis Radix	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Smilax Scodinicaulis C.H. Wrisht?	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Figwort Root	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Citri Exocarpium Rubrum	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Ephedra Herba	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Achyranthis Bidentatae Radix	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Radix Clematidis	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Citrus Reticulata	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Drynariae Rhizoma	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000748	0.8777	0.1223	0.9530	Codonopsis Radix	HMF	237332	FALSE	o1c(ccc1CO)C=O
MOL000749	0.7705	0.2295	0.6325	Chrysanthemi Indici Flos	Linoleic	5282457	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)O
MOL000749	0.7705	0.2295	0.6325	Sparganii Rhizoma	Linoleic	5282457	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)O
MOL000749	0.7705	0.2295	0.6325	Spirodelae Herba	Linoleic	5282457	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)O
MOL000749	0.7705	0.2295	0.6325	Chebulae Fructus	Linoleic	5282457	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)O
MOL000749	0.7705	0.2295	0.6325	Echinopsis Radix	Linoleic	5282457	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)O
MOL000749	0.7705	0.2295	0.6325	Eriocauli Flos	Linoleic	5282457	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)O
MOL000749	0.7705	0.2295	0.6325	Houttuyniae Herba	Linoleic	5282457	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)O
MOL000749	0.7705	0.2295	0.6325	Panax Ginseng C. A. Mey.	Linoleic	5282457	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)O
MOL000749	0.7705	0.2295	0.6325	Panacis Quinquefolii Radix	Linoleic	5282457	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)O
MOL000749	0.7705	0.2295	0.6325	Farfarae Flos	Linoleic	5282457	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)O
MOL000749	0.7705	0.2295	0.6325	Jujubae Fructus	Linoleic	5282457	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)O
MOL000749	0.7705	0.2295	0.6325	Alpiniae Oxyphyliae Fructus	Linoleic	5282457	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)O
MOL000749	0.7705	0.2295	0.6325	Lycii Cortex	Linoleic	5282457	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)O
MOL000749	0.7705	0.2295	0.6325	Lycii Fructus	Linoleic	5282457	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)O
MOL000749	0.7705	0.2295	0.6325	Cornus Officinalis Sieb. Et Zucc.	Linoleic	5282457	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)O

MOL000749	0.7705	0.2295	0.6325	Ginkgo Semen	Linoleic	5282457	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)O
MOL000749	0.7705	0.2295	0.6325	Polygonati Odorati Rhizoma	Linoleic	5282457	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)O
MOL000749	0.7705	0.2295	0.6325	Corayceps	Linoleic	5282457	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)O
MOL000749	0.7705	0.2295	0.6325	Smilax Scodinicaulis C.H. Wrisht?	Linoleic	5282457	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)O
MOL000750	0.9304	0.0696	0.7352	Smilax Scodinicaulis C.H. Wrisht?	Anemonin	71676052	FALSE	C1CC2(C31C=CC(=O)O3)C=CC(=O)O2
MOL000751	0.4913	0.5087	0.8090	Smilax Scodinicaulis C.H. Wrisht?	clemaphenolA	46173999	FALSE	c1(cc(ccc1OC)C1OCC2C1COC2c1cc(c(cc1)OC)O)O
MOL000751	0.4913	0.5087	0.8090	Radix Clematidis	clemaphenolA	46173999	FALSE	c1(cc(ccc1OC)C1OCC2C1COC2c1cc(c(cc1)OC)O)O
MOL000752	0.4873	0.5127	0.7540	Smilax Scodinicaulis C.H. Wrisht?	clematichinenoside AR	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(OC2C(O)C(O)C(O)C(O2)C)C(O1)CO)C)C)C)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)OC1OCC(C(C1O)O)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)C)O)C)O)O
MOL000753	0.6631	0.3369	0.7696	Smilax Scodinicaulis C.H. Wrisht?	clematichinenoside AR2	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)OC1OCC(C(C1O)O)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)C)O)C)O)O
MOL000754	0.7341	0.2659	0.8358	Smilax Scodinicaulis C.H. Wrisht?	clematichinenoside AR2_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)OC1OCC(C(C1O)O)O)O)C)O)O
MOL000755	0.4896	0.5104	0.7529	Smilax Scodinicaulis C.H. Wrisht?	clematichinenoside AR6	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CC(C(C1)(C)C)O)C(=O)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(OC2C(O)C(O)C(O)C(O2)C)C(O1)CO)C)C)C)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)OC1OCC(C(C1O)O)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)C)O)C)O)O
MOL000756	0.5180	0.4820	0.7603	Smilax Scodinicaulis C.H. Wrisht?	clematichinenoside AR7	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(OC2C(O)C(O)C(O)C(O2)C)C(O1)CO)C)C)C)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)OC1OCC(C(C1O)O)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)CO)O)C)O)O
MOL000757	0.5966	0.4034	0.7663	Smilax Scodinicaulis C.H. Wrisht?	Clematichinenoside C	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(OC2C(O)C(O)C(O)C(O2)C)C(O1)CO)C)C)C)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)OC1OCC(C(C1O)O)OC1C(O)C(O)C(O)C(O1)CO)O)C)O)O

MOL000758	0.9068	0.0932	0.9580	Smilax Scodinicaulis C.H. Wrisht?	Deoxyribonolactone	161815	FALSE	C1C(C(OC1=O)CO)O
MOL000759	0.9296	0.0704	0.9430	Smilax Scodinicaulis C.H. Wrisht?	dihydro-4-hydroxy-5-hydroxymethyl-2(3H)-furanone	Not Available	FALSE	O1C(=O)CCC1(C(=O)OCC)O
MOL000760	0.7069	0.2931	0.7770	Smilax Scodinicaulis C.H. Wrisht?	hederasaponin B	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(OC2C(O)C(O)C(O)C(O2)C)C(O1)CO)C)C)C)(CO)C)OC1OCC(C(C1OC1OC(C(C(C1O)OC1OCC(C(C1O)O)O)O)C)O)O
MOL000761	0.6980	0.3020	0.7756	Smilax Scodinicaulis C.H. Wrisht?	huzhangoside B	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(OC2C(O)C(O)C(O)C(O2)C)C(O1)CO)C)C)C)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)OC1OCC(C(C1O)O)O)O)C)O)O
MOL000762	0.5863	0.4137	0.6493	Phellodendri Chinrnsis Cortex	Palmidin A	Not Available	FALSE	c12c(C(c3c(C1=O)c(cc(c3)C)O)C1c3c(C(=O)c4c1cc(cc4O)CO)c(ccc3)O)cc(cc2O)O
MOL000762	0.5863	0.4137	0.6493	Coptidis Rhizoma	Palmidin A	Not Available	FALSE	c12c(C(c3c(C1=O)c(cc(c3)C)O)C1c3c(C(=O)c4c1cc(cc4O)CO)c(ccc3)O)cc(cc2O)O
MOL000762	0.5863	0.4137	0.6493	Caulis Aristolochiae	Palmidin A	Not Available	FALSE	c12c(C(c3c(C1=O)c(cc(c3)C)O)C1c3c(C(=O)c4c1cc(cc4O)CO)c(ccc3)O)cc(cc2O)O
MOL000763	0.8889	0.1111	0.6437	Aristolochiae Fructus	Aristoloside_qt	161218	FALSE	c12c(c(cc3c1cc(cc3OC)O)[N+](=O)O)c(cc1c2OCO1)C(=O)O
MOL000763	0.8889	0.1111	0.6437	Caulis Akebiae	Aristoloside_qt	161218	FALSE	c12c(c(cc3c1cc(cc3OC)O)[N+](=O)O)c(cc1c2OCO1)C(=O)O
MOL000763	0.8889	0.1111	0.6437	Rhizoma Seu Herba Aristolochiae Mollissimae	Aristoloside_qt	161218	FALSE	c12c(c(cc3c1cc(cc3OC)O)[N+](=O)O)c(cc1c2OCO1)C(=O)O
MOL000763	0.8889	0.1111	0.6437	Caulis Aristolochiae	Aristoloside_qt	161218	FALSE	c12c(c(cc3c1cc(cc3OC)O)[N+](=O)O)c(cc1c2OCO1)C(=O)O
MOL000764	0.6627	0.3373	0.7711	Caulis Aristolochiae	magnoflorine	929259	FALSE	c12c3c4c(CC1[N+](CCc2cc(c3O)OC)(C)C)ccc(c4O)OC
MOL000764	0.6627	0.3373	0.7711	Zanthoxylum Nitidum	magnoflorine	929259	FALSE	c12c3c4c(CC1[N+](CCc2cc(c3O)OC)(C)C)ccc(c4O)OC
MOL000764	0.6627	0.3373	0.7711	Phellodendri Chinrnsis Cortex	magnoflorine	929259	FALSE	c12c3c4c(CC1[N+](CCc2cc(c3O)OC)(C)C)ccc(c4O)OC
MOL000764	0.6627	0.3373	0.7711	Stephaniae Tetrandrae Radix	magnoflorine	929259	FALSE	c12c3c4c(CC1[N+](CCc2cc(c3O)OC)(C)C)ccc(c4O)OC

MOL000768	0.8825	0.1175	0.8741	Cymbopon Citratus(D C.) Stapf	luteolin-7-O-α-L-rhamnopyranosyl(1→2)-β-D-glucopyransside	25203781	FALSE	c1(cc(=O)c2c(cc(cc2o1)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO)O)c1cc(c(cc1)O)O
MOL000768	0.8825	0.1175	0.8741	Chrysanthemi Flos	luteolin-7-O-α-L-rhamnopyranosyl(1→2)-β-D-glucopyransside	25203781	FALSE	c1(cc(=O)c2c(cc(cc2o1)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO)O)c1cc(c(cc1)O)O
MOL000770	0.9234	0.0766	0.9505	Cymbopon Citratus(D C.) Stapf	3-Hepten-2-one, 3-methyl-	5364798	FALSE	C(=C\CCC)(/C(=O)C)\C
MOL000771	0.9297	0.0703	0.8613	Schizonepetae Herba	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Inulae Herba	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Oroxyli Semen	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Aristolochiae Fructus	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Cinnamomi Ramulus	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Imperatae Rhizoma	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Radix Cirsii Japonici	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Semen Lini	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Polygoni Avicularis Herba	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Scutellariae Barbatae Herba	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Cnidii Fructus	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Rhizoma Fagopyri Cymosi	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Ranunculi Ternati Radix	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O

MOL000771	0.9297	0.0703	0.8613	Acoritataninowii Rhizoma	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Commelinae Herba	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Citrus Reticulata	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Maydis Seigma	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Lygodii Spora	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Allium Azureum Ledeb.	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Menthae Herba	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Drynariae Rhizoma	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Jujubae Fructus	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Sennae Folium	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Pollen Typhae	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Cymbopon Citratus(D C.) Stapf	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Fritiliariae Irrhosae Bulbus	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Crataegi Folium	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Prunellae Spica	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Microctis Folium	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Hedyotis Diffusae Herba	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Schizonepetae Spica	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Calendula Officinalis	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Curcumae Radix	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Boehmeriae Rhizoma Et Radix	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O

MOL000771	0.9297	0.0703	0.8613	Plantaginis Herba	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Ginkgo Folium	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Phragmitis Rhizoma	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Lonicerae Japonicae Flos	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Eucommiae Cortex	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Ephedra Herba	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Aloe	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Notopterygii Rhizoma Et Radix	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000771	0.9297	0.0703	0.8613	Puerariae Flos	p-coumaric acid	637542	FALSE	C(=O)(/C=C/c1ccc(cc1)O)O
MOL000773	0.3527	0.6473	0.7032	Cymbopon Citratus(D C.) Stapf	cymbopogne	Not Available	FALSE	C1(=O)CCC2C(C1C)(CCC1C3(C)CCC4(C)CCC(C(C)C)C4C3(CCC21C)C)C
MOL000774	0.9331	0.0669	0.9423	Hippophae Fructus	(-)-Citronellal	443157	FALSE	C(CCC=C(C)C)(CC=O)C
MOL000774	0.9331	0.0669	0.9423	Zingiberis Rhizoma	(-)-Citronellal	443157	FALSE	C(CCC=C(C)C)(CC=O)C
MOL000774	0.9331	0.0669	0.9423	Zingiber Officinale Roscoe	(-)-Citronellal	443157	FALSE	C(CCC=C(C)C)(CC=O)C
MOL000774	0.9331	0.0669	0.9423	Cymbopon Citratus(D C.) Stapf	(-)-Citronellal	443157	FALSE	C(CCC=C(C)C)(CC=O)C
MOL000774	0.9331	0.0669	0.9423	Citri Fructus	(-)-Citronellal	443157	FALSE	C(CCC=C(C)C)(CC=O)C
MOL000774	0.9331	0.0669	0.9423	Arum Ternatum Thunb.	(-)-Citronellal	443157	FALSE	C(CCC=C(C)C)(CC=O)C
MOL000774	0.9331	0.0669	0.9423	Zanthoxyli Pericarpium	(-)-Citronellal	443157	FALSE	C(CCC=C(C)C)(CC=O)C
MOL000774	0.9331	0.0669	0.9423	Myristicae Semen	(-)-Citronellal	443157	FALSE	C(CCC=C(C)C)(CC=O)C
MOL000774	0.9331	0.0669	0.9423	Mori Cortex	(-)-Citronellal	443157	FALSE	C(CCC=C(C)C)(CC=O)C
MOL000774	0.9331	0.0669	0.9423	Geranium Wilfordii Maxim.	(-)-Citronellal	443157	FALSE	C(CCC=C(C)C)(CC=O)C
MOL000774	0.9331	0.0669	0.9423	Capsici Fructus	(-)-Citronellal	443157	FALSE	C(CCC=C(C)C)(CC=O)C
MOL000775	0.9178	0.0822	0.9694	Carthami Flos	EEE	8857	TRUE	O(C(=O)C)CC
MOL000775	0.9178	0.0822	0.9694	Paederiae Scandentis Herba	EEE	8857	TRUE	O(C(=O)C)CC
MOL000775	0.9178	0.0822	0.9694	Ardisiae Japonicae Herba	EEE	8857	TRUE	O(C(=O)C)CC
MOL000775	0.9178	0.0822	0.9694	Folium Artemisiae Argyi	EEE	8857	TRUE	O(C(=O)C)CC
MOL000775	0.9178	0.0822	0.9694	Paeoniae Radix Alba	EEE	8857	TRUE	O(C(=O)C)CC
MOL000775	0.9178	0.0822	0.9694	Cymbopon Citratus(D C.) Stapf	EEE	8857	TRUE	O(C(=O)C)CC
MOL000775	0.9178	0.0822	0.9694	Achyranthis Bidentatae Radix	EEE	8857	TRUE	O(C(=O)C)CC
MOL000775	0.9178	0.0822	0.9694	Oroxyli Semen	EEE	8857	TRUE	O(C(=O)C)CC

MOL000775	0.9178	0.0822	0.9694	Morindae Officinalis Radix	EEE	8857	TRUE	O(C(=O)C)CC
MOL000775	0.9178	0.0822	0.9694	Cornus Officinalis Sieb. Et Zucc.	EEE	8857	TRUE	O(C(=O)C)CC
MOL000775	0.9178	0.0822	0.9694	Ephedra Herba	EEE	8857	TRUE	O(C(=O)C)CC
MOL000775	0.9178	0.0822	0.9694	Sesami Nigrum Semen	EEE	8857	TRUE	O(C(=O)C)CC
MOL000775	0.9178	0.0822	0.9694	Rubi Fructus	EEE	8857	TRUE	O(C(=O)C)CC
MOL000775	0.9178	0.0822	0.9694	Hippophae Fructus	EEE	8857	TRUE	O(C(=O)C)CC
MOL000775	0.9178	0.0822	0.9694	Allii Sativi Bulbus	EEE	8857	TRUE	O(C(=O)C)CC
MOL000775	0.9178	0.0822	0.9694	Capsici Fructus	EEE	8857	TRUE	O(C(=O)C)CC
MOL000775	0.9178	0.0822	0.9694	Campsis Flos	EEE	8857	TRUE	O(C(=O)C)CC
MOL000775	0.9178	0.0822	0.9694	Santalum Album L.	EEE	8857	TRUE	O(C(=O)C)CC
MOL000775	0.9178	0.0822	0.9694	Notoginseng Flos	EEE	8857	TRUE	O(C(=O)C)CC
MOL000775	0.9178	0.0822	0.9694	A. Dahurica (Fisch.) Benth. Et Hook	EEE	8857	TRUE	O(C(=O)C)CC
MOL000776	0.8580	0.1420	0.6689	Cymbopon Citratus(D C.) Stapf	OXA	702	TRUE	C(C)O
MOL000776	0.8580	0.1420	0.6689	Capsici Fructus	OXA	702	TRUE	C(C)O
MOL000776	0.8580	0.1420	0.6689	Eucommiae Folium	OXA	702	TRUE	C(C)O
MOL000776	0.8580	0.1420	0.6689	Ephedra Herba	OXA	702	TRUE	C(C)O
MOL000776	0.8580	0.1420	0.6689	Achyranthis Bidentatae Radix	OXA	702	TRUE	C(C)O
MOL000777	0.9254	0.0746	0.9672	Mori Fructus	(2S)-2-methylbutan-1-ol	2723602	FALSE	C(CC)(CO)C
MOL000777	0.9254	0.0746	0.9672	Maydis Seigma	(2S)-2-methylbutan-1-ol	2723602	FALSE	C(CC)(CO)C
MOL000777	0.9254	0.0746	0.9672	Folium Artemisiae Argyi	(2S)-2-methylbutan-1-ol	2723602	FALSE	C(CC)(CO)C
MOL000777	0.9254	0.0746	0.9672	Cymbopon Citratus(D C.) Stapf	(2S)-2-methylbutan-1-ol	2723602	FALSE	C(CC)(CO)C
MOL000777	0.9254	0.0746	0.9672	Lonicerae Japonicae Flos	(2S)-2-methylbutan-1-ol	2723602	FALSE	C(CC)(CO)C
MOL000777	0.9254	0.0746	0.9672	Paederiae Scandentis Herba	(2S)-2-methylbutan-1-ol	2723602	FALSE	C(CC)(CO)C
MOL000778	0.7534	0.2466	0.7106	Corydalis Decumbens(Thunb.)Pers.	6-O-E-Feruloylajugol	Not Available	FALSE	COc1c(O)ccc(c1)/C=C/C(=O)OC1CC(C2C1C=COC2OC1OC(C(C(C1O)O)O)CO)(C)O
MOL000778	0.7534	0.2466	0.7106	Coptidis Rhizoma	6-O-E-Feruloylajugol	Not Available	FALSE	COc1c(O)ccc(c1)/C=C/C(=O)OC1CC(C2C1C=COC2OC1OC(C(C(C1O)O)O)CO)(C)O

MOL000778	0.7534	0.2466	0.7106	Inulae Flos	6-O-E-Feruloylajugol	Not Available	FALSE	COc1c(O)ccc(c1)/C=C/C(=O)OC1CC(C2C1C=COC2OC1OC(C(C(C1O)O)O)CO)(C)O
MOL000778	0.7534	0.2466	0.7106	Rhizome Of Whiteback Greenbrier	6-O-E-Feruloylajugol	Not Available	FALSE	COc1c(O)ccc(c1)/C=C/C(=O)OC1CC(C2C1C=COC2OC1OC(C(C(C1O)O)O)CO)(C)O
MOL000779	0.6976	0.3024	0.6871	Coptidis Rhizoma	6-O-E-Feruloylajugol_qt	Not Available	FALSE	COc1c(O)ccc(c1)/C=C/C(=O)OC1CC(C2C1C=COC2O)(C)O
MOL000779	0.6976	0.3024	0.6871	Rhizome Of Whiteback Greenbrier	6-O-E-Feruloylajugol_qt	Not Available	FALSE	COc1c(O)ccc(c1)/C=C/C(=O)OC1CC(C2C1C=COC2O)(C)O
MOL000779	0.6976	0.3024	0.6871	Corydalis Decumbens(Thunb.)Pers.	6-O-E-Feruloylajugol_qt	Not Available	FALSE	COc1c(O)ccc(c1)/C=C/C(=O)OC1CC(C2C1C=COC2O)(C)O
MOL000780	0.6550	0.3450	0.7267	Corydalis Decumbens(Thunb.)Pers.	Adlumidine	120734	FALSE	c12c(cc3c(c1)CCN(C3C1c3c(C(=O)O1)c1c(cc3)OCO1)C)OCO2
MOL000781	0.7613	0.2387	0.8467	Corydalis Decumbens(Thunb.)Pers.	PDSP1_000624	Not Available	FALSE	c12c(cc3c4c1c1c(CC4N(CC3)C)ccc(c1O)OC)OCO2
MOL000782	0.7343	0.2657	0.8365	Corydalis Decumbens(Thunb.)Pers.	Menisporphine	Not Available	FALSE	c1(c(c2c3c(c1)ccnc3c1c(C2=O)cc(cc1)OC)OC)OC
MOL000782	0.7343	0.2657	0.8365	Phellodendri Chinrnsis Cortex	Menisporphine	Not Available	FALSE	c1(c(c2c3c(c1)ccnc3c1c(C2=O)cc(cc1)OC)OC)OC
MOL000782	0.7343	0.2657	0.8365	Menispermi Rhizoma	Menisporphine	Not Available	FALSE	c1(c(c2c3c(c1)ccnc3c1c(C2=O)cc(cc1)OC)OC)OC
MOL000783	0.4388	0.5612	0.6364	Jujubae Fructus	Protoporphyrin	Not Available	FALSE	c\1/2=C\C3=N/C(=C\c4[nH]c(/C=C/5\N=C(/C=c(\[nH]1)/c(c2C)C=C)C(=C5C=C)C)c(c4CCC(=O)O)C)/C(=C3C)CCC(=O)O
MOL000783	0.4388	0.5612	0.6364	Corydalis Decumbens(Thunb.)Pers.	Protoporphyrin	Not Available	FALSE	c\1/2=C\C3=N/C(=C\c4[nH]c(/C=C/5\N=C(/C=c(\[nH]1)/c(c2C)C=C)C(=C5C=C)C)c(c4CCC(=O)O)C)/C(=C3C)CCC(=O)O
MOL000784	0.9524	0.0476	0.9201	Corydalis Decumbens(Thunb.)Pers.	Tetrahydropiperic acid	5321853	FALSE	c1(ccc2c(c1)OCO2)CCCCC(=O)O
MOL000785	0.4620	0.5380	0.7406	Mahoniae Caulis	palmatine	19009	FALSE	c12c3c(cc(c(c3)OC)OC)CC[n+]1cc1c(c2)ccc(c1OC)OC
MOL000785	0.4620	0.5380	0.7406	Phellodendri Amurensis Cortex	palmatine	19009	FALSE	c12c3c(cc(c(c3)OC)OC)CC[n+]1cc1c(c2)ccc(c1OC)OC
MOL000785	0.4620	0.5380	0.7406	Mahoniae Eadix	palmatine	19009	FALSE	c12c3c(cc(c(c3)OC)OC)CC[n+]1cc1c(c2)ccc(c1OC)OC
MOL000785	0.4620	0.5380	0.7406	Mahoniae Folum	palmatine	19009	FALSE	c12c3c(cc(c(c3)OC)OC)CC[n+]1cc1c(c2)ccc(c1OC)OC
MOL000785	0.4620	0.5380	0.7406	Tinosporae Radix	palmatine	19009	FALSE	c12c3c(cc(c(c3)OC)OC)CC[n+]1cc1c(c2)ccc(c1OC)OC
MOL000785	0.4620	0.5380	0.7406	Corydalis Decumbens(Thunb.)Pers.	palmatine	19009	FALSE	c12c3c(cc(c(c3)OC)OC)CC[n+]1cc1c(c2)ccc(c1OC)OC
MOL000785	0.4620	0.5380	0.7406	Achyranthis Bidentatae Radix	palmatine	19009	FALSE	c12c3c(cc(c(c3)OC)OC)CC[n+]1cc1c(c2)ccc(c1OC)OC
MOL000785	0.4620	0.5380	0.7406	Phellodendri Chinrnsis Cortex	palmatine	19009	FALSE	c12c3c(cc(c(c3)OC)OC)CC[n+]1cc1c(c2)ccc(c1OC)OC

MOL000785	0.4620	0.5380	0.7406	Corydalis Rhizoma	palmatine	19009	FALSE	c12c3c(cc(c(c3)OC)OC)CC[n+]1cc1c(c2)ccc(c1OC)OC
MOL000785	0.4620	0.5380	0.7406	Thalictri Glandulosissimi Et	palmatine	19009	FALSE	c12c3c(cc(c(c3)OC)OC)CC[n+]1cc1c(c2)ccc(c1OC)OC
MOL000785	0.4620	0.5380	0.7406	Coptidis Rhizoma	palmatine	19009	FALSE	c12c3c(cc(c(c3)OC)OC)CC[n+]1cc1c(c2)ccc(c1OC)OC
MOL000786	0.3741	0.6259	0.7535	Corydalis Rhizoma	STOCK1N-14407	969488	FALSE	C12c3c(cc(c(c3)OC)OC)CCN1Cc1c(C2)ccc(c1OC)OC
MOL000786	0.3741	0.6259	0.7535	Corydalis Decumbens(Thunb.)Pers.	STOCK1N-14407	969488	FALSE	C12c3c(cc(c(c3)OC)OC)CCN1Cc1c(C2)ccc(c1OC)OC
MOL000788	0.6632	0.3368	0.6813	Corydalis Decumbens(Thunb.)Pers.	119736-65-1	189686	FALSE	O1COc2c1ccc1c2C(OC1C1N(CCc2cc3c(cc12)OCO3)C)O
MOL000789	0.5778	0.4222	0.7454	Mahoniae Caulis	jatrorrizine	72323	FALSE	c12c3c(CC[n+]1cc1c(c2)ccc(c1OC)OC)cc(c(c3)OC)O
MOL000789	0.5778	0.4222	0.7454	Mahoniae Folum	jatrorrizine	72323	FALSE	c12c3c(CC[n+]1cc1c(c2)ccc(c1OC)OC)cc(c(c3)OC)O
MOL000789	0.5778	0.4222	0.7454	Thalictri Glandulosissimi Et	jatrorrizine	72323	FALSE	c12c3c(CC[n+]1cc1c(c2)ccc(c1OC)OC)cc(c(c3)OC)O
MOL000789	0.5778	0.4222	0.7454	Corydalis Decumbens(Thunb.)Pers.	jatrorrizine	72323	FALSE	c12c3c(CC[n+]1cc1c(c2)ccc(c1OC)OC)cc(c(c3)OC)O
MOL000789	0.5778	0.4222	0.7454	Tinosporae Radix	jatrorrizine	72323	FALSE	c12c3c(CC[n+]1cc1c(c2)ccc(c1OC)OC)cc(c(c3)OC)O
MOL000789	0.5778	0.4222	0.7454	Mahoniae Eadix	jatrorrizine	72323	FALSE	c12c3c(CC[n+]1cc1c(c2)ccc(c1OC)OC)cc(c(c3)OC)O
MOL000789	0.5778	0.4222	0.7454	Coptidis Rhizoma	jatrorrizine	72323	FALSE	c12c3c(CC[n+]1cc1c(c2)ccc(c1OC)OC)cc(c(c3)OC)O
MOL000790	0.5377	0.4623	0.7611	Phellodendri Chinrnsis Cortex	Isocorypalmine	440229	FALSE	c12c(CCN3Cc4c(CC13)ccc(c4OC)OC)cc(c(c2)O)OC
MOL000790	0.5377	0.4623	0.7611	Corydalis Rhizoma	Isocorypalmine	440229	FALSE	c12c(CCN3Cc4c(CC13)ccc(c4OC)OC)cc(c(c2)O)OC
MOL000790	0.5377	0.4623	0.7611	Corydalis Decumbens(Thunb.)Pers.	Isocorypalmine	440229	FALSE	c12c(CCN3Cc4c(CC13)ccc(c4OC)OC)cc(c(c2)O)OC
MOL000791	0.6550	0.3450	0.7267	Forsythiae Fructus	bicuculline	10237	FALSE	C1(c2c(C(=O)O1)c1c(cc2)OCO1)C1c2c(cc3c(c2)OCO3)CCN1C
MOL000791	0.6550	0.3450	0.7267	Corydalis Bungeanae Herba	bicuculline	10237	FALSE	C1(c2c(C(=O)O1)c1c(cc2)OCO1)C1c2c(cc3c(c2)OCO3)CCN1C
MOL000791	0.6550	0.3450	0.7267	Corydalis Rhizoma	bicuculline	10237	FALSE	C1(c2c(C(=O)O1)c1c(cc2)OCO1)C1c2c(cc3c(c2)OCO3)CCN1C
MOL000791	0.6550	0.3450	0.7267	Corydalis Decumbens(Thunb.)Pers.	bicuculline	10237	FALSE	C1(c2c(C(=O)O1)c1c(cc2)OCO1)C1c2c(cc3c(c2)OCO3)CCN1C
MOL000793	0.7613	0.2387	0.8467	Corydalis Rhizoma	C09367	Not Available	FALSE	c12c3C(Cc4c1c(c(cc4)OC)O)N(CCc3cc1c2OCO1)C
MOL000793	0.7613	0.2387	0.8467	Corydalis Decumbens(Thunb.)Pers.	C09367	Not Available	FALSE	c12c3C(Cc4c1c(c(cc4)OC)O)N(CCc3cc1c2OCO1)C
MOL000794	0.4972	0.5028	0.7067	Menispermi Rhizoma	menisperine	161487	FALSE	c12c3C(Cc4c1c(c(cc4)OC)O)[N+](CCc3cc(c2OC)OC)(C)C
MOL000794	0.4972	0.5028	0.7067	Corydalis Decumbens(Thunb.)Pers.	menisperine	161487	FALSE	c12c3C(Cc4c1c(c(cc4)OC)O)[N+](CCc3cc(c2OC)OC)(C)C
MOL000794	0.4972	0.5028	0.7067	Stephaniae Tetrandrae Radix	menisperine	161487	FALSE	c12c3C(Cc4c1c(c(cc4)OC)O)[N+](CCc3cc(c2OC)OC)(C)C

MOL000794	0.4972	0.5028	0.7067	Chelidonii Herba	menisperine	161487	FALSE	c12c3C(Cc4c1c(c(cc4)OC)O)[N+](CCc3cc(c2OC)OC)(C)C
MOL000794	0.4972	0.5028	0.7067	Tinosporae Radix	menisperine	161487	FALSE	c12c3C(Cc4c1c(c(cc4)OC)O)[N+](CCc3cc(c2OC)OC)(C)C
MOL000795	0.5017	0.4983	0.6935	Polyporus Umbellatus(Pers)Fr.	(20s,22r,24r)-16,22-epoxy-3beta,14alpha,23beta,25-tetrahydroxyergost-7-en-6-one	Not Available	FALSE	C1C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C)C1C(C2)OC(C1C)C(C(C(C)(C)O)C)O)O)C)O
MOL000796	0.2471	0.7529	0.6241	Polyporus Umbellatus(Pers)Fr.	(22e,24r)-ergosta-6-en-3beta,5alpha,6beta-triol	14236575	FALSE	C1C(CC2(C(C1)(C1C(=CC2O)C2C(CC1)(C(CC2)C(CCC(C(C)C)C)C)C)C)O)O
MOL000797	0.1926	0.8074	0.6142	Polyporus Umbellatus(Pers)Fr.	(22e,24r)-ergosta-7,22-dien-3-one	Not Available	FALSE	C1C(=O)CC2C(C1)(C1C(=CC2)C2C(CC1)(C(CC2)C(/C=C/C(C(C)C)C)C)C)C
MOL000799	0.3419	0.6581	0.6498	Polyporus Umbellatus(Pers)Fr.	(23r,24r,25r)-23,26-epoxy-3beta,14alpha,21alpha,22alpha-tetrahydroxyergost-7-en-6-one	Not Available	FALSE	C1C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C)C(CC2)C(O)(C)C(C1OCC(C1C)C)O)O)C)O
MOL000800	0.3614	0.6386	0.6688	Polyporus Umbellatus(Pers)Fr.	22,23-epoxy-3beta,14alpha,,20beta,24beta-tetrahydroxy-7-en-6-one	Not Available	FALSE	C1C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C)C(CC2)C(C)(O)C1C(O1)C(C(C)C)(O)C)O)C)O
MOL000801	0.2819	0.7181	0.7257	Polyporus Umbellatus(Pers)Fr.	5alpha,8alpha-epidioxy-(22e,24r)-ergosta-6,22-dien-3beta-ol	Not Available	FALSE	C1C(CC23C(C1)(C1C(C=C2)(C2C(CC1)(C(CC2)C(/C=C/C(C(C)C)C)C)C)OO3)C)O
MOL000802	0.1772	0.8228	0.6464	Ailanthi Cortex	27625-48-5	6441416	FALSE	C1C(=O)C=C2C(C1)(C1C(=C3C(CC1)(C)C(CC3)C(C)/C=C/C(C(C)C)C)C=C2)C
MOL000802	0.1772	0.8228	0.6464	Lasiosphaera Seu Calvatia	27625-48-5	6441416	FALSE	C1C(=O)C=C2C(C1)(C1C(=C3C(CC1)(C)C(CC3)C(C)/C=C/C(C(C)C)C)C=C2)C
MOL000802	0.1772	0.8228	0.6464	Ranunculi Ternati Radix	27625-48-5	6441416	FALSE	C1C(=O)C=C2C(C1)(C1C(=C3C(CC1)(C)C(CC3)C(C)/C=C/C(C(C)C)C)C=C2)C

MOL000802	0.1772	0.8228	0.6464	Polyporus Umbellatus(Pers)Fr.	27625-48-5	6441416	FALSE	C1C(=O)C=C2C(C1)(C1C(=C3C(CC1)(C)C(CC3)C(C)/C=C/C(C(C)C)C)C=C2)C
MOL000805	0.3937	0.6063	0.6146	Polyporus Umbellatus(Pers)Fr.	polyorusterone,f	Not Available	FALSE	C1(C(CC2(C(C1)(C1C(=CC2=O)C2(C(CC1)(C(CC2)C(C(CC(C(C)C)C)O)C)C)O)C)O)O)O
MOL000806	0.6288	0.3712	0.7219	Polyporus Umbellatus(Pers)Fr.	polyporoid,a	Not Available	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C)C1C(C2)OC(C1(O)C)C(C(C)C(C)C)O)O)C)O)O
MOL000807	0.4772	0.5228	0.6805	Polyporus Umbellatus(Pers)Fr.	polyporoid,b	44450001	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C)C(CC2)C(O)(C)C(C1OCC(C1C)C)O)O)C)O)O
MOL000808	0.5334	0.4666	0.6649	Polyporus Umbellatus(Pers)Fr.	polyporoid,c	Not Available	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C)C(C(C2)O)C(O)(C)C(CC(C(C)C)C)O)O)C)O)O
MOL000809	0.3955	0.6045	0.6277	Polyporus Umbellatus(Pers)Fr.	polyporusterone,a	15168039	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C)C(CC2)C(O)(C)C(CC(C(C)C)C)O)O)C)O)O
MOL000810	0.4029	0.5971	0.6491	Polyporus Umbellatus(Pers)Fr.	polyporusterone,b	15168041	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C)C(CC2)C(O)(C)C(CC(=C)C(C)C)O)O)C)O)O
MOL000811	0.3573	0.6427	0.6892	Polyporus Umbellatus(Pers)Fr.	polyporusterone,c	44575600	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C)C(CC2)C(O)(C)C1C(C(C)C)C)O1)O)C)O)O
MOL000812	0.3435	0.6565	0.6548	Polyporus Umbellatus(Pers)Fr.	polyporusterone,g	44449940	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C)C(CC2)C(C)C(CC(=C)C(C)C)O)O)C)O)O
MOL000813	0.9388	0.0612	0.9616	Bamusaeconcretiosilicea	MAN	185698	FALSE	C1(C(C(C(C(O1)O)O)O)O)CO
MOL000813	0.9388	0.0612	0.9616	Polyporus Umbellatus(Pers)Fr.	MAN	185698	FALSE	C1(C(C(C(C(O1)O)O)O)O)CO
MOL000813	0.9388	0.0612	0.9616	Arecae Semen	MAN	185698	FALSE	C1(C(C(C(C(O1)O)O)O)O)CO
MOL000814	0.9388	0.0612	0.9616	Abrus Precatorius L.	GLA	439357	FALSE	C1(C(C(C(C(O1)O)O)O)O)CO
MOL000814	0.9388	0.0612	0.9616	Bamusaeconcretiosilicea	GLA	439357	FALSE	C1(C(C(C(C(O1)O)O)O)O)CO
MOL000814	0.9388	0.0612	0.9616	Sterculiae Lychnophorae Semen	GLA	439357	FALSE	C1(C(C(C(C(O1)O)O)O)O)CO
MOL000814	0.9388	0.0612	0.9616	Polyporus Umbellatus(Pers)Fr.	GLA	439357	FALSE	C1(C(C(C(C(O1)O)O)O)O)CO
MOL000814	0.9388	0.0612	0.9616	Hippophae Fructus	GLA	439357	FALSE	C1(C(C(C(C(O1)O)O)O)O)CO

MOL000815	0.3955	0.6045	0.6277	Polyporus Umbellatus(Pers)Fr.	(2S,3R,5R,9R,10R,13R,14S,17S)-17-[(1R,2R,4S)-1,2-dihydroxy-1,4,5-trimethylhexyl]-2,3,14-trihydroxy-10,13-dimethyl-2,3,4,5,9,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-6-one	10814524	FALSE	C1(C(CC2(C(C1)C(=O)C=C1C3(CCC(C(C(CC(C)C(C)C)O)(C)O)C3(C)CCC21)O)C)O)O
MOL000816	0.1926	0.8074	0.6142	Lasiosphaera Seu Calvatia	ergosta-7,22-dien-3-one	Not Available	FALSE	C1(=O)CCC2(C(C1)CC=C1C3CCC(C(/C=C/C(C)C(C)C)C)C3(C)CCC21)C
MOL000816	0.1926	0.8074	0.6142	Polyporus Umbellatus(Pers)Fr.	ergosta-7,22-dien-3-one	Not Available	FALSE	C1(=O)CCC2(C(C1)CC=C1C3CCC(C(/C=C/C(C)C(C)C)C)C3(C)CCC21)C
MOL000817	0.2032	0.7968	0.6108	Polyporus Umbellatus(Pers)Fr.	ergosta-5,7,22-trien-3-ol	Not Available	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC23)C1)C)O
MOL000819	0.3407	0.6593	0.6608	Polyporus Umbellatus(Pers)Fr.	polyporusterone D	44575601	FALSE	C1(C(CC2(C(C1)C(=O)C=C1C3(CCC(C(=C)C(CC(C)C(C)C)O)C3(C)CCC21)O)C)O)O
MOL000820	0.2985	0.7015	0.6884	Polyporus Umbellatus(Pers)Fr.	polyporusterone E	44575602	FALSE	C1(C(CC2(C(C1)C(=O)C=C1C3(CCC(C(C4C(C(C)C(C)C)O4)C)C3(C)CCC21)O)C)O)O
MOL000821	0.3416	0.6584	0.6348	Polyporus Umbellatus(Pers)Fr.	polyporusterone F	44575603	FALSE	C1(C(CC2(C(C1)C(=O)C=C1C3(CCC(C(C(CC(C)C(C)C)O)C)C3(C)CCC21)O)C)O)O
MOL000822	0.2414	0.7586	0.6450	Polyporus Umbellatus(Pers)Fr.	polyporusterone G	Not Available	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C(CC2)C(C(CC(=C)C(C)C)C)C)C)O)C)O)O
MOL000823	0.9384	0.0616	0.8513	Alisma Orientale (Sam.) Juz.	1h-indole-3-carboxylic,acid	Not Available	FALSE	[nH]1cc(c2ccccc12)C(=O)O

MOL000824	0.8800	0.1200	0.7456	Alisma Orientale (Sam.) Juz.	(1R,3aS,8aR)-7-isopropyl-1-methyl-4-methylene-2,3,3a,5,6,8a-hexahydroazulen-1-ol	15934381	FALSE	C12C(C=C(CCC1=C)C(C)C)C(CC2)(O)C
MOL000825	0.8914	0.1086	0.7800	Alisma Orientale (Sam.) Juz.	(1R,3aR,4S,7R,8S,8aS)-7-isopropyl-1,4-dimethyl-3,3a,5,6,8,8a-hexahydro-2H-azulene-1,4,7,8-tetrol	16742799	FALSE	C12C(C(C(CCC1(C)O)(C(C)C)O)O)C(CC2)(C)O
MOL000826	0.8915	0.1085	0.8028	Alisma Orientale (Sam.) Juz.	(1R,3aS,4S,8aR)-7-(2-hydroxypropan-2-yl)-1,4-dimethyl-2,3,3a,5,6,8a-hexahydroazulene-1,4-diol	16742798	FALSE	C12C(C=C(CCC1(C)O)C(O)(C)C)C(CC2)(C)O
MOL000827	0.8626	0.1374	0.7837	Alisma Orientale (Sam.) Juz.	(1S,3aR,4R,8aS)-7-isopropyl-1,4-dimethyl-2,3,3a,5,6,8a-hexahydroazulene-1,4-diol	10988340	FALSE	C12C(C=C(CCC1(O)C)C(C)C)C(CC2)(O)C
MOL000827	0.8626	0.1374	0.7837	Curcumae Radix	(1S,3aR,4R,8aS)-7-isopropyl-1,4-dimethyl-2,3,3a,5,6,8a-hexahydroazulene-1,4-diol	10988340	FALSE	C12C(C=C(CCC1(O)C)C(C)C)C(CC2)(O)C
MOL000828	0.2620	0.7380	0.6556	Alisma Orientale (Sam.) Juz.	Alisol A	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2(C(=C(CC2)C(CC(O)C(O)C(C)(O)C)C)CC1O)C)C)(C)C
MOL000829	0.1705	0.8295	0.7220	Alisma Orientale (Sam.) Juz.	Alisol A monoacetate	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2(C(=C(CC2)C(CC(O)C(OC(=O)C)C(C)(O)C)C)CC1O)C)C)(C)C
MOL000830	0.1863	0.8137	0.7337	Alisma Orientale (Sam.) Juz.	Alisol B	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2(C(=C(CC2)C(CC(C2C(C)(C)O2)O)C)CC1O)C)C)(C)C

MOL000831	0.1344	0.8656	0.7486	Alisma Orientale (Sam.) Juz.	Alisol B monoacetate	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2(C(=C(CC2)C(CC(OC(=O)C)C2C(O2)(C)C)C)CC1O)C)C)(C)C
MOL000832	0.2395	0.7605	0.6976	Alisma Orientale (Sam.) Juz.	alisol,b,23-acetate	Not Available	FALSE	C1C(=O)CC2C(C1)(C1C(CC2)(C2(C(CC1O)C(CC2)C(CC(O)C1C(O1)(C)C)C)C)C)C
MOL000833	0.2740	0.7260	0.7784	Alisma Orientale (Sam.) Juz.	alisol,f	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2(C(=C3C(C2)OC(CC3C)C(C(C)(C)O)CC(=O)C)CC1O)C)C)(C)C
MOL000834	0.9264	0.0736	0.9436	Alisma Orientale (Sam.) Juz.	alpha-D-fructofuranose	11105942	FALSE	OCC1(C(O)C(O)C(O1)CO)O
MOL000835	0.9401	0.0599	0.8917	Semiaquilegiae Radix	EA-fructofuranoside	133590	FALSE	OCC1(C(O)C(O)C(O1)CO)OCC
MOL000835	0.9401	0.0599	0.8917	Alisma Orientale (Sam.) Juz.	EA-fructofuranoside	133590	FALSE	OCC1(C(O)C(O)C(O1)CO)OCC
MOL000835	0.9401	0.0599	0.8917	Codonopsis Radix	EA-fructofuranoside	133590	FALSE	OCC1(C(O)C(O)C(O1)CO)OCC
MOL000836	0.9401	0.0599	0.8917	Dioscoreaebulbiferae	(2R,3S,4S,5R)-2-ethoxy-2,5-bis(hydroxymethyl)oxolane-3,4-diol	11769694	FALSE	OCC1(C(O)C(O)C(O1)CO)OCC
MOL000836	0.9401	0.0599	0.8917	Alisma Orientale (Sam.) Juz.	(2R,3S,4S,5R)-2-ethoxy-2,5-bis(hydroxymethyl)oxolane-3,4-diol	11769694	FALSE	OCC1(C(O)C(O)C(O1)CO)OCC
MOL000837	0.8800	0.1200	0.7456	Alisma Orientale (Sam.) Juz.	lismol	Not Available	FALSE	C12C(C=C(CCC1=C)C(C)C)C(CC2)(O)C
MOL000838	0.8734	0.1266	0.8002	Alisma Orientale (Sam.) Juz.	alpha-D-Galp-(1->6)-alpha-D-Galp-(1->6)-D-Glu	5461026	FALSE	C1(C(C(C(C(O1)OCC1C(C(C(C(O1)OCC(O)C(O)C(O)C(C=O)O)O)O)O)O)O)O)CO
MOL000839	0.8891	0.1109	0.7588	Alisma Orientale (Sam.) Juz.	rel-(1R,3aS,4S,7S,8R,8aS)-7-isopropyl-1,4-dimethyldecahydro-4,7-epoxyazulene-1,8-diol	Not Available	FALSE	C12C(C(C3(CCC1(C)O3)C(C)C)O)C(CC2)(O)C

MOL000840	0.8881	0.1119	0.7609	Alisma Orientale (Sam.) Juz.	orientalol,f	Not Available	FALSE	C12C(=C(CC2)C)C(C2(CCC1(O2)C)C(C)C)O
MOL000841	0.8947	0.1053	0.8286	Rehmanniae Radix Praeparata	raffinose	439242	FALSE	OCC1OC(OCC2OC(OC3(CO)C(O)C(O)C(CO)O3)C(O)C(O)C2O)C(O)C(O)C1O
MOL000841	0.8947	0.1053	0.8286	Cassiae Semen	raffinose	439242	FALSE	OCC1OC(OCC2OC(OC3(CO)C(O)C(O)C(CO)O3)C(O)C(O)C2O)C(O)C(O)C1O
MOL000841	0.8947	0.1053	0.8286	Plantaginis Herba	raffinose	439242	FALSE	OCC1OC(OCC2OC(OC3(CO)C(O)C(O)C(CO)O3)C(O)C(O)C2O)C(O)C(O)C1O
MOL000841	0.8947	0.1053	0.8286	Lablab Semen Album	raffinose	439242	FALSE	OCC1OC(OCC2OC(OC3(CO)C(O)C(O)C(CO)O3)C(O)C(O)C2O)C(O)C(O)C1O
MOL000841	0.8947	0.1053	0.8286	Alisma Orientale (Sam.) Juz.	raffinose	439242	FALSE	OCC1OC(OCC2OC(OC3(CO)C(O)C(O)C(CO)O3)C(O)C(O)C2O)C(O)C(O)C1O
MOL000842	0.9075	0.0925	0.8754	Jujubae Fructus	sucrose	5988	FALSE	OCC1OC(OC2(CO)C(O)C(O)C(CO)O2)C(O)C(O)C1O
MOL000842	0.9075	0.0925	0.8754	Isatdis Radix	sucrose	5988	FALSE	OCC1OC(OC2(CO)C(O)C(O)C(CO)O2)C(O)C(O)C1O
MOL000842	0.9075	0.0925	0.8754	Sapindi Mukorossiperic Arpium	sucrose	5988	FALSE	OCC1OC(OC2(CO)C(O)C(O)C(CO)O2)C(O)C(O)C1O
MOL000842	0.9075	0.0925	0.8754	Notopterygii Rhizoma Et Radix	sucrose	5988	FALSE	OCC1OC(OC2(CO)C(O)C(O)C(CO)O2)C(O)C(O)C1O
MOL000842	0.9075	0.0925	0.8754	Dioscoreaebulbiferae	sucrose	5988	FALSE	OCC1OC(OC2(CO)C(O)C(O)C(CO)O2)C(O)C(O)C1O
MOL000842	0.9075	0.0925	0.8754	Fructus Ligustri Lucidi	sucrose	5988	FALSE	OCC1OC(OC2(CO)C(O)C(O)C(CO)O2)C(O)C(O)C1O
MOL000842	0.9075	0.0925	0.8754	Fritiliariae Irrhosae Bulbus	sucrose	5988	FALSE	OCC1OC(OC2(CO)C(O)C(O)C(CO)O2)C(O)C(O)C1O
MOL000842	0.9075	0.0925	0.8754	Actinidia Chinensis Planch	sucrose	5988	FALSE	OCC1OC(OC2(CO)C(O)C(O)C(CO)O2)C(O)C(O)C1O
MOL000842	0.9075	0.0925	0.8754	Sterculiae Lychnophorae Semen	sucrose	5988	FALSE	OCC1OC(OC2(CO)C(O)C(O)C(CO)O2)C(O)C(O)C1O
MOL000842	0.9075	0.0925	0.8754	Rehmanniae Radix Praeparata	sucrose	5988	FALSE	OCC1OC(OC2(CO)C(O)C(O)C(CO)O2)C(O)C(O)C1O
MOL000842	0.9075	0.0925	0.8754	Plantaginis Herba	sucrose	5988	FALSE	OCC1OC(OC2(CO)C(O)C(O)C(CO)O2)C(O)C(O)C1O
MOL000842	0.9075	0.0925	0.8754	Chuanxiong Rhizoma	sucrose	5988	FALSE	OCC1OC(OC2(CO)C(O)C(O)C(CO)O2)C(O)C(O)C1O
MOL000842	0.9075	0.0925	0.8754	Hippophae Fructus	sucrose	5988	FALSE	OCC1OC(OC2(CO)C(O)C(O)C(CO)O2)C(O)C(O)C1O
MOL000842	0.9075	0.0925	0.8754	Alisma Orientale (Sam.) Juz.	sucrose	5988	FALSE	OCC1OC(OC2(CO)C(O)C(O)C(CO)O2)C(O)C(O)C1O
MOL000842	0.9075	0.0925	0.8754	Gynostemmae Pentaphylli Herba	sucrose	5988	FALSE	OCC1OC(OC2(CO)C(O)C(O)C(CO)O2)C(O)C(O)C1O
MOL000842	0.9075	0.0925	0.8754	Bolbostemae Paniculati Bulbus	sucrose	5988	FALSE	OCC1OC(OC2(CO)C(O)C(O)C(CO)O2)C(O)C(O)C1O
MOL000842	0.9075	0.0925	0.8754	Farfarae Flos	sucrose	5988	FALSE	OCC1OC(OC2(CO)C(O)C(O)C(CO)O2)C(O)C(O)C1O
MOL000843	0.8524	0.1476	0.7737	Alisma Orientale (Sam.) Juz.	stachyose	Not Available	FALSE	OC1C(CO)OC(OCC2OC(OC3C(OC4(CO)OC(CO)C(O)C4O)OC(CO)C(O)C3O)C(O)C(O)C2O)C(O)C1O
MOL000844	0.8511	0.1489	0.6141	Alisma Orientale (Sam.) Juz.	Sulfoorientalol A	Not Available	FALSE	C12CCC(C1C=C(CCC2(O)C)C(C)C)(S(=O)(=O)O)C
MOL000844	0.8511	0.1489	0.6141	Capsellae Herba	Sulfoorientalol A	Not Available	FALSE	C12CCC(C1C=C(CCC2(O)C)C(C)C)(S(=O)(=O)O)C

MOL000845	0.8289	0.1711	0.6209	Alisma Orientale (Sam.) Juz.	Sulfoorientalol B	Not Available	FALSE	C12CCC(C1C=C(CCC2(CS(=O)(=O)O)O)C(C)C)(O)C
MOL000846	0.8266	0.1734	0.6668	Alisma Orientale (Sam.) Juz.	Sulfoorientalol C	Not Available	FALSE	C12CCC(C1C=C(CC/C/2=C/S(=O)(=O)O)C(C)C)(O)C
MOL000847	0.8632	0.1368	0.6488	Alisma Orientale (Sam.) Juz.	Sulfoorientalol D	Not Available	FALSE	C1C(C2C(C1)C1(CCC(C2O)(C(C)C)O1)C)(C)S(=O)(=O)O
MOL000848	0.8844	0.1156	0.7351	Alisma Orientale (Sam.) Juz.	verbascose	Not Available	FALSE	C1(C(C(C(OC1CO)OCC1C(C(C(C(O1)OCC1C(C(C(O1)COC1C(C(C(C(O1)OOC1(C(C(C(C1)CO)O)O)CO)O)O)O)O)O)O)O)O)O)O)O
MOL000849	0.1016	0.8984	0.7327	Alisma Orientale (Sam.) Juz.	16β-methoxyalisol B monoacetate	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C)C3(C)CC(C(=C3CC(C21)O)C(CC(C1C(C)(C)O1)OC(=O)C)C)OC)C
MOL000850	0.2620	0.7380	0.6556	Alisma Orientale (Sam.) Juz.	alisol A	15558616	FALSE	C12=C(CCC1(C1(C(C3(C(C(C(=O)CC3)(C)C)CC1)C)C(C2)O)C)C)C(CC(C(C(O)(C)C)O)O)C
MOL000851	0.1705	0.8295	0.7220	Alisma Orientale (Sam.) Juz.	alisol A(B,C)monoacetate	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2(C(=C(CC2)C(CC(C(C)(C)C)O)OC(=O)C)O)C)CC1O)C)C)(C)C
MOL000852	0.1348	0.8652	0.7648	Alisma Orientale (Sam.) Juz.	16β-hydroxyalisol B monoacetate	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C)C3(C)CC(C(=C3CC(C21)O)C(CC(C1C(C)(C)O1)OC(=O)C)C)O)C
MOL000853	0.2217	0.7783	0.7201	Alisma Orientale (Sam.) Juz.	alisol B	Not Available	FALSE	C12=C(CCC1(C1(C(C3(C(CC(=O)CC3)CC1)C)C(C2)O)C)C)C(CC(C1OC1(C)C)O)C
MOL000854	0.1904	0.8096	0.7602	Alisma Orientale (Sam.) Juz.	alisol C	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C)C3(C)CC(=O)C(=C3CC(C21)O)C(CC(C1C(C)(C)O1)O)C)C
MOL000855	0.5544	0.4456	0.7456	Alisma Orientale (Sam.) Juz.	alisol B monoacetate	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1C3(C)CCC(=C3CC(C21)O)C(CC(C1C(C)(C)O1)(CC(=O)O)O)C)C
MOL000856	0.1241	0.8759	0.7492	Alisma Orientale (Sam.) Juz.	alisol C monoacetate	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)C2(C(=C(C(=O)C2)C(CC(OC(=O)C)C2OC2(C)C)C)CC1O)C)C)(C)C
MOL000857	0.8937	0.1063	0.9519	Hippophae Fructus	NCA	936	FALSE	c1(cccnc1)C(=O)N
MOL000857	0.8937	0.1063	0.9519	Alisma Orientale (Sam.) Juz.	NCA	936	FALSE	c1(cccnc1)C(=O)N
MOL000857	0.8937	0.1063	0.9519	Corayceps	NCA	936	FALSE	c1(cccnc1)C(=O)N
MOL000857	0.8937	0.1063	0.9519	Vigna Radiata	NCA	936	FALSE	c1(cccnc1)C(=O)N
MOL000857	0.8937	0.1063	0.9519	Smilacis Glabrae Rhixoma	NCA	936	FALSE	c1(cccnc1)C(=O)N
MOL000858	0.6054	0.3946	0.6301	Alisma Orientale (Sam.) Juz.	Glycerol palmitate	3084463	FALSE	C(C(O)CO)OC(=O)CCCCCCCCCCCCCCC
MOL000858	0.6054	0.3946	0.6301	Fritiliariae Irrhosae Bulbus	Glycerol palmitate	3084463	FALSE	C(C(O)CO)OC(=O)CCCCCCCCCCCCCCC
MOL000858	0.6054	0.3946	0.6301	Olibanun	Glycerol palmitate	3084463	FALSE	C(C(O)CO)OC(=O)CCCCCCCCCCCCCCC

MOL000858	0.6054	0.3946	0.6301	Uncariae Ramulus Cumuncis	Glycerol palmitate	3084463	FALSE	C(C(O)CO)OC(=O)CCCCCCCCCCCCCCC
MOL000858	0.6054	0.3946	0.6301	Arum Ternatum Thunb.	Glycerol palmitate	3084463	FALSE	C(C(O)CO)OC(=O)CCCCCCCCCCCCCCC
MOL000858	0.6054	0.3946	0.6301	Rhizoma Fagopyri Cymosi	Glycerol palmitate	3084463	FALSE	C(C(O)CO)OC(=O)CCCCCCCCCCCCCCC
MOL000858	0.6054	0.3946	0.6301	Spirodelae Herba	Glycerol palmitate	3084463	FALSE	C(C(O)CO)OC(=O)CCCCCCCCCCCCCCC
MOL000862	0.1344	0.8656	0.7486	Alisma Orientale (Sam.) Juz.	[(1S,3R)-1-[(2R)-3,3-dimethyloxiran-2-yl]-3-[(5R,8S,9S,10S,11S,14R)-11-hydroxy-4,4,8,10,14-pentamethyl-3-oxo-1,2,5,6,7,9,11,12,15,16-decahydrocyclopenta[a]phenanthren-17-yl]butyl] acetate	14036811	FALSE	C12(C(C3(C(CC2)C(C(=O)CC3)(C)C)C)C(CC2=C(CCC12C)C(CC(C1C(O1)(C)C)OC(=O)C)C)O)C
MOL000863	0.9102	0.0898	0.8905	Achyranthis Bidentatae Radix	Dekan	15600	FALSE	CCCCCCCCCC
MOL000863	0.9102	0.0898	0.8905	Radix Angelicae Biseratae	Dekan	15600	FALSE	CCCCCCCCCC
MOL000863	0.9102	0.0898	0.8905	Viticis Negundo Folium	Dekan	15600	FALSE	CCCCCCCCCC
MOL000863	0.9102	0.0898	0.8905	Lysimachiae Foenigraeci Herba	Dekan	15600	FALSE	CCCCCCCCCC
MOL000863	0.9102	0.0898	0.8905	Ginseng Folium	Dekan	15600	FALSE	CCCCCCCCCC
MOL000863	0.9102	0.0898	0.8905	Leonuri Fructus	Dekan	15600	FALSE	CCCCCCCCCC
MOL000863	0.9102	0.0898	0.8905	Zingiberis Rhizoma	Dekan	15600	FALSE	CCCCCCCCCC
MOL000866	0.8540	0.1460	0.7003	Leonuri Fructus	2,4,4,6-tetramethylhept-2-ene	566184	FALSE	CC(=CC(CC(C)C)(C)C)C
MOL000870	0.5610	0.4390	0.6116	Prunellae Spica	HEXATRIACONTANE	12412	FALSE	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
MOL000870	0.5610	0.4390	0.6116	Sojae Semen Nigrum	HEXATRIACONTANE	12412	FALSE	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
MOL000870	0.5610	0.4390	0.6116	Canarii Fructus	HEXATRIACONTANE	12412	FALSE	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC

MOL000870	0.5610	0.4390	0.6116	Citrus Aurantium	HEXATRIACONTANE	12412	FALSE	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
MOL000870	0.5610	0.4390	0.6116	Microctis Folium	HEXATRIACONTANE	12412	FALSE	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
MOL000870	0.5610	0.4390	0.6116	Leonuri Fructus	HEXATRIACONTANE	12412	FALSE	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
MOL000870	0.5610	0.4390	0.6116	Maydis Seigma	HEXATRIACONTANE	12412	FALSE	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
MOL000870	0.5610	0.4390	0.6116	Semen Euphorbiae	HEXATRIACONTANE	12412	FALSE	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
MOL000870	0.5610	0.4390	0.6116	Capsici Fructus	HEXATRIACONTANE	12412	FALSE	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
MOL000871	0.9336	0.0664	0.9671	Equiseti Hiemalis Herba	Butylacetat	31272	FALSE	C(=O)(C)OCCCC
MOL000871	0.9336	0.0664	0.9671	Allii Fistulost Bulbus	Butylacetat	31272	FALSE	C(=O)(C)OCCCC
MOL000871	0.9336	0.0664	0.9671	Leonuri Fructus	Butylacetat	31272	FALSE	C(=O)(C)OCCCC
MOL000871	0.9336	0.0664	0.9671	Momordicae Fructus	Butylacetat	31272	FALSE	C(=O)(C)OCCCC
MOL000872	0.9181	0.0819	0.8978	Eriobotryae Folium	(6R)-2,6-dimethyloctane	11413903	FALSE	CC(CCCC(CC)C)C
MOL000872	0.9181	0.0819	0.8978	Radix Bupleuri	(6R)-2,6-dimethyloctane	11413903	FALSE	CC(CCCC(CC)C)C
MOL000872	0.9181	0.0819	0.8978	Leonuri Fructus	(6R)-2,6-dimethyloctane	11413903	FALSE	CC(CCCC(CC)C)C
MOL000873	0.8891	0.1109	0.9717	Leonuri Fructus	CYH	7967	FALSE	C1(=O)CCCCC1
MOL000873	0.8891	0.1109	0.9717	Cornus Officinalis Sieb. Et Zucc.	CYH	7967	FALSE	C1(=O)CCCCC1
MOL000873	0.8891	0.1109	0.9717	Capsici Fructus	CYH	7967	FALSE	C1(=O)CCCCC1
MOL000873	0.8891	0.1109	0.9717	Schizonepetae Herba	CYH	7967	FALSE	C1(=O)CCCCC1
MOL000873	0.8891	0.1109	0.9717	Eriobotryae Folium	CYH	7967	FALSE	C1(=O)CCCCC1
MOL000873	0.8891	0.1109	0.9717	Radix Bupleuri	CYH	7967	FALSE	C1(=O)CCCCC1
MOL000873	0.8891	0.1109	0.9717	Rhododendri Daurici Folium	CYH	7967	FALSE	C1(=O)CCCCC1
MOL000873	0.8891	0.1109	0.9717	Stephaniae Tetrandrae Radix	CYH	7967	FALSE	C1(=O)CCCCC1
MOL000874	0.9438	0.0562	0.9616	Ardisiae Japonicae Herba	paeonol	11092	FALSE	C(=O)(C)c1c(cc(cc1)OC)O
MOL000874	0.9438	0.0562	0.9616	A. Dahurica (Fisch.) Benth. Et Hook	paeonol	11092	FALSE	C(=O)(C)c1c(cc(cc1)OC)O
MOL000874	0.9438	0.0562	0.9616	Platycladi Cacumen	paeonol	11092	FALSE	C(=O)(C)c1c(cc(cc1)OC)O
MOL000874	0.9438	0.0562	0.9616	Cassiae Semen	paeonol	11092	FALSE	C(=O)(C)c1c(cc(cc1)OC)O
MOL000874	0.9438	0.0562	0.9616	Paeoniae Radix Alba	paeonol	11092	FALSE	C(=O)(C)c1c(cc(cc1)OC)O
MOL000874	0.9438	0.0562	0.9616	Leonuri Fructus	paeonol	11092	FALSE	C(=O)(C)c1c(cc(cc1)OC)O

MOL000874	0.9438	0.0562	0.9616	Ginkgo Folium	paeonol	11092	FALSE	C(=O)(C)c1c(cc(cc1)OC)O
MOL000874	0.9438	0.0562	0.9616	Scutellariae Barbatae Herba	paeonol	11092	FALSE	C(=O)(C)c1c(cc(cc1)OC)O
MOL000874	0.9438	0.0562	0.9616	Cannabis Sativa L.	paeonol	11092	FALSE	C(=O)(C)c1c(cc(cc1)OC)O
MOL000874	0.9438	0.0562	0.9616	Mori Follum	paeonol	11092	FALSE	C(=O)(C)c1c(cc(cc1)OC)O
MOL000874	0.9438	0.0562	0.9616	Radix Cynanchi Paniculati	paeonol	11092	FALSE	C(=O)(C)c1c(cc(cc1)OC)O
MOL000874	0.9438	0.0562	0.9616	Radix Paeoniae Rubra	paeonol	11092	FALSE	C(=O)(C)c1c(cc(cc1)OC)O
MOL000874	0.9438	0.0562	0.9616	Arisaematis Rhizoma	paeonol	11092	FALSE	C(=O)(C)c1c(cc(cc1)OC)O
MOL000874	0.9438	0.0562	0.9616	Cortex Moutan	paeonol	11092	FALSE	C(=O)(C)c1c(cc(cc1)OC)O
MOL000874	0.9438	0.0562	0.9616	Semen Firmianae	paeonol	11092	FALSE	C(=O)(C)c1c(cc(cc1)OC)O
MOL000874	0.9438	0.0562	0.9616	Campsis Flos	paeonol	11092	FALSE	C(=O)(C)c1c(cc(cc1)OC)O
MOL000874	0.9438	0.0562	0.9616	Allii Fistulost Bulbus	paeonol	11092	FALSE	C(=O)(C)c1c(cc(cc1)OC)O
MOL000874	0.9438	0.0562	0.9616	Panax Ginseng C. A. Mey.	paeonol	11092	FALSE	C(=O)(C)c1c(cc(cc1)OC)O
MOL000874	0.9438	0.0562	0.9616	Lycii Fructus	paeonol	11092	FALSE	C(=O)(C)c1c(cc(cc1)OC)O
MOL000874	0.9438	0.0562	0.9616	Magnolia Officinalis Rehd Et Wils.	paeonol	11092	FALSE	C(=O)(C)c1c(cc(cc1)OC)O
MOL000875	0.8683	0.1317	0.6011	Allii Fistulost Bulbus	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Paederiae Scandentis Herba	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Paeoniae Radix Alba	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Capsici Fructus	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Tamaricis Cacumen	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Morindae Officinalis Radix	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Rubi Fructus	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Arum Ternatum Thunb.	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Lysimachiae Foenigraeci Herba	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Ganoderma	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Fructus Ligustri Lucidi	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Phragmitis Rhizoma	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Siphonostegiae Herba	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Smilacis Glabrae Rhixoma	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Rhizome Of Whiteback Greenbrier	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Gossampiniflos	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Platycladi Semen	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Platycladi Cacumen	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Polygonati Odorati Rhizoma	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Leonuri Fructus	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Alpiniae Officinarum Rhizome	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Herba Patriniae	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Figwort Root	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Lycii Fructus	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C

MOL000875	0.8683	0.1317	0.6011	Benzoinum	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Ginkgo Folium	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Viticis Negundo Folium	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Aucklandiae Radix	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Lysimachiae Herba	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Viticis Fructus	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Celastri Orbiculati Fructus	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Mahoniae Caulis	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Ginsen Radix Et Rhizoma Rubra	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Sedi Herba	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Magnolia Officinalis Rehd Et Wils.	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Anisi Stellati Fructus	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Gnaphalii Affinis Herba	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000875	0.8683	0.1317	0.6011	Lonicerae Japonicae Flos	Cedrol	Not Available	FALSE	C1CC(C23CCC(C(C(C12)(C)C)C3)(O)C)C
MOL000877	0.9012	0.0988	0.8697	Leonuri Fructus	2-butyl-1-octanol	Not Available	FALSE	C(C(CCCCCC)CCCC)O
MOL000877	0.9012	0.0988	0.8697	Capsici Fructus	2-butyl-1-octanol	Not Available	FALSE	C(C(CCCCCC)CCCC)O
MOL000878	0.5569	0.4431	0.6604	Radix Bupleuri	Farnesylacetone	1711945	FALSE	CC(=O)CC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C
MOL000878	0.5569	0.4431	0.6604	Eriobotryae Folium	Farnesylacetone	1711945	FALSE	CC(=O)CC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C
MOL000878	0.5569	0.4431	0.6604	Millettiae Speciosae Radix	Farnesylacetone	1711945	FALSE	CC(=O)CC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C
MOL000878	0.5569	0.4431	0.6604	Sedi Herba	Farnesylacetone	1711945	FALSE	CC(=O)CC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C
MOL000878	0.5569	0.4431	0.6604	Ephedra Herba	Farnesylacetone	1711945	FALSE	CC(=O)CC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C
MOL000878	0.5569	0.4431	0.6604	Caryophylliflos	Farnesylacetone	1711945	FALSE	CC(=O)CC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C
MOL000878	0.5569	0.4431	0.6604	Rhododendri Daurici Folium	Farnesylacetone	1711945	FALSE	CC(=O)CC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C
MOL000878	0.5569	0.4431	0.6604	Leonuri Fructus	Farnesylacetone	1711945	FALSE	CC(=O)CC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C
MOL000878	0.5569	0.4431	0.6604	Ginkgo Folium	Farnesylacetone	1711945	FALSE	CC(=O)CC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C
MOL000878	0.5569	0.4431	0.6604	Aauropi Folium	Farnesylacetone	1711945	FALSE	CC(=O)CC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C
MOL000878	0.5569	0.4431	0.6604	Campsis Flos	Farnesylacetone	1711945	FALSE	CC(=O)CC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C

MOL000878	0.5569	0.4431	0.6604	Lycii Fructus	Farnesylacetone	1711945	FALSE	CC(=O)CC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C
MOL000879	0.6571	0.3429	0.6259	Notoginseng Flos	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Lygodii Spora	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Achyranthis Bidentatae Radix	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Puerariae Flos	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Curculiginis Rhizome	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Mahoniae Folum	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Calyx Seu Fructus Physalis	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Ginkgo Folium	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Chuanxiong Rhizoma	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Cayratiae Japonicae Herba	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Radix Cirsii Japonici	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Trichosanthes Kirilowii Maxim	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Rhizome Of Whiteback Greenbrier	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Platycladi Semen	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Cornus Officinalis Sieb. Et Zucc.	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Alpiniae Officinarum Rhizome	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Litchi Semen	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Verbenae Herb	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Leonuri Herba	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OC

MOL000879	0.6571	0.3429	0.6259	Croci Stigma	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Polygoni Orientalis Fructus	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Codonopsis Radix	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Farfarae Flos	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Notopterygii Rhizoma Et Radix	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Pollen Typhae	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Raphani Semen	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Humulus Scandens (Lour.) Merr.	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Leonuri Fructus	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Violsse Herba	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Mori Cortex	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Isatdis Radix	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Maydis Seigma	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Peucedani Radix	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Amygdalus Communis Vas	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Lonicerae Japonicae Flos	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Lepidii Semen Descurainiae Semen	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Magnolia Officinalis Rehd Et Wils.	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Cynanchistauntonii Rhizoma Et Radix	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Ephedra Herba	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Lycii Fructus	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC

MOL000879	0.6571	0.3429	0.6259	Hedysari Radix	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Zingiberis Rhizoma	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Broussonetiae Fructus	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Gossampiniflos	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Momordicae Fructus	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Citri Grandis Exocarpium	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Meliae Azedarach Fructus	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Panax Ginseng C. A. Mey.	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Allii Fistulost Bulbus	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Radix Clematidis	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Peucedanidecursivi Radix	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Mahoniae Caulis	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Cassiae Semen	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Radix Angelicae Biseratae	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Hippophae Fructus	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Campsis Flos	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000879	0.6571	0.3429	0.6259	Sterculiae Lychnophorae Semen	methyl palmitate	8181	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC
MOL000881	0.9139	0.0861	0.9308	Leonuri Fructus	o-Toluene diamine	13205	FALSE	c1(c(cccc1N)N)C
MOL000882	0.9159	0.0841	0.8607	Mahoniae Caulis	1,1-dimethylbutyl benzene	16136	FALSE	c1(ccccc1)C(CCC)(C)C
MOL000882	0.9159	0.0841	0.8607	Morindae Officinalis Radix	1,1-dimethylbutyl benzene	16136	FALSE	c1(ccccc1)C(CCC)(C)C

MOL000882	0.9159	0.0841	0.8607	Leonuri Fructus	1,1-dimethylbutyl benzene	16136	FALSE	c1(ccccc1)C(CCC)(C)C
MOL000883	0.8948	0.1052	0.9647	Eucommiae Folium	3,3-Dimethylcyclohexanol	59649284	FALSE	C1(CC(CCC1)(C)C)O
MOL000883	0.8948	0.1052	0.9647	Leonuri Fructus	3,3-Dimethylcyclohexanol	59649284	FALSE	C1(CC(CCC1)(C)C)O
MOL000884	0.9290	0.0710	0.7600	Notoginseng Flos	Azulen	9231	FALSE	c12c(ccccc1)ccc2
MOL000884	0.9290	0.0710	0.7600	Acoritataninowii Rhizoma	Azulen	9231	FALSE	c12c(ccccc1)ccc2
MOL000884	0.9290	0.0710	0.7600	Momordicae Fructus	Azulen	9231	FALSE	c12c(ccccc1)ccc2
MOL000884	0.9290	0.0710	0.7600	Leonuri Fructus	Azulen	9231	FALSE	c12c(ccccc1)ccc2
MOL000885	0.8772	0.1228	0.7847	Viticis Negundo Folium	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Farfarae Flos	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Smilacis Glabrae Rhixoma	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Hippophae Fructus	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Cornus Officinalis Sieb. Et Zucc.	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Pteridis Multifidae Herba	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Leonuri Fructus	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Panacis Quinquefolii Radix	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Cinnanmomi Cortex	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Sesami Nigrum Semen	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Angelicae Sinensis Radix	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Litchi Semen	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Panacis Japonici Rhizoma	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Capsici Fructus	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Achyranthis Bidentatae Radix	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Mori Fructus	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Arisaematis Rhizoma	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Radix Cirsii Japonici	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Ginseng Folium	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Zanthoxyli Pericarpium	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Apocyniveneti Folium	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Cuscutae Semen	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Menthae Herba	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Momordicae Fructus	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Flos Genkwa	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Lysimachiae Foenigraeci Herba	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Morindae Officinalis Radix	Dodekan	8182	FALSE	CCCCCCCCCCCC

MOL000885	0.8772	0.1228	0.7847	Codonopsis Radix	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000885	0.8772	0.1228	0.7847	Lonicerae Japonicae Flos	Dodekan	8182	FALSE	CCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Radix Bupleuri	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Hippophae Fructus	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Mori Fructus	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Cornus Officinalis Sieb. Et Zucc.	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Maydis Seigma	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Morindae Officinalis Radix	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Achyranthis Bidentatae Radix	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Momordicae Fructus	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Leonuri Fructus	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Magnolia Officinalis Rehd Et Wils.	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Capsici Fructus	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Gnaphalii Affinis Herba	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Chuanxiong Rhizoma	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Panax Ginseng C. A. Mey.	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Rhododendri Daurici Folium	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Lysimachiae Foenigraeci Herba	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Cynanchistauntonii Rhizoma Et Radix	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Mahoniae Caulis	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Allii Tuberosi Semen	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Zingiberis Rhizoma	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Radix Cirsii Japonici	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Adenophprae Ae Radix	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Apocyniveneti Folium	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Arisaematis Rhizoma	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Ginkgo Folium	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Radix Angelicae Biseratae	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Amygdalus Communis Vas	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Campsis Flos	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Rose Rugosae Flos	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Microctis Folium	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Lonicerae Japonicae Flos	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Farfarae Flos	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Celastri Orbiculati Fructus	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Ephedra Herba	tetradecane	12389	FALSE	CCCCCCCCCCCCCC
MOL000886	0.8012	0.1988	0.6375	Lycii Fructus	tetradecane	12389	FALSE	CCCCCCCCCCCCCC

MOL000887	0.5485	0.4515	0.6702	Curcumae Rhizoma	demethoxycurcumin	Not Available	FALSE	C(=C\C(=O)/C=C(/C=C\c1cc(c(cc1)O)OC)\O)\c1ccc(cc1)O
MOL000888	0.5485	0.4515	0.6702	Curcumae Rhizoma	demethoxycurcumin	Not Available	FALSE	C(=C\C(=O)CC(=O)/C=C\c1ccc(cc1)O)\c1cc(c(cc1)O)OC
MOL000888	0.5485	0.4515	0.6702	Curcumaelongae Rhizoma	demethoxycurcumin	Not Available	FALSE	C(=C\C(=O)CC(=O)/C=C\c1ccc(cc1)O)\c1cc(c(cc1)O)OC
MOL000889	0.8871	0.1129	0.7818	Curcumae Rhizoma	Isocurcumenol	Not Available	FALSE	C1CC(C23CC(=C(C)C)C(CC(=C)C12)(O3)O)C
MOL000889	0.8871	0.1129	0.7818	Curcumae Radix	Isocurcumenol	Not Available	FALSE	C1CC(C23CC(=C(C)C)C(CC(=C)C12)(O3)O)C
MOL000889	0.8871	0.1129	0.7818	Cyperi Rhizoma	Isocurcumenol	Not Available	FALSE	C1CC(C23CC(=C(C)C)C(CC(=C)C12)(O3)O)C
MOL000890	0.8816	0.1184	0.7446	Curcumaelongae Rhizoma	(+)-alpha-Curcumene	3083834	FALSE	c1(ccc(cc1)C(C)CCC=C(C)C)C
MOL000890	0.8816	0.1184	0.7446	Polygoni Orientalis Fructus	(+)-alpha-Curcumene	3083834	FALSE	c1(ccc(cc1)C(C)CCC=C(C)C)C
MOL000890	0.8816	0.1184	0.7446	Cornus Officinalis Sieb. Et Zucc.	(+)-alpha-Curcumene	3083834	FALSE	c1(ccc(cc1)C(C)CCC=C(C)C)C
MOL000890	0.8816	0.1184	0.7446	Rhododendri Daurici Folium	(+)-alpha-Curcumene	3083834	FALSE	c1(ccc(cc1)C(C)CCC=C(C)C)C
MOL000890	0.8816	0.1184	0.7446	Folium Artemisiae Argyi	(+)-alpha-Curcumene	3083834	FALSE	c1(ccc(cc1)C(C)CCC=C(C)C)C
MOL000890	0.8816	0.1184	0.7446	Codonopsis Radix	(+)-alpha-Curcumene	3083834	FALSE	c1(ccc(cc1)C(C)CCC=C(C)C)C
MOL000890	0.8816	0.1184	0.7446	Ganoderma	(+)-alpha-Curcumene	3083834	FALSE	c1(ccc(cc1)C(C)CCC=C(C)C)C
MOL000890	0.8816	0.1184	0.7446	Panacis Quinquefolii Radix	(+)-alpha-Curcumene	3083834	FALSE	c1(ccc(cc1)C(C)CCC=C(C)C)C
MOL000890	0.8816	0.1184	0.7446	Curcumae Radix	(+)-alpha-Curcumene	3083834	FALSE	c1(ccc(cc1)C(C)CCC=C(C)C)C
MOL000890	0.8816	0.1184	0.7446	Ardisiae Japonicae Herba	(+)-alpha-Curcumene	3083834	FALSE	c1(ccc(cc1)C(C)CCC=C(C)C)C
MOL000890	0.8816	0.1184	0.7446	Zingiberis Rhizoma	(+)-alpha-Curcumene	3083834	FALSE	c1(ccc(cc1)C(C)CCC=C(C)C)C
MOL000890	0.8816	0.1184	0.7446	Curcumae Rhizoma	(+)-alpha-Curcumene	3083834	FALSE	c1(ccc(cc1)C(C)CCC=C(C)C)C
MOL000890	0.8816	0.1184	0.7446	Verbenae Herb	(+)-alpha-Curcumene	3083834	FALSE	c1(ccc(cc1)C(C)CCC=C(C)C)C
MOL000890	0.8816	0.1184	0.7446	Ailanthi Cortex	(+)-alpha-Curcumene	3083834	FALSE	c1(ccc(cc1)C(C)CCC=C(C)C)C
MOL000890	0.8816	0.1184	0.7446	Campsis Flos	(+)-alpha-Curcumene	3083834	FALSE	c1(ccc(cc1)C(C)CCC=C(C)C)C

MOL000891	0.8410	0.1590	0.7763	Curcumae Rhizoma	(1R,10R)-epoxy-1,10-dihydrocurdione	Not Available	FALSE	C1CC2C(CC(=O)C(CC(=O)C1C)C(C)C)(C)O2
MOL000892	0.5271	0.4729	0.7282	Curcumae Rhizoma	TNP00001	6604598	FALSE	C(=C\C(=O)CC(=O)/C=C\c1cc(c(cc1)O)OC)\c1cc(c(cc1)O)OC
MOL000892	0.5271	0.4729	0.7282	Curcumaelongae Rhizoma	TNP00001	6604598	FALSE	C(=C\C(=O)CC(=O)/C=C\c1cc(c(cc1)O)OC)\c1cc(c(cc1)O)OC
MOL000893	0.3692	0.6308	0.7663	Curcumae Rhizoma	difurocumenone	Not Available	FALSE	o1c2c(c(c1)C)C(=O)C1C(CC/C=C(/C2)\C)(C2C3=C(C1(C2)C)Cc1c(CC3C)occ1C)C
MOL000893	0.3692	0.6308	0.7663	Curcumae Radix	difurocumenone	Not Available	FALSE	o1c2c(c(c1)C)C(=O)C1C(CC/C=C(/C2)\C)(C2C3=C(C1(C2)C)Cc1c(CC3C)occ1C)C
MOL000894	0.8792	0.1208	0.8323	Curcumae Rhizoma	turmerone	Not Available	FALSE	CC1CCC(CC1)C(C)CC(=O)C=C(C)C
MOL000895	0.8753	0.1247	0.7985	Morindae Officinalis Radix	Zingiberene	92776	FALSE	C1=C(C=CC(C1)C(C)CCC=C(C)C)C
MOL000895	0.8753	0.1247	0.7985	Lonicerae Japonicae Flos	Zingiberene	92776	FALSE	C1=C(C=CC(C1)C(C)CCC=C(C)C)C
MOL000895	0.8753	0.1247	0.7985	Curcumae Rhizoma	Zingiberene	92776	FALSE	C1=C(C=CC(C1)C(C)CCC=C(C)C)C
MOL000895	0.8753	0.1247	0.7985	Curcumae Radix	Zingiberene	92776	FALSE	C1=C(C=CC(C1)C(C)CCC=C(C)C)C
MOL000895	0.8753	0.1247	0.7985	Zingiberis Rhizoma	Zingiberene	92776	FALSE	C1=C(C=CC(C1)C(C)CCC=C(C)C)C
MOL000895	0.8753	0.1247	0.7985	Zingiber Officinale Roscoe	Zingiberene	92776	FALSE	C1=C(C=CC(C1)C(C)CCC=C(C)C)C
MOL000896	0.8619	0.1381	0.8526	Curcumae Rhizoma	13657-68-6	6441391	FALSE	C1(=O)CC(C(=O)C/C(=C/CCC1C)/C)C(C)C
MOL000897	0.9071	0.0929	0.8240	Curcumae Rhizoma	(3S,3aR,8aR)-3,8a-dihydroxy-5-isopropylidene-3,8-dimethyl-1,2,3a,4-tetrahydroazulen-6-one	11776892	FALSE	C1(CCC2(C(=CC(=O)C(=C(C)C)CC12)C)O)(C)O
MOL000897	0.9071	0.0929	0.8240	Curcumae Radix	(3S,3aR,8aR)-3,8a-dihydroxy-5-isopropylidene-3,8-dimethyl-1,2,3a,4-tetrahydroazulen-6-one	11776892	FALSE	C1(CCC2(C(=CC(=O)C(=C(C)C)CC12)C)O)(C)O

MOL000898	0.8700	0.1300	0.7960	Curcumae Rhizoma	(1S,6R,7R)-4-isopropylidene-1-methyl-7-(3-oxobutyl)norcaran-3-one	153845	FALSE	C12(CC(=O)C(=C(C)C)CC1C2CCC(=O)C)C
MOL000898	0.8700	0.1300	0.7960	Curcumaelongae Rhizoma	(1S,6R,7R)-4-isopropylidene-1-methyl-7-(3-oxobutyl)norcaran-3-one	153845	FALSE	C12(CC(=O)C(=C(C)C)CC1C2CCC(=O)C)C
MOL000898	0.8700	0.1300	0.7960	Curcumae Radix	(1S,6R,7R)-4-isopropylidene-1-methyl-7-(3-oxobutyl)norcaran-3-one	153845	FALSE	C12(CC(=O)C(=C(C)C)CC1C2CCC(=O)C)C
MOL000899	0.8073	0.1927	0.6924	Codonopsis Radix	Furanodiene	636458	FALSE	C1C/C=C(/Cc2c(C/C=C/1\C)c(co2)C)\C
MOL000899	0.8073	0.1927	0.6924	Curcumae Rhizoma	Furanodiene	636458	FALSE	C1C/C=C(/Cc2c(C/C=C/1\C)c(co2)C)\C
MOL000900	0.8890	0.1110	0.8341	Curcumaelongae Rhizoma	(5R,6R)-5-isopropenyl-3,6-dimethyl-6-vinyl-5,7-dihydrobenzofuran-4-one	3081930	FALSE	o1cc(c2c1CC(C(C2=O)C(=C)C)(C=C)C)C
MOL000900	0.8890	0.1110	0.8341	Curcumae Rhizoma	(5R,6R)-5-isopropenyl-3,6-dimethyl-6-vinyl-5,7-dihydrobenzofuran-4-one	3081930	FALSE	o1cc(c2c1CC(C(C2=O)C(=C)C)(C=C)C)C
MOL000900	0.8890	0.1110	0.8341	Curcumae Radix	(5R,6R)-5-isopropenyl-3,6-dimethyl-6-vinyl-5,7-dihydrobenzofuran-4-one	3081930	FALSE	o1cc(c2c1CC(C(C2=O)C(=C)C)(C=C)C)C
MOL000901	0.8935	0.1065	0.7768	Curcumae Radix	BRN 2004585	Not Available	FALSE	C1CC(C23CC(=C(C)C)C(C=C(C12)C)(O3)O)C
MOL000901	0.8935	0.1065	0.7768	Curcumaelongae Rhizoma	BRN 2004585	Not Available	FALSE	C1CC(C23CC(=C(C)C)C(C=C(C12)C)(O3)O)C
MOL000901	0.8935	0.1065	0.7768	Curcumae Rhizoma	BRN 2004585	Not Available	FALSE	C1CC(C23CC(=C(C)C)C(C=C(C12)C)(O3)O)C
MOL000902	0.8695	0.1305	0.7531	Curcumae Rhizoma	curcumol	Not Available	FALSE	C1CC(C23CC(C(CC(=C)C12)(O3)O)C(C)C)C
MOL000902	0.8695	0.1305	0.7531	Curcumaelongae Rhizoma	curcumol	Not Available	FALSE	C1CC(C23CC(C(CC(=C)C12)(O3)O)C(C)C)C

MOL000903	0.8250	0.1750	0.7437	Curcumae Radix	Gweicurculactone	130117	FALSE	o1c2c(c(c1=O)C)cc1C(CCc1c(c2)C)C
MOL000903	0.8250	0.1750	0.7437	Curcumae Rhizoma	Gweicurculactone	130117	FALSE	o1c2c(c(c1=O)C)cc1C(CCc1c(c2)C)C
MOL000904	0.9653	0.0347	0.8601	Zanthoxyli Pericarpium	cineole	Not Available	FALSE	C12(OCC(CC1(C)C)CC2)C
MOL000904	0.9653	0.0347	0.8601	Curcumae Rhizoma	cineole	Not Available	FALSE	C12(OCC(CC1(C)C)CC2)C
MOL000904	0.9653	0.0347	0.8601	Acoritataninowii Rhizoma	cineole	Not Available	FALSE	C12(OCC(CC1(C)C)CC2)C
MOL000905	0.9548	0.0452	0.7808	Platycladi Cacumen	()-beta-Pinene	10290825	FALSE	C12C(=C)CCC(C1(C)C)C2
MOL000905	0.9548	0.0452	0.7808	Asari Radix Et Rhizoma	()-beta-Pinene	10290825	FALSE	C12C(=C)CCC(C1(C)C)C2
MOL000905	0.9548	0.0452	0.7808	Olibanun	()-beta-Pinene	10290825	FALSE	C12C(=C)CCC(C1(C)C)C2
MOL000905	0.9548	0.0452	0.7808	Curcumae Rhizoma	()-beta-Pinene	10290825	FALSE	C12C(=C)CCC(C1(C)C)C2
MOL000905	0.9548	0.0452	0.7808	Codonopsis Radix	()-beta-Pinene	10290825	FALSE	C12C(=C)CCC(C1(C)C)C2
MOL000905	0.9548	0.0452	0.7808	Coriandri Sativi Herba	()-beta-Pinene	10290825	FALSE	C12C(=C)CCC(C1(C)C)C2
MOL000905	0.9548	0.0452	0.7808	Curcumaelongae Rhizoma	()-beta-Pinene	10290825	FALSE	C12C(=C)CCC(C1(C)C)C2
MOL000905	0.9548	0.0452	0.7808	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	()-beta-Pinene	10290825	FALSE	C12C(=C)CCC(C1(C)C)C2
MOL000905	0.9548	0.0452	0.7808	Schizonepetae Herba	()-beta-Pinene	10290825	FALSE	C12C(=C)CCC(C1(C)C)C2
MOL000905	0.9548	0.0452	0.7808	Canarii Fructus	()-beta-Pinene	10290825	FALSE	C12C(=C)CCC(C1(C)C)C2
MOL000905	0.9548	0.0452	0.7808	Houttuyniae Herba	()-beta-Pinene	10290825	FALSE	C12C(=C)CCC(C1(C)C)C2
MOL000905	0.9548	0.0452	0.7808	Moslae Herba	()-beta-Pinene	10290825	FALSE	C12C(=C)CCC(C1(C)C)C2
MOL000905	0.9548	0.0452	0.7808	Borneolum Syntheticum	()-beta-Pinene	10290825	FALSE	C12C(=C)CCC(C1(C)C)C2
MOL000905	0.9548	0.0452	0.7808	Myristicae Semen	()-beta-Pinene	10290825	FALSE	C12C(=C)CCC(C1(C)C)C2
MOL000905	0.9548	0.0452	0.7808	Schisandrae Chinensis Fructus	()-beta-Pinene	10290825	FALSE	C12C(=C)CCC(C1(C)C)C2
MOL000906	0.8531	0.1469	0.6602	Curcumae Rhizoma	wenjine	Not Available	FALSE	C12(C(/C=C\3/C(CC4(C(CC1)O4)C)(OC(=O)C)C)O)O2)C
MOL000907	0.8848	0.1152	0.6967	Curcumae Rhizoma	curcumalactone	Not Available	FALSE	O1C(=O)C(CC21C(CCC2C(=C)C)C)C(C)C
MOL000908	0.8619	0.1381	0.6520	Piperis Fructus	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Cyperi Rhizoma	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Linderae Radix	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Rubi Fructus	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Panax Ginseng C. A. Mey.	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Schizonepetae Spica	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Cnidii Fructus	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Rhizome Of Whiteback Greenbrier	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Ginsen Radix Et Rhizoma Rubra	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Arum Ternatum Thunb.	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Farfarae Flos	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Zingiber Officinale Roscoe	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C

MOL000908	0.8619	0.1381	0.6520	Artemisiae Scopariae Herba	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Chuanxiong Rhizoma	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Artemisia Annua L.	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Myrrha	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Gnaphalii Affinis Herba	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Ginseng Folium	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Notoginseng Flos	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Alpiniae Officinarum Rhizome	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Phellodendri Chinrnsis Cortex	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Campsis Flos	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Ailanthi Cortex	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Aristolochiae Fructus	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Zanthoxyli Pericarpium	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Curcumae Radix	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Hippophae Fructus	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Cayratiae Japonicae Herba	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Curcumae Rhizoma	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Arisaematis Rhizoma	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Kaempferiae Rhizoma	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Lysimachiae Herba	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Platycladi Cacumen	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Borneolum Syntheticum	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000908	0.8619	0.1381	0.6520	Lonicerae Japonicae Flos	beta-elemene	6918391	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C=C)C
MOL000909	0.8553	0.1447	0.6660	Solidaginis Herba	(3S,4R)-3-isopropenyl-1-isopropyl-4-methyl-4-vinylcyclohexene	12004383	FALSE	C1(=CC(C(CC1)(C)C=C)C(=C)C)C(C)C
MOL000909	0.8553	0.1447	0.6660	Curcumae Rhizoma	(3S,4R)-3-isopropenyl-1-isopropyl-4-methyl-4-vinylcyclohexene	12004383	FALSE	C1(=CC(C(CC1)(C)C=C)C(=C)C)C(C)C

MOL000909	0.8553	0.1447	0.6660	Viticis Negundo Folium	(3S,4R)-3-isopropenyl-1-isopropyl-4-methyl-4-vinylcyclohexene	12004383	FALSE	C1(=CC(C(CC1)(C)C=C)C(=C)C)C(C)C
MOL000909	0.8553	0.1447	0.6660	Perillae Fructus	(3S,4R)-3-isopropenyl-1-isopropyl-4-methyl-4-vinylcyclohexene	12004383	FALSE	C1(=CC(C(CC1)(C)C=C)C(=C)C)C(C)C
MOL000909	0.8553	0.1447	0.6660	Rubi Fructus	(3S,4R)-3-isopropenyl-1-isopropyl-4-methyl-4-vinylcyclohexene	12004383	FALSE	C1(=CC(C(CC1)(C)C=C)C(=C)C)C(C)C
MOL000910	0.8684	0.1316	0.8662	Curcumaelongae Rhizoma	Germacron	6436348	FALSE	C1(=O)C/C(=C/CC/C(=C/CC1=C(C)C)/C)/C
MOL000910	0.8684	0.1316	0.8662	Curcumae Rhizoma	Germacron	6436348	FALSE	C1(=O)C/C(=C/CC/C(=C/CC1=C(C)C)/C)/C
MOL000910	0.8684	0.1316	0.8662	Geranium Wilfordii Maxim.	Germacron	6436348	FALSE	C1(=O)C/C(=C/CC/C(=C/CC1=C(C)C)/C)/C
MOL000910	0.8684	0.1316	0.8662	Curcumae Radix	Germacron	6436348	FALSE	C1(=O)C/C(=C/CC/C(=C/CC1=C(C)C)/C)/C
MOL000910	0.8684	0.1316	0.8662	Perilla Frutescens	Germacron	6436348	FALSE	C1(=O)C/C(=C/CC/C(=C/CC1=C(C)C)/C)/C
MOL000910	0.8684	0.1316	0.8662	Rhododendri Daurici Folium	Germacron	6436348	FALSE	C1(=O)C/C(=C/CC/C(=C/CC1=C(C)C)/C)/C
MOL000911	0.9536	0.0464	0.9572	Schisandrae Chinensis Fructus	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Zanthoxyli Pericarpium	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Ligustici Rhizoma Et Radix	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Citrus Aurantium	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Anisi Stellati Fructus	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Fructus Carotae	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Cinnanmomi Cortex	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Citri Fructus Retinervus	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Evodiae Fructus	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Platycladi Cacumen	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Kadsurae Coccineae Radix Et Caulis	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Rhododendri Daurici Folium	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C

MOL000911	0.9536	0.0464	0.9572	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Piperis Fructus	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Forsythiae Fructus	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Et Radix Patriniae Rhizoma	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Chuanxiong Rhizoma	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Viticis Negundo Folium	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Rubi Fructus	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Rhizome Of Whiteback Greenbrier	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Ginkgo Folium	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Apocyniveneti Folium	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Citri Reticulatae Pericarpium Viride	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Viticis Fructus	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Moslae Herba	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Sennae Folium	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Citri Reticulatae Folium	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Zingiberis Rhizoma	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Magnolia Officinalis Rehd Et Wils.	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Curcumae Radix	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Folium Artemisiae Argyi	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Herba Clinopodii Polycephali.	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000911	0.9536	0.0464	0.9572	Curcumae Rhizoma	Terpilene	7462	FALSE	C1(=CC=C(CC1)C)C(C)C
MOL000912	0.9343	0.0657	0.9527	Curcumae Rhizoma	(2S)-heptan-2-ol	2724897	FALSE	CC(CCCCC)O
MOL000912	0.9343	0.0657	0.9527	Zingiber Officinale Roscoe	(2S)-heptan-2-ol	2724897	FALSE	CC(CCCCC)O
MOL000913	0.9082	0.0918	0.6986	Folium Artemisiae Argyi	tricyclene	55250308	FALSE	CC12C3C1CC(C3)C2(C)C
MOL000913	0.9082	0.0918	0.6986	Zanthoxyli Pericarpium	tricyclene	55250308	FALSE	CC12C3C1CC(C3)C2(C)C
MOL000913	0.9082	0.0918	0.6986	Magnolia Officinalis Rehd Et Wils.	tricyclene	55250308	FALSE	CC12C3C1CC(C3)C2(C)C
MOL000913	0.9082	0.0918	0.6986	Piperis Longi Fructus	tricyclene	55250308	FALSE	CC12C3C1CC(C3)C2(C)C
MOL000913	0.9082	0.0918	0.6986	Curcumae Rhizoma	tricyclene	55250308	FALSE	CC12C3C1CC(C3)C2(C)C
MOL000913	0.9082	0.0918	0.6986	Zingiberis Rhizoma	tricyclene	55250308	FALSE	CC12C3C1CC(C3)C2(C)C
MOL000913	0.9082	0.0918	0.6986	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	tricyclene	55250308	FALSE	CC12C3C1CC(C3)C2(C)C
MOL000913	0.9082	0.0918	0.6986	Artemisia Annua L.	tricyclene	55250308	FALSE	CC12C3C1CC(C3)C2(C)C
MOL000913	0.9082	0.0918	0.6986	Cnidii Fructus	tricyclene	55250308	FALSE	CC12C3C1CC(C3)C2(C)C

MOL000914	0.9537	0.0463	0.7528	Borneolum Syntheticum	(5S)-1-isopropyl-4-methylbicyclo[3.1.0]hex-3-ene	12444324	FALSE	C1=C(C2C(C1)(C(C)C)C2)C
MOL000914	0.9537	0.0463	0.7528	Artemisia Annua L.	(5S)-1-isopropyl-4-methylbicyclo[3.1.0]hex-3-ene	12444324	FALSE	C1=C(C2C(C1)(C(C)C)C2)C
MOL000914	0.9537	0.0463	0.7528	Kaempferiae Rhizoma	(5S)-1-isopropyl-4-methylbicyclo[3.1.0]hex-3-ene	12444324	FALSE	C1=C(C2C(C1)(C(C)C)C2)C
MOL000914	0.9537	0.0463	0.7528	Bidentis Bipinnatae Herba	(5S)-1-isopropyl-4-methylbicyclo[3.1.0]hex-3-ene	12444324	FALSE	C1=C(C2C(C1)(C(C)C)C2)C
MOL000914	0.9537	0.0463	0.7528	Curcumae Rhizoma	(5S)-1-isopropyl-4-methylbicyclo[3.1.0]hex-3-ene	12444324	FALSE	C1=C(C2C(C1)(C(C)C)C2)C
MOL000914	0.9537	0.0463	0.7528	Olibanun	(5S)-1-isopropyl-4-methylbicyclo[3.1.0]hex-3-ene	12444324	FALSE	C1=C(C2C(C1)(C(C)C)C2)C
MOL000914	0.9537	0.0463	0.7528	Coriandri Sativi Herba	(5S)-1-isopropyl-4-methylbicyclo[3.1.0]hex-3-ene	12444324	FALSE	C1=C(C2C(C1)(C(C)C)C2)C
MOL000915	0.8624	0.1376	0.8464	Curcumae Rhizoma	(1S,10S),(4S,5S)-germacrone-1(10),4-diepoxide	Not Available	FALSE	C1CC2C(CC(=O)/C(=C(/C)\C=O)/CC3C1(C)O3)(O2)C
MOL000916	0.9541	0.0459	0.7681	Olibanun	Car-3-ene	442461	FALSE	C12CC(=CCC1C2(C)C)C
MOL000916	0.9541	0.0459	0.7681	Rubi Fructus	Car-3-ene	442461	FALSE	C12CC(=CCC1C2(C)C)C
MOL000916	0.9541	0.0459	0.7681	Moslae Herba	Car-3-ene	442461	FALSE	C12CC(=CCC1C2(C)C)C

MOL000916	0.9541	0.0459	0.7681	Artemisiae Scopariae Herba	Car-3-ene	442461	FALSE	C12CC(=CCC1C2(C)C)C
MOL000916	0.9541	0.0459	0.7681	Zanthoxyli Pericarpium	Car-3-ene	442461	FALSE	C12CC(=CCC1C2(C)C)C
MOL000916	0.9541	0.0459	0.7681	Citri Sarcodactylis Fructus	Car-3-ene	442461	FALSE	C12CC(=CCC1C2(C)C)C
MOL000916	0.9541	0.0459	0.7681	Coriandri Sativi Herba	Car-3-ene	442461	FALSE	C12CC(=CCC1C2(C)C)C
MOL000916	0.9541	0.0459	0.7681	Citri Fructus	Car-3-ene	442461	FALSE	C12CC(=CCC1C2(C)C)C
MOL000916	0.9541	0.0459	0.7681	Radix Angelicae Biseratae	Car-3-ene	442461	FALSE	C12CC(=CCC1C2(C)C)C
MOL000916	0.9541	0.0459	0.7681	Curcumae Rhizoma	Car-3-ene	442461	FALSE	C12CC(=CCC1C2(C)C)C
MOL000917	0.9653	0.0347	0.8601	Curcumae Rhizoma	cineole	Not Available	FALSE	C1C2COC(CC2)(C)C1(C)C
MOL000917	0.9653	0.0347	0.8601	Curcumaelongae Rhizoma	cineole	Not Available	FALSE	C1C2COC(CC2)(C)C1(C)C
MOL000917	0.9653	0.0347	0.8601	Olibanun	cineole	Not Available	FALSE	C1C2COC(CC2)(C)C1(C)C
MOL000917	0.9653	0.0347	0.8601	Zanthoxyli Pericarpium	cineole	Not Available	FALSE	C1C2COC(CC2)(C)C1(C)C
MOL000918	0.9323	0.0677	0.9381	Notoginseng Flos	2-NONANONE	13187	FALSE	C(=O)(CCCCCCC)C
MOL000918	0.9323	0.0677	0.9381	Adenophprae Ae Radix	2-NONANONE	13187	FALSE	C(=O)(CCCCCCC)C
MOL000918	0.9323	0.0677	0.9381	Zingiber Officinale Roscoe	2-NONANONE	13187	FALSE	C(=O)(CCCCCCC)C
MOL000918	0.9323	0.0677	0.9381	Curcumae Rhizoma	2-NONANONE	13187	FALSE	C(=O)(CCCCCCC)C
MOL000918	0.9323	0.0677	0.9381	Radix Bupleuri	2-NONANONE	13187	FALSE	C(=O)(CCCCCCC)C
MOL000918	0.9323	0.0677	0.9381	Momordicae Fructus	2-NONANONE	13187	FALSE	C(=O)(CCCCCCC)C
MOL000918	0.9323	0.0677	0.9381	Radix Angelicae Biseratae	2-NONANONE	13187	FALSE	C(=O)(CCCCCCC)C
MOL000918	0.9323	0.0677	0.9381	Caryophylliflos	2-NONANONE	13187	FALSE	C(=O)(CCCCCCC)C
MOL000918	0.9323	0.0677	0.9381	Zingiberis Rhizoma	2-NONANONE	13187	FALSE	C(=O)(CCCCCCC)C
MOL000918	0.9323	0.0677	0.9381	Artemisiae Scopariae Herba	2-NONANONE	13187	FALSE	C(=O)(CCCCCCC)C
MOL000918	0.9323	0.0677	0.9381	Rose Rugosae Flos	2-NONANONE	13187	FALSE	C(=O)(CCCCCCC)C
MOL000919	0.9313	0.0687	0.9384	Radix Angelicae Biseratae	(S)-()-2-Nonanol	11094753	FALSE	C(CCCCCCC)(O)C
MOL000919	0.9313	0.0687	0.9384	Curcumae Rhizoma	(S)-()-2-Nonanol	11094753	FALSE	C(CCCCCCC)(O)C
MOL000920	0.9299	0.0701	0.9389	Aristolochiae Fructus	LINALOOL (D)	67179	FALSE	CC(=CCCC(C=C)(O)C)C
MOL000920	0.9299	0.0701	0.9389	Olibanun	LINALOOL (D)	67179	FALSE	CC(=CCCC(C=C)(O)C)C

MOL000920	0.9299	0.0701	0.9389	Dianthi Herba	LINALOOL (D)	67179	FALSE	CC(=CCCC(C=C)(O)C)C
MOL000920	0.9299	0.0701	0.9389	Mori Follum	LINALOOL (D)	67179	FALSE	CC(=CCCC(C=C)(O)C)C
MOL000920	0.9299	0.0701	0.9389	Platycladi Cacumen	LINALOOL (D)	67179	FALSE	CC(=CCCC(C=C)(O)C)C
MOL000920	0.9299	0.0701	0.9389	Forsythiae Fructus	LINALOOL (D)	67179	FALSE	CC(=CCCC(C=C)(O)C)C
MOL000920	0.9299	0.0701	0.9389	Ganoderma	LINALOOL (D)	67179	FALSE	CC(=CCCC(C=C)(O)C)C
MOL000920	0.9299	0.0701	0.9389	Leonuri Herba	LINALOOL (D)	67179	FALSE	CC(=CCCC(C=C)(O)C)C
MOL000920	0.9299	0.0701	0.9389	Alpiniae Oxyphyliae Fructus	LINALOOL (D)	67179	FALSE	CC(=CCCC(C=C)(O)C)C
MOL000920	0.9299	0.0701	0.9389	Bidentis Bipinnatae Herba	LINALOOL (D)	67179	FALSE	CC(=CCCC(C=C)(O)C)C
MOL000920	0.9299	0.0701	0.9389	Siphonostegiae Herba	LINALOOL (D)	67179	FALSE	CC(=CCCC(C=C)(O)C)C
MOL000920	0.9299	0.0701	0.9389	Borneolum Syntheticum	LINALOOL (D)	67179	FALSE	CC(=CCCC(C=C)(O)C)C
MOL000920	0.9299	0.0701	0.9389	Croci Stigma	LINALOOL (D)	67179	FALSE	CC(=CCCC(C=C)(O)C)C
MOL000920	0.9299	0.0701	0.9389	Zingiber Officinale Roscoe	LINALOOL (D)	67179	FALSE	CC(=CCCC(C=C)(O)C)C
MOL000920	0.9299	0.0701	0.9389	Lonicerae Japonicae Flos	LINALOOL (D)	67179	FALSE	CC(=CCCC(C=C)(O)C)C
MOL000920	0.9299	0.0701	0.9389	Curcumae Rhizoma	LINALOOL (D)	67179	FALSE	CC(=CCCC(C=C)(O)C)C
MOL000920	0.9299	0.0701	0.9389	Piperis Longi Fructus	LINALOOL (D)	67179	FALSE	CC(=CCCC(C=C)(O)C)C
MOL000921	0.8449	0.1551	0.8410	Curcumae Rhizoma	(1S,4E,10S)-8-isopropylidene-1,5-dimethyl-11-oxabicyclo[8.1.0]undec-4-en-7-one	11637239	FALSE	C12CC(=C(C)C)C(=O)C/C(=C/CCC1(O2)C)/C

MOL000921	0.8449	0.1551	0.8410	Curcumaelongae Rhizoma	(1S,4E,10S)-8-isopropylidene-1,5-dimethyl-11-oxabicyclo[8.1.0]undec-4-en-7-one	11637239	FALSE	C12CC(=C(C)C)C(=O)C/C(=C/CCC1(O2)C)/C
MOL000922	0.9498	0.0502	0.9678	Myristicae Semen	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Peucedani Radix	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Radix Salviae	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Aucklandiae Radix	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Curcumae Rhizoma	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Moslae Herba	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	A. Dahurica (Fisch.) Benth. Et Hook	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Coriandri Sativi Herba	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Aristolochiae Fructus	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Ganoderma	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Olibanun	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Rhododendri Daurici Folium	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Alpiniae Officinarum Rhizome	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Myrrha	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Platycladi Cacumen	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Citri Sarcodactylis Fructus	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Cyperi Rhizoma	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C

MOL000922	0.9498	0.0502	0.9678	Radix Bupleuri	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Ardisiae Japonicae Herba	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Alpiniae Oxyphyliae Fructus	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Magnolia Officinalis Rehd Et Wils.	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Caryophylliflos	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Citrus Reticulata	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Chuanxiong Rhizoma	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Peucedanidecursivi Radix	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000922	0.9498	0.0502	0.9678	Lilii Bulbus	(R)-p-Menth-1-en-4-ol	5325830	FALSE	C1(CC=C(CC1)C)(O)C(C)C
MOL000923	0.9586	0.0414	0.7752	Evodiae Fructus	ACETIC ACID,BORNYL ESTER	637531	FALSE	C12(C(CC(CC1)C2(C)C)OC(=O)C)C
MOL000923	0.9586	0.0414	0.7752	Asari Radix Et Rhizoma	ACETIC ACID,BORNYL ESTER	637531	FALSE	C12(C(CC(CC1)C2(C)C)OC(=O)C)C
MOL000923	0.9586	0.0414	0.7752	Houttuyniae Herba	ACETIC ACID,BORNYL ESTER	637531	FALSE	C12(C(CC(CC1)C2(C)C)OC(=O)C)C
MOL000923	0.9586	0.0414	0.7752	Rhododendri Daurici Folium	ACETIC ACID,BORNYL ESTER	637531	FALSE	C12(C(CC(CC1)C2(C)C)OC(=O)C)C
MOL000923	0.9586	0.0414	0.7752	Curcumae Rhizoma	ACETIC ACID,BORNYL ESTER	637531	FALSE	C12(C(CC(CC1)C2(C)C)OC(=O)C)C
MOL000923	0.9586	0.0414	0.7752	Schisandrae Chinensis Fructus	ACETIC ACID,BORNYL ESTER	637531	FALSE	C12(C(CC(CC1)C2(C)C)OC(=O)C)C
MOL000923	0.9586	0.0414	0.7752	Citri Sarcodactylis Fructus	ACETIC ACID,BORNYL ESTER	637531	FALSE	C12(C(CC(CC1)C2(C)C)OC(=O)C)C
MOL000923	0.9586	0.0414	0.7752	Magnolia Officinalis Rehd Et Wils.	ACETIC ACID,BORNYL ESTER	637531	FALSE	C12(C(CC(CC1)C2(C)C)OC(=O)C)C
MOL000924	0.9042	0.0958	0.9033	Ganoderma	Mnk	8163	FALSE	CC(=O)CCCCCCCCC

MOL000924	0.9042	0.0958	0.9033	Arum Ternatum Thunb.	Mnk	8163	FALSE	CC(=O)CCCCCCCCC
MOL000924	0.9042	0.0958	0.9033	Morindae Officinalis Radix	Mnk	8163	FALSE	CC(=O)CCCCCCCCC
MOL000924	0.9042	0.0958	0.9033	Radix Bupleuri	Mnk	8163	FALSE	CC(=O)CCCCCCCCC
MOL000924	0.9042	0.0958	0.9033	Zingiberis Rhizoma	Mnk	8163	FALSE	CC(=O)CCCCCCCCC
MOL000924	0.9042	0.0958	0.9033	Rose Rugosae Flos	Mnk	8163	FALSE	CC(=O)CCCCCCCCC
MOL000924	0.9042	0.0958	0.9033	Caryophylliflos	Mnk	8163	FALSE	CC(=O)CCCCCCCCC
MOL000924	0.9042	0.0958	0.9033	Ardisiae Japonicae Herba	Mnk	8163	FALSE	CC(=O)CCCCCCCCC
MOL000924	0.9042	0.0958	0.9033	Momordicae Fructus	Mnk	8163	FALSE	CC(=O)CCCCCCCCC
MOL000924	0.9042	0.0958	0.9033	Junci Medulla	Mnk	8163	FALSE	CC(=O)CCCCCCCCC
MOL000924	0.9042	0.0958	0.9033	Zanthoxyli Pericarpium	Mnk	8163	FALSE	CC(=O)CCCCCCCCC
MOL000924	0.9042	0.0958	0.9033	Curcumae Rhizoma	Mnk	8163	FALSE	CC(=O)CCCCCCCCC
MOL000924	0.9042	0.0958	0.9033	Zingiber Officinale Roscoe	Mnk	8163	FALSE	CC(=O)CCCCCCCCC
MOL000924	0.9042	0.0958	0.9033	Saururi Herba	Mnk	8163	FALSE	CC(=O)CCCCCCCCC
MOL000924	0.9042	0.0958	0.9033	Capsici Fructus	Mnk	8163	FALSE	CC(=O)CCCCCCCCC
MOL000924	0.9042	0.0958	0.9033	Mahoniae Folum	Mnk	8163	FALSE	CC(=O)CCCCCCCCC
MOL000924	0.9042	0.0958	0.9033	Allii Fistulost Bulbus	Mnk	8163	FALSE	CC(=O)CCCCCCCCC
MOL000924	0.9042	0.0958	0.9033	Phellodendri Amurensis Cortex	Mnk	8163	FALSE	CC(=O)CCCCCCCCC
MOL000924	0.9042	0.0958	0.9033	Houttuyniae Herba	Mnk	8163	FALSE	CC(=O)CCCCCCCCC
MOL000925	0.8553	0.1447	0.6660	Myrrha	δ-elemene	Not Available	FALSE	C1(=CC(C(CC1)(C)C=C)C(=C)C)C(C)C
MOL000925	0.8553	0.1447	0.6660	Curcumae Rhizoma	δ-elemene	Not Available	FALSE	C1(=CC(C(CC1)(C)C=C)C(=C)C)C(C)C
MOL000926	0.8298	0.1702	0.7447	Zingiberis Rhizoma	cis-beta-farnesene	5317319	FALSE	C=CC(=C)CC/C=C(\CCC=C(C)C)/C
MOL000926	0.8298	0.1702	0.7447	Broussonetiae Fructus	cis-beta-farnesene	5317319	FALSE	C=CC(=C)CC/C=C(\CCC=C(C)C)/C
MOL000926	0.8298	0.1702	0.7447	Farfarae Flos	cis-beta-farnesene	5317319	FALSE	C=CC(=C)CC/C=C(\CCC=C(C)C)/C
MOL000926	0.8298	0.1702	0.7447	Echinopsis Radix	cis-beta-farnesene	5317319	FALSE	C=CC(=C)CC/C=C(\CCC=C(C)C)/C
MOL000926	0.8298	0.1702	0.7447	Moslae Herba	cis-beta-farnesene	5317319	FALSE	C=CC(=C)CC/C=C(\CCC=C(C)C)/C
MOL000926	0.8298	0.1702	0.7447	Curcumae Rhizoma	cis-beta-farnesene	5317319	FALSE	C=CC(=C)CC/C=C(\CCC=C(C)C)/C
MOL000926	0.8298	0.1702	0.7447	Anisi Stellati Fructus	cis-beta-farnesene	5317319	FALSE	C=CC(=C)CC/C=C(\CCC=C(C)C)/C
MOL000927	0.8553	0.1447	0.6426	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	α-muurolene	Not Available	FALSE	C1(CC=C(C2CCC(=CC12)C)C)C(C)C
MOL000927	0.8553	0.1447	0.6426	Lysimachiae Herba	α-muurolene	Not Available	FALSE	C1(CC=C(C2CCC(=CC12)C)C)C(C)C
MOL000927	0.8553	0.1447	0.6426	Cinnanmomi Cortex	α-muurolene	Not Available	FALSE	C1(CC=C(C2CCC(=CC12)C)C)C(C)C
MOL000927	0.8553	0.1447	0.6426	Curcumae Rhizoma	α-muurolene	Not Available	FALSE	C1(CC=C(C2CCC(=CC12)C)C)C(C)C
MOL000927	0.8553	0.1447	0.6426	Meliae Azedarach Fructus	α-muurolene	Not Available	FALSE	C1(CC=C(C2CCC(=CC12)C)C)C(C)C
MOL000927	0.8553	0.1447	0.6426	Rhododendri Daurici Folium	α-muurolene	Not Available	FALSE	C1(CC=C(C2CCC(=CC12)C)C)C(C)C

MOL000929	0.8753	0.1247	0.7985	Platycladi Cacumen	(5S)-5-[(1R)-1,5-dimethylhex-4-enyl]-2-methylcyclohexa-1,3-diene	11127403	FALSE	C1=C(C=CC(C1)C(CCC=C(C)C)C)C
MOL000929	0.8753	0.1247	0.7985	Curcumaelongae Rhizoma	(5S)-5-[(1R)-1,5-dimethylhex-4-enyl]-2-methylcyclohexa-1,3-diene	11127403	FALSE	C1=C(C=CC(C1)C(CCC=C(C)C)C)C
MOL000929	0.8753	0.1247	0.7985	Piperis Longi Fructus	(5S)-5-[(1R)-1,5-dimethylhex-4-enyl]-2-methylcyclohexa-1,3-diene	11127403	FALSE	C1=C(C=CC(C1)C(CCC=C(C)C)C)C
MOL000929	0.8753	0.1247	0.7985	Curcumae Rhizoma	(5S)-5-[(1R)-1,5-dimethylhex-4-enyl]-2-methylcyclohexa-1,3-diene	11127403	FALSE	C1=C(C=CC(C1)C(CCC=C(C)C)C)C
MOL000930	0.8363	0.1637	0.7550	Ardisiae Japonicae Herba	cis-.alpha.-Farnesene	5362889	FALSE	C=C/C(=C\C/C=C(/CCC=C(C)C)\C)/C
MOL000930	0.8363	0.1637	0.7550	Curcumae Rhizoma	cis-.alpha.-Farnesene	5362889	FALSE	C=C/C(=C\C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Cinnanmomi Cortex	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Kadsurae Coccineae Radix Et Caulis	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Zingiber Officinale Roscoe	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Et Radix Patriniae Rhizoma	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Meliae Azedarach Fructus	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Curcumae Rhizoma	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Caryophylliflos	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C

MOL000932	0.8363	0.1637	0.7550	Ginseng Folium	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Dalbergiae Odoriferae Lignum	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Zingiberis Rhizoma	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Perillae Fructus	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Citri Reticulatae Folium	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Folium Nelumbinis	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Ligustici Rhizoma Et Radix	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Ephedra Herba	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Perilla Frutescens	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Citri Fructus Retinervus	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Radix Bupleuri	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Alpiniae Officinarum Rhizome	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Zanthoxyli Pericarpium	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Lysimachiae Herba	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Radix Salviae	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Piperis Longi Fructus	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Cnidii Fructus	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Solidaginis Herba	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Evodiae Fructus	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Piperis Fructus	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Myrrha	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C

MOL000932	0.8363	0.1637	0.7550	Sennae Folium	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000932	0.8363	0.1637	0.7550	Chuanxiong Rhizoma	alpha-Farnesene	5281516	FALSE	C=C/C(=C/C/C=C(/CCC=C(C)C)\C)/C
MOL000933	0.8614	0.1386	0.8269	Chuanxiong Rhizoma	.gamma.-Bisabolene	5352437	FALSE	C1C=C(CC/C/1=C(\CCC=C(C)C)/C)C
MOL000933	0.8614	0.1386	0.8269	Curcumae Rhizoma	.gamma.-Bisabolene	5352437	FALSE	C1C=C(CC/C/1=C(\CCC=C(C)C)/C)C
MOL000934	0.8711	0.1289	0.7791	Ginkgo Folium	β-seisquiphellandrene	Not Available	FALSE	CC(=CCCC(C)C1C=CC(=C)CC1)C
MOL000934	0.8711	0.1289	0.7791	Curcumae Rhizoma	β-seisquiphellandrene	Not Available	FALSE	CC(=CCCC(C)C1C=CC(=C)CC1)C
MOL000934	0.8711	0.1289	0.7791	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	β-seisquiphellandrene	Not Available	FALSE	CC(=CCCC(C)C1C=CC(=C)CC1)C
MOL000936	0.8616	0.1384	0.8179	Cnidii Fructus	Germacrene B	5281519	FALSE	C\1(=C/CC/C(=C/CC(=C(C)C)CC1)/C)/C
MOL000936	0.8616	0.1384	0.8179	Curcumae Rhizoma	Germacrene B	5281519	FALSE	C\1(=C/CC/C(=C/CC(=C(C)C)CC1)/C)/C
MOL000936	0.8616	0.1384	0.8179	Curcumae Radix	Germacrene B	5281519	FALSE	C\1(=C/CC/C(=C/CC(=C(C)C)CC1)/C)/C
MOL000936	0.8616	0.1384	0.8179	Myrrha	Germacrene B	5281519	FALSE	C\1(=C/CC/C(=C/CC(=C(C)C)CC1)/C)/C
MOL000936	0.8616	0.1384	0.8179	Viticis Negundo Folium	Germacrene B	5281519	FALSE	C\1(=C/CC/C(=C/CC(=C(C)C)CC1)/C)/C
MOL000936	0.8616	0.1384	0.8179	Bidentis Bipinnatae Herba	Germacrene B	5281519	FALSE	C\1(=C/CC/C(=C/CC(=C(C)C)CC1)/C)/C
MOL000936	0.8616	0.1384	0.8179	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Germacrene B	5281519	FALSE	C\1(=C/CC/C(=C/CC(=C(C)C)CC1)/C)/C
MOL000936	0.8616	0.1384	0.8179	Ailanthi Cortex	Germacrene B	5281519	FALSE	C\1(=C/CC/C(=C/CC(=C(C)C)CC1)/C)/C
MOL000936	0.8616	0.1384	0.8179	Asari Radix Et Rhizoma	Germacrene B	5281519	FALSE	C\1(=C/CC/C(=C/CC(=C(C)C)CC1)/C)/C
MOL000939	0.8484	0.1516	0.6928	Curcumae Rhizoma	(1S,3E,7E,11S)-1,5,5,8-tetramethyl-12-oxabicyclo[9.1.0]dodeca-3,7-diene	12900741	FALSE	C12(C/C=C/C(C/C=C(/CCC1O2)\C)(C)C)C
MOL000941	0.8991	0.1009	0.8310	Curcumae Rhizoma	Zingiberenol	Not Available	FALSE	C1(C=CC(CC1)C(CCC=C(C)C)C)(O)C

MOL000942	0.8265	0.1735	0.6775	Curcumae Rhizoma	(1R,4S,4aR,8aR)-4-isopropyl-1,6-dimethyl-3,4,4a,7,8,8a-hexahydro-2H-naphthalen-1-ol	10398656	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C
MOL000942	0.8265	0.1735	0.6775	Croci Stigma	(1R,4S,4aR,8aR)-4-isopropyl-1,6-dimethyl-3,4,4a,7,8,8a-hexahydro-2H-naphthalen-1-ol	10398656	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C
MOL000942	0.8265	0.1735	0.6775	Panax Ginseng C. A. Mey.	(1R,4S,4aR,8aR)-4-isopropyl-1,6-dimethyl-3,4,4a,7,8,8a-hexahydro-2H-naphthalen-1-ol	10398656	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C
MOL000942	0.8265	0.1735	0.6775	Radix Salviae	(1R,4S,4aR,8aR)-4-isopropyl-1,6-dimethyl-3,4,4a,7,8,8a-hexahydro-2H-naphthalen-1-ol	10398656	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C
MOL000943	0.8362	0.1638	0.7638	Magnolia Officinalis Rehd Et Wils.	epi-10-.gamma.-Eudesmol	6430754	FALSE	C1CC(=C2C(C1)(CCC(C2)C(C)(O)C)C)C
MOL000943	0.8362	0.1638	0.7638	Curcumae Radix	epi-10-.gamma.-Eudesmol	6430754	FALSE	C1CC(=C2C(C1)(CCC(C2)C(C)(O)C)C)C

MOL000943	0.8362	0.1638	0.7638	Curcumae Rhizoma	epi-10-.gamma.-Eudesmol	6430754	FALSE	C1CC(=C2C(C1)(CCC(C2)C(C)(O)C)C)C
MOL000944	0.8876	0.1124	0.8394	Curcumaelongae Rhizoma	(6R)-2-methyl-6-(4-methylphenyl)hept-2-en-4-one	11736067	FALSE	CC(=CC(=O)CC(C)c1ccc(cc1)C)C
MOL000944	0.8876	0.1124	0.8394	Dalbergiae Odoriferae Lignum	(6R)-2-methyl-6-(4-methylphenyl)hept-2-en-4-one	11736067	FALSE	CC(=CC(=O)CC(C)c1ccc(cc1)C)C
MOL000944	0.8876	0.1124	0.8394	Curcumae Rhizoma	(6R)-2-methyl-6-(4-methylphenyl)hept-2-en-4-one	11736067	FALSE	CC(=CC(=O)CC(C)c1ccc(cc1)C)C
MOL000946	0.5485	0.4515	0.6702	Curcumae Radix	demethoxycurcumin	5469424	FALSE	c1(ccc(cc1)/C=C/C(=O)CC(=O)/C=C/c1ccc(c(c1)OC)O)O
MOL000946	0.5485	0.4515	0.6702	Curcumaelongae Rhizoma	demethoxycurcumin	5469424	FALSE	c1(ccc(cc1)/C=C/C(=O)CC(=O)/C=C/c1ccc(c(c1)OC)O)O
MOL000947	0.8834	0.1166	0.8625	Curcumaelongae Rhizoma	(6Z,10S)-3-isopropylidene-6,10-dimethyl-cyclodec-6-ene-1,4-quinone	6442617	FALSE	C1(=O)CC(=C(C)C)C(=O)C/C(=C/CCC1C)/C
MOL000948	0.8670	0.1330	0.8516	Curcumaelongae Rhizoma	4-methoxy-5-hydroxybis	Not Available	FALSE	C(=O)(CC(C1CC(C(C=C1)(OC)C)O)C)C=C(C)C
MOL000949	0.9057	0.0943	0.8094	Curcumaelongae Rhizoma	(3S,3aS,8aR)-3-hydroxy-5-isopropylidene-3-methyl-8-methylene-2,3a,4,8a-tetrahydro-1H-azulen-6-one	14543198	FALSE	C1(CCC2C(=C)CC(=O)C(=C(C)C)CC12)(C)O

MOL000949	0.9057	0.0943	0.8094	Curcumae Radix	(3S,3aS,8aR)-3-hydroxy-5-isopropylidene-3-methyl-8-methylene-2,3a,4,8a-tetrahydro-1H-azulen-6-one	14543198	FALSE	C1(CCC2C(=C)CC(=O)C(=C(C)C)CC12)(C)O
MOL000950	0.7868	0.2132	0.7261	Curcumaelongae Rhizoma	ar-tumerone	Not Available	FALSE	C(=C)(CC(c1ccc(C)cc1)C)C=C(C)C
MOL000951	0.5470	0.4530	0.7508	Curcumaelongae Rhizoma	dihydrocurcumin	Not Available	FALSE	C(CC(=O)/C=C(/C=C\c1cc(c(cc1)O)OC)\O)c1cc(c(cc1)O)OC
MOL000952	0.9110	0.0890	0.7922	Curcumaelongae Rhizoma	(3S,3aS,8aS)-3-hydroxy-5-isopropylidene-3,8-dimethyl-2,3a,4,8a-tetrahydro-1H-azulen-6-one	10263440	FALSE	C1(CCC2C(=CC(=O)C(=C(C)C)CC12)C)(C)O
MOL000953	0.2185	0.7815	0.6135	Lycii Fructus	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Cassiae Semen	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Semen Lini	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Curcumaelongae Rhizoma	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Tamaricis Cacumen	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Rhizoma Dioscoreae	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Amygdalus Communis Vas	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Hippophae Fructus	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Carthami Flos	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Thalluslaminariae	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Coicis Semen	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O

MOL000953	0.2185	0.7815	0.6135	Perillae Fructus	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Isatdis Radix	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Calendula Officinalis	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Arisaematis Rhizoma	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Gynostemmae Pentaphylli Herba	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Corayceps	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Abrus Precatorius L.	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Mume Fructus	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Silybum Marianum	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Scutellariae Barbatae Herba	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Bovis Calculus	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Cuscutae Semen	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Solanum Nigrum Linn.	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Capsici Fructus	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Ranunculi Ternati Radix	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Aloe	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Bombyx Mori L.	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Melo Semen	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000953	0.2185	0.7815	0.6135	Lycii Cortex	CLR	5997	TRUE	C1(CCC2(C(=CCC3C4CCC(C(CCCC(C)C)C)C4(C)CCC23)C1)C)O
MOL000954	0.9025	0.0975	0.8750	Curcumaelongae Rhizoma	α-turmerone	Not Available	FALSE	CC(=CC(=O)CC(C)C1C=CC(=CC1)C)C
MOL000955	0.9087	0.0913	0.8818	Curcumaelongae Rhizoma	turmeronol A	Not Available	FALSE	CC(=CC(=O)CC(C)c1cc(c(cc1)C)O)C
MOL000955	0.9087	0.0913	0.8818	Curcumae Radix	turmeronol A	Not Available	FALSE	CC(=CC(=O)CC(C)c1cc(c(cc1)C)O)C

MOL000956	0.8822	0.1178	0.8604	Curcumaelongae Rhizoma	(6S)-2-methyl-6-[(1S)-4-methylene-1-cyclohex-2-enyl]hept-2-en-4-one	14287405	FALSE	CC(=CC(=O)CC(C)C1C=CC(=C)CC1)C
MOL000957	0.8619	0.1381	0.8526	Perilla Frutescens	(3R,6E,10S)-3-isopropyl-6,10-dimethylcyclodec-6-ene-1,4-dione	10466651	FALSE	C\1=C(/CC(=O)C(CC(=O)C(CC1)C)C(C)C)\C
MOL000957	0.8619	0.1381	0.8526	Curcumaelongae Rhizoma	(3R,6E,10S)-3-isopropyl-6,10-dimethylcyclodec-6-ene-1,4-dione	10466651	FALSE	C\1=C(/CC(=O)C(CC(=O)C(CC1)C)C(C)C)\C
MOL000958	0.9217	0.0783	0.8874	Curcumaelongae Rhizoma	2,5-dihydroxybisabola-3,10-diene	Not Available	FALSE	C(CC(C1CC(C=CC1O)O)C)C=C(C)C
MOL000959	0.8970	0.1030	0.8021	Curcumaelongae Rhizoma	zedoarondiol	24834047	FALSE	C1(CCC2C(CC(=O)C(=C(C)C)CC12)(C)O)(C)O
MOL000959	0.8970	0.1030	0.8021	Curcumae Radix	zedoarondiol	24834047	FALSE	C1(CCC2C(CC(=O)C(=C(C)C)CC12)(C)O)(C)O
MOL000960	0.8793	0.1207	0.7987	Curcumaelongae Rhizoma	procurcumadiol	14633012	FALSE	C1CC(C2(CC(=C(C)C)C(=O)C=C(C12)C)O)(C)O
MOL000960	0.8793	0.1207	0.7987	Curcumae Radix	procurcumadiol	14633012	FALSE	C1CC(C2(CC(=C(C)C)C(=O)C=C(C12)C)O)(C)O
MOL000961	0.9110	0.0890	0.7922	Curcumaelongae Rhizoma	(3S,3aS,8aR)-3-hydroxy-5-isopropylidene-3,8-dimethyl-2,3a,4,8a-tetrahydro-1H-azulen-6-one	189061	FALSE	C1(CCC2C(=CC(=O)C(=C(C)C)CC12)C)(C)O

MOL000961	0.9110	0.0890	0.7922	Curcumae Radix	(3S,3aS,8aR)-3-hydroxy-5-isopropylidene-3,8-dimethyl-2,3a,4,8a-tetrahydro-1H-azulen-6-one	189061	FALSE	C1(CCC2C(=CC(=O)C(=C(C)C)CC12)C)(C)O
MOL000962	0.9183	0.0817	0.8570	Curcumaelongae Rhizoma	(6S)-6-[(1R,4S,5S)-4,5-dihydroxy-4-methyl-1-cyclohex-2-enyl]-2-methylhept-2-en-4-one	14287397	FALSE	CC(=CC(=O)CC(C)C1C=CC(C(C1)O)(C)O)C
MOL000962	0.9183	0.0817	0.8570	Curcumae Radix	(6S)-6-[(1R,4S,5S)-4,5-dihydroxy-4-methyl-1-cyclohex-2-enyl]-2-methylhept-2-en-4-one	14287397	FALSE	CC(=CC(=O)CC(C)C1C=CC(C(C1)O)(C)O)C
MOL000963	0.8988	0.1012	0.8367	Curcumae Radix	bisacumol	Not Available	FALSE	c1c(ccc(c1)C(CC(C=C(C)C)O)C)C
MOL000963	0.8988	0.1012	0.8367	Curcumaelongae Rhizoma	bisacumol	Not Available	FALSE	c1c(ccc(c1)C(CC(C=C(C)C)O)C)C
MOL000964	0.6869	0.3131	0.6431	Curcumaelongae Rhizoma	4-hydroxybisabola-2,10-diene-9-one	Not Available	FALSE	C(=C)(CC(C1CCC(C=C1)(C)C)C)C=C(C)C
MOL000965	0.9189	0.0811	0.8628	Curcumaelongae Rhizoma	4,5-dihydroxybisabola-2,10-diene	Not Available	FALSE	C(CC(C1CC(C(C=C1)(O)C)O)C)C=C(C)C
MOL000966	0.9029	0.0971	0.8702	Curcumae Radix	turmeronol B	Not Available	FALSE	CC(=CC(=O)CC(C)c1c(cc(cc1)C)O)C
MOL000966	0.9029	0.0971	0.8702	Curcumaelongae Rhizoma	turmeronol B	Not Available	FALSE	CC(=CC(=O)CC(C)c1c(cc(cc1)C)O)C
MOL000968	0.8659	0.1341	0.8062	Panacis Quinquefolii Radix	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Cinnamomi Ramulus	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C

MOL000968	0.8659	0.1341	0.8062	Ephedra Herba	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Moslae Herba	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Junci Medulla	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Asari Radix Et Rhizoma	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Radix Angelicae Biseratae	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Verbenae Herb	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Viticis Negundo Folium	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Piperis Longi Fructus	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Ginseng Folium	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Aucklandiae Radix	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Zingiberis Rhizoma	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Folium Artemisiae Argyi	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Curcumaelongae Rhizoma	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Anisi Stellati Fructus	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Schisandrae Chinensis Fructus	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Curcumae Radix	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Magnoliae Flos	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Saposhnikoviae Radix	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Tamaricis Cacumen	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000968	0.8659	0.1341	0.8062	Panax Ginseng C. A. Mey.	beta-Bisabolene	68128	FALSE	C=C(CCC=C(C)C)C1CC=C(CC1)C
MOL000970	0.8822	0.1178	0.8604	Curcumae Radix	Curlone	Not Available	FALSE	CC(=CC(=O)CC(C)C1C=CC(=C)CC1)C

MOL000970	0.8822	0.1178	0.8604	Curcumaelongae Rhizoma	Curlone	Not Available	FALSE	CC(=CC(=O)CC(C)C1C=CC(=C)CC1)C
MOL000971	0.5346	0.4654	0.6149	Phytolaccae Radix	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Cornus Officinalis Sieb. Et Zucc.	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Eriobotryae Folium	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Folium Artemisiae Argyi	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Curculiginis Rhizome	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Dalbergiae Odoriferae Lignum	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Crotonis Fructus	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Ephedra Herba	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Cnidii Fructus	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Radix Cynanchi	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Trichosanthes Kirilowii Maxim	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Equiseti Hiemalis Herba	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Calyx Seu Fructus Physalis	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Toosendan Fructus	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Ginseng Folium	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Impatientis Semen	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Allii Fistulost Bulbus	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Capsici Fructus	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Saussureae Involucratae Herba	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCCC)OCC

MOL000971	0.5346	0.4654	0.6149	Ginkgo Folium	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Broussonetiae Fructus	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Morindae Officinalis Radix	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Millettiae Speciosae Radix	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Mahoniae Caulis	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Schizonepetae Spica	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Folium Nelumbinis	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Mahoniae Folum	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Curcumaelongae Rhizoma	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Chuanxiong Rhizoma	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Lycii Fructus	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Radix Cirsii Japonici	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Momordicae Fructus	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Ranunculi Ternati Radix	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Maydis Seigma	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Prunellae Spica	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Semen Firmianae	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Lonicerae Japonicae Flos	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Gynostemmae Pentaphylli Herba	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Gossampiniflos	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Arum Ternatum Thunb.	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC

MOL000971	0.5346	0.4654	0.6149	Isatdis Radix	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Hippophae Fructus	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Verbenae Herb	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Campsis Flos	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Saxifraga Stolonifera	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Coicis Semen	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Adenophprae Ae Radix	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Ardisiae Japonicae Herba	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000971	0.5346	0.4654	0.6149	Lygodii Spora	Ethylpalmitate	12366	FALSE	C(=O)(CCCCCCCCCCCCCCC)OCC
MOL000972	0.8689	0.1311	0.8712	Curcumaelongae Rhizoma	germacrone-13-al	Not Available	FALSE	C(=O)/C(=C\1/C(=O)C/C(=C/CC/C(=C/C1)/C)/C)/C
MOL000973	0.4373	0.5627	0.6910	Myrrha	8α-acetylfuranodiene	Not Available	FALSE	O=C(OC1C/C(=C/Cc2c(C/C(=C/1)/C)occ2C)/C)C
MOL000974	0.9628	0.0372	0.9395	Zanthoxyli Pericarpium	cuminal	326	FALSE	C(=O)c1ccc(cc1)C(C)C
MOL000974	0.9628	0.0372	0.9395	Ephedra Herba	cuminal	326	FALSE	C(=O)c1ccc(cc1)C(C)C
MOL000974	0.9628	0.0372	0.9395	Folium Artemisiae Argyi	cuminal	326	FALSE	C(=O)c1ccc(cc1)C(C)C
MOL000974	0.9628	0.0372	0.9395	Myrrha	cuminal	326	FALSE	C(=O)c1ccc(cc1)C(C)C
MOL000974	0.9628	0.0372	0.9395	Radix Angelicae Biseratae	cuminal	326	FALSE	C(=O)c1ccc(cc1)C(C)C
MOL000974	0.9628	0.0372	0.9395	Curcumae Radix	cuminal	326	FALSE	C(=O)c1ccc(cc1)C(C)C
MOL000974	0.9628	0.0372	0.9395	Olibanun	cuminal	326	FALSE	C(=O)c1ccc(cc1)C(C)C
MOL000974	0.9628	0.0372	0.9395	Linderae Radix	cuminal	326	FALSE	C(=O)c1ccc(cc1)C(C)C
MOL000974	0.9628	0.0372	0.9395	Magnolia Officinalis Rehd Et Wils.	cuminal	326	FALSE	C(=O)c1ccc(cc1)C(C)C
MOL000974	0.9628	0.0372	0.9395	Radix Bupleuri	cuminal	326	FALSE	C(=O)c1ccc(cc1)C(C)C
MOL000974	0.9628	0.0372	0.9395	Rubi Fructus	cuminal	326	FALSE	C(=O)c1ccc(cc1)C(C)C
MOL000974	0.9628	0.0372	0.9395	Angelicae Sinensis Radix	cuminal	326	FALSE	C(=O)c1ccc(cc1)C(C)C
MOL000975	0.8777	0.1223	0.6026	Myrrha	(E)-α-santalal	Not Available	FALSE	C12C3C1(C(C(C2)C3)(C)CC/C=C(/C)\C=O)C
MOL000976	0.7429	0.2571	0.8319	Myrrha	myrrhone	71349601	FALSE	C1(=O)CC(Cc2c1c(cc1c2c(co1)C)C)C
MOL000977	0.8114	0.1886	0.8130	Myrrha	furanogermacra-1E,10(15)-dien-6-one	Not Available	FALSE	C\1=C\C(=C)Cc2c(C(=O)CC(C1)C)c(co2)C

MOL000978	0.8081	0.1919	0.8175	Myrrha	furanoeudesma- 1,4-diene-6-one	Not Available	FALSE	C1=CC2(C(=C(C1)C)C(=O)c1c(C2)occ1C)C
MOL000979	0.7713	0.2287	0.7871	Myrrha	2-methoxyfuranoguaia-9-ene-8-one	Not Available	FALSE	C1(=CC(=O)c2c(C3C1C(CC3C)OC)occ2C)C
MOL000980	0.8581	0.1419	0.8103	Myrrha	(4S)-4-[(1Z)-1,5-dimethylhexa-1,4-dienyl]-1-methylcyclohexene	24798702	FALSE	C(=C(\C)/C1CCC(=CC1)C)/CC=C(C)C
MOL000980	0.8581	0.1419	0.8103	Cinnamomi Ramulus	(4S)-4-[(1Z)-1,5-dimethylhexa-1,4-dienyl]-1-methylcyclohexene	24798702	FALSE	C(=C(\C)/C1CCC(=CC1)C)/CC=C(C)C
MOL000981	0.4235	0.5765	0.6649	Myrrha	camphorene	Not Available	FALSE	C(C1=CCC(CC1)C(=C)CCC=C(C)C)CC=C(C)C
MOL000982	0.7946	0.2054	0.6419	Myrrha	isofuranogermacrene	Not Available	FALSE	C1(C(CC2=C(C1)CC=C2C)C(=C)C)(C=C)C
MOL000986	0.4331	0.5669	0.7622	Myrrha	1-Asarinine	101612	FALSE	c12c(ccc(c1)C1C3C(CO1)C(OC3)c1cc3c(cc1)OCO3)OCO2
MOL000986	0.4331	0.5669	0.7622	Zanthoxylum Nitidum	1-Asarinine	101612	FALSE	c12c(ccc(c1)C1C3C(CO1)C(OC3)c1cc3c(cc1)OCO3)OCO2
MOL000987	0.2427	0.7573	0.6138	Myrrha	cholesterol	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CCC1C(C)CCCC(C)C)C)C
MOL000988	0.2462	0.7538	0.8541	Myrrha	4,17(20)-(cis)-pregnadiene-3,16-dione	Not Available	FALSE	C1C(=O)C=C2C(C1)(C1C(CC2)C2C(CC1)(C(=C(C)C)C(=O)C2)C)C
MOL000989	0.2045	0.7955	0.6917	Myrrha	guggulsterol-I	Not Available	FALSE	C1C(=C)C=C2C(C1)(C1C(CC2)C2C(CC1)(C(C(C2)O)C(O)(C)C(O)CCC(C)C)C)C
MOL000990	0.2360	0.7640	0.7125	Myrrha	guggulsterol-II	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC(C1C(O)(C)CCCC(C)C)O)C)O
MOL000991	0.9278	0.0722	0.9097	Myrrha	cinnamaldehyde	637511	FALSE	C(=O)/C=C/c1ccccc1
MOL000991	0.9278	0.0722	0.9097	Cinnanmomi Cortex	cinnamaldehyde	637511	FALSE	C(=O)/C=C/c1ccccc1
MOL000991	0.9278	0.0722	0.9097	Ginkgo Folium	cinnamaldehyde	637511	FALSE	C(=O)/C=C/c1ccccc1

MOL000991	0.9278	0.0722	0.9097	Ardisiae Japonicae Herba	cinnamaldehyde	637511	FALSE	C(=O)/C=C/c1ccccc1
MOL000991	0.9278	0.0722	0.9097	Benzoinum	cinnamaldehyde	637511	FALSE	C(=O)/C=C/c1ccccc1
MOL000991	0.9278	0.0722	0.9097	Ephedra Herba	cinnamaldehyde	637511	FALSE	C(=O)/C=C/c1ccccc1
MOL000991	0.9278	0.0722	0.9097	Aucklandiae Radix	cinnamaldehyde	637511	FALSE	C(=O)/C=C/c1ccccc1
MOL000991	0.9278	0.0722	0.9097	Cinnamomi Ramulus	cinnamaldehyde	637511	FALSE	C(=O)/C=C/c1ccccc1
MOL000991	0.9278	0.0722	0.9097	Scutellariae Barbatae Herba	cinnamaldehyde	637511	FALSE	C(=O)/C=C/c1ccccc1
MOL000991	0.9278	0.0722	0.9097	Styrax	cinnamaldehyde	637511	FALSE	C(=O)/C=C/c1ccccc1
MOL000991	0.9278	0.0722	0.9097	Eriobotryae Folium	cinnamaldehyde	637511	FALSE	C(=O)/C=C/c1ccccc1
MOL000991	0.9278	0.0722	0.9097	Curcumae Radix	cinnamaldehyde	637511	FALSE	C(=O)/C=C/c1ccccc1
MOL000991	0.9278	0.0722	0.9097	Corayceps	cinnamaldehyde	637511	FALSE	C(=O)/C=C/c1ccccc1
MOL000992	0.1958	0.8042	0.7313	Myrrha	guggulsterol-III	Not Available	FALSE	C1C(=C)C=C2C(C1)(C1C(CC2)C2C(CC1)(C(C(C2)O)C(O)(C)CCCC(C)C)C)C
MOL000994	0.7385	0.2615	0.6541	Myrrha	(2S,3S,4R)-octadecane-1,2,3,4-tetrol	16046590	FALSE	C(C(C(C(CO)O)O)O)CCCCCCCCCCCCC
MOL000995	0.6559	0.3441	0.6078	Myrrha	eicosan-1,2,3,4-tetrol	Not Available	FALSE	C(C(C(CO)O)O)(O)CCCCCCCCCCCCCCCC
MOL000996	0.1940	0.8060	0.6772	Myrrha	Guggulsterol IV	Not Available	FALSE	C1C(=O)CC2(C(C1)(C1C(CC2=O)C2C(CC1)(C(CC2)C(C)CCCC(C)C)C)C)C
MOL000997	0.1772	0.8228	0.6937	Myrrha	guggulsterol V	51521444	FALSE	C1C(CC2(C(C1)(C1C(CC2OC(=O)C)C2C(CC1)(C(CC2)C(C)CCCC(C)C)C)C)O)O
MOL000998	0.9208	0.0792	0.7851	Codonopsis Radix	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-[(2R,3R,4S,5S)-3,4,5-trihydroxytetrahydropyran-2-yl]oxy-chromone	5317847	FALSE	c1(c(OC2OCC(C(C2O)O)O)c(=O)c2c(O)cc(O)cc2o1)c1cc(O)c(O)cc1

MOL000998	0.9208	0.0792	0.7851	Myrrha	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-[(2R,3R,4S,5S)-3,4,5-trihydroxytetrahydropyran-2-yl]oxy-chromone	5317847	FALSE	c1(c(OC2OCC(C(C2O)O)O)c(=O)c2c(O)cc(O)cc2o1)c1cc(O)c(O)cc1
MOL000999	0.9265	0.0735	0.8040	Myrrha	quercetin-3-O-β-D-galactoside	12304325	FALSE	c1(c(OC2OC(C(C(C2O)O)O)CO)c(=O)c2c(O)cc(O)cc2o1)c1cc(O)c(O)cc1
MOL001000	0.9133	0.0867	0.8176	Myrrha	quercetin-3-O-α-L-rhamnoside	12314859	FALSE	c1(c(OC2C(C(C(C(O2)C)O)O)O)c(=O)c2c(O)cc(O)cc2o1)c1cc(O)c(O)cc1
MOL001001	0.9345	0.0655	0.7751	Myrrha	quercetin-3-O-β-D-glucuronide	Not Available	FALSE	c1(c(OC2OC(C(C(C2O)O)O)O)c(=O)c2c(O)cc(O)cc2o1)c1cc(O)c(O)cc1
MOL001002	0.9305	0.0695	0.9000	Radix Paeoniae Rubra	ellagic acid	Not Available	TRUE	c1(c(c2c3c(c1)c(=O)oc1c3c(cc(c1O)O)c(=O)o2)O)O
MOL001002	0.9305	0.0695	0.9000	Juglandis Semen	ellagic acid	Not Available	TRUE	c1(c(c2c3c(c1)c(=O)oc1c3c(cc(c1O)O)c(=O)o2)O)O
MOL001002	0.9305	0.0695	0.9000	Choerospondiatis Fructus	ellagic acid	Not Available	TRUE	c1(c(c2c3c(c1)c(=O)oc1c3c(cc(c1O)O)c(=O)o2)O)O
MOL001002	0.9305	0.0695	0.9000	Myrrha	ellagic acid	Not Available	TRUE	c1(c(c2c3c(c1)c(=O)oc1c3c(cc(c1O)O)c(=O)o2)O)O
MOL001002	0.9305	0.0695	0.9000	Quisqualis Indica	ellagic acid	Not Available	TRUE	c1(c(c2c3c(c1)c(=O)oc1c3c(cc(c1O)O)c(=O)o2)O)O
MOL001002	0.9305	0.0695	0.9000	Rubi Fructus	ellagic acid	Not Available	TRUE	c1(c(c2c3c(c1)c(=O)oc1c3c(cc(c1O)O)c(=O)o2)O)O
MOL001002	0.9305	0.0695	0.9000	Granati Pericarpium	ellagic acid	Not Available	TRUE	c1(c(c2c3c(c1)c(=O)oc1c3c(cc(c1O)O)c(=O)o2)O)O
MOL001002	0.9305	0.0695	0.9000	Euphorbiae Humifusae Herba	ellagic acid	Not Available	TRUE	c1(c(c2c3c(c1)c(=O)oc1c3c(cc(c1O)O)c(=O)o2)O)O
MOL001002	0.9305	0.0695	0.9000	Phyllanthi Fructus	ellagic acid	Not Available	TRUE	c1(c(c2c3c(c1)c(=O)oc1c3c(cc(c1O)O)c(=O)o2)O)O
MOL001002	0.9305	0.0695	0.9000	Potentillae Chinensis Herba	ellagic acid	Not Available	TRUE	c1(c(c2c3c(c1)c(=O)oc1c3c(cc(c1O)O)c(=O)o2)O)O
MOL001002	0.9305	0.0695	0.9000	Chebulae Fructus	ellagic acid	Not Available	TRUE	c1(c(c2c3c(c1)c(=O)oc1c3c(cc(c1O)O)c(=O)o2)O)O
MOL001002	0.9305	0.0695	0.9000	Geranium Wilfordii Maxim.	ellagic acid	Not Available	TRUE	c1(c(c2c3c(c1)c(=O)oc1c3c(cc(c1O)O)c(=O)o2)O)O
MOL001002	0.9305	0.0695	0.9000	Canarii Fructus	ellagic acid	Not Available	TRUE	c1(c(c2c3c(c1)c(=O)oc1c3c(cc(c1O)O)c(=O)o2)O)O
MOL001002	0.9305	0.0695	0.9000	Bistortae Rhizoma	ellagic acid	Not Available	TRUE	c1(c(c2c3c(c1)c(=O)oc1c3c(cc(c1O)O)c(=O)o2)O)O
MOL001002	0.9305	0.0695	0.9000	Oroxyli Semen	ellagic acid	Not Available	TRUE	c1(c(c2c3c(c1)c(=O)oc1c3c(cc(c1O)O)c(=O)o2)O)O
MOL001002	0.9305	0.0695	0.9000	Agrimonia Eupatoria	ellagic acid	Not Available	TRUE	c1(c(c2c3c(c1)c(=O)oc1c3c(cc(c1O)O)c(=O)o2)O)O
MOL001006	0.2168	0.7832	0.6260	Codonopsis Radix	poriferasta-7,22E-dien-3beta-ol	5283663	FALSE	C1C(CC2C(C1)(C1C(=CC2)C2C(CC1)(C(CC2)C(/C=C/C(C(C)C)CC)C)C)C)O

MOL001006	0.2168	0.7832	0.6260	Myrrha	poriferasta-7,22E-dien-3beta-ol	5283663	FALSE	C1C(CC2C(C1)(C1C(=CC2)C2C(CC1)(C(CC2)C(/C=C/C(C(C)C)CC)C)C)C)O
MOL001006	0.2168	0.7832	0.6260	Benincasae Exocarpium	poriferasta-7,22E-dien-3beta-ol	5283663	FALSE	C1C(CC2C(C1)(C1C(=CC2)C2C(CC1)(C(CC2)C(/C=C/C(C(C)C)CC)C)C)C)O
MOL001006	0.2168	0.7832	0.6260	Achyranthis Bidentatae Radix	poriferasta-7,22E-dien-3beta-ol	5283663	FALSE	C1C(CC2C(C1)(C1C(=CC2)C2C(CC1)(C(CC2)C(/C=C/C(C(C)C)CC)C)C)C)O
MOL001007	0.1678	0.8322	0.6095	Myrrha	16β-hydroxy-4,17(20)Z-pregnadien-3-one	Not Available	FALSE	C1C(=C)C=C2C(C1)(C1C(CC2)C2C(CC1)(C(=C(C)C)C(C2)C)C)C
MOL001008	0.1743	0.8257	0.6810	Myrrha	20α-hydroxy-4-pregnen-3-one	Not Available	FALSE	C1C(=O)C=C2C(C1)(C1C(CC2)C2C(CC1)(C(CC2)C(C)(C)C)C)C
MOL001009	0.3727	0.6273	0.9401	Myrrha	guggulsterol-VI	69232409	FALSE	C1(=O)CCC2(C(=C1)CCC1C3CC(C(CC)C3(C)CCC21)O)C
MOL001012	0.2298	0.7702	0.7517	Myrrha	(5R,8R,9R,10R,13R,14R)-4,4,8,10,14-pentamethyl-1,2,5,6,7,9,11,12,13,15-decahydrocyclopenta[a]phenanthren-3-one	12071382	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2(C(CC1)C=CC2)C)C)C)(C)C
MOL001013	0.5019	0.4981	0.6486	Myrrha	mansumbinoic acid	Not Available	FALSE	C(CC1(C(C(=C)C)CCC2(C1CCC1C2(CC=C1)C)C)C)C(=O)O
MOL001014	0.9291	0.0709	0.9327	Myrrha	methylheptanone	Not Available	FALSE	CCC(=C)C(CCC)C
MOL001015	0.9586	0.0414	0.7752	Folium Artemisiae Argyi	ZINC00388662	6950273	FALSE	C1C2(C(CC(C1)C2(C)C)OC(=O)C)C
MOL001015	0.9586	0.0414	0.7752	Linderae Radix	ZINC00388662	6950273	FALSE	C1C2(C(CC(C1)C2(C)C)OC(=O)C)C
MOL001015	0.9586	0.0414	0.7752	Artemisia Annua L.	ZINC00388662	6950273	FALSE	C1C2(C(CC(C1)C2(C)C)OC(=O)C)C
MOL001015	0.9586	0.0414	0.7752	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	ZINC00388662	6950273	FALSE	C1C2(C(CC(C1)C2(C)C)OC(=O)C)C
MOL001015	0.9586	0.0414	0.7752	Myrrha	ZINC00388662	6950273	FALSE	C1C2(C(CC(C1)C2(C)C)OC(=O)C)C
MOL001016	0.9513	0.0487	0.7420	Myrrha	1,8-cineole	15775266	FALSE	C1CC2CCC1(CC2(C)C)C

MOL001017	0.9132	0.0868	0.8991	Campsis Flos	3,3,7-trimethylocta-1,6-diene	10986446	FALSE	CC(=CCCC(C=C)(C)C)C
MOL001017	0.9132	0.0868	0.8991	Violsse Herba	3,3,7-trimethylocta-1,6-diene	10986446	FALSE	CC(=CCCC(C=C)(C)C)C
MOL001017	0.9132	0.0868	0.8991	Myrrha	3,3,7-trimethylocta-1,6-diene	10986446	FALSE	CC(=CCCC(C=C)(C)C)C
MOL001017	0.9132	0.0868	0.8991	Sennae Folium	3,3,7-trimethylocta-1,6-diene	10986446	FALSE	CC(=CCCC(C=C)(C)C)C
MOL001018	0.9272	0.0728	0.8978	Myrrha	1-allyl-4-ethylbenzene	2758890	FALSE	c1cc(ccc1CC)CC=C
MOL001019	0.4157	0.5843	0.9073	Myrrha	(7S,8R,9S,10R,13S,14S,17Z)-17-ethylidene-7-hydroxy-10,13-dimethyl-1,2,6,7,8,9,11,12,14,15-decahydrocyclopenta[a]phenanthrene-3,16-dione	10496532	FALSE	C1C(=O)C=C2C(C1)(C1C(C(C2)O)C2C(CC1)(/C(=C/C)/C(=O)C2)C)C
MOL001020	0.4386	0.5614	0.9284	Myrrha	(7S,8S,9S,10R,13S,14S,17R)-17-ethyl-7-hydroxy-10,13-dimethyl-2,6,7,8,9,11,12,14,15,17-decahydro-1H-cyclopenta[a]phenanthrene-3,16-dione	10711515	FALSE	C1C(=O)C=C2C(C1)(C1C(C(C2)O)C2C(CC1)(C(C(=O)C2)CC)C)C

MOL001021	0.3111	0.6889	0.9073	Myrrha	7β,15β-dihydroxypregn-4-ene-3,16-dione	Not Available	FALSE	C1C(=O)C=C2C(C1)(C1C(C(C2)O)C2C(CC1)(C(C(=O)C2C)CC)C)C
MOL001022	0.2018	0.7982	0.8461	Myrrha	11α-hydroxypregna-4,17(20)-trans-diene-3,16-dione	Not Available	FALSE	C1C(=O)C=C2C(C1)(C1C(CC2)C2C(CC1C)(/C(=C\C)/C(=O)C2)C)C
MOL001023	0.4326	0.5674	0.8957	Myrrha	(8S,9S,10R,11R,13S,14S,17E)-17-ethylidene-11-hydroxy-10,13-dimethyl-1,2,6,7,8,9,11,12,14,15-decahydrocyclopenta[a]phenanthrene-3,16-dione	10568300	FALSE	C1C(=O)C=C2C(C1)(C1C(CC2)C2C(CC1O)(/C(=C\C)/C(=O)C2)C)C
MOL001024	0.5602	0.4398	0.9113	Myrrha	(8R,9S,10R,11R,13S,14S,15S,17E)-17-ethylidene-11,15-dihydroxy-10,13-dimethyl-1,2,6,7,8,9,11,12,14,15-decahydrocyclopenta[a]phenanthrene-3,16-dione	10831307	FALSE	C1C(=O)C=C2C(C1)(C1C(CC2)C2C(CC1O)(/C(=C\C)/C(=O)C2O)C)C
MOL001030	0.9378	0.0622	0.8872	Myrrha	Propenylbenzene	252325	FALSE	c1ccc(cc1)/C=C/C
MOL001031	0.2695	0.7305	0.7312	Myrrha	epimansumbinol	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C=CC2)C)C)C)(C)C)O
MOL001036	0.2312	0.7688	0.9018	Myrrha	Guggulsterone-M	Not Available	FALSE	C1C(=O)C=C2C(C1)(C1C(CC2)C2C(CC1)(/C(=C(\C)/OC)/C(=O)C2)C)C

MOL001037	0.2527	0.7473	0.8945	Myrrha	dehydroguggulsterone-M	Not Available	FALSE	C1=CC2(C(=CC1=O)CCC1C2CCC2(C1CC(=O)/C/2=C(\C)/OC)C)C
MOL001038	0.2962	0.7038	0.6596	Myrrha	guggulsterol-Y	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC(C1C(CCCC(C)(C)O)(C)O)O)C)O
MOL001040	0.9396	0.0604	0.8008	Scutellariae Barbatae Herba	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	667495	TRUE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL001040	0.9396	0.0604	0.8008	Pollen Typhae	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	667495	TRUE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL001040	0.9396	0.0604	0.8008	Euonymi Alati Ramulus	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	667495	TRUE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL001040	0.9396	0.0604	0.8008	Nardostachyos Radix Et Rhizoma	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	667495	TRUE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL001040	0.9396	0.0604	0.8008	Choerospondiatis Fructus	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	667495	TRUE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL001040	0.9396	0.0604	0.8008	Sophorae Flavescentis Radix	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	667495	TRUE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O

MOL001040	0.9396	0.0604	0.8008	Flos Genkwa	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	667495	TRUE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL001040	0.9396	0.0604	0.8008	Mume Fructus	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	667495	TRUE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL001040	0.9396	0.0604	0.8008	Myrrha	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	667495	TRUE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL001040	0.9396	0.0604	0.8008	Drynariae Rhizoma	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	667495	TRUE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL001040	0.9396	0.0604	0.8008	Fortunes Bossfern Rhizome	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	667495	TRUE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL001040	0.9396	0.0604	0.8008	Dalbergiae Odoriferae Lignum	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	667495	TRUE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL001040	0.9396	0.0604	0.8008	Polygoni Orientalis Fructus	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	667495	TRUE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O

MOL001040	0.9396	0.0604	0.8008	Strychni Semen	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	667495	TRUE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL001040	0.9396	0.0604	0.8008	Citri Exocarpium Rubrum	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	667495	TRUE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL001040	0.9396	0.0604	0.8008	Folium Artemisiae Argyi	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	667495	TRUE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL001044	0.3357	0.6643	0.9526	Myrrha	pregn-4-ene-3,16-dione	Not Available	FALSE	C1C(=O)C=C2C(C1)(C1C(CC2)C2C(CC1)(C(C(=O)C2)CC)C)C
MOL001047	0.4691	0.5309	0.6726	Myrrha	(+)-Epiexcelsin	489948	FALSE	c12c(cc(cc1OC)C1C3C(CO1)C(OC3)c1cc(c3c(c1)OCO3)OC)OCO2
MOL001048	0.2876	0.7124	0.7191	Myrrha	16-hydroperoxymansumbin-13(17)- en-3-one	Not Available	FALSE	C1C(=C)C(C2C(C1)(C1C(CC2)(C2(C(CC1)C=C(C2)OO)C)C)C)(C)C
MOL001049	0.3873	0.6127	0.8009	Myrrha	16-hydroperoxymansumbin-13(17)-en-3β-ol	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C=C(C2)OO)C)C)C)(C)C)O
MOL001050	0.8856	0.1144	0.9569	Myrrha	CRS	342	FALSE	c1ccc(cc1O)C
MOL001050	0.8856	0.1144	0.9569	Bomboo Juice	CRS	342	FALSE	c1ccc(cc1O)C
MOL001050	0.8856	0.1144	0.9569	Sojae Semen Nigrum	CRS	342	FALSE	c1ccc(cc1O)C
MOL001050	0.8856	0.1144	0.9569	Arisaematis Rhizoma	CRS	342	FALSE	c1ccc(cc1O)C
MOL001050	0.8856	0.1144	0.9569	Cassiae Semen	CRS	342	FALSE	c1ccc(cc1O)C
MOL001050	0.8856	0.1144	0.9569	Aucklandiae Radix	CRS	342	FALSE	c1ccc(cc1O)C
MOL001050	0.8856	0.1144	0.9569	Radix Angelicae Biseratae	CRS	342	FALSE	c1ccc(cc1O)C

MOL001051	0.6043	0.3957	0.6904	Myrrha	16-hydroperoxy-3,4-seco-mansumbin-3(28),13(17)-dien-3-oic acid	Not Available	FALSE	C(C(=O)O)CC1(C(C(=C)C)CCC2(C1CCC1C2(CC(=C1)OO)C)C)C
MOL001052	0.2395	0.7605	0.8481	Myrrha	mansumbin-13(17)-en-3,16-dione	Not Available	FALSE	C1CC2(C(C(C1=O)(C)C)CCC1(C2CCC2=CC(=O)CC12C)C)C
MOL001053	0.3058	0.6942	0.8352	Myrrha	3β-hydroxymansumbin-13(17)-en-16-one	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC(=O)C2)CC1)C)C)C)(C)C)O
MOL001055	0.9537	0.0463	0.7528	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C
MOL001055	0.9537	0.0463	0.7528	Evodiae Fructus	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C
MOL001055	0.9537	0.0463	0.7528	Coriandri Sativi Herba	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C
MOL001055	0.9537	0.0463	0.7528	Platycladi Cacumen	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C
MOL001055	0.9537	0.0463	0.7528	Asari Radix Et Rhizoma	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C

MOL001055	0.9537	0.0463	0.7528	Olibanun	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C
MOL001055	0.9537	0.0463	0.7528	Sesami Nigrum Semen	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C
MOL001055	0.9537	0.0463	0.7528	Notopterygii Rhizoma Et Radix	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C
MOL001055	0.9537	0.0463	0.7528	Viticis Fructus	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C
MOL001055	0.9537	0.0463	0.7528	Radix Salviae	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C
MOL001055	0.9537	0.0463	0.7528	Menthae Herba	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C
MOL001055	0.9537	0.0463	0.7528	Citri Sarcodactylis Fructus	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C
MOL001055	0.9537	0.0463	0.7528	Viticis Negundo Folium	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C

MOL001055	0.9537	0.0463	0.7528	Magnoliae Flos	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C
MOL001055	0.9537	0.0463	0.7528	Chrysanthemi Flos	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C
MOL001055	0.9537	0.0463	0.7528	Zingiberis Rhizoma	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C
MOL001055	0.9537	0.0463	0.7528	Myrrha	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C
MOL001055	0.9537	0.0463	0.7528	Lysimachiae Herba	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C
MOL001055	0.9537	0.0463	0.7528	Chuanxiong Rhizoma	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C
MOL001055	0.9537	0.0463	0.7528	Piperis Fructus	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C
MOL001055	0.9537	0.0463	0.7528	Citrus Reticulata	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C

MOL001055	0.9537	0.0463	0.7528	Rubi Fructus	5-isopropyl-2-methylbicyclo[3.1.0]hex-2-ene	637518	FALSE	C1(=CCC2(C1C2)C(C)C)C
MOL001057	0.8670	0.1330	0.7405	Myrrha	2- methyl-5-(5 ' -hydroxy-1 ' ,5 ' -dimethyl-3 ' -hexenyl)phenol	Not Available	FALSE	c1cc(cc(c1C)O)C(C)C/C=C/C(C)(C)C
MOL001058	0.5781	0.4219	0.8501	Myrrha	picropolygamain	Not Available	FALSE	c12c(cc3c(c1)CC1C(C3c3cc4c(cc3)OCO4)C(=O)OC1)OCO2
MOL001059	0.9086	0.0914	0.9013	Myrrha	isolinalyl acetate	Not Available	FALSE	CC(=C)CCCC(OC(=O)C)(C=C)C
MOL001060	0.2695	0.7305	0.7312	Myrrha	mansumbinol	12071383	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C=CC2)C)C)C)(C)C)O
MOL001061	0.1869	0.8131	0.7773	Myrrha	(16S, 20R)-dihydroxydammar-24-en-3-one	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(C(C2)(O)C)C(C)(O)CCC=C(C)C)C)C)(C)C
MOL001062	0.1892	0.8108	0.6766	Myrrha	15α-hydroxymansumbinone	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2(C(CC1)C=CC2C)C)C)C)(C)C
MOL001063	0.1533	0.8467	0.7774	Myrrha	28-acetoxy-15α-hydroxymansumbinone	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2(C(CC1)C=CC2O)C)C)C)(C)COC(=O)CC
MOL001064	0.9020	0.0980	0.8241	Myrrha	3-[(E,1R)-5-hydroxy-1,5-dimethyl-hex-3-enyl]-6-methyl-pyrocatechol	11021311	FALSE	c1cc(c(c(c1C)O)O)C(C)C/C=C/C(C)(C)O
MOL001065	0.9329	0.0671	0.7389	Myrrha	2-methyl- 5-(4'(S)-hydroxy 1'(R),5'-dimethylhex-5'-enyl)-phenol	Not Available	FALSE	c1cc(cc(c1C)O)C(C)CCC(C(=C)C)O

MOL001066	0.2439	0.7561	0.6858	Myrrha	3β,16 β,20(S),25-tetrahydroxydammar-23-ene	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(C(C2)O)C(O)(C)C/C=C\C(C)(C)O)C)C)C)(C)C)O
MOL001067	0.1916	0.8084	0.7176	Myrrha	3β-acetoxy-16 β,20(S),25-trihydroxydammar-23-ene	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(C(C2)O)C(O)(C)C/C=C/C(C)(C)O)C)C)(C)C)OC(=C)C
MOL001068	0.2264	0.7736	0.7810	Myrrha	3β,16β,20(R)-trihydroxydammar-24-ene	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(C(C2)O)C(C)(O)C/C=C/C(C)C)C)C)(C)C)O
MOL001069	0.1930	0.8070	0.7298	Myrrha	3β-acetoxy-16 β,20(R)-dihydroxydammar-24-ene	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(C(C2)O)C(C)(O)C/C=C/C(C)C)C)C)(C)C)OC(=C)C
MOL001070	0.3521	0.6479	0.7433	Myrrha	3-epi-lupenyl acetate	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=C)C)C)C)C)(C)C)(C)OC(=O)C
MOL001071	0.7487	0.2513	0.8599	Myrrha	methyl commate B	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1C)C)C)C)C)(C(=O)O)C)O
MOL001072	0.7465	0.2535	0.7683	Myrrha	methyl commate C	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C)C)C)(C)C(=O)O)O)O
MOL001073	0.6793	0.3207	0.8060	Myrrha	methyl commate D	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1C)C)C)C)C)(C)C(=O)O)O)C
MOL001074	0.7503	0.2497	0.7994	Myrrha	methyl commate E	Not Available	FALSE	C1(C(C(C2C(C1C)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1C)C)C)C)C)(C)C(=O)O)O)O
MOL001075	0.8860	0.1140	0.7557	Myrrha	cadinanetriol	Not Available	FALSE	C1C(C(C2C(C1)C(CCC2C(C)C)(C)O)O)(C)O
MOL001076	0.8704	0.1296	0.7910	Myrrha	guaiane	Not Available	FALSE	C12C(C(C(CCC1(C)O)C(C)C)O)C(=C)CC2
MOL001077	0.8583	0.1417	0.7720	Myrrha	3α- Hydroxy-T-cadinol	44566715	FALSE	C1(C(=CC2C(C1)C(CCC2C(C)C)(O)C)C)O
MOL001078	0.9051	0.0949	0.8097	Myrrha	3-oxo-T-cadinol	Not Available	FALSE	C1(=O)C(=CC2C(C1)C(CCC2C(C)C)(O)C)C
MOL001079	0.4016	0.5984	0.7287	Myrrha	lupeone	Not Available	FALSE	C1C(=C)C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=C)C)C)C)C)(C)C
MOL001081	0.8544	0.1456	0.7963	Myrrha	eudesm-4(15)-ene-1β,6α-diol	14137571	FALSE	C1CC(=C)C2C(C1O)(CCC(C2O)C(C)C)C
MOL001082	0.7615	0.2385	0.7680	Myrrha	α-oxobisabolene	Not Available	FALSE	C(CC=C(C)C)C(C1CCC(=CC1=C)C)C
MOL001085	0.7932	0.2068	0.6633	Myrrha	α-bisabolol	Not Available	FALSE	C(CC=C(C)C)C(C1CCC(=CC1)C)(C)C
MOL001086	0.9420	0.0580	0.9186	Myrrha	DMT	8441	FALSE	c1cc(ccc1C(=O)OC)C(=O)OC
MOL001086	0.9420	0.0580	0.9186	Ligustici Rhizoma Et Radix	DMT	8441	FALSE	c1cc(ccc1C(=O)OC)C(=O)OC

MOL001087	0.4918	0.5082	0.6641	Myrrha	3-epi-α-amirin	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1C)C)C)C)C)(C)C)(C)C
MOL001088	0.3450	0.6550	0.7026	Myrrha	1α-acetoxy-9,19-cyclolanost-24-en-3β-ol	Not Available	FALSE	C1C(C(C2C3(C1OC(=C)C)C1(C(CC2)C2(C(CC1)(C(CC2)C(C)CCC=C(C)C)C)C)C3)(C)C)O
MOL001089	0.2325	0.7675	0.6497	Myrrha	29-norlanost-8,24-dien-1α,2α,3β- triol	Not Available	FALSE	C1(C(C(C2C(C1O)(C1=C(CC2)C2(C(CC1)(C(CC2)C(C)CCC=C(C)C)C)C)C)O)O
MOL001090	0.4084	0.5916	0.7243	Myrrha	2 α , 3 β , 2 3 - trihydroxyolean-12-ene	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C)C)C)(CO)C)O)O
MOL001091	0.4263	0.5737	0.7145	Myrrha	lupeol	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=C)C)C)C)C)(C)C)C
MOL001092	0.1872	0.8128	0.6993	Myrrha	[(3R,5R,8R,9R,10R,13R,14R,17S)-17-[(2S,5S)-5-(2-hydroxypropan-2-yl)-2-methyloxolan-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-yl] acetate	12019028	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C1(CCC(O1)C(C)(C)O)C)C)C)(C)C)OC(=O)C
MOL001093	0.2014	0.7986	0.7339	Myrrha	cabraleone	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C1(CCC(O1)C(C)(C)O)C)C)C)(C)C
MOL001094	0.2728	0.7272	0.6957	Myrrha	cabraleadiol	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C1(CCC(O1)C(C)(C)O)C)C)C)(C)C)(O)C
MOL001095	0.2044	0.7956	0.7280	Myrrha	isofouquieron e	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(C)(O)C/C=C/C(C)(C)C)C)C)(C)C
MOL001096	0.4152	0.5848	0.6833	Myrrha	α-amirone	Not Available	FALSE	C1C(=C)C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1C)C)C)C)C)(C)C
MOL001097	0.9171	0.0829	0.9273	Magnolia Officinalis Rehd Et Wils.	o-xylene	7237	FALSE	c1cccc(c1C)C

MOL001097	0.9171	0.0829	0.9273	Radix Cirsii Japonici	o-xylene	7237	FALSE	c1cccc(c1C)C
MOL001097	0.9171	0.0829	0.9273	Capsici Fructus	o-xylene	7237	FALSE	c1cccc(c1C)C
MOL001097	0.9171	0.0829	0.9273	licorice	o-xylene	7237	FALSE	c1cccc(c1C)C
MOL001097	0.9171	0.0829	0.9273	Myrrha	o-xylene	7237	FALSE	c1cccc(c1C)C
MOL001097	0.9171	0.0829	0.9273	Thalluslaminariae	o-xylene	7237	FALSE	c1cccc(c1C)C
MOL001097	0.9171	0.0829	0.9273	Carthami Flos	o-xylene	7237	FALSE	c1cccc(c1C)C
MOL001097	0.9171	0.0829	0.9273	Gynostemmae Pentaphylli Herba	o-xylene	7237	FALSE	c1cccc(c1C)C
MOL001097	0.9171	0.0829	0.9273	Radix Angelicae Biseratae	o-xylene	7237	FALSE	c1cccc(c1C)C
MOL001097	0.9171	0.0829	0.9273	Sterculiae Lychnophorae Semen	o-xylene	7237	FALSE	c1cccc(c1C)C
MOL001097	0.9171	0.0829	0.9273	Chaenomeles Sinensis (Thouin) Koehne	o-xylene	7237	FALSE	c1cccc(c1C)C
MOL001097	0.9171	0.0829	0.9273	Ginseng Folium	o-xylene	7237	FALSE	c1cccc(c1C)C
MOL001098	0.9005	0.0995	0.9077	Eriobotryae Folium	m-xylene	7929	FALSE	c1ccc(cc1C)C
MOL001098	0.9005	0.0995	0.9077	Perillae Fructus	m-xylene	7929	FALSE	c1ccc(cc1C)C
MOL001098	0.9005	0.0995	0.9077	Arisaematis Rhizoma	m-xylene	7929	FALSE	c1ccc(cc1C)C
MOL001098	0.9005	0.0995	0.9077	Sesami Nigrum Semen	m-xylene	7929	FALSE	c1ccc(cc1C)C
MOL001098	0.9005	0.0995	0.9077	Curcumae Radix	m-xylene	7929	FALSE	c1ccc(cc1C)C
MOL001098	0.9005	0.0995	0.9077	Ginseng Folium	m-xylene	7929	FALSE	c1ccc(cc1C)C
MOL001098	0.9005	0.0995	0.9077	Myrrha	m-xylene	7929	FALSE	c1ccc(cc1C)C
MOL001098	0.9005	0.0995	0.9077	Momordicae Fructus	m-xylene	7929	FALSE	c1ccc(cc1C)C
MOL001098	0.9005	0.0995	0.9077	Sojae Semen Nigrum	m-xylene	7929	FALSE	c1ccc(cc1C)C
MOL001098	0.9005	0.0995	0.9077	licorice	m-xylene	7929	FALSE	c1ccc(cc1C)C
MOL001098	0.9005	0.0995	0.9077	Typhonii Rhizoma	m-xylene	7929	FALSE	c1ccc(cc1C)C
MOL001099	0.9228	0.0772	0.9345	Mori Fructus	p-xylene	7809	FALSE	c1cc(ccc1C)C
MOL001099	0.9228	0.0772	0.9345	Carthami Flos	p-xylene	7809	FALSE	c1cc(ccc1C)C
MOL001099	0.9228	0.0772	0.9345	Panacis Japonici Rhizoma	p-xylene	7809	FALSE	c1cc(ccc1C)C
MOL001099	0.9228	0.0772	0.9345	Ephedra Herba	p-xylene	7809	FALSE	c1cc(ccc1C)C
MOL001099	0.9228	0.0772	0.9345	Oroxyli Semen	p-xylene	7809	FALSE	c1cc(ccc1C)C
MOL001099	0.9228	0.0772	0.9345	Rubi Fructus	p-xylene	7809	FALSE	c1cc(ccc1C)C
MOL001099	0.9228	0.0772	0.9345	Maydis Seigma	p-xylene	7809	FALSE	c1cc(ccc1C)C
MOL001099	0.9228	0.0772	0.9345	Flos Genkwa	p-xylene	7809	FALSE	c1cc(ccc1C)C
MOL001099	0.9228	0.0772	0.9345	Arisaematis Rhizoma	p-xylene	7809	FALSE	c1cc(ccc1C)C
MOL001099	0.9228	0.0772	0.9345	Sesami Nigrum Semen	p-xylene	7809	FALSE	c1cc(ccc1C)C
MOL001099	0.9228	0.0772	0.9345	Chaenomeles Sinensis (Thouin) Koehne	p-xylene	7809	FALSE	c1cc(ccc1C)C
MOL001099	0.9228	0.0772	0.9345	Myrrha	p-xylene	7809	FALSE	c1cc(ccc1C)C
MOL001099	0.9228	0.0772	0.9345	licorice	p-xylene	7809	FALSE	c1cc(ccc1C)C
MOL001099	0.9228	0.0772	0.9345	Eriobotryae Folium	p-xylene	7809	FALSE	c1cc(ccc1C)C
MOL001100	0.8928	0.1072	0.8795	Myrrha	Decatriene	6365714	FALSE	C(CC/C=C/C=C/C=C)C
MOL001101	0.9188	0.0812	0.9182	Citrus Reticulata	alpha-Ocimene	5320249	FALSE	C(=C)(CC/C=C(/C=C)\C)C

MOL001101	0.9188	0.0812	0.9182	Myrrha	alpha-Ocimene	5320249	FALSE	C(=C)(CC/C=C(/C=C)\C)C
MOL001101	0.9188	0.0812	0.9182	Lilii Bulbus	alpha-Ocimene	5320249	FALSE	C(=C)(CC/C=C(/C=C)\C)C
MOL001101	0.9188	0.0812	0.9182	Citrus Aurantium	alpha-Ocimene	5320249	FALSE	C(=C)(CC/C=C(/C=C)\C)C
MOL001101	0.9188	0.0812	0.9182	Ligustici Rhizoma Et Radix	alpha-Ocimene	5320249	FALSE	C(=C)(CC/C=C(/C=C)\C)C
MOL001102	0.9052	0.0948	0.9218	Myrrha	2,6-Dimethylhepta-1,5-diene	81203	FALSE	C(CC=C(C)C)C(=C)C
MOL001103	0.9139	0.0861	0.9101	Myrrha	[(3R)-3,7-dimethylocta-1,6-dien-3-yl] acetate	442474	FALSE	C(OC(=O)C)(CCC=C(C)C)(C=C)C
MOL001103	0.9139	0.0861	0.9101	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	[(3R)-3,7-dimethylocta-1,6-dien-3-yl] acetate	442474	FALSE	C(OC(=O)C)(CCC=C(C)C)(C=C)C
MOL001103	0.9139	0.0861	0.9101	Ephedra Herba	[(3R)-3,7-dimethylocta-1,6-dien-3-yl] acetate	442474	FALSE	C(OC(=O)C)(CCC=C(C)C)(C=C)C
MOL001103	0.9139	0.0861	0.9101	Viticis Fructus	[(3R)-3,7-dimethylocta-1,6-dien-3-yl] acetate	442474	FALSE	C(OC(=O)C)(CCC=C(C)C)(C=C)C
MOL001103	0.9139	0.0861	0.9101	Coriandri Sativi Herba	[(3R)-3,7-dimethylocta-1,6-dien-3-yl] acetate	442474	FALSE	C(OC(=O)C)(CCC=C(C)C)(C=C)C
MOL001103	0.9139	0.0861	0.9101	Rhizome Of Whiteback Greenbrier	[(3R)-3,7-dimethylocta-1,6-dien-3-yl] acetate	442474	FALSE	C(OC(=O)C)(CCC=C(C)C)(C=C)C
MOL001103	0.9139	0.0861	0.9101	Centipedae Herba	[(3R)-3,7-dimethylocta-1,6-dien-3-yl] acetate	442474	FALSE	C(OC(=O)C)(CCC=C(C)C)(C=C)C
MOL001103	0.9139	0.0861	0.9101	Herba Sarcandrae	[(3R)-3,7-dimethylocta-1,6-dien-3-yl] acetate	442474	FALSE	C(OC(=O)C)(CCC=C(C)C)(C=C)C

MOL001103	0.9139	0.0861	0.9101	Artemisia Annua L.	[(3R)-3,7-dimethylocta-1,6-dien-3-yl] acetate	442474	FALSE	C(OC(=O)C)(CCC=C(C)C)(C=C)C
MOL001103	0.9139	0.0861	0.9101	Radix Salviae	[(3R)-3,7-dimethylocta-1,6-dien-3-yl] acetate	442474	FALSE	C(OC(=O)C)(CCC=C(C)C)(C=C)C
MOL001105	0.9105	0.0895	0.6495	Myrrha	(+)-aromadendrene	Not Available	FALSE	C12C(C3C(CCC1=C)C3)C(CC2)C
MOL001106	0.9129	0.0871	0.7039	Myrrha	ledene	Not Available	FALSE	C12=C(CCC3C(C1C(CC2)C)C3)C
MOL001108	0.9141	0.0859	0.8397	Myrrha	(E)-isoeugenol	Not Available	FALSE	c1cc(cc(c1C)CC)/C=C\C
MOL001109	0.9619	0.0381	0.7507	Mori Fructus	β-thujene	Not Available	FALSE	C1(C=CC2(C1C2)C(C)C)C
MOL001109	0.9619	0.0381	0.7507	Radix Bupleuri	β-thujene	Not Available	FALSE	C1(C=CC2(C1C2)C(C)C)C
MOL001109	0.9619	0.0381	0.7507	Myrrha	β-thujene	Not Available	FALSE	C1(C=CC2(C1C2)C(C)C)C
MOL001110	0.9237	0.0763	0.9230	Magnolia Officinalis Rehd Et Wils.	cis-beta-Ocimene	5320250	FALSE	C(=C(\C=C)/C)\CC=C(C)C
MOL001110	0.9237	0.0763	0.9230	Citrus Reticulata	cis-beta-Ocimene	5320250	FALSE	C(=C(\C=C)/C)\CC=C(C)C
MOL001110	0.9237	0.0763	0.9230	Evodiae Fructus	cis-beta-Ocimene	5320250	FALSE	C(=C(\C=C)/C)\CC=C(C)C
MOL001110	0.9237	0.0763	0.9230	Campsis Flos	cis-beta-Ocimene	5320250	FALSE	C(=C(\C=C)/C)\CC=C(C)C
MOL001110	0.9237	0.0763	0.9230	Olibanun	cis-beta-Ocimene	5320250	FALSE	C(=C(\C=C)/C)\CC=C(C)C
MOL001110	0.9237	0.0763	0.9230	Zanthoxyli Pericarpium	cis-beta-Ocimene	5320250	FALSE	C(=C(\C=C)/C)\CC=C(C)C
MOL001110	0.9237	0.0763	0.9230	Capsici Fructus	cis-beta-Ocimene	5320250	FALSE	C(=C(\C=C)/C)\CC=C(C)C
MOL001110	0.9237	0.0763	0.9230	Curcumae Radix	cis-beta-Ocimene	5320250	FALSE	C(=C(\C=C)/C)\CC=C(C)C
MOL001110	0.9237	0.0763	0.9230	Myrrha	cis-beta-Ocimene	5320250	FALSE	C(=C(\C=C)/C)\CC=C(C)C
MOL001111	0.9384	0.0616	0.7202	Myrrha	α-pinene-epoxide	Not Available	FALSE	C12C(C(CC3C1(C)C3)C2)(C)C
MOL001113	0.9304	0.0696	0.6645	Myrrha	α-thujone	Not Available	FALSE	C12(CC1(CC(=C)C2C)C(C)C)C
MOL001114	0.9609	0.0391	0.9166	Radix Angelicae Biseratae	2-[(1R)-2,2,3-trimethyl-1-cyclopent-3-enyl]ethanal	1252759	FALSE	C1(=CCC(C1(C)C)CC=O)C

MOL001114	0.9609	0.0391	0.9166	Platycladi Cacumen	2-[(1R)-2,2,3-trimethyl-1-cyclopent-3-enyl]ethanal	1252759	FALSE	C1(=CCC(C1(C)C)CC=O)C
MOL001114	0.9609	0.0391	0.9166	Myrrha	2-[(1R)-2,2,3-trimethyl-1-cyclopent-3-enyl]ethanal	1252759	FALSE	C1(=CCC(C1(C)C)CC=O)C
MOL001115	0.9613	0.0387	0.8133	Magnolia Officinalis Rehd Et Wils.	cis-Verbenol	164888	FALSE	C12CC(C(C=C1C)O)C2(C)C
MOL001115	0.9613	0.0387	0.8133	Centipedae Herba	cis-Verbenol	164888	FALSE	C12CC(C(C=C1C)O)C2(C)C
MOL001115	0.9613	0.0387	0.8133	Myrrha	cis-Verbenol	164888	FALSE	C12CC(C(C=C1C)O)C2(C)C
MOL001116	0.9374	0.0626	0.7538	Myrrha	pinocarvone	Not Available	FALSE	C1(=C)CC2CC(C1=C)C2(C)C
MOL001117	0.9245	0.0755	0.9336	Myrrha	p-mentha-1,5-dien-8-ol	Not Available	FALSE	C1=C(C=CC(C1)C(C)(C)C)C
MOL001118	0.9459	0.0541	0.9643	Myrrha	p-mentha-1(7)-dien-8-ol	Not Available	FALSE	C1=CC(CCC1=C)C(C)(C)O
MOL001119	0.9260	0.0740	0.8738	Myrrha	TBT	7390	FALSE	c1cc(ccc1C)C(C)(C)C
MOL001120	0.9363	0.0637	0.7401	Myrrha	myrtenal	Not Available	FALSE	C12C(C(CC=C1C=O)C2(C)C)(C)C
MOL001121	0.9569	0.0431	0.8088	Nardostachyos Radix Et Rhizoma	19894-97-4	88301	FALSE	C12CC(CC=C1CO)C2(C)C
MOL001121	0.9569	0.0431	0.8088	Ligustici Rhizoma Et Radix	19894-97-4	88301	FALSE	C12CC(CC=C1CO)C2(C)C
MOL001121	0.9569	0.0431	0.8088	Zingiberis Rhizoma	19894-97-4	88301	FALSE	C12CC(CC=C1CO)C2(C)C
MOL001121	0.9569	0.0431	0.8088	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	19894-97-4	88301	FALSE	C12CC(CC=C1CO)C2(C)C
MOL001121	0.9569	0.0431	0.8088	Cyperi Rhizoma	19894-97-4	88301	FALSE	C12CC(CC=C1CO)C2(C)C
MOL001121	0.9569	0.0431	0.8088	Radix Bupleuri	19894-97-4	88301	FALSE	C12CC(CC=C1CO)C2(C)C
MOL001121	0.9569	0.0431	0.8088	Cinnamomi Ramulus	19894-97-4	88301	FALSE	C12CC(CC=C1CO)C2(C)C
MOL001121	0.9569	0.0431	0.8088	Folium Artemisiae Argyi	19894-97-4	88301	FALSE	C12CC(CC=C1CO)C2(C)C
MOL001121	0.9569	0.0431	0.8088	Ephedra Herba	19894-97-4	88301	FALSE	C12CC(CC=C1CO)C2(C)C
MOL001121	0.9569	0.0431	0.8088	Myrrha	19894-97-4	88301	FALSE	C12CC(CC=C1CO)C2(C)C
MOL001122	0.7275	0.2725	0.7097	Myrrha	(4aS,8aS)-3,5,8a-trimethyl-4a,9-dihydro-4H-benzo[f]benzofuran	643237	FALSE	C1=CC2(C(C(=C1)C)Cc1c(C2)occ1C)C
MOL001123	0.8553	0.1447	0.6426	Farfarae Flos	muurolene	12306047	FALSE	C1C(=CC2C(C1)C(=CCC2C(C)C)C)C
MOL001123	0.8553	0.1447	0.6426	Lonicerae Japonicae Flos	muurolene	12306047	FALSE	C1C(=CC2C(C1)C(=CCC2C(C)C)C)C
MOL001123	0.8553	0.1447	0.6426	Cnidii Fructus	muurolene	12306047	FALSE	C1C(=CC2C(C1)C(=CCC2C(C)C)C)C
MOL001123	0.8553	0.1447	0.6426	Myrrha	muurolene	12306047	FALSE	C1C(=CC2C(C1)C(=CCC2C(C)C)C)C

MOL001123	0.8553	0.1447	0.6426	Tamaricis Cacumen	muurolene	12306047	FALSE	C1C(=CC2C(C1)C(=CCC2C(C)C)C)C
MOL001123	0.8553	0.1447	0.6426	Caryophylliflos	muurolene	12306047	FALSE	C1C(=CC2C(C1)C(=CCC2C(C)C)C)C
MOL001123	0.8553	0.1447	0.6426	Alpiniae Officinarum Rhizome	muurolene	12306047	FALSE	C1C(=CC2C(C1)C(=CCC2C(C)C)C)C
MOL001123	0.8553	0.1447	0.6426	Rhododendri Daurici Folium	muurolene	12306047	FALSE	C1C(=CC2C(C1)C(=CCC2C(C)C)C)C
MOL001123	0.8553	0.1447	0.6426	Solidaginis Herba	muurolene	12306047	FALSE	C1C(=CC2C(C1)C(=CCC2C(C)C)C)C
MOL001123	0.8553	0.1447	0.6426	Stephaniae Tetrandrae Radix	muurolene	12306047	FALSE	C1C(=CC2C(C1)C(=CCC2C(C)C)C)C
MOL001123	0.8553	0.1447	0.6426	Rhizome Of Whiteback Greenbrier	muurolene	12306047	FALSE	C1C(=CC2C(C1)C(=CCC2C(C)C)C)C
MOL001123	0.8553	0.1447	0.6426	Magnolia Officinalis Rehd Et Wils.	muurolene	12306047	FALSE	C1C(=CC2C(C1)C(=CCC2C(C)C)C)C
MOL001123	0.8553	0.1447	0.6426	Gossampiniflos	muurolene	12306047	FALSE	C1C(=CC2C(C1)C(=CCC2C(C)C)C)C
MOL001123	0.8553	0.1447	0.6426	Evodiae Fructus	muurolene	12306047	FALSE	C1C(=CC2C(C1)C(=CCC2C(C)C)C)C
MOL001123	0.8553	0.1447	0.6426	Cinnamomi Ramulus	muurolene	12306047	FALSE	C1C(=CC2C(C1)C(=CCC2C(C)C)C)C
MOL001123	0.8553	0.1447	0.6426	Cyperi Rhizoma	muurolene	12306047	FALSE	C1C(=CC2C(C1)C(=CCC2C(C)C)C)C
MOL001123	0.8553	0.1447	0.6426	Cinnanmomi Cortex	muurolene	12306047	FALSE	C1C(=CC2C(C1)C(=CCC2C(C)C)C)C
MOL001124	0.5449	0.4551	0.6971	Myrrha	erlangerin A	Not Available	FALSE	c1(c(c(c2c(c1)C1C3(C(C2c2cc4c(cc2)OCO4)(C(=O)OC3/C(=C/C)/C(=O)O1)O)O)OC)OC)OC
MOL001125	0.2400	0.7600	0.7125	Myrrha	erlangerin B	Not Available	FALSE	c1(c(c(c2c(c1)CC1C(C2c2ccc3c(c2)OCO3)(C(=O)OC1)OC(=C)C)OC)OC)OC
MOL001126	0.4152	0.5848	0.7176	Myrrha	[(5aS,8aR,9R)-8-oxo-9-(3,4,5-trimethoxyphenyl)-5,5a,6,9-tetrahydroisobenzofurano[6,5-f][1,3]benzodioxol-8a-yl] acetate	11004967	FALSE	c12c(cc3c(c1)CC1C(C3c3cc(c(c(c3)OC)OC)OC)(C(=O)OC1)OC(=O)C)OCO2
MOL001127	0.4152	0.5848	0.7176	Myrrha	erlangerin D	Not Available	FALSE	c12c(cc3c(c1)CC1C(C3c3cc(c(c(c3)OC)OC)OC)(C(=O)OC1)OC(=O)C)OCO2
MOL001128	0.3882	0.6118	0.6977	Myrrha	7-O-methylaloeresin A	Not Available	FALSE	c1c(ccc(c1)/C=C\C(=O)OC1C(C(C(OC1c1c(cc(c2c1oc(cc2=O)CC(=O)C)C)OC)CO)O)O)O
MOL001129	0.9569	0.0431	0.8029	Folium Artemisiae Argyi	l-Verbenone	92874	FALSE	C12C(C(C(=O)C=C1C)C2)(C)C
MOL001129	0.9569	0.0431	0.8029	Eriobotryae Folium	l-Verbenone	92874	FALSE	C12C(C(C(=O)C=C1C)C2)(C)C
MOL001129	0.9569	0.0431	0.8029	Caryophylliflos	l-Verbenone	92874	FALSE	C12C(C(C(=O)C=C1C)C2)(C)C
MOL001129	0.9569	0.0431	0.8029	Myrrha	l-Verbenone	92874	FALSE	C12C(C(C(=O)C=C1C)C2)(C)C

MOL001129	0.9569	0.0431	0.8029	Ligustici Rhizoma Et Radix	l-Verbenone	92874	FALSE	C12C(C(C(=O)C=C1C)C2)(C)C
MOL001129	0.9569	0.0431	0.8029	Carthami Flos	l-Verbenone	92874	FALSE	C12C(C(C(=O)C=C1C)C2)(C)C
MOL001129	0.9569	0.0431	0.8029	Schizonepetae Herba	l-Verbenone	92874	FALSE	C12C(C(C(=O)C=C1C)C2)(C)C
MOL001129	0.9569	0.0431	0.8029	Verbenae Herb	l-Verbenone	92874	FALSE	C12C(C(C(=O)C=C1C)C2)(C)C
MOL001130	0.7173	0.2827	0.7650	Myrrha	Fellavine	193876	FALSE	C1(C(C(C(OC1CO)Oc1cc(c2c(c1CC=C(C)C)OC(C(C2=O)O)c1ccc(cc1)O)O)O)O)O
MOL001130	0.7173	0.2827	0.7650	Phellodendri Amurensis Cortex	Fellavine	193876	FALSE	C1(C(C(C(OC1CO)Oc1cc(c2c(c1CC=C(C)C)OC(C(C2=O)O)c1ccc(cc1)O)O)O)O)O
MOL001131	0.5911	0.4089	0.7961	Phellodendri Amurensis Cortex	phellamurin_qt	Not Available	FALSE	Oc1cc(c2c(c1CC=C(C)C)OC(C(C2=O)O)c1ccc(cc1)O)O
MOL001131	0.5911	0.4089	0.7961	Myrrha	phellamurin_qt	Not Available	FALSE	Oc1cc(c2c(c1CC=C(C)C)OC(C(C2=O)O)c1ccc(cc1)O)O
MOL001132	0.8318	0.1682	0.6026	Myrrha	longipinene	Not Available	FALSE	C1CC(C2C3C(C1)(C2C(=CC3)C)C)(C)C
MOL001132	0.8318	0.1682	0.6026	Ardisiae Japonicae Herba	longipinene	Not Available	FALSE	C1CC(C2C3C(C1)(C2C(=CC3)C)C)(C)C
MOL001132	0.8318	0.1682	0.6026	Achyranthis Asperae Herba	longipinene	Not Available	FALSE	C1CC(C2C3C(C1)(C2C(=CC3)C)C)(C)C
MOL001132	0.8318	0.1682	0.6026	Styrax	longipinene	Not Available	FALSE	C1CC(C2C3C(C1)(C2C(=CC3)C)C)(C)C
MOL001133	0.8341	0.1659	0.8004	Myrrha	1,10(15)-furanodien-6-one	Not Available	FALSE	C\1=C/C(=C)Cc2c(C(=O)CC(C1O)C)c(co2)C
MOL001135	0.3706	0.6294	0.7418	Myrrha	cedrelone	Not Available	FALSE	C1=CC2(C(=C(C(=O)C3(C2CCC2(C43CC4CC2c2cocc2)C)C)O)C(C1=O)(C)C)C
MOL001136	0.7464	0.2536	0.7908	Myrrha	1,2-epoxyfurano-10(15)-germacren-6-one	Not Available	FALSE	C12CC(CC(=O)c3c(CC(=C)C1O2)occ3C)C
MOL001137	0.9694	0.0306	0.8737	Myrrha	4,7-dimethoxy-5-methyl-coumarin	185740	FALSE	c1c(cc2c(c1C)c(cc(=O)o2)OC)OC
MOL001138	0.2968	0.7032	0.6853	Myrrha	(3R,20S)-3,20-dihydroxydammar- 24-ene	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(C)(O)CCC=C(C)C)C)C)C)(C)C)C
MOL001139	0.1836	0.8164	0.7220	Myrrha	(3R,20S)-3-acetoxy-20-hydroxydammar-24- ene	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(C)(O)CCC=C(C)C)C)C)C)(C)C)OC(=O)C

MOL001141	0.1905	0.8095	0.7624	Myrrha	(20S)-3β-acetoxy- 12 β,16β-trihydroxydammar-24-ene	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(C(C2)O)C(O)(C)CCC=C(C)C)C)C)(C)C)OC(=O)C
MOL001142	0.3753	0.6247	0.7843	Myrrha	(20S)12β,16β-trihydroxydammar-24-ene-3β-O-β-glucopyranoside	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(C(C2)O)C(O)(C)CCC=C(C)C)C)C)(C)C)OC1C(O)C(O)C(O)C(O1)CO
MOL001143	0.2561	0.7439	0.7131	Myrrha	(20S)12β,16β-trihydroxydammar-24-ene-3β-O-β-glucopyranoside_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(C(C2)O)C(O)(C)CCC=C(C)C)C)C)(C)C)O
MOL001144	0.4773	0.5227	0.6193	Myrrha	lindestrene	Not Available	FALSE	C1=CC2(C(C(=C)C1)(CC1=C(C2)CC=C1C)C)C
MOL001145	0.1846	0.8154	0.7664	Myrrha	(20S)-3β-acetoxy-12 β,16β,25-tetrahydroxydammar-23-ene	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(C(C2)O)C(C)(O)CCC=C(C)C)C)C)(C)C)OC(=O)C
MOL001146	0.2391	0.7609	0.7038	Myrrha	(20S)-3β,12 β,16β,25-pentahydroxydammar-23-ene	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(C)CCC=C(C)C)C)C)(C)C)O
MOL001147	0.2159	0.7841	0.6910	Myrrha	(20R)-3β-acetoxy-16β-dihydroxydammar-24-ene	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(C)CCC=C(C)C)C)C)(C)C)OC(=O)C
MOL001148	0.1844	0.8156	0.7292	Myrrha	3β-hydroxydammar-24-ene	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(C(C2)O)C(C)CCC=C(C)C)C)C)(C)C)OC(=O)C
MOL001149	0.2334	0.7666	0.7607	Myrrha	3β-acetoxydammar-24-ene	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(C(C2)O)C(C)(O)CCC=C(C)C)C)C)(C)C)O

MOL001150	0.1943	0.8057	0.7370	Myrrha	3β-acetoxy-16β-hydroxydammar-24-ene	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(C(C2)O)C(O)(C)C/C=C/C(C)(C)O)C)C)(C)C)OC(=O)C
MOL001151	0.2919	0.7081	0.6710	Myrrha	(20R)- 3β,16β-trihydroxydammar-24-ene	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(C(C2)O)C(O)(C)C/C=C/C(C)(C)O)C)C)(C)C)O
MOL001152	0.8890	0.1110	0.8341	Myrrha	(5S,6S)-5-isopropenyl-3,6-dimethyl-6-vinyl-5,7-dihydrobenzofuran-4-one	10376566	FALSE	C=CC1(C(C(=C)C)C(=O)c2c(C1)occ2C)C
MOL001153	0.8250	0.1750	0.8098	Myrrha	(5E,9E)-3,6,10-trimethyl-8,11-dihydro-7H-cyclodeca[b]furan-4-one	6506548	FALSE	C1C/C(=C/C(=O)c2c(C/C(=C/1)/C)occ2C)/C
MOL001154	0.7533	0.2467	0.6231	Myrrha	dihydropyrocurzerenone	Not Available	FALSE	C1C(Cc2c(C1)c(cc1c2c(co1)C)C)C
MOL001155	0.7113	0.2887	0.7923	Myrrha	3-methoxy-10(15)-dihydrofuranodien-6-one	Not Available	FALSE	C1C(C(CC(=O)c2c(CC(=C)C1)occ2C)C)OC
MOL001156	0.7825	0.2175	0.7873	Myrrha	3-methoxyfuranoguaia-9- en-8-one	Not Available	FALSE	C1(=CC(=O)c2c(C3C1CC(C3C)OC)occ2C)C
MOL001157	0.7231	0.2769	0.7892	Myrrha	(6R,8R,9E)-8-methoxy-3,6,10-trimethyl-6,7,8,11-tetrahydro-5H-cyclodeca[b]furan-4-one	11747425	FALSE	C1(CC(CC(=O)c2c(C/C(=C/1)/C)occ2C)C)OC

MOL001158	0.7345	0.2655	0.7180	Myrrha	3-methoxy-10-methylenefuranogermacra-1- en-6-one	Not Available	FALSE	C\1=C\C(C(CC(=O)c2c(CC1=C)occ2C)C)OC
MOL001159	0.4373	0.5627	0.6910	Myrrha	2-acetoxyfuranodiene	Not Available	FALSE	C1(C/C(=C/Cc2c(C/C(=C/1)/C)occ2C)/C)OC(=O)C
MOL001160	0.7197	0.2803	0.7906	Codonopsis Radix	2-methoxyfuranodiene	Not Available	FALSE	C1(C/C(=C/Cc2c(C/C(=C/1)/C)occ2C)/C)OC
MOL001160	0.7197	0.2803	0.7906	Myrrha	2-methoxyfuranodiene	Not Available	FALSE	C1(C/C(=C/Cc2c(C/C(=C/1)/C)occ2C)/C)OC
MOL001161	0.7103	0.2897	0.7279	Myrrha	lindestrene	Not Available	FALSE	C1=CC2(C(C(=C)C1)Cc1c(C2)occ1C)C
MOL001162	0.8270	0.1730	0.7269	Myrrha	commiferin	Not Available	FALSE	C1(CC(=C)C2C(C1)(CC1C(=C(C(=O)O1)C)C2)C)O
MOL001163	0.8846	0.1154	0.8512	Myrrha	germacrone	Not Available	FALSE	C1CC(=C2C(=C1)CC(=O)C(=C(C)C)C2)C
MOL001164	0.5330	0.4670	0.6641	Myrrha	[(5S,6R,8R,9Z)-8-methoxy-3,6,10-trimethyl-4-oxo-6,7,8,11-tetrahydro-5H-cyclodeca[b]furan-5-yl] acetate	10870920	FALSE	C1(CC(C(C(=O)c2c(C/C(=C\1)/C)occ2C)OC(=O)C)C)OC
MOL001165	0.7197	0.2803	0.6662	Myrrha	furanodiene	Not Available	FALSE	C1C/C(=C/CC2=C(C/C(=C/1)/C)CC=C2C)/C
MOL001166	0.8108	0.1892	0.8116	Myrrha	4,5-dihydrofuranodiene-6-one	Not Available	FALSE	C1CC(CC(=O)c2c(C/C(=C/1)/C)occ2C)C
MOL001168	0.8647	0.1353	0.6853	Fritillariaeussuriensis Bulbus	(1S,2S)-2-isopropenyl-4-isopropylidene-1-methyl-1-vinylcyclohexane	6432312	FALSE	C=CC1(C(C(=C)C)CC(=C(C)C)CC1)C

MOL001168	0.8647	0.1353	0.6853	Menthae Herba	(1S,2S)-2-isopropenyl-4-isopropylidene-1-methyl-1-vinylcyclohexane	6432312	FALSE	C=CC1(C(C(=C)C)CC(=C(C)C)CC1)C
MOL001168	0.8647	0.1353	0.6853	Myrrha	(1S,2S)-2-isopropenyl-4-isopropylidene-1-methyl-1-vinylcyclohexane	6432312	FALSE	C=CC1(C(C(=C)C)CC(=C(C)C)CC1)C
MOL001168	0.8647	0.1353	0.6853	Rhododendri Daurici Folium	(1S,2S)-2-isopropenyl-4-isopropylidene-1-methyl-1-vinylcyclohexane	6432312	FALSE	C=CC1(C(C(=C)C)CC(=C(C)C)CC1)C
MOL001168	0.8647	0.1353	0.6853	Ginsen Radix Et Rhizoma Rubra	(1S,2S)-2-isopropenyl-4-isopropylidene-1-methyl-1-vinylcyclohexane	6432312	FALSE	C=CC1(C(C(=C)C)CC(=C(C)C)CC1)C
MOL001168	0.8647	0.1353	0.6853	Zanthoxyli Pericarpium	(1S,2S)-2-isopropenyl-4-isopropylidene-1-methyl-1-vinylcyclohexane	6432312	FALSE	C=CC1(C(C(=C)C)CC(=C(C)C)CC1)C
MOL001168	0.8647	0.1353	0.6853	Solidaginis Herba	(1S,2S)-2-isopropenyl-4-isopropylidene-1-methyl-1-vinylcyclohexane	6432312	FALSE	C=CC1(C(C(=C)C)CC(=C(C)C)CC1)C

MOL001168	0.8647	0.1353	0.6853	Hippophae Fructus	(1S,2S)-2-isopropenyl-4-isopropylidene-1-methyl-1-vinylcyclohexane	6432312	FALSE	C=CC1(C(C(=C)C)CC(=C(C)C)CC1)C
MOL001168	0.8647	0.1353	0.6853	Et Radix Patriniae Rhizoma	(1S,2S)-2-isopropenyl-4-isopropylidene-1-methyl-1-vinylcyclohexane	6432312	FALSE	C=CC1(C(C(=C)C)CC(=C(C)C)CC1)C
MOL001168	0.8647	0.1353	0.6853	Stephaniae Tetrandrae Radix	(1S,2S)-2-isopropenyl-4-isopropylidene-1-methyl-1-vinylcyclohexane	6432312	FALSE	C=CC1(C(C(=C)C)CC(=C(C)C)CC1)C
MOL001168	0.8647	0.1353	0.6853	Lonicerae Japonicae Flos	(1S,2S)-2-isopropenyl-4-isopropylidene-1-methyl-1-vinylcyclohexane	6432312	FALSE	C=CC1(C(C(=C)C)CC(=C(C)C)CC1)C
MOL001169	0.3587	0.6413	0.7898	Myrrha	8α-methoxyfuranodiene	Not Available	FALSE	C1C(/C=C(/CC2=C(C/C=C/1\C)C(=CC2)C)\C)CC
MOL001171	0.7856	0.2144	0.7151	Myrrha	β-bisabolene	Not Available	FALSE	C(CC=C(C)C)C(=C)C1(CCC(=CC1)C)C
MOL001172	0.8250	0.1750	0.8098	Curcumae Radix	24268-41-5	6442374	FALSE	C1c2c(C(=O)/C=C(\CC/C=C\1/C)/C)c(co2)C
MOL001172	0.8250	0.1750	0.8098	Myrrha	24268-41-5	6442374	FALSE	C1c2c(C(=O)/C=C(\CC/C=C\1/C)/C)c(co2)C
MOL001173	0.7345	0.2655	0.7180	Myrrha	(6S,7R,8E)-7-methoxy-3,6-dimethyl-10-methylidene-5,6,7,11-tetrahydrocyclodeca[b]furan-4-one	10923274	FALSE	C\1=C/C(=C)Cc2c(C(=O)CC(C1OC)C)c(co2)C

MOL001174	0.7464	0.2536	0.7908	Myrrha	rel-1S,2S-epoxy- 4R-furanogermacr-10(15)-en-6-one	Not Available	FALSE	C12CC(CC(=O)c3c(CC(=C)C1O2)occ3C)C
MOL001175	0.2637	0.7363	0.9644	Myrrha	Guggulsterone	6439929	FALSE	C1(=O)CCC2(C(=C1)CCC1C3CC(=O)/C(=C/C)/C3(C)CCC21)C
MOL001178	0.8824	0.1176	0.6432	Myrrha	α-gurjunene	Not Available	FALSE	C12(C(=C(CC2)C)C2C(CCC1C)C2)C
MOL001180	0.8550	0.1450	0.6445	Solidaginis Herba	γ-muurolene	12313020	FALSE	C1C(=CC2C(C1)C(=C)CCC2C(C)C)C
MOL001180	0.8550	0.1450	0.6445	Myrrha	γ-muurolene	12313020	FALSE	C1C(=CC2C(C1)C(=C)CCC2C(C)C)C
MOL001180	0.8550	0.1450	0.6445	Cnidii Fructus	γ-muurolene	12313020	FALSE	C1C(=CC2C(C1)C(=C)CCC2C(C)C)C
MOL001180	0.8550	0.1450	0.6445	Rubi Fructus	γ-muurolene	12313020	FALSE	C1C(=CC2C(C1)C(=C)CCC2C(C)C)C
MOL001180	0.8550	0.1450	0.6445	Lonicerae Japonicae Flos	γ-muurolene	12313020	FALSE	C1C(=CC2C(C1)C(=C)CCC2C(C)C)C
MOL001182	0.6405	0.3595	0.6287	Myrrha	1,3-furanoeudesma-diene	Not Available	FALSE	C1=C(C2(C(C=C1)(Cc1c(C2)c(co1)C)C)C)C
MOL001183	0.8219	0.1781	0.6554	Myrrha	(3R,4aS,8aR)-3-isopropenyl-5,8a-dimethyl-2,3,4,4a,7,8-hexahydro-1H-naphthalene	11052745	FALSE	C1C=C(C2C(C1)(CCC(C2)C(=C)C)C)C
MOL001184	0.8598	0.1402	0.6769	Viticis Fructus	bicyclogermacrene	13894537	FALSE	C1C/C(=C/C2C(CC/C(=C/1)/C)C2(C)C)/C
MOL001184	0.8598	0.1402	0.6769	Myrrha	bicyclogermacrene	13894537	FALSE	C1C/C(=C/C2C(CC/C(=C/1)/C)C2(C)C)/C
MOL001184	0.8598	0.1402	0.6769	Ailanthi Cortex	bicyclogermacrene	13894537	FALSE	C1C/C(=C/C2C(CC/C(=C/1)/C)C2(C)C)/C
MOL001184	0.8598	0.1402	0.6769	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	bicyclogermacrene	13894537	FALSE	C1C/C(=C/C2C(CC/C(=C/1)/C)C2(C)C)/C
MOL001185	0.6583	0.3417	0.7180	Myrrha	furanoeudesma-1,4-diene	Not Available	FALSE	C1=CC2(C(=C(C1)C)CC1=C(C2)CC=C1C)C
MOL001186	0.8031	0.1969	0.6041	Myrrha	β-eudesmol	Not Available	FALSE	C1CC(=C)C2C(C1)(CCC(C2)C(C)C)C
MOL001189	0.8418	0.1582	0.6717	Polygoni Orientalis Fructus	cis-caryophyllene	5498519	FALSE	C1(CC2C1CC/C(=C\CCC2=C)/C)(C)C
MOL001189	0.8418	0.1582	0.6717	Myrrha	cis-caryophyllene	5498519	FALSE	C1(CC2C1CC/C(=C\CCC2=C)/C)(C)C
MOL001189	0.8418	0.1582	0.6717	Leonuri Herba	cis-caryophyllene	5498519	FALSE	C1(CC2C1CC/C(=C\CCC2=C)/C)(C)C

MOL001189	0.8418	0.1582	0.6717	Rhododendri Daurici Folium	cis-caryophyllene	5498519	FALSE	C1(CC2C1CC/C(=C\CCC2=C)/C)(C)C
MOL001190	0.7841	0.2159	0.6759	Myrrha	β-sesquiphellandrene	Not Available	FALSE	C(CC=C(C)C)C(C1(C=CC(=C)CC1)C)C
MOL001191	0.8356	0.1644	0.6683	Myrrha	(4aR,8aR)-3-isopropylidene-5,8a-dimethyl-1,2,4,4a,7,8-hexahydronaphthalene	6432648	FALSE	C1C=C(C2C(C1)(CCC(=C(C)C)C2)C)C
MOL001193	0.8731	0.1269	0.7548	Myrrha	caryophyllene oxide	Not Available	FALSE	C1(CC2(C1CCC1(C(CCC2=C)O1)C)O)(C)C
MOL001196	0.8475	0.1525	0.7107	Myrrha	7-epi-α-eudesmol	12304196	FALSE	C1C=C(C2C(C1)(CCC(C2)C(C)(C)O)C)C
MOL001197	0.7060	0.2940	0.7400	Myrrha	2-hydroxyfuranodiene	Not Available	FALSE	C1(C/C(=C/CC2=C(C/C(=C/1)/C)CC=C2)/C)C
MOL001198	0.6955	0.3045	0.7516	Myrrha	10-epi-γ-eudesmol acetate	57407173	FALSE	C1CC(=C2C(C1)(CCC(C2)C(C)(C)OC(=O)C)C)C
MOL001199	0.8270	0.1730	0.7269	Myrrha	commiferin	Not Available	FALSE	O1C2C(=C(C1=O)C)CC1C(=C)CC(CC1(C2)C)O
MOL001200	0.9454	0.0546	0.8773	Myrrha	(E)-β-ocimene epoxide	Not Available	FALSE	C(=C(\C)/C=C)\CC1C(C1)(C)C
MOL001202	0.9476	0.0524	0.9749	Myrrha	1-[(1R)-4-methyl-1-cyclohex-3-enyl]ethanone	10909635	FALSE	C1C=C(CCC1C(=O)C)C
MOL001205	0.8786	0.1214	0.8706	Myrrha	6-methyl-3,5-heptadiene-2-one	Not Available	FALSE	C(=C\C=C(C)C)\C(=C)C
MOL001206	0.8396	0.1604	0.6091	Myrrha	Santalene (minor)	6431197	FALSE	C1C2C(C(=C)C(C1)C2)(C)CCC=C(C)C
MOL001207	0.8818	0.1182	0.7316	Myrrha	(Z)-β-santalene	Not Available	FALSE	C1CC2C(C(=C)C1C2)CCC=C(C)C
MOL001208	0.8516	0.1484	0.8080	Myrrha	2,6-dimethyl-3(E),5(E),7-octatrien- 2-ol	Not Available	FALSE	C(=C(\C=C\C)/C)\C=C\C(C)(C)C

MOL001209	0.9175	0.0825	0.9388	Olibanun	1-acetyl-4-isopropenylcyclopentene	45085864	FALSE	C(=O)(C)C1=CCC(C1)C(=C)C
MOL001210	0.9558	0.0442	0.9779	Ephedra Herba	(4S)-4-isopropylcyclohexene-1-carbaldehyde	11842593	FALSE	C1(=CCC(CC1)C(C)C)C=O
MOL001210	0.9558	0.0442	0.9779	Chuanxiong Rhizoma	(4S)-4-isopropylcyclohexene-1-carbaldehyde	11842593	FALSE	C1(=CCC(CC1)C(C)C)C=O
MOL001210	0.9558	0.0442	0.9779	Zingiberis Rhizoma	(4S)-4-isopropylcyclohexene-1-carbaldehyde	11842593	FALSE	C1(=CCC(CC1)C(C)C)C=O
MOL001210	0.9558	0.0442	0.9779	Evodiae Fructus	(4S)-4-isopropylcyclohexene-1-carbaldehyde	11842593	FALSE	C1(=CCC(CC1)C(C)C)C=O
MOL001210	0.9558	0.0442	0.9779	Olibanun	(4S)-4-isopropylcyclohexene-1-carbaldehyde	11842593	FALSE	C1(=CCC(CC1)C(C)C)C=O
MOL001211	0.9022	0.0978	0.8489	Olibanun	cis-lanceol	Not Available	FALSE	C(/C(=C\CCC(=C)C1CC=C(CC1)C)/C)O
MOL001212	0.8284	0.1716	0.7450	Capsici Fructus	Loxanol V	8209	FALSE	C(CCCCCCCCCCCCC)O
MOL001212	0.8284	0.1716	0.7450	Olibanun	Loxanol V	8209	FALSE	C(CCCCCCCCCCCCC)O
MOL001212	0.8284	0.1716	0.7450	Angelicae Sinensis Radix	Loxanol V	8209	FALSE	C(CCCCCCCCCCCCC)O
MOL001212	0.8284	0.1716	0.7450	Panax Ginseng C. A. Mey.	Loxanol V	8209	FALSE	C(CCCCCCCCCCCCC)O
MOL001212	0.8284	0.1716	0.7450	A. Dahurica (Fisch.) Benth. Et Hook	Loxanol V	8209	FALSE	C(CCCCCCCCCCCCC)O
MOL001213	0.8881	0.1119	0.8560	Olibanun	linalyl butyrate	36690113	FALSE	C(=O)(CCC)OC(CCC=C(C)C)(C)C=C
MOL001214	0.9396	0.0604	0.9372	Olibanun	Rystal	12124	FALSE	C(=O)(C)Nc1cc(ccc1)O
MOL001215	0.2068	0.7932	0.7271	Olibanun	tirucallol	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1=C2CCC2(C1(C)CCC2C(CCC=C(C)C)C)C)C)O
MOL001216	0.9649	0.0351	0.9175	Olibanun	amantadine	2130	FALSE	NC12CC3CC(C1)CC(C3)C2
MOL001217	0.9586	0.0414	0.7752	Folium Artemisiae Argyi	()-Bornyl acetate	6950274	FALSE	C12(C(CC(CC1)C2(C)C)OC(=O)C)C
MOL001217	0.9586	0.0414	0.7752	Olibanun	()-Bornyl acetate	6950274	FALSE	C12(C(CC(CC1)C2(C)C)OC(=O)C)C
MOL001217	0.9586	0.0414	0.7752	Cinnamomi Ramulus	()-Bornyl acetate	6950274	FALSE	C12(C(CC(CC1)C2(C)C)OC(=O)C)C

MOL001217	0.9586	0.0414	0.7752	Stephaniae Tetrandrae Radix	()-Bornyl acetate	6950274	FALSE	C12(C(CC(CC1)C2(C)C)OC(=O)C)C
MOL001217	0.9586	0.0414	0.7752	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	()-Bornyl acetate	6950274	FALSE	C12(C(CC(CC1)C2(C)C)OC(=O)C)C
MOL001217	0.9586	0.0414	0.7752	Zingiber Officinale Roscoe	()-Bornyl acetate	6950274	FALSE	C12(C(CC(CC1)C2(C)C)OC(=O)C)C
MOL001217	0.9586	0.0414	0.7752	Agrimonia Eupatoria	()-Bornyl acetate	6950274	FALSE	C12(C(CC(CC1)C2(C)C)OC(=O)C)C
MOL001218	0.8888	0.1112	0.8590	Paeoniae Radix Alba	Pisol	8193	FALSE	C(CCCCCCCCCCC)O
MOL001218	0.8888	0.1112	0.8590	Olibanun	Pisol	8193	FALSE	C(CCCCCCCCCCC)O
MOL001218	0.8888	0.1112	0.8590	Panax Ginseng C. A. Mey.	Pisol	8193	FALSE	C(CCCCCCCCCCC)O
MOL001218	0.8888	0.1112	0.8590	Panacis Quinquefolii Radix	Pisol	8193	FALSE	C(CCCCCCCCCCC)O
MOL001218	0.8888	0.1112	0.8590	A. Dahurica (Fisch.) Benth. Et Hook	Pisol	8193	FALSE	C(CCCCCCCCCCC)O
MOL001218	0.8888	0.1112	0.8590	Piperis Longi Fructus	Pisol	8193	FALSE	C(CCCCCCCCCCC)O
MOL001221	0.8205	0.1795	0.6754	Polygonati Odorati Rhizoma	7-TETRADECENE	5364651	FALSE	CCCCCC/C=C/CCCCCC
MOL001221	0.8205	0.1795	0.6754	Olibanun	7-TETRADECENE	5364651	FALSE	CCCCCC/C=C/CCCCCC
MOL001222	0.3548	0.6452	0.7817	Olibanun	Estan	6010	FALSE	C1(=O)CCC2(C(=C1)CCC1C3CCC(C3(C)CCC21)C)O)C
MOL001223	0.9609	0.0391	0.9166	Magnolia Officinalis Rehd Et Wils.	(S)-2,2,3-Trimethylcyclopent-3-ene-1-acetaldehyde	90969	FALSE	C1(C(C(=CC1)C)(C)C)CC=O
MOL001223	0.9609	0.0391	0.9166	Folium Nelumbinis	(S)-2,2,3-Trimethylcyclopent-3-ene-1-acetaldehyde	90969	FALSE	C1(C(C(=CC1)C)(C)C)CC=O
MOL001223	0.9609	0.0391	0.9166	Radix Clematidis	(S)-2,2,3-Trimethylcyclopent-3-ene-1-acetaldehyde	90969	FALSE	C1(C(C(=CC1)C)(C)C)CC=O
MOL001223	0.9609	0.0391	0.9166	Chuanxiong Rhizoma	(S)-2,2,3-Trimethylcyclopent-3-ene-1-acetaldehyde	90969	FALSE	C1(C(C(=CC1)C)(C)C)CC=O

MOL001223	0.9609	0.0391	0.9166	Olibanun	(S)-2,2,3-Trimethylcyclopent-3-ene-1-acetaldehyde	90969	FALSE	C1(C(C(=CC1)C)(C)C)CC=O
MOL001224	0.8519	0.1481	0.7206	Angelicae Sinensis Radix	Tridecylene	17095	FALSE	C=CCCCCCCCCCCC
MOL001224	0.8519	0.1481	0.7206	Piperis Longi Fructus	Tridecylene	17095	FALSE	C=CCCCCCCCCCCC
MOL001224	0.8519	0.1481	0.7206	Physochlainae Radix	Tridecylene	17095	FALSE	C=CCCCCCCCCCCC
MOL001224	0.8519	0.1481	0.7206	Olibanun	Tridecylene	17095	FALSE	C=CCCCCCCCCCCC
MOL001224	0.8519	0.1481	0.7206	Farfarae Flos	Tridecylene	17095	FALSE	C=CCCCCCCCCCCC
MOL001224	0.8519	0.1481	0.7206	Capsici Fructus	Tridecylene	17095	FALSE	C=CCCCCCCCCCCC
MOL001225	0.8841	0.1159	0.8926	Chaenomeles Sinensis (Thouin) Koehne	Butyl octanoate	11517	FALSE	C(=O)(CCCCCCC)OCCCC
MOL001225	0.8841	0.1159	0.8926	Olibanun	Butyl octanoate	11517	FALSE	C(=O)(CCCCCCC)OCCCC
MOL001226	0.9055	0.0945	0.9293	Olibanun	alpha-terpineol	Not Available	FALSE	C1CC(=CCC1C(C)(C)C)C
MOL001227	0.8834	0.1166	0.8824	Notopterygii Rhizoma Et Radix	Decyl acetate	8167	FALSE	C(CCCCCCCCC)OC(=O)C
MOL001227	0.8834	0.1166	0.8824	Radix Angelicae Biseratae	Decyl acetate	8167	FALSE	C(CCCCCCCCC)OC(=O)C
MOL001227	0.8834	0.1166	0.8824	Olibanun	Decyl acetate	8167	FALSE	C(CCCCCCCCC)OC(=O)C
MOL001227	0.8834	0.1166	0.8824	Menthae Herba	Decyl acetate	8167	FALSE	C(CCCCCCCCC)OC(=O)C
MOL001228	0.9488	0.0512	0.8405	Olibanun	Medilla	5280567	FALSE	c1(=O)cc(c2ccc(O)cc2o1)C
MOL001229	0.9051	0.0949	0.9491	Mori Fructus	cis-resveratrol	1548910	FALSE	c1(cc(cc(c1)/C=C\c1ccc(cc1)O)O)O
MOL001229	0.9051	0.0949	0.9491	Boehmeriae Rhizoma Et Radix	cis-resveratrol	1548910	FALSE	c1(cc(cc(c1)/C=C\c1ccc(cc1)O)O)O
MOL001229	0.9051	0.0949	0.9491	Olibanun	cis-resveratrol	1548910	FALSE	c1(cc(cc(c1)/C=C\c1ccc(cc1)O)O)O
MOL001229	0.9051	0.0949	0.9491	Smilax China	cis-resveratrol	1548910	FALSE	c1(cc(cc(c1)/C=C\c1ccc(cc1)O)O)O
MOL001229	0.9051	0.0949	0.9491	Ampelopsis Japonica	cis-resveratrol	1548910	FALSE	c1(cc(cc(c1)/C=C\c1ccc(cc1)O)O)O
MOL001229	0.9051	0.0949	0.9491	Belamcandae Rhizome	cis-resveratrol	1548910	FALSE	c1(cc(cc(c1)/C=C\c1ccc(cc1)O)O)O
MOL001229	0.9051	0.0949	0.9491	Polygoni Cuspidati Rhizoma Et Radix	cis-resveratrol	1548910	FALSE	c1(cc(cc(c1)/C=C\c1ccc(cc1)O)O)O
MOL001230	0.9041	0.0959	0.8950	Folium Nelumbinis	Tip-Nip	8184	FALSE	C(CCCCCCCCCC)O
MOL001230	0.9041	0.0959	0.8950	Olibanun	Tip-Nip	8184	FALSE	C(CCCCCCCCCC)O
MOL001231	0.9513	0.0487	0.9506	Olibanun	(5R)-Menth-2-enone	11205871	FALSE	C1(=O)C(=CCC(C1)C)C(C)C
MOL001232	0.3513	0.6487	0.9500	Ecliptae Herba	TES	6013	TRUE	C1(=O)CCC2(C(=C1)CCC1C3CCC(C3(C)CCC21)O)C
MOL001232	0.3513	0.6487	0.9500	Alpiniae Officinarum Rhizome	TES	6013	TRUE	C1(=O)CCC2(C(=C1)CCC1C3CCC(C3(C)CCC21)O)C
MOL001232	0.3513	0.6487	0.9500	Olibanun	TES	6013	TRUE	C1(=O)CCC2(C(=C1)CCC1C3CCC(C3(C)CCC21)O)C
MOL001233	0.9745	0.0255	0.7453	Olibanun	Penconazol	40427894	FALSE	n1(ncnc1)CC(CCC)c1c(cc(cc1)Cl)Cl
MOL001235	0.4722	0.5278	0.7941	Olibanun	9-C-Retinal	6436082	FALSE	C1(=C(C(CCC1)(C)C)/C=C/C(=C\C=C\C(=C\C=O)\C)/C)C

MOL001236	0.9323	0.0677	0.9620	Olibanun	isopropyliden ecyclohexane	138578	FALSE	C1(=C(C)C)CCCCC1
MOL001237	0.9438	0.0562	0.9322	Olibanun	o-Acetyltoluene	11340	FALSE	C(=O)(C)c1c(cccc1)C
MOL001237	0.9438	0.0562	0.9322	Cinnanmomi Cortex	o-Acetyltoluene	11340	FALSE	C(=O)(C)c1c(cccc1)C
MOL001237	0.9438	0.0562	0.9322	Radix Rhei Et Rhizome	o-Acetyltoluene	11340	FALSE	C(=O)(C)c1c(cccc1)C
MOL001237	0.9438	0.0562	0.9322	Zanthoxyli Pericarpium	o-Acetyltoluene	11340	FALSE	C(=O)(C)c1c(cccc1)C
MOL001238	0.3812	0.6188	0.7418	Verbenae Herb	3-Epilupeol	5270628	FALSE	C12C(CCC3(C4(CCC5C(C(CCC5(C4CCC13)C)O)(C)C)C)C)(CCC2C(=C)C)C
MOL001238	0.3812	0.6188	0.7418	Olibanun	3-Epilupeol	5270628	FALSE	C12C(CCC3(C4(CCC5C(C(CCC5(C4CCC13)C)O)(C)C)C)C)(CCC2C(=C)C)C
MOL001239	0.3048	0.6952	0.7437	Olibanun	epilupeol acetate	40884505	FALSE	C(=O)(C)OC1CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C(=C)C)C4C3CCC21)C
MOL001240	0.9612	0.0388	0.8272	Olibanun	trans-pinocamphone (pinocamphone)	6430551	FALSE	C12C(C(=O)CC(C1(C)C)C2)C
MOL001240	0.9612	0.0388	0.8272	Glechomae Herba	trans-pinocamphone (pinocamphone)	6430551	FALSE	C12C(C(=O)CC(C1(C)C)C2)C
MOL001240	0.9612	0.0388	0.8272	Cyperi Rhizoma	trans-pinocamphone (pinocamphone)	6430551	FALSE	C12C(C(=O)CC(C1(C)C)C2)C
MOL001241	0.6543	0.3457	0.8196	Olibanun	O-acetyl-α-boswellic acid	Not Available	FALSE	O=C(OC1CCC2(C(C1(C)C(=O)O)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C)C)C)C)C)C
MOL001242	0.9660	0.0340	0.8024	Ganoderma	dl-Thujone	261491	FALSE	C12(CC(=O)C(C1C2)C)C(C)C
MOL001242	0.9660	0.0340	0.8024	Folium Artemisiae Argyi	dl-Thujone	261491	FALSE	C12(CC(=O)C(C1C2)C)C(C)C
MOL001242	0.9660	0.0340	0.8024	Olibanun	dl-Thujone	261491	FALSE	C12(CC(=O)C(C1C2)C)C(C)C
MOL001242	0.9660	0.0340	0.8024	Platycladi Cacumen	dl-Thujone	261491	FALSE	C12(CC(=O)C(C1C2)C)C(C)C
MOL001243	0.7483	0.2517	0.8900	Olibanun	3alpha-Hydroxy-olean-12-en-24-oic-acid	637234	FALSE	C12C(C3(C(=CC2)C2C(CC3)(CCC(C2)(C)C)C)C)(CCC2C1(CCC(C2(C(=O)O)C)O)C)C

MOL001243	0.7483	0.2517	0.8900	Hemerocallis Radix	3alpha-Hydroxy-olean-12-en-24-oic-acid	637234	FALSE	C12C(C3(C(=CC2)C2C(CC3)(CCC(C2)(C)C)C)C)(CCC2C1(CCC(C2(C(=O)O)C)O)C)C
MOL001244	0.3541	0.6459	0.6890	Olibanun	α-amyrenone	12306155	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(=O)CC1)(C)C)C)C1C(CC3)(CCC(C1C)C)C)C)C
MOL001245	0.9554	0.0446	0.8004	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(1S,5R)-7,7-dimethyl-4-bicyclo[3.1.1]hept-3-enecarboxaldehyde	1201529	FALSE	C12C(=CCC(C1(C)C)C2)C=O
MOL001245	0.9554	0.0446	0.8004	Olibanun	(1S,5R)-7,7-dimethyl-4-bicyclo[3.1.1]hept-3-enecarboxaldehyde	1201529	FALSE	C12C(=CCC(C1(C)C)C2)C=O
MOL001245	0.9554	0.0446	0.8004	Cyperi Rhizoma	(1S,5R)-7,7-dimethyl-4-bicyclo[3.1.1]hept-3-enecarboxaldehyde	1201529	FALSE	C12C(=CCC(C1(C)C)C2)C=O
MOL001245	0.9554	0.0446	0.8004	Folium Artemisiae Argyi	(1S,5R)-7,7-dimethyl-4-bicyclo[3.1.1]hept-3-enecarboxaldehyde	1201529	FALSE	C12C(=CCC(C1(C)C)C2)C=O
MOL001246	0.9594	0.0406	0.8168	Cortex Moutan	(1R)-()-Nopinone	157139	FALSE	C12C(=O)CCC(C1(C)C)C2
MOL001246	0.9594	0.0406	0.8168	Paeoniae Radix Alba	(1R)-()-Nopinone	157139	FALSE	C12C(=O)CCC(C1(C)C)C2
MOL001246	0.9594	0.0406	0.8168	Olibanun	(1R)-()-Nopinone	157139	FALSE	C12C(=O)CCC(C1(C)C)C2
MOL001247	0.9481	0.0519	0.8245	Olibanun	myrtenic acid	Not Available	FALSE	C12C(=CCC(C1(C)C)C2)C(=O)O
MOL001248	0.9552	0.0448	0.9671	Olibanun	cis-5-Hydroxy-p-menth-1(6)-en-2-one	6429208	FALSE	C1C(C(C=C(C1=O)C)O)C(C)C

MOL001249	0.9051	0.0949	0.8097	Olibanun	(4aR,5S,8R,8aR)-8-hydroxy-5-isopropyl-3,8-dimethyl-1,4a,5,6,7,8a-hexahydronaphthalen-2-one	15275959	FALSE	C1C(=O)C(=CC2C(CCC(C12)(C)O)C(C)C)C
MOL001250	0.6410	0.3590	0.8114	Olibanun	O-acetyl-β-boswellic acid	Not Available	FALSE	O=C(OC1CCC2(C(C1(C)C(=O)O)CCC1(C2CC=C2C1(CCC1(C2C(C(CC1)C)C)C)C)C)C)C
MOL001251	0.5517	0.4483	0.7655	Olibanun	dihydroroburic acid	Not Available	FALSE	CC(C1C(CCC(=O)O)(C2C(CC1)(C1(C(=CC2)C2C(CC1)(CCC(C2C)C)C)C)C)C)C
MOL001252	0.9555	0.0445	0.9729	Olibanun	4-isopropylcyclohex-2-en-1-one	642520	FALSE	C1(=O)C=CC(CC1)C(C)C
MOL001252	0.9555	0.0445	0.9729	Piperis Fructus	4-isopropylcyclohex-2-en-1-one	642520	FALSE	C1(=O)C=CC(CC1)C(C)C
MOL001252	0.9555	0.0445	0.9729	Zanthoxyli Pericarpium	4-isopropylcyclohex-2-en-1-one	642520	FALSE	C1(=O)C=CC(CC1)C(C)C
MOL001252	0.9555	0.0445	0.9729	Evodiae Fructus	4-isopropylcyclohex-2-en-1-one	642520	FALSE	C1(=O)C=CC(CC1)C(C)C
MOL001253	0.3062	0.6938	0.7312	Olibanun	11-keto-α-amyrenone	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C2C(=O)C=C2C1(CCC1(C2C(C(CC1)C)C)C)C)C)C
MOL001254	0.9544	0.0456	0.9777	Zingiber Officinale Roscoe	(S)-p-Mentha-1,8-dien-7-al	2724159	FALSE	C1(CCC(=CC1)C=O)C(=C)C
MOL001254	0.9544	0.0456	0.9777	Olibanun	(S)-p-Mentha-1,8-dien-7-al	2724159	FALSE	C1(CCC(=CC1)C=O)C(=C)C
MOL001254	0.9544	0.0456	0.9777	Herba Patriniae	(S)-p-Mentha-1,8-dien-7-al	2724159	FALSE	C1(CCC(=CC1)C=O)C(=C)C
MOL001254	0.9544	0.0456	0.9777	Ephedra Herba	(S)-p-Mentha-1,8-dien-7-al	2724159	FALSE	C1(CCC(=CC1)C=O)C(=C)C
MOL001254	0.9544	0.0456	0.9777	Adenophprae Ae Radix	(S)-p-Mentha-1,8-dien-7-al	2724159	FALSE	C1(CCC(=CC1)C=O)C(=C)C
MOL001254	0.9544	0.0456	0.9777	Folium Artemisiae Argyi	(S)-p-Mentha-1,8-dien-7-al	2724159	FALSE	C1(CCC(=CC1)C=O)C(=C)C

MOL001255	0.7487	0.2513	0.8599	Hemerocallis Radix	Boswellic acid	168928	FALSE	C12C(C3(C(=CC2)C2C(CC3)(CCC(C2C)C)C)C)(CCC2C1(CCC(C2(C(=O)O)C)O)C)C
MOL001255	0.7487	0.2513	0.8599	Olibanun	Boswellic acid	168928	FALSE	C12C(C3(C(=CC2)C2C(CC3)(CCC(C2C)C)C)C)(CCC2C1(CCC(C2(C(=O)O)C)O)C)C
MOL001256	0.9424	0.0576	0.8744	Olibanun	α-campholenaldehyde	Not Available	FALSE	C1=C(C(C(C1)CC=C)(C)C)C
MOL001257	0.9076	0.0924	0.9621	Olibanun	D-arabinonic acid	122045	FALSE	C(C(C(=O)O)O)(C(CO)O)O
MOL001258	0.9453	0.0547	0.9737	Olibanun	trans-Sobrerol	854498	FALSE	C1(CC(CC=C1C)C(C)(C)O)O
MOL001259	0.7148	0.2852	0.8064	Olibanun	(3R,4R,4aR,6aR,6bS,8aR,11R,12S,12aR,14aR,14bS)-3-hydroxy-4,6a,6b,8a,11,12,14b-heptamethyl-14-oxo-1,2,3,4a,5,6,7,8,9,10,11,12,12a,14a-tetradecahydropicene-4-carboxylic acid	9847548	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1=O)C1C(CC2)(CCC(C1C)C)C)C)C)C)(C)C(=O)O)O
MOL001260	0.9531	0.0469	0.9642	Olibanun	3,6-dihydroxy-p-menth-1-ene	13919075	FALSE	C1=C(C(CC(C1O)C(C)C)O)C
MOL001261	0.9556	0.0444	0.8860	Olibanun	Acetyl-m-xylene	6985	FALSE	c1(c(cc(cc1)C)C)C(=O)C
MOL001262	0.2068	0.7932	0.7271	Olibanun	3-hydroxy-tirucallic,acid	40469707	FALSE	C1C(C(C2C(C1)(C1=C(CC2)C2(C(CC1)(C(CC2)C(C)CCC=C(C)C)C)C)C)(C)C)O
MOL001263	0.5755	0.4245	0.7720	Olibanun	3-oxo-tirucallic,acid	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=C(CC2)C2(C(CC1)(C(CC2)C(CCC=C(C)C)C(=O)O)C)C)(C)C
MOL001264	0.6444	0.3556	0.8037	Olibanun	acetyl-11-keto-beta-boswellic,acid	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1=O)C1C(CC2)(CCC(C1C)C)C)C)C)C)(C)C(=O)O)OC(=O)C
MOL001265	0.6543	0.3457	0.8196	Olibanun	acetyl-alpha-boswellic,acid	15181201	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C)C)C)C)(C(=O)O)C)OC(=O)C
MOL001266	0.6410	0.3590	0.8114	Olibanun	acetyl-beta-boswellic,acid	Not Available	FALSE	C1CC(C(C2C1(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1C)C)C)C)C)C)(C)C(=O)O)OC(=O)C

MOL001267	0.9618	0.0382	0.8292	Olibanun	(1S,3S,5R)-3,6,6-trimethylnorpinan-2-one	21675519	FALSE	C1(=O)C(CC2CC1C2(C)C)C
MOL001268	0.7487	0.2513	0.8599	Olibanun	beta-boswellic,acid	Not Available	FALSE	C1CC(C(C2C1(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1C)C)C)C)C)C)(C)C(=O)O)O
MOL001271	0.3812	0.6188	0.7418	Olibanun	epilupeol	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=C)C)C)C)C)C)(C)C)O
MOL001273	0.9569	0.0431	0.8029	Peucedanidecursivi Radix	80-57-9	65724	FALSE	C12C(=O)C=C(C(C1(C)C)C2)C
MOL001273	0.9569	0.0431	0.8029	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	80-57-9	65724	FALSE	C12C(=O)C=C(C(C1(C)C)C2)C
MOL001273	0.9569	0.0431	0.8029	Peucedani Radix	80-57-9	65724	FALSE	C12C(=O)C=C(C(C1(C)C)C2)C
MOL001273	0.9569	0.0431	0.8029	Olibanun	80-57-9	65724	FALSE	C12C(=O)C=C(C(C1(C)C)C2)C
MOL001273	0.9569	0.0431	0.8029	Angelicae Sinensis Radix	80-57-9	65724	FALSE	C12C(=O)C=C(C(C1(C)C)C2)C
MOL001273	0.9569	0.0431	0.8029	Campsis Flos	80-57-9	65724	FALSE	C12C(=O)C=C(C(C1(C)C)C2)C
MOL001273	0.9569	0.0431	0.8029	Radix Bupleuri	80-57-9	65724	FALSE	C12C(=O)C=C(C(C1(C)C)C2)C
MOL001273	0.9569	0.0431	0.8029	Schizonepetae Spica	80-57-9	65724	FALSE	C12C(=O)C=C(C(C1(C)C)C2)C
MOL001276	0.1603	0.8397	0.7219	Olibanun	isocembrene	Not Available	FALSE	C1(=C)CCC2=C(C3C(C(C2=C1)C(C)C)CC(=CC3)C)C
MOL001277	0.2251	0.7749	0.7475	Olibanun	isofpuquierol	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(C)(O)C/C=C/C(C)(C)O)C)C)(C)C)O
MOL001281	0.6054	0.3946	0.6301	Quisqualis Indica	L-alpha-Palmitin	11359451	FALSE	CCCCCCCCCCCCCCCC(=O)OCC(CO)O
MOL001281	0.6054	0.3946	0.6301	Carthami Flos	L-alpha-Palmitin	11359451	FALSE	CCCCCCCCCCCCCCCC(=O)OCC(CO)O
MOL001281	0.6054	0.3946	0.6301	Siegesbeckiae Herba	L-alpha-Palmitin	11359451	FALSE	CCCCCCCCCCCCCCCC(=O)OCC(CO)O
MOL001281	0.6054	0.3946	0.6301	Sparganii Rhizoma	L-alpha-Palmitin	11359451	FALSE	CCCCCCCCCCCCCCCC(=O)OCC(CO)O
MOL001281	0.6054	0.3946	0.6301	Citri Sarcodactylis Fructus	L-alpha-Palmitin	11359451	FALSE	CCCCCCCCCCCCCCCC(=O)OCC(CO)O
MOL001281	0.6054	0.3946	0.6301	Arum Ternatum Thunb.	L-alpha-Palmitin	11359451	FALSE	CCCCCCCCCCCCCCCC(=O)OCC(CO)O
MOL001281	0.6054	0.3946	0.6301	Olibanun	L-alpha-Palmitin	11359451	FALSE	CCCCCCCCCCCCCCCC(=O)OCC(CO)O
MOL001281	0.6054	0.3946	0.6301	Arisaematis Rhizoma	L-alpha-Palmitin	11359451	FALSE	CCCCCCCCCCCCCCCC(=O)OCC(CO)O
MOL001281	0.6054	0.3946	0.6301	Isatdis Radix	L-alpha-Palmitin	11359451	FALSE	CCCCCCCCCCCCCCCC(=O)OCC(CO)O
MOL001282	0.3812	0.6188	0.7418	Olibanun	lup-20(29)-en-3-ol	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=C)C)C)C)C)C)(C)C)O
MOL001283	0.8642	0.1358	0.7920	Campsis Flos	C09704	5281525	FALSE	C(C)(C=C)(CC/C=C(\C)/CCC=C(C)C)O
MOL001283	0.8642	0.1358	0.7920	Perillae Fructus	C09704	5281525	FALSE	C(C)(C=C)(CC/C=C(\C)/CCC=C(C)C)O
MOL001283	0.8642	0.1358	0.7920	Eriobotryae Folium	C09704	5281525	FALSE	C(C)(C=C)(CC/C=C(\C)/CCC=C(C)C)O

MOL001283	0.8642	0.1358	0.7920	Lonicerae Japonicae Flos	C09704	5281525	FALSE	C(C)(C=C)(CC/C=C(\C)/CCC=C(C)C)O
MOL001283	0.8642	0.1358	0.7920	Ganoderma	C09704	5281525	FALSE	C(C)(C=C)(CC/C=C(\C)/CCC=C(C)C)O
MOL001283	0.8642	0.1358	0.7920	Radix Bupleuri	C09704	5281525	FALSE	C(C)(C=C)(CC/C=C(\C)/CCC=C(C)C)O
MOL001283	0.8642	0.1358	0.7920	Viticis Negundo Folium	C09704	5281525	FALSE	C(C)(C=C)(CC/C=C(\C)/CCC=C(C)C)O
MOL001283	0.8642	0.1358	0.7920	Olibanun	C09704	5281525	FALSE	C(C)(C=C)(CC/C=C(\C)/CCC=C(C)C)O
MOL001284	0.9068	0.0932	0.8907	Olibanun	neryl,acetate	Not Available	FALSE	CC(=CCC/C(=C\COC(=C)C)/C)C
MOL001285	0.9339	0.0661	0.9484	Raphani Semen	octanol	957	FALSE	C(CCCCCCC)O
MOL001285	0.9339	0.0661	0.9484	Ephedra Herba	octanol	957	FALSE	C(CCCCCCC)O
MOL001285	0.9339	0.0661	0.9484	Dianthi Herba	octanol	957	FALSE	C(CCCCCCC)O
MOL001285	0.9339	0.0661	0.9484	Achyranthis Bidentatae Radix	octanol	957	FALSE	C(CCCCCCC)O
MOL001285	0.9339	0.0661	0.9484	Panacis Quinquefolii Radix	octanol	957	FALSE	C(CCCCCCC)O
MOL001285	0.9339	0.0661	0.9484	Meliae Azedarach Fructus	octanol	957	FALSE	C(CCCCCCC)O
MOL001285	0.9339	0.0661	0.9484	Radix Angelicae Biseratae	octanol	957	FALSE	C(CCCCCCC)O
MOL001285	0.9339	0.0661	0.9484	Morindae Officinalis Radix	octanol	957	FALSE	C(CCCCCCC)O
MOL001285	0.9339	0.0661	0.9484	Ginkgo Folium	octanol	957	FALSE	C(CCCCCCC)O
MOL001285	0.9339	0.0661	0.9484	Lonicerae Japonicae Flos	octanol	957	FALSE	C(CCCCCCC)O
MOL001285	0.9339	0.0661	0.9484	Olibanun	octanol	957	FALSE	C(CCCCCCC)O
MOL001285	0.9339	0.0661	0.9484	Arisaematis Rhizoma	octanol	957	FALSE	C(CCCCCCC)O
MOL001286	0.9446	0.0554	0.8450	Olibanun	olibanumol,a	44233146	FALSE	C12C(C(CC(C1(O)C)O)C(C)C)O2
MOL001287	0.9511	0.0489	0.8058	Olibanun	olibanumol,b	44233147	FALSE	C12CC1(CC(C2(O)C)O)C(C)C
MOL001288	0.9445	0.0555	0.9758	Olibanun	olibanumol,c	15512326	FALSE	C1C(=CCC(C(C)C)(C1)O)CO
MOL001289	0.3783	0.6217	0.7784	Olibanun	olibanumol,h	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(C)(C)CO)C)C)C)(C)C)O
MOL001290	0.3424	0.6576	0.7567	Olibanun	olibanumol,i	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=O)C)C)C)C)(C)C)O
MOL001291	0.2593	0.7407	0.6694	Olibanun	olibanumol,j	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C(CC2)C(CCC(O)C(C)(C)O)C)C)C)(C)C)O
MOL001292	0.9485	0.0515	0.9731	Olibanun	(1R,3S)-1-isopropyl-4-methylcyclohex-4-ene-1,3-diol	11789644	FALSE	C1=C(C(CC(C1)(C(C)C)O)O)C
MOL001293	0.9509	0.0491	0.9695	Olibanun	p-menth-4-en-1,2-diol	Not Available	FALSE	C1C=C(CC(C1(C)O)O)C(C)C
MOL001294	0.9496	0.0504	0.9665	Olibanun	p-menth-5-en-1,2-diol	26176656	FALSE	C1=CC(CC(C1(C)O)O)C(C)C
MOL001295	0.2054	0.7946	0.6534	Olibanun	phyllocladene	Not Available	FALSE	C12CCC3C(CC1=C)(CCC1C3(CCCC1(C)C)C)C2
MOL001296	0.9619	0.0381	0.7610	Curcumae Radix	(1R,5R)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	10887971	FALSE	C1C(=C)C2C(C1)(C(C)C)C2

MOL001296	0.9619	0.0381	0.7610	Coriandri Sativi Herba	(1R,5R)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	10887971	FALSE	C1C(=C)C2C(C1)(C(C)C)C2
MOL001296	0.9619	0.0381	0.7610	Olibanun	(1R,5R)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	10887971	FALSE	C1C(=C)C2C(C1)(C(C)C)C2
MOL001296	0.9619	0.0381	0.7610	Litseae Fructus	(1R,5R)-1-isopropyl-4-methylenebicyclo[3.1.0]hexane	10887971	FALSE	C1C(=C)C2C(C1)(C(C)C)C2
MOL001298	0.7954	0.2046	0.7567	Sparganii Rhizoma	dehydrocostus lactone	73174	FALSE	O1C2C(C(=C)C1=O)CCC(=C)C1CCC(=C)C21
MOL001298	0.7954	0.2046	0.7567	Saussureae Involucratae Herba	dehydrocostus lactone	73174	FALSE	O1C2C(C(=C)C1=O)CCC(=C)C1CCC(=C)C21
MOL001299	0.9167	0.0833	0.8980	Sparganii Rhizoma	(1S,2S)-1,2-bis(2-furyl)ethane-1,2-diol	10607833	FALSE	C(O)(c1occc1)C(O)c1occc1
MOL001300	0.9359	0.0641	0.9554	Platycladi Cacumen	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Cinnanmomi Cortex	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Fructus Ligustri Lucidi	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Uncariae Ramulus Cumuncis	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Lysimachiae Foenigraeci Herba	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Bombyx Mori L.	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Dysosmae Verspiellis Rhixoma Et Radix	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Siphonostegiae Herba	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Ilicis Purpureae Folium	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Morindae Officinalis Radix	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Paederiae Scandentis Herba	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Eriobotryae Folium	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Junci Medulla	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Dianthi Herba	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Daturae Flos	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Cornus Officinalis Sieb. Et Zucc.	PEL	6054	FALSE	C(Cc1ccccc1)O

MOL001300	0.9359	0.0641	0.9554	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Humulus Scandens (Lour.) Merr.	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Ginkgo Folium	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Litchi Semen	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Lonicerae Japonicae Flos	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Ilicis Cornutae Folium Immayuri	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Rose Rugosae Flos	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Scutellariae Barbatae Herba	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Radix Clematidis	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Mume Flos	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Cinnamomi Ramulus	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Hippophae Fructus	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Caryophylliflos	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Flos Genkwa	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Violsse Herba	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Ardisiae Japonicae Herba	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Campsis Flos	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Oroxyli Semen	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Sparganii Rhizoma	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Scutellariae Radix	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Farfarae Flos	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001300	0.9359	0.0641	0.9554	Buddlejae Flos	PEL	6054	FALSE	C(Cc1ccccc1)O
MOL001301	0.9278	0.0722	0.9110	Radix Rhei Et Rhizome	cis-Zimtsaeure	5372954	FALSE	C(=O)(/C=C\c1ccccc1)O
MOL001301	0.9278	0.0722	0.9110	Selaginella Doederleinii Hieron	cis-Zimtsaeure	5372954	FALSE	C(=O)(/C=C\c1ccccc1)O
MOL001301	0.9278	0.0722	0.9110	Picrorhizae Rhizoma	cis-Zimtsaeure	5372954	FALSE	C(=O)(/C=C\c1ccccc1)O
MOL001301	0.9278	0.0722	0.9110	Figwort Root	cis-Zimtsaeure	5372954	FALSE	C(=O)(/C=C\c1ccccc1)O
MOL001301	0.9278	0.0722	0.9110	Sparganii Rhizoma	cis-Zimtsaeure	5372954	FALSE	C(=O)(/C=C\c1ccccc1)O
MOL001301	0.9278	0.0722	0.9110	Cinnamomi Ramulus	cis-Zimtsaeure	5372954	FALSE	C(=O)(/C=C\c1ccccc1)O
MOL001301	0.9278	0.0722	0.9110	Lycii Cortex	cis-Zimtsaeure	5372954	FALSE	C(=O)(/C=C\c1ccccc1)O
MOL001301	0.9278	0.0722	0.9110	Curcumae Radix	cis-Zimtsaeure	5372954	FALSE	C(=O)(/C=C\c1ccccc1)O
MOL001302	0.9276	0.0724	0.9413	Angelicae Sinensis Radix	Usaf hc-1	5192	FALSE	C(=O)(CCCCCCCCC(=O)O)O
MOL001302	0.9276	0.0724	0.9413	Sparganii Rhizoma	Usaf hc-1	5192	FALSE	C(=O)(CCCCCCCCC(=O)O)O
MOL001302	0.9276	0.0724	0.9413	Ranunculi Ternati Radix	Usaf hc-1	5192	FALSE	C(=O)(CCCCCCCCC(=O)O)O
MOL001302	0.9276	0.0724	0.9413	Isatdis Radix	Usaf hc-1	5192	FALSE	C(=O)(CCCCCCCCC(=O)O)O

MOL001303	0.8619	0.1381	0.6520	Folium Artemisiae Argyi	(1R,2R,4S)-2,4-diisopropenyl-1-methyl-1-vinylcyclohexane	9859094	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C)C=C
MOL001303	0.8619	0.1381	0.6520	Leonuri Herba	(1R,2R,4S)-2,4-diisopropenyl-1-methyl-1-vinylcyclohexane	9859094	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C)C=C
MOL001303	0.8619	0.1381	0.6520	Radix Bupleuri	(1R,2R,4S)-2,4-diisopropenyl-1-methyl-1-vinylcyclohexane	9859094	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C)C=C
MOL001303	0.8619	0.1381	0.6520	Sparganii Rhizoma	(1R,2R,4S)-2,4-diisopropenyl-1-methyl-1-vinylcyclohexane	9859094	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C)C=C
MOL001303	0.8619	0.1381	0.6520	Radix Salviae	(1R,2R,4S)-2,4-diisopropenyl-1-methyl-1-vinylcyclohexane	9859094	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C)C=C
MOL001304	0.8782	0.1218	0.9292	Sparganii Rhizoma	2-ACETYLPYRROLE	14079	FALSE	[nH]1c(ccc1)C(=O)C
MOL001304	0.8782	0.1218	0.9292	Bombyx Mori L.	2-ACETYLPYRROLE	14079	FALSE	[nH]1c(ccc1)C(=O)C
MOL001304	0.8782	0.1218	0.9292	Radix Clematidis	2-ACETYLPYRROLE	14079	FALSE	[nH]1c(ccc1)C(=O)C
MOL001304	0.8782	0.1218	0.9292	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	2-ACETYLPYRROLE	14079	FALSE	[nH]1c(ccc1)C(=O)C

MOL001304	0.8782	0.1218	0.9292	Campsis Flos	2-ACETYLPYRROLE	14079	FALSE	[nH]1c(ccc1)C(=O)C
MOL001304	0.8782	0.1218	0.9292	Bolbostemae Paniculati Bulbus	2-ACETYLPYRROLE	14079	FALSE	[nH]1c(ccc1)C(=O)C
MOL001304	0.8782	0.1218	0.9292	Momordicae Fructus	2-ACETYLPYRROLE	14079	FALSE	[nH]1c(ccc1)C(=O)C
MOL001305	0.9541	0.0459	0.8843	Sparganii Rhizoma	3,4-dihydro-8-hydroxy-3-methyl-1H-2-benzopyran-4-one	Not Available	FALSE	C1(C(=O)c2c(CO1)c(ccc2)O)C
MOL001306	0.9345	0.0655	0.9238	Evodiae Fructus	o-Acetyl-p-cresol	15068	FALSE	c1(c(cc(cc1)C)C(=O)C)O
MOL001306	0.9345	0.0655	0.9238	Radix Clematidis	o-Acetyl-p-cresol	15068	FALSE	c1(c(cc(cc1)C)C(=O)C)O
MOL001306	0.9345	0.0655	0.9238	Lysimachiae Herba	o-Acetyl-p-cresol	15068	FALSE	c1(c(cc(cc1)C)C(=O)C)O
MOL001306	0.9345	0.0655	0.9238	Sparganii Rhizoma	o-Acetyl-p-cresol	15068	FALSE	c1(c(cc(cc1)C)C(=O)C)O
MOL001306	0.9345	0.0655	0.9238	Chuanxiong Rhizoma	o-Acetyl-p-cresol	15068	FALSE	c1(c(cc(cc1)C)C(=O)C)O
MOL001306	0.9345	0.0655	0.9238	Radix Angelicae Biseratae	o-Acetyl-p-cresol	15068	FALSE	c1(c(cc(cc1)C)C(=O)C)O
MOL001306	0.9345	0.0655	0.9238	Angelicae Sinensis Radix	o-Acetyl-p-cresol	15068	FALSE	c1(c(cc(cc1)C)C(=O)C)O
MOL001307	0.8755	0.1245	0.7188	Sparganii Rhizoma	6,7,10-Trihydroxy-8-octadecenoic acid	Not Available	FALSE	C(=O)(CCCCC(C(/C=C/C(CCCCCCCC)O)O)O)O
MOL001308	0.7657	0.2343	0.6074	Radix Cynanchi	oleic acid	637517	FALSE	C(=O)(CCCCCCC/C=C/CCCCCCCC)O
MOL001308	0.7657	0.2343	0.6074	Croci Stigma	oleic acid	637517	FALSE	C(=O)(CCCCCCC/C=C/CCCCCCCC)O
MOL001308	0.7657	0.2343	0.6074	Semen Firmianae	oleic acid	637517	FALSE	C(=O)(CCCCCCC/C=C/CCCCCCCC)O
MOL001308	0.7657	0.2343	0.6074	Semen Lini	oleic acid	637517	FALSE	C(=O)(CCCCCCC/C=C/CCCCCCCC)O
MOL001308	0.7657	0.2343	0.6074	Mylabris	oleic acid	637517	FALSE	C(=O)(CCCCCCC/C=C/CCCCCCCC)O
MOL001308	0.7657	0.2343	0.6074	Myristicae Semen	oleic acid	637517	FALSE	C(=O)(CCCCCCC/C=C/CCCCCCCC)O
MOL001308	0.7657	0.2343	0.6074	Citri Sarcodactylis Fructus	oleic acid	637517	FALSE	C(=O)(CCCCCCC/C=C/CCCCCCCC)O
MOL001308	0.7657	0.2343	0.6074	Et Radix Patriniae Rhizoma	oleic acid	637517	FALSE	C(=O)(CCCCCCC/C=C/CCCCCCCC)O

MOL001308	0.7657	0.2343	0.6074	Alpiniae Oxyphyliae Fructus	oleic acid	637517	FALSE	C(=O)(CCCCCCC/C=C/CCCCCCCC)O
MOL001308	0.7657	0.2343	0.6074	Lablab Semen Album	oleic acid	637517	FALSE	C(=O)(CCCCCCC/C=C/CCCCCCCC)O
MOL001308	0.7657	0.2343	0.6074	Ginkgo Semen	oleic acid	637517	FALSE	C(=O)(CCCCCCC/C=C/CCCCCCCC)O
MOL001308	0.7657	0.2343	0.6074	Sparganii Rhizoma	oleic acid	637517	FALSE	C(=O)(CCCCCCC/C=C/CCCCCCCC)O
MOL001308	0.7657	0.2343	0.6074	Polygonati Odorati Rhizoma	oleic acid	637517	FALSE	C(=O)(CCCCCCC/C=C/CCCCCCCC)O
MOL001308	0.7657	0.2343	0.6074	Eriocauli Flos	oleic acid	637517	FALSE	C(=O)(CCCCCCC/C=C/CCCCCCCC)O
MOL001308	0.7657	0.2343	0.6074	Corayceps	oleic acid	637517	FALSE	C(=O)(CCCCCCC/C=C/CCCCCCCC)O
MOL001309	0.9018	0.0982	0.9389	Codonopsis Radix	6-methylolpyridin-3-ol	419490	FALSE	c1(ccc(cn1)O)CO
MOL001309	0.9018	0.0982	0.9389	Sparganii Rhizoma	6-methylolpyridin-3-ol	419490	FALSE	c1(ccc(cn1)O)CO
MOL001310	0.7391	0.2609	0.9223	Lycopi Herba	Epibetulinic acid	485711	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C(=C)C)C4C3CCC21)C)O
MOL001310	0.7391	0.2609	0.9223	Sparganii Rhizoma	Epibetulinic acid	485711	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C(=C)C)C4C3CCC21)C)O
MOL001311	0.7715	0.2285	0.6306	Sparganii Rhizoma	Ricineic acid	5282796	FALSE	C(=O)(CCCCCCC/C=C/C=C/CCCCCC)O
MOL001312	0.8576	0.1424	0.6905	Ardisiae Japonicae Herba	9-HEXADECENOIC ACID	5282745	FALSE	C(=O)(CCCCCCC/C=C/CCCCCC)O
MOL001312	0.8576	0.1424	0.6905	Viticis Fructus	9-HEXADECENOIC ACID	5282745	FALSE	C(=O)(CCCCCCC/C=C/CCCCCC)O
MOL001312	0.8576	0.1424	0.6905	Sparganii Rhizoma	9-HEXADECENOIC ACID	5282745	FALSE	C(=O)(CCCCCCC/C=C/CCCCCC)O
MOL001312	0.8576	0.1424	0.6905	Oroxyli Semen	9-HEXADECENOIC ACID	5282745	FALSE	C(=O)(CCCCCCC/C=C/CCCCCC)O
MOL001312	0.8576	0.1424	0.6905	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	9-HEXADECENOIC ACID	5282745	FALSE	C(=O)(CCCCCCC/C=C/CCCCCC)O
MOL001312	0.8576	0.1424	0.6905	Panax Ginseng C. A. Mey.	9-HEXADECENOIC ACID	5282745	FALSE	C(=O)(CCCCCCC/C=C/CCCCCC)O
MOL001313	0.8883	0.1117	0.7199	Sparganii Rhizoma	sanleng	Not Available	FALSE	C(=O)(CCCCC(/C=C/C(C(CCCCCCCC)O)O)O)O
MOL001314	0.9297	0.0703	0.9549	Arisaematis Rhizoma	Azelex	19347555	FALSE	C(=O)(CCCCCCCC(=O)O)O
MOL001314	0.9297	0.0703	0.9549	Cichorii Radix	Azelex	19347555	FALSE	C(=O)(CCCCCCCC(=O)O)O
MOL001314	0.9297	0.0703	0.9549	Sparganii Rhizoma	Azelex	19347555	FALSE	C(=O)(CCCCCCCC(=O)O)O

MOL001314	0.9297	0.0703	0.9549	Cynanchistauntonii Rhizoma Et Radix	Azelex	19347555	FALSE	C(=O)(CCCCCCCC(=O)O)O
MOL001314	0.9297	0.0703	0.9549	Codonopsis Radix	Azelex	19347555	FALSE	C(=O)(CCCCCCCC(=O)O)O
MOL001314	0.9297	0.0703	0.9549	Hordei Fructus Germinatus	Azelex	19347555	FALSE	C(=O)(CCCCCCCC(=O)O)O
MOL001314	0.9297	0.0703	0.9549	Ranunculi Ternati Radix	Azelex	19347555	FALSE	C(=O)(CCCCCCCC(=O)O)O
MOL001314	0.9297	0.0703	0.9549	Cortex Hibisci	Azelex	19347555	FALSE	C(=O)(CCCCCCCC(=O)O)O
MOL001314	0.9297	0.0703	0.9549	Mahoniae Caulis	Azelex	19347555	FALSE	C(=O)(CCCCCCCC(=O)O)O
MOL001314	0.9297	0.0703	0.9549	Angelicae Sinensis Radix	Azelex	19347555	FALSE	C(=O)(CCCCCCCC(=O)O)O
MOL001314	0.9297	0.0703	0.9549	Achyranthis Bidentatae Radix	Azelex	19347555	FALSE	C(=O)(CCCCCCCC(=O)O)O
MOL001314	0.9297	0.0703	0.9549	Cortex Periplocae Radicis	Azelex	19347555	FALSE	C(=O)(CCCCCCCC(=O)O)O
MOL001314	0.9297	0.0703	0.9549	Radix Cynanchi	Azelex	19347555	FALSE	C(=O)(CCCCCCCC(=O)O)O
MOL001314	0.9297	0.0703	0.9549	Ailanthi Cortex	Azelex	19347555	FALSE	C(=O)(CCCCCCCC(=O)O)O
MOL001314	0.9297	0.0703	0.9549	Broussonetiae Fructus	Azelex	19347555	FALSE	C(=O)(CCCCCCCC(=O)O)O
MOL001314	0.9297	0.0703	0.9549	Artemisiae Scopariae Herba	Azelex	19347555	FALSE	C(=O)(CCCCCCCC(=O)O)O
MOL001319	0.9499	0.0501	0.8968	Persicae Semen	3-feruloylquinic acid	Not Available	FALSE	c1(c(cc(cc1)/C=C/C(=O)OC1C(C(CC(C1)(O)C(=O)O)O)O)O)OC)O
MOL001320	0.9169	0.0831	0.8031	Eriobotryae Folium	Amygdalin	656516	FALSE	c1(ccccc1)C(C#N)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)CO
MOL001320	0.9169	0.0831	0.8031	Amygdalus Communis Vas	Amygdalin	656516	FALSE	c1(ccccc1)C(C#N)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)CO
MOL001320	0.9169	0.0831	0.8031	Chaenomeles Sinensis (Thouin) Koehne	Amygdalin	656516	FALSE	c1(ccccc1)C(C#N)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)CO
MOL001320	0.9169	0.0831	0.8031	Mume Fructus	Amygdalin	656516	FALSE	c1(ccccc1)C(C#N)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)CO
MOL001320	0.9169	0.0831	0.8031	Semen Pruni	Amygdalin	656516	FALSE	c1(ccccc1)C(C#N)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)CO
MOL001320	0.9169	0.0831	0.8031	Persicae Semen	Amygdalin	656516	FALSE	c1(ccccc1)C(C#N)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)CO
MOL001321	0.9367	0.0633	0.9676	Persicae Semen	d-mandelonitrile	9548674	FALSE	c1(ccccc1)C(C#N)O
MOL001321	0.9367	0.0633	0.9676	Perilla Frutescens	d-mandelonitrile	9548674	FALSE	c1(ccccc1)C(C#N)O
MOL001321	0.9367	0.0633	0.9676	Amygdalus Communis Vas	d-mandelonitrile	9548674	FALSE	c1(ccccc1)C(C#N)O
MOL001323	0.2190	0.7810	0.6457	Citri Sarcodactylis Fructus	Sitosterol alpha1	9548595	FALSE	C1(CCC2(C(C1C)CC=C1C3CCC(C(CC/C(=C/C)/C(C)C)C)C3(C)CCC21)C)O
MOL001323	0.2190	0.7810	0.6457	Lycii Fructus	Sitosterol alpha1	9548595	FALSE	C1(CCC2(C(C1C)CC=C1C3CCC(C(CC/C(=C/C)/C(C)C)C)C3(C)CCC21)C)O
MOL001323	0.2190	0.7810	0.6457	Persicae Semen	Sitosterol alpha1	9548595	FALSE	C1(CCC2(C(C1C)CC=C1C3CCC(C(CC/C(=C/C)/C(C)C)C)C3(C)CCC21)C)O

MOL001323	0.2190	0.7810	0.6457	Coicis Semen	Sitosterol alpha1	9548595	FALSE	C1(CCC2(C(C1C)CC=C1C3CCC(C(CC/C(=C/C)/C(C)C)C)C3(C)CCC21)C)O
MOL001327	0.8346	0.1654	0.8197	Persicae Semen	2,3-didehydro GA69	Not Available	FALSE	C1C=CC2(C3C1(C1C4(C3C(=O)O)CC(C(C1)O)C(=C)C4)OC2=O)C
MOL001328	0.8346	0.1654	0.8197	Persicae Semen	2,3-didehydro GA70	Not Available	FALSE	C1C=CC2(C3C1(C1C4(C3C(=O)O)CC(C(C1)O)C(=C)C4)OC2=O)C
MOL001329	0.8694	0.1306	0.8322	Persicae Semen	2,3-didehydro GA77	Not Available	FALSE	C1C=CC2(C3C1(C1C4(C3C(=O)O)CC(C(C1)O)(O)C(=C)C4)OC2=O)C
MOL001330	0.7830	0.2170	0.8258	Persicae Semen	2,3-didehydro GA9	Not Available	FALSE	C1C=CC2(C3C1(C1C4(C3C(=O)O)CC(CC1)C(=C)C4)OC2=O)C
MOL001331	0.8972	0.1028	0.8208	Persicae Semen	Amygdalinic acid	Not Available	FALSE	c1ccc(cc1)C(C(=O)O)OC1C(C(C(C(O1)COC1C(C(C(C(O1)CO)O)O)O)O)O)O
MOL001332	0.9513	0.0487	0.9659	Persicae Semen	RMN	11914	FALSE	c1ccc(cc1)C(C(=O)O)O
MOL001333	0.2107	0.7893	0.6251	Persicae Semen	7-dehydroavenasterol	12795736	FALSE	C1(CCC2(C(C1)CC=C1C3CCC(C(CC/C(=C/C)/C(C)C)C)C3(C)CCC21)C)O
MOL001334	0.9269	0.0731	0.8229	Persicae Semen	Benzyl Beta -gentiobioside	Not Available	FALSE	c1ccc(cc1)COC1C(C(C(C(O1)COC1C(C(C(C(O1)CO)O)O)O)O)O)O)O
MOL001335	0.8932	0.1068	0.9598	Morindae Officinalis Radix	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Rhododendri Daurici Folium	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Radix Clematidis	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Dioscoreaebulbiferae	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Chuanxiong Rhizoma	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Persicae Semen	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Ranunculi Ternati Radix	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Farfarae Flos	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Daturae Flos	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Bombyx Mori L.	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Campsis Flos	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Rose Rugosae Flos	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Humulus Scandens (Lour.) Merr.	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Ilicis Cornutae Folium Immayuri	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Litchi Semen	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Mume Flos	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Hippophae Fructus	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Ephedra Herba	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Ilicis Purpureae Folium	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Scutellariae Barbatae Herba	WLN: Q1R	244	FALSE	c1ccc(cc1)CO

MOL001335	0.8932	0.1068	0.9598	Eriobotryae Folium	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Acoritataninowii Rhizoma	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Caryophylliflos	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Cistanches Herba	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Ginkgo Folium	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Mori Fructus	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Momordicae Fructus	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001335	0.8932	0.1068	0.9598	Jujubae Fructus	WLN: Q1R	244	FALSE	c1ccc(cc1)CO
MOL001336	0.9313	0.0687	0.9044	Persicae Semen	(2S,3R,4S,5S,6R)-2-(benzyloxy)-6-methylol-tetrahydropyran-3,4,5-triol	7918796	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)Cc1ccccc1
MOL001336	0.9313	0.0687	0.9044	Ranunculi Ternati Radix	(2S,3R,4S,5S,6R)-2-(benzyloxy)-6-methylol-tetrahydropyran-3,4,5-triol	7918796	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)Cc1ccccc1
MOL001337	0.9313	0.0687	0.9044	Carthami Flos	Benzyl glucopyranoside	188977	FALSE	c1cc(ccc1)COC1C(O)C(O)C(O)C(O1)CO
MOL001337	0.9313	0.0687	0.9044	Persicae Semen	Benzyl glucopyranoside	188977	FALSE	c1cc(ccc1)COC1C(O)C(O)C(O)C(O1)CO
MOL001337	0.9313	0.0687	0.9044	Dioscoreaebulbiferae	Benzyl glucopyranoside	188977	FALSE	c1cc(ccc1)COC1C(O)C(O)C(O)C(O1)CO
MOL001338	0.8644	0.1356	0.7969	Persicae Semen	GA118	Not Available	FALSE	C1CC2(C3C(C1O)(C1C4(C3C(=O)O)CC(CC1)(C(=C)C4)O)OC2=O)C
MOL001339	0.8396	0.1604	0.8341	Persicae Semen	GA119	Not Available	FALSE	C1CC2(C3C(C1O)(C1C4(C3C(=O)O)CC(CC1)C(=C)C4)OC2=O)C
MOL001340	0.7863	0.2137	0.8261	Persicae Semen	GA120	Not Available	FALSE	C1=CCC2(C3C1(C1C4(C3C(=O)O)CC(CC1)C(=C)C4)OC2=O)C
MOL001341	0.8361	0.1639	0.8185	Persicae Semen	GA121	Not Available	FALSE	C1=CCC2(C3C1(C1C4(C3C(=O)O)CC(C(C1)O)C(=C)C4)OC2=O)C
MOL001342	0.8489	0.1511	0.7970	Persicae Semen	GA121-isolactone	Not Available	FALSE	C1=C2C(C3(CC1OC3=O)C)C(C13C2CC(C(C1)C(=C)C3)O)C(=O)O
MOL001343	0.8361	0.1639	0.8185	Persicae Semen	GA122	Not Available	FALSE	C1=CCC2(C3C1(C1C4(C3C(=O)O)CC(C(C1)O)C(=C)C4)OC2=O)C
MOL001344	0.8489	0.1511	0.7970	Persicae Semen	GA122-isolactone	Not Available	FALSE	C1=C2C(C3(CC1OC3=O)C)C(C13C2CC(C(C1)C(=C)C3)O)C(=O)O

MOL001345	0.9377	0.0623	0.9142	Dioscoreaebulbiferae	Methyl-alpha-D-fructofuranoside	6325664	FALSE	OCC1(C(O)C(O)C(O1)CO)OC
MOL001345	0.9377	0.0623	0.9142	Persicae Semen	Methyl-alpha-D-fructofuranoside	6325664	FALSE	OCC1(C(O)C(O)C(O1)CO)OC
MOL001346	0.8683	0.1317	0.8340	Persicae Semen	GA126	Not Available	FALSE	C1=CCC2(C3C1(C1C4(C3C(=O)O)CC(C(C1)O)(O)C(=C)C4)OC2=O)C
MOL001347	0.8622	0.1378	0.8112	Persicae Semen	GA16	Not Available	FALSE	C1C(C2(C3C(C1O)(C1C4(C3C(=O)O)CC(CC1)C(=C)C4)OC2=O)C)O
MOL001348	0.8621	0.1379	0.7691	Semen Pharbitidis	gibberellin 17	Not Available	FALSE	C1CC(C2C(C1)(C1C3(C2C(=O)O)CC(CC1)(C(=C)C3)O)C(=O)O)(C)C(=O)O
MOL001348	0.8621	0.1379	0.7691	Persicae Semen	gibberellin 17	Not Available	FALSE	C1CC(C2C(C1)(C1C3(C2C(=O)O)CC(CC1)(C(=C)C3)O)C(=O)O)(C)C(=O)O
MOL001349	0.8327	0.1673	0.7738	Semen Pharbitidis	4a-formyl-7alpha-hydroxy-1-methyl-8-methylidene-4aalpha,4bbeta-gibbane-1alpha,10beta-dicarboxylic acid	Not Available	FALSE	C1CC(C2C(C1)(C1C3(C2C(=O)O)CC(CC1)(C(=C)C3)O)C=O)(C)C(=O)O
MOL001349	0.8327	0.1673	0.7738	Persicae Semen	4a-formyl-7alpha-hydroxy-1-methyl-8-methylidene-4aalpha,4bbeta-gibbane-1alpha,10beta-dicarboxylic acid	Not Available	FALSE	C1CC(C2C(C1)(C1C3(C2C(=O)O)CC(CC1)(C(=C)C3)O)C=O)(C)C(=O)O
MOL001350	0.8691	0.1309	0.7918	Persicae Semen	GA30	Not Available	FALSE	C1=CC(C2(C3C1(C1C4(C3C(=O)O)CC(C(C1)O)C(=C)C4)OC2=O)C)O
MOL001351	0.8023	0.1977	0.8010	Semen Pharbitidis	Gibberellin A44	Not Available	FALSE	C1CC2(C3C(C1)(C1C4(C3C(=O)O)CC(CC1)(C(=C)C4)O)COC2=O)C
MOL001351	0.8023	0.1977	0.8010	Persicae Semen	Gibberellin A44	Not Available	FALSE	C1CC2(C3C(C1)(C1C4(C3C(=O)O)CC(CC1)(C(=C)C4)O)COC2=O)C

MOL001352	0.8622	0.1378	0.8112	Persicae Semen	GA54	Not Available	FALSE	C1C(C2(C3C(C1O)(C1C4(C3C(=O)O)CC(CC1)C(=C)C4)OC2=O)C)O
MOL001353	0.8644	0.1356	0.7969	Persicae Semen	GA60	Not Available	FALSE	C1CC2(C3C(C1O)(C1C4(C3C(=O)O)CC(CC1)(C(=C)C4)O)OC2=O)C
MOL001354	0.8396	0.1604	0.8341	Persicae Semen	GA61	Not Available	FALSE	C1CC2(C3C(C1O)(C1C4(C3C(=O)O)CC(CC1)C(=C)C4)OC2=O)C
MOL001355	0.8687	0.1313	0.8016	Persicae Semen	GA63	Not Available	FALSE	C1C(C2(C3C(C1)(C1C4(C3C(=O)O)CC(CC1)C(=C)C4O)OC2=O)C)O
MOL001356	0.9353	0.0647	0.9514	Persicae Semen	MGL	445238	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)C
MOL001357	0.8413	0.1587	0.8232	Persicae Semen	GA69	Not Available	FALSE	C1CCC2(C3C1(C1C4(C3C(=O)O)CC(C(C1)O)C(=C)C4)OC2=O)C
MOL001358	0.8384	0.1616	0.8249	Persicae Semen	gibberellin 7	Not Available	FALSE	C1=CC(C2(C3C1(C1C4(C3C(=O)O)CC(CC1)C(=C)C4)OC2=O)C)O
MOL001359	0.8413	0.1587	0.8232	Persicae Semen	GA70	Not Available	FALSE	C1CCC2(C3C1(C1C4(C3C(=O)O)CC(C(C1)O)C(=C)C4)OC2=O)C
MOL001360	0.8719	0.1281	0.8326	Persicae Semen	GA77	Not Available	FALSE	C1CCC2(C3C1(C1C4(C3C(=O)O)CC(C(C1)O)(O)C(=C)C4)OC2=O)C
MOL001361	0.8873	0.1127	0.8709	Persicae Semen	GA87	Not Available	FALSE	C1=CC(C2(C3C1(C1C4(C3C(=O)O)CC(C(C1)O)(O)C(=C)C4)OC2=O)C)O
MOL001362	0.8352	0.1648	0.7917	Persicae Semen	GA95	Not Available	FALSE	C1=CCC2(C3C1(C1C4(C3C(=O)O)CC(CC1)(O)C(=C)C4)OC2=O)C
MOL001363	0.8261	0.1739	0.7621	Persicae Semen	GA97	Not Available	FALSE	C1(CC(C2C(C1)(C1C3(C2C(=O)O)CC(CC1)(C(=C)C3)O)C)(C)C(=O)O)O
MOL001364	0.9203	0.0797	0.8953	Persicae Semen	(2S)-2-phenyl-2-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyacetic acid	10125665	FALSE	C(=O)(C(c1ccccc1)OC1C(O)C(O)C(O)C(O1)CO)O
MOL001365	0.9187	0.0813	0.8740	Persicae Semen	prunasin	Not Available	FALSE	C1(C(C(C(C(O1)OC(c1ccccc1)C#N)O)O)O)O)CO
MOL001366	0.9367	0.0633	0.9676	Chaenomeles Sinensis (Thouin) Koehne	MNN	439767	FALSE	OC(c1ccccc1)C#N
MOL001366	0.9367	0.0633	0.9676	Amygdalus Communis Vas	MNN	439767	FALSE	OC(c1ccccc1)C#N
MOL001366	0.9367	0.0633	0.9676	Perilla Frutescens	MNN	439767	FALSE	OC(c1ccccc1)C#N
MOL001366	0.9367	0.0633	0.9676	Persicae Semen	MNN	439767	FALSE	OC(c1ccccc1)C#N
MOL001366	0.9367	0.0633	0.9676	Eriobotryae Folium	MNN	439767	FALSE	OC(c1ccccc1)C#N
MOL001366	0.9367	0.0633	0.9676	Semen Pruni	MNN	439767	FALSE	OC(c1ccccc1)C#N
MOL001366	0.9367	0.0633	0.9676	Mume Fructus	MNN	439767	FALSE	OC(c1ccccc1)C#N

MOL001367	0.9315	0.0685	0.9359	Persicae Semen	[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl] (E)-3-(4-hydroxyphenyl)prop-2-enoate	14158117	FALSE	O1C(C(C(C(C1OC(=O)/C=C/c1ccc(cc1)O)O)O)O)C O
MOL001368	0.9511	0.0489	0.9318	Persicae Semen	3-O-p-coumaroylquinic acid	Not Available	FALSE	C1(CC(C(C(C1)OC(=O)/C=C\c1ccc(cc1)O)O)O)(C(=O)O)O
MOL001369	0.8441	0.1559	0.7239	Persicae Semen	Grandidentatin	52041673	FALSE	C1CCC(C(C1)O)OC1C(C(C(C(O1)CO)O)O)OC(=O)/C=C/c1ccc(cc1)O
MOL001370	0.7093	0.2907	0.7113	Persicae Semen	[2-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl] methyl (E)-3-(3,4-dihydroxyphenyl)prop-2-enoate	23872119	FALSE	c1ccc(c(c1)COC(=O)/C=C/c1cc(c(cc1)O)O)OC1C(C(C(C(O1)CO)O)O)O
MOL001371	0.9030	0.0970	0.8798	Persicae Semen	Populoside_qt	Not Available	FALSE	c1ccc(c(c1)COC(=O)/C=C/c1cc(c(cc1)O)O)O
MOL001372	0.8443	0.1557	0.7948	Persicae Semen	beta-D-Glucopyranoside, 2-((benzoyloxy) methyl)-4-hydroxyphenyl	117440	FALSE	c1ccc(cc1)C(=O)OCc1c(ccc(c1)O)OC1C(C(C(C(O1)CO)O)O)O
MOL001373	0.9175	0.0825	0.9240	Persicae Semen	Salireposide_qt	12300041	FALSE	c1ccc(cc1)C(=O)OCc1c(ccc(c1)O)O
MOL001375	0.8778	0.1222	0.9514	Apocyniveneti Folium	4,4-dimethylcyclopent-2-en-1-one	140955	FALSE	C1(=O)C=CC(C1)(C)C

MOL001375	0.8778	0.1222	0.9514	Croci Stigma	4,4-dimethylcyclopent-2-en-1-one	140955	FALSE	C1(=O)C=CC(C1)(C)C
MOL001376	0.9018	0.0982	0.9009	Mylabris	Foron	10438	FALSE	CC(=CC(=O)C=C(C)C)C
MOL001376	0.9018	0.0982	0.9009	Croci Stigma	Foron	10438	FALSE	CC(=CC(=O)C=C(C)C)C
MOL001377	0.9219	0.0781	0.9095	Croci Stigma	Oxophorone	62374	FALSE	C1(=O)C(=CC(=O)CC1(C)C)C
MOL001377	0.9219	0.0781	0.9095	Dysosmae Verspiellis Rhixoma Et Radix	Oxophorone	62374	FALSE	C1(=O)C(=CC(=O)CC1(C)C)C
MOL001378	0.9388	0.0612	0.8551	Croci Stigma	3,5-Dimethylbenzaldehyde	34225	FALSE	C(=O)c1cc(cc(c1)C)C
MOL001379	0.9213	0.0787	0.9554	Croci Stigma	(4S)-4-hydroxy-3,5,5-trimethylcyclohex-2-en-1-one	11367121	FALSE	C1(=O)C=C(C(C(C1)(C)C)O)C
MOL001380	0.9237	0.0763	0.9193	Croci Stigma	Allyl heptoate	8878	FALSE	C(=O)(CCCCCC)OCC=C
MOL001381	0.9254	0.0746	0.9307	Croci Stigma	Isodecanoic acid	111470	FALSE	OC(=O)CCCCCCC(C)C
MOL001382	0.8949	0.1051	0.9087	Ginkgo Folium	Methylheptadienone	5370101	FALSE	CC(=O)/C=C/C=C(C)C
MOL001382	0.8949	0.1051	0.9087	Evodiae Fructus	Methylheptadienone	5370101	FALSE	CC(=O)/C=C/C=C(C)C
MOL001382	0.8949	0.1051	0.9087	Siphonostegiae Herba	Methylheptadienone	5370101	FALSE	CC(=O)/C=C/C=C(C)C
MOL001382	0.8949	0.1051	0.9087	Croci Stigma	Methylheptadienone	5370101	FALSE	CC(=O)/C=C/C=C(C)C
MOL001383	0.9250	0.0750	0.8837	Croci Stigma	ZINC04661833	7312691	FALSE	CC(/C=C/C1=C(CCCC1(C)C)C)O
MOL001384	0.9322	0.0678	0.7665	Ginkgo Folium	(E)-4-[(1R,6S)-2,2,6-trimethyl-7-oxabicyclo[4.1.0]heptan-1-yl]but-3-en-2-one	10798423	FALSE	CC(=O)/C=C/C12C(CCCC1(O2)C)(C)C

MOL001384	0.9322	0.0678	0.7665	Croci Stigma	(E)-4-[(1R,6S)-2,2,6-trimethyl-7-oxabicyclo[4.1.0]heptan-1-yl]but-3-en-2-one	10798423	FALSE	CC(=O)/C=C/C12C(CCCC1(O2)C)(C)C
MOL001385	0.9291	0.0709	0.9508	Arum Ternatum Thunb.	9-Oxononanoic acid	75704	FALSE	C(=O)(CCCCCCCC=O)O
MOL001385	0.9291	0.0709	0.9508	Radix Cynanchi	9-Oxononanoic acid	75704	FALSE	C(=O)(CCCCCCCC=O)O
MOL001385	0.9291	0.0709	0.9508	Arecae Semen	9-Oxononanoic acid	75704	FALSE	C(=O)(CCCCCCCC=O)O
MOL001385	0.9291	0.0709	0.9508	Croci Stigma	9-Oxononanoic acid	75704	FALSE	C(=O)(CCCCCCCC=O)O
MOL001386	0.8807	0.1193	0.8474	Croci Stigma	Methyl laurate	8139	FALSE	C(=O)(CCCCCCCCCCC)OC
MOL001386	0.8807	0.1193	0.8474	Broussonetiae Fructus	Methyl laurate	8139	FALSE	C(=O)(CCCCCCCCCCC)OC
MOL001386	0.8807	0.1193	0.8474	Ephedra Herba	Methyl laurate	8139	FALSE	C(=O)(CCCCCCCCCCC)OC
MOL001386	0.8807	0.1193	0.8474	Radix Bupleuri	Methyl laurate	8139	FALSE	C(=O)(CCCCCCCCCCC)OC
MOL001387	0.9666	0.0334	0.8450	Eriobotryae Folium	(7aS)-4,4,7a-trimethyl-6,7-dihydro-5H-benzofuran-2-one	157995	FALSE	O1C(=O)C=C2C1(CCCC2(C)C)C
MOL001387	0.9666	0.0334	0.8450	Lysimachiae Foenigraeci Herba	(7aS)-4,4,7a-trimethyl-6,7-dihydro-5H-benzofuran-2-one	157995	FALSE	O1C(=O)C=C2C1(CCCC2(C)C)C
MOL001387	0.9666	0.0334	0.8450	Carthami Flos	(7aS)-4,4,7a-trimethyl-6,7-dihydro-5H-benzofuran-2-one	157995	FALSE	O1C(=O)C=C2C1(CCCC2(C)C)C

MOL001387	0.9666	0.0334	0.8450	Ginkgo Folium	(7aS)-4,4,7a-trimethyl-6,7-dihydro-5H-benzofuran-2-one	157995	FALSE	O1C(=O)C=C2C1(CCCC2(C)C)C
MOL001387	0.9666	0.0334	0.8450	Millettiae Speciosae Radix	(7aS)-4,4,7a-trimethyl-6,7-dihydro-5H-benzofuran-2-one	157995	FALSE	O1C(=O)C=C2C1(CCCC2(C)C)C
MOL001387	0.9666	0.0334	0.8450	Siphonostegiae Herba	(7aS)-4,4,7a-trimethyl-6,7-dihydro-5H-benzofuran-2-one	157995	FALSE	O1C(=O)C=C2C1(CCCC2(C)C)C
MOL001387	0.9666	0.0334	0.8450	Cassiae Semen	(7aS)-4,4,7a-trimethyl-6,7-dihydro-5H-benzofuran-2-one	157995	FALSE	O1C(=O)C=C2C1(CCCC2(C)C)C
MOL001387	0.9666	0.0334	0.8450	Croci Stigma	(7aS)-4,4,7a-trimethyl-6,7-dihydro-5H-benzofuran-2-one	157995	FALSE	O1C(=O)C=C2C1(CCCC2(C)C)C
MOL001388	0.8608	0.1392	0.6197	Caryophylliflos	(+)-Ledol	92812	FALSE	C12C(C3C(CCC1(C)O)C3(C)C)C(CC2)C
MOL001388	0.8608	0.1392	0.6197	Linderae Radix	(+)-Ledol	92812	FALSE	C12C(C3C(CCC1(C)O)C3(C)C)C(CC2)C
MOL001388	0.8608	0.1392	0.6197	Rhododendri Daurici Folium	(+)-Ledol	92812	FALSE	C12C(C3C(CCC1(C)O)C3(C)C)C(CC2)C
MOL001388	0.8608	0.1392	0.6197	Folium Artemisiae Argyi	(+)-Ledol	92812	FALSE	C12C(C3C(CCC1(C)O)C3(C)C)C(CC2)C
MOL001388	0.8608	0.1392	0.6197	Croci Stigma	(+)-Ledol	92812	FALSE	C12C(C3C(CCC1(C)O)C3(C)C)C(CC2)C
MOL001388	0.8608	0.1392	0.6197	Viticis Negundo Folium	(+)-Ledol	92812	FALSE	C12C(C3C(CCC1(C)O)C3(C)C)C(CC2)C
MOL001388	0.8608	0.1392	0.6197	Cistanches Herba	(+)-Ledol	92812	FALSE	C12C(C3C(CCC1(C)O)C3(C)C)C(CC2)C
MOL001388	0.8608	0.1392	0.6197	Santalum Album L.	(+)-Ledol	92812	FALSE	C12C(C3C(CCC1(C)O)C3(C)C)C(CC2)C
MOL001388	0.8608	0.1392	0.6197	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	(+)-Ledol	92812	FALSE	C12C(C3C(CCC1(C)O)C3(C)C)C(CC2)C
MOL001388	0.8608	0.1392	0.6197	Lonicerae Japonicae Flos	(+)-Ledol	92812	FALSE	C12C(C3C(CCC1(C)O)C3(C)C)C(CC2)C
MOL001388	0.8608	0.1392	0.6197	Angelicae Sinensis Radix	(+)-Ledol	92812	FALSE	C12C(C3C(CCC1(C)O)C3(C)C)C(CC2)C
MOL001388	0.8608	0.1392	0.6197	Chrysanthemi Flos	(+)-Ledol	92812	FALSE	C12C(C3C(CCC1(C)O)C3(C)C)C(CC2)C
MOL001388	0.8608	0.1392	0.6197	Litchi Semen	(+)-Ledol	92812	FALSE	C12C(C3C(CCC1(C)O)C3(C)C)C(CC2)C
MOL001388	0.8608	0.1392	0.6197	Zanthoxyli Pericarpium	(+)-Ledol	92812	FALSE	C12C(C3C(CCC1(C)O)C3(C)C)C(CC2)C

MOL001390	0.8608	0.1392	0.6197	Croci Stigma	49070_FLUKA	12304985	FALSE	C1CC(C2C3C(CCC(C12)(O)C)C3(C)C)C
MOL001390	0.8608	0.1392	0.6197	Aucklandiae Radix	49070_FLUKA	12304985	FALSE	C1CC(C2C3C(CCC(C12)(O)C)C3(C)C)C
MOL001390	0.8608	0.1392	0.6197	Radix Angelicae Biseratae	49070_FLUKA	12304985	FALSE	C1CC(C2C3C(CCC(C12)(O)C)C3(C)C)C
MOL001390	0.8608	0.1392	0.6197	Chuanxiong Rhizoma	49070_FLUKA	12304985	FALSE	C1CC(C2C3C(CCC(C12)(O)C)C3(C)C)C
MOL001390	0.8608	0.1392	0.6197	Pogostemon Cablin (Blanco) Benth.	49070_FLUKA	12304985	FALSE	C1CC(C2C3C(CCC(C12)(O)C)C3(C)C)C
MOL001390	0.8608	0.1392	0.6197	Caryophylliflos	49070_FLUKA	12304985	FALSE	C1CC(C2C3C(CCC(C12)(O)C)C3(C)C)C
MOL001390	0.8608	0.1392	0.6197	Lysimachiae Herba	49070_FLUKA	12304985	FALSE	C1CC(C2C3C(CCC(C12)(O)C)C3(C)C)C
MOL001390	0.8608	0.1392	0.6197	Stephaniae Tetrandrae Radix	49070_FLUKA	12304985	FALSE	C1CC(C2C3C(CCC(C12)(O)C)C3(C)C)C
MOL001390	0.8608	0.1392	0.6197	Viticis Negundo Folium	49070_FLUKA	12304985	FALSE	C1CC(C2C3C(CCC(C12)(O)C)C3(C)C)C
MOL001391	0.9292	0.0708	0.9064	Croci Stigma	3-Oxo-.beta.-ionone	5363876	FALSE	C1(=O)C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL001392	0.7983	0.2017	0.7472	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Methyl myristate	31284	FALSE	C(=O)(CCCCCCCCCCCCC)OC
MOL001392	0.7983	0.2017	0.7472	Sojae Semen Nigrum	Methyl myristate	31284	FALSE	C(=O)(CCCCCCCCCCCCC)OC
MOL001392	0.7983	0.2017	0.7472	Lonicerae Japonicae Flos	Methyl myristate	31284	FALSE	C(=O)(CCCCCCCCCCCCC)OC
MOL001392	0.7983	0.2017	0.7472	Platycladi Semen	Methyl myristate	31284	FALSE	C(=O)(CCCCCCCCCCCCC)OC
MOL001392	0.7983	0.2017	0.7472	Perillae Fructus	Methyl myristate	31284	FALSE	C(=O)(CCCCCCCCCCCCC)OC
MOL001392	0.7983	0.2017	0.7472	Isatdis Radix	Methyl myristate	31284	FALSE	C(=O)(CCCCCCCCCCCCC)OC
MOL001392	0.7983	0.2017	0.7472	Herba Patriniae	Methyl myristate	31284	FALSE	C(=O)(CCCCCCCCCCCCC)OC
MOL001392	0.7983	0.2017	0.7472	Panax Ginseng C. A. Mey.	Methyl myristate	31284	FALSE	C(=O)(CCCCCCCCCCCCC)OC
MOL001392	0.7983	0.2017	0.7472	Broussonetiae Fructus	Methyl myristate	31284	FALSE	C(=O)(CCCCCCCCCCCCC)OC
MOL001392	0.7983	0.2017	0.7472	Notopterygii Rhizoma Et Radix	Methyl myristate	31284	FALSE	C(=O)(CCCCCCCCCCCCC)OC
MOL001392	0.7983	0.2017	0.7472	Hoveniae Dulcis Semen	Methyl myristate	31284	FALSE	C(=O)(CCCCCCCCCCCCC)OC

MOL001392	0.7983	0.2017	0.7472	Sterculiae Lychnophorae Semen	Methyl myristate	31284	FALSE	C(=O)(CCCCCCCCCCCCC)OC
MOL001392	0.7983	0.2017	0.7472	Croci Stigma	Methyl myristate	31284	FALSE	C(=O)(CCCCCCCCCCCCC)OC
MOL001392	0.7983	0.2017	0.7472	Codonopsis Radix	Methyl myristate	31284	FALSE	C(=O)(CCCCCCCCCCCCC)OC
MOL001392	0.7983	0.2017	0.7472	Radix Bupleuri	Methyl myristate	31284	FALSE	C(=O)(CCCCCCCCCCCCC)OC
MOL001392	0.7983	0.2017	0.7472	Impatientis Semen	Methyl myristate	31284	FALSE	C(=O)(CCCCCCCCCCCCC)OC
MOL001392	0.7983	0.2017	0.7472	Iridis Tectori Rhizoma	Methyl myristate	31284	FALSE	C(=O)(CCCCCCCCCCCCC)OC
MOL001393	0.8919	0.1081	0.7814	Cortex Periplocae Radicis	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Crotonis Fructus	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Mahoniae Caulis	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Capsici Fructus	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Smilacis Glabrae Rhixoma	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Farfarae Flos	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Choerospondiatis Fructus	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Oroxyli Semen	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Cucurbitae Moschatae Semen	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Ginkgo Folium	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Allium Azureum Ledeb.	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Kochiae Fructus	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Iridis Tectori Rhizoma	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Folium Nelumbinis	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Scutellariae Barbatae Herba	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Et Radix Patriniae Rhizoma	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Phytolaccae Radix	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Eriobotryae Folium	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Dalbergiae Odoriferae Lignum	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Puerariae Flos	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Trichosanthes Kirilowii Maxim	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Citri Grandis Exocarpium	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Maydis Seigma	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Foeniculi Fructus	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Paeoniae Radix Alba	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Rhizome Of Whiteback Greenbrier	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O

MOL001393	0.8919	0.1081	0.7814	Calyx Seu Fructus Physalis	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Litchi Semen	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Achyranthis Bidentatae Radix	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Citri Sarcodactylis Fructus	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Lonicerae Japonicae Flos	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Ganoderma	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Gnaphalii Affinis Herba	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Broussonetiae Fructus	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Ranunculi Ternati Radix	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Myristicae Semen	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Quisqualis Indica	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Arecae Semen	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Radix Clematidis	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Aconiti Lateralis Radix Praeparata	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Cortex Hibisci	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Cnidii Fructus	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Hippophae Fructus	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Morindae Officinalis Radix	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Radix Cynanchi Paniculati	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Platycladi Semen	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Alpiniae Officinarum Rhizome	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Piperis Fructus	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Radix Bupleuri	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Semen Lini	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Linderae Radix	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Codonopsis Radix	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Mahoniae Folum	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Ginsen Radix Et Rhizoma Rubra	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Silybum Marianum	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Millettiae Speciosae Radix	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Curcumae Radix	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Cinnanmomi Cortex	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Mori Fructus	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Ardisiae Japonicae Herba	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Croci Stigma	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Aucklandiae Radix	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Meliae Azedarach Fructus	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCC)O

MOL001393	0.8919	0.1081	0.7814	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Allii Tuberosi Semen	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Linderae Radix	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Thalluslaminariae	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Magnolia Officinalis Rehd Et Wils.	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Portulacae Herba	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Viticis Fructus	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Cannabis Sativa L.	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Lepidii Semen Descurainiae Semen	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Hyoscyami Semen	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Melo Semen	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Eriocauli Flos	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Cornus Officinalis Sieb. Et Zucc.	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Carthami Flos	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Gossampiniflos	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Junci Medulla	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Rhododendri Daurici Folium	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Violsse Herba	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Astragali Cpmplanatisemen	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Mori Cortex	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Ephedra Herba	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Semen Euphorbiae	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Acoritataninowii Rhizoma	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Momordicae Fructus	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Santalum Album L.	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Trollius Chinensis	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Prunellae Spica	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Platycladi Cacumen	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Phyllanthi Fructus	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Coicis Semen	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Tamaricis Cacumen	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Schizonepetae Spica	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Ilicis Purpureae Folium	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Lycii Fructus	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O

MOL001393	0.8919	0.1081	0.7814	Amygdalus Communis Vas	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Curculiginis Rhizome	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Abutili Semen	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Herbahypericiperforati	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Paederiae Scandentis Herba	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001393	0.8919	0.1081	0.7814	Citri Reticulatae Semen	myristic acid	11005	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Malvae Fructus	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Broussonetiae Fructus	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Momordicae Semen	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Puerariae Flos	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Capsici Fructus	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Citri Grandis Exocarpium	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Radix Clematidis	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Semiaquilegiae Radix	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Santalum Album L.	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Quisqualis Indica	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Cortex Periplocae Radicis	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Radix Cynanchi Paniculati	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Arecae Semen	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Ginkgo Folium	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Arisaematis Rhizoma	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Isatdis Radix	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Mori Cortex	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Astragali Cpmplanatisemen	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O

MOL001396	0.8751	0.1249	0.7287	Rhizome Of Whiteback Greenbrier	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Saxifraga Stolonifera	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Lycii Fructus	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Paeoniae Radix Alba	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Gossampiniflos	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Ardisiae Japonicae Herba	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Morindae Officinalis Radix	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Arum Ternatum Thunb.	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Radix Bupleuri	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Tamaricis Cacumen	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Croci Stigma	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Zingiberis Rhizoma	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Codonopsis Radix	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Ganoderma	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Herba Sarcandrae	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Magnolia Officinalis Rehd Et Wils.	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Momordicae Fructus	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Curculiginis Rhizome	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Linderae Radix	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Ephedra Herba	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Allium Azureum Ledeb.	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCCC)O

MOL001396	0.8751	0.1249	0.7287	Asari Radix Et Rhizoma	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Ginsen Radix Et Rhizoma Rubra	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Eriocauli Flos	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Farfarae Flos	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Allii Tuberosi Semen	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Rehmanniae Radix Praeparata	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Cucurbitae Moschatae Semen	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Panax Ginseng C. A. Mey.	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Oroxyli Semen	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Aristolochiae Fructus	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Foeniculi Fructus	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Carthami Flos	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001396	0.8751	0.1249	0.7287	Polygonati Odorati Rhizoma	PENTADECYLIC ACID	13849	FALSE	C(=O)(CCCCCCCCCCCCCC)O
MOL001397	0.9321	0.0679	0.9460	Croci Stigma	cis-Hept-2-enal	5362616	FALSE	C(=O)/C=C\CCCC
MOL001398	0.5096	0.4904	0.6647	Cornus Officinalis Sieb. Et Zucc.	Methyllinolenate	5319706	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)OC
MOL001398	0.5096	0.4904	0.6647	Trichosanthes Kirilowii Maxim	Methyllinolenate	5319706	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)OC
MOL001398	0.5096	0.4904	0.6647	Campsis Flos	Methyllinolenate	5319706	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)OC
MOL001398	0.5096	0.4904	0.6647	Ginseng Folium	Methyllinolenate	5319706	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)OC
MOL001398	0.5096	0.4904	0.6647	Smilacis Glabrae Rhixoma	Methyllinolenate	5319706	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)OC
MOL001398	0.5096	0.4904	0.6647	Croci Stigma	Methyllinolenate	5319706	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)OC
MOL001398	0.5096	0.4904	0.6647	Farfarae Flos	Methyllinolenate	5319706	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)OC

MOL001398	0.5096	0.4904	0.6647	Raphani Semen	Methyllinolenate	5319706	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)OC
MOL001398	0.5096	0.4904	0.6647	Carthami Flos	Methyllinolenate	5319706	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)OC
MOL001398	0.5096	0.4904	0.6647	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Methyllinolenate	5319706	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)OC
MOL001398	0.5096	0.4904	0.6647	Platycladi Cacumen	Methyllinolenate	5319706	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)OC
MOL001398	0.5096	0.4904	0.6647	Lonicerae Japonicae Flos	Methyllinolenate	5319706	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)OC
MOL001398	0.5096	0.4904	0.6647	Ginkgo Folium	Methyllinolenate	5319706	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)OC
MOL001398	0.5096	0.4904	0.6647	Isatdis Radix	Methyllinolenate	5319706	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)OC
MOL001398	0.5096	0.4904	0.6647	Millettiae Speciosae Radix	Methyllinolenate	5319706	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)OC
MOL001398	0.5096	0.4904	0.6647	Impatientis Semen	Methyllinolenate	5319706	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)OC
MOL001398	0.5096	0.4904	0.6647	Hedysari Radix	Methyllinolenate	5319706	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)OC
MOL001404	0.5607	0.4393	0.6097	Ginseng Folium	Pentatriacontane	12413	FALSE	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
MOL001404	0.5607	0.4393	0.6097	Croci Stigma	Pentatriacontane	12413	FALSE	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
MOL001404	0.5607	0.4393	0.6097	Microctis Folium	Pentatriacontane	12413	FALSE	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
MOL001404	0.5607	0.4393	0.6097	Siphonostegiae Herba	Pentatriacontane	12413	FALSE	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
MOL001404	0.5607	0.4393	0.6097	Fritiliariae Irrhosae Bulbus	Pentatriacontane	12413	FALSE	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
MOL001404	0.5607	0.4393	0.6097	Amygdalus Communis Vas	Pentatriacontane	12413	FALSE	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
MOL001404	0.5607	0.4393	0.6097	Viticis Negundo Folium	Pentatriacontane	12413	FALSE	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
MOL001405	0.6188	0.3812	0.7566	Croci Stigma	crocin I	Not Available	FALSE	C1(C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)CO)OC(=O)/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(\C)/C(=O)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)CO)\C)/C)/C
MOL001407	0.5911	0.4089	0.7288	Croci Stigma	Crocin 2	Not Available	FALSE	C/C(=C\C=C\C=C(/C)\C=C\C=C(/C)\C(=O)OC1C((C(C(O1)COC1C(C(C(C(O1)CO)O)O)O)O)O)O)/C=C/C=C(\C)/C(=O)OC1C(C(C(C(O1)CO)O)O)O

MOL001408	0.9227	0.0773	0.8097	Croci Stigma	4-(beta-D-Glucopyranosyloxy)-2,6,6-trimethyl-1-cyclohexene-1-carboxaldehyde	130796	FALSE	C1(=C(CC(CC1(C)C)OC1C(O)C(O)C(O)C(O1)CO)C)C=O
MOL001409	0.9525	0.0475	0.8898	Croci Stigma	picrocrocin_qt	25201359	FALSE	C1(=C(CC(CC1(C)C)O)C)C=O
MOL001411	0.7171	0.2829	0.7214	Croci Stigma	helichrysoside	Not Available	FALSE	C(=O)(/C=C\c1ccc(cc1)O)OCC1OC(C(C(C1O)O)O)Oc1c(oc2c(c1=O)c(cc(c2)O)O)c1cc(c(cc1)O)O
MOL001412	0.8620	0.1380	0.8451	Croci Stigma	crosatoside A	Not Available	FALSE	c1(c(c(=O)c2c(cc(cc2o1)O)O)O)c1cc(c(cc1)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO)OC
MOL001413	0.7422	0.2578	0.7464	Croci Stigma	carthamin	Not Available	FALSE	C1(=O)/C(=C\C2=C(C(C(=C(C2=O)C(=O)/C=C\c2ccc(cc2)O)O)(O)C2C(O)C(O)C(O)C(O2)CO)O)/C(=O)C(=C(C1(O)C1C(O)C(O)C(O)C(O1)CO)O)C(=O)/C=C/c1ccc(cc1)O
MOL001414	0.8774	0.1226	0.8128	Croci Stigma	safflor yellow A	Not Available	FALSE	O1C2C(C3=C1C(C(=C(C3=O)C(=O)/C=C\c1ccc(cc1)O)O)(O)C1C(O)C(O)C(O)C(O1)CO)OC(C(C2O)O)CO
MOL001415	0.9140	0.0860	0.8280	Croci Stigma	Kaempferol-3-glucoside	Not Available	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)O
MOL001415	0.9140	0.0860	0.8280	Phyllanthi Fructus	Kaempferol-3-glucoside	Not Available	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)O
MOL001416	0.8959	0.1041	0.8039	Croci Stigma	beta-Phorone	10108	FALSE	C1(=O)CC(=CC(C1)(C)C)C
MOL001416	0.8959	0.1041	0.8039	Celastri Orbiculati Fructus	beta-Phorone	10108	FALSE	C1(=O)CC(=CC(C1)(C)C)C
MOL001417	0.9236	0.0764	0.9438	Radix Bupleuri	OCTENAL	5283324	FALSE	C(=O)/C=C/CCCCC
MOL001417	0.9236	0.0764	0.9438	Morindae Officinalis Radix	OCTENAL	5283324	FALSE	C(=O)/C=C/CCCCC
MOL001417	0.9236	0.0764	0.9438	Croci Stigma	OCTENAL	5283324	FALSE	C(=O)/C=C/CCCCC
MOL001417	0.9236	0.0764	0.9438	Ganoderma	OCTENAL	5283324	FALSE	C(=O)/C=C/CCCCC
MOL001417	0.9236	0.0764	0.9438	Malvae Fructus	OCTENAL	5283324	FALSE	C(=O)/C=C/CCCCC
MOL001417	0.9236	0.0764	0.9438	Coriandri Sativi Herba	OCTENAL	5283324	FALSE	C(=O)/C=C/CCCCC
MOL001417	0.9236	0.0764	0.9438	Thalluslaminariae	OCTENAL	5283324	FALSE	C(=O)/C=C/CCCCC
MOL001417	0.9236	0.0764	0.9438	Adenophprae Ae Radix	OCTENAL	5283324	FALSE	C(=O)/C=C/CCCCC
MOL001417	0.9236	0.0764	0.9438	Panacis Japonici Rhizoma	OCTENAL	5283324	FALSE	C(=O)/C=C/CCCCC
MOL001418	0.2148	0.7852	0.6012	Leonuri Herba	galeopsin	Not Available	FALSE	C1C(=O)C(C(C2(CCCC(C12)(C)C)C)(O)CCc1cocc1)(C)OC(=O)C
MOL001420	0.2190	0.7810	0.6041	Leonuri Herba	ZINC04073977	9801811	FALSE	C1C(=O)CC2=CCC3C(C2(C1)C)CCC1(C3CCC1C(CCC(CC)C(C)C)C)C
MOL001420	0.2190	0.7810	0.6041	Euonymi Alati Ramulus	ZINC04073977	9801811	FALSE	C1C(=O)CC2=CCC3C(C2(C1)C)CCC1(C3CCC1C(CCC(CC)C(C)C)C)C
MOL001420	0.2190	0.7810	0.6041	Hippophae Fructus	ZINC04073977	9801811	FALSE	C1C(=O)CC2=CCC3C(C2(C1)C)CCC1(C3CCC1C(CCC(CC)C(C)C)C)C

MOL001420	0.2190	0.7810	0.6041	Bistortae Rhizoma	ZINC04073977	9801811	FALSE	C1C(=O)CC2=CCC3C(C2(C1)C)CCC1(C3CCC1C(CCC(CC)C(C)C)C)C
MOL001421	0.3762	0.6238	0.6975	Leonuri Herba	preleoheterin	Not Available	FALSE	C1CC(C2C(C1)(C1(C(C(C2=O)O)C)CCC2(O1)C=COC2)C)(C)C
MOL001422	0.3735	0.6265	0.6715	Leonuri Herba	iso-preleoheterin	Not Available	FALSE	C1CC(C2C(C1)(C1(C(C(=O)C2O)C)CCC2(O1)COC=C2)C)(C)C
MOL001423	0.8764	0.1236	0.8492	Leonuri Herba	isorhamnetin-3-o-beta-d-rutinoside	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)C)c1ccc(c(c1)OC)O)O)O
MOL001424	0.8763	0.1237	0.8456	Leonuri Herba	isorhamnetin, 3-o-rutinoside	Not Available	FALSE	c1c(c(cc(c1)c1c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)C)OC)O
MOL001426	0.2704	0.7296	0.7034	Leonuri Herba	Hispanolone	5458747	FALSE	C1C(=O)C(C(C2(CCCC(C12)(C)C)C)(CCC1(CC1)C)C)C
MOL001427	0.2855	0.7145	0.7564	Leonuri Herba	leojaponin	Not Available	FALSE	C1CC(C2=C(C(=O)C(=C(C2(C1)C)CCC1=CC=[O+]C1)C)O)(C)C
MOL001428	0.9293	0.0707	0.8664	Leonuri Herba	ACon1_000342	14237626	FALSE	c1c(c(c(cc1O)OC)OC1OC(C(C(C1O)O)O)CO)OC
MOL001429	0.9058	0.0942	0.9503	Leonuri Herba	2,6-Dimethoxyquinol	96038	FALSE	c1c(c(c(cc1O)OC)O)OC
MOL001430	0.8669	0.1331	0.7372	Leonuri Herba	leonuriside,b	Not Available	FALSE	C1(OC(C(C(C1O)OC1C(C(C(C(O1)C)O)O)OC1OCC(C(C1O)O)O)O)CO)OCCc1cc(c(cc1)O)O
MOL001431	0.9272	0.0728	0.8736	Leonuri Herba	melatonin	Not Available	FALSE	c12c([nH]cc1CCNC(=O)C)ccc(c2)OC
MOL001436	0.9318	0.0682	0.8690	Rehmanniae Radix Praeparata	leonuride	46227138	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)C1C2C(C=CO1)C(CC2(C)O)O
MOL001436	0.9318	0.0682	0.8690	Leonuri Herba	leonuride	46227138	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)C1C2C(C=CO1)C(CC2(C)O)O
MOL001437	0.9456	0.0544	0.8249	Leonuri Herba	leonurinine_q+	Not Available	FALSE	OC1C2C(C=CO1)C(CC2(C)O)O
MOL001438	0.3018	0.6982	0.6635	Leonuri Herba	leosibiricin	Not Available	FALSE	O1C2C3C(C1=O)(CCCC3(C(C(C2=O)(C)OC(=O)C)(O)CCc1cocc1)C)C
MOL001439	0.7149	0.2851	0.6020	Leonuri Herba	arachidonic acid	444899	FALSE	C(=O)(CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC)O
MOL001439	0.7149	0.2851	0.6020	Cannabis Sativa L.	arachidonic acid	444899	FALSE	C(=O)(CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC)O
MOL001439	0.7149	0.2851	0.6020	Litseae Fructus	arachidonic acid	444899	FALSE	C(=O)(CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC)O
MOL001439	0.7149	0.2851	0.6020	Platycladi Semen	arachidonic acid	444899	FALSE	C(=O)(CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC)O
MOL001439	0.7149	0.2851	0.6020	Thalluslaminariae	arachidonic acid	444899	FALSE	C(=O)(CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC)O
MOL001439	0.7149	0.2851	0.6020	Quisqualis Indica	arachidonic acid	444899	FALSE	C(=O)(CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC)O
MOL001439	0.7149	0.2851	0.6020	Pollen Typhae	arachidonic acid	444899	FALSE	C(=O)(CCC/C=C\C/C=C\C/C=C\C/C=C\CCCCC)O

MOL001439	0.7149	0.2851	0.6020	Corayceps	arachidonic acid	444899	FALSE	C(=O)(CCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCCCC)O
MOL001439	0.7149	0.2851	0.6020	Portulacae Herba	arachidonic acid	444899	FALSE	C(=O)(CCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCCCC)O
MOL001439	0.7149	0.2851	0.6020	Silybum Marianum	arachidonic acid	444899	FALSE	C(=O)(CCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCCCC)O
MOL001439	0.7149	0.2851	0.6020	Perillae Fructus	arachidonic acid	444899	FALSE	C(=O)(CCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCCCC)O
MOL001439	0.7149	0.2851	0.6020	Aloe	arachidonic acid	444899	FALSE	C(=O)(CCC/C=C\C/C=C\C/C=C\C/C=C\C/C=C\CCCCC)O
MOL001441	0.8830	0.1170	0.9643	Leonuri Herba	4-Guanidinobutanoate	25200642	FALSE	C(=O)(CCCNC(=N)N)O
MOL001443	0.9164	0.0836	0.9747	Leonuri Herba	4-Guanidino-1-butanol	5317848	FALSE	N(C(=N)N)CCCCO
MOL001444	0.2429	0.7571	0.6442	Leonuri Herba	LC 5504	Not Available	FALSE	C1CC(C2C(C1)(C1(C(C(=O)C2)C)OC2(CC1)C=COC2)C)(C)C
MOL001444	0.2429	0.7571	0.6442	Schisandrae Chinensis Fructus	LC 5504	Not Available	FALSE	C1CC(C2C(C1)(C1(C(C(=O)C2)C)OC2(CC1)C=COC2)C)(C)C
MOL001445	0.9419	0.0581	0.8926	Leonuri Herba	Leonurine	161464	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)OCCCCNC(=N)N
MOL001445	0.9419	0.0581	0.8926	Cistanches Herba	Leonurine	161464	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)OCCCCNC(=N)N
MOL001446	0.4090	0.5910	0.7039	Abrus Precatorius L.	Cholanoic acid	92803	FALSE	C1CCC2(C(C1)CCC1C3CCC(C(CCC(=O)O)C)C3(C)CCC21)C
MOL001446	0.4090	0.5910	0.7039	Lycopi Herba	Cholanoic acid	92803	FALSE	C1CCC2(C(C1)CCC1C3CCC(C(CCC(=O)O)C)C3(C)CCC21)C
MOL001447	0.7225	0.2775	0.8528	Lycopi Herba	oleanolic acid	14208454	FALSE	C(=O)(C12CCC3(C4(CCC5C(CCCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)C)C)C)O
MOL001448	0.6295	0.3705	0.7590	Lycopi Herba	arjunetin	Not Available	FALSE	C1(C(CC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)OC5C(O)C(O)C(O)C(O5)CO)CCC(C)(C)C(C4C3=CCC21)O)C)O)O
MOL001449	0.7405	0.2595	0.7570	Rosae Laevigatae Fructus	arjunetin_qt	Not Available	FALSE	C1(C(CC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C)(C)C(C4C3=CCC21)O)C)O)O
MOL001449	0.7405	0.2595	0.7570	Lycopi Herba	arjunetin_qt	Not Available	FALSE	C1(C(CC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C)(C)C(C4C3=CCC21)O)C)O)O
MOL001452	0.9008	0.0992	0.9674	Maydis Seigma	protocatechualdehyde	8768	FALSE	C(=O)c1cc(c(cc1)O)O
MOL001452	0.9008	0.0992	0.9674	Cicadae Periostracum	protocatechualdehyde	8768	FALSE	C(=O)c1cc(c(cc1)O)O
MOL001452	0.9008	0.0992	0.9674	Salviae Chinensis Herba	protocatechualdehyde	8768	FALSE	C(=O)c1cc(c(cc1)O)O
MOL001452	0.9008	0.0992	0.9674	Ilicis Purpureae Folium	protocatechualdehyde	8768	FALSE	C(=O)c1cc(c(cc1)O)O

MOL001452	0.9008	0.0992	0.9674	Perilla Frutescens	protocatechualdehyde	8768	FALSE	C(=O)c1cc(c(cc1)O)O
MOL001452	0.9008	0.0992	0.9674	Litchi Semen	protocatechualdehyde	8768	FALSE	C(=O)c1cc(c(cc1)O)O
MOL001452	0.9008	0.0992	0.9674	Radix Salviae	protocatechualdehyde	8768	FALSE	C(=O)c1cc(c(cc1)O)O
MOL001452	0.9008	0.0992	0.9674	Lycopi Herba	protocatechualdehyde	8768	FALSE	C(=O)c1cc(c(cc1)O)O
MOL001452	0.9008	0.0992	0.9674	Arisaematis Rhizoma	protocatechualdehyde	8768	FALSE	C(=O)c1cc(c(cc1)O)O
MOL001452	0.9008	0.0992	0.9674	Tripterygii Radix	protocatechualdehyde	8768	FALSE	C(=O)c1cc(c(cc1)O)O
MOL001452	0.9008	0.0992	0.9674	Glechomae Herba	protocatechualdehyde	8768	FALSE	C(=O)c1cc(c(cc1)O)O
MOL001452	0.9008	0.0992	0.9674	Cinnamomi Ramulus	protocatechualdehyde	8768	FALSE	C(=O)c1cc(c(cc1)O)O
MOL001452	0.9008	0.0992	0.9674	Arum Ternatum Thunb.	protocatechualdehyde	8768	FALSE	C(=O)c1cc(c(cc1)O)O
MOL001453	0.9136	0.0864	0.8056	Lycopi Herba	Rosmarinate	639655	FALSE	C(=C\C(=O)OC(C(=O)O)Cc1ccc(c(c1)O)O)/c1cc(c(cc1)O)O
MOL001454	0.7572	0.2428	0.8317	Radix Stephaniae Cepharanthae.	berberine	Not Available	FALSE	O1c2cc3CC[n+]4c(c3cc2OC1)cc1c(c4)c(OC)c(OC)cc1
MOL001454	0.7572	0.2428	0.8317	Corydalis Rhizoma	berberine	Not Available	FALSE	O1c2cc3CC[n+]4c(c3cc2OC1)cc1c(c4)c(OC)c(OC)cc1
MOL001454	0.7572	0.2428	0.8317	Phellodendri Amurensis Cortex	berberine	Not Available	FALSE	O1c2cc3CC[n+]4c(c3cc2OC1)cc1c(c4)c(OC)c(OC)cc1
MOL001454	0.7572	0.2428	0.8317	Coptidis Rhizoma	berberine	Not Available	FALSE	O1c2cc3CC[n+]4c(c3cc2OC1)cc1c(c4)c(OC)c(OC)cc1
MOL001454	0.7572	0.2428	0.8317	Jujubae Fructus	berberine	Not Available	FALSE	O1c2cc3CC[n+]4c(c3cc2OC1)cc1c(c4)c(OC)c(OC)cc1
MOL001454	0.7572	0.2428	0.8317	Phellodendri Chinrnsis Cortex	berberine	Not Available	FALSE	O1c2cc3CC[n+]4c(c3cc2OC1)cc1c(c4)c(OC)c(OC)cc1
MOL001454	0.7572	0.2428	0.8317	Thalictri Glandulosissimi Et	berberine	Not Available	FALSE	O1c2cc3CC[n+]4c(c3cc2OC1)cc1c(c4)c(OC)c(OC)cc1
MOL001454	0.7572	0.2428	0.8317	Achyranthis Bidentatae Radix	berberine	Not Available	FALSE	O1c2cc3CC[n+]4c(c3cc2OC1)cc1c(c4)c(OC)c(OC)cc1
MOL001454	0.7572	0.2428	0.8317	Mahoniae Eadix	berberine	Not Available	FALSE	O1c2cc3CC[n+]4c(c3cc2OC1)cc1c(c4)c(OC)c(OC)cc1
MOL001454	0.7572	0.2428	0.8317	Mahoniae Folum	berberine	Not Available	FALSE	O1c2cc3CC[n+]4c(c3cc2OC1)cc1c(c4)c(OC)c(OC)cc1
MOL001454	0.7572	0.2428	0.8317	Evodiae Fructus	berberine	Not Available	FALSE	O1c2cc3CC[n+]4c(c3cc2OC1)cc1c(c4)c(OC)c(OC)cc1
MOL001454	0.7572	0.2428	0.8317	Chelidonii Herba	berberine	Not Available	FALSE	O1c2cc3CC[n+]4c(c3cc2OC1)cc1c(c4)c(OC)c(OC)cc1
MOL001455	0.7381	0.2619	0.9085	Phellodendri Amurensis Cortex	(S)-Canadine	Not Available	TRUE	O1c2cc3C4N(CCc3cc2OC1)Cc1c(C4)ccc(OC)c1OC
MOL001455	0.7381	0.2619	0.9085	Chelidonii Herba	(S)-Canadine	Not Available	TRUE	O1c2cc3C4N(CCc3cc2OC1)Cc1c(C4)ccc(OC)c1OC
MOL001456	0.9133	0.0867	0.9545	Hippophae Fructus	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Kansui Radix	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Cichorii Radix	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O

MOL001456	0.9133	0.0867	0.9545	Mori Fructus	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Ranunculi Ternati Radix	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Rosae Laevigatae Fructus	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Rose Rugosae Flos	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Capsici Fructus	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Stemonae Radix	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Portulacae Herba	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Semen Pini Koraiensis	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Morindae Officinalis Radix	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Folium Nelumbinis	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Rubi Fructus	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Chaenomeles Sinensis (Thouin) Koehne	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Isatidis Folium	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Maydis Seigma	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Mume Fructus	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Radix Rhei Et Rhizome	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Quisqualis Indica	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Citrus Aurantium	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Lycii Fructus	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Polygoni Cuspidati Rhizoma Et Radix	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Citri Fructus	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Aloe	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Eriobotryae Folium	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Pollen Typhae	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Chelidonii Herba	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Choerospondiatis Fructus	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001456	0.9133	0.0867	0.9545	Evodiae Fructus	citric acid	19782904	FALSE	OC(CC(=O)O)(CC(=O)O)C(=O)O
MOL001457	0.5867	0.4133	0.7503	Tinosporae Radix	columbamine	72310	FALSE	O(c1c2c[n+]3CCc4c(c3cc2ccc1OC)cc(O)c(OC)c4)C
MOL001457	0.5867	0.4133	0.7503	Thalictri Glandulosissimi Et	columbamine	72310	FALSE	O(c1c2c[n+]3CCc4c(c3cc2ccc1OC)cc(O)c(OC)c4)C
MOL001457	0.5867	0.4133	0.7503	Mahoniae Caulis	columbamine	72310	FALSE	O(c1c2c[n+]3CCc4c(c3cc2ccc1OC)cc(O)c(OC)c4)C
MOL001457	0.5867	0.4133	0.7503	Coptidis Rhizoma	columbamine	72310	FALSE	O(c1c2c[n+]3CCc4c(c3cc2ccc1OC)cc(O)c(OC)c4)C
MOL001457	0.5867	0.4133	0.7503	Corydalis Rhizoma	columbamine	72310	FALSE	O(c1c2c[n+]3CCc4c(c3cc2ccc1OC)cc(O)c(OC)c4)C
MOL001457	0.5867	0.4133	0.7503	Chelidonii Herba	columbamine	72310	FALSE	O(c1c2c[n+]3CCc4c(c3cc2ccc1OC)cc(O)c(OC)c4)C
MOL001458	0.8731	0.1269	0.7286	Mahoniae Caulis	coptisine	Not Available	FALSE	O1c2cc3c4[n+](CCc3cc2OC1)cc1c(c4)ccc2OCOc12
MOL001458	0.8731	0.1269	0.7286	Corydalis Bungeanae Herba	coptisine	Not Available	FALSE	O1c2cc3c4[n+](CCc3cc2OC1)cc1c(c4)ccc2OCOc12
MOL001458	0.8731	0.1269	0.7286	Corydalis Rhizoma	coptisine	Not Available	FALSE	O1c2cc3c4[n+](CCc3cc2OC1)cc1c(c4)ccc2OCOc12
MOL001458	0.8731	0.1269	0.7286	Zanthoxylum Nitidum	coptisine	Not Available	FALSE	O1c2cc3c4[n+](CCc3cc2OC1)cc1c(c4)ccc2OCOc12
MOL001458	0.8731	0.1269	0.7286	Thalictri Glandulosissimi Et	coptisine	Not Available	FALSE	O1c2cc3c4[n+](CCc3cc2OC1)cc1c(c4)ccc2OCOc12

MOL001458	0.8731	0.1269	0.7286	Achyranthis Bidentatae Radix	coptisine	Not Available	FALSE	O1c2cc3c4[n+](CCc3cc2OC1)cc1c(c4)ccc2OCOc12
MOL001458	0.8731	0.1269	0.7286	Phellodendri Chinrnsis Cortex	coptisine	Not Available	FALSE	O1c2cc3c4[n+](CCc3cc2OC1)cc1c(c4)ccc2OCOc12
MOL001458	0.8731	0.1269	0.7286	Phellodendri Amurensis Cortex	coptisine	Not Available	FALSE	O1c2cc3c4[n+](CCc3cc2OC1)cc1c(c4)ccc2OCOc12
MOL001458	0.8731	0.1269	0.7286	Chelidonii Herba	coptisine	Not Available	FALSE	O1c2cc3c4[n+](CCc3cc2OC1)cc1c(c4)ccc2OCOc12
MOL001459	0.7985	0.2015	0.7871	Chelidonii Herba	corysamine	Not Available	FALSE	O1c2c3c(c(c4[n+](CCc3c4cc4OCOc4c3)c3)C)ccc2OC1
MOL001461	0.6599	0.3401	0.8435	Zanthoxylum Nitidum	Dihydrocheler ythrine	485077	FALSE	O1c2cc3c4N(Cc5c(c4ccc3cc2OC1)ccc(OC)c5OC)C
MOL001461	0.6599	0.3401	0.8435	Chelidonii Herba	Dihydrocheler ythrine	485077	FALSE	O1c2cc3c4N(Cc5c(c4ccc3cc2OC1)ccc(OC)c5OC)C
MOL001461	0.6599	0.3401	0.8435	Corydalis Rhizoma	Dihydrocheler ythrine	485077	FALSE	O1c2cc3c4N(Cc5c(c4ccc3cc2OC1)ccc(OC)c5OC)C
MOL001462	0.7847	0.2153	0.7731	Chelidonii Herba	Dihydrochelir ubine	Not Available	FALSE	O1c2c3CN(c4c(c3c(OC)cc2OC1)ccc1c4cc2OCOc2c1)C
MOL001463	0.8207	0.1793	0.7761	Corydalis Bungeanae Herba	Dihydrosangu inarine	Not Available	FALSE	O1c2c3CN(c4c(c3ccc2OC1)ccc1c4cc2OCOc2c1)C
MOL001463	0.8207	0.1793	0.7761	Chelidonii Herba	Dihydrosangu inarine	Not Available	FALSE	O1c2c3CN(c4c(c3ccc2OC1)ccc1c4cc2OCOc2c1)C
MOL001463	0.8207	0.1793	0.7761	Corydalis Rhizoma	Dihydrosangu inarine	Not Available	FALSE	O1c2c3CN(c4c(c3ccc2OC1)ccc1c4cc2OCOc2c1)C
MOL001464	0.8757	0.1243	0.9442	Chelidonii Herba	histamine	774	FALSE	[nH]1c(CCN)cnc1
MOL001464	0.8757	0.1243	0.9442	Phytolaccae Radix	histamine	774	FALSE	[nH]1c(CCN)cnc1
MOL001465	0.7731	0.2269	0.7215	Chelidonii Herba	chelamidine	15160109	FALSE	c1c(c(c2c(c1)C1C(N(C2)C)c2c(C(C1O)O)cc1c(c2)OCO1)OC)OC
MOL001466	0.6627	0.3373	0.8262	Chelidonii Herba	(+/-)-Homochelido nine	164609	FALSE	OC1C2C(N(Cc3c2ccc(OC)c3OC)C)c2c(C1)cc1OCOc1c2
MOL001467	0.6202	0.3798	0.8157	Chelidonii Herba	Luteanin	10143	TRUE	O(c1c2c3C(N(CCc3cc1OC)C)Cc1c2c(O)c(OC)cc1)C
MOL001467	0.6202	0.3798	0.8157	Radix Stephaniae Cepharanthae.	Luteanin	10143	TRUE	O(c1c2c3C(N(CCc3cc1OC)C)Cc1c2c(O)c(OC)cc1)C
MOL001468	0.8998	0.1002	0.9695	Capsici Fructus	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Mume Fructus	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Maydis Seigma	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Chelidonii Herba	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Hippophae Fructus	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Pollen Typhae	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Isatidis Folium	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Polygoni Cuspidati Rhizoma Et Radix	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Rose Rugosae Flos	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Aloe	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O

MOL001468	0.8998	0.1002	0.9695	Quisqualis Indica	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Imperatae Rhizoma	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Eriobotryae Folium	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Portulacae Herba	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Cichorii Radix	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Capsellae Herba	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Jujubae Fructus	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Cornus Officinalis Sieb. Et Zucc.	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Mori Fructus	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Rosae Laevigatae Fructus	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Citrus Aurantium	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Rubi Fructus	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Folium Nelumbinis	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Xanthii Fructus	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Farfarae Flos	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Lycii Fructus	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Choerospondiatis Fructus	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001468	0.8998	0.1002	0.9695	Chaenomeles Sinensis (Thouin) Koehne	MLT	222656	FALSE	OC(CC(=O)O)C(=O)O
MOL001469	0.7877	0.2123	0.7457	Chelidonii Herba	methoxychelidonine	Not Available	FALSE	c1c2c(c3c(c1)C1C(N(C3)C)c3c(CC1O)cc1c(c3OC)OCO1)OCO2
MOL001470	0.8515	0.1485	0.6687	Chelidonii Herba	NME	6329	TRUE	NC
MOL001471	0.8217	0.1783	0.6825	Chelidonii Herba	oxychleidonine	Not Available	FALSE	OC1C2C(N(C(=O)c3c2ccc2OCOc32)C)c2c(C1)cc1OCOc1c2
MOL001472	0.8698	0.1302	0.6883	Chelidonii Herba	chelamine	Not Available	FALSE	c12c(cc3c(c1)C1C(C(C3O)O)c3c(CN1C)c1c(cc3)OCO1)OCO2
MOL001473	0.8187	0.1813	0.7733	Chelidonii Herba	rhoeadine	Not Available	FALSE	O1C2C(N(CCc3c2cc2OCOc2c3)C)c2c(C1OC)c1OCOc1cc2
MOL001474	0.8351	0.1649	0.7408	Corydalis Rhizoma	sanguinarine	Not Available	FALSE	O1c2c3c(c4c([n+](c3)C)c3c(cc4)cc4OCOc4c3)ccc2OC1
MOL001474	0.8351	0.1649	0.7408	Chelidonii Herba	sanguinarine	Not Available	FALSE	O1c2c3c(c4c([n+](c3)C)c3c(cc4)cc4OCOc4c3)ccc2OC1
MOL001474	0.8351	0.1649	0.7408	Zanthoxylum Nitidum	sanguinarine	Not Available	FALSE	O1c2c3c(c4c([n+](c3)C)c3c(cc4)cc4OCOc4c3)ccc2OC1
MOL001474	0.8351	0.1649	0.7408	Mori Cortex	sanguinarine	Not Available	FALSE	O1c2c3c(c4c([n+](c3)C)c3c(cc4)cc4OCOc4c3)ccc2OC1
MOL001476	0.8577	0.1423	0.7648	Chelidonii Herba	(S)-Stylopine	Not Available	FALSE	O1c2c3CN4C(Cc3ccc2OC1)c1c(CC4)cc2OCOc2c1
MOL001476	0.8577	0.1423	0.7648	Strychni Semen	(S)-Stylopine	Not Available	FALSE	O1c2c3CN4C(Cc3ccc2OC1)c1c(CC4)cc2OCOc2c1
MOL001477	0.9491	0.0509	0.9665	Daturae Flos	tyramine	5610	FALSE	Oc1ccc(CCN)cc1
MOL001477	0.9491	0.0509	0.9665	Crataegi Folium	tyramine	5610	FALSE	Oc1ccc(CCN)cc1
MOL001477	0.9491	0.0509	0.9665	Silybum Marianum	tyramine	5610	FALSE	Oc1ccc(CCN)cc1
MOL001477	0.9491	0.0509	0.9665	Herba Cirsii	tyramine	5610	FALSE	Oc1ccc(CCN)cc1
MOL001477	0.9491	0.0509	0.9665	Hordei Fructus Germinatus	tyramine	5610	FALSE	Oc1ccc(CCN)cc1
MOL001477	0.9491	0.0509	0.9665	Chelidonii Herba	tyramine	5610	FALSE	Oc1ccc(CCN)cc1

MOL001478	0.7331	0.2669	0.8729	Chelidonii Herba	toddaline	2703	FALSE	O1c2cc3c4[n+](cc5c(c4ccc3cc2OC1)ccc(OC)c5OC)C
MOL001478	0.7331	0.2669	0.8729	Zanthoxylum Nitidum	toddaline	2703	FALSE	O1c2cc3c4[n+](cc5c(c4ccc3cc2OC1)ccc(OC)c5OC)C
MOL001479	0.2633	0.7367	0.7180	Chelidonii Herba	chelidimerine	Not Available	FALSE	O1c2c3c(N(c4c(c3ccc2OC1)ccc1c4cc2OCOc2c1)C)CC(=O)CC1N(c2c(c3c1c1OCOc1cc3)ccc1c2cc2OCOc2c1)C
MOL001480	0.9091	0.0909	0.8977	Chelidonii Herba	Jerva acid	7431	FALSE	o1c(cc(=O)cc1C(=O)O)C(=O)O
MOL001481	0.8095	0.1905	0.7667	Chelidonii Herba	chelidonine	Not Available	FALSE	OC1c2c(N(Cc3c2ccc2OCOc32)C)c2c(c1)cc1OCOc1c2
MOL001482	0.6302	0.3698	0.7749	Chelidonii Herba	chelilutine	443720	FALSE	O1c2cc3c4[n+](cc5c(c4ccc3cc2OC1)c(OC)cc(OC)c5OC)C
MOL001483	0.7817	0.2183	0.7460	Chelidonii Herba	bocconine	Not Available	FALSE	O1c2c3c(c4c([n+](c3)C)c3c(cc4)cc4OCOc4c3)c(OC)cc2OC1
MOL001484	0.9187	0.0813	0.7311	Sophorae Tonkinensis Radix Et Rhizome	Inermine	Not Available	FALSE	O1C2C(c3c1cc1OCOc1c3)COc1c2ccc(O)c1
MOL001484	0.9187	0.0813	0.7311	Sophorae Flavescentis Radix	Inermine	Not Available	FALSE	O1C2C(c3c1cc1OCOc1c3)COc1c2ccc(O)c1
MOL001484	0.9187	0.0813	0.7311	Radix Euphorbiae Pekinensis	Inermine	Not Available	FALSE	O1C2C(c3c1cc1OCOc1c3)COc1c2ccc(O)c1
MOL001484	0.9187	0.0813	0.7311	Millettiae Speciosae Radix	Inermine	Not Available	FALSE	O1C2C(c3c1cc1OCOc1c3)COc1c2ccc(O)c1
MOL001484	0.9187	0.0813	0.7311	licorice	Inermine	Not Available	FALSE	O1C2C(c3c1cc1OCOc1c3)COc1c2ccc(O)c1
MOL001490	0.2777	0.7223	0.6107	Ginkgo Folium	bis[(2S)-2-ethylhexyl] benzene-1,2-dicarboxylate	7057920	FALSE	O(CC(CCCC)CC)C(=O)c1c(C(=O)OCC(CCCC)CC)cccc1
MOL001490	0.2777	0.7223	0.6107	Choerospondiatis Fructus	bis[(2S)-2-ethylhexyl] benzene-1,2-dicarboxylate	7057920	FALSE	O(CC(CCCC)CC)C(=O)c1c(C(=O)OCC(CCCC)CC)cccc1
MOL001490	0.2777	0.7223	0.6107	Millettiae Speciosae Radix	bis[(2S)-2-ethylhexyl] benzene-1,2-dicarboxylate	7057920	FALSE	O(CC(CCCC)CC)C(=O)c1c(C(=O)OCC(CCCC)CC)cccc1
MOL001491	0.5161	0.4839	0.6983	Millettiae Speciosae Radix	(-)-(7R,8S)-Dihydrodehydrodiconiferyl alcohol	5274623	FALSE	O1C(C(c2c1c(OC)cc(c2)CCCO)CO)c1cc(OC)c(O)cc1
MOL001494	0.4321	0.5679	0.6275	Lithospermum Erythrorhizon	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Lycii Fructus	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Millettiae Speciosae Radix	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Campsis Flos	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Equiseti Hiemalis Herba	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Semen Firmianae	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Litchi Semen	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Folium Artemisiae Argyi	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC

MOL001494	0.4321	0.5679	0.6275	Adenophprae Ae Radix	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Cornus Officinalis Sieb. Et Zucc.	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Ginkgo Folium	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Mahoniae Caulis	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Chuanxiong Rhizoma	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Broussonetiae Fructus	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Canarii Fructus	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Lonicerae Japonicae Flos	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Hippophae Fructus	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	A. Dahurica (Fisch.) Benth. Et Hook	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Trichosanthes Kirilowii Maxim	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Gossampiniflos	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Momordicae Fructus	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Typhonii Rhizoma	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Rosae Laevigatae Fructus	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Maydis Seigma	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Ranunculi Ternati Radix	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Achyranthis Asperae Herba	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Toosendan Fructus	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001494	0.4321	0.5679	0.6275	Coicis Semen	Mandenol	5282184	FALSE	O(C(=O)CCCCCCC/C=C\C/C=C\CCCCC)CC
MOL001495	0.4112	0.5888	0.6385	Toosendan Fructus	Ethyl linolenate	6371716	FALSE	O(C(=O)CCCCCCC/C=C/C/C=C/C/C=C/CC)CC
MOL001495	0.4112	0.5888	0.6385	Millettiae Speciosae Radix	Ethyl linolenate	6371716	FALSE	O(C(=O)CCCCCCC/C=C/C/C=C/C/C=C/CC)CC
MOL001495	0.4112	0.5888	0.6385	Mahoniae Folum	Ethyl linolenate	6371716	FALSE	O(C(=O)CCCCCCC/C=C/C/C=C/C/C=C/CC)CC
MOL001495	0.4112	0.5888	0.6385	Cornus Officinalis Sieb. Et Zucc.	Ethyl linolenate	6371716	FALSE	O(C(=O)CCCCCCC/C=C/C/C=C/C/C=C/CC)CC
MOL001495	0.4112	0.5888	0.6385	Lycii Fructus	Ethyl linolenate	6371716	FALSE	O(C(=O)CCCCCCC/C=C/C/C=C/C/C=C/CC)CC
MOL001495	0.4112	0.5888	0.6385	Lonicerae Japonicae Flos	Ethyl linolenate	6371716	FALSE	O(C(=O)CCCCCCC/C=C/C/C=C/C/C=C/CC)CC
MOL001496	0.7586	0.2414	0.6845	Hippophae Fructus	ETHYLMYRISTATE	31283	FALSE	O(C(=O)CCCCCCCCCCCCC)CC
MOL001496	0.7586	0.2414	0.6845	Gossampiniflos	ETHYLMYRISTATE	31283	FALSE	O(C(=O)CCCCCCCCCCCCC)CC

MOL001496	0.7586	0.2414	0.6845	Mahoniae Caulis	ETHYLMYRISTATE	31283	FALSE	O(C(=O)CCCCCCCCCCCCCC)CC
MOL001496	0.7586	0.2414	0.6845	Saussureae Involucratae Herba	ETHYLMYRISTATE	31283	FALSE	O(C(=O)CCCCCCCCCCCCCC)CC
MOL001496	0.7586	0.2414	0.6845	Lycii Fructus	ETHYLMYRISTATE	31283	FALSE	O(C(=O)CCCCCCCCCCCCCC)CC
MOL001496	0.7586	0.2414	0.6845	Millettiae Speciosae Radix	ETHYLMYRISTATE	31283	FALSE	O(C(=O)CCCCCCCCCCCCCC)CC
MOL001496	0.7586	0.2414	0.6845	Crotonis Fructus	ETHYLMYRISTATE	31283	FALSE	O(C(=O)CCCCCCCCCCCCCC)CC
MOL001497	0.6577	0.3423	0.6513	Paederiae Scandentis Herba	Ethylpentadecanoate	38762	FALSE	O(C(=O)CCCCCCCCCCCCCC)CC
MOL001497	0.6577	0.3423	0.6513	Morindae Officinalis Radix	Ethylpentadecanoate	38762	FALSE	O(C(=O)CCCCCCCCCCCCCC)CC
MOL001497	0.6577	0.3423	0.6513	Saussureae Involucratae Herba	Ethylpentadecanoate	38762	FALSE	O(C(=O)CCCCCCCCCCCCCC)CC
MOL001497	0.6577	0.3423	0.6513	Adenophprae Ae Radix	Ethylpentadecanoate	38762	FALSE	O(C(=O)CCCCCCCCCCCCCC)CC
MOL001497	0.6577	0.3423	0.6513	Ranunculi Ternati Radix	Ethylpentadecanoate	38762	FALSE	O(C(=O)CCCCCCCCCCCCCC)CC
MOL001497	0.6577	0.3423	0.6513	Maydis Seigma	Ethylpentadecanoate	38762	FALSE	O(C(=O)CCCCCCCCCCCCCC)CC
MOL001497	0.6577	0.3423	0.6513	Millettiae Speciosae Radix	Ethylpentadecanoate	38762	FALSE	O(C(=O)CCCCCCCCCCCCCC)CC
MOL001500	0.9675	0.0325	0.8388	Commelinae Herba	LOLIOLIDE	100332	FALSE	O1C2(C(=CC1=O)C(CC(O)C2)(C)C)C
MOL001500	0.9675	0.0325	0.8388	Millettiae Speciosae Radix	LOLIOLIDE	100332	FALSE	O1C2(C(=CC1=O)C(CC(O)C2)(C)C)C
MOL001500	0.9675	0.0325	0.8388	Polygoni Avicularis Herba	LOLIOLIDE	100332	FALSE	O1C2(C(=CC1=O)C(CC(O)C2)(C)C)C
MOL001500	0.9675	0.0325	0.8388	Eucommiae Cortex	LOLIOLIDE	100332	FALSE	O1C2(C(=CC1=O)C(CC(O)C2)(C)C)C
MOL001500	0.9675	0.0325	0.8388	Siphonostegiae Herba	LOLIOLIDE	100332	FALSE	O1C2(C(=CC1=O)C(CC(O)C2)(C)C)C
MOL001500	0.9675	0.0325	0.8388	Capsici Fructus	LOLIOLIDE	100332	FALSE	O1C2(C(=CC1=O)C(CC(O)C2)(C)C)C
MOL001500	0.9675	0.0325	0.8388	Bombyx Mori L.	LOLIOLIDE	100332	FALSE	O1C2(C(=CC1=O)C(CC(O)C2)(C)C)C
MOL001500	0.9675	0.0325	0.8388	Plantaginis Herba	LOLIOLIDE	100332	FALSE	O1C2(C(=CC1=O)C(CC(O)C2)(C)C)C
MOL001501	0.8143	0.1857	0.6081	Maydis Seigma	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Tamaricis Cacumen	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Rehmanniae Radix Praeparata	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Curculiginis Rhizome	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Broussonetiae Fructus	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Millettiae Speciosae Radix	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Amygdalus Communis Vas	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC

MOL001501	0.8143	0.1857	0.6081	Panacis Quinquefolii Radix	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Perillae Fructus	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Alpiniae Officinarum Rhizome	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Aloe	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Allium Azureum Ledeb.	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Semiaquilegiae Radix	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Carthami Flos	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Jujubae Fructus	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Citri Reticulatae Semen	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Cortex Periplocae Radicis	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Malvae Fructus	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Fritillariaeussuriensis Bulbus	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Aconitum Kusnezoffii Reichb	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Ginsen Radix Et Rhizoma Rubra	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Cucurbitae Moschatae Semen	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Kochiae Fructus	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Ginkgo Folium	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Arisaematis Rhizoma	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Allii Tuberosi Semen	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Oroxyli Semen	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Lysimachiae Foenigraeci Herba	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Schizonepetae Spica	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Arecae Semen	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Momordicae Semen	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Isatdis Radix	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001501	0.8143	0.1857	0.6081	Portulacae Herba	Daturic acid	10465	FALSE	OC(=O)CCCCCCCCCCCCCCCC
MOL001505	0.6599	0.3401	0.7130	Millettiae Speciosae Radix	Pyracrenic acid	6439576	FALSE	O(C1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)C(=O)O)CC3)C)(CC2)C)(CC1)C)(C)C)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001508	0.4108	0.5892	0.7050	Millettiae Speciosae Radix	Isolactucerol	115250	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC(=C)C5C)C)CC3)C)(CC2)C)(CC1)C)(C)C
MOL001509	0.8968	0.1032	0.8864	Aauropi Folium	ZINC01081275	5498521	FALSE	O=C(/C=C/C1C(CCC=C1C)(C)C)C
MOL001509	0.8968	0.1032	0.8864	Acoritataninowii Rhizoma	ZINC01081275	5498521	FALSE	O=C(/C=C/C1C(CCC=C1C)(C)C)C
MOL001509	0.8968	0.1032	0.8864	Mume Flos	ZINC01081275	5498521	FALSE	O=C(/C=C/C1C(CCC=C1C)(C)C)C

MOL001509	0.8968	0.1032	0.8864	Junci Medulla	ZINC01081275	5498521	FALSE	O=C(/C=C/C1C(CCC=C1C)(C)C)C
MOL001509	0.8968	0.1032	0.8864	Millettiae Speciosae Radix	ZINC01081275	5498521	FALSE	O=C(/C=C/C1C(CCC=C1C)(C)C)C
MOL001511	0.8617	0.1383	0.7003	Gomphrenae Globosae Flos Seu Herba	(E)-1-((E)-2-(2,6-dicarboxy-2,3-dihydropyridin-4(1H)-ylidene)ethylidene)-6-hydroxy-5-((2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yloxy)indolinium-2-carboxylate	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2CC(/[N+](=C\C=C\3/CC(NC(=C3)C(=O)O)C(=O)O)/c2cc1O)C(=O)O)CO
MOL001512	0.9369	0.0631	0.6193	Gomphrenae Globosae Flos Seu Herba	amaranthin_qt	Not Available	FALSE	Oc1cc2CC(/[N+](=C/C=C\3/CC(NC(=C3)C(=O)O)C(=O)O)/c2cc1O)C(=O)O
MOL001513	0.8645	0.1355	0.6952	Gomphrenae Globosae Flos Seu Herba	amaranthin	Not Available	FALSE	O(C1C(O)C(O)C(OC1Oc1cc2CC(/[N+](=C\C=C\3/CC(NC(=C3)C(=O)O)C(=O)O)/c2cc1O)C(=O)O)CO)C1OC(C(O)C(O)C1O)C(=O)O
MOL001514	0.6861	0.3139	0.6383	Gomphrenae Globosae Flos Seu Herba	gomphrenin V	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2/[N+](=C/C=C\3/CC(NC(=C3)C(=O)O)C(=O)O)/C(Cc2cc1O)C(=O)O)COC(=O)/C=C/c1cc(OC)c(O)cc1
MOL001515	0.8604	0.1396	0.7005	Gomphrenae Globosae Flos Seu Herba	gomphreninI	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2/[N+](=C/C=C/3\CC(NC(=C3)C(=O)O)C(=O)O)/C(Cc2cc1O)C(=O)O)CO
MOL001516	0.8547	0.1453	0.7895	Gomphrenae Globosae Flos Seu Herba	7,9-dihydroxy-6-(4-hydroxyphenyl)pyrano[2,3-f][1,3]benzodioxol-8-one	9883305	FALSE	o1c2c(c(O)c3OCOc3c2)c(=O)c(O)c1c1ccc(O)cc1

MOL001516	0.8547	0.1453	0.7895	Polygoni Tinctorii Foliu	7,9-dihydroxy-6-(4-hydroxyphenyl)pyrano[2,3-f][1,3]benzodioxol-8-one	9883305	FALSE	o1c2c(c(O)c3OCOc3c2)c(=O)c(O)c1c1ccc(O)cc1
MOL001517	0.8529	0.1471	0.6964	Gomphrenae Globosae Flos Seu Herba	isogomphrenin I	Not Available	FALSE	C1(C(OC(C(C1O)O)Oc1c(cc2c(c1)N(C(C2)C(=O)O)/C=C/C1=CC(=NC(C1)C(=O)O)C(=O)O)O)CO)O
MOL001518	0.9238	0.0762	0.7185	Gomphrenae Globosae Flos Seu Herba	isogomphrenin I_qt	Not Available	FALSE	C1/C(=C/C(=C/O)/O)/CC(N1/C=C/C1=CC(=NC(C1)C(=O)O)C(=O)O)C(=O)O
MOL001519	0.6617	0.3383	0.6287	Gomphrenae Globosae Flos Seu Herba	isogomphrenin II	Not Available	FALSE	c1(ccc(cc1)/C=C/C(=O)OCC1OC(C(C(C1O)O)O)Oc1c(cc2c(c1)N(C(C2)C(=O)O)/C=C/C1=CC(=NC(C1)C(=O)O)C(=O)O)O)O
MOL001520	0.6430	0.3570	0.6298	Gomphrenae Globosae Flos Seu Herba	isogomphrenin III	Not Available	FALSE	c1c(c(cc(c1)/C=C/C(=O)OCC1C(C(C(C(O1)Oc1c(cc2c(c1)N(C(C2)C(=O)O)/C=C/C1=CC(=NC(C1)C(=O)O)C(=O)O)O)O)O)O)OC)O
MOL001521	0.7038	0.2962	0.7941	Ziziphi Spinosae Semen	ceanothic acid	Not Available	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)C(=O)O)CC3)C)(CC2)C)(C1C(=O)O)C)(C)C
MOL001522	0.8117	0.1883	0.8275	Jujubae Fructus	(3)-Coclaurine	160487	FALSE	O(c1cc2c(C(NCC2)Cc2ccc(O)cc2)cc1O)C
MOL001522	0.8117	0.1883	0.8275	Ziziphi Spinosae Semen	(3)-Coclaurine	160487	FALSE	O(c1cc2c(C(NCC2)Cc2ccc(O)cc2)cc1O)C
MOL001526	0.7399	0.2601	0.8072	Ziziphi Spinosae Semen	jujuboside A	Not Available	FALSE	O1C23OC(CC(O)(C2C2C(C4(C(C5(C(CC4)C(C(OC4OCC(O)C(OC6OC(C(O)C(O)C6OC6OCC(O)C(O)C6O)COC6OC(C(O)C(O)C6O)CO)C4OC4OC(C(O)C(O)C4O)C)CC5)(C)C)C)CC2)C)(C3)C1)C)C=C(C)C
MOL001527	0.3975	0.6025	0.7953	Ziziphi Spinosae Semen	jujuboside A_qt	Not Available	FALSE	O1C23OC(CC(O)(C2C2C(C4(C(C5(C(CC4)C(C(O)CC5)(C)C)C)CC2)C)(C3)C1)C)C=C(C)C
MOL001528	0.6895	0.3105	0.8303	Ziziphi Spinosae Semen	jujuboside B	Not Available	FALSE	O1C23C(C4C(C5(C(C6(C(CC5)C(C(OC5OCC(O)C(OC7OC(C(O)C(O)C7OC7OCC(O)C(O)C7O)CO)C5OC5OC(C(O)C(O)C5O)C)CC6)(C)C)C)CC4)C)C2)C(O)(CC1(OC3)C=C(C)C)C
MOL001529	0.3522	0.6478	0.7951	Ziziphi Spinosae Semen	jujuboside B_qt	Not Available	FALSE	O1C23C(C4C(C5(C(C6(C(CC5)C(C(O)CC6)(C)C)C)CC4)C)C2)C(O)(CC1(OC3)C=C(C)C)C
MOL001530	0.6987	0.3013	0.7929	Folium Nelumbinis	n-methylasimilobine	Not Available	FALSE	O(c1c2c3C(N(CCc3cc1O)C)Cc1c2cccc1)C
MOL001530	0.6987	0.3013	0.7929	Ziziphi Spinosae Semen	n-methylasimilobine	Not Available	FALSE	O(c1c2c3C(N(CCc3cc1O)C)Cc1c2cccc1)C
MOL001531	0.5920	0.4080	0.7436	Ziziphi Spinosae Semen	dl-Nuciferine	22156	FALSE	O(c1c2c3C(N(CCc3cc1OC)C)Cc1c2cccc1)C
MOL001533	0.0481	0.9519	0.6424	Ziziphi Spinosae Semen	sanjoinine A	Not Available	FALSE	c1cc2ccc1OC(C(C(=O)NC(C(=O)N/C=C/2)CC(C)C)NC(=O)C(Cc1ccccc1)N(C)C)C(C)C

MOL001535	0.0434	0.9566	0.6284	Ziziphi Spinosae Semen	sanjoinine D	Not Available	FALSE	c1cc2ccc1OC(C(C(=O)NC(C(=O)NCC2OC)CC(C)C)NC(=O)C(Cc1ccccc1)N(C)C)C(C)C
MOL001536	0.0600	0.9400	0.6544	Ziziphi Spinosae Semen	sanjoinine F	Not Available	FALSE	c1cc2ccc1OC(C(C(=O)NC(C(=O)N/C=C/2)C(CC(C)C)O)NC(=O)C(Cc1ccccc1)N(C)C)C(C)C
MOL001537	0.0551	0.9449	0.6317	Ziziphi Spinosae Semen	sanjoinine G1	Not Available	FALSE	c1cc2ccc1OC(C(C(=O)NC(C(=O)NCC2O)CC(C)C)NC(=O)C(Cc1ccccc1)N(C)C)C(C)C
MOL001540	0.8533	0.1467	0.8421	Jujubae Fructus	Spinosin	155692	FALSE	O(C1C(O)C(O)C(OC1c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1OC)CO)C1OC(C(O)C(O)C1O)CO
MOL001540	0.8533	0.1467	0.8421	Ziziphi Spinosae Semen	Spinosin	155692	FALSE	O(C1C(O)C(O)C(OC1c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1OC)CO)C1OC(C(O)C(O)C1O)CO
MOL001541	0.7963	0.2037	0.8488	Ziziphi Spinosae Semen	4H-Benzopyran-4-one, 6-beta-D-glucopyranosyl-5-hydroxy-2-(4-hydroxyphenyl)-7-methoxy-	124034	FALSE	OC1C(O)C(O)C(OC1c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1OC)CO
MOL001541	0.7963	0.2037	0.8488	Swertiae Mileensis Herba	4H-Benzopyran-4-one, 6-beta-D-glucopyranosyl-5-hydroxy-2-(4-hydroxyphenyl)-7-methoxy-	124034	FALSE	OC1C(O)C(O)C(OC1c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1OC)CO
MOL001542	0.7963	0.2037	0.8488	Ziziphi Spinosae Semen	swertisin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1OC
MOL001543	0.8728	0.1272	0.7911	Trigonellae Semen	Vicenin-2	442664	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c(C2OC(C(O)C(O)C2O)CO)c(O)c2c1oc(cc2=O)c1ccc(O)cc1
MOL001543	0.8728	0.1272	0.7911	Lysimachiae Herba	Vicenin-2	442664	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c(C2OC(C(O)C(O)C2O)CO)c(O)c2c1oc(cc2=O)c1ccc(O)cc1
MOL001543	0.8728	0.1272	0.7911	licorice	Vicenin-2	442664	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c(C2OC(C(O)C(O)C2O)CO)c(O)c2c1oc(cc2=O)c1ccc(O)cc1
MOL001543	0.8728	0.1272	0.7911	Santalum Album L.	Vicenin-2	442664	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c(C2OC(C(O)C(O)C2O)CO)c(O)c2c1oc(cc2=O)c1ccc(O)cc1
MOL001543	0.8728	0.1272	0.7911	Ziziphi Spinosae Semen	Vicenin-2	442664	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c(C2OC(C(O)C(O)C2O)CO)c(O)c2c1oc(cc2=O)c1ccc(O)cc1

MOL001543	0.8728	0.1272	0.7911	Artemisia Annua L.	Vicenin-2	442664	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c(C2OC(C(O)C(O)C2O)CO)c(O)c2c1oc(cc2=O)c1ccc(O)cc1
MOL001544	0.8505	0.1495	0.8131	Ziziphi Spinosae Semen	zivulgarin	Not Available	FALSE	O(C1C(O)C(O)C(OC1CO)c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1OC)C1OC(C(O)C(O)C1O)CO
MOL001545	0.7963	0.2037	0.8488	Ziziphi Spinosae Semen	zivulgarin_qt	Not Available	FALSE	OC1C(O)C(O)C(OC1CO)c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1OC
MOL001546	0.6389	0.3611	0.6894	Ziziphi Spinosae Semen	zizyphusine	Not Available	FALSE	c1(ccc2c(c1OC)c1c3C(C2)[N+](CCc3cc(c1O)O)(C)C)OC
MOL001547	0.5508	0.4492	0.7593	Ziziphi Spinosae Semen	6'-p-coumaroylspinosin	Not Available	FALSE	c1(c(ccc(c1)/C=C/C(=O)OCC1C(C(C(C(O1)OC1C(OC(C(C1O)O)CO)c1c(c2c(cc1C)oc(cc2=O)c1ccc(cc1)O)O)O)O)O)O)OC
MOL001548	0.5244	0.4756	0.7581	Ziziphi Spinosae Semen	6'-sinapoylspinosin	Not Available	FALSE	c1(c(c(cc(c1)/C=C/C(=O)OCC1C(C(C(C(O1)OC1C(OC(C(C1O)O)CO)C1Cc2c(C=C1OC)oc(cc2=O)c1ccc(cc1)O)O)O)O)OC)O)OC
MOL001549	0.6885	0.3115	0.7662	Ziziphi Spinosae Semen	alphitolic acid	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC3C(=C)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C
MOL001550	0.0641	0.9359	0.7995	Ziziphi Spinosae Semen	amphibine D	Not Available	FALSE	O1C2C(N(CC2)C(=O)C(NC(=O)C(N(C)C)Cc2ccccc2)C(CC)C)C(=O)NC(C(CC)C)C(=O)N/C=C\c2ccc1cc2
MOL001551	0.3664	0.6336	0.7896	Jujubae Fructus	Trochol	72326	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)CO)CC3)C)(CC2)C)(CC1)C)(C)C
MOL001551	0.3664	0.6336	0.7896	Cortex Moutan	Trochol	72326	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)CO)CC3)C)(CC2)C)(CC1)C)(C)C
MOL001551	0.3664	0.6336	0.7896	Ziziphi Spinosae Semen	Trochol	72326	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)CO)CC3)C)(CC2)C)(CC1)C)(C)C
MOL001551	0.3664	0.6336	0.7896	Trigonellae Semen	Trochol	72326	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)CO)CC3)C)(CC2)C)(CC1)C)(C)C
MOL001551	0.3664	0.6336	0.7896	Glehniae Radix	Trochol	72326	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)CO)CC3)C)(CC2)C)(CC1)C)(C)C
MOL001551	0.3664	0.6336	0.7896	Platycodon Grandiforus	Trochol	72326	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)CO)CC3)C)(CC2)C)(CC1)C)(C)C
MOL001551	0.3664	0.6336	0.7896	Glechomae Herba	Trochol	72326	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)CO)CC3)C)(CC2)C)(CC1)C)(C)C
MOL001551	0.3664	0.6336	0.7896	Lysimachiae Foenigraeci Herba	Trochol	72326	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)CO)CC3)C)(CC2)C)(CC1)C)(C)C
MOL001551	0.3664	0.6336	0.7896	Ilicis Cornutae Folium Immayuri	Trochol	72326	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)CO)CC3)C)(CC2)C)(CC1)C)(C)C
MOL001551	0.3664	0.6336	0.7896	Aucklandiae Radix	Trochol	72326	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)CO)CC3)C)(CC2)C)(CC1)C)(C)C
MOL001551	0.3664	0.6336	0.7896	Euonymi Alati Ramulus	Trochol	72326	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)CO)CC3)C)(CC2)C)(CC1)C)(C)C
MOL001551	0.3664	0.6336	0.7896	Tamaricis Cacumen	Trochol	72326	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)CO)CC3)C)(CC2)C)(CC1)C)(C)C
MOL001551	0.3664	0.6336	0.7896	Cortex Hibisci	Trochol	72326	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)CO)CC3)C)(CC2)C)(CC1)C)(C)C

MOL001551	0.3664	0.6336	0.7896	Semen Euphorbiae	Trochol	72326	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)CO)CC3)C)(CC2)C)(CC1)C)(C)C
MOL001551	0.3664	0.6336	0.7896	Isatdis Radix	Trochol	72326	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)CO)CC3)C)(CC2)C)(CC1)C)(C)C
MOL001551	0.3664	0.6336	0.7896	Eucommiae Cortex	Trochol	72326	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)CO)CC3)C)(CC2)C)(CC1)C)(C)C
MOL001551	0.3664	0.6336	0.7896	Hoveniae Dulcis Semen	Trochol	72326	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)CO)CC3)C)(CC2)C)(CC1)C)(C)C
MOL001551	0.3664	0.6336	0.7896	Sophora Japonica L.	Trochol	72326	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)CO)CC3)C)(CC2)C)(CC1)C)(C)C
MOL001551	0.3664	0.6336	0.7896	Caulis Akebiae	Trochol	72326	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)CO)CC3)C)(CC2)C)(CC1)C)(C)C
MOL001552	0.8739	0.1261	0.9139	Hyoscyami Semen	OIN	154417	FALSE	O(C1CC2N(C(CC2)C1)C)C(=O)C(c1ccccc1)CO
MOL001552	0.8739	0.1261	0.9139	Lycii Cortex	OIN	154417	FALSE	O(C1CC2N(C(CC2)C1)C)C(=O)C(c1ccccc1)CO
MOL001553	0.8182	0.1818	0.7586	Hyoscyami Semen	atroscine	Not Available	FALSE	O1C2C1C1N(C2CC(OC(=O)C(CO)c2ccccc2)C1)C
MOL001554	0.8182	0.1818	0.7586	Physochlainae Radix	Scopolamine	Not Available	FALSE	O1C2C1C1N(C2CC(OC(=O)C(CO)c2ccccc2)C1)C
MOL001554	0.8182	0.1818	0.7586	Hyoscyami Semen	Scopolamine	Not Available	FALSE	O1C2C1C1N(C2CC(OC(=O)C(CO)c2ccccc2)C1)C
MOL001554	0.8182	0.1818	0.7586	Daturae Flos	Scopolamine	Not Available	FALSE	O1C2C1C1N(C2CC(OC(=O)C(CO)c2ccccc2)C1)C
MOL001555	0.2663	0.7337	0.6910	Piperis Longi Fructus	ZINC03996196	7299790	FALSE	C12C(C(OC2)c2cc(c(cc2)OC)OC)COC1c1cc(c(cc1)OC)OC
MOL001556	0.8418	0.1582	0.6717	Piperis Longi Fructus	Isocaryophyllene	5281522	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(\CC2)/C
MOL001556	0.8418	0.1582	0.6717	Panacis Quinquefolii Radix	Isocaryophyllene	5281522	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(\CC2)/C
MOL001556	0.8418	0.1582	0.6717	Fritillariaeussuriensis Bulbus	Isocaryophyllene	5281522	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(\CC2)/C
MOL001556	0.8418	0.1582	0.6717	Ardisiae Japonicae Herba	Isocaryophyllene	5281522	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(\CC2)/C
MOL001556	0.8418	0.1582	0.6717	Cnidii Fructus	Isocaryophyllene	5281522	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(\CC2)/C
MOL001556	0.8418	0.1582	0.6717	Rhododendri Daurici Folium	Isocaryophyllene	5281522	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(\CC2)/C
MOL001556	0.8418	0.1582	0.6717	Moslae Herba	Isocaryophyllene	5281522	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(\CC2)/C
MOL001556	0.8418	0.1582	0.6717	Farfarae Flos	Isocaryophyllene	5281522	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(\CC2)/C
MOL001556	0.8418	0.1582	0.6717	Houttuyniae Herba	Isocaryophyllene	5281522	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(\CC2)/C
MOL001556	0.8418	0.1582	0.6717	Ailanthi Cortex	Isocaryophyllene	5281522	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(\CC2)/C
MOL001556	0.8418	0.1582	0.6717	Anisi Stellati Fructus	Isocaryophyllene	5281522	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(\CC2)/C

MOL001556	0.8418	0.1582	0.6717	Kadsurae Coccineae Radix Et Caulis	Isocaryophyllene	5281522	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(\CC2)/C
MOL001556	0.8418	0.1582	0.6717	Aristolochiae Fructus	Isocaryophyllene	5281522	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(\CC2)/C
MOL001556	0.8418	0.1582	0.6717	Cinnamomi Ramulus	Isocaryophyllene	5281522	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(\CC2)/C
MOL001556	0.8418	0.1582	0.6717	Centipedae Herba	Isocaryophyllene	5281522	FALSE	C12C(CC1(C)C)C(=C)CC/C=C(\CC2)/C
MOL001557	0.9454	0.0546	0.8813	Piperis Longi Fructus	CIS-DECAHYDRONAPHTHALENE	7044	FALSE	C12C(CCCC1)CCCC2
MOL001558	0.4331	0.5669	0.7622	Ginkgo Folium	sesamin	72307	FALSE	C12C(C(OC2)c2cc3c(cc2)OCO3)COC1c1cc2c(cc1)OCO2
MOL001558	0.4331	0.5669	0.7622	Gentianae Radix Et Rhozima	sesamin	72307	FALSE	C12C(C(OC2)c2cc3c(cc2)OCO3)COC1c1cc2c(cc1)OCO2
MOL001558	0.4331	0.5669	0.7622	Piperis Longi Fructus	sesamin	72307	FALSE	C12C(C(OC2)c2cc3c(cc2)OCO3)COC1c1cc2c(cc1)OCO2
MOL001558	0.4331	0.5669	0.7622	Cuscutae Semen	sesamin	72307	FALSE	C12C(C(OC2)c2cc3c(cc2)OCO3)COC1c1cc2c(cc1)OCO2
MOL001558	0.4331	0.5669	0.7622	Asari Radix Et Rhizoma	sesamin	72307	FALSE	C12C(C(OC2)c2cc3c(cc2)OCO3)COC1c1cc2c(cc1)OCO2
MOL001558	0.4331	0.5669	0.7622	Zanthoxylum Nitidum	sesamin	72307	FALSE	C12C(C(OC2)c2cc3c(cc2)OCO3)COC1c1cc2c(cc1)OCO2
MOL001558	0.4331	0.5669	0.7622	Stemonae Radix	sesamin	72307	FALSE	C12C(C(OC2)c2cc3c(cc2)OCO3)COC1c1cc2c(cc1)OCO2
MOL001559	0.8015	0.1985	0.9013	Piperis Longi Fructus	piperlongumine	5320621	FALSE	C(=O)(/C=C/C=C/c1cc2OCOc2cc1)NCC(C)C
MOL001559	0.8015	0.1985	0.9013	Rhizoma Dioscoreae	piperlongumine	5320621	FALSE	C(=O)(/C=C/C=C/c1cc2OCOc2cc1)NCC(C)C
MOL001560	0.1658	0.8342	0.8534	Piperis Longi Fructus	pipernonaline	Not Available	FALSE	C1CCN(CC1)C(=O)/C=C/CCCC/C=C\c1ccc2c(c1)OCO2
MOL001561	0.2328	0.7672	0.8311	Piperis Longi Fructus	dehydropipernonaline	Not Available	FALSE	C1CCN(CC1)C(=O)/C=C/C=C/CC/C=C\c1ccc2c(c1)OCO2
MOL001563	0.0536	0.9464	0.8127	Piperis Longi Fructus	piperundecalidine	Not Available	FALSE	C1CCN(CC1)C(=O)/C=C/C=C/CCCC/C=C\c1ccc2c(c1)OCO2
MOL001564	0.8975	0.1025	0.9697	Piperis Fructus	PIP	8082	FALSE	C1NCCCC1
MOL001564	0.8975	0.1025	0.9697	Piperis Longi Fructus	PIP	8082	FALSE	C1NCCCC1
MOL001564	0.8975	0.1025	0.9697	Capsici Fructus	PIP	8082	FALSE	C1NCCCC1
MOL001567	0.9614	0.0386	0.9710	Piperis Longi Fructus	2,4-Dimethoxytoluene	96403	FALSE	c1(cc(ccc1C)OC)OC
MOL001569	0.6682	0.3318	0.6719	Piperis Longi Fructus	3-phenylundecane	Not Available	FALSE	C(CC)CCCCCC(CC)c1ccccc1
MOL001569	0.6682	0.3318	0.6719	Panacis Quinquefolii Radix	3-phenylundecane	Not Available	FALSE	C(CC)CCCCCC(CC)c1ccccc1

MOL001570	0.8420	0.1580	0.7243	Rhododendri Daurici Folium	1,4,7,-Cycloundecatriene, 1,5,9,9-tetramethyl-, Z,Z,Z-	5368784	FALSE	C1(CC/C(=C\C/C=C(\C/C=C\1)/C)/C)(C)C
MOL001570	0.8420	0.1580	0.7243	Piperis Longi Fructus	1,4,7,-Cycloundecatriene, 1,5,9,9-tetramethyl-, Z,Z,Z-	5368784	FALSE	C1(CC/C(=C\C/C=C(\C/C=C\1)/C)/C)(C)C
MOL001571	0.9268	0.0732	0.9340	Piperis Longi Fructus	4-[(1-Carboxy-2-methylbutyl)amino]-2(1H)-pyrimidinone	Not Available	FALSE	c1(=O)nc(cc[nH]1)NC(C(CC)C)C(=O)O
MOL001573	0.9401	0.0599	0.9437	Piperis Longi Fructus	Methyl hydrocinnamate	7643	FALSE	c1(CCC(=O)OC)ccccc1
MOL001574	0.9386	0.0614	0.9228	Piperis Longi Fructus	Bicyclo[3. 2. 2]non-6-en-3-one	Not Available	FALSE	C12CC(=O)CC(C=C1)CC2
MOL001575	0.6482	0.3518	0.6228	Platycladi Cacumen	cedryl acetate	Not Available	FALSE	C(=O)(C)OC1(C)CCC2C(C)(C)C3CC12CCC3C
MOL001575	0.6482	0.3518	0.6228	Radix Angelicae Biseratae	cedryl acetate	Not Available	FALSE	C(=O)(C)OC1(C)CCC2C(C)(C)C3CC12CCC3C
MOL001575	0.6482	0.3518	0.6228	Piperis Longi Fructus	cedryl acetate	Not Available	FALSE	C(=O)(C)OC1(C)CCC2C(C)(C)C3CC12CCC3C
MOL001575	0.6482	0.3518	0.6228	Agrimonia Eupatoria	cedryl acetate	Not Available	FALSE	C(=O)(C)OC1(C)CCC2C(C)(C)C3CC12CCC3C
MOL001575	0.6482	0.3518	0.6228	Viticis Fructus	cedryl acetate	Not Available	FALSE	C(=O)(C)OC1(C)CCC2C(C)(C)C3CC12CCC3C
MOL001576	0.9466	0.0534	0.8411	Piperis Longi Fructus	(2R,4aR,8aR)-2-methyldecalin	12816526	FALSE	C1C(CCC2CCCCC12)C
MOL001577	0.8295	0.1705	0.7346	Piperis Longi Fructus	Dodecahydro pyrido [1,2-b]isoquinolin-6-one	Not Available	FALSE	C1(=O)N2C(CC3CCCCC13)CCCC2
MOL001578	0.9221	0.0779	0.9505	Ephedra Herba	Hypnon	7410	FALSE	c1(ccccc1)C(=O)C
MOL001578	0.9221	0.0779	0.9505	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	Hypnon	7410	FALSE	c1(ccccc1)C(=O)C
MOL001578	0.9221	0.0779	0.9505	Angelicae Sinensis Radix	Hypnon	7410	FALSE	c1(ccccc1)C(=O)C
MOL001578	0.9221	0.0779	0.9505	Cinnamomi Ramulus	Hypnon	7410	FALSE	c1(ccccc1)C(=O)C
MOL001578	0.9221	0.0779	0.9505	Radix Cynanchi Paniculati	Hypnon	7410	FALSE	c1(ccccc1)C(=O)C
MOL001578	0.9221	0.0779	0.9505	Oroxyli Semen	Hypnon	7410	FALSE	c1(ccccc1)C(=O)C
MOL001578	0.9221	0.0779	0.9505	Piperis Longi Fructus	Hypnon	7410	FALSE	c1(ccccc1)C(=O)C
MOL001578	0.9221	0.0779	0.9505	Cinnanmomi Cortex	Hypnon	7410	FALSE	c1(ccccc1)C(=O)C

MOL001578	0.9221	0.0779	0.9505	Moslae Herba	Hypnon	7410	FALSE	c1(ccccc1)C(=O)C
MOL001579	0.8154	0.1846	0.6964	Bidentis Bipinnatae Herba	germacrene	Not Available	FALSE	C\1=C\CC(C)CCC(C(C)C)CCC1C
MOL001579	0.8154	0.1846	0.6964	Evodiae Fructus	germacrene	Not Available	FALSE	C\1=C\CC(C)CCC(C(C)C)CCC1C
MOL001579	0.8154	0.1846	0.6964	Cinnanmomi Cortex	germacrene	Not Available	FALSE	C\1=C\CC(C)CCC(C(C)C)CCC1C
MOL001579	0.8154	0.1846	0.6964	Viticis Fructus	germacrene	Not Available	FALSE	C\1=C\CC(C)CCC(C(C)C)CCC1C
MOL001579	0.8154	0.1846	0.6964	Solidaginis Herba	germacrene	Not Available	FALSE	C\1=C\CC(C)CCC(C(C)C)CCC1C
MOL001579	0.8154	0.1846	0.6964	Chuanxiong Rhizoma	germacrene	Not Available	FALSE	C\1=C\CC(C)CCC(C(C)C)CCC1C
MOL001579	0.8154	0.1846	0.6964	Viticis Negundo Folium	germacrene	Not Available	FALSE	C\1=C\CC(C)CCC(C(C)C)CCC1C
MOL001579	0.8154	0.1846	0.6964	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	germacrene	Not Available	FALSE	C\1=C\CC(C)CCC(C(C)C)CCC1C
MOL001579	0.8154	0.1846	0.6964	Meliae Azedarach Fructus	germacrene	Not Available	FALSE	C\1=C\CC(C)CCC(C(C)C)CCC1C
MOL001579	0.8154	0.1846	0.6964	Curcumae Radix	germacrene	Not Available	FALSE	C\1=C\CC(C)CCC(C(C)C)CCC1C
MOL001579	0.8154	0.1846	0.6964	Calyx Seu Fructus Physalis	germacrene	Not Available	FALSE	C\1=C\CC(C)CCC(C(C)C)CCC1C
MOL001579	0.8154	0.1846	0.6964	Gynostemmae Pentaphylli Herba	germacrene	Not Available	FALSE	C\1=C\CC(C)CCC(C(C)C)CCC1C
MOL001579	0.8154	0.1846	0.6964	Piperis Longi Fructus	germacrene	Not Available	FALSE	C\1=C\CC(C)CCC(C(C)C)CCC1C
MOL001579	0.8154	0.1846	0.6964	Cannabis Sativa L.	germacrene	Not Available	FALSE	C\1=C\CC(C)CCC(C(C)C)CCC1C
MOL001579	0.8154	0.1846	0.6964	Piperis Fructus	germacrene	Not Available	FALSE	C\1=C\CC(C)CCC(C(C)C)CCC1C
MOL001579	0.8154	0.1846	0.6964	Epimrdii Herba	germacrene	Not Available	FALSE	C\1=C\CC(C)CCC(C(C)C)CCC1C
MOL001580	0.9345	0.0655	0.9010	Piperis Fructus	Piperonal	8438	FALSE	c12c(ccc(c1)C=O)OCO2
MOL001580	0.9345	0.0655	0.9010	Ginsen Radix Et Rhizoma Rubra	Piperonal	8438	FALSE	c12c(ccc(c1)C=O)OCO2
MOL001580	0.9345	0.0655	0.9010	Piperis Longi Fructus	Piperonal	8438	FALSE	c12c(ccc(c1)C=O)OCO2
MOL001581	0.9251	0.0749	0.9376	Piperis Longi Fructus	Isobutylisovalerate	11514	FALSE	C(CC(=O)OCC(C)C)(C)C
MOL001583	0.9403	0.0597	0.7988	Piperis Longi Fructus	Lawsone	6755	FALSE	c1cc2c(cc1)C(=O)C(=CC2=O)O
MOL001584	0.8760	0.1240	0.8713	Piperis Longi Fructus	[(3S)-3,7-dimethylocta-1,6-dien-3-yl] propanoate	1616358	FALSE	C(OC(=O)CC)(CCC=C(C)C)(C=C)C
MOL001584	0.8760	0.1240	0.8713	Coriandri Sativi Herba	[(3S)-3,7-dimethylocta-1,6-dien-3-yl] propanoate	1616358	FALSE	C(OC(=O)CC)(CCC=C(C)C)(C=C)C
MOL001585	0.5692	0.4308	0.6233	Piperis Longi Fructus	9,17-OCTADECADIENAL (Z)	5365667	FALSE	C(=O)CCCCCCC/C=C\CCCCCCC=C
MOL001585	0.5692	0.4308	0.6233	Lycii Fructus	9,17-OCTADECADIENAL (Z)	5365667	FALSE	C(=O)CCCCCCC/C=C\CCCCCCC=C

MOL001586	0.8927	0.1073	0.8997	Piperis Longi Fructus	N-(2,5-dimethoxyphenyl)-4-methoxybenzamide	532276	FALSE	C(=O)(c1ccc(cc1)OC)Nc1c(ccc(c1)OC)OC
MOL001587	0.7866	0.2134	0.9396	Piperis Longi Fructus	(E)-5-(4-hydroxy-3-methoxy-phenyl)-1-piperidino-pent-2-en-1-one	11630663	FALSE	N1(CCCCC1)C(=O)/C=C/CCc1cc(c(cc1)O)OC
MOL001590	0.8576	0.1424	0.8172	Piperis Longi Fructus	N-isobutyl-decatrans-2-trans-4-dienamide	Not Available	FALSE	CC(CNC(=O)/C=C/C=C/CCCC)C
MOL001591	0.9111	0.0889	0.9394	Piperis Longi Fructus	p-Amino-o-cresol	76081	FALSE	c1(c(cc(cc1)N)C)O
MOL001592	0.7530	0.2470	0.8510	Piperis Longi Fructus	piperine	638024	TRUE	C1Oc2c(O1)cc(cc2)/C=C/C=C/C(=O)N1CCCCC1
MOL001593	0.9582	0.0418	0.9574	Menthae Herba	Piperitenone	381152	FALSE	C1(=CC(=O)C(=C(C)C)CC1)C
MOL001593	0.9582	0.0418	0.9574	Piperis Fructus	Piperitenone	381152	FALSE	C1(=CC(=O)C(=C(C)C)CC1)C
MOL001593	0.9582	0.0418	0.9574	Piperis Longi Fructus	Piperitenone	381152	FALSE	C1(=CC(=O)C(=C(C)C)CC1)C
MOL001593	0.9582	0.0418	0.9574	Ligustici Rhizoma Et Radix	Piperitenone	381152	FALSE	C1(=CC(=O)C(=C(C)C)CC1)C
MOL001593	0.9582	0.0418	0.9574	Schizonepetae Herba	Piperitenone	381152	FALSE	C1(=CC(=O)C(=C(C)C)CC1)C
MOL001594	0.8549	0.1451	0.7208	Piperis Longi Fructus	Pisatin	Not Available	FALSE	c1cc2c(cc1OC)OCC1(C2Oc2c1cc1c(c2)OCO1)O
MOL001595	0.8733	0.1267	0.9011	Asari Radix Et Rhizoma	sesamol	68289	FALSE	c12c(ccc(c1)O)OCO2
MOL001595	0.8733	0.1267	0.9011	Piperis Longi Fructus	sesamol	68289	FALSE	c12c(ccc(c1)O)OCO2
MOL001595	0.8733	0.1267	0.9011	Sesami Nigrum Semen	sesamol	68289	FALSE	c12c(ccc(c1)O)OCO2
MOL001596	0.8066	0.1934	0.6678	Piperis Longi Fructus	tetradecadiene-1,13	30875	FALSE	C(CCCCCC=C)CCCCC=C
MOL001596	0.8066	0.1934	0.6678	Farfarae Flos	tetradecadiene-1,13	30875	FALSE	C(CCCCCC=C)CCCCC=C
MOL001598	0.7576	0.2424	0.7432	Piperis Longi Fructus	Undulatone	Not Available	FALSE	C1(=O)C=C(C2C(C1O)(C1C34C(C2OC(=O)/C(=C/C)/C)OC(=O)C(C3C(C(C1(O)OC4)O)C)OC(=O)C)C)C
MOL001599	0.9060	0.0940	0.7345	Perilla Frutescens	α-cubebol	Not Available	FALSE	C1(CCC(C2C=C(CCC12)C)(C)C)(O)C
MOL001599	0.9060	0.0940	0.7345	Litchi Semen	α-cubebol	Not Available	FALSE	C1(CCC(C2C=C(CCC12)C)(C)C)(O)C
MOL001599	0.9060	0.0940	0.7345	Curcumae Radix	α-cubebol	Not Available	FALSE	C1(CCC(C2C=C(CCC12)C)(C)C)(O)C
MOL001599	0.9060	0.0940	0.7345	Rhizome Of Whiteback Greenbrier	α-cubebol	Not Available	FALSE	C1(CCC(C2C=C(CCC12)C)(C)C)(O)C
MOL001599	0.9060	0.0940	0.7345	Piperis Longi Fructus	α-cubebol	Not Available	FALSE	C1(CCC(C2C=C(CCC12)C)(C)C)(O)C
MOL001599	0.9060	0.0940	0.7345	Tamaricis Cacumen	α-cubebol	Not Available	FALSE	C1(CCC(C2C=C(CCC12)C)(C)C)(O)C

MOL001599	0.9060	0.0940	0.7345	Kadsurae Coccineae Radix Et Caulis	α-cubebol	Not Available	FALSE	C1(CCC(C2C=C(CCC12)C)(C)C)(O)C
MOL001599	0.9060	0.0940	0.7345	Cornus Officinalis Sieb. Et Zucc.	α-cubebol	Not Available	FALSE	C1(CCC(C2C=C(CCC12)C)(C)C)(O)C
MOL001599	0.9060	0.0940	0.7345	Acoritataninowii Rhizoma	α-cubebol	Not Available	FALSE	C1(CCC(C2C=C(CCC12)C)(C)C)(O)C
MOL001599	0.9060	0.0940	0.7345	Cinnamomi Ramulus	α-cubebol	Not Available	FALSE	C1(CCC(C2C=C(CCC12)C)(C)C)(O)C
MOL001599	0.9060	0.0940	0.7345	licorice	α-cubebol	Not Available	FALSE	C1(CCC(C2C=C(CCC12)C)(C)C)(O)C
MOL001599	0.9060	0.0940	0.7345	Alpiniae Officinarum Rhizome	α-cubebol	Not Available	FALSE	C1(CCC(C2C=C(CCC12)C)(C)C)(O)C
MOL001599	0.9060	0.0940	0.7345	Meliae Azedarach Fructus	α-cubebol	Not Available	FALSE	C1(CCC(C2C=C(CCC12)C)(C)C)(O)C
MOL001599	0.9060	0.0940	0.7345	Bidentis Bipinnatae Herba	α-cubebol	Not Available	FALSE	C1(CCC(C2C=C(CCC12)C)(C)C)(O)C
MOL001599	0.9060	0.0940	0.7345	Cinnanmomi Cortex	α-cubebol	Not Available	FALSE	C1(CCC(C2C=C(CCC12)C)(C)C)(O)C
MOL001601	0.7151	0.2849	0.8455	Piperis Longi Fructus	1,2,5,6-tetrahydrotanshinone	Not Available	FALSE	c12c(ccc3c1C(=O)C(=O)C1=C3OCC1C)C(=CCC2)C
MOL001601	0.7151	0.2849	0.8455	Radix Salviae	1,2,5,6-tetrahydrotanshinone	Not Available	FALSE	c12c(ccc3c1C(=O)C(=O)C1=C3OCC1C)C(=CCC2)C
MOL001602	0.8477	0.1523	0.6782	Piperis Longi Fructus	1,4-cadinadiene	50986185	FALSE	C1(CCC(C2=CCC(=CC12)C)C)C(C)C
MOL001602	0.8477	0.1523	0.6782	Cinnanmomi Cortex	1,4-cadinadiene	50986185	FALSE	C1(CCC(C2=CCC(=CC12)C)C)C(C)C
MOL001602	0.8477	0.1523	0.6782	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	1,4-cadinadiene	50986185	FALSE	C1(CCC(C2=CCC(=CC12)C)C)C(C)C
MOL001603	0.5485	0.4515	0.6702	Piperis Longi Fructus	demethoxycurcumin	Not Available	FALSE	c1(cc(c(cc1)O)OC)/C=C/C(=O)CC(=O)/C=C\c1ccc(cc1)O
MOL001604	0.9491	0.0509	0.9656	Lonicerae Japonicae Flos	Linalool	Not Available	FALSE	C(CCC1C(C)(C)O1)(C=C)(C)O
MOL001604	0.9491	0.0509	0.9656	Lygodii Spora	Linalool	Not Available	FALSE	C(CCC1C(C)(C)O1)(C=C)(C)O
MOL001604	0.9491	0.0509	0.9656	Ephedra Herba	Linalool	Not Available	FALSE	C(CCC1C(C)(C)O1)(C=C)(C)O
MOL001604	0.9491	0.0509	0.9656	Schisandrae Chinensis Fructus	Linalool	Not Available	FALSE	C(CCC1C(C)(C)O1)(C=C)(C)O
MOL001604	0.9491	0.0509	0.9656	Piperis Longi Fructus	Linalool	Not Available	FALSE	C(CCC1C(C)(C)O1)(C=C)(C)O
MOL001604	0.9491	0.0509	0.9656	Lysimachiae Foenigraeci Herba	Linalool	Not Available	FALSE	C(CCC1C(C)(C)O1)(C=C)(C)O
MOL001604	0.9491	0.0509	0.9656	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Linalool	Not Available	FALSE	C(CCC1C(C)(C)O1)(C=C)(C)O
MOL001604	0.9491	0.0509	0.9656	Paederiae Scandentis Herba	Linalool	Not Available	FALSE	C(CCC1C(C)(C)O1)(C=C)(C)O
MOL001604	0.9491	0.0509	0.9656	Cornus Officinalis Sieb. Et Zucc.	Linalool	Not Available	FALSE	C(CCC1C(C)(C)O1)(C=C)(C)O
MOL001604	0.9491	0.0509	0.9656	Evodiae Fructus	Linalool	Not Available	FALSE	C(CCC1C(C)(C)O1)(C=C)(C)O
MOL001604	0.9491	0.0509	0.9656	Chaenomeles Sinensis (Thouin) Koehne	Linalool	Not Available	FALSE	C(CCC1C(C)(C)O1)(C=C)(C)O

MOL001605	0.9647	0.0353	0.9194	Piperis Longi Fructus	cis-2-Decalone	246289	FALSE	C1C(=O)CCC2CCCCC12
MOL001606	0.8009	0.1991	0.6810	Stephaniae Tetrandrae Radix	BB_NC-0668	9855795	FALSE	C12(C(=CCCC2C)CCC(C1)C(=C)C)C
MOL001606	0.8009	0.1991	0.6810	Linderae Radix	BB_NC-0668	9855795	FALSE	C12(C(=CCCC2C)CCC(C1)C(=C)C)C
MOL001606	0.8009	0.1991	0.6810	Piperis Longi Fructus	BB_NC-0668	9855795	FALSE	C12(C(=CCCC2C)CCC(C1)C(=C)C)C
MOL001606	0.8009	0.1991	0.6810	Alpiniae Oxyphyliae Fructus	BB_NC-0668	9855795	FALSE	C12(C(=CCCC2C)CCC(C1)C(=C)C)C
MOL001606	0.8009	0.1991	0.6810	Meliae Azedarach Fructus	BB_NC-0668	9855795	FALSE	C12(C(=CCCC2C)CCC(C1)C(=C)C)C
MOL001606	0.8009	0.1991	0.6810	Linderae Radix	BB_NC-0668	9855795	FALSE	C12(C(=CCCC2C)CCC(C1)C(=C)C)C
MOL001606	0.8009	0.1991	0.6810	Cornus Officinalis Sieb. Et Zucc.	BB_NC-0668	9855795	FALSE	C12(C(=CCCC2C)CCC(C1)C(=C)C)C
MOL001606	0.8009	0.1991	0.6810	Solidaginis Herba	BB_NC-0668	9855795	FALSE	C12(C(=CCCC2C)CCC(C1)C(=C)C)C
MOL001606	0.8009	0.1991	0.6810	Magnolia Officinalis Rehd Et Wils.	BB_NC-0668	9855795	FALSE	C12(C(=CCCC2C)CCC(C1)C(=C)C)C
MOL001606	0.8009	0.1991	0.6810	Alpiniae Officinarum Rhizome	BB_NC-0668	9855795	FALSE	C12(C(=CCCC2C)CCC(C1)C(=C)C)C
MOL001606	0.8009	0.1991	0.6810	Lignum Pini Nodi	BB_NC-0668	9855795	FALSE	C12(C(=CCCC2C)CCC(C1)C(=C)C)C
MOL001606	0.8009	0.1991	0.6810	Rhododendri Daurici Folium	BB_NC-0668	9855795	FALSE	C12(C(=CCCC2C)CCC(C1)C(=C)C)C
MOL001606	0.8009	0.1991	0.6810	Pogostemon Cablin (Blanco) Benth.	BB_NC-0668	9855795	FALSE	C12(C(=CCCC2C)CCC(C1)C(=C)C)C
MOL001608	0.8553	0.1447	0.6660	Ailanthi Cortex	delta-elemene	12309449	FALSE	C1(C=C(CCC1(C=C)C)C(C)C)C(=C)C
MOL001608	0.8553	0.1447	0.6660	Piperis Longi Fructus	delta-elemene	12309449	FALSE	C1(C=C(CCC1(C=C)C)C(C)C)C(=C)C
MOL001608	0.8553	0.1447	0.6660	Campsis Flos	delta-elemene	12309449	FALSE	C1(C=C(CCC1(C=C)C)C(C)C)C(=C)C
MOL001608	0.8553	0.1447	0.6660	Et Radix Patriniae Rhizoma	delta-elemene	12309449	FALSE	C1(C=C(CCC1(C=C)C)C(C)C)C(=C)C
MOL001609	0.9036	0.0964	0.8757	Piperis Longi Fructus	Cyclodecene, 1-methyl-	5367581	FALSE	C\1(=C\CCCCCCCC1)/C
MOL001610	0.2377	0.7623	0.6618	Piperis Longi Fructus	sylvatine	Not Available	FALSE	C(=O)(/C=C/C=C\c1cc2OCOc2cc1)NCCCC/C=C/CCCC(C)C
MOL001611	0.8199	0.1801	0.9271	Piperis Longi Fructus	dihydropiperlonguminine	12682184	FALSE	C(=O)(/C=C/CCc1cc2OCOc2cc1)NCC(C)C
MOL001612	0.9373	0.0627	0.8948	Piperis Longi Fructus	PIPERONYLIC ACID	7196	FALSE	c12c(ccc(c1)C(=O)O)OCO2
MOL001614	0.1900	0.8100	0.6938	Piperis Longi Fructus	(E,E,E)-11-(1,3-Benzodioxol-5-yl)-N-(2-methylpropyl)-2,4,10-undecatrienenamide	6453083	FALSE	C(=O)(/C=C/C=C/C=C/CC/C=C/c1cc2OCOc2cc1)NCC(C)C

MOL001616	0.2692	0.7308	0.8489	Piperis Longi Fructus	1-[1-oxo-9(3,4-methylenedioxyphenyl)-2E,8E-nonadienyl] pyrrolidine	Not Available	FALSE	N1(CCCC1)C(=O)/C=C/CCCC/C=C\c1cc2c(cc1)OCO2
MOL001617	0.2056	0.7944	0.6437	Piperis Longi Fructus	guineensine	Not Available	FALSE	c1(c(cc(cc1)/C=C/CCCCCC/C=C/C=C/C(=O)NCC(C)C)OC)O
MOL001618	0.8247	0.1753	0.7836	Piperis Longi Fructus	Pellitorin	5318516	FALSE	C(=C\C=C\CCCCC)/C(=O)NCC(C)C
MOL001618	0.8247	0.1753	0.7836	Rhizoma Dioscoreae	Pellitorin	5318516	FALSE	C(=C\C=C\CCCCC)/C(=O)NCC(C)C
MOL001618	0.8247	0.1753	0.7836	Piperis Fructus	Pellitorin	5318516	FALSE	C(=C\C=C\CCCCC)/C(=O)NCC(C)C
MOL001618	0.8247	0.1753	0.7836	Cornus Officinalis Sieb. Et Zucc.	Pellitorin	5318516	FALSE	C(=C\C=C\CCCCC)/C(=O)NCC(C)C
MOL001620	0.7321	0.2679	0.6026	Codonopsis Radix	Pentadecene	25913	FALSE	C(CCCCCCC)CCCCCC=C
MOL001620	0.7321	0.2679	0.6026	Ginkgo Folium	Pentadecene	25913	FALSE	C(CCCCCCC)CCCCCC=C
MOL001620	0.7321	0.2679	0.6026	Rose Rugosae Flos	Pentadecene	25913	FALSE	C(CCCCCCC)CCCCCC=C
MOL001620	0.7321	0.2679	0.6026	Lonicerae Japonicae Flos	Pentadecene	25913	FALSE	C(CCCCCCC)CCCCCC=C
MOL001620	0.7321	0.2679	0.6026	Farfarae Flos	Pentadecene	25913	FALSE	C(CCCCCCC)CCCCCC=C
MOL001620	0.7321	0.2679	0.6026	Puerariae Flos	Pentadecene	25913	FALSE	C(CCCCCCC)CCCCCC=C
MOL001620	0.7321	0.2679	0.6026	Saussureae Involucratae Herba	Pentadecene	25913	FALSE	C(CCCCCCC)CCCCCC=C
MOL001620	0.7321	0.2679	0.6026	Aucklandiae Radix	Pentadecene	25913	FALSE	C(CCCCCCC)CCCCCC=C
MOL001620	0.7321	0.2679	0.6026	Carthami Flos	Pentadecene	25913	FALSE	C(CCCCCCC)CCCCCC=C
MOL001620	0.7321	0.2679	0.6026	Capsici Fructus	Pentadecene	25913	FALSE	C(CCCCCCC)CCCCCC=C
MOL001620	0.7321	0.2679	0.6026	Piperis Longi Fructus	Pentadecene	25913	FALSE	C(CCCCCCC)CCCCCC=C
MOL001620	0.7321	0.2679	0.6026	Microctis Folium	Pentadecene	25913	FALSE	C(CCCCCCC)CCCCCC=C
MOL001620	0.7321	0.2679	0.6026	Bidentis Bipinnatae Herba	Pentadecene	25913	FALSE	C(CCCCCCC)CCCCCC=C
MOL001621	0.4772	0.5228	0.8483	Piperis Longi Fructus	l-undecylenyl-3,4-methylenedioxybenzene	Not Available	FALSE	c12c(cc(cc1)/C=C/CCCCCCCCC)OCO2
MOL001622	0.8090	0.1910	0.6483	Farfarae Flos	1-Tetradecene	14260	FALSE	C(CCCCCC=C)CCCCCC
MOL001622	0.8090	0.1910	0.6483	Radix Angelicae Biseratae	1-Tetradecene	14260	FALSE	C(CCCCCC=C)CCCCCC
MOL001622	0.8090	0.1910	0.6483	Crotonis Fructus	1-Tetradecene	14260	FALSE	C(CCCCCC=C)CCCCCC
MOL001622	0.8090	0.1910	0.6483	Carthami Flos	1-Tetradecene	14260	FALSE	C(CCCCCC=C)CCCCCC
MOL001623	0.8799	0.1201	0.7782	Crotonis Fructus	Phlorizin	6072	FALSE	c1(cc(c(c(c1)O)C(=O)CCc1ccc(cc1)O)OC1OC(C(C(C1O)O)O)CO)O
MOL001624	0.9066	0.0934	0.7831	Crotonis Fructus	Phloretol	4788	TRUE	c1(cc(c(c(c1)O)C(=O)CCc1ccc(cc1)O)O)O
MOL001624	0.9066	0.0934	0.7831	Rubi Fructus	Phloretol	4788	TRUE	c1(cc(c(c(c1)O)C(=O)CCc1ccc(cc1)O)O)O
MOL001625	0.1503	0.8497	0.7663	Crotonis Fructus	Phorbol caprate, tiglate	Not Available	FALSE	C1(C2(C(C3C(C1OC(=O)/C(=C/C)/C)(C3(C)C)OC(=O)CCCCCCCCC)C=C(CC1(C2C=C(C1=O)C)O)CO)O)C

MOL001627	0.9279	0.0721	0.8994	Crotonis Fructus	[(1R,5S)-8-methyl-8-azabicyclo[3.2.1]octan-3-yl] (E)-2-methylbut-2-enoate	Not Available	FALSE	C1(OC(=O)/C(=C/C)/C)CC2N(C(C1)CC2)C
MOL001627	0.9279	0.0721	0.8994	Daturae Flos	[(1R,5S)-8-methyl-8-azabicyclo[3.2.1]octan-3-yl] (E)-2-methylbut-2-enoate	Not Available	FALSE	C1(OC(=O)/C(=C/C)/C)CC2N(C(C1)CC2)C
MOL001628	0.5335	0.4665	0.6958	Crotonis Fructus	3-(3,4-dihydroxyphenyl)-1-(5-hydroxy-2,2-dimethylchromen-6-yl)propan-1-one	11473265	FALSE	O1C(C=Cc2c1ccc(c2O)C(=O)CCc1cc(O)c(O)cc1)(C)C
MOL001629	0.9003	0.0997	0.9686	Crotonis Fructus	BEO	637090	FALSE	C(=O)(/C=C/C)O
MOL001629	0.9003	0.0997	0.9686	Chaenomeles Sinensis (Thouin) Koehne	BEO	637090	FALSE	C(=O)(/C=C/C)O
MOL001629	0.9003	0.0997	0.9686	Capsici Fructus	BEO	637090	FALSE	C(=O)(/C=C/C)O
MOL001630	0.8797	0.1203	0.8396	Crotonis Fructus	Crotonoside	65085	FALSE	O1C(n2c3nc(=O)[nH]c(N)c3nc2)C(O)C(O)C1CO
MOL001632	0.8480	0.1520	0.7879	Crotonis Fructus	Isoguanine	76900	FALSE	c12c(c(nc(n1)O)N)[nH]cn2
MOL001633	0.7564	0.2436	0.8929	Crotonis Fructus	AIDS161753	Not Available	FALSE	OC12C(C1(C)C)C1C(O)(C(C2O)C)C2C(CC(=C1)CO)C(=O)C(=C2)C
MOL001634	0.1761	0.8239	0.7325	Crotonis Fructus	Phorbol acetate, caprate	Not Available	FALSE	C12(C(C(C3(C(C1C2(C)C)C=C(CO)CC1(C3C=C(C)C1=O)O)O)C)OC(=O)C)OC(=O)CCCCCCCCC
MOL001635	0.1492	0.8508	0.7440	Crotonis Fructus	AIDS161963	Not Available	FALSE	C12(C(C(C3(C(C1C2(C)C)C=C(CO)CC1(C3C=C(C)C1=O)O)O)C)OC(=O)C)OC(=O)CCCCCCCCCCC
MOL001636	0.1608	0.8392	0.7394	Crotonis Fructus	phorbol-12-butyrate-13-laurate	Not Available	FALSE	C12(C(C(C3(C(C1C2(C)C)C=C(CO)CC1(C3C=C(C)C1=O)O)O)C)OC(=O)CCC)OC(=O)CCCCCCCCCCC
MOL001637	0.1840	0.8160	0.7355	Crotonis Fructus	phorbol-12-tiglate-13-laurate	Not Available	FALSE	C12(C(C(C3(C(C1C2(C)C)C=C(CO)CC1(C3C=C(C)C1=O)O)O)C)OC(=O)/C(=C/C)/C)OC(=O)CCCCCCCCCCCC
MOL001638	0.8812	0.1188	0.9388	Crotonis Fructus	Phorbol	Not Available	FALSE	C12C3C(C4C(CC(=C3)CO)(C(=O)C(=C4)C)O)(C(C(C1(C2(C)C)O)O)C)O

MOL001639	0.9009	0.0991	0.9657	Achyranthis Asperae Herba	Tiglic acid	125468	FALSE	C(=O)(/C(=C/C)/C)O
MOL001639	0.9009	0.0991	0.9657	Crotonis Fructus	Tiglic acid	125468	FALSE	C(=O)(/C(=C/C)/C)O
MOL001639	0.9009	0.0991	0.9657	Fructus Carotae	Tiglic acid	125468	FALSE	C(=O)(/C(=C/C)/C)O
MOL001639	0.9009	0.0991	0.9657	Capsici Fructus	Tiglic acid	125468	FALSE	C(=O)(/C(=C/C)/C)O
MOL001639	0.9009	0.0991	0.9657	Semen Pharbitidis	Tiglic acid	125468	FALSE	C(=O)(/C(=C/C)/C)O
MOL001640	0.9243	0.0757	0.9258	Trichosanthes Kirilowii Maxim	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Momordicae Fructus	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Linderae Radix	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Phyllanthi Fructus	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Aloe	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Portulacae Herba	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Carthami Flos	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Humulus Scandens (Lour.) Merr.	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Campsis Flos	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Gossampiniflos	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Ranunculi Ternati Radix	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Ginkgo Folium	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Junci Medulla	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Sedi Herba	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Momordicae Semen	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Mori Fructus	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Folium Artemisiae Argyi	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Tamaricis Cacumen	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Hippophae Fructus	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Crotonis Fructus	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Morindae Officinalis Radix	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	A. Dahurica (Fisch.) Benth. Et Hook	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Paederiae Scandentis Herba	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Canarii Fructus	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Lonicerae Japonicae Flos	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Angelicae Sinensis Radix	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Epimrdii Herba	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Rhizome Of Whiteback Greenbrier	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Ephedra Herba	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Platycladi Cacumen	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001640	0.9243	0.0757	0.9258	Meliae Azedarach Fructus	NON	2969	FALSE	C(CCCCCC)CCC(=O)O
MOL001641	0.4777	0.5223	0.6406	Citri Grandis Exocarpium	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC

MOL001641	0.4777	0.5223	0.6406	Allii Fistulost Bulbus	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Ginkgo Folium	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Litchi Semen	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Codonopsis Radix	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Magnolia Officinalis Rehd Et Wils.	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Asteris Radix Et Rhizoma	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Aconitum Kusnezoffii Reichb	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Lonicerae Japonicae Flos	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Crotonis Fructus	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Panax Ginseng C. A. Mey.	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Sterculiae Lychnophorae Semen	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Amygdalus Communis Vas	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Campsis Flos	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Trichosanthes Kirilowii Maxim	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Mori Cortex	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Coicis Semen	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Semen Firmianae	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Chuanxiong Rhizoma	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Raphani Semen	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Arisaematis Rhizoma	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Ginseng Folium	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC

MOL001641	0.4777	0.5223	0.6406	Broussonetiae Fructus	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Platycladi Cacumen	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Farfarae Flos	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Radix Cirsii Japonici	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Mahoniae Folum	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Canarii Fructus	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Radix Clematidis	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001641	0.4777	0.5223	0.6406	Rhododendri Daurici Folium	METHYL LINOLEATE	5284421	FALSE	C(CC/C=C\C/C=C\CCCCC)CCCCC(=O)OC
MOL001642	0.8805	0.1195	0.8365	Crotonis Fructus	Crotonside	Not Available	FALSE	n1c(=O)[nH]c2c(c1N)ncn2C1OC(C(C1O)O)CO
MOL001643	0.9700	0.0300	0.8329	Crotonis Fructus	Croweacin	5316141	FALSE	c1cc2c(c(c1CC=C)OC)OCO2
MOL001643	0.9700	0.0300	0.8329	Asari Radix Et Rhizoma	Croweacin	5316141	FALSE	c1cc2c(c(c1CC=C)OC)OCO2
MOL001643	0.9700	0.0300	0.8329	Magnoliae Flos	Croweacin	5316141	FALSE	c1cc2c(c(c1CC=C)OC)OCO2
MOL001644	0.8831	0.1169	0.8621	Eucommiae Folium	Dodecanal	8194	FALSE	CCCCCCCCCCCC=O
MOL001644	0.8831	0.1169	0.8621	Flos Genkwa	Dodecanal	8194	FALSE	CCCCCCCCCCCC=O
MOL001644	0.8831	0.1169	0.8621	Codonopsis Radix	Dodecanal	8194	FALSE	CCCCCCCCCCCC=O
MOL001644	0.8831	0.1169	0.8621	Coriandri Sativi Herba	Dodecanal	8194	FALSE	CCCCCCCCCCCC=O
MOL001644	0.8831	0.1169	0.8621	Meliae Azedarach Fructus	Dodecanal	8194	FALSE	CCCCCCCCCCCC=O
MOL001644	0.8831	0.1169	0.8621	Gnaphalii Affinis Herba	Dodecanal	8194	FALSE	CCCCCCCCCCCC=O
MOL001644	0.8831	0.1169	0.8621	Hippophae Fructus	Dodecanal	8194	FALSE	CCCCCCCCCCCC=O
MOL001644	0.8831	0.1169	0.8621	Momordicae Fructus	Dodecanal	8194	FALSE	CCCCCCCCCCCC=O
MOL001644	0.8831	0.1169	0.8621	Cnidii Fructus	Dodecanal	8194	FALSE	CCCCCCCCCCCC=O
MOL001644	0.8831	0.1169	0.8621	Campsis Flos	Dodecanal	8194	FALSE	CCCCCCCCCCCC=O
MOL001644	0.8831	0.1169	0.8621	Crotonis Fructus	Dodecanal	8194	FALSE	CCCCCCCCCCCC=O
MOL001644	0.8831	0.1169	0.8621	Linderae Radix	Dodecanal	8194	FALSE	CCCCCCCCCCCC=O
MOL001644	0.8831	0.1169	0.8621	Paeoniae Radix Alba	Dodecanal	8194	FALSE	CCCCCCCCCCCC=O
MOL001644	0.8831	0.1169	0.8621	A. Dahurica (Fisch.) Benth. Et Hook	Dodecanal	8194	FALSE	CCCCCCCCCCCC=O
MOL001644	0.8831	0.1169	0.8621	Houttuyniae Herba	Dodecanal	8194	FALSE	CCCCCCCCCCCC=O
MOL001645	0.4245	0.5755	0.6020	Crotonis Fructus	Linoleyl acetate	5319042	FALSE	C(CCC/C=C/C/C=C/CCCCCCCCOC(=O)C)C
MOL001645	0.4245	0.5755	0.6020	Epimrdii Herba	Linoleyl acetate	5319042	FALSE	C(CCC/C=C/C/C=C/CCCCCCCCOC(=O)C)C
MOL001645	0.4245	0.5755	0.6020	Radix Bupleuri	Linoleyl acetate	5319042	FALSE	C(CCC/C=C/C/C=C/CCCCCCCCOC(=O)C)C

MOL001645	0.4245	0.5755	0.6020	Lycii Cortex	Linoleyl acetate	5319042	FALSE	C(CCC/C=C/C/C=C/CCCCCCCCOC(=O)C)C
MOL001645	0.4245	0.5755	0.6020	Corayceps	Linoleyl acetate	5319042	FALSE	C(CCC/C=C/C/C=C/CCCCCCCCOC(=O)C)C
MOL001646	0.6222	0.3778	0.8515	Hedyotis Diffusae Herba	2,3-dimethoxy-6-methyanthraquinone	Not Available	FALSE	c12c(c(ccc1)C)C(=O)c1c(C2=O)cc(c(c1)OC)OC
MOL001648	0.9559	0.0441	0.8681	Eucommiae Cortex	genipin	442424	FALSE	OC1OC=C(C2C1C(=CC2)CO)C(=O)OC
MOL001648	0.9559	0.0441	0.8681	Hedyotis Diffusae Herba	genipin	442424	FALSE	OC1OC=C(C2C1C(=CC2)CO)C(=O)OC
MOL001648	0.9559	0.0441	0.8681	Gardeniae Fructus	genipin	442424	FALSE	OC1OC=C(C2C1C(=CC2)CO)C(=O)OC
MOL001649	0.7977	0.2023	0.7912	Morindae Officinalis Radix	2-hydroxy-3-methylanthraquinone	10889963	FALSE	c12c(cccc1)C(=O)c1c(C2=O)cc(c(c1)C)O
MOL001649	0.7977	0.2023	0.7912	Hedyotis Diffusae Herba	2-hydroxy-3-methylanthraquinone	10889963	FALSE	c12c(cccc1)C(=O)c1c(C2=O)cc(c(c1)C)O
MOL001649	0.7977	0.2023	0.7912	Scutellariae Barbatae Herba	2-hydroxy-3-methylanthraquinone	10889963	FALSE	c12c(cccc1)C(=O)c1c(C2=O)cc(c(c1)C)O
MOL001650	0.7765	0.2235	0.7551	Hedyotis Diffusae Herba	E-6-O-p-methoxycinnamoyl scandoside methyl ester	Not Available	FALSE	C1(C2C(C(=CO1)C(=O)OC)C(C=C2CO)OC(=O)/C=C\c1ccc(cc1)O)OC1C(O)C(O)C(O)C(O1)CO
MOL001652	0.8628	0.1372	0.7153	Morindae Officinalis Radix	1H-2,6-dioxacyclopent(cd)inden-1-one, 4-((acetyloxy)methyl)-5-(beta-D-glucopyranosyloxy)-2a,4a,5,7b-tetrahydro-, (2aS-(2aalpha,5alpha,7balpha))-	Not Available	FALSE	O1C2C3C(C(OC4OC(C(O)C(O)C4O)CO)OC=C3C1=O)C(=C2)COC(=O)C

MOL001652	0.8628	0.1372	0.7153	Hedyotis Diffusae Herba	1H-2,6-dioxacyclopent(cd)inden-1-one, 4-((acetyloxy)methyl)-5-(beta-D-glucopyranosyloxy)-2a,4a,5,7b-tetrahydro-, (2aS-(2aalpha,5alpha,7balpha))-	Not Available	FALSE	O1C2C3C(C(OC4OC(C(O)C(O)C4O)CO)OC=C3C1=O)C(=C2)COC(=O)C
MOL001653	0.9246	0.0754	0.7598	Hedyotis Diffusae Herba	asperuloside_qt	Not Available	FALSE	O1C2C3C(C(O)OC=C3C1=O)C(=C2)COC(=O)C
MOL001654	0.4426	0.5574	0.7474	Prunellae Spica	Oleanolic acid-28-O-beta-D-glucopyranoside	Not Available	FALSE	C1(CC2C(CC1)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C)C(=O)OC1OC(C(C(C1O)O)O)CO)(C)C
MOL001654	0.4426	0.5574	0.7474	Caryophylliflos	Oleanolic acid-28-O-beta-D-glucopyranoside	Not Available	FALSE	C1(CC2C(CC1)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C)C(=O)OC1OC(C(C(C1O)O)O)CO)(C)C
MOL001654	0.4426	0.5574	0.7474	Fructus Ligustri Lucidi	Oleanolic acid-28-O-beta-D-glucopyranoside	Not Available	FALSE	C1(CC2C(CC1)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C)C(=O)OC1OC(C(C(C1O)O)O)CO)(C)C
MOL001654	0.4426	0.5574	0.7474	Caulis Akebiae	Oleanolic acid-28-O-beta-D-glucopyranoside	Not Available	FALSE	C1(CC2C(CC1)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C)C(=O)OC1OC(C(C(C1O)O)O)CO)(C)C
MOL001654	0.4426	0.5574	0.7474	Hedyotis Diffusae Herba	Oleanolic acid-28-O-beta-D-glucopyranoside	Not Available	FALSE	C1(CC2C(CC1)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C)C(=O)OC1OC(C(C(C1O)O)O)CO)(C)C

MOL001655	0.7553	0.2447	0.9079	Caryophylliflos	oleanolic acid-3-O-β-D-glucuronopyranoside_qt	25728252	FALSE	C1(CC2C(CC1)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C)C(=O)O)(C)C
MOL001655	0.7553	0.2447	0.9079	Fructus Ligustri Lucidi	oleanolic acid-3-O-β-D-glucuronopyranoside_qt	25728252	FALSE	C1(CC2C(CC1)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C)C(=O)O)(C)C
MOL001655	0.7553	0.2447	0.9079	Achyranthis Bidentatae Radix	oleanolic acid-3-O-β-D-glucuronopyranoside_qt	25728252	FALSE	C1(CC2C(CC1)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C)C(=O)O)(C)C
MOL001655	0.7553	0.2447	0.9079	Hedyotis Diffusae Herba	oleanolic acid-3-O-β-D-glucuronopyranoside_qt	25728252	FALSE	C1(CC2C(CC1)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C)C(=O)O)(C)C
MOL001655	0.7553	0.2447	0.9079	Caulis Akebiae	oleanolic acid-3-O-β-D-glucuronopyranoside_qt	25728252	FALSE	C1(CC2C(CC1)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C)C(=O)O)(C)C
MOL001656	0.9210	0.0790	0.8818	Hedyotis Diffusae Herba	(1S,4aS,5R,7aS)-5-hydroxy-7-methylol-1-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]oxy-1,4a,5,7a-tetrahydrocyclopenta[d]pyran-4-carboxylic acid	21602023	FALSE	O(C1OC=C(C2C1C(=CC2O)CO)C(=O)O)C1OC(C(O)C(O)C1O)CO

MOL001656	0.9210	0.0790	0.8818	Paederiae Scandentis Herba	(1S,4aS,5R,7aS)-5-hydroxy-7-methylol-1-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]oxy-1,4a,5,7a-tetrahydrocyclopenta[d]pyran-4-carboxylic acid	21602023	FALSE	O(C1OC=C(C2C1C(=CC2O)CO)C(=O)O)C1OC(C(O)C(O)C1O)CO
MOL001656	0.9210	0.0790	0.8818	Morindae Officinalis Radix	(1S,4aS,5R,7aS)-5-hydroxy-7-methylol-1-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]oxy-1,4a,5,7a-tetrahydrocyclopenta[d]pyran-4-carboxylic acid	21602023	FALSE	O(C1OC=C(C2C1C(=CC2O)CO)C(=O)O)C1OC(C(O)C(O)C1O)CO
MOL001657	0.9468	0.0532	0.8480	Morindae Officinalis Radix	scandoside_qt	Not Available	FALSE	OC1OC=C(C2C1C(=CC2O)CO)C(=O)O
MOL001657	0.9468	0.0532	0.8480	Hedyotis Diffusae Herba	scandoside_qt	Not Available	FALSE	OC1OC=C(C2C1C(=CC2O)CO)C(=O)O
MOL001657	0.9468	0.0532	0.8480	Paederiae Scandentis Herba	scandoside_qt	Not Available	FALSE	OC1OC=C(C2C1C(=CC2O)CO)C(=O)O
MOL001658	0.9404	0.0596	0.8880	Hedyotis Diffusae Herba	3'-Hydroxyanethole	5314180	FALSE	c1c(ccc(c1)/C=C/CO)OC
MOL001660	0.9444	0.0556	0.9017	Hedyotis Diffusae Herba	p-MCA	699414	FALSE	c1c(ccc(c1)/C=C/C(=O)O)OC
MOL001660	0.9444	0.0556	0.9017	Figwort Root	p-MCA	699414	FALSE	c1c(ccc(c1)/C=C/C(=O)O)OC
MOL001660	0.9444	0.0556	0.9017	Acoritataninowii Rhizoma	p-MCA	699414	FALSE	c1c(ccc(c1)/C=C/C(=O)O)OC
MOL001660	0.9444	0.0556	0.9017	Equiseti Hiemalis Herba	p-MCA	699414	FALSE	c1c(ccc(c1)/C=C/C(=O)O)OC
MOL001661	0.9185	0.0815	0.8425	Paederiae Scandentis Herba	Scandoside methyl ester	442433	FALSE	O(C1OC=C(C2C1C(=CC2O)CO)C(=O)OC)C1OC(C(O)C(O)C1O)CO

MOL001661	0.9185	0.0815	0.8425	Hedyotis Diffusae Herba	Scandoside methyl ester	442433	FALSE	O(C1OC=C(C2C1C(=CC2O)CO)C(=O)OC)C1OC(C(O)C(O)C1O)CO
MOL001662	0.9477	0.0523	0.8365	Paederiae Scandentis Herba	scandoside_qt	71577496	FALSE	OC1OC=C(C2C1C(=CC2O)CO)C(=O)OC
MOL001662	0.9477	0.0523	0.8365	Hedyotis Diffusae Herba	scandoside_qt	71577496	FALSE	OC1OC=C(C2C1C(=CC2O)CO)C(=O)OC
MOL001663	0.7553	0.2447	0.9079	Plantaginis Semen	(4aS,6aR,6aS,6bR,8aR,10R,12aR,14bS)-10-hydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	11869658	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O
MOL001663	0.7553	0.2447	0.9079	Verbenae Herb	(4aS,6aR,6aS,6bR,8aR,10R,12aR,14bS)-10-hydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	11869658	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O

MOL001663	0.7553	0.2447	0.9079	Ardisiae Japonicae Herba	(4aS,6aR,6aS,6bR,8aR,10R,12aR,14bS)-10-hydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	11869658	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O
MOL001663	0.7553	0.2447	0.9079	Radix Clematidis	(4aS,6aR,6aS,6bR,8aR,10R,12aR,14bS)-10-hydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	11869658	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O
MOL001663	0.7553	0.2447	0.9079	Styrax	(4aS,6aR,6aS,6bR,8aR,10R,12aR,14bS)-10-hydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	11869658	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O

MOL001663	0.7553	0.2447	0.9079	Hedyotis Diffusae Herba	(4aS,6aR,6aS,6bR,8aR,10R,12aR,14bS)-10-hydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	11869658	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O
MOL001663	0.7553	0.2447	0.9079	Gardeniae Fructus	(4aS,6aR,6aS,6bR,8aR,10R,12aR,14bS)-10-hydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	11869658	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O
MOL001664	0.9210	0.0790	0.8818	Paederiae Scandentis Herba	deacetylasperulosidic acid	12315350	FALSE	C1(C(C(C(OC1CO)OC1OC=C(C2C1C(=CC2O)CO)C(=O)O)O)O)O
MOL001664	0.9210	0.0790	0.8818	Hedyotis Diffusae Herba	deacetylasperulosidic acid	12315350	FALSE	C1(C(C(C(OC1CO)OC1OC=C(C2C1C(=CC2O)CO)C(=O)O)O)O)O
MOL001665	0.9468	0.0532	0.8480	Paederiae Scandentis Herba	deacetylasperulosidic acid _qt	Not Available	FALSE	OC1OC=C(C2C1C(=CC2O)CO)C(=O)O
MOL001665	0.9468	0.0532	0.8480	Hedyotis Diffusae Herba	deacetylasperulosidic acid _qt	Not Available	FALSE	OC1OC=C(C2C1C(=CC2O)CO)C(=O)O
MOL001666	0.9185	0.0815	0.8425	Paederiae Scandentis Herba	Deacetyl asperulosidic acid methyl ester	6325021	FALSE	C1(C(C(C(OC1CO)OC1OC=C(C2C1C(=CC2O)CO)C(=O)OC)O)O)O

MOL001666	0.9185	0.0815	0.8425	Hedyotis Diffusae Herba	Deacetyl asperulosidic acid methyl ester	6325021	FALSE	C1(C(C(C(OC1CO)OC1OC=C(C2C1C(=CC2O)CO)C(=O)OC)O)O)O
MOL001667	0.9477	0.0523	0.8365	Hedyotis Diffusae Herba	deacetyl asperuloside acid_qt	Not Available	FALSE	OC1OC=C(C2C1C(=CC2O)CO)C(=O)OC
MOL001667	0.9477	0.0523	0.8365	Paederiae Scandentis Herba	deacetyl asperuloside acid_qt	Not Available	FALSE	OC1OC=C(C2C1C(=CC2O)CO)C(=O)OC
MOL001668	0.9326	0.0674	0.8877	Hedyotis Diffusae Herba	Geniposidic acid	443354	FALSE	O(C1OC=C(C2C1C(=CC2)CO)C(=O)O)C1OC(C(O)C(O)C1O)CO
MOL001668	0.9326	0.0674	0.8877	Cistanches Herba	Geniposidic acid	443354	FALSE	O(C1OC=C(C2C1C(=CC2)CO)C(=O)O)C1OC(C(O)C(O)C1O)CO
MOL001668	0.9326	0.0674	0.8877	Plantaginis Semen	Geniposidic acid	443354	FALSE	O(C1OC=C(C2C1C(=CC2)CO)C(=O)O)C1OC(C(O)C(O)C1O)CO
MOL001668	0.9326	0.0674	0.8877	Eucommiae Folium	Geniposidic acid	443354	FALSE	O(C1OC=C(C2C1C(=CC2)CO)C(=O)O)C1OC(C(O)C(O)C1O)CO
MOL001668	0.9326	0.0674	0.8877	Eucommiae Cortex	Geniposidic acid	443354	FALSE	O(C1OC=C(C2C1C(=CC2)CO)C(=O)O)C1OC(C(O)C(O)C1O)CO
MOL001669	0.9508	0.0492	0.8597	Plantaginis Semen	geniposidie acid_qt	Not Available	FALSE	OC1OC=C(C2C1C(=CC2)CO)C(=O)O
MOL001669	0.9508	0.0492	0.8597	Eucommiae Folium	geniposidie acid_qt	Not Available	FALSE	OC1OC=C(C2C1C(=CC2)CO)C(=O)O
MOL001669	0.9508	0.0492	0.8597	Eucommiae Cortex	geniposidie acid_qt	Not Available	FALSE	OC1OC=C(C2C1C(=CC2)CO)C(=O)O
MOL001669	0.9508	0.0492	0.8597	Hedyotis Diffusae Herba	geniposidie acid_qt	Not Available	FALSE	OC1OC=C(C2C1C(=CC2)CO)C(=O)O
MOL001669	0.9508	0.0492	0.8597	Cistanches Herba	geniposidie acid_qt	Not Available	FALSE	OC1OC=C(C2C1C(=CC2)CO)C(=O)O
MOL001670	0.6574	0.3426	0.8649	Hedyotis Diffusae Herba	2-methoxy-3-methyl-9,10-anthraquinone	10514946	FALSE	c12c(cccc1)C(=O)c1c(C2=O)cc(c(c1)OC)C
MOL001671	0.6385	0.3615	0.8469	Hedyotis Diffusae Herba	Digitolutein	160475	FALSE	c12c(cccc1)C(=O)c1c(C2=O)cc(c(c1OC)O)C
MOL001672	0.9143	0.0857	0.9281	Herba Patriniae	Hexylthiol	8106	FALSE	C(CCC)CCS
MOL001673	0.8934	0.1066	0.9306	Herba Patriniae	2-Ethyl-5-methylfuran	74346	FALSE	c1(oc(cc1)C)CC
MOL001674	0.9323	0.0677	0.8644	Herba Patriniae	Villosolside	Not Available	FALSE	C12C(COC(=O)C1C)C(C(C2)O)(C)OC1OC(C(C(C1O)O)O)CO
MOL001675	0.9449	0.0551	0.8821	Herba Patriniae	Villosol	Not Available	FALSE	C12C(COC(=O)C1C)C(C(C2)O)(C)O
MOL001676	0.1805	0.8195	0.6361	Herba Patriniae	Vilmorrianine C	Not Available	FALSE	C1(ccc(c1)OC)C(=O)OC1C2CC3C1(CC2OC)(C1C(C2C43C(CCC2(COC)CN(C14)CC)OC)OC)OC(=O)
MOL001678	0.6396	0.3604	0.7861	Herba Patriniae	bolusanthol B	Not Available	FALSE	C1(c2(cc1O)OCC(c2=O)C1cc(c(c(c1)O)O)CC=C(C)C)O

MOL001679	0.9660	0.0340	0.8024	Sinapis Semen	(1S,4S)-1-isopropyl-4-methyl-3-bicyclo[3.1.0]hexanone	6432452	FALSE	O=C1C(C2C(C2)(C1)C(C)C)C
MOL001679	0.9660	0.0340	0.8024	Herba Patriniae	(1S,4S)-1-isopropyl-4-methyl-3-bicyclo[3.1.0]hexanone	6432452	FALSE	O=C1C(C2C(C2)(C1)C(C)C)C
MOL001680	0.9130	0.0870	0.8362	Gentianae Radix Et Rhozima	Loganin	87691	FALSE	C12C(C(=COC1OC1OC(C(C(C1O)O)O)CO)C(=O)OC)CC(C2C)O
MOL001680	0.9130	0.0870	0.8362	Herba Patriniae	Loganin	87691	FALSE	C12C(C(=COC1OC1OC(C(C(C1O)O)O)CO)C(=O)OC)CC(C2C)O
MOL001680	0.9130	0.0870	0.8362	Strychni Semen	Loganin	87691	FALSE	C12C(C(=COC1OC1OC(C(C(C1O)O)O)CO)C(=O)OC)CC(C2C)O
MOL001680	0.9130	0.0870	0.8362	Dipsaci Radix	Loganin	87691	FALSE	C12C(C(=COC1OC1OC(C(C(C1O)O)O)CO)C(=O)OC)CC(C2C)O
MOL001680	0.9130	0.0870	0.8362	Lonicerae Japonicae Flos	Loganin	87691	FALSE	C12C(C(=COC1OC1OC(C(C(C1O)O)O)CO)C(=O)OC)CC(C2C)O
MOL001680	0.9130	0.0870	0.8362	Cornus Officinalis Sieb. Et Zucc.	Loganin	87691	FALSE	C12C(C(=COC1OC1OC(C(C(C1O)O)O)CO)C(=O)OC)CC(C2C)O
MOL001681	0.9569	0.0431	0.8722	Strychni Semen	methyl (1R,4aS,6S,7R,7aS)-1,6-dihydroxy-7-methyl-1,4a,5,6,7,7a-hexahydrocyclopenta[d]pyran-4-carboxylate	10466307	FALSE	C12C(C(=COC1O)C(=O)OC)CC(C2C)O
MOL001681	0.9569	0.0431	0.8722	Lonicerae Japonicae Flos	methyl (1R,4aS,6S,7R,7aS)-1,6-dihydroxy-7-methyl-1,4a,5,6,7,7a-hexahydrocyclopenta[d]pyran-4-carboxylate	10466307	FALSE	C12C(C(=COC1O)C(=O)OC)CC(C2C)O

MOL001681	0.9569	0.0431	0.8722	Dipsaci Radix	methyl (1R,4aS,6S,7R,7aS)-1,6-dihydroxy-7-methyl-1,4a,5,6,7,7a-hexahydrocyclopenta[d]pyran-4-carboxylate	10466307	FALSE	C12C(C(=COC1O)C(=O)OC)CC(C2C)O
MOL001681	0.9569	0.0431	0.8722	Herba Patriniae	methyl (1R,4aS,6S,7R,7aS)-1,6-dihydroxy-7-methyl-1,4a,5,6,7,7a-hexahydrocyclopenta[d]pyran-4-carboxylate	10466307	FALSE	C12C(C(=COC1O)C(=O)OC)CC(C2C)O
MOL001681	0.9569	0.0431	0.8722	Cornus Officinalis Sieb. Et Zucc.	methyl (1R,4aS,6S,7R,7aS)-1,6-dihydroxy-7-methyl-1,4a,5,6,7,7a-hexahydrocyclopenta[d]pyran-4-carboxylate	10466307	FALSE	C12C(C(=COC1O)C(=O)OC)CC(C2C)O

MOL001682	0.8849	0.1151	0.7198	Herba Patriniae	(1S,4aS,6R,8S,8aS)-6-hydroxy-8-methyl-1-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]oxy-1,4a,5,6,8,8a-hexahydropyrano[4,3-d]pyran-4-carboxylic acid methyl ester	11228693	FALSE	C12C(C(=COC1OC1OC(C(C(C1O)O)O)CO)C(=O)OC)CC(OC2C)O
MOL001682	0.8849	0.1151	0.7198	Cornus Officinalis Sieb. Et Zucc.	(1S,4aS,6R,8S,8aS)-6-hydroxy-8-methyl-1-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]oxy-1,4a,5,6,8,8a-hexahydropyrano[4,3-d]pyran-4-carboxylic acid methyl ester	11228693	FALSE	C12C(C(=COC1OC1OC(C(C(C1O)O)O)CO)C(=O)OC)CC(OC2C)O
MOL001683	0.9243	0.0757	0.8120	Cornus Officinalis Sieb. Et Zucc.	morroniside_qt	Not Available	FALSE	C12C(C(=COC1O)C(=O)OC)CC(OC2C)O
MOL001683	0.9243	0.0757	0.8120	Herba Patriniae	morroniside_qt	Not Available	FALSE	C12C(C(=COC1O)C(=O)OC)CC(OC2C)O
MOL001684	0.9388	0.0612	0.8720	Herba Patriniae	6-isoquinolylamine	588991	FALSE	c12cc(N)ccc1cncc2
MOL001685	0.3550	0.6450	0.6048	Herba Patriniae	orotinin	Not Available	FALSE	O1C(CC(=O)c2c1c(c1OC(C=Cc1c2O)(C)C)CC=C(C)C)c1c(O)cccc1O

MOL001686	0.8292	0.1708	0.6361	Herba Patriniae	patrinalloside	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)CC1=COC(C2C1CC(C2CO)O)OC(=O)CC(C)C
MOL001687	0.9137	0.0863	0.7414	Herba Patriniae	Patrinoside-aglycone	3059326	FALSE	OCC1=COC(C2C1CC(C2CO)O)OC(=O)CC(C)C
MOL001689	0.9198	0.0802	0.9763	Menthae Herba	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001689	0.9198	0.0802	0.9763	Trollius Chinensis	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001689	0.9198	0.0802	0.9763	Glechomae Herba	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001689	0.9198	0.0802	0.9763	Lygodii Spora	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001689	0.9198	0.0802	0.9763	Paederiae Scandentis Herba	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001689	0.9198	0.0802	0.9763	Nardostachyos Radix Et Rhizoma	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001689	0.9198	0.0802	0.9763	Chrysanthemi Flos	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001689	0.9198	0.0802	0.9763	Platycodon Grandiforus	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001689	0.9198	0.0802	0.9763	Schizonepetae Spica	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001689	0.9198	0.0802	0.9763	Moslae Herba	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001689	0.9198	0.0802	0.9763	Pseudostellariae Radix	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001689	0.9198	0.0802	0.9763	Herba Cirsii	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001689	0.9198	0.0802	0.9763	Ecliptae Herba	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001689	0.9198	0.0802	0.9763	Lysimachiae Herba	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001689	0.9198	0.0802	0.9763	Chrysanthemi Indici Flos	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001689	0.9198	0.0802	0.9763	Isatdis Radix	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001689	0.9198	0.0802	0.9763	Herba Patriniae	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001689	0.9198	0.0802	0.9763	Lycii Cortex	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001689	0.9198	0.0802	0.9763	Buddlejae Flos	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001689	0.9198	0.0802	0.9763	Lobeliae Chinensis Herba	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001689	0.9198	0.0802	0.9763	Scutellariae Radix	acacetin	5280442	TRUE	Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1
MOL001690	0.9247	0.0753	0.9448	Caulis Akebiae	Inositol-b	892	FALSE	C1(C(C(C(C(C1O)O)O)O)O)O
MOL001690	0.9247	0.0753	0.9448	Maydis Seigma	Inositol-b	892	FALSE	C1(C(C(C(C(C1O)O)O)O)O)O
MOL001690	0.9247	0.0753	0.9448	Herba Patriniae	Inositol-b	892	FALSE	C1(C(C(C(C(C1O)O)O)O)O)O
MOL001691	0.9367	0.0633	0.9775	Humulus Scandens (Lour.) Merr.	vitamin c	54670067	TRUE	C1(=C(C(OC1=O)C(CO)O)O)O
MOL001691	0.9367	0.0633	0.9775	Herba Patriniae	vitamin c	54670067	TRUE	C1(=C(C(OC1=O)C(CO)O)O)O
MOL001691	0.9367	0.0633	0.9775	Raphani Semen	vitamin c	54670067	TRUE	C1(=C(C(OC1=O)C(CO)O)O)O
MOL001691	0.9367	0.0633	0.9775	Lycii Fructus	vitamin c	54670067	TRUE	C1(=C(C(OC1=O)C(CO)O)O)O
MOL001691	0.9367	0.0633	0.9775	Vigna Radiata	vitamin c	54670067	TRUE	C1(=C(C(OC1=O)C(CO)O)O)O
MOL001691	0.9367	0.0633	0.9775	Platycodon Grandiforus	vitamin c	54670067	TRUE	C1(=C(C(OC1=O)C(CO)O)O)O
MOL001691	0.9367	0.0633	0.9775	Rosae Laevigatae Fructus	vitamin c	54670067	TRUE	C1(=C(C(OC1=O)C(CO)O)O)O
MOL001691	0.9367	0.0633	0.9775	Ginkgo Folium	vitamin c	54670067	TRUE	C1(=C(C(OC1=O)C(CO)O)O)O
MOL001691	0.9367	0.0633	0.9775	Hippophae Fructus	vitamin c	54670067	TRUE	C1(=C(C(OC1=O)C(CO)O)O)O
MOL001691	0.9367	0.0633	0.9775	Portulacae Herba	vitamin c	54670067	TRUE	C1(=C(C(OC1=O)C(CO)O)O)O
MOL001691	0.9367	0.0633	0.9775	Crataegi Folium	vitamin c	54670067	TRUE	C1(=C(C(OC1=O)C(CO)O)O)O
MOL001691	0.9367	0.0633	0.9775	Ginkgo Semen	vitamin c	54670067	TRUE	C1(=C(C(OC1=O)C(CO)O)O)O

MOL001691	0.9367	0.0633	0.9775	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	vitamin c	54670067	TRUE	C1(=C(C(OC1=O)C(CO)O)O)O
MOL001691	0.9367	0.0633	0.9775	Corayceps	vitamin c	54670067	TRUE	C1(=C(C(OC1=O)C(CO)O)O)O
MOL001691	0.9367	0.0633	0.9775	Euryales Semen	vitamin c	54670067	TRUE	C1(=C(C(OC1=O)C(CO)O)O)O
MOL001691	0.9367	0.0633	0.9775	Gnaphalii Affinis Herba	vitamin c	54670067	TRUE	C1(=C(C(OC1=O)C(CO)O)O)O
MOL001692	0.9344	0.0656	0.9643	Herba Patriniae	beta-D-Apiose	441474	FALSE	C1(C(C(OC1)O)O)(O)CO
MOL001692	0.9344	0.0656	0.9643	Cortex Moutan	beta-D-Apiose	441474	FALSE	C1(C(C(OC1)O)O)(O)CO
MOL001692	0.9344	0.0656	0.9643	Abrus Precatorius L.	beta-D-Apiose	441474	FALSE	C1(C(C(OC1)O)O)(O)CO
MOL001694	0.9527	0.0473	0.9767	Perilla Frutescens	Perillyl alcohol	369312	FALSE	C1(CCC(=CC1)CO)C(=C)C
MOL001694	0.9527	0.0473	0.9767	Evodiae Fructus	Perillyl alcohol	369312	FALSE	C1(CCC(=CC1)CO)C(=C)C
MOL001694	0.9527	0.0473	0.9767	Lysimachiae Herba	Perillyl alcohol	369312	FALSE	C1(CCC(=CC1)CO)C(=C)C
MOL001694	0.9527	0.0473	0.9767	Cortex Periplocae Radicis	Perillyl alcohol	369312	FALSE	C1(CCC(=CC1)CO)C(=C)C
MOL001694	0.9527	0.0473	0.9767	Cnidii Fructus	Perillyl alcohol	369312	FALSE	C1(CCC(=CC1)CO)C(=C)C
MOL001694	0.9527	0.0473	0.9767	Herba Patriniae	Perillyl alcohol	369312	FALSE	C1(CCC(=CC1)CO)C(=C)C
MOL001695	0.9182	0.0818	0.7903	Paederiae Scandentis Herba	Quercimeritrin (6CI,7CI,8CI)	5282160	FALSE	C1(C(C(OC(C1O)Oc1cc(c2c(c1)oc(c(c2=O)O)c1cc(cc1)O)O)O)CO)O)O
MOL001695	0.9182	0.0818	0.7903	Inulae Herba	Quercimeritrin (6CI,7CI,8CI)	5282160	FALSE	C1(C(C(OC(C1O)Oc1cc(c2c(c1)oc(c(c2=O)O)c1cc(cc1)O)O)O)CO)O)O
MOL001695	0.9182	0.0818	0.7903	Carthami Flos	Quercimeritrin (6CI,7CI,8CI)	5282160	FALSE	C1(C(C(OC(C1O)Oc1cc(c2c(c1)oc(c(c2=O)O)c1cc(cc1)O)O)O)CO)O)O
MOL001695	0.9182	0.0818	0.7903	Daturae Flos	Quercimeritrin (6CI,7CI,8CI)	5282160	FALSE	C1(C(C(OC(C1O)Oc1cc(c2c(c1)oc(c(c2=O)O)c1cc(cc1)O)O)O)CO)O)O
MOL001695	0.9182	0.0818	0.7903	Celastri Orbiculati Fructus	Quercimeritrin (6CI,7CI,8CI)	5282160	FALSE	C1(C(C(OC(C1O)Oc1cc(c2c(c1)oc(c(c2=O)O)c1cc(cc1)O)O)O)CO)O)O
MOL001695	0.9182	0.0818	0.7903	Gnaphalii Affinis Herba	Quercimeritrin (6CI,7CI,8CI)	5282160	FALSE	C1(C(C(OC(C1O)Oc1cc(c2c(c1)oc(c(c2=O)O)c1cc(cc1)O)O)O)CO)O)O
MOL001695	0.9182	0.0818	0.7903	Saururi Herba	Quercimeritrin (6CI,7CI,8CI)	5282160	FALSE	C1(C(C(OC(C1O)Oc1cc(c2c(c1)oc(c(c2=O)O)c1cc(cc1)O)O)O)CO)O)O

MOL001695	0.9182	0.0818	0.7903	Herba Patriniae	Quercimeritrin (6CI,7CI,8CI)	5282160	FALSE	C1(C(C(OC(C1O)Oc1cc(c2c(c1)oc(c(c2=O)O)c1cc(cc(cc1)O)O)O)CO)O)O
MOL001695	0.9182	0.0818	0.7903	Geranium Wilfordii Maxim.	Quercimeritrin (6CI,7CI,8CI)	5282160	FALSE	C1(C(C(OC(C1O)Oc1cc(c2c(c1)oc(c(c2=O)O)c1cc(cc(cc1)O)O)O)CO)O)O
MOL001696	0.3089	0.6911	0.6067	Hydnocarpi Anthelminticae Semen	Morusin	5281671	FALSE	O1c2c(C=CC1(C)C)c1c(c(c2)O)c(=O)c(c(o1)c1ccc(cc1O)O)CC=C(C)C
MOL001696	0.3089	0.6911	0.6067	Cornus Officinalis Sieb. Et Zucc.	Morusin	5281671	FALSE	O1c2c(C=CC1(C)C)c1c(c(c2)O)c(=O)c(c(o1)c1ccc(cc1O)O)CC=C(C)C
MOL001696	0.3089	0.6911	0.6067	licorice	Morusin	5281671	FALSE	O1c2c(C=CC1(C)C)c1c(c(c2)O)c(=O)c(c(o1)c1ccc(cc1O)O)CC=C(C)C
MOL001696	0.3089	0.6911	0.6067	Mori Cortex	Morusin	5281671	FALSE	O1c2c(C=CC1(C)C)c1c(c(c2)O)c(=O)c(c(o1)c1ccc(cc1O)O)CC=C(C)C
MOL001696	0.3089	0.6911	0.6067	Herba Patriniae	Morusin	5281671	FALSE	O1c2c(C=CC1(C)C)c1c(c(c2)O)c(=O)c(c(o1)c1ccc(cc1O)O)CC=C(C)C
MOL001697	0.6826	0.3174	0.7922	Capsellae Herba	Sinoacutine	Not Available	FALSE	C12C3(c4c(C5(C1=CC(=O)C(=C5)OC)C3)c(c(cc4)OC)O)CN2C
MOL001697	0.6826	0.3174	0.7922	Sinapis Semen	Sinoacutine	Not Available	FALSE	C12C3(c4c(C5(C1=CC(=O)C(=C5)OC)C3)c(c(cc4)OC)O)CN2C
MOL001697	0.6826	0.3174	0.7922	Herba Patriniae	Sinoacutine	Not Available	FALSE	C12C3(c4c(C5(C1=CC(=O)C(=C5)OC)C3)c(c(cc4)OC)O)CN2C
MOL001698	0.6756	0.3244	0.6855	Dysosmae Verspiellis Rhixoma Et Radix	Clei B	119458	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(c(c3c1cc(OC)c(OC)c3)c1cc3OCOc3cc1)C(=O)OC2)CO
MOL001699	0.6084	0.3916	0.7642	Dysosmae Verspiellis Rhixoma Et Radix	Diphyllin	100492	FALSE	Oc1c2c(c(c3c1cc(OC)c(OC)c3)c1cc3OCOc3cc1)C(=O)OC2
MOL001700	0.4655	0.5345	0.8310	Dysosmae Verspiellis Rhixoma Et Radix	deoxypodophyllotoxin	345501	FALSE	O1CC2C(C(c3c(C2)cc2OCOc2c3)c2cc(OC)c(OC)c(OC)c2)C1=O
MOL001701	0.9506	0.0494	0.7917	Dysosmae Verspiellis Rhixoma Et Radix	7-[(2S)-2,3-dihydroxypropyl]-1,3-dimethylpurine-2,6-dione	688352	FALSE	c12c(n(c(=O)n(c2=O)C)C)ncn1CC(CO)O
MOL001702	0.8224	0.1776	0.7326	Dysosmae Verspiellis Rhixoma Et Radix	dysoanthraquinone	Not Available	FALSE	O1COc2c1cc1C(=O)c3cc(c(c(c3C(=O)c1c2)OC)OC)OC

MOL001703	0.7255	0.2745	0.6308	Dysosmae Verspiellis Rhixoma Et Radix	4-[(2R,3S,4S)-4-[(S)-hydroxy-(3-hydroxy-5-methoxyphenyl)methyl]-3-(hydroxymethyl)oxolan-2-yl]-2-methoxyphenol	16109834	FALSE	O1C(C(C(C1)C(O)c1cc(OC)cc(O)c1)CO)c1cc(OC)c(O)cc1
MOL001704	0.8470	0.1530	0.7740	Dysosmae Verspiellis Rhixoma Et Radix	E-7-Tetradecenol	5362726	FALSE	OCCCCCC/C=C/CCCCCC
MOL001705	0.8470	0.1530	0.8324	Evodiae Fructus	Neryl isovalerate	5362830	FALSE	O(C(=O)CC(C)C)C/C=C(/CCC=C(C)C)\C
MOL001705	0.8470	0.1530	0.8324	Dysosmae Verspiellis Rhixoma Et Radix	Neryl isovalerate	5362830	FALSE	O(C(=O)CC(C)C)C/C=C(/CCC=C(C)C)\C
MOL001706	0.9262	0.0738	0.9386	Dysosmae Verspiellis Rhixoma Et Radix	2,6-dimethyl-3,7-octadiene-2,6-diol	Not Available	FALSE	CC(/C=C/CC(C=C)(O)C)(O)C
MOL001706	0.9262	0.0738	0.9386	Panax Ginseng C. A. Mey.	2,6-dimethyl-3,7-octadiene-2,6-diol	Not Available	FALSE	CC(/C=C/CC(C=C)(O)C)(O)C
MOL001707	0.8968	0.1032	0.8864	Eriobotryae Folium	24190-29-2	638013	FALSE	O=C(/C=C/C1C(CCC=C1C)(C)C)C
MOL001707	0.8968	0.1032	0.8864	Epimrdii Herba	24190-29-2	638013	FALSE	O=C(/C=C/C1C(CCC=C1C)(C)C)C
MOL001707	0.8968	0.1032	0.8864	Lysimachiae Foenigraeci Herba	24190-29-2	638013	FALSE	O=C(/C=C/C1C(CCC=C1C)(C)C)C
MOL001707	0.8968	0.1032	0.8864	Dysosmae Verspiellis Rhixoma Et Radix	24190-29-2	638013	FALSE	O=C(/C=C/C1C(CCC=C1C)(C)C)C
MOL001707	0.8968	0.1032	0.8864	Hippophae Fructus	24190-29-2	638013	FALSE	O=C(/C=C/C1C(CCC=C1C)(C)C)C
MOL001707	0.8968	0.1032	0.8864	Ginkgo Folium	24190-29-2	638013	FALSE	O=C(/C=C/C1C(CCC=C1C)(C)C)C
MOL001708	0.5442	0.4558	0.7879	Dysosmae Verspiellis Rhixoma Et Radix	picropodophyllone	1618391	FALSE	O1CC2C(C(c3c(C2=O)cc2OCOc2c3)c2cc(OC)c(OC)c(OC)c2)C1=O
MOL001709	0.6809	0.3191	0.6625	Dysosmae Verspiellis Rhixoma Et Radix	methyl (2E,4E)-hexadeca-2,4-dienoate	6443015	FALSE	C(=O)(/C=C/C=C/CCCCCCCCCCC)OC
MOL001709	0.6809	0.3191	0.6625	Rehmanniae Radix Praeparata	methyl (2E,4E)-hexadeca-2,4-dienoate	6443015	FALSE	C(=O)(/C=C/C=C/CCCCCCCCCCC)OC
MOL001710	0.5659	0.4341	0.6661	Dysosmae Verspiellis Rhixoma Et Radix	picropodophyllin	72435	FALSE	O1CC2C(C(c3c(C2O)cc2OCOc2c3)c2cc(OC)c(OC)c(OC)c2)C1=O

MOL001711	0.8254	0.1746	0.6793	Sedi Herba	3,7,11-trimethyl-1-dodecanol	12944527	FALSE	C(CCCC(CCO)C)(CCCC(C)C)C
MOL001711	0.8254	0.1746	0.6793	Dysosmae Verspiellis Rhixoma Et Radix	3,7,11-trimethyl-1-dodecanol	12944527	FALSE	C(CCCC(CCO)C)(CCCC(C)C)C
MOL001712	0.7074	0.2926	0.7233	Dysosmae Verspiellis Rhixoma Et Radix	PGB	161177	FALSE	O(C1C2C(C(c3c1cc1OCOc1c3)c1cc(OC)c(OC)c(OC)c1)C(=O)OC2)C1OC(C(O)C(O)C1O)CO
MOL001713	0.5659	0.4341	0.6661	Dysosmae Verspiellis Rhixoma Et Radix	(5R,5aR,8aR,9S)-5-hydroxy-9-(3,4,5-trimethoxyphenyl)-5a,6,8a,9-tetrahydro-5H-isobenzofurano[5,6-f][1,3]benzodioxol-8-one	11047943	FALSE	OC1C2C(C(c3c1cc1OCOc1c3)c1cc(OC)c(OC)c(OC)c1)C(=O)OC2
MOL001714	0.5659	0.4341	0.6661	Dysosmae Verspiellis Rhixoma Et Radix	podophyllotoxin	10607	FALSE	O1CC2C(C(c3c(C2O)cc2OCOc2c3)c2cc(OC)c(OC)c(OC)c2)C1=O
MOL001715	0.5442	0.4558	0.7879	Dysosmae Verspiellis Rhixoma Et Radix	Podophylloto xone	443014	FALSE	O1CC2C(C(c3c(C2=O)cc2OCOc2c3)c2cc(OC)c(OC)c(OC)c2)C1=O
MOL001716	0.7067	0.2933	0.8023	Dysosmae Verspiellis Rhixoma Et Radix	4'-Demethylpodophyllotoxin	122667	FALSE	O1CC2C(C(c3c(C2O)cc2OCOc2c3)c2cc(OC)c(O)c(OC)c2)C1=O
MOL001717	0.5750	0.4250	0.6895	Dysosmae Verspiellis Rhixoma Et Radix	PELTATIN B	92122	FALSE	O1CC2C(C(c3c(C2)c(O)c2OCOc2c3)c2cc(OC)c(OC)c(OC)c2)C1=O
MOL001717	0.5750	0.4250	0.6895	Granati Pericarpium	PELTATIN B	92122	FALSE	O1CC2C(C(c3c(C2)c(O)c2OCOc2c3)c2cc(OC)c(OC)c(OC)c2)C1=O
MOL001718	0.8820	0.1180	0.9625	Dysosmae Verspiellis Rhixoma Et Radix	cis-1,3-dimethyl-cyclohexanol	13435948	FALSE	C1(CC(CCC1)C)(O)C
MOL001719	0.9246	0.0754	0.9150	Lonicerae Japonicae Flos	2-[(2S,5R)-5-ethenyl-5-methyloxolan-2-yl]propan-2-ol	11116492	FALSE	O1C(CCC1(C=C)C)C(O)(C)C

MOL001719	0.9246	0.0754	0.9150	Paederiae Scandentis Herba	2-[(2S,5R)-5-ethenyl-5-methyloxolan-2-yl]propan-2-ol	11116492	FALSE	O1C(CCC1(C=C)C)C(O)(C)C
MOL001719	0.9246	0.0754	0.9150	Dysosmae Verspiellis Rhixoma Et Radix	2-[(2S,5R)-5-ethenyl-5-methyloxolan-2-yl]propan-2-ol	11116492	FALSE	O1C(CCC1(C=C)C)C(O)(C)C
MOL001719	0.9246	0.0754	0.9150	Zingiberis Rhizoma	2-[(2S,5R)-5-ethenyl-5-methyloxolan-2-yl]propan-2-ol	11116492	FALSE	O1C(CCC1(C=C)C)C(O)(C)C
MOL001719	0.9246	0.0754	0.9150	Rhododendri Daurici Folium	2-[(2S,5R)-5-ethenyl-5-methyloxolan-2-yl]propan-2-ol	11116492	FALSE	O1C(CCC1(C=C)C)C(O)(C)C
MOL001719	0.9246	0.0754	0.9150	Capsici Fructus	2-[(2S,5R)-5-ethenyl-5-methyloxolan-2-yl]propan-2-ol	11116492	FALSE	O1C(CCC1(C=C)C)C(O)(C)C
MOL001720	0.9123	0.0877	0.8481	Isatdis Radix	4-hydroxy-1H-indole-3-carbaldehyde	9815282	FALSE	c1ccc2c(c1O)c(c[nH]2)C=O
MOL001721	0.8005	0.1995	0.6808	Isatdis Radix	Isaindigodione	Not Available	FALSE	N1c2ccccc2C2(C1=O)CCCC1CC(=O)C(=C(N21)C)C(=O)O
MOL001722	0.9006	0.0994	0.8293	Isatdis Radix	2-O-beta-D-glucopyranosyl-2H-1,4-benzoxazin-3(4H)-one	38356372	FALSE	c1ccc2c(c1)OC(C(=O)N2)OC1C(C(C(C(O1)CO)O)O)O
MOL001723	0.9301	0.0699	0.8388	Isatdis Radix	2-O-beta-D-glucopyranosyl-2H-1,4-benzoxazin-3(4H)-one_qt	40532717	FALSE	OC1C(=O)Nc2ccccc2O1

MOL001724	0.8951	0.1049	0.8265	Isatdis Radix	2-O-beta-D-glucopyranosyl-4-hydroxy-2H-1,4-benzoxazin-3(4H)-one	Not Available	FALSE	O1C(C(O)C(O)C(O)C1OC1Oc2c(N(O)C1=O)cccc2)CO
MOL001725	0.9263	0.0737	0.8555	Isatdis Radix	2-O-beta-D-glucopyranosyl-4-hydroxy-2H-1,4-benzoxazin-3(4H)-one_qt	40572506	FALSE	OC1Oc2c(N(O)C1=O)cccc2
MOL001726	0.3841	0.6159	0.7072	Isatdis Radix	pinoresinol-4-O-beta-D-apiosyl-beta-D-glucopyranoside	Not Available	FALSE	C1C(C(C(C1)OC1C(C(CCC1Oc1ccc(cc1OC)C1C2C(CO1)C(OC2)c1cc(c(cc1)O)OC)O)O)O)(O)CO
MOL001727	0.8942	0.1058	0.7033	Isatdis Radix	3-[2′ -(5′ -hydroxymethyl) furyl] -1 (2H) -isoquinolinone-7-O-BETA-D-glucoside	Not Available	FALSE	C1(C(C(C(C(O1)Oc1ccc2c(c1)c(=O)[nH]c(c2)c1ccc(o1)CO)O)O)O)CO
MOL001728	0.9189	0.0811	0.7395	Isatdis Radix	3-[2′ -(5′ -hydroxymethyl) furyl] -1 (2H) -isoquinolinone-7-O-BETA-D-glucoside_qt	Not Available	FALSE	Oc1ccc2c(c1)c(=O)[nH]c(c2)c1ccc(o1)CO
MOL001729	0.8511	0.1489	0.8134	Radix Rhei Et Rhizome	Crysophanol	10208	FALSE	c12c(C(=O)c3c(C1=O)cccc3O)c(cc(c2)C)O
MOL001729	0.8511	0.1489	0.8134	Xanthii Fructus	Crysophanol	10208	FALSE	c12c(C(=O)c3c(C1=O)cccc3O)c(cc(c2)C)O
MOL001729	0.8511	0.1489	0.8134	Menthae Herba	Crysophanol	10208	FALSE	c12c(C(=O)c3c(C1=O)cccc3O)c(cc(c2)C)O
MOL001729	0.8511	0.1489	0.8134	Sargentodoxae Caulis	Crysophanol	10208	FALSE	c12c(C(=O)c3c(C1=O)cccc3O)c(cc(c2)C)O
MOL001729	0.8511	0.1489	0.8134	Chuanxiong Rhizoma	Crysophanol	10208	FALSE	c12c(C(=O)c3c(C1=O)cccc3O)c(cc(c2)C)O
MOL001729	0.8511	0.1489	0.8134	Achyranthis Bidentatae Radix	Crysophanol	10208	FALSE	c12c(C(=O)c3c(C1=O)cccc3O)c(cc(c2)C)O
MOL001729	0.8511	0.1489	0.8134	Areca Catechu L.	Crysophanol	10208	FALSE	c12c(C(=O)c3c(C1=O)cccc3O)c(cc(c2)C)O

MOL001729	0.8511	0.1489	0.8134	Asteris Radix Et Rhizoma	Crysophanol	10208	FALSE	c12c(C(=O)c3c(C1=O)cccc3O)c(cc(c2)C)O
MOL001729	0.8511	0.1489	0.8134	Isatdis Radix	Crysophanol	10208	FALSE	c12c(C(=O)c3c(C1=O)cccc3O)c(cc(c2)C)O
MOL001729	0.8511	0.1489	0.8134	Abri Herba	Crysophanol	10208	FALSE	c12c(C(=O)c3c(C1=O)cccc3O)c(cc(c2)C)O
MOL001729	0.8511	0.1489	0.8134	Hemerocallis Radix	Crysophanol	10208	FALSE	c12c(C(=O)c3c(C1=O)cccc3O)c(cc(c2)C)O
MOL001729	0.8511	0.1489	0.8134	Ampelopsis Japonica	Crysophanol	10208	FALSE	c12c(C(=O)c3c(C1=O)cccc3O)c(cc(c2)C)O
MOL001729	0.8511	0.1489	0.8134	Glechomae Herba	Crysophanol	10208	FALSE	c12c(C(=O)c3c(C1=O)cccc3O)c(cc(c2)C)O
MOL001729	0.8511	0.1489	0.8134	Sennae Folium	Crysophanol	10208	FALSE	c12c(C(=O)c3c(C1=O)cccc3O)c(cc(c2)C)O
MOL001729	0.8511	0.1489	0.8134	Polygoni Cuspidati Rhizoma Et Radix	Crysophanol	10208	FALSE	c12c(C(=O)c3c(C1=O)cccc3O)c(cc(c2)C)O
MOL001729	0.8511	0.1489	0.8134	Aucklandiae Radix	Crysophanol	10208	FALSE	c12c(C(=O)c3c(C1=O)cccc3O)c(cc(c2)C)O
MOL001729	0.8511	0.1489	0.8134	Arum Ternatum Thunb.	Crysophanol	10208	FALSE	c12c(C(=O)c3c(C1=O)cccc3O)c(cc(c2)C)O
MOL001729	0.8511	0.1489	0.8134	Cassiae Semen	Crysophanol	10208	FALSE	c12c(C(=O)c3c(C1=O)cccc3O)c(cc(c2)C)O
MOL001729	0.8511	0.1489	0.8134	Semen Pharbitidis	Crysophanol	10208	FALSE	c12c(C(=O)c3c(C1=O)cccc3O)c(cc(c2)C)O
MOL001730	0.9067	0.0933	0.8404	Isatdis Radix	6-Hydroxyindole	524508	FALSE	Oc1cc2[nH]ccc2cc1
MOL001731	0.9388	0.0612	0.9616	Radix Bupleuri	Dextrin Corn	79025	FALSE	O1C(C(O)C(O)C(O)C1O)CO
MOL001731	0.9388	0.0612	0.9616	Isatdis Radix	Dextrin Corn	79025	FALSE	O1C(C(O)C(O)C(O)C1O)CO
MOL001732	0.9295	0.0705	0.9606	Lygodii Spora	IFP	753	FALSE	OC(CO)CO
MOL001732	0.9295	0.0705	0.9606	Mori Fructus	IFP	753	FALSE	OC(CO)CO
MOL001732	0.9295	0.0705	0.9606	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	IFP	753	FALSE	OC(CO)CO
MOL001732	0.9295	0.0705	0.9606	Ginseng Folium	IFP	753	FALSE	OC(CO)CO
MOL001732	0.9295	0.0705	0.9606	Typhonii Rhizoma	IFP	753	FALSE	OC(CO)CO
MOL001732	0.9295	0.0705	0.9606	Hippophae Fructus	IFP	753	FALSE	OC(CO)CO
MOL001732	0.9295	0.0705	0.9606	Lilii Bulbus	IFP	753	FALSE	OC(CO)CO
MOL001732	0.9295	0.0705	0.9606	Isatdis Radix	IFP	753	FALSE	OC(CO)CO
MOL001732	0.9295	0.0705	0.9606	Chaenomeles Sinensis (Thouin) Koehne	IFP	753	FALSE	OC(CO)CO
MOL001732	0.9295	0.0705	0.9606	Aucklandiae Radix	IFP	753	FALSE	OC(CO)CO
MOL001733	0.7794	0.2206	0.9116	Siphonostegiae Herba	EUPATORIN	97214	FALSE	c12c(c(c(c2OC)OC)O)C(=O)cc(o1)c1cc(c(cc1)OC)O
MOL001733	0.7794	0.2206	0.9116	Isatdis Radix	EUPATORIN	97214	FALSE	c12c(c(c(c2OC)OC)O)C(=O)cc(o1)c1cc(c(cc1)OC)O
MOL001734	0.9028	0.0972	0.7399	Isatdis Radix	3-[[(2R,3R,5R,6S)-3,5-dihydroxy-6-(1H-indol-3-yloxy)-4-oxooxan-2-yl]methoxy]-3-oxopropanoic acid	641608	FALSE	O1C(C(O)C(=O)C(O)C1Oc1c2c([nH]c1)cccc2)COC(=O)CC(=O)O

MOL001735	0.8665	0.1335	0.9073	Wikstroemiae Indicae Rasix	Dinatin	5281628	FALSE	c12c(oc(cc2=O)c2ccc(cc2)O)cc(c(c1O)OC)O
MOL001735	0.8665	0.1335	0.9073	Saussureae Involucratae Herba	Dinatin	5281628	FALSE	c12c(oc(cc2=O)c2ccc(cc2)O)cc(c(c1O)OC)O
MOL001735	0.8665	0.1335	0.9073	Belamcandae Rhizome	Dinatin	5281628	FALSE	c12c(oc(cc2=O)c2ccc(cc2)O)cc(c(c1O)OC)O
MOL001735	0.8665	0.1335	0.9073	Isatdis Radix	Dinatin	5281628	FALSE	c12c(oc(cc2=O)c2ccc(cc2)O)cc(c(c1O)OC)O
MOL001735	0.8665	0.1335	0.9073	Plantaginis Herba	Dinatin	5281628	FALSE	c12c(oc(cc2=O)c2ccc(cc2)O)cc(c(c1O)OC)O
MOL001735	0.8665	0.1335	0.9073	Oroxyli Semen	Dinatin	5281628	FALSE	c12c(oc(cc2=O)c2ccc(cc2)O)cc(c(c1O)OC)O
MOL001735	0.8665	0.1335	0.9073	Radix Cirsii Japonici	Dinatin	5281628	FALSE	c12c(oc(cc2=O)c2ccc(cc2)O)cc(c(c1O)OC)O
MOL001735	0.8665	0.1335	0.9073	Scutellariae Barbatae Herba	Dinatin	5281628	FALSE	c12c(oc(cc2=O)c2ccc(cc2)O)cc(c(c1O)OC)O
MOL001735	0.8665	0.1335	0.9073	Eriocauli Flos	Dinatin	5281628	FALSE	c12c(oc(cc2=O)c2ccc(cc2)O)cc(c(c1O)OC)O
MOL001735	0.8665	0.1335	0.9073	Plantaginis Semen	Dinatin	5281628	FALSE	c12c(oc(cc2=O)c2ccc(cc2)O)cc(c(c1O)OC)O
MOL001736	0.9461	0.0539	0.9148	Isatdis Radix	(-)-taxifolin	712316	FALSE	c1(cc(c2c(c1)OC(C(C2=O)O)c1ccc(c(c1)O)O)O)O
MOL001736	0.9461	0.0539	0.9148	Smilacis Glabrae Rhixoma	(-)-taxifolin	712316	FALSE	c1(cc(c2c(c1)OC(C(C2=O)O)c1ccc(c(c1)O)O)O)O
MOL001736	0.9461	0.0539	0.9148	Polygoni Orientalis Fructus	(-)-taxifolin	712316	FALSE	c1(cc(c2c(c1)OC(C(C2=O)O)c1ccc(c(c1)O)O)O)O
MOL001736	0.9461	0.0539	0.9148	Cinnamomi Ramulus	(-)-taxifolin	712316	FALSE	c1(cc(c2c(c1)OC(C(C2=O)O)c1ccc(c(c1)O)O)O)O
MOL001736	0.9461	0.0539	0.9148	Rhizoma Dioscoreae	(-)-taxifolin	712316	FALSE	c1(cc(c2c(c1)OC(C(C2=O)O)c1ccc(c(c1)O)O)O)O
MOL001736	0.9461	0.0539	0.9148	Gleditsiae Spina	(-)-taxifolin	712316	FALSE	c1(cc(c2c(c1)OC(C(C2=O)O)c1ccc(c(c1)O)O)O)O
MOL001736	0.9461	0.0539	0.9148	Silybum Marianum	(-)-taxifolin	712316	FALSE	c1(cc(c2c(c1)OC(C(C2=O)O)c1ccc(c(c1)O)O)O)O
MOL001736	0.9461	0.0539	0.9148	Choerospondiatis Fructus	(-)-taxifolin	712316	FALSE	c1(cc(c2c(c1)OC(C(C2=O)O)c1ccc(c(c1)O)O)O)O
MOL001736	0.9461	0.0539	0.9148	Rhododendri Daurici Folium	(-)-taxifolin	712316	FALSE	c1(cc(c2c(c1)OC(C(C2=O)O)c1ccc(c(c1)O)O)O)O
MOL001737	0.9384	0.0616	0.8513	licorice	ICO	69867	FALSE	c12c([nH]cc1C(=O)O)cccc2
MOL001737	0.9384	0.0616	0.8513	Isatdis Radix	ICO	69867	FALSE	c12c([nH]cc1C(=O)O)cccc2
MOL001738	0.8798	0.1202	0.9520	Hordei Fructus Germinatus	MLI	23511544	FALSE	OC(=O)CC(=O)O
MOL001738	0.8798	0.1202	0.9520	Panax Ginseng C. A. Mey.	MLI	23511544	FALSE	OC(=O)CC(=O)O
MOL001738	0.8798	0.1202	0.9520	Isatdis Radix	MLI	23511544	FALSE	OC(=O)CC(=O)O
MOL001738	0.8798	0.1202	0.9520	Gynostemmae Pentaphylli Herba	MLI	23511544	FALSE	OC(=O)CC(=O)O
MOL001739	0.8576	0.1424	0.6905	Arum Ternatum Thunb.	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Gossampiniflos	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Ginsen Radix Et Rhizoma Rubra	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Rehmanniae Radix Praeparata	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Morindae Officinalis Radix	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Cortex Periplocae Radicis	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Broussonetiae Fructus	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Tamaricis Cacumen	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Ginkgo Folium	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Zanthoxyli Pericarpium	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Amygdalus Communis Vas	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC

MOL001739	0.8576	0.1424	0.6905	Capsici Fructus	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Citri Reticulatae Semen	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Polygonati Odorati Rhizoma	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Cannabis Sativa L.	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Momordicae Fructus	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Cinnanmomi Cortex	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Oroxyli Semen	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Et Radix Patriniae Rhizoma	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Ginkgo Semen	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Trichosanthes Kirilowii Maxim	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Cornus Officinalis Sieb. Et Zucc.	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Arecae Semen	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Choerospondiatis Fructus	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Aloe	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Kochiae Fructus	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Meliae Azedarach Fructus	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Curcumae Radix	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Isatdis Radix	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Carthami Flos	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Perillae Fructus	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Cucurbitae Moschatae Semen	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Linderae Radix	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Hippophae Fructus	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Jujubae Fructus	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001739	0.8576	0.1424	0.6905	Tripterygii Radix	zoomaric acid	445638	FALSE	OC(=O)CCCCCCC/C=C\CCCCCC
MOL001740	0.8958	0.1042	0.9172	Sinapis Semen	4-Methylpentyl isothiocyanate	519452	FALSE	S=C=NCCCC(C)C
MOL001740	0.8958	0.1042	0.9172	Isatdis Radix	4-Methylpentyl isothiocyanate	519452	FALSE	S=C=NCCCC(C)C

MOL001741	0.9121	0.0879	0.9378	Sinapis Semen	3-Butenyl isothiocyanate	76922	FALSE	C(CC=C)N=C=S
MOL001741	0.9121	0.0879	0.9378	Isatdis Radix	3-Butenyl isothiocyanate	76922	FALSE	C(CC=C)N=C=S
MOL001742	0.9436	0.0564	0.9712	Isatdis Radix	ASO	64960	FALSE	C1(C(C(C(CO1)O)O)O)CO
MOL001743	0.9341	0.0659	0.8962	Picrorhizae Rhizoma	1-[(2R,3S,4S,5S)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]pyrimidine-2,4-dione	7059439	FALSE	C1(n2c(=O)[nH]c(=O)cc2)OC(C(C1O)O)CO
MOL001743	0.9341	0.0659	0.8962	Isatdis Radix	1-[(2R,3S,4S,5S)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]pyrimidine-2,4-dione	7059439	FALSE	C1(n2c(=O)[nH]c(=O)cc2)OC(C(C1O)O)CO
MOL001744	0.8841	0.1159	0.9618	Corayceps	uracil	1174	FALSE	[nH]1c(=O)[nH]c(=O)cc1
MOL001744	0.8841	0.1159	0.9618	Arum Ternatum Thunb.	uracil	1174	FALSE	[nH]1c(=O)[nH]c(=O)cc1
MOL001744	0.8841	0.1159	0.9618	Bombyx Mori L.	uracil	1174	FALSE	[nH]1c(=O)[nH]c(=O)cc1
MOL001744	0.8841	0.1159	0.9618	Fritiliariae Irrhosae Bulbus	uracil	1174	FALSE	[nH]1c(=O)[nH]c(=O)cc1
MOL001744	0.8841	0.1159	0.9618	Cotyledon Fimbriata Turcz.	uracil	1174	FALSE	[nH]1c(=O)[nH]c(=O)cc1
MOL001744	0.8841	0.1159	0.9618	Aconiti Lateralis Radix Praeparata	uracil	1174	FALSE	[nH]1c(=O)[nH]c(=O)cc1
MOL001744	0.8841	0.1159	0.9618	Sargassum	uracil	1174	FALSE	[nH]1c(=O)[nH]c(=O)cc1
MOL001744	0.8841	0.1159	0.9618	Chuanxiong Rhizoma	uracil	1174	FALSE	[nH]1c(=O)[nH]c(=O)cc1
MOL001744	0.8841	0.1159	0.9618	Farfarae Flos	uracil	1174	FALSE	[nH]1c(=O)[nH]c(=O)cc1
MOL001744	0.8841	0.1159	0.9618	Evodiae Fructus	uracil	1174	FALSE	[nH]1c(=O)[nH]c(=O)cc1
MOL001744	0.8841	0.1159	0.9618	Isatdis Radix	uracil	1174	FALSE	[nH]1c(=O)[nH]c(=O)cc1
MOL001745	0.4699	0.5301	0.6100	Isatdis Radix	Methyl vaccenate	5364432	FALSE	C(=O)(CCCCCCCCC/C=C/CCCCCC)OC
MOL001746	0.5898	0.4102	0.6068	Folium Ilicis Cornutae	ELD	5283387	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)N
MOL001746	0.5898	0.4102	0.6068	Mahoniae Folum	ELD	5283387	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)N
MOL001746	0.5898	0.4102	0.6068	Uncariae Ramulus Cumuncis	ELD	5283387	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)N
MOL001746	0.5898	0.4102	0.6068	Momordicae Fructus	ELD	5283387	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)N

MOL001746	0.5898	0.4102	0.6068	Gynostemmae Pentaphylli Herba	ELD	5283387	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)N
MOL001746	0.5898	0.4102	0.6068	Cornus Officinalis Sieb. Et Zucc.	ELD	5283387	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)N
MOL001746	0.5898	0.4102	0.6068	Isatdis Radix	ELD	5283387	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)N
MOL001746	0.5898	0.4102	0.6068	Cinnamomi Ramulus	ELD	5283387	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)N
MOL001746	0.5898	0.4102	0.6068	Evodiae Fructus	ELD	5283387	FALSE	C(C/C=C\CCCCCCCC)CCCCCC(=O)N
MOL001748	0.4755	0.5245	0.6128	Isatdis Radix	methyl (E)-octadec-8-enoate	5364422	FALSE	C(=O)(CCCCCC/C=C/CCCCCCCCC)OC
MOL001748	0.4755	0.5245	0.6128	Alpiniae Officinarum Rhizome	methyl (E)-octadec-8-enoate	5364422	FALSE	C(=O)(CCCCCC/C=C/CCCCCCCCC)OC
MOL001749	0.2777	0.7223	0.6107	Caryophylliflos	ZINC03860434	7057921	FALSE	c1(c(C(=O)OCC(CCCC)CC)cccc1)C(=O)OCC(CCCC)CC
MOL001749	0.2777	0.7223	0.6107	Achyranthis Asperae Herba	ZINC03860434	7057921	FALSE	c1(c(C(=O)OCC(CCCC)CC)cccc1)C(=O)OCC(CCCC)CC
MOL001749	0.2777	0.7223	0.6107	Allii Fistulost Bulbus	ZINC03860434	7057921	FALSE	c1(c(C(=O)OCC(CCCC)CC)cccc1)C(=O)OCC(CCCC)CC
MOL001749	0.2777	0.7223	0.6107	Fritiliariae Irrhosae Bulbus	ZINC03860434	7057921	FALSE	c1(c(C(=O)OCC(CCCC)CC)cccc1)C(=O)OCC(CCCC)CC
MOL001749	0.2777	0.7223	0.6107	Folium Ilicis Cornutae	ZINC03860434	7057921	FALSE	c1(c(C(=O)OCC(CCCC)CC)cccc1)C(=O)OCC(CCCC)CC
MOL001749	0.2777	0.7223	0.6107	Radix Cirsii Japonici	ZINC03860434	7057921	FALSE	c1(c(C(=O)OCC(CCCC)CC)cccc1)C(=O)OCC(CCCC)CC
MOL001749	0.2777	0.7223	0.6107	Momordicae Fructus	ZINC03860434	7057921	FALSE	c1(c(C(=O)OCC(CCCC)CC)cccc1)C(=O)OCC(CCCC)CC
MOL001749	0.2777	0.7223	0.6107	Arecae Semen	ZINC03860434	7057921	FALSE	c1(c(C(=O)OCC(CCCC)CC)cccc1)C(=O)OCC(CCCC)CC
MOL001749	0.2777	0.7223	0.6107	Maydis Seigma	ZINC03860434	7057921	FALSE	c1(c(C(=O)OCC(CCCC)CC)cccc1)C(=O)OCC(CCCC)CC
MOL001749	0.2777	0.7223	0.6107	Ephedrae Radix Et Rhizoma	ZINC03860434	7057921	FALSE	c1(c(C(=O)OCC(CCCC)CC)cccc1)C(=O)OCC(CCCC)CC
MOL001749	0.2777	0.7223	0.6107	Isatdis Radix	ZINC03860434	7057921	FALSE	c1(c(C(=O)OCC(CCCC)CC)cccc1)C(=O)OCC(CCCC)CC
MOL001751	0.8791	0.1209	0.6094	Isatdis Radix	glucobrassicin_qt	25202091	FALSE	S/C(=N/OS(=O)(=O)O)/Cc1c2c([nH]c1)cccc2
MOL001752	0.9472	0.0528	0.9560	Lilii Bulbus	EUG	332	FALSE	c1(cc(ccc1O)C=C)OC
MOL001752	0.9472	0.0528	0.9560	Radix Clematidis	EUG	332	FALSE	c1(cc(ccc1O)C=C)OC
MOL001752	0.9472	0.0528	0.9560	Chuanxiong Rhizoma	EUG	332	FALSE	c1(cc(ccc1O)C=C)OC
MOL001752	0.9472	0.0528	0.9560	Eriobotryae Folium	EUG	332	FALSE	c1(cc(ccc1O)C=C)OC
MOL001752	0.9472	0.0528	0.9560	Campsis Flos	EUG	332	FALSE	c1(cc(ccc1O)C=C)OC
MOL001752	0.9472	0.0528	0.9560	Momordicae Fructus	EUG	332	FALSE	c1(cc(ccc1O)C=C)OC

MOL001752	0.9472	0.0528	0.9560	Caryophylliflos	EUG	332	FALSE	c1(cc(ccc1O)C=C)OC
MOL001752	0.9472	0.0528	0.9560	Meliae Azedarach Fructus	EUG	332	FALSE	c1(cc(ccc1O)C=C)OC
MOL001752	0.9472	0.0528	0.9560	Radix Angelicae Biseratae	EUG	332	FALSE	c1(cc(ccc1O)C=C)OC
MOL001752	0.9472	0.0528	0.9560	Microctis Folium	EUG	332	FALSE	c1(cc(ccc1O)C=C)OC
MOL001752	0.9472	0.0528	0.9560	Lysimachiae Foenigraeci Herba	EUG	332	FALSE	c1(cc(ccc1O)C=C)OC
MOL001752	0.9472	0.0528	0.9560	Paederiae Scandentis Herba	EUG	332	FALSE	c1(cc(ccc1O)C=C)OC
MOL001752	0.9472	0.0528	0.9560	Isatdis Radix	EUG	332	FALSE	c1(cc(ccc1O)C=C)OC
MOL001752	0.9472	0.0528	0.9560	Magnolia Officinalis Rehd Et Wils.	EUG	332	FALSE	c1(cc(ccc1O)C=C)OC
MOL001752	0.9472	0.0528	0.9560	Ginkgo Folium	EUG	332	FALSE	c1(cc(ccc1O)C=C)OC
MOL001752	0.9472	0.0528	0.9560	Lycii Fructus	EUG	332	FALSE	c1(cc(ccc1O)C=C)OC
MOL001752	0.9472	0.0528	0.9560	Lygodii Spora	EUG	332	FALSE	c1(cc(ccc1O)C=C)OC
MOL001752	0.9472	0.0528	0.9560	Evodiae Fructus	EUG	332	FALSE	c1(cc(ccc1O)C=C)OC
MOL001754	0.6575	0.3425	0.7331	Isatdis Radix	2-Methoxy-4-vinylphenol_qt	Not Available	FALSE	c1(c(ccc(c1)CC1COCC1C(O)c1ccc(c(c1)OC)O)O)OC
MOL001756	0.7957	0.2043	0.6575	Isatdis Radix	quindoline	98912	FALSE	n1c2c(cc3ccccc13)[nH]c1c2cccc1
MOL001757	0.8638	0.1362	0.8547	Isatdis Radix	GUN	764	FALSE	c12c(c(=O)[nH]c(n1)N)[nH]cn2
MOL001757	0.8638	0.1362	0.8547	Arum Ternatum Thunb.	GUN	764	FALSE	c12c(c(=O)[nH]c(n1)N)[nH]cn2
MOL001758	0.9422	0.0578	0.9309	Isatdis Radix	Hydroxyterephthalic acid	97257	FALSE	c1(c(cc(cc1)C(=O)O)O)C(=O)O
MOL001759	0.9330	0.0670	0.7996	Isatdis Radix	Methyl indole-3-carboxylate	589098	FALSE	c1cc2c(cc1)[nH]cc2C(=O)OC
MOL001760	0.8286	0.1714	0.7204	Lepidii Semen Descurainiae Semen	Myronate	6911854	FALSE	C1(OC(C(C(C1O)O)O)O)CO)S/C(=N/OS(=O)(=O)O)/CC=C
MOL001760	0.8286	0.1714	0.7204	Sinapis Semen	Myronate	6911854	FALSE	C1(OC(C(C(C1O)O)O)O)CO)S/C(=N/OS(=O)(=O)O)/CC=C
MOL001760	0.8286	0.1714	0.7204	Isatdis Radix	Myronate	6911854	FALSE	C1(OC(C(C(C1O)O)O)O)CO)S/C(=N/OS(=O)(=O)O)/CC=C
MOL001761	0.7801	0.2199	0.7989	Isatdis Radix	sinigrin	45479598	FALSE	S/C(=N/OS(=O)(=O)O)/CC=C
MOL001761	0.7801	0.2199	0.7989	Sinapis Semen	sinigrin	45479598	FALSE	S/C(=N/OS(=O)(=O)O)/CC=C
MOL001762	0.8822	0.1178	0.8492	Isatdis Radix	3-Formylindole	10256	FALSE	c1cc2c(cc1)[nH]cc2C=O
MOL001763	0.9218	0.0782	0.8072	Isatdis Radix	3-(2-hydroxyphenyl)quinazolin-4-one	611001	FALSE	n1cn(c(=O)c2ccccc12)c1c(cccc1)O
MOL001764	0.8990	0.1010	0.8832	Dichroae Radix	4-Quinazolone	63112	FALSE	n1c[nH]c(=O)c2ccccc12
MOL001764	0.8990	0.1010	0.8832	Isatidis Folium	4-Quinazolone	63112	FALSE	n1c[nH]c(=O)c2ccccc12
MOL001764	0.8990	0.1010	0.8832	Isatdis Radix	4-Quinazolone	63112	FALSE	n1c[nH]c(=O)c2ccccc12

MOL001765	0.9483	0.0517	0.8156	Isatdis Radix	2-(1-methoxyindol-3-yl)acetonitrile	11954881	FALSE	c1cc2c(cc1)n(cc2CC#N)OC
MOL001766	0.9272	0.0728	0.8613	Isatidis Folium	5-hydroxyoxindole	76955	FALSE	c1cc2c(cc1O)CC(=O)N2
MOL001766	0.9272	0.0728	0.8613	Isatdis Radix	5-hydroxyoxindole	76955	FALSE	c1cc2c(cc1O)CC(=O)N2
MOL001767	0.8753	0.1247	0.6096	Isatdis Radix	hydroxyindirubin	Not Available	FALSE	C\1(=C/2\Nc3c(C2=O)ccc(c3)O)/c2c(NC1=O)cccc2
MOL001768	0.9111	0.0889	0.9557	Rehmanniae Radix Praeparata	Sumiki's acid	80642	FALSE	o1c(ccc1CO)C(=O)O
MOL001768	0.9111	0.0889	0.9557	Isatdis Radix	Sumiki's acid	80642	FALSE	o1c(ccc1CO)C(=O)O
MOL001768	0.9111	0.0889	0.9557	Momordicae Fructus	Sumiki's acid	80642	FALSE	o1c(ccc1CO)C(=O)O
MOL001772	0.9194	0.0806	0.8939	Smilacis Glabrae Rhixoma	Dihydro-beta-ionone	519382	FALSE	O=C(CCC1=C(CCCC1(C)C)C)C
MOL001772	0.9194	0.0806	0.8939	Isatdis Radix	Dihydro-beta-ionone	519382	FALSE	O=C(CCC1=C(CCCC1(C)C)C)C
MOL001772	0.9194	0.0806	0.8939	Ephedra Herba	Dihydro-beta-ionone	519382	FALSE	O=C(CCC1=C(CCCC1(C)C)C)C
MOL001772	0.9194	0.0806	0.8939	Rehmanniae Radix Praeparata	Dihydro-beta-ionone	519382	FALSE	O=C(CCC1=C(CCCC1(C)C)C)C
MOL001773	0.8894	0.1106	0.8234	Lonicerae Japonicae Flos	indole	798	FALSE	[nH]1c2c(cc1)cccc2
MOL001773	0.8894	0.1106	0.8234	Eriobotryae Folium	indole	798	FALSE	[nH]1c2c(cc1)cccc2
MOL001773	0.8894	0.1106	0.8234	Morindae Officinalis Radix	indole	798	FALSE	[nH]1c2c(cc1)cccc2
MOL001773	0.8894	0.1106	0.8234	Bombyx Mori L.	indole	798	FALSE	[nH]1c2c(cc1)cccc2
MOL001773	0.8894	0.1106	0.8234	Momordicae Fructus	indole	798	FALSE	[nH]1c2c(cc1)cccc2
MOL001773	0.8894	0.1106	0.8234	Isatdis Radix	indole	798	FALSE	[nH]1c2c(cc1)cccc2
MOL001773	0.8894	0.1106	0.8234	Dalbergiae Odoriferae Lignum	indole	798	FALSE	[nH]1c2c(cc1)cccc2
MOL001774	0.2410	0.7590	0.7758	Isatdis Radix	Ineketone	188456	FALSE	OC12C(C3(C(O)CC(C=C3C(=O)C2)(C)C=C)C)CCCC1(C)C
MOL001775	0.8243	0.1757	0.7764	Isatdis Radix	Isoacolamone	71587143	FALSE	C1C=C(C2C(C1)(CCC(C2=O)C(C)C)C)C
MOL001776	0.8722	0.1278	0.6915	Isatdis Radix	Kingiside	Not Available	FALSE	C1(=O)OC(C2C(C1)C(=COC2OC1OC(C(C(C1O)O)O)CO)OC(=O)C)C
MOL001777	0.9174	0.0826	0.7760	Isatdis Radix	Kingiside_qt	Not Available	FALSE	C1(=O)OC(C2C(C1)C(=COC2O)OC(=O)C)C
MOL001778	0.9256	0.0744	0.9133	Isatdis Radix	Sinapaldehyde	5280802	FALSE	O(c1c(O)c(OC)cc(c1)/C=C/C=O)C
MOL001778	0.9256	0.0744	0.9133	Lepidii Semen Descurainiae Semen	Sinapaldehyde	5280802	FALSE	O(c1c(O)c(OC)cc(c1)/C=C/C=O)C
MOL001778	0.9256	0.0744	0.9133	Fraxini Cortex	Sinapaldehyde	5280802	FALSE	O(c1c(O)c(OC)cc(c1)/C=C/C=O)C
MOL001779	0.6338	0.3662	0.7751	Isatdis Radix	Sinoacutine	Not Available	FALSE	OC12C34C(=CC(=O)C(=C4)OC)C(N(CC3)C)CC2CC1OC

MOL001780	0.9508	0.0492	0.9234	Isatidis Folium	WV	6923516	TRUE	c12c(CC(C(=O)O)N)c[nH]c1cccc2
MOL001780	0.9508	0.0492	0.9234	Allium Azureum Ledeb.	WV	6923516	TRUE	c12c(CC(C(=O)O)N)c[nH]c1cccc2
MOL001780	0.9508	0.0492	0.9234	Isatdis Radix	WV	6923516	TRUE	c12c(CC(C(=O)O)N)c[nH]c1cccc2
MOL001780	0.9508	0.0492	0.9234	Evodiae Fructus	WV	6923516	TRUE	c12c(CC(C(=O)O)N)c[nH]c1cccc2
MOL001781	0.7584	0.2416	0.7576	Polygoni Tinctorii Foliu	Indigo	5318432	FALSE	C\1(=C/2\C(=O)c3c(N2)cccc3)/C(=O)c2c(N1)cccc2
MOL001781	0.7584	0.2416	0.7576	Isatidis Folium	Indigo	5318432	FALSE	C\1(=C/2\C(=O)c3c(N2)cccc3)/C(=O)c2c(N1)cccc2
MOL001781	0.7584	0.2416	0.7576	Indigo Naturalis	Indigo	5318432	FALSE	C\1(=C/2\C(=O)c3c(N2)cccc3)/C(=O)c2c(N1)cccc2
MOL001781	0.7584	0.2416	0.7576	Isatdis Radix	Indigo	5318432	FALSE	C\1(=C/2\C(=O)c3c(N2)cccc3)/C(=O)c2c(N1)cccc2
MOL001782	0.8181	0.1819	0.7480	Isatdis Radix	(2Z)-2-(2-oxoindolin-3-ylidene)indolin-3-one	5318433	FALSE	C\1(=C/2\Nc3c(C2=O)cccc3)/c2c(NC1=O)cccc2
MOL001782	0.8181	0.1819	0.7480	Polygoni Tinctorii Foliu	(2Z)-2-(2-oxoindolin-3-ylidene)indolin-3-one	5318433	FALSE	C\1(=C/2\Nc3c(C2=O)cccc3)/c2c(NC1=O)cccc2
MOL001784	0.9273	0.0727	0.9245	Isatdis Radix	1-thiocyanato-2-hydroxy-3-butene	Not Available	FALSE	C(C(C=C)O)SC#N
MOL001785	0.9049	0.0951	0.8563	Polygoni Tinctorii Foliu	ISN	7054	FALSE	N1C(=O)C(=O)c2ccccc12
MOL001785	0.9049	0.0951	0.8563	Indigo Naturalis	ISN	7054	FALSE	N1C(=O)C(=O)c2ccccc12
MOL001785	0.9049	0.0951	0.8563	Isatdis Radix	ISN	7054	FALSE	N1C(=O)C(=O)c2ccccc12
MOL001786	0.6905	0.3095	0.7091	Isatdis Radix	(+)-isolariciresinol	12311071	FALSE	OCC1C(Cc2c(C1c1cc(OC)c(O)cc1)cc(O)c(OC)c2)CO
MOL001787	0.9273	0.0727	0.9000	Lobeliae Chinensis Herba	ADO	60961	FALSE	OCC1C(O)C(O)C(O1)n1cnc2c(N)ncnc12
MOL001787	0.9273	0.0727	0.9000	Hordei Fructus Germinatus	ADO	60961	FALSE	OCC1C(O)C(O)C(O1)n1cnc2c(N)ncnc12
MOL001787	0.9273	0.0727	0.9000	Carthami Flos	ADO	60961	FALSE	OCC1C(O)C(O)C(O1)n1cnc2c(N)ncnc12
MOL001787	0.9273	0.0727	0.9000	Commelinae Herba	ADO	60961	FALSE	OCC1C(O)C(O)C(O1)n1cnc2c(N)ncnc12
MOL001787	0.9273	0.0727	0.9000	Bolbostemae Paniculati Bulbus	ADO	60961	FALSE	OCC1C(O)C(O)C(O1)n1cnc2c(N)ncnc12
MOL001787	0.9273	0.0727	0.9000	Solanum Nigrum Linn.	ADO	60961	FALSE	OCC1C(O)C(O)C(O1)n1cnc2c(N)ncnc12
MOL001787	0.9273	0.0727	0.9000	Saposhnikoviae Radix	ADO	60961	FALSE	OCC1C(O)C(O)C(O1)n1cnc2c(N)ncnc12
MOL001787	0.9273	0.0727	0.9000	Chuanxiong Rhizoma	ADO	60961	FALSE	OCC1C(O)C(O)C(O1)n1cnc2c(N)ncnc12
MOL001787	0.9273	0.0727	0.9000	Lasiosphaera Seu Calvatia	ADO	60961	FALSE	OCC1C(O)C(O)C(O1)n1cnc2c(N)ncnc12
MOL001787	0.9273	0.0727	0.9000	Isatdis Radix	ADO	60961	FALSE	OCC1C(O)C(O)C(O1)n1cnc2c(N)ncnc12
MOL001787	0.9273	0.0727	0.9000	Allium Azureum Ledeb.	ADO	60961	FALSE	OCC1C(O)C(O)C(O1)n1cnc2c(N)ncnc12
MOL001787	0.9273	0.0727	0.9000	Abri Herba	ADO	60961	FALSE	OCC1C(O)C(O)C(O1)n1cnc2c(N)ncnc12
MOL001787	0.9273	0.0727	0.9000	Fritiliariae Irrhosae Bulbus	ADO	60961	FALSE	OCC1C(O)C(O)C(O1)n1cnc2c(N)ncnc12
MOL001787	0.9273	0.0727	0.9000	Farfarae Flos	ADO	60961	FALSE	OCC1C(O)C(O)C(O1)n1cnc2c(N)ncnc12
MOL001787	0.9273	0.0727	0.9000	Folium Ilicis Cornutae	ADO	60961	FALSE	OCC1C(O)C(O)C(O1)n1cnc2c(N)ncnc12
MOL001787	0.9273	0.0727	0.9000	Ampelopsis Japonica	ADO	60961	FALSE	OCC1C(O)C(O)C(O1)n1cnc2c(N)ncnc12

MOL001787	0.9273	0.0727	0.9000	Fritillariaeussuriensis Bulbus	ADO	60961	FALSE	OCC1C(O)C(O)C(O1)n1cnc2c(N)ncnc12
MOL001788	0.8328	0.1672	0.8309	Abri Herba	adenine	190	FALSE	[nH]1cnc2c(N)ncnc12
MOL001788	0.8328	0.1672	0.8309	Corayceps	adenine	190	FALSE	[nH]1cnc2c(N)ncnc12
MOL001788	0.8328	0.1672	0.8309	Arum Ternatum Thunb.	adenine	190	FALSE	[nH]1cnc2c(N)ncnc12
MOL001788	0.8328	0.1672	0.8309	Carthami Flos	adenine	190	FALSE	[nH]1cnc2c(N)ncnc12
MOL001788	0.8328	0.1672	0.8309	Hordei Fructus Germinatus	adenine	190	FALSE	[nH]1cnc2c(N)ncnc12
MOL001788	0.8328	0.1672	0.8309	Chuanxiong Rhizoma	adenine	190	FALSE	[nH]1cnc2c(N)ncnc12
MOL001788	0.8328	0.1672	0.8309	Lobeliae Chinensis Herba	adenine	190	FALSE	[nH]1cnc2c(N)ncnc12
MOL001788	0.8328	0.1672	0.8309	Isatdis Radix	adenine	190	FALSE	[nH]1cnc2c(N)ncnc12
MOL001788	0.8328	0.1672	0.8309	Angelicae Sinensis Radix	adenine	190	FALSE	[nH]1cnc2c(N)ncnc12
MOL001789	0.9030	0.0970	0.8088	Sedi Herba	isoliquiritigenin	638278	FALSE	c1(C(=O)/C=C/c2ccc(cc2)O)c(cc(cc1)O)O
MOL001789	0.9030	0.0970	0.8088	Polygonati Rhizoma	isoliquiritigenin	638278	FALSE	c1(C(=O)/C=C/c2ccc(cc2)O)c(cc(cc1)O)O
MOL001789	0.9030	0.0970	0.8088	Radix Bupleuri	isoliquiritigenin	638278	FALSE	c1(C(=O)/C=C/c2ccc(cc2)O)c(cc(cc1)O)O
MOL001789	0.9030	0.0970	0.8088	Allium Azureum Ledeb.	isoliquiritigenin	638278	FALSE	c1(C(=O)/C=C/c2ccc(cc2)O)c(cc(cc1)O)O
MOL001789	0.9030	0.0970	0.8088	Myristicae Semen	isoliquiritigenin	638278	FALSE	c1(C(=O)/C=C/c2ccc(cc2)O)c(cc(cc1)O)O
MOL001789	0.9030	0.0970	0.8088	licorice	isoliquiritigenin	638278	FALSE	c1(C(=O)/C=C/c2ccc(cc2)O)c(cc(cc1)O)O
MOL001789	0.9030	0.0970	0.8088	Isatdis Radix	isoliquiritigenin	638278	FALSE	c1(C(=O)/C=C/c2ccc(cc2)O)c(cc(cc1)O)O
MOL001789	0.9030	0.0970	0.8088	Epimrdii Herba	isoliquiritigenin	638278	FALSE	c1(C(=O)/C=C/c2ccc(cc2)O)c(cc(cc1)O)O
MOL001790	0.7934	0.2066	0.8315	Lobeliae Chinensis Herba	Linarin	5317025	FALSE	c12c(oc(cc1=O)c1ccc(cc1)OC)cc(cc2O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL001790	0.7934	0.2066	0.8315	Ecliptae Herba	Linarin	5317025	FALSE	c12c(oc(cc1=O)c1ccc(cc1)OC)cc(cc2O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL001790	0.7934	0.2066	0.8315	Lygodii Spora	Linarin	5317025	FALSE	c12c(oc(cc1=O)c1ccc(cc1)OC)cc(cc2O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL001790	0.7934	0.2066	0.8315	Lysimachiae Herba	Linarin	5317025	FALSE	c12c(oc(cc1=O)c1ccc(cc1)OC)cc(cc2O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL001790	0.7934	0.2066	0.8315	Glechomae Herba	Linarin	5317025	FALSE	c12c(oc(cc1=O)c1ccc(cc1)OC)cc(cc2O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL001790	0.7934	0.2066	0.8315	Paederiae Scandentis Herba	Linarin	5317025	FALSE	c12c(oc(cc1=O)c1ccc(cc1)OC)cc(cc2O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL001790	0.7934	0.2066	0.8315	Lycii Cortex	Linarin	5317025	FALSE	c12c(oc(cc1=O)c1ccc(cc1)OC)cc(cc2O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL001790	0.7934	0.2066	0.8315	Pseudostellariae Radix	Linarin	5317025	FALSE	c12c(oc(cc1=O)c1ccc(cc1)OC)cc(cc2O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O

MOL001790	0.7934	0.2066	0.8315	Herba Patriniae	Linarin	5317025	FALSE	c12c(oc(cc1=O)c1ccc(cc1)OC)cc(cc2O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL001790	0.7934	0.2066	0.8315	Herba Cirsii	Linarin	5317025	FALSE	c12c(oc(cc1=O)c1ccc(cc1)OC)cc(cc2O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL001790	0.7934	0.2066	0.8315	Menthae Herba	Linarin	5317025	FALSE	c12c(oc(cc1=O)c1ccc(cc1)OC)cc(cc2O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL001790	0.7934	0.2066	0.8315	Chrysanthemi Indici Flos	Linarin	5317025	FALSE	c12c(oc(cc1=O)c1ccc(cc1)OC)cc(cc2O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL001790	0.7934	0.2066	0.8315	Isatdis Radix	Linarin	5317025	FALSE	c12c(oc(cc1=O)c1ccc(cc1)OC)cc(cc2O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL001790	0.7934	0.2066	0.8315	Chrysanthemi Flos	Linarin	5317025	FALSE	c12c(oc(cc1=O)c1ccc(cc1)OC)cc(cc2O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL001790	0.7934	0.2066	0.8315	Buddlejae Flos	Linarin	5317025	FALSE	c12c(oc(cc1=O)c1ccc(cc1)OC)cc(cc2O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL001791	0.9424	0.0576	0.8350	Isatdis Radix	2,3-dihydro-4-hydroxy-2-oxo-indole-3-acetonitrile	60156058	FALSE	c1cc(c2c(c1)NC(=O)C2CC#N)O
MOL001792	0.9203	0.0797	0.7746	Isatdis Radix	DFV	114829	FALSE	C1(CC(=O)c2c(O1)cc(cc2)O)c1ccc(cc1)O
MOL001792	0.9203	0.0797	0.7746	Polygonati Rhizoma	DFV	114829	FALSE	C1(CC(=O)c2c(O1)cc(cc2)O)c1ccc(cc1)O
MOL001792	0.9203	0.0797	0.7746	licorice	DFV	114829	FALSE	C1(CC(=O)c2c(O1)cc(cc2)O)c1ccc(cc1)O
MOL001792	0.9203	0.0797	0.7746	Epimrdii Herba	DFV	114829	FALSE	C1(CC(=O)c2c(O1)cc(cc2)O)c1ccc(cc1)O
MOL001792	0.9203	0.0797	0.7746	Dalbergiae Odoriferae Lignum	DFV	114829	FALSE	C1(CC(=O)c2c(O1)cc(cc2)O)c1ccc(cc1)O
MOL001792	0.9203	0.0797	0.7746	Hedysari Radix	DFV	114829	FALSE	C1(CC(=O)c2c(O1)cc(cc2)O)c1ccc(cc1)O
MOL001792	0.9203	0.0797	0.7746	Sedi Herba	DFV	114829	FALSE	C1(CC(=O)c2c(O1)cc(cc2)O)c1ccc(cc1)O
MOL001792	0.9203	0.0797	0.7746	Rhapontici Radix	DFV	114829	FALSE	C1(CC(=O)c2c(O1)cc(cc2)O)c1ccc(cc1)O
MOL001792	0.9203	0.0797	0.7746	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	DFV	114829	FALSE	C1(CC(=O)c2c(O1)cc(cc2)O)c1ccc(cc1)O
MOL001794	0.9023	0.0977	0.9675	Isatidis Folium	MAE	444266	FALSE	C(=O)(/C=C\C(=O)O)O
MOL001794	0.9023	0.0977	0.9675	Eucommiae Cortex	MAE	444266	FALSE	C(=O)(/C=C\C(=O)O)O
MOL001794	0.9023	0.0977	0.9675	Isatdis Radix	MAE	444266	FALSE	C(=O)(/C=C\C(=O)O)O
MOL001794	0.9023	0.0977	0.9675	Mahoniae Caulis	MAE	444266	FALSE	C(=O)(/C=C\C(=O)O)O
MOL001794	0.9023	0.0977	0.9675	Radix Rhei Et Rhizome	MAE	444266	FALSE	C(=O)(/C=C\C(=O)O)O
MOL001794	0.9023	0.0977	0.9675	Glechomae Herba	MAE	444266	FALSE	C(=O)(/C=C\C(=O)O)O

MOL001797	0.8490	0.1510	0.8596	Citrus Aurantium	(2S)-7-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-6-methylol-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-tetrahydropyran-2-yl]oxy-5-hydroxy-2-(3-hydroxy-5-methoxy-phenyl)chroman-4-one	24721685	FALSE	c12c(C(=O)CC(O1)c1cc(cc(c1)O)OC)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL001797	0.8490	0.1510	0.8596	Citri Grandis Exocarpium	(2S)-7-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-6-methylol-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-tetrahydropyran-2-yl]oxy-5-hydroxy-2-(3-hydroxy-5-methoxy-phenyl)chroman-4-one	24721685	FALSE	c12c(C(=O)CC(O1)c1cc(cc(c1)O)OC)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O

MOL001797	0.8490	0.1510	0.8596	Citri Exocarpium Rubrum	(2S)-7-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-6-methylol-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-tetrahydropyran-2-yl]oxy-5-hydroxy-2-(3-hydroxy-5-methoxy-phenyl)chroman-4-one	24721685	FALSE	c12c(C(=O)CC(O1)c1cc(cc(c1)O)OC)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL001797	0.8490	0.1510	0.8596	Citrus Reticulata	(2S)-7-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-6-methylol-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-tetrahydropyran-2-yl]oxy-5-hydroxy-2-(3-hydroxy-5-methoxy-phenyl)chroman-4-one	24721685	FALSE	c12c(C(=O)CC(O1)c1cc(cc(c1)O)OC)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O

MOL001797	0.8490	0.1510	0.8596	Aurantii Fructus Immaturus	(2S)-7-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-6-methylol-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-tetrahydropyran-2-yl]oxy-5-hydroxy-2-(3-hydroxy-5-methoxy-phenyl)chroman-4-one	24721685	FALSE	c12c(C(=O)CC(O1)c1cc(cc(c1)O)OC)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL001797	0.8490	0.1510	0.8596	Isatdis Radix	(2S)-7-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-6-methylol-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-tetrahydropyran-2-yl]oxy-5-hydroxy-2-(3-hydroxy-5-methoxy-phenyl)chroman-4-one	24721685	FALSE	c12c(C(=O)CC(O1)c1cc(cc(c1)O)OC)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O

MOL001797	0.8490	0.1510	0.8596	Citri Reticulatae Pericarpium Viride	(2S)-7-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-6-methylol-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-tetrahydropyran-2-yl]oxy-5-hydroxy-2-(3-hydroxy-5-methoxy-phenyl)chroman-4-one	24721685	FALSE	c12c(C(=O)CC(O1)c1cc(cc(c1)O)OC)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL001798	0.9099	0.0901	0.8942	Citri Grandis Exocarpium	neohesperidin_qt	42607889	FALSE	c12c(C(=O)CC(O1)c1cc(cc(c1)O)OC)c(cc(c2)O)O
MOL001798	0.9099	0.0901	0.8942	Isatdis Radix	neohesperidin_qt	42607889	FALSE	c12c(C(=O)CC(O1)c1cc(cc(c1)O)OC)c(cc(c2)O)O
MOL001798	0.9099	0.0901	0.8942	Citrus Aurantium	neohesperidin_qt	42607889	FALSE	c12c(C(=O)CC(O1)c1cc(cc(c1)O)OC)c(cc(c2)O)O
MOL001798	0.9099	0.0901	0.8942	Aurantii Fructus Immaturus	neohesperidin_qt	42607889	FALSE	c12c(C(=O)CC(O1)c1cc(cc(c1)O)OC)c(cc(c2)O)O
MOL001798	0.9099	0.0901	0.8942	Citri Exocarpium Rubrum	neohesperidin_qt	42607889	FALSE	c12c(C(=O)CC(O1)c1cc(cc(c1)O)OC)c(cc(c2)O)O
MOL001798	0.9099	0.0901	0.8942	Citri Reticulatae Pericarpium Viride	neohesperidin_qt	42607889	FALSE	c12c(C(=O)CC(O1)c1cc(cc(c1)O)OC)c(cc(c2)O)O
MOL001799	0.2267	0.7733	0.7806	Isatdis Radix	Pyropheophorbide α Methyl Ester	Not Available	FALSE	c12=C3C4=N/C(=C\c5[nH]c(/C=C/6\N=C(/C=c(\[nH]2)/c(c1C(=O)C3)C)C(=C6C)CC)c(c5C)C=C)/C(C4CCC(=O)OC)C
MOL001801	0.9310	0.0690	0.9606	Isatdis Radix	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Celastri Orbiculati Fructus	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Cyperi Rhizoma	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Artemisia Annua L.	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Paeoniae Radix Alba	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Choerospondiatis Fructus	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Bomboo Juice	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Gentianae Radix Et Rhozima	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Citrus Aurantium	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O

MOL001801	0.9310	0.0690	0.9606	Carthami Flos	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Canarii Fructus	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Asteris Radix Et Rhizoma	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Solidaginis Herba	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Bidentis Bipinnatae Herba	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Radix Paeoniae Rubra	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Calendula Officinalis	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Artemisiae Scopariae Herba	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Folium Nelumbinis	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Herba Clematidis Aethusaefoliae	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Anisi Stellati Fructus	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Plantaginis Herba	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Isatidis Folium	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Inulae Herba	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Polygonati Rhizoma	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001801	0.9310	0.0690	0.9606	Glehniae Radix	salicylic acid	338	FALSE	C(=O)(c1c(O)cccc1)O
MOL001802	0.8987	0.1013	0.8390	Isatdis Radix	Benzouracil	64048	FALSE	c1(=O)[nH]c(=O)c2ccccc2[nH]1
MOL001802	0.8987	0.1013	0.8390	Isatidis Folium	Benzouracil	64048	FALSE	c1(=O)[nH]c(=O)c2ccccc2[nH]1
MOL001803	0.7053	0.2947	0.9658	Isatdis Radix	Sinensetin	145659	TRUE	c12c(c(c(cc1oc(cc2=O)c1cc(c(cc1)OC)OC)OC)OC)O C
MOL001803	0.7053	0.2947	0.9658	Citri Grandis Exocarpium	Sinensetin	145659	TRUE	c12c(c(c(cc1oc(cc2=O)c1cc(c(cc1)OC)OC)OC)OC)O C
MOL001803	0.7053	0.2947	0.9658	Aurantii Fructus Immaturus	Sinensetin	145659	TRUE	c12c(c(c(cc1oc(cc2=O)c1cc(c(cc1)OC)OC)OC)OC)O C
MOL001803	0.7053	0.2947	0.9658	Citri Reticulatae Pericarpium Viride	Sinensetin	145659	TRUE	c12c(c(c(cc1oc(cc2=O)c1cc(c(cc1)OC)OC)OC)OC)O C
MOL001804	0.2561	0.7439	0.6673	Isatdis Radix	Stigmasta-5,22-diene-3beta,7alpha-diol	Not Available	FALSE	C1(CCC2(C(=CC(C3C4CCC(C(/C=C\CC(CC)C(C)C)C)C4(C)CCC23)C)C1)C)O
MOL001805	0.9415	0.0585	0.7838	Isatdis Radix	1-methoxyindole-3-carbaldehyde	398554	FALSE	c1cc2c(cc1)n(cc2C=O)OC
MOL001806	0.2745	0.7255	0.6618	Isatdis Radix	Stigmasta-5,22-diene-3beta,7beta-diol	Not Available	FALSE	C1(CCC2(C(=CC(C3C4CCC(C(/C=C\CC(CC)C(C)C)C)C4(C)CCC23)CC)C1)C)O
MOL001807	0.9265	0.0735	0.9278	Sedi Herba	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Coriolus	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Lepidii Semen Descurainiae Semen	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Inulae Herba	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O

MOL001807	0.9265	0.0735	0.9278	Viticis Cannabifoliae Fructus	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Rhizoma Fagopyri Cymosi	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Stemonae Radix	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Uncariae Ramulus Cumuncis	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Polygoni Orientalis Fructus	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Smilacis Glabrae Rhixoma	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Radix Cynanchi	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Plantaginis Herba	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Cotyledon Fimbriata Turcz.	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Herba Sarcandrae	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Isatdis Radix	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Sargentodoxae Caulis	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Zanthoxylum Nitidum	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Toosendan Fructus	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Isatidis Folium	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Herba Selaginellae Moellendorfii	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Tripterygii Radix	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Rhododendri Daurici Folium	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Hordei Fructus Germinatus	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Aristolochiae Fructus	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Kaki Calyx	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001807	0.9265	0.0735	0.9278	Curcumae Radix	Cedar acid	10742	FALSE	C(=O)(c1cc(c(O)c(OC)c1)OC)O
MOL001810	0.5240	0.4760	0.6906	Isatdis Radix	6-(3-oxoindolin-2-ylidene)indolo[2,1-b]quinazolin-12-one	3035728	FALSE	O=c1n2c(nc3c1cccc3)/c(=C\1/Nc3c(C1=O)cccc3)/c1c2cccc1
MOL001810	0.5240	0.4760	0.6906	Indigo Naturalis	6-(3-oxoindolin-2-ylidene)indolo[2,1-b]quinazolin-12-one	3035728	FALSE	O=c1n2c(nc3c1cccc3)/c(=C\1/Nc3c(C1=O)cccc3)/c1c2cccc1

MOL001810	0.5240	0.4760	0.6906	Isatidis Folium	6-(3-oxoindolin-2-ylidene)indolo[2,1-b]quinazolin-12-one	3035728	FALSE	O=c1n2c(nc3c1cccc3)/c(=C\1/Nc3c(C1=O)cccc3)/c1c2cccc1
MOL001811	0.9112	0.0888	0.9767	Isatdis Radix	VTO	3032313	FALSE	C1(OC(=S)NC1)C=C
MOL001812	0.9083	0.0917	0.8426	Isatdis Radix	2,5-dihydroxy-indole	45082883	FALSE	c1(O)cc2c(cc1)[nH]c(c2)O
MOL001814	0.8684	0.1316	0.8737	Isatdis Radix	(E)-3-(3,5-dimethoxy-4-hydroxy-benzylidene)-2-indolinone	Not Available	FALSE	c1cc2c(cc1)/C(=C(\c1cc(cc(c1)OC)OC)/O)/C(=O)N2
MOL001816	0.7692	0.2308	0.6569	Cucurbitae Moschatae Semen	Amide HPL	69421	FALSE	C(CCCCCCCCCC)CCCCC(=O)N
MOL001816	0.7692	0.2308	0.6569	Evodiae Fructus	Amide HPL	69421	FALSE	C(CCCCCCCCCC)CCCCC(=O)N
MOL001816	0.7692	0.2308	0.6569	Cornus Officinalis Sieb. Et Zucc.	Amide HPL	69421	FALSE	C(CCCCCCCCCC)CCCCC(=O)N
MOL001816	0.7692	0.2308	0.6569	Arum Ternatum Thunb.	Amide HPL	69421	FALSE	C(CCCCCCCCCC)CCCCC(=O)N
MOL001816	0.7692	0.2308	0.6569	Isatdis Radix	Amide HPL	69421	FALSE	C(CCCCCCCCCC)CCCCC(=O)N
MOL001818	0.6603	0.3397	0.6582	Hippophae Fructus	Methyl palmitelaidate	638303	FALSE	C(=O)(CCCCCCC/C=C/CCCCCC)OC
MOL001818	0.6603	0.3397	0.6582	Isatdis Radix	Methyl palmitelaidate	638303	FALSE	C(=O)(CCCCCCC/C=C/CCCCCC)OC
MOL001818	0.6603	0.3397	0.6582	Sapindi Mukorossi Semen	Methyl palmitelaidate	638303	FALSE	C(=O)(CCCCCCC/C=C/CCCCCC)OC
MOL001818	0.6603	0.3397	0.6582	Arum Ternatum Thunb.	Methyl palmitelaidate	638303	FALSE	C(=O)(CCCCCCC/C=C/CCCCCC)OC
MOL001818	0.6603	0.3397	0.6582	Panax Ginseng C. A. Mey.	Methyl palmitelaidate	638303	FALSE	C(=O)(CCCCCCC/C=C/CCCCCC)OC
MOL001819	0.7552	0.2448	0.6750	Hoveniae Dulcis Semen	METHYL PENTADECANOATE	23518	FALSE	C(CCCCCCCCCCC)CCC(=O)OC
MOL001819	0.7552	0.2448	0.6750	Perillae Fructus	METHYL PENTADECANOATE	23518	FALSE	C(CCCCCCCCCCC)CCC(=O)OC
MOL001819	0.7552	0.2448	0.6750	Isatdis Radix	METHYL PENTADECANOATE	23518	FALSE	C(CCCCCCCCCCC)CCC(=O)OC

MOL001819	0.7552	0.2448	0.6750	Radix Bupleuri	METHYL PENTADECANOATE	23518	FALSE	C(CCCCCCCCCCC)CCC(=O)OC
MOL001819	0.7552	0.2448	0.6750	Panax Ginseng C. A. Mey.	METHYL PENTADECANOATE	23518	FALSE	C(CCCCCCCCCCC)CCC(=O)OC
MOL001819	0.7552	0.2448	0.6750	Evodiae Fructus	METHYL PENTADECANOATE	23518	FALSE	C(CCCCCCCCCCC)CCC(=O)OC
MOL001819	0.7552	0.2448	0.6750	Codonopsis Radix	METHYL PENTADECANOATE	23518	FALSE	C(CCCCCCCCCCC)CCC(=O)OC
MOL001819	0.7552	0.2448	0.6750	Arisaematis Rhizoma	METHYL PENTADECANOATE	23518	FALSE	C(CCCCCCCCCCC)CCC(=O)OC
MOL001819	0.7552	0.2448	0.6750	Gossampiniflos	METHYL PENTADECANOATE	23518	FALSE	C(CCCCCCCCCCC)CCC(=O)OC
MOL001819	0.7552	0.2448	0.6750	Impatientis Semen	METHYL PENTADECANOATE	23518	FALSE	C(CCCCCCCCCCC)CCC(=O)OC
MOL001819	0.7552	0.2448	0.6750	Sojae Semen Nigrum	METHYL PENTADECANOATE	23518	FALSE	C(CCCCCCCCCCC)CCC(=O)OC
MOL001819	0.7552	0.2448	0.6750	Hedysari Radix	METHYL PENTADECANOATE	23518	FALSE	C(CCCCCCCCCCC)CCC(=O)OC
MOL001819	0.7552	0.2448	0.6750	Chuanxiong Rhizoma	METHYL PENTADECANOATE	23518	FALSE	C(CCCCCCCCCCC)CCC(=O)OC
MOL001819	0.7552	0.2448	0.6750	Broussonetiae Fructus	METHYL PENTADECANOATE	23518	FALSE	C(CCCCCCCCCCC)CCC(=O)OC
MOL001820	0.8490	0.1510	0.6395	Isatdis Radix	(E)-3-(3,5-dimethoxy-4-hydroxyb-enzylidene)-2-indolinone	Not Available	FALSE	c1cc2c(cc1)C(C(=O)N2)c1cc(c(c(c1)OC)CO)OC
MOL001821	0.8127	0.1873	0.9265	Isatdis Radix	Methyl 2-ethylhexyl phthalate	Not Available	FALSE	O(CC(CCCC)CC)C(=O)c1c(cccc1)C(=O)OC

MOL001822	0.9170	0.0830	0.9242	Isatdis Radix	5-(methoxymethyl)-2-furoic acid	1125227	FALSE	c1(oc(cc1)COC)C(=O)O
MOL001823	0.9206	0.0794	0.8045	Isatdis Radix	isatan B	Not Available	FALSE	O1C(C(O)C(=O)C(O)C1Oc1c2c([nH]c1)cccc2)CO
MOL001824	0.9436	0.0564	0.7627	Isatdis Radix	Indole-3-acetonitrile-6-O-beta-D-glucopyranoside	5318434	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2[nH]cc(c2cc1)CC#N)CO
MOL001825	0.9288	0.0712	0.8859	Isatdis Radix	indole-3-acetonitrile-6-o-β-D-glucopyranoside_qt	Not Available	FALSE	Oc1cc2[nH]cc(c2cc1)CC#N
MOL001826	0.9219	0.0781	0.8199	Isatdis Radix	Indican, plant	441564	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c([nH]c1)cccc2)CO
MOL001827	0.9033	0.0967	0.8187	Isatdis Radix	Indoxyl	50591	FALSE	Oc1c2c([nH]c1)cccc2
MOL001827	0.9033	0.0967	0.8187	Indigo Naturalis	Indoxyl	50591	FALSE	Oc1c2c([nH]c1)cccc2
MOL001827	0.9033	0.0967	0.8187	Polygoni Tinctorii Foliu	Indoxyl	50591	FALSE	Oc1c2c([nH]c1)cccc2
MOL001828	0.4542	0.5458	0.6519	Isatdis Radix	3-[(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)methyl]-2,4-dihydro-1H-pyrrolo[2,1-b]quinazolin-9-one	10405595	FALSE	O=c1n2CCC(=c2[nH]c2c1cccc2)/C=C\1/C=C(OC)C(=O)C(=C1)OC
MOL001829	0.8632	0.1368	0.8717	Isatdis Radix	Glucofranguli n	99649	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(C(=O)c3c(C2=O)c(O)cc(c3)C)cc(O)c1)CO
MOL001829	0.8632	0.1368	0.8717	Sennae Folium	Glucofranguli n	99649	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(C(=O)c3c(C2=O)c(O)cc(c3)C)cc(O)c1)CO
MOL001829	0.8632	0.1368	0.8717	Dianthi Herba	Glucofranguli n	99649	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(C(=O)c3c(C2=O)c(O)cc(c3)C)cc(O)c1)CO
MOL001829	0.8632	0.1368	0.8717	Polygoni Cuspidati Rhizoma Et Radix	Glucofranguli n	99649	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(C(=O)c3c(C2=O)c(O)cc(c3)C)cc(O)c1)CO
MOL001829	0.8632	0.1368	0.8717	Boehmeriae Rhizoma Et Radix	Glucofranguli n	99649	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(C(=O)c3c(C2=O)c(O)cc(c3)C)cc(O)c1)CO

MOL001830	0.9216	0.0784	0.9005	Isatdis Radix	(E)-4-(4-hydroxy-3,5-dimethoxyphenyl)but-3-en-2-one	10727728	FALSE	c1(c(cc(cc1OC)/C=C/C(=O)C)OC)O
MOL001831	0.8627	0.1373	0.8788	Arum Ternatum Thunb.	HX	790	FALSE	O=c1nc[nH]c2nc[nH]c12
MOL001831	0.8627	0.1373	0.8788	Tripterygii Radix	HX	790	FALSE	O=c1nc[nH]c2nc[nH]c12
MOL001831	0.8627	0.1373	0.8788	Isatdis Radix	HX	790	FALSE	O=c1nc[nH]c2nc[nH]c12
MOL001832	0.7499	0.2501	0.6019	Isatdis Radix	1-sulpho-3-indolylmethyl-glucosinolate	Not Available	FALSE	S(/C(=N\OS(=O)(=O)O)/Cc1c2c(n(c1)S(=O)(=O)O)cccc2)C1C(C(C(C(O1)CO)O)O)O
MOL001834	0.5066	0.4934	0.6290	Isatdis Radix	(+)-Lariciresinol-4-beta-D-glucopyranoside	11972394	FALSE	O1C(C(C(C1)Cc1cc(OC)c(OC2OC(C(O)C(O)C2O)CO)cc1)CO)c1cc(OC)c(O)cc1
MOL001835	0.9040	0.0960	0.7113	Isatdis Radix	BB_NC-1530	677114	FALSE	N1C(=O)C2N(C(=O)c3c1cccc3)CCC2
MOL001836	0.9358	0.0642	0.9195	Lobeliae Chinensis Herba	n-butyl-β-D-fructopyranoside	50914217	FALSE	C1C(C(C(C(O1)(CO)OCCCC)O)O)O
MOL001836	0.9358	0.0642	0.9195	Achyranthis Bidentatae Radix	n-butyl-β-D-fructopyranoside	50914217	FALSE	C1C(C(C(C(O1)(CO)OCCCC)O)O)O
MOL001836	0.9358	0.0642	0.9195	Smilacis Glabrae Rhixoma	n-butyl-β-D-fructopyranoside	50914217	FALSE	C1C(C(C(C(O1)(CO)OCCCC)O)O)O
MOL001836	0.9358	0.0642	0.9195	Isatdis Radix	n-butyl-β-D-fructopyranoside	50914217	FALSE	C1C(C(C(C(O1)(CO)OCCCC)O)O)O
MOL001837	0.9183	0.0817	0.8513	Nelumbinis Plumula	Methyl-p-coumarate	5319562	FALSE	C(=O)(/C=C/c1ccc(cc1)O)OC
MOL001837	0.9183	0.0817	0.8513	Fritiliariae Irrhosae Bulbus	Methyl-p-coumarate	5319562	FALSE	C(=O)(/C=C/c1ccc(cc1)O)OC
MOL001837	0.9183	0.0817	0.8513	Uncariae Ramulus Cumuncis	Methyl-p-coumarate	5319562	FALSE	C(=O)(/C=C/c1ccc(cc1)O)OC
MOL001837	0.9183	0.0817	0.8513	Lonicerae Japonicae Flos	Methyl-p-coumarate	5319562	FALSE	C(=O)(/C=C/c1ccc(cc1)O)OC
MOL001837	0.9183	0.0817	0.8513	Isatdis Radix	Methyl-p-coumarate	5319562	FALSE	C(=O)(/C=C/c1ccc(cc1)O)OC
MOL001837	0.9183	0.0817	0.8513	Flos Genkwa	Methyl-p-coumarate	5319562	FALSE	C(=O)(/C=C/c1ccc(cc1)O)OC

MOL001840	0.4635	0.5365	0.6205	Isatdis Radix	(+)-1-Lariciresinol-4'-beta-D-glucopyranoside	Not Available	FALSE	O1C(C(C(C1)Cc1cc(OC)c(O)cc1)CO)c1cc(OC)c(OC2OC(C(O)C(O)C2O)CO)cc1
MOL001841	0.9394	0.0606	0.8474	Jujubae Fructus	IES	802	FALSE	c12c([nH]cc1CC(=O)O)cccc2
MOL001841	0.9394	0.0606	0.8474	Fritillariae Pallidiflorae Bulbus	IES	802	FALSE	c12c([nH]cc1CC(=O)O)cccc2
MOL001841	0.9394	0.0606	0.8474	Isatdis Radix	IES	802	FALSE	c12c([nH]cc1CC(=O)O)cccc2
MOL001841	0.9394	0.0606	0.8474	Bombyx Mori L.	IES	802	FALSE	c12c([nH]cc1CC(=O)O)cccc2
MOL001842	0.5013	0.4987	0.7652	Cuscutae Semen	Pinoresinol	73399	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(O)cc1
MOL001842	0.5013	0.4987	0.7652	Wikstroemiae Indicae Rasix	Pinoresinol	73399	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(O)cc1
MOL001842	0.5013	0.4987	0.7652	Eucommiae Folium	Pinoresinol	73399	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(O)cc1
MOL001842	0.5013	0.4987	0.7652	Forsythiae Fructus	Pinoresinol	73399	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(O)cc1
MOL001842	0.5013	0.4987	0.7652	Drynariae Rhizoma	Pinoresinol	73399	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(O)cc1
MOL001842	0.5013	0.4987	0.7652	Cistanches Herba	Pinoresinol	73399	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(O)cc1
MOL001842	0.5013	0.4987	0.7652	Solanum Nigrum Linn.	Pinoresinol	73399	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(O)cc1
MOL001842	0.5013	0.4987	0.7652	Lobeliae Chinensis Herba	Pinoresinol	73399	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(O)cc1
MOL001842	0.5013	0.4987	0.7652	Eucommiae Cortex	Pinoresinol	73399	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(O)cc1
MOL001842	0.5013	0.4987	0.7652	Daturae Flos	Pinoresinol	73399	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(O)cc1
MOL001842	0.5013	0.4987	0.7652	Isatdis Radix	Pinoresinol	73399	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(O)cc1
MOL001842	0.5013	0.4987	0.7652	Pulsatilliae Radix	Pinoresinol	73399	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(O)cc1
MOL001843	0.9117	0.0883	0.9640	Equiseti Hiemalis Herba	HBA	126	FALSE	c1(ccc(cc1)O)C=O
MOL001843	0.9117	0.0883	0.9640	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	HBA	126	FALSE	c1(ccc(cc1)O)C=O
MOL001843	0.9117	0.0883	0.9640	Flos Genkwa	HBA	126	FALSE	c1(ccc(cc1)O)C=O
MOL001843	0.9117	0.0883	0.9640	Lilii Bulbus	HBA	126	FALSE	c1(ccc(cc1)O)C=O
MOL001843	0.9117	0.0883	0.9640	Pine Pollen	HBA	126	FALSE	c1(ccc(cc1)O)C=O
MOL001843	0.9117	0.0883	0.9640	Isatdis Radix	HBA	126	FALSE	c1(ccc(cc1)O)C=O
MOL001843	0.9117	0.0883	0.9640	Ranunculi Ternati Radix	HBA	126	FALSE	c1(ccc(cc1)O)C=O
MOL001843	0.9117	0.0883	0.9640	Phragmitis Rhizoma	HBA	126	FALSE	c1(ccc(cc1)O)C=O
MOL001843	0.9117	0.0883	0.9640	Lepidii Semen Descurainiae Semen	HBA	126	FALSE	c1(ccc(cc1)O)C=O
MOL001843	0.9117	0.0883	0.9640	Salviae Chinensis Herba	HBA	126	FALSE	c1(ccc(cc1)O)C=O
MOL001843	0.9117	0.0883	0.9640	Scutellariae Barbatae Herba	HBA	126	FALSE	c1(ccc(cc1)O)C=O
MOL001843	0.9117	0.0883	0.9640	Semiaquilegiae Radix	HBA	126	FALSE	c1(ccc(cc1)O)C=O
MOL001843	0.9117	0.0883	0.9640	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	HBA	126	FALSE	c1(ccc(cc1)O)C=O
MOL001843	0.9117	0.0883	0.9640	Rhizoma Fagopyri Cymosi	HBA	126	FALSE	c1(ccc(cc1)O)C=O
MOL001843	0.9117	0.0883	0.9640	Toosendan Fructus	HBA	126	FALSE	c1(ccc(cc1)O)C=O
MOL001843	0.9117	0.0883	0.9640	Pollen Typhae	HBA	126	FALSE	c1(ccc(cc1)O)C=O

MOL001844	0.5766	0.4234	0.6867	Isatdis Radix	clemastanin B	Not Available	FALSE	C1(C(C(C(C(O1)Oc1ccc(cc1OC)C1OCC(Cc2ccc(c(c2)OC)OC2C(O)C(C(C(O2)CO)O)O)C1CO)O)O)O)CO
MOL001845	0.6977	0.3023	0.6636	Isatdis Radix	clemastanin B_qt	56850102	FALSE	Oc1ccc(cc1OC)C1OCC(Cc2ccc(c(c2)OC)O)C1CO
MOL001846	0.6719	0.3281	0.6609	Mylabris	1,2,3,4,5,6,7,8-octahydro-1-methylphenanthrene	Not Available	FALSE	C1CC(c2c(C1)c1c(cc2)CCCC1)C
MOL001847	0.9052	0.0948	0.7349	Mylabris	2-Isopropenyl-1,3,5-trimethylbenzene	518986	FALSE	c1(c(cc(cc1C)C)C)C(=C)C
MOL001849	0.9160	0.0840	0.9390	Mylabris	2,6-dimethyl-6-nitro-2-hepten-4-one	557916	FALSE	C(=CC(=O)CC(C)(C)[N+](=O)O)(C)C
MOL001850	0.8714	0.1286	0.8241	Morindae Officinalis Radix	Izoforon	6544	FALSE	C1(CC(=CC(=O)C1)C)(C)C
MOL001850	0.8714	0.1286	0.8241	Ephedra Herba	Izoforon	6544	FALSE	C1(CC(=CC(=O)C1)C)(C)C
MOL001850	0.8714	0.1286	0.8241	licorice	Izoforon	6544	FALSE	C1(CC(=CC(=O)C1)C)(C)C
MOL001850	0.8714	0.1286	0.8241	Celastri Orbiculati Fructus	Izoforon	6544	FALSE	C1(CC(=CC(=O)C1)C)(C)C
MOL001850	0.8714	0.1286	0.8241	Mylabris	Izoforon	6544	FALSE	C1(CC(=CC(=O)C1)C)(C)C
MOL001850	0.8714	0.1286	0.8241	Paederiae Scandentis Herba	Izoforon	6544	FALSE	C1(CC(=CC(=O)C1)C)(C)C
MOL001851	0.5088	0.4912	0.6400	Mylabris	3-Phenyl-4-azafluorene	618317	FALSE	c1ccc2c(c1)Cc1c2nc(cc1)c1ccccc1
MOL001852	0.8980	0.1020	0.8120	Mylabris	4-(3-methylbut-2-enyl)-1H-indole	598515	FALSE	c12c(cccc1CC=C(C)C)[nH]cc2
MOL001853	0.9252	0.0748	0.8351	Mylabris	2-Acetyl-6-methoxynaphthalene	77506	FALSE	c12c(cc(cc2)OC)ccc(c1)C(=O)C
MOL001853	0.9252	0.0748	0.8351	Cinnanmomi Cortex	2-Acetyl-6-methoxynaphthalene	77506	FALSE	c12c(cc(cc2)OC)ccc(c1)C(=O)C
MOL001854	0.9279	0.0721	0.9485	Mylabris	6-methyl-3-heptanol	Not Available	FALSE	C(CCC(C)C)(CC)O
MOL001855	0.7656	0.2344	0.6051	Mylabris	octadec-7-enoic acid	5282756	FALSE	C(=O)(CCCCC/C=C/CCCCCCCCC)O
MOL001856	0.9058	0.0942	0.8351	Oroxyli Semen	Fleet-X	7947	FALSE	c1c(cc(cc1C)C)C
MOL001856	0.9058	0.0942	0.8351	Chaenomeles Sinensis (Thouin) Koehne	Fleet-X	7947	FALSE	c1c(cc(cc1C)C)C
MOL001856	0.9058	0.0942	0.8351	Sojae Semen Nigrum	Fleet-X	7947	FALSE	c1c(cc(cc1C)C)C

MOL001856	0.9058	0.0942	0.8351	Mylabris	Fleet-X	7947	FALSE	c1c(cc(cc1C)C)C
MOL001857	0.9002	0.0998	0.7719	Mylabris	norcantharidin	Not Available	FALSE	O1C2C3C(C1CC2)C(=O)OC3=O
MOL001858	0.9503	0.0497	0.8021	Mylabris	cantharidin	Not Available	FALSE	C12(C(C3OC1CC3)(C(=O)OC2=O)C)C
MOL001859	0.8574	0.1426	0.6722	Ephedra Herba	FMT	18971002	FALSE	C(=O)O
MOL001859	0.8574	0.1426	0.6722	Maydis Seigma	FMT	18971002	FALSE	C(=O)O
MOL001859	0.8574	0.1426	0.6722	Bomboo Juice	FMT	18971002	FALSE	C(=O)O
MOL001859	0.8574	0.1426	0.6722	Mori Fructus	FMT	18971002	FALSE	C(=O)O
MOL001859	0.8574	0.1426	0.6722	Mylabris	FMT	18971002	FALSE	C(=O)O
MOL001859	0.8574	0.1426	0.6722	Pollen Typhae	FMT	18971002	FALSE	C(=O)O
MOL001859	0.8574	0.1426	0.6722	Stemonae Radix	FMT	18971002	FALSE	C(=O)O
MOL001859	0.8574	0.1426	0.6722	Ginkgo Semen	FMT	18971002	FALSE	C(=O)O
MOL001860	0.9048	0.0952	0.8408	Mylabris	2-isobutyl-1,4-dimethylbenzene	41508	FALSE	c1(c(ccc(c1)C)C)CC(C)C
MOL001861	0.9254	0.0746	0.7701	Mylabris	1,6,8-trimethyl-1,2,3,4-tetrahydronaphthalene	Not Available	FALSE	c1(cc(c2c(c1)CCCC2C)C)C
MOL001862	0.8655	0.1345	0.6352	Alpiniae Officinarum Rhizome	Cadalin	10225	FALSE	c1(ccc(c2cc(ccc12)C)C(C)C)C
MOL001862	0.8655	0.1345	0.6352	Sedi Herba	Cadalin	10225	FALSE	c1(ccc(c2cc(ccc12)C)C(C)C)C
MOL001862	0.8655	0.1345	0.6352	Rhododendri Daurici Folium	Cadalin	10225	FALSE	c1(ccc(c2cc(ccc12)C)C(C)C)C
MOL001862	0.8655	0.1345	0.6352	Cinnanmomi Cortex	Cadalin	10225	FALSE	c1(ccc(c2cc(ccc12)C)C(C)C)C
MOL001862	0.8655	0.1345	0.6352	Tamaricis Cacumen	Cadalin	10225	FALSE	c1(ccc(c2cc(ccc12)C)C(C)C)C
MOL001862	0.8655	0.1345	0.6352	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	Cadalin	10225	FALSE	c1(ccc(c2cc(ccc12)C)C(C)C)C
MOL001862	0.8655	0.1345	0.6352	Ailanthi Cortex	Cadalin	10225	FALSE	c1(ccc(c2cc(ccc12)C)C(C)C)C
MOL001862	0.8655	0.1345	0.6352	Magnolia Officinalis Rehd Et Wils.	Cadalin	10225	FALSE	c1(ccc(c2cc(ccc12)C)C(C)C)C
MOL001862	0.8655	0.1345	0.6352	Cinnamomi Ramulus	Cadalin	10225	FALSE	c1(ccc(c2cc(ccc12)C)C(C)C)C
MOL001862	0.8655	0.1345	0.6352	Adenophprae Ae Radix	Cadalin	10225	FALSE	c1(ccc(c2cc(ccc12)C)C(C)C)C
MOL001862	0.8655	0.1345	0.6352	Gossampiniflos	Cadalin	10225	FALSE	c1(ccc(c2cc(ccc12)C)C(C)C)C
MOL001862	0.8655	0.1345	0.6352	Ardisiae Japonicae Herba	Cadalin	10225	FALSE	c1(ccc(c2cc(ccc12)C)C(C)C)C
MOL001862	0.8655	0.1345	0.6352	Cyperi Rhizoma	Cadalin	10225	FALSE	c1(ccc(c2cc(ccc12)C)C(C)C)C
MOL001862	0.8655	0.1345	0.6352	Mylabris	Cadalin	10225	FALSE	c1(ccc(c2cc(ccc12)C)C(C)C)C
MOL001863	0.6563	0.3437	0.6249	Aristolochiae Fructus	METHYL ISOPALMITATE	21205	FALSE	C(=O)(CCCCCCCCCCCCC(C)C)OC

MOL001863	0.6563	0.3437	0.6249	Lycii Fructus	METHYL ISOPALMITATE	21205	FALSE	C(=O)(CCCCCCCCCCCCC(C)C)OC
MOL001863	0.6563	0.3437	0.6249	Caryophylliflos	METHYL ISOPALMITATE	21205	FALSE	C(=O)(CCCCCCCCCCCCC(C)C)OC
MOL001863	0.6563	0.3437	0.6249	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	METHYL ISOPALMITATE	21205	FALSE	C(=O)(CCCCCCCCCCCCC(C)C)OC
MOL001863	0.6563	0.3437	0.6249	Magnolia Officinalis Rehd Et Wils.	METHYL ISOPALMITATE	21205	FALSE	C(=O)(CCCCCCCCCCCCC(C)C)OC
MOL001863	0.6563	0.3437	0.6249	Mylabris	METHYL ISOPALMITATE	21205	FALSE	C(=O)(CCCCCCCCCCCCC(C)C)OC
MOL001864	0.8596	0.1404	0.8496	Mylabris	Benztriazole	7220	FALSE	n1[nH]nc2c1cccc2
MOL001866	0.9496	0.0504	0.8616	Mylabris	Benzene, 1-(2-butenyl)-2,3-dimethyl-	5372817	FALSE	c1(c(c(ccc1)C)C)C/C=C/C
MOL001867	0.9446	0.0554	0.9653	Imperatae Rhizoma	Isovanillin	12127	FALSE	Oc1cc(C=O)ccc1OC
MOL001867	0.9446	0.0554	0.9653	Coptidis Rhizoma	Isovanillin	12127	FALSE	Oc1cc(C=O)ccc1OC
MOL001867	0.9446	0.0554	0.9653	Polygoni Orientalis Fructus	Isovanillin	12127	FALSE	Oc1cc(C=O)ccc1OC
MOL001867	0.9446	0.0554	0.9653	Evodiae Fructus	Isovanillin	12127	FALSE	Oc1cc(C=O)ccc1OC
MOL001867	0.9446	0.0554	0.9653	Dichroae Radix	Isovanillin	12127	FALSE	Oc1cc(C=O)ccc1OC
MOL001867	0.9446	0.0554	0.9653	Myristicae Semen	Isovanillin	12127	FALSE	Oc1cc(C=O)ccc1OC
MOL001867	0.9446	0.0554	0.9653	Cortex Periplocae Radicis	Isovanillin	12127	FALSE	Oc1cc(C=O)ccc1OC
MOL001867	0.9446	0.0554	0.9653	Alpiniae Oxyphyliae Fructus	Isovanillin	12127	FALSE	Oc1cc(C=O)ccc1OC
MOL001868	0.9575	0.0425	0.8157	Imperatae Rhizoma	4-Methyllimetol	5354284	FALSE	c1(=O)cc(c2c(o1)cc(cc2O)O)C
MOL001869	0.3825	0.6175	0.7070	Strychni Semen	fernenol	Not Available	FALSE	C1C(C(C2C(C1)(C1=CCC3(C(C1CC2)(CCC1(C3CCC1C(C)C)C)C)C)(C)C)O
MOL001869	0.3825	0.6175	0.7070	Imperatae Rhizoma	fernenol	Not Available	FALSE	C1C(C(C2C(C1)(C1=CCC3(C(C1CC2)(CCC1(C3CCC1C(C)C)C)C)C)(C)C)O
MOL001871	0.3815	0.6185	0.7162	Imperatae Rhizoma	simiarenol	12442794	FALSE	OC1C(C2=CCC3C4(C(C5C(CC4)(C(CC5)C(C)C)C)(CCC3(C2CC1)C)C)C)(C)C
MOL001871	0.3815	0.6185	0.7162	Benincasae Exocarpium	simiarenol	12442794	FALSE	OC1C(C2=CCC3C4(C(C5C(CC4)(C(CC5)C(C)C)C)(CCC3(C2CC1)C)C)C)(C)C
MOL001871	0.3815	0.6185	0.7162	Folium Artemisiae Argyi	simiarenol	12442794	FALSE	OC1C(C2=CCC3C4(C(C5C(CC4)(C(CC5)C(C)C)C)(CCC3(C2CC1)C)C)C)(C)C
MOL001871	0.3815	0.6185	0.7162	Benincasae Semen	simiarenol	12442794	FALSE	OC1C(C2=CCC3C4(C(C5C(CC4)(C(CC5)C(C)C)C)(CCC3(C2CC1)C)C)C)(C)C

MOL001872	0.3364	0.6636	0.6653	Imperatae Rhizoma	Hollow cylinder protein complex	189045	FALSE	O(C1C(C2C(C3=CCC4(C(C3CC2)(CCC2(C4CCC2C(C)C)C)C)C)(CC1)C)(C)C)C
MOL001873	0.9418	0.0582	0.9590	Imperatae Rhizoma	Sobrol A	8434	FALSE	C(=O)(c1ccc(cc1)O)OCC
MOL001873	0.9418	0.0582	0.9590	Flos Genkwa	Sobrol A	8434	FALSE	C(=O)(c1ccc(cc1)O)OCC
MOL001873	0.9418	0.0582	0.9590	Mori Cortex	Sobrol A	8434	FALSE	C(=O)(c1ccc(cc1)O)OCC
MOL001873	0.9418	0.0582	0.9590	Evodiae Fructus	Sobrol A	8434	FALSE	C(=O)(c1ccc(cc1)O)OCC
MOL001873	0.9418	0.0582	0.9590	Allii Sativi Bulbus	Sobrol A	8434	FALSE	C(=O)(c1ccc(cc1)O)OCC
MOL001873	0.9418	0.0582	0.9590	Sinapis Semen	Sobrol A	8434	FALSE	C(=O)(c1ccc(cc1)O)OCC
MOL001874	0.3825	0.6175	0.7070	Imperatae Rhizoma	isoarborinol	12305182	FALSE	OC1C(C2C(C3=CCC4(C(C3CC2)(CCC2(C4CCC2C(C)C)C)C)C)(CC1)C)(C)C
MOL001874	0.3825	0.6175	0.7070	Coicis Semen	isoarborinol	12305182	FALSE	OC1C(C2C(C3=CCC4(C(C3CC2)(CCC2(C4CCC2C(C)C)C)C)C)(CC1)C)(C)C
MOL001875	0.8390	0.1610	0.7279	Lonicerae Japonicae Flos	isochlorogenic,acid	Not Available	FALSE	C1(C(C(CC(C1)(C(=O)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)O)OC(=O)/C=C\c1cc(c(cc1)O)O
MOL001875	0.8390	0.1610	0.7279	Imperatae Rhizoma	isochlorogenic,acid	Not Available	FALSE	C1(C(C(CC(C1)(C(=O)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)O)OC(=O)/C=C\c1cc(c(cc1)O)O
MOL001875	0.8390	0.1610	0.7279	Inulae Herba	isochlorogenic,acid	Not Available	FALSE	C1(C(C(CC(C1)(C(=O)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)O)OC(=O)/C=C\c1cc(c(cc1)O)O
MOL001875	0.8390	0.1610	0.7279	Folium Ilicis Cornutae	isochlorogenic,acid	Not Available	FALSE	C1(C(C(CC(C1)(C(=O)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)O)OC(=O)/C=C\c1cc(c(cc1)O)O
MOL001875	0.8390	0.1610	0.7279	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	isochlorogenic,acid	Not Available	FALSE	C1(C(C(CC(C1)(C(=O)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)O)OC(=O)/C=C\c1cc(c(cc1)O)O
MOL001875	0.8390	0.1610	0.7279	Artemisia Annua L.	isochlorogenic,acid	Not Available	FALSE	C1(C(C(CC(C1)(C(=O)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)O)OC(=O)/C=C\c1cc(c(cc1)O)O
MOL001875	0.8390	0.1610	0.7279	Chrysanthemi Flos	isochlorogenic,acid	Not Available	FALSE	C1(C(C(CC(C1)(C(=O)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)O)OC(=O)/C=C\c1cc(c(cc1)O)O
MOL001876	0.8811	0.1189	0.9661	Imperatae Rhizoma	6-Methoxyflavone	147157	TRUE	c1(cc(=O)c2c(o1)ccc(c2)OC)c1ccccc1
MOL001877	0.8368	0.1632	0.7310	Imperatae Rhizoma	Isochlorogenic acid B	Not Available	FALSE	C1C(CC(C(C1O)OC(=O)/C=C/c1ccc(c(c1)O)O)OC(=O)/C=C\c1cc(c(cc1)O)O)(O)C(=O)O
MOL001878	0.8368	0.1632	0.7310	Imperatae Rhizoma	4,5-Di-O-caffeoylquinic acid	6474309	FALSE	C1(CC(C(C(C1)O)OC(=O)/C=C/c1cc(c(cc1)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)(C(=O)O)O
MOL001878	0.8368	0.1632	0.7310	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	4,5-Di-O-caffeoylquinic acid	6474309	FALSE	C1(CC(C(C(C1)O)OC(=O)/C=C/c1cc(c(cc1)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)(C(=O)O)O
MOL001878	0.8368	0.1632	0.7310	Xanthii Fructus	4,5-Di-O-caffeoylquinic acid	6474309	FALSE	C1(CC(C(C(C1)O)OC(=O)/C=C/c1cc(c(cc1)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)(C(=O)O)O

MOL001878	0.8368	0.1632	0.7310	Folium Artemisiae Argyi	4,5-Di-O-caffeoylquinic acid	6474309	FALSE	C1(CC(C(C(C1)O)OC(=O)/C=C/c1cc(c(cc1)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)(C(=O)O)O
MOL001879	0.3364	0.6636	0.6653	Imperatae Rhizoma	cylindrin	12308619	FALSE	O(C1C(C2C(C3=CCC4(C(C3CC2)(CCC2(C4CCC2C(C)C)C)C)C)(CC1)C)(C)C)C
MOL001880	0.8881	0.1119	0.9473	Cotyledon Fimbriata Turcz.	OXL	18676629	FALSE	C(=O)(C(=O)O)O
MOL001880	0.8881	0.1119	0.9473	Stemonae Radix	OXL	18676629	FALSE	C(=O)(C(=O)O)O
MOL001880	0.8881	0.1119	0.9473	Coriolus	OXL	18676629	FALSE	C(=O)(C(=O)O)O
MOL001880	0.8881	0.1119	0.9473	Imperatae Rhizoma	OXL	18676629	FALSE	C(=O)(C(=O)O)O
MOL001880	0.8881	0.1119	0.9473	Polygoni Avicularis Herba	OXL	18676629	FALSE	C(=O)(C(=O)O)O
MOL001880	0.8881	0.1119	0.9473	Polygoni Cuspidati Rhizoma Et Radix	OXL	18676629	FALSE	C(=O)(C(=O)O)O
MOL001880	0.8881	0.1119	0.9473	Equiseti Hiemalis Herba	OXL	18676629	FALSE	C(=O)(C(=O)O)O
MOL001880	0.8881	0.1119	0.9473	Kansui Radix	OXL	18676629	FALSE	C(=O)(C(=O)O)O
MOL001880	0.8881	0.1119	0.9473	Allii Fistulost Bulbus	OXL	18676629	FALSE	C(=O)(C(=O)O)O
MOL001880	0.8881	0.1119	0.9473	Verbenae Herb	OXL	18676629	FALSE	C(=O)(C(=O)O)O
MOL001880	0.8881	0.1119	0.9473	Capsellae Herba	OXL	18676629	FALSE	C(=O)(C(=O)O)O
MOL001880	0.8881	0.1119	0.9473	Radix Rhei Et Rhizome	OXL	18676629	FALSE	C(=O)(C(=O)O)O
MOL001880	0.8881	0.1119	0.9473	Maydis Seigma	OXL	18676629	FALSE	C(=O)(C(=O)O)O
MOL001880	0.8881	0.1119	0.9473	Lycii Fructus	OXL	18676629	FALSE	C(=O)(C(=O)O)O
MOL001880	0.8881	0.1119	0.9473	Hippophae Fructus	OXL	18676629	FALSE	C(=O)(C(=O)O)O
MOL001880	0.8881	0.1119	0.9473	Folium Nelumbinis	OXL	18676629	FALSE	C(=O)(C(=O)O)O
MOL001880	0.8881	0.1119	0.9473	Artemisiae Scopariae Herba	OXL	18676629	FALSE	C(=O)(C(=O)O)O
MOL001880	0.8881	0.1119	0.9473	Choerospondiatis Fructus	OXL	18676629	FALSE	C(=O)(C(=O)O)O
MOL001880	0.8881	0.1119	0.9473	Portulacae Herba	OXL	18676629	FALSE	C(=O)(C(=O)O)O
MOL001880	0.8881	0.1119	0.9473	Mori Fructus	OXL	18676629	FALSE	C(=O)(C(=O)O)O
MOL001881	0.9098	0.0902	0.8304	Coicis Semen	MBOA	10772	FALSE	o1c(=O)[nH]c2c1cc(cc2)OC
MOL001881	0.9098	0.0902	0.8304	Imperatae Rhizoma	MBOA	10772	FALSE	o1c(=O)[nH]c2c1cc(cc2)OC
MOL001881	0.9098	0.0902	0.8304	Phragmitis Rhizoma	MBOA	10772	FALSE	o1c(=O)[nH]c2c1cc(cc2)OC
MOL001882	0.9114	0.0886	0.9647	Lygodii Spora	Tricine	6992779	FALSE	C(=O)(CNC(CO)(CO)CO)O
MOL001882	0.9114	0.0886	0.9647	Imperatae Rhizoma	Tricine	6992779	FALSE	C(=O)(CNC(CO)(CO)CO)O
MOL001883	0.9304	0.0696	0.7352	Imperatae Rhizoma	anemonin	Not Available	FALSE	O1C(=O)C=CC21C1(OC(=O)C=C1)CC2
MOL001883	0.9304	0.0696	0.7352	Pulsatilliae Radix	anemonin	Not Available	FALSE	O1C(=O)C=CC21C1(OC(=O)C=C1)CC2
MOL001883	0.9304	0.0696	0.7352	Radix Clematidis	anemonin	Not Available	FALSE	O1C(=O)C=CC21C1(OC(=O)C=C1)CC2
MOL001884	0.3904	0.6096	0.8410	Phragmitis Rhizoma	Omaine	220401	FALSE	COc1c(OC)c(c2c(c1)CCC(c1c2ccc(c(=O)c1)OC)NC)OC
MOL001884	0.3904	0.6096	0.8410	Imperatae Rhizoma	Omaine	220401	FALSE	COc1c(OC)c(c2c(c1)CCC(c1c2ccc(c(=O)c1)OC)NC)OC
MOL001884	0.3904	0.6096	0.8410	Gentianae Radix Et Rhozima	Omaine	220401	FALSE	COc1c(OC)c(c2c(c1)CCC(c1c2ccc(c(=O)c1)OC)NC)OC
MOL001884	0.3904	0.6096	0.8410	Coicis Semen	Omaine	220401	FALSE	COc1c(OC)c(c2c(c1)CCC(c1c2ccc(c(=O)c1)OC)NC)OC
MOL001885	0.3217	0.6783	0.6705	Imperatae Rhizoma	Cymarin	Not Available	FALSE	C1(CC2(C(CC1)(C1C(CC2)C2(C(CC1)(C)C(CC2)C1=CC(=O)OC1)O)C=O)O)OC1OC(C(C(C1)OC)O)C

MOL001886	0.9023	0.0977	0.9553	Chaenomeles Sinensis (Thouin) Koehne	Tar	439655	FALSE	C(=O)(C(C(C(=O)O)O)O)O
MOL001886	0.9023	0.0977	0.9553	Hippophae Fructus	Tar	439655	FALSE	C(=O)(C(C(C(=O)O)O)O)O
MOL001886	0.9023	0.0977	0.9553	Folium Nelumbinis	Tar	439655	FALSE	C(=O)(C(C(C(=O)O)O)O)O
MOL001886	0.9023	0.0977	0.9553	Eucommiae Folium	Tar	439655	FALSE	C(=O)(C(C(C(=O)O)O)O)O
MOL001886	0.9023	0.0977	0.9553	Maydis Seigma	Tar	439655	FALSE	C(=O)(C(C(C(=O)O)O)O)O
MOL001886	0.9023	0.0977	0.9553	Capsici Fructus	Tar	439655	FALSE	C(=O)(C(C(C(=O)O)O)O)O
MOL001886	0.9023	0.0977	0.9553	Capsellae Herba	Tar	439655	FALSE	C(=O)(C(C(C(=O)O)O)O)O
MOL001886	0.9023	0.0977	0.9553	Polygoni Cuspidati Rhizoma Et Radix	Tar	439655	FALSE	C(=O)(C(C(C(=O)O)O)O)O
MOL001886	0.9023	0.0977	0.9553	Mori Fructus	Tar	439655	FALSE	C(=O)(C(C(C(=O)O)O)O)O
MOL001886	0.9023	0.0977	0.9553	Eucommiae Cortex	Tar	439655	FALSE	C(=O)(C(C(C(=O)O)O)O)O
MOL001886	0.9023	0.0977	0.9553	Imperatae Rhizoma	Tar	439655	FALSE	C(=O)(C(C(C(=O)O)O)O)O
MOL001886	0.9023	0.0977	0.9553	Cornus Officinalis Sieb. Et Zucc.	Tar	439655	FALSE	C(=O)(C(C(C(=O)O)O)O)O
MOL001886	0.9023	0.0977	0.9553	Aloe	Tar	439655	FALSE	C(=O)(C(C(C(=O)O)O)O)O
MOL001886	0.9023	0.0977	0.9553	Farfarae Flos	Tar	439655	FALSE	C(=O)(C(C(C(=O)O)O)O)O
MOL001886	0.9023	0.0977	0.9553	Jujubae Fructus	Tar	439655	FALSE	C(=O)(C(C(C(=O)O)O)O)O
MOL001886	0.9023	0.0977	0.9553	Xanthii Fructus	Tar	439655	FALSE	C(=O)(C(C(C(=O)O)O)O)O
MOL001886	0.9023	0.0977	0.9553	Rubi Fructus	Tar	439655	FALSE	C(=O)(C(C(C(=O)O)O)O)O
MOL001886	0.9023	0.0977	0.9553	Ampelopsis Japonica	Tar	439655	FALSE	C(=O)(C(C(C(=O)O)O)O)O
MOL001887	0.9023	0.0977	0.9553	Codonopsis Radix	SRT	447315	FALSE	C(=O)(C(O)C(O)C(=O)O)O
MOL001887	0.9023	0.0977	0.9553	Imperatae Rhizoma	SRT	447315	FALSE	C(=O)(C(O)C(O)C(=O)O)O
MOL001887	0.9023	0.0977	0.9553	Choerospondiatis Fructus	SRT	447315	FALSE	C(=O)(C(O)C(O)C(=O)O)O
MOL001887	0.9023	0.0977	0.9553	Eriobotryae Folium	SRT	447315	FALSE	C(=O)(C(O)C(O)C(=O)O)O
MOL001888	0.9030	0.0970	0.9647	Paeoniae Radix Alba	2,2-dimethylcyclohexanol	638180	FALSE	C1(C(CCCC1)(C)C)O
MOL001889	0.4777	0.5223	0.6406	Broussonetiae Fructus	Methyl linolelaidate	5362793	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)OC
MOL001889	0.4777	0.5223	0.6406	Momordicae Fructus	Methyl linolelaidate	5362793	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)OC
MOL001889	0.4777	0.5223	0.6406	Paeoniae Radix Alba	Methyl linolelaidate	5362793	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)OC
MOL001889	0.4777	0.5223	0.6406	Cornus Officinalis Sieb. Et Zucc.	Methyl linolelaidate	5362793	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)OC
MOL001889	0.4777	0.5223	0.6406	Magnolia Officinalis Rehd Et Wils.	Methyl linolelaidate	5362793	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)OC
MOL001889	0.4777	0.5223	0.6406	Et Radix Patriniae Rhizoma	Methyl linolelaidate	5362793	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)OC
MOL001889	0.4777	0.5223	0.6406	Echinopsis Radix	Methyl linolelaidate	5362793	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)OC

MOL001889	0.4777	0.5223	0.6406	Lycii Fructus	Methyl linolelaidate	5362793	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)OC
MOL001889	0.4777	0.5223	0.6406	Puerariae Flos	Methyl linolelaidate	5362793	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)OC
MOL001889	0.4777	0.5223	0.6406	Aristolochiae Fructus	Methyl linolelaidate	5362793	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)OC
MOL001891	0.7595	0.2405	0.6595	Paeoniae Radix Alba	9-methylenefluorene	78147	FALSE	C1(=C)c2ccccc2c2ccccc12
MOL001891	0.7595	0.2405	0.6595	Ardisiae Japonicae Herba	9-methylenefluorene	78147	FALSE	C1(=C)c2ccccc2c2ccccc12
MOL001892	0.9227	0.0773	0.9101	Paeoniae Radix Alba	Dipropyl phthalate	8559	FALSE	c1(c(C(=O)OCCC)cccc1)C(=O)OCCC
MOL001893	0.9288	0.0712	0.9706	Sesami Nigrum Semen	BU3	225936	FALSE	C(C(C)O)(C)O
MOL001893	0.9288	0.0712	0.9706	Cornus Officinalis Sieb. Et Zucc.	BU3	225936	FALSE	C(C(C)O)(C)O
MOL001893	0.9288	0.0712	0.9706	Chaenomeles Sinensis (Thouin) Koehne	BU3	225936	FALSE	C(C(C)O)(C)O
MOL001893	0.9288	0.0712	0.9706	Magnolia Officinalis Rehd Et Wils.	BU3	225936	FALSE	C(C(C)O)(C)O
MOL001893	0.9288	0.0712	0.9706	Hordei Fructus Germinatus	BU3	225936	FALSE	C(C(C)O)(C)O
MOL001893	0.9288	0.0712	0.9706	Paeoniae Radix Alba	BU3	225936	FALSE	C(C(C)O)(C)O
MOL001893	0.9288	0.0712	0.9706	Mori Fructus	BU3	225936	FALSE	C(C(C)O)(C)O
MOL001893	0.9288	0.0712	0.9706	Litchi Semen	BU3	225936	FALSE	C(C(C)O)(C)O
MOL001893	0.9288	0.0712	0.9706	Caryophylliflos	BU3	225936	FALSE	C(C(C)O)(C)O
MOL001895	0.9110	0.0890	0.6442	Paeoniae Radix Alba	Dibutylphenol	31405	FALSE	c1(c(c(C(C)(C)C)ccc1)O)C(C)(C)C
MOL001896	0.9569	0.0431	0.8088	Forsythiae Fructus	bicyclo[3.1.1]hept-2-ene-2-methanol, 6,6-dimethyl-	636475	FALSE	OCC1=CCC2C(C1C2)(C)C
MOL001896	0.9569	0.0431	0.8088	Perillae Fructus	bicyclo[3.1.1]hept-2-ene-2-methanol, 6,6-dimethyl-	636475	FALSE	OCC1=CCC2C(C1C2)(C)C
MOL001896	0.9569	0.0431	0.8088	Aristolochiae Fructus	bicyclo[3.1.1]hept-2-ene-2-methanol, 6,6-dimethyl-	636475	FALSE	OCC1=CCC2C(C1C2)(C)C
MOL001896	0.9569	0.0431	0.8088	Paeoniae Radix Alba	bicyclo[3.1.1]hept-2-ene-2-methanol, 6,6-dimethyl-	636475	FALSE	OCC1=CCC2C(C1C2)(C)C

MOL001896	0.9569	0.0431	0.8088	Citri Sarcodactylis Fructus	bicyclo[3.1.1]hept-2-ene-2-methanol, 6,6-dimethyl-	636475	FALSE	OCC1=CCC2C(C1C2)(C)C
MOL001897	0.9582	0.0418	0.8162	Paeoniae Radix Alba	()-trans-Myrtanol	84880	FALSE	OCC1C2C(C(C2)CC1)(C)C
MOL001898	0.9252	0.0748	0.9658	Paeoniae Radix Alba	Acetyl oxide	7918	FALSE	C(=O)(OC(=O)C)C
MOL001900	0.7411	0.2589	0.8486	Paeoniae Radix Alba	Pulchinenoside A_qt	21672692	FALSE	C1(CCC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C(=C)C)C4C3CCC21)C)O
MOL001900	0.7411	0.2589	0.8486	Pulsatilliae Radix	Pulchinenoside A_qt	21672692	FALSE	C1(CCC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C(=C)C)C4C3CCC21)C)O
MOL001901	0.3698	0.6302	0.6857	Persicae Semen	24-Methylenecycloartanol	Not Available	FALSE	OC1C(C2C3(C4(C3)C(C3(C(CC4)(C(CC3)C(CCC(=C)C(C)C)C)C)C)CC2)CC1)(C)C
MOL001901	0.3698	0.6302	0.6857	Semen Lini	24-Methylenecycloartanol	Not Available	FALSE	OC1C(C2C3(C4(C3)C(C3(C(CC4)(C(CC3)C(CCC(=C)C(C)C)C)C)C)CC2)CC1)(C)C
MOL001901	0.3698	0.6302	0.6857	Kansui Radix	24-Methylenecycloartanol	Not Available	FALSE	OC1C(C2C3(C4(C3)C(C3(C(CC4)(C(CC3)C(CCC(=C)C(C)C)C)C)C)CC2)CC1)(C)C
MOL001901	0.3698	0.6302	0.6857	Lycii Fructus	24-Methylenecycloartanol	Not Available	FALSE	OC1C(C2C3(C4(C3)C(C3(C(CC4)(C(CC3)C(CCC(=C)C(C)C)C)C)C)CC2)CC1)(C)C
MOL001901	0.3698	0.6302	0.6857	Paeoniae Radix Alba	24-Methylenecycloartanol	Not Available	FALSE	OC1C(C2C3(C4(C3)C(C3(C(CC4)(C(CC3)C(CCC(=C)C(C)C)C)C)C)CC2)CC1)(C)C
MOL001901	0.3698	0.6302	0.6857	Lobeliae Chinensis Herba	24-Methylenecycloartanol	Not Available	FALSE	OC1C(C2C3(C4(C3)C(C3(C(CC4)(C(CC3)C(CCC(=C)C(C)C)C)C)C)CC2)CC1)(C)C
MOL001901	0.3698	0.6302	0.6857	Capsici Fructus	24-Methylenecycloartanol	Not Available	FALSE	OC1C(C2C3(C4(C3)C(C3(C(CC4)(C(CC3)C(CCC(=C)C(C)C)C)C)C)CC2)CC1)(C)C
MOL001901	0.3698	0.6302	0.6857	Perillae Fructus	24-Methylenecycloartanol	Not Available	FALSE	OC1C(C2C3(C4(C3)C(C3(C(CC4)(C(CC3)C(CCC(=C)C(C)C)C)C)C)CC2)CC1)(C)C
MOL001901	0.3698	0.6302	0.6857	Phellodendri Amurensis Cortex	24-Methylenecycloartanol	Not Available	FALSE	OC1C(C2C3(C4(C3)C(C3(C(CC4)(C(CC3)C(CCC(=C)C(C)C)C)C)C)CC2)CC1)(C)C

MOL001902	0.7167	0.2833	0.8120	Paeoniae Radix Alba	3β,23-dihydroxy-oleana-11,13(18)-dien-28-oic acid	Not Available	FALSE	C1(CCC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C)(C)CC4=C3C=CC21)C)O
MOL001903	0.7382	0.2618	0.8502	Paeoniae Radix Alba	3β-hydroxy-11-oxo-olean-12-en-28-oic acid	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C)(C)CC4C3=CC(=O)C21)C)O
MOL001904	0.9686	0.0314	0.9429	Paeoniae Radix Alba	2 - methyl - 3 - (2 - propenyl) - phenol	19854132	FALSE	c1(c(c(ccc1)CC=C)C)O
MOL001905	0.7031	0.2969	0.8652	Paeoniae Radix Alba	3β-hydroxy-oleana-11,13(18)-dien-28-oic acid?	15226483	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C)(C)CC4=C3C=CC21)C)O
MOL001906	0.9287	0.0713	0.9406	Canavaliae Semen	Methylgallate	7428	FALSE	Oc1cc(cc(O)c1O)C(=O)OC
MOL001906	0.9287	0.0713	0.9406	Phyllanthi Fructus	Methylgallate	7428	FALSE	Oc1cc(cc(O)c1O)C(=O)OC
MOL001906	0.9287	0.0713	0.9406	Euphorbiae Humifusae Herba	Methylgallate	7428	FALSE	Oc1cc(cc(O)c1O)C(=O)OC
MOL001906	0.9287	0.0713	0.9406	Radix Paeoniae Rubra	Methylgallate	7428	FALSE	Oc1cc(cc(O)c1O)C(=O)OC
MOL001906	0.9287	0.0713	0.9406	Galla Chinensis	Methylgallate	7428	FALSE	Oc1cc(cc(O)c1O)C(=O)OC
MOL001906	0.9287	0.0713	0.9406	Anemarrhenae Rhizoma	Methylgallate	7428	FALSE	Oc1cc(cc(O)c1O)C(=O)OC
MOL001906	0.9287	0.0713	0.9406	Granati Pericarpium	Methylgallate	7428	FALSE	Oc1cc(cc(O)c1O)C(=O)OC
MOL001906	0.9287	0.0713	0.9406	Paeoniae Radix Alba	Methylgallate	7428	FALSE	Oc1cc(cc(O)c1O)C(=O)OC
MOL001906	0.9287	0.0713	0.9406	Euphorbiae Helioscopiae Herba	Methylgallate	7428	FALSE	Oc1cc(cc(O)c1O)C(=O)OC
MOL001906	0.9287	0.0713	0.9406	Cornus Officinalis Sieb. Et Zucc.	Methylgallate	7428	FALSE	Oc1cc(cc(O)c1O)C(=O)OC
MOL001907	0.9359	0.0641	0.9349	Canarii Fructus	Progallin A	13250	FALSE	O(C(=O)c1cc(O)c(O)c(O)c1)CC
MOL001907	0.9359	0.0641	0.9349	Gleditsiae Spina	Progallin A	13250	FALSE	O(C(=O)c1cc(O)c(O)c(O)c1)CC
MOL001907	0.9359	0.0641	0.9349	Radix Paeoniae Rubra	Progallin A	13250	FALSE	O(C(=O)c1cc(O)c(O)c(O)c1)CC
MOL001907	0.9359	0.0641	0.9349	Phyllanthi Fructus	Progallin A	13250	FALSE	O(C(=O)c1cc(O)c(O)c(O)c1)CC
MOL001907	0.9359	0.0641	0.9349	Paeoniae Radix Alba	Progallin A	13250	FALSE	O(C(=O)c1cc(O)c(O)c(O)c1)CC
MOL001907	0.9359	0.0641	0.9349	Saussureae Involucratae Herba	Progallin A	13250	FALSE	O(C(=O)c1cc(O)c(O)c(O)c1)CC
MOL001907	0.9359	0.0641	0.9349	Quisqualis Indica	Progallin A	13250	FALSE	O(C(=O)c1cc(O)c(O)c(O)c1)CC
MOL001907	0.9359	0.0641	0.9349	Euphorbiae Helioscopiae Herba	Progallin A	13250	FALSE	O(C(=O)c1cc(O)c(O)c(O)c1)CC
MOL001907	0.9359	0.0641	0.9349	Kaki Calyx	Progallin A	13250	FALSE	O(C(=O)c1cc(O)c(O)c(O)c1)CC

MOL001907	0.9359	0.0641	0.9349	Arisaematis Rhizoma	Progallin A	13250	FALSE	O(C(=O)c1cc(O)c(O)c(O)c1)CC
MOL001907	0.9359	0.0641	0.9349	Mori Cortex	Progallin A	13250	FALSE	O(C(=O)c1cc(O)c(O)c(O)c1)CC
MOL001907	0.9359	0.0641	0.9349	Gleditsiae Fructus	Progallin A	13250	FALSE	O(C(=O)c1cc(O)c(O)c(O)c1)CC
MOL001908	0.8731	0.1269	0.7113	Schizonepetae Herba	(Z)-(1S,5R)-beta-pinen-10-yl-beta-vicianoside	Not Available	FALSE	O(/C=C/1\C2C(C(C2)CC1)(C)C)C1OC(C(O)C(O)C1O)COC1OCC(O)C(O)C1O
MOL001908	0.8731	0.1269	0.7113	Paeoniae Radix Alba	(Z)-(1S,5R)-beta-pinen-10-yl-beta-vicianoside	Not Available	FALSE	O(/C=C/1\C2C(C(C2)CC1)(C)C)C1OC(C(O)C(O)C1O)COC1OCC(O)C(O)C1O
MOL001909	0.9622	0.0378	0.8112	Paeoniae Radix Alba	(Z)-(1S,5R)-beta-pinen-10-yl-beta-vicianoside_qt	Not Available	FALSE	O/C=C/1\C2C(C(C2)CC1)(C)C
MOL001910	0.6130	0.3870	0.7143	Paeoniae Radix Alba	11alpha,12alpha-epoxy-3beta-23-dihydroxy-30-norolean-20-en-28,12beta-olide	Not Available	FALSE	C1(CCC2(C(C1(CO)C)CCC1(C)C3(C)CCC45C(=O)OC6(C3C5CC(=CC4)C)C(C21)O6)C)O
MOL001911	0.8561	0.1439	0.8139	Paeoniae Radix Alba	albiflorin R1	Not Available	FALSE	O1C2C3(C(O)(CC3C(=O)C2)C1(OC1OC(C(O)C(O)C1O)CO)C)COC(=O)c1ccccc1
MOL001912	0.8334	0.1666	0.7860	Paeoniae Radix Alba	albiflorin R1_qt	Not Available	FALSE	O1C2C3(C(O)(CC3C(=O)C2)C1(O)C)COC(=O)c1ccccc1
MOL001913	0.8686	0.1314	0.8891	Paeoniae Radix Alba	propyl (2R)-2-hydroxypropanoate	10654258	FALSE	C(=O)(C(C)O)OCCC
MOL001914	0.7482	0.2518	0.7320	Paeoniae Radix Alba	gallotannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1
MOL001915	0.8733	0.1267	0.8062	Paeoniae Radix Alba	paeonoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL001915	0.8733	0.1267	0.8062	Cortex Moutan	paeonoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1

MOL001917	0.9421	0.0579	0.9004	Paeoniae Radix Alba	(3S,3aR,5S,6S,7aR)-5,6-dihydroxy-3,6-dimethyl-3,3a,4,5,7,7a-hexahydrobenzofuran-2-one	21630941	FALSE	O1C2C(CC(C(C2)(O)C)O)C(C1=O)C
MOL001918	0.7783	0.2217	0.6849	Paeoniae Radix Alba	paeoniflorgenone	Not Available	FALSE	O1C2(C3(OC1C(C(C3)C(=O)C2)COC(=O)c1ccccc1)O)C
MOL001918	0.7783	0.2217	0.6849	Radix Paeoniae Rubra	paeoniflorgenone	Not Available	FALSE	O1C2(C3(OC1C(C(C3)C(=O)C2)COC(=O)c1ccccc1)O)C
MOL001919	0.3949	0.6051	0.9382	Paeoniae Radix Alba	(3S,5R,8R,9R,10S,14S)-3,17-dihydroxy-4,4,8,10,14-pentamethyl-2,3,5,6,7,9-hexahydro-1H-cyclopenta[a]phenanthrene-15,16-dione	9841735	FALSE	OC1C(C2C(C3C(CC2)(C2(C(=C(O)C(=O)C2=O)C=C3)C)C)(CC1)C)(C)C
MOL001921	0.8669	0.1331	0.8199	Radix Paeoniae Rubra	Lactiflorin	Not Available	FALSE	O1C23C4(C(C2)C(OC4=O)(CC3OC2OC(C(O)C(O)C12)CO)C)COC(=O)c1ccccc1
MOL001921	0.8669	0.1331	0.8199	Paeoniae Radix Alba	Lactiflorin	Not Available	FALSE	O1C23C4(C(C2)C(OC4=O)(CC3OC2OC(C(O)C(O)C12)CO)C)COC(=O)c1ccccc1
MOL001922	0.7398	0.2602	0.6244	Maydis Seigma	2-Hexyl-1-decanol	Not Available	FALSE	C(CCCCCCCC)(CCCCCC)CO
MOL001922	0.7398	0.2602	0.6244	Allii Fistulost Bulbus	2-Hexyl-1-decanol	Not Available	FALSE	C(CCCCCCCC)(CCCCCC)CO
MOL001922	0.7398	0.2602	0.6244	Paeoniae Radix Alba	2-Hexyl-1-decanol	Not Available	FALSE	C(CCCCCCCC)(CCCCCC)CO

MOL001923	0.8181	0.1819	0.7616	Paeoniae Radix Alba	[(3S,3aR,6S,7aR)-6-hydroxy-6-methyl-2,5-dioxo-3a,4,7,7a-tetrahydro-3H-benzofuran-3-yl]methyl benzoate	10471123	FALSE	O1C2C(C(C1=O)COC(=O)c1ccccc1)CC(=O)C(O)(C2)C
MOL001924	0.8609	0.1391	0.8300	Cimicifugae Rhizoma	paeoniflorin	Not Available	FALSE	O1C2(C3(OC4OC(C(O)C(O)C4O)CO)C4(C(C3)C(OC14)(O)C2)COC(=O)c1ccccc1)C
MOL001924	0.8609	0.1391	0.8300	Paeoniae Radix Alba	paeoniflorin	Not Available	FALSE	O1C2(C3(OC4OC(C(O)C(O)C4O)CO)C4(C(C3)C(OC14)(O)C2)COC(=O)c1ccccc1)C
MOL001924	0.8609	0.1391	0.8300	Radix Paeoniae Rubra	paeoniflorin	Not Available	FALSE	O1C2(C3(OC4OC(C(O)C(O)C4O)CO)C4(C(C3)C(OC14)(O)C2)COC(=O)c1ccccc1)C
MOL001925	0.8886	0.1114	0.7846	Radix Paeoniae Rubra	paeoniflorin_qt	Not Available	FALSE	O1C2(C3(O)C4(C(C3)C(OC14)(O)C2)COC(=O)c1ccccc1)C
MOL001925	0.8886	0.1114	0.7846	Cortex Moutan	paeoniflorin_qt	Not Available	FALSE	O1C2(C3(O)C4(C(C3)C(OC14)(O)C2)COC(=O)c1ccccc1)C
MOL001925	0.8886	0.1114	0.7846	Figwort Root	paeoniflorin_qt	Not Available	FALSE	O1C2(C3(O)C4(C(C3)C(OC14)(O)C2)COC(=O)c1ccccc1)C
MOL001925	0.8886	0.1114	0.7846	Cimicifugae Rhizoma	paeoniflorin_qt	Not Available	FALSE	O1C2(C3(O)C4(C(C3)C(OC14)(O)C2)COC(=O)c1ccccc1)C
MOL001925	0.8886	0.1114	0.7846	Paeoniae Radix Alba	paeoniflorin_qt	Not Available	FALSE	O1C2(C3(O)C4(C(C3)C(OC14)(O)C2)COC(=O)c1ccccc1)C
MOL001926	0.8542	0.1458	0.6300	Phyllanthi Fructus	1,2,3,6-tetra-O-galloylglucose	Not Available	FALSE	O=C(C(O)(C(O)(C(O)C(O)C(O)C(=O)c1cc(O)c(O)c(O)c1)C(=O)c1cc(O)c(O)c(O)c1)C(=O)c1cc(O)c(O)c(O)c(O)c1)C(=O)c1cc(O)c(O)c(O)c1
MOL001926	0.8542	0.1458	0.6300	Euphorbiae Helioscopiae Herba	1,2,3,6-tetra-O-galloylglucose	Not Available	FALSE	O=C(C(O)(C(O)(C(O)C(O)C(O)C(=O)c1cc(O)c(O)c(O)c1)C(=O)c1cc(O)c(O)c(O)c1)C(=O)c1cc(O)c(O)c(O)c(O)c1)C(=O)c1cc(O)c(O)c(O)c1
MOL001926	0.8542	0.1458	0.6300	Paeoniae Radix Alba	1,2,3,6-tetra-O-galloylglucose	Not Available	FALSE	O=C(C(O)(C(O)(C(O)C(O)C(O)C(=O)c1cc(O)c(O)c(O)c1)C(=O)c1cc(O)c(O)c(O)c1)C(=O)c1cc(O)c(O)c(O)c(O)c1)C(=O)c1cc(O)c(O)c(O)c1
MOL001927	0.8571	0.1429	0.8299	Paeoniae Radix Alba	albiflorin	Not Available	FALSE	O1C2(C3(OC4OC(C(O)C(O)C4O)CO)C(C(C3)C(O)C2)(C1=O)COC(=O)c1ccccc1)C
MOL001928	0.8788	0.1212	0.7799	Paeoniae Radix Alba	albiflorin_qt	Not Available	FALSE	O1C2(C3(O)C(C(C3)C(O)C2)(C1=O)COC(=O)c1ccccc1)C
MOL001931	0.9013	0.0987	0.9725	Paeoniae Radix Alba	4-Chlorobutyric acid	12300	FALSE	C(C(=O)O)CCCl

MOL001932	0.8069	0.1931	0.8074	Paeoniae Radix Alba	galloylpaeoniflorin	Not Available	FALSE	O1C2(C3(OC4OC(C(O)C(O)C4O)COC(=O)c4cc(O)c(O)c(O)c4)C4(C(C3)C(OC14)(O)C2)COC(=O)c1ccccc1)C
MOL001932	0.8069	0.1931	0.8074	Radix Paeoniae Rubra	galloylpaeoniflorin	Not Available	FALSE	O1C2(C3(OC4OC(C(O)C(O)C4O)COC(=O)c4cc(O)c(O)c(O)c4)C4(C(C3)C(OC14)(O)C2)COC(=O)c1ccccc1)C
MOL001933	0.8857	0.1143	0.8322	Paeoniae Radix Alba	oxypaeoniflorin	Not Available	FALSE	O1C2(C3(OC4OC(C(O)C(O)C4O)CO)C4(C(C3)C(OC14)(O)C2)COC(=O)c1ccc(O)cc1)C
MOL001934	0.9336	0.0664	0.8879	Paeoniae Radix Alba	(3R,3aR,6S,7aR)-6-hydroxy-3,6-dimethyl-3a,4,7,7a-tetrahydro-3H-benzofuran-2,5-dione	10081437	FALSE	O1C2C(C(C1=O)C)CC(=O)C(O)(C2)C
MOL001935	0.9335	0.0665	0.8933	Paeoniae Radix Alba	(3aR,6S,7aR)-6-hydroxy-6-methyl-3-methylene-3a,4,7,7a-tetrahydrobenzofuran-2,5-dione	10375422	FALSE	O1C2C(CC(=O)C(O)(C2)C)C(=C)C1=O
MOL001936	0.9241	0.0759	0.9423	Paeoniae Radix Alba	cis-5-Octen-1-ol	5352837	FALSE	C(/C=C\CC)CCCO
MOL001937	0.9265	0.0735	0.9552	Paeoniae Radix Alba	24253-30-3	141082	FALSE	CCC(=O)CC=C
MOL001938	0.7778	0.2222	0.6850	Forsythiae Fructus	Secoisolariciresinol	65373	FALSE	OCC(C(Cc1cc(OC)c(O)cc1)CO)Cc1cc(OC)c(O)cc1
MOL001938	0.7778	0.2222	0.6850	Glehniae Radix	Secoisolariciresinol	65373	FALSE	OCC(C(Cc1cc(OC)c(O)cc1)CO)Cc1cc(OC)c(O)cc1
MOL001938	0.7778	0.2222	0.6850	Drynariae Rhizoma	Secoisolariciresinol	65373	FALSE	OCC(C(Cc1cc(OC)c(O)cc1)CO)Cc1cc(OC)c(O)cc1
MOL001939	0.7737	0.2263	0.8981	Glehniae Radix	Alloisoimperatorin	5317436	FALSE	c1(=O)ccc2c(o1)c(c1c(c2O)cco1)CC=C(C)C
MOL001939	0.7737	0.2263	0.8981	A. Dahurica (Fisch.) Benth. Et Hook	Alloisoimperatorin	5317436	FALSE	c1(=O)ccc2c(o1)c(c1c(c2O)cco1)CC=C(C)C
MOL001939	0.7737	0.2263	0.8981	Saussureae Involucratae Herba	Alloisoimperatorin	5317436	FALSE	c1(=O)ccc2c(o1)c(c1c(c2O)cco1)CC=C(C)C
MOL001940	0.7023	0.2977	0.6696	Notopterygii Rhizoma Et Radix	Falcarindiol	5281148	FALSE	OC(/C=C\CCCCCCC)C#CC#CC(O)C=C
MOL001940	0.7023	0.2977	0.6696	Peucedani Radix	Falcarindiol	5281148	FALSE	OC(/C=C\CCCCCCC)C#CC#CC(O)C=C
MOL001940	0.7023	0.2977	0.6696	Glehniae Radix	Falcarindiol	5281148	FALSE	OC(/C=C\CCCCCCC)C#CC#CC(O)C=C

MOL001940	0.7023	0.2977	0.6696	A. Dahurica (Fisch.) Benth. Et Hook	Falcarindiol	5281148	FALSE	OC(/C=C\CCCCCCC)C#CC#CC(O)C=C
MOL001940	0.7023	0.2977	0.6696	Saposhnikoviae Radix	Falcarindiol	5281148	FALSE	OC(/C=C\CCCCCCC)C#CC#CC(O)C=C
MOL001941	0.7499	0.2501	0.7918	Notopterygii Rhizoma Et Radix	Ammidin	10212	FALSE	O(c1c2occc2cc2c1oc(=O)cc2)CC=C(C)C
MOL001941	0.7499	0.2501	0.7918	Coriandri Sativi Herba	Ammidin	10212	FALSE	O(c1c2occc2cc2c1oc(=O)cc2)CC=C(C)C
MOL001941	0.7499	0.2501	0.7918	Saposhnikoviae Radix	Ammidin	10212	FALSE	O(c1c2occc2cc2c1oc(=O)cc2)CC=C(C)C
MOL001941	0.7499	0.2501	0.7918	Cnidii Fructus	Ammidin	10212	FALSE	O(c1c2occc2cc2c1oc(=O)cc2)CC=C(C)C
MOL001941	0.7499	0.2501	0.7918	Glehniae Radix	Ammidin	10212	FALSE	O(c1c2occc2cc2c1oc(=O)cc2)CC=C(C)C
MOL001941	0.7499	0.2501	0.7918	A. Dahurica (Fisch.) Benth. Et Hook	Ammidin	10212	FALSE	O(c1c2occc2cc2c1oc(=O)cc2)CC=C(C)C
MOL001941	0.7499	0.2501	0.7918	Rubi Fructus	Ammidin	10212	FALSE	O(c1c2occc2cc2c1oc(=O)cc2)CC=C(C)C
MOL001941	0.7499	0.2501	0.7918	Gardeniae Fructus	Ammidin	10212	FALSE	O(c1c2occc2cc2c1oc(=O)cc2)CC=C(C)C
MOL001941	0.7499	0.2501	0.7918	Peucedanidecursivi Radix	Ammidin	10212	FALSE	O(c1c2occc2cc2c1oc(=O)cc2)CC=C(C)C
MOL001941	0.7499	0.2501	0.7918	Foeniculi Fructus	Ammidin	10212	FALSE	O(c1c2occc2cc2c1oc(=O)cc2)CC=C(C)C
MOL001941	0.7499	0.2501	0.7918	Peucedani Radix	Ammidin	10212	FALSE	O(c1c2occc2cc2c1oc(=O)cc2)CC=C(C)C
MOL001941	0.7499	0.2501	0.7918	Radix Angelicae Biseratae	Ammidin	10212	FALSE	O(c1c2occc2cc2c1oc(=O)cc2)CC=C(C)C
MOL001941	0.7499	0.2501	0.7918	Aurantii Fructus Immaturus	Ammidin	10212	FALSE	O(c1c2occc2cc2c1oc(=O)cc2)CC=C(C)C
MOL001942	0.7394	0.2606	0.8281	A. Dahurica (Fisch.) Benth. Et Hook	isoimperatorin	68081	FALSE	O(c1c2c(occ2)cc2oc(=O)ccc12)CC=C(C)C
MOL001942	0.7394	0.2606	0.8281	Radix Salviae	isoimperatorin	68081	FALSE	O(c1c2c(occ2)cc2oc(=O)ccc12)CC=C(C)C
MOL001942	0.7394	0.2606	0.8281	Glehniae Radix	isoimperatorin	68081	FALSE	O(c1c2c(occ2)cc2oc(=O)ccc12)CC=C(C)C
MOL001942	0.7394	0.2606	0.8281	Citri Exocarpium Rubrum	isoimperatorin	68081	FALSE	O(c1c2c(occ2)cc2oc(=O)ccc12)CC=C(C)C
MOL001942	0.7394	0.2606	0.8281	Rhododendri Daurici Folium	isoimperatorin	68081	FALSE	O(c1c2c(occ2)cc2oc(=O)ccc12)CC=C(C)C
MOL001942	0.7394	0.2606	0.8281	Radix Angelicae Biseratae	isoimperatorin	68081	FALSE	O(c1c2c(occ2)cc2oc(=O)ccc12)CC=C(C)C
MOL001942	0.7394	0.2606	0.8281	Peucedani Radix	isoimperatorin	68081	FALSE	O(c1c2c(occ2)cc2oc(=O)ccc12)CC=C(C)C
MOL001942	0.7394	0.2606	0.8281	Peucedanidecursivi Radix	isoimperatorin	68081	FALSE	O(c1c2c(occ2)cc2oc(=O)ccc12)CC=C(C)C
MOL001944	0.8901	0.1099	0.8313	Anemarrhenae Rhizoma	Marmesin	334704	FALSE	O1C(C(O)(C)C)Cc2c1cc1oc(=O)ccc1c2
MOL001944	0.8901	0.1099	0.8313	Notopterygii Rhizoma Et Radix	Marmesin	334704	FALSE	O1C(C(O)(C)C)Cc2c1cc1oc(=O)ccc1c2
MOL001944	0.8901	0.1099	0.8313	Saposhnikoviae Radix	Marmesin	334704	FALSE	O1C(C(O)(C)C)Cc2c1cc1oc(=O)ccc1c2
MOL001944	0.8901	0.1099	0.8313	Acoritataninowii Rhizoma	Marmesin	334704	FALSE	O1C(C(O)(C)C)Cc2c1cc1oc(=O)ccc1c2
MOL001944	0.8901	0.1099	0.8313	Peucedani Radix	Marmesin	334704	FALSE	O1C(C(O)(C)C)Cc2c1cc1oc(=O)ccc1c2
MOL001944	0.8901	0.1099	0.8313	Radix Angelicae Biseratae	Marmesin	334704	FALSE	O1C(C(O)(C)C)Cc2c1cc1oc(=O)ccc1c2
MOL001944	0.8901	0.1099	0.8313	Glehniae Radix	Marmesin	334704	FALSE	O1C(C(O)(C)C)Cc2c1cc1oc(=O)ccc1c2

MOL001945	0.9178	0.0822	0.7970	Foeniculi Fructus	Majudin	2355	FALSE	o1c2c(c(OC)c3c(oc(=O)cc3)c2)cc1
MOL001945	0.9178	0.0822	0.7970	Peucedani Radix	Majudin	2355	FALSE	o1c2c(c(OC)c3c(oc(=O)cc3)c2)cc1
MOL001945	0.9178	0.0822	0.7970	Peucedanidecursivi Radix	Majudin	2355	FALSE	o1c2c(c(OC)c3c(oc(=O)cc3)c2)cc1
MOL001945	0.9178	0.0822	0.7970	Cnidii Fructus	Majudin	2355	FALSE	o1c2c(c(OC)c3c(oc(=O)cc3)c2)cc1
MOL001945	0.9178	0.0822	0.7970	Santalum Album L.	Majudin	2355	FALSE	o1c2c(c(OC)c3c(oc(=O)cc3)c2)cc1
MOL001945	0.9178	0.0822	0.7970	Acoritataninowii Rhizoma	Majudin	2355	FALSE	o1c2c(c(OC)c3c(oc(=O)cc3)c2)cc1
MOL001945	0.9178	0.0822	0.7970	Radix Angelicae Biseratae	Majudin	2355	FALSE	o1c2c(c(OC)c3c(oc(=O)cc3)c2)cc1
MOL001945	0.9178	0.0822	0.7970	Saposhnikoviae Radix	Majudin	2355	FALSE	o1c2c(c(OC)c3c(oc(=O)cc3)c2)cc1
MOL001945	0.9178	0.0822	0.7970	Zanthoxyli Pericarpium	Majudin	2355	FALSE	o1c2c(c(OC)c3c(oc(=O)cc3)c2)cc1
MOL001945	0.9178	0.0822	0.7970	Notopterygii Rhizoma Et Radix	Majudin	2355	FALSE	o1c2c(c(OC)c3c(oc(=O)cc3)c2)cc1
MOL001945	0.9178	0.0822	0.7970	Phytolaccae Radix	Majudin	2355	FALSE	o1c2c(c(OC)c3c(oc(=O)cc3)c2)cc1
MOL001945	0.9178	0.0822	0.7970	Glehniae Radix	Majudin	2355	FALSE	o1c2c(c(OC)c3c(oc(=O)cc3)c2)cc1
MOL001945	0.9178	0.0822	0.7970	Saussureae Involucratae Herba	Majudin	2355	FALSE	o1c2c(c(OC)c3c(oc(=O)cc3)c2)cc1
MOL001945	0.9178	0.0822	0.7970	Portulacae Herba	Majudin	2355	FALSE	o1c2c(c(OC)c3c(oc(=O)cc3)c2)cc1
MOL001945	0.9178	0.0822	0.7970	Citri Grandis Exocarpium	Majudin	2355	FALSE	o1c2c(c(OC)c3c(oc(=O)cc3)c2)cc1
MOL001945	0.9178	0.0822	0.7970	Aurantii Fructus Immaturus	Majudin	2355	FALSE	o1c2c(c(OC)c3c(oc(=O)cc3)c2)cc1
MOL001945	0.9178	0.0822	0.7970	A. Dahurica (Fisch.) Benth. Et Hook	Majudin	2355	FALSE	o1c2c(c(OC)c3c(oc(=O)cc3)c2)cc1
MOL001945	0.9178	0.0822	0.7970	Coriandri Sativi Herba	Majudin	2355	FALSE	o1c2c(c(OC)c3c(oc(=O)cc3)c2)cc1
MOL001945	0.9178	0.0822	0.7970	Citri Exocarpium Rubrum	Majudin	2355	FALSE	o1c2c(c(OC)c3c(oc(=O)cc3)c2)cc1
MOL001946	0.7905	0.2095	0.7355	Saposhnikoviae Radix	Ammijin	216283	FALSE	O(C(C1Oc2c(C1)cc1c(oc(=O)cc1)c2)(C)C)C1OC(C(O)C(O)C1O)CO
MOL001946	0.7905	0.2095	0.7355	Radix Angelicae Biseratae	Ammijin	216283	FALSE	O(C(C1Oc2c(C1)cc1c(oc(=O)cc1)c2)(C)C)C1OC(C(O)C(O)C1O)CO
MOL001946	0.7905	0.2095	0.7355	Glehniae Radix	Ammijin	216283	FALSE	O(C(C1Oc2c(C1)cc1c(oc(=O)cc1)c2)(C)C)C1OC(C(O)C(O)C1O)CO
MOL001946	0.7905	0.2095	0.7355	Peucedani Radix	Ammijin	216283	FALSE	O(C(C1Oc2c(C1)cc1c(oc(=O)cc1)c2)(C)C)C1OC(C(O)C(O)C1O)CO
MOL001947	0.9389	0.0611	0.8981	Dioscoreaebulbiferae	n-butyl-β-D-fructoufranoside	13386213	FALSE	O1C(OCCCC)(C(O)C(O)C1CO)CO
MOL001947	0.9389	0.0611	0.8981	Bolbostemae Paniculati Bulbus	n-butyl-β-D-fructoufranoside	13386213	FALSE	O1C(OCCCC)(C(O)C(O)C1CO)CO
MOL001947	0.9389	0.0611	0.8981	Smilacis Glabrae Rhixoma	n-butyl-β-D-fructoufranoside	13386213	FALSE	O1C(OCCCC)(C(O)C(O)C1CO)CO
MOL001947	0.9389	0.0611	0.8981	Lobeliae Chinensis Herba	n-butyl-β-D-fructoufranoside	13386213	FALSE	O1C(OCCCC)(C(O)C(O)C1CO)CO

MOL001947	0.9389	0.0611	0.8981	Lilii Bulbus	n-butyl-β-D-fructoufranoside	13386213	FALSE	O1C(OCCCC)(C(O)C(O)C1CO)CO
MOL001947	0.9389	0.0611	0.8981	Semiaquilegiae Radix	n-butyl-β-D-fructoufranoside	13386213	FALSE	O1C(OCCCC)(C(O)C(O)C1CO)CO
MOL001947	0.9389	0.0611	0.8981	Glehniae Radix	n-butyl-β-D-fructoufranoside	13386213	FALSE	O1C(OCCCC)(C(O)C(O)C1CO)CO
MOL001948	0.8661	0.1339	0.8895	Schisandrae Chinensis Fructus	Nootkatin	238797	FALSE	Oc1c(=O)cc(C(C)C)c(CC=C(C)C)cc1
MOL001948	0.8661	0.1339	0.8895	Glehniae Radix	Nootkatin	238797	FALSE	Oc1c(=O)cc(C(C)C)c(CC=C(C)C)cc1
MOL001949	0.6294	0.3706	0.6584	Adenophprae Ae Radix	panaxynol	5281149	FALSE	OC(C#CC#CC/C=C\CCCCCCC)C=C
MOL001949	0.6294	0.3706	0.6584	Panax Ginseng C. A. Mey.	panaxynol	5281149	FALSE	OC(C#CC#CC/C=C\CCCCCCC)C=C
MOL001949	0.6294	0.3706	0.6584	Ginsen Radix Et Rhizoma Rubra	panaxynol	5281149	FALSE	OC(C#CC#CC/C=C\CCCCCCC)C=C
MOL001949	0.6294	0.3706	0.6584	Panacis Quinquefolii Radix	panaxynol	5281149	FALSE	OC(C#CC#CC/C=C\CCCCCCC)C=C
MOL001949	0.6294	0.3706	0.6584	Glehniae Radix	panaxynol	5281149	FALSE	OC(C#CC#CC/C=C\CCCCCCC)C=C
MOL001950	0.9555	0.0445	0.7255	Glehniae Radix	psoralen	6199	TRUE	o1c2c(cc3c(oc(=O)cc3)c2)cc1
MOL001950	0.9555	0.0445	0.7255	Radix Angelicae Biseratae	psoralen	6199	TRUE	o1c2c(cc3c(oc(=O)cc3)c2)cc1
MOL001950	0.9555	0.0445	0.7255	Dictamni Cortex	psoralen	6199	TRUE	o1c2c(cc3c(oc(=O)cc3)c2)cc1
MOL001950	0.9555	0.0445	0.7255	Saposhnikoviae Radix	psoralen	6199	TRUE	o1c2c(cc3c(oc(=O)cc3)c2)cc1
MOL001950	0.9555	0.0445	0.7255	Peucedani Radix	psoralen	6199	TRUE	o1c2c(cc3c(oc(=O)cc3)c2)cc1
MOL001951	0.1467	0.8533	0.6643	Notopterygii Rhizoma Et Radix	Bergaptin	5471349	FALSE	O(c1c2c(occ2)cc2oc(=O)ccc12)C/C=C(/CCC=C(C)C)\C
MOL001951	0.1467	0.8533	0.6643	Glehniae Radix	Bergaptin	5471349	FALSE	O(c1c2c(occ2)cc2oc(=O)ccc12)C/C=C(/CCC=C(C)C)\C
MOL001952	0.9154	0.0846	0.9154	Fructus Ligustri Lucidi	Sinapyl alcohol	5280507	FALSE	Oc1c(OC)cc(cc1OC)/C=C/CO
MOL001952	0.9154	0.0846	0.9154	Jujubae Fructus	Sinapyl alcohol	5280507	FALSE	Oc1c(OC)cc(cc1OC)/C=C/CO
MOL001952	0.9154	0.0846	0.9154	Fraxini Cortex	Sinapyl alcohol	5280507	FALSE	Oc1c(OC)cc(cc1OC)/C=C/CO
MOL001952	0.9154	0.0846	0.9154	Tinosporae Radix	Sinapyl alcohol	5280507	FALSE	Oc1c(OC)cc(cc1OC)/C=C/CO
MOL001952	0.9154	0.0846	0.9154	Ilicis Purpureae Folium	Sinapyl alcohol	5280507	FALSE	Oc1c(OC)cc(cc1OC)/C=C/CO
MOL001952	0.9154	0.0846	0.9154	Glehniae Radix	Sinapyl alcohol	5280507	FALSE	Oc1c(OC)cc(cc1OC)/C=C/CO
MOL001952	0.9154	0.0846	0.9154	Bistortae Rhizoma	Sinapyl alcohol	5280507	FALSE	Oc1c(OC)cc(cc1OC)/C=C/CO
MOL001952	0.9154	0.0846	0.9154	Eucommiae Cortex	Sinapyl alcohol	5280507	FALSE	Oc1c(OC)cc(cc1OC)/C=C/CO

MOL001952	0.9154	0.0846	0.9154	Saussureae Involucratae Herba	Sinapyl alcohol	5280507	FALSE	Oc1c(OC)cc(cc1OC)/C=C/CO
MOL001953	0.9276	0.0724	0.7909	Cnidii Fructus	Uvadex	4114	FALSE	o1c2c(cc3c(oc(=O)cc3)c2OC)cc1
MOL001953	0.9276	0.0724	0.7909	Foeniculi Fructus	Uvadex	4114	FALSE	o1c2c(cc3c(oc(=O)cc3)c2OC)cc1
MOL001953	0.9276	0.0724	0.7909	Glehniae Radix	Uvadex	4114	FALSE	o1c2c(cc3c(oc(=O)cc3)c2OC)cc1
MOL001953	0.9276	0.0724	0.7909	Peucedani Radix	Uvadex	4114	FALSE	o1c2c(cc3c(oc(=O)cc3)c2OC)cc1
MOL001953	0.9276	0.0724	0.7909	A. Dahurica (Fisch.) Benth. Et Hook	Uvadex	4114	FALSE	o1c2c(cc3c(oc(=O)cc3)c2OC)cc1
MOL001953	0.9276	0.0724	0.7909	Saposhnikoviae Radix	Uvadex	4114	FALSE	o1c2c(cc3c(oc(=O)cc3)c2OC)cc1
MOL001953	0.9276	0.0724	0.7909	Dictamni Cortex	Uvadex	4114	FALSE	o1c2c(cc3c(oc(=O)cc3)c2OC)cc1
MOL001953	0.9276	0.0724	0.7909	Radix Angelicae Biseratae	Uvadex	4114	FALSE	o1c2c(cc3c(oc(=O)cc3)c2OC)cc1
MOL001954	0.8884	0.1116	0.7810	Citri Exocarpium Rubrum	Xanthotoxol	65090	FALSE	o1c2c(cc3c(oc(=O)cc3)c2O)cc1
MOL001954	0.8884	0.1116	0.7810	Notopterygii Rhizoma Et Radix	Xanthotoxol	65090	FALSE	o1c2c(cc3c(oc(=O)cc3)c2O)cc1
MOL001954	0.8884	0.1116	0.7810	Cnidii Fructus	Xanthotoxol	65090	FALSE	o1c2c(cc3c(oc(=O)cc3)c2O)cc1
MOL001954	0.8884	0.1116	0.7810	Glehniae Radix	Xanthotoxol	65090	FALSE	o1c2c(cc3c(oc(=O)cc3)c2O)cc1
MOL001954	0.8884	0.1116	0.7810	A. Dahurica (Fisch.) Benth. Et Hook	Xanthotoxol	65090	FALSE	o1c2c(cc3c(oc(=O)cc3)c2O)cc1
MOL001954	0.8884	0.1116	0.7810	Coriandri Sativi Herba	Xanthotoxol	65090	FALSE	o1c2c(cc3c(oc(=O)cc3)c2O)cc1
MOL001955	0.9497	0.0503	0.9440	Calendula Officinalis	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Saussureae Involucratae Herba	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Chaenomeles Sinensis (Thouin) Koehne	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Persicae Semen	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Lonicerae Japonicae Flos	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Ilicis Cornutae Folium Immayuri	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Ginkgo Folium	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Hyperici Japonici Herber	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Inulae Herba	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Coptidis Rhizoma	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1

MOL001955	0.9497	0.0503	0.9440	Uncariae Ramulus Cumuncis	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Anisi Stellati Fructus	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Phellodendri Amurensis Cortex	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Polygoni Avicularis Herba	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Andrographis Herba	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Eucommiae Folium	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Pyrrosiae Folium	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Apocyniveneti Folium	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Eucommiae Cortex	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Evodiae Fructus	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Maydis Seigma	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Solidaginis Herba	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Inulae Flos	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Herbahypericiperforati	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Eriobotryae Folium	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Herba Cirsii	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Cichorii Radix	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Glehniae Radix	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Houttuyniae Herba	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Aucklandiae Radix	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Hedysarum Multijugum Maxim.	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1

MOL001955	0.9497	0.0503	0.9440	Saxifraga Stolonifera	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Ilicis Purpureae Folium	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Gnaphalii Affinis Herba	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Erycibe Obtusifolia Benth	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Croci Stigma	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Cymbopon Citratus(D C.) Stapf	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Stemonae Radix	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Hippophae Fructus	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Radix Salviae	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Hordei Fructus Germinatus	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Boehmeriae Rhizoma Et Radix	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Semen Pharbitidis	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Artemisiae Scopariae Herba	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Notopterygii Rhizoma Et Radix	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Imperatae Rhizoma	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Amygdalus Communis Vas	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Farfarae Flos	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Cyperi Rhizoma	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Plantaginis Herba	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Crataegi Folium	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Bistortae Rhizoma	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1

MOL001955	0.9497	0.0503	0.9440	Gardeniae Fructus	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001955	0.9497	0.0503	0.9440	Carthami Flos	Heriguard	1794427	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL001956	0.7022	0.2978	0.8320	Notopterygii Rhizoma Et Radix	Cnidilin	821449	FALSE	c1(=O)ccc2c(o1)c(c1c(c2OCC=C(C)C)cco1)OC
MOL001956	0.7022	0.2978	0.8320	A. Dahurica (Fisch.) Benth. Et Hook	Cnidilin	821449	FALSE	c1(=O)ccc2c(o1)c(c1c(c2OCC=C(C)C)cco1)OC
MOL001956	0.7022	0.2978	0.8320	Glehniae Radix	Cnidilin	821449	FALSE	c1(=O)ccc2c(o1)c(c1c(c2OCC=C(C)C)cco1)OC
MOL001957	0.7411	0.2589	0.8486	Pulsatilliae Radix	Anemosapogenin	11812750	FALSE	C1(CCC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C(=C)C)C4C3CCC21)C)O
MOL001957	0.7411	0.2589	0.8486	Abri Herba	Anemosapogenin	11812750	FALSE	C1(CCC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C(=C)C)C4C3CCC21)C)O
MOL001958	0.6921	0.3079	0.7683	Pulsatilliae Radix	3-O-alpha-L-Arabinopyranosyl-3 beta,23-dihydroxy-lup-20(29)-en-28-oic acid	Not Available	FALSE	C1(C(C(OCC1O)OC1C(C2C(CC1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=C)C)C(=O)O)C)C)C)(C)CO)O)O
MOL001959	0.7411	0.2589	0.8486	Pulsatilliae Radix	3-O-alpha-L-Arabinopyranosyl-3 beta,23-dihydroxy-lup-20(29)-en-28-oic acid_qt	Not Available	FALSE	OC1C(C2C(CC1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=C)C)C(=O)O)C)C)C)(C)CO
MOL001960	0.7411	0.2589	0.8486	Pulsatilliae Radix	Anemosapogenin	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=C)C)C(=O)O)C)C)C)(C)CO)O
MOL001961	0.6858	0.3142	0.8313	Pulsatilliae Radix	Anemoside A3	Not Available	FALSE	C1C(C(C(C(O1)OC1C(OC(C(C1O)O)C)OC1C(C2C(CC1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(C(=O)O)CCC1C(=C)C)C)C)(CO)C)O)O)O
MOL001962	0.7411	0.2589	0.8486	Pulsatilliae Radix	Anemoside B4_qt	Not Available	FALSE	OC1C(C2C(CC1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(C(=O)O)CCC1C(=C)C)C)C)(CO)C
MOL001963	0.7705	0.2295	0.7996	Pulsatilliae Radix	Anemoside B4	Not Available	FALSE	C1(C(C(C(OC1)OC1C(OC(C(C1O)O)C)OC1C(C2C(CC1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=C)C)C(=O)OC1OC(C(C(C1O)O)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)C)C)C)(C)CO)O)
MOL001964	0.7022	0.2978	0.7632	Caulis Akebiae	Cauloside A	441928	FALSE	C1C(CC2C(C1)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(CO)C)OC1OCC(C(C1O)O)O)C)C)C)C)C(=O)O)(C)C
MOL001964	0.7022	0.2978	0.7632	Pulsatilliae Radix	Cauloside A	441928	FALSE	C1C(CC2C(C1)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(CO)C)OC1OCC(C(C1O)O)O)C)C)C)C)C(=O)O)(C)C

MOL001965	0.1194	0.8806	0.9113	Boschniakia Rossica Herba	Dauricine (8CI)	73400	FALSE	C1N(C(c2c(C1)cc(c(c2)OC)OC)Cc1cc(Oc2ccc(CC3c4cc(c(OC)cc4CCN3C)OC)cc2)c(cc1)O)C
MOL001965	0.1194	0.8806	0.9113	Menispermi Rhizoma	Dauricine (8CI)	73400	FALSE	C1N(C(c2c(C1)cc(c(c2)OC)OC)Cc1cc(Oc2ccc(CC3c4cc(c(OC)cc4CCN3C)OC)cc2)c(cc1)O)C
MOL001965	0.1194	0.8806	0.9113	Cistanches Herba	Dauricine (8CI)	73400	FALSE	C1N(C(c2c(C1)cc(c(c2)OC)OC)Cc1cc(Oc2ccc(CC3c4cc(c(OC)cc4CCN3C)OC)cc2)c(cc1)O)C
MOL001965	0.1194	0.8806	0.9113	Pulsatilliae Radix	Dauricine (8CI)	73400	FALSE	C1N(C(c2c(C1)cc(c(c2)OC)OC)Cc1cc(Oc2ccc(CC3c4cc(c(OC)cc4CCN3C)OC)cc2)c(cc1)O)C
MOL001965	0.1194	0.8806	0.9113	Caulis Akebiae	Dauricine (8CI)	73400	FALSE	C1N(C(c2c(C1)cc(c(c2)OC)OC)Cc1cc(Oc2ccc(CC3c4cc(c(OC)cc4CCN3C)OC)cc2)c(cc1)O)C
MOL001965	0.1194	0.8806	0.9113	Panax Ginseng C. A. Mey.	Dauricine (8CI)	73400	FALSE	C1N(C(c2c(C1)cc(c(c2)OC)OC)Cc1cc(Oc2ccc(CC3c4cc(c(OC)cc4CCN3C)OC)cc2)c(cc1)O)C
MOL001965	0.1194	0.8806	0.9113	Phellodendri Chinrnsis Cortex	Dauricine (8CI)	73400	FALSE	C1N(C(c2c(C1)cc(c(c2)OC)OC)Cc1cc(Oc2ccc(CC3c4cc(c(OC)cc4CCN3C)OC)cc2)c(cc1)O)C
MOL001965	0.1194	0.8806	0.9113	Andrographis Herba	Dauricine (8CI)	73400	FALSE	C1N(C(c2c(C1)cc(c(c2)OC)OC)Cc1cc(Oc2ccc(CC3c4cc(c(OC)cc4CCN3C)OC)cc2)c(cc1)O)C
MOL001966	0.7443	0.2557	0.8531	Pulsatilliae Radix	Hederagenin 3-O-arabinoside	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1OC(C(C(C1O)O)OC1OC(C(C(C1O)O)O)C(=O)O)CO)C)C)(C)CO)O
MOL001966	0.7443	0.2557	0.8531	Radix Clematidis	Hederagenin 3-O-arabinoside	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1OC(C(C(C1O)O)OC1OC(C(C(C1O)O)O)C(=O)O)CO)C)C)(C)CO)O
MOL001967	0.6877	0.3123	0.8326	Pulsatilliae Radix	Hederagenin-28-O-beta-D-glucuronopyranosyl-(1-4)-beta-D-glucopyranoside	11721847	FALSE	C1(CCC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C(=C)C)C4C3CCC21)C)OC1C(OC2C(O)C(O)C(O)C(O2)C)C(O)C(O)CO1
MOL001968	0.7613	0.2387	0.8412	Pulsatilliae Radix	Hederagenin-28-O-beta-D-glucuronopyranosyl-(1-4)-beta-D-glucopyranoside_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)CO)O
MOL001969	0.7705	0.2295	0.7877	Pulsatilliae Radix	Pulchinenoside A	Not Available	FALSE	C1(C(C(C(O1)OC1C(C(COC1OC1C(CC)(C2C(CC1)(C1C(CC2)(CCC1C(=C)C)C(=O)OC1C(C(C(C(C1)COC1C(C(C(C(O1)CO)OC1OC(C(C(C1O)O)O)C)O)O)O)O)O)C)C)C)O)O)O)O)O)C
MOL001970	0.7760	0.2240	0.8338	Pulsatilliae Radix	Pulchinenoside C	Not Available	FALSE	C1CC(C(C2C1(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1C(C(C(C(O1)COC1OC(C(C(C1O)O)OC1C(C(C(C(O1)C)O)O)O)O)CO)O)O)O)C)C)C)(CO)C)O

MOL001971	0.7112	0.2888	0.8716	Pulsatilliae Radix	Pulchinenoside C_qt	Not Available	FALSE	OC1C(CC)(C2C(CC1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=C)C)C(=O)O)C)C)C)C
MOL001972	0.9571	0.0429	0.9601	Cistanches Herba	Pulegone	442495	FALSE	C1C(CCC(=C(C)C)C1=O)C
MOL001972	0.9571	0.0429	0.9601	Pulsatilliae Radix	Pulegone	442495	FALSE	C1C(CCC(=C(C)C)C1=O)C
MOL001972	0.9571	0.0429	0.9601	Epimrdii Herba	Pulegone	442495	FALSE	C1C(CCC(=C(C)C)C1=O)C
MOL001972	0.9571	0.0429	0.9601	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	Pulegone	442495	FALSE	C1C(CCC(=C(C)C)C1=O)C
MOL001972	0.9571	0.0429	0.9601	Menthae Herba	Pulegone	442495	FALSE	C1C(CCC(=C(C)C)C1=O)C
MOL001972	0.9571	0.0429	0.9601	Siphonostegiae Herba	Pulegone	442495	FALSE	C1C(CCC(=C(C)C)C1=O)C
MOL001972	0.9571	0.0429	0.9601	Panacis Quinquefolii Radix	Pulegone	442495	FALSE	C1C(CCC(=C(C)C)C1=O)C
MOL001972	0.9571	0.0429	0.9601	Radix Bupleuri	Pulegone	442495	FALSE	C1C(CCC(=C(C)C)C1=O)C
MOL001972	0.9571	0.0429	0.9601	Lysimachiae Herba	Pulegone	442495	FALSE	C1C(CCC(=C(C)C)C1=O)C
MOL001973	0.2058	0.7942	0.6203	Lysimachiae Foenigraeci Herba	Sitosteryl acetate	5354503	FALSE	C12C(C3(C(=CC2)CC(CC3)OC(=O)C)C)CCC2(C1CCC2C(CCC(C(C)C)CC)C)C
MOL001973	0.2058	0.7942	0.6203	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Sitosteryl acetate	5354503	FALSE	C12C(C3(C(=CC2)CC(CC3)OC(=O)C)C)CCC2(C1CCC2C(CCC(C(C)C)CC)C)C
MOL001973	0.2058	0.7942	0.6203	Scutellariae Barbatae Herba	Sitosteryl acetate	5354503	FALSE	C12C(C3(C(=CC2)CC(CC3)OC(=O)C)C)CCC2(C1CCC2C(CCC(C(C)C)CC)C)C
MOL001973	0.2058	0.7942	0.6203	Allium Azureum Ledeb.	Sitosteryl acetate	5354503	FALSE	C12C(C3(C(=CC2)CC(CC3)OC(=O)C)C)CCC2(C1CCC2C(CCC(C(C)C)CC)C)C
MOL001973	0.2058	0.7942	0.6203	Pulsatilliae Radix	Sitosteryl acetate	5354503	FALSE	C12C(C3(C(=CC2)CC(CC3)OC(=O)C)C)CCC2(C1CCC2C(CCC(C(C)C)CC)C)C
MOL001973	0.2058	0.7942	0.6203	Ranunculi Ternati Radix	Sitosteryl acetate	5354503	FALSE	C12C(C3(C(=CC2)CC(CC3)OC(=O)C)C)CCC2(C1CCC2C(CCC(C(C)C)CC)C)C

MOL001974	0.7765	0.2235	0.8032	Pulsatilliae Radix	[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydropyran-2-yl]oxymethyl]tetrahydropyran-2-yl](4aS,6aR,6aS,6bR,8aR,9R,10S,12aR,14bS)-10-[(2S,3R,4S,5S)-4,5-dihydroxy-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-me	21627940	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(CO)C)OC1C(OC3C(C(C(C(O3)C)O)O)O)C(C(CO1)O)O)C)CC(CC2)(C)C)C(=O)OC1OC(COC2OC(C(C(C2O)O)O)CO)C(C(C1O)O)O
MOL001976	0.5677	0.4323	0.7791	Pulsatilliae Radix	androstane-3,11,17-triol	58857078	FALSE	OC1C2C(C3C(C1)(C(O)CC3)C)CCC1C2(CCC(O)C1)C
MOL001977	0.9121	0.0879	0.8283	Pulsatilliae Radix	cernuoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(O/C(=C/c3cc(O)c(O)cc3)/C2=O)cc(O)c1)CO
MOL001978	0.9298	0.0702	0.8874	Pulsatilliae Radix	Aureusidin	5281220	FALSE	Oc1c2c(O/C(=C\c3cc(O)c(O)cc3)/C2=O)cc(O)c1
MOL001978	0.9298	0.0702	0.8874	Drynariae Rhizoma	Aureusidin	5281220	FALSE	Oc1c2c(O/C(=C\c3cc(O)c(O)cc3)/C2=O)cc(O)c1
MOL001979	0.2068	0.7932	0.7271	Lycii Fructus	LAN	246983	FALSE	C12=C(C3(C(CC2)C(C(CC3)O)(C)C)C)CCC2(C1(CCC2C(CCC=C(C)C)C)C)C
MOL001979	0.2068	0.7932	0.7271	Hippophae Fructus	LAN	246983	FALSE	C12=C(C3(C(CC2)C(C(CC3)O)(C)C)C)CCC2(C1(CCC2C(CCC=C(C)C)C)C)C
MOL001979	0.2068	0.7932	0.7271	Pulsatilliae Radix	LAN	246983	FALSE	C12=C(C3(C(CC2)C(C(CC3)O)(C)C)C)CCC2(C1(CCC2C(CCC=C(C)C)C)C)C
MOL001979	0.2068	0.7932	0.7271	Radix Euphorbiae Pekinensis	LAN	246983	FALSE	C12=C(C3(C(CC2)C(C(CC3)O)(C)C)C)CCC2(C1(CCC2C(CCC=C(C)C)C)C)C
MOL001980	0.7028	0.2972	0.8314	Dipsaci Radix	Helixin	73296	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1OC1OC(C(O)C(O)C1O)C
MOL001980	0.7028	0.2972	0.8314	Lonicerae Japonicae Flos	Helixin	73296	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1OC1OC(C(O)C(O)C1O)C

MOL001980	0.7028	0.2972	0.8314	Pulsatilliae Radix	Helixin	73296	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1OC1OC(C(O)C(O)C1O)C
MOL001981	0.7403	0.2597	0.8448	Pulsatilliae Radix	pulsatilla saponin D	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C)C1OCC(OC2OC(C(O)C(O)C2O)CO)C(O)C1OC1OC(C(O)C(O)C1O)C
MOL001982	0.7613	0.2387	0.8412	Dipsaci Radix	disacoside B_qt	40469778	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C
MOL001982	0.7613	0.2387	0.8412	Pulsatilliae Radix	disacoside B_qt	40469778	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C
MOL001982	0.7613	0.2387	0.8412	Lonicerae Japonicae Flos	disacoside B_qt	40469778	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C
MOL001983	0.7617	0.2383	0.8543	Pulsatilliae Radix	3beta,23-Dihydroxy-lup-20(29)-ene-28-O-alpha-L-rhamnopyranosyl-(1-4)-beta-D-glucopyranosyl(1-6)-beta-D-glucopyranoside	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=C)C)OC1C(C(C(C(COC2C(C(C(C(CO)O2)OC2OC(C(C(C2O)O)O)C)O)O)O)O1)O)O)O)C)C)(O)C)O
MOL001984	0.3873	0.6127	0.7005	Pulsatilliae Radix	3beta,23-Dihydroxy-lup-20(29)-ene-28-O-alpha-L-rhamnopyranosyl-(1-4)-beta-D-glucopyranosyl(1-6)-beta-D-glucopyranoside_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=C)C)O)C)C)C)(O)C)O
MOL001985	0.5750	0.4250	0.6895	Pulsatilliae Radix	ZINC01615307	11862128	FALSE	O1CC2C(C(c3c(C2)c(O)c2OCOc2c3)c2cc(OC)c(OC)c(OC)c2)C1=O
MOL001987	0.6562	0.3438	0.6630	Pulsatilliae Radix	β-sitosterol	Not Available	FALSE	C1(OC(C(C1O)O)Oc1c2c(cc3c1CC1C(C3c3cc(c(c(c3)OC)OC)OC)C(=O)OC1)OCO2)CO
MOL001988	0.5750	0.4250	0.6895	Pulsatilliae Radix	AIDS045703	466155	FALSE	Oc1c2c(cc3c1CC1C(C3c3cc(c(c(c3)OC)OC)OC)C(=O)OC1)OCO2

MOL001989	0.7520	0.2480	0.8051	Pulsatilliae Radix	Anemoside A	Not Available	FALSE	C1CCC2(C(C1C(=C)C)C1C(CC2)(C2C(CC1)C1(C(CC2)C(C(CC1)OC1OCC(C(C1CC1CC(C(C(C1O)O)O)C)O)O)CO)C)C)C(=O)O
MOL001990	0.7724	0.2276	0.7975	Pulsatilliae Radix	Anemoside B	71307558	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=C)C)C(=O)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)OC1C(C(C(C(O1)C)O)O)O)CO)C)C)(CO)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)C)O)O
MOL001991	0.7411	0.2589	0.8486	Pulsatilliae Radix	Anemoside B_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=C)C)C(=O)O)C)C)(CO)C)O
MOL001994	0.9621	0.0379	0.8052	Pulsatilliae Radix	3-Methylcoumarin	17130	FALSE	c12c(oc(=O)c(c1)C)cccc2
MOL001995	0.8958	0.1042	0.8907	Pulsatilliae Radix	2,5-Furandione	7923	FALSE	C1(=O)C=CC(=O)O1
MOL001996	0.7018	0.2982	0.8872	Anisi Stellati Fructus	Betulonic acid	122844	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C2CCC2C1(CCC1(C2C(CC1)C(=C)C)C(=O)O)C)C)C
MOL001996	0.7018	0.2982	0.8872	Gleditsiae Fructus	Betulonic acid	122844	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C2CCC2C1(CCC1(C2C(CC1)C(=C)C)C(=O)O)C)C)C
MOL001996	0.7018	0.2982	0.8872	Jujubae Fructus	Betulonic acid	122844	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C2CCC2C1(CCC1(C2C(CC1)C(=C)C)C(=O)O)C)C)C
MOL001996	0.7018	0.2982	0.8872	Fructuslipuidambaris	Betulonic acid	122844	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C2CCC2C1(CCC1(C2C(CC1)C(=C)C)C(=O)O)C)C)C
MOL001996	0.7018	0.2982	0.8872	Humulus Scandens (Lour.) Merr.	Betulonic acid	122844	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C2CCC2C1(CCC1(C2C(CC1)C(=C)C)C(=O)O)C)C)C
MOL001996	0.7018	0.2982	0.8872	Pulsatilliae Radix	Betulonic acid	122844	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C2CCC2C1(CCC1(C2C(CC1)C(=C)C)C(=O)O)C)C)C
MOL001996	0.7018	0.2982	0.8872	Gleditsiae Spina	Betulonic acid	122844	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C2CCC2C1(CCC1(C2C(CC1)C(=C)C)C(=O)O)C)C)C
MOL001996	0.7018	0.2982	0.8872	Gnaphalii Affinis Herba	Betulonic acid	122844	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C2CCC2C1(CCC1(C2C(CC1)C(=C)C)C(=O)O)C)C)C
MOL001996	0.7018	0.2982	0.8872	Rosae Laevigatae Fructus	Betulonic acid	122844	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C2CCC2C1(CCC1(C2C(CC1)C(=C)C)C(=O)O)C)C)C
MOL001996	0.7018	0.2982	0.8872	Cornus Officinalis Sieb. Et Zucc.	Betulonic acid	122844	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C2CCC2C1(CCC1(C2C(CC1)C(=C)C)C(=O)O)C)C)C
MOL001996	0.7018	0.2982	0.8872	Herba Sarcandrae	Betulonic acid	122844	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C2CCC2C1(CCC1(C2C(CC1)C(=C)C)C(=O)O)C)C)C
MOL001996	0.7018	0.2982	0.8872	Forsythiae Fructus	Betulonic acid	122844	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C2CCC2C1(CCC1(C2C(CC1)C(=C)C)C(=O)O)C)C)C
MOL001997	0.9700	0.0300	0.8005	Zanthoxylum Nitidum	5,6,7-Trimethoxycoumarin	148724	FALSE	o1c(=O)ccc2c(c(c(cc12)OC)OC)OC

MOL001997	0.9700	0.0300	0.8005	Pulsatilliae Radix	5,6,7-Trimethoxycoumarin	148724	FALSE	o1c(=O)ccc2c(c(c(cc12)OC)OC)OC
MOL001999	0.9562	0.0438	0.8392	Herba Sarcandrae	scoparone	8417	FALSE	c12c(cc(c(c1)OC)OC)oc(=O)cc2
MOL001999	0.9562	0.0438	0.8392	Folium Ilicis Cornutae	scoparone	8417	FALSE	c12c(cc(c(c1)OC)OC)oc(=O)cc2
MOL001999	0.9562	0.0438	0.8392	Cyathulae Radix	scoparone	8417	FALSE	c12c(cc(c(c1)OC)OC)oc(=O)cc2
MOL001999	0.9562	0.0438	0.8392	Citri Sarcodactylis Fructus	scoparone	8417	FALSE	c12c(cc(c(c1)OC)OC)oc(=O)cc2
MOL001999	0.9562	0.0438	0.8392	Radix Bupleuri	scoparone	8417	FALSE	c12c(cc(c(c1)OC)OC)oc(=O)cc2
MOL001999	0.9562	0.0438	0.8392	Lobeliae Chinensis Herba	scoparone	8417	FALSE	c12c(cc(c(c1)OC)OC)oc(=O)cc2
MOL001999	0.9562	0.0438	0.8392	Pulsatilliae Radix	scoparone	8417	FALSE	c12c(cc(c(c1)OC)OC)oc(=O)cc2
MOL001999	0.9562	0.0438	0.8392	Artemisiae Scopariae Herba	scoparone	8417	FALSE	c12c(cc(c(c1)OC)OC)oc(=O)cc2
MOL001999	0.9562	0.0438	0.8392	Radix Puerariae	scoparone	8417	FALSE	c12c(cc(c(c1)OC)OC)oc(=O)cc2
MOL001999	0.9562	0.0438	0.8392	Canarii Fructus	scoparone	8417	FALSE	c12c(cc(c(c1)OC)OC)oc(=O)cc2
MOL001999	0.9562	0.0438	0.8392	Artemisia Annua L.	scoparone	8417	FALSE	c12c(cc(c(c1)OC)OC)oc(=O)cc2
MOL001999	0.9562	0.0438	0.8392	Folium Artemisiae Argyi	scoparone	8417	FALSE	c12c(cc(c(c1)OC)OC)oc(=O)cc2
MOL002000	0.9298	0.0702	0.7749	Pulsatilliae Radix	Fraxinol	3047739	FALSE	o1c(=O)ccc2c(c(c(cc12)OC)O)OC
MOL002000	0.9298	0.0702	0.7749	Lobeliae Chinensis Herba	Fraxinol	3047739	FALSE	o1c(=O)ccc2c(c(c(cc12)OC)O)OC
MOL002001	0.6382	0.3618	0.8180	Radix Salviae	Oleanolic acid deriv.	151202	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)OC(=O)C
MOL002001	0.6382	0.3618	0.8180	Rubia Cordifolia	Oleanolic acid deriv.	151202	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)OC(=O)C
MOL002001	0.6382	0.3618	0.8180	Gleditsiae Spina	Oleanolic acid deriv.	151202	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)OC(=O)C
MOL002001	0.6382	0.3618	0.8180	Boschniakia Rossica Herba	Oleanolic acid deriv.	151202	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)OC(=O)C
MOL002001	0.6382	0.3618	0.8180	Fructus Ligustri Lucidi	Oleanolic acid deriv.	151202	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)OC(=O)C
MOL002001	0.6382	0.3618	0.8180	Pulsatilliae Radix	Oleanolic acid deriv.	151202	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)OC(=O)C
MOL002002	0.9566	0.0434	0.9769	Artemisia Annua L.	cis-Carveol	330573	FALSE	C1(C(=CCC(C1)C(=C)C)C)O
MOL002002	0.9566	0.0434	0.9769	Stephaniae Tetrandrae Radix	cis-Carveol	330573	FALSE	C1(C(=CCC(C1)C(=C)C)C)O
MOL002002	0.9566	0.0434	0.9769	Folium Artemisiae Argyi	cis-Carveol	330573	FALSE	C1(C(=CCC(C1)C(=C)C)C)O
MOL002002	0.9566	0.0434	0.9769	Canarii Fructus	cis-Carveol	330573	FALSE	C1(C(=CCC(C1)C(=C)C)C)O
MOL002002	0.9566	0.0434	0.9769	Magnolia Officinalis Rehd Et Wils.	cis-Carveol	330573	FALSE	C1(C(=CCC(C1)C(=C)C)C)O
MOL002002	0.9566	0.0434	0.9769	Radix Bupleuri	cis-Carveol	330573	FALSE	C1(C(=CCC(C1)C(=C)C)C)O
MOL002002	0.9566	0.0434	0.9769	Citri Fructus Retinervus	cis-Carveol	330573	FALSE	C1(C(=CCC(C1)C(=C)C)C)O
MOL002002	0.9566	0.0434	0.9769	Kadsurae Coccineae Radix Et Caulis	cis-Carveol	330573	FALSE	C1(C(=CCC(C1)C(=C)C)C)O
MOL002002	0.9566	0.0434	0.9769	Rhododendri Daurici Folium	cis-Carveol	330573	FALSE	C1(C(=CCC(C1)C(=C)C)C)O

MOL002002	0.9566	0.0434	0.9769	Platycladi Cacumen	cis-Carveol	330573	FALSE	C1(C(=CCC(C1)C(=C)C)C)O
MOL002002	0.9566	0.0434	0.9769	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	cis-Carveol	330573	FALSE	C1(C(=CCC(C1)C(=C)C)C)O
MOL002003	0.8035	0.1965	0.6474	Citri Grandis Exocarpium	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Evodiae Fructus	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Aucklandiae Radix	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Viticis Fructus	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Calyx Seu Fructus Physalis	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Menthae Herba	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Rhizome Of Whiteback Greenbrier	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Rhododendri Daurici Folium	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Ecliptae Herba	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Folium Artemisiae Argyi	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Radix Cynanchi Paniculati	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Semen Euphorbiae	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Caryophylliflos	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C

MOL002003	0.8035	0.1965	0.6474	Lonicerae Japonicae Flos	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Litchi Semen	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Perilla Frutescens	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Cannabis Sativa L.	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Linderae Radix	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Peucedanidecursivi Radix	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Piperis Longi Fructus	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Cinnamomi Ramulus	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Carthami Flos	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Cynanchistauntonii Rhizoma Et Radix	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Platycladi Cacumen	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Acoritataninowii Rhizoma	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Dalbergiae Odoriferae Lignum	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Pogostemon Cablin (Blanco) Benth.	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C

MOL002003	0.8035	0.1965	0.6474	Peucedani Radix	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Kadsurae Coccineae Radix Et Caulis	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Eupatorium Fortunei Turcz	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Apocyniveneti Folium	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Fructuslipuidambaris	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Viticis Negundo Folium	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Anemarrhenae Rhizoma	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Rhapontici Radix	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Arisaematis Rhizoma	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Magnolia Officinalis Rehd Et Wils.	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Lysimachiae Herba	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Solidaginis Herba	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Humulus Scandens (Lour.) Merr.	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002003	0.8035	0.1965	0.6474	Cinnanmomi Cortex	(-)-Caryophyllene oxide	Not Available	FALSE	C1CC2C(C(=C)CCC3C1(O3)C)CC2(C)C
MOL002004	0.9487	0.0513	0.8045	Platycladi Cacumen	endo-fenchol	439711	FALSE	C12C(C(C(CC1)(C)C2)O)(C)C

MOL002004	0.9487	0.0513	0.8045	Prunellae Spica	endo-fenchol	439711	FALSE	C12C(C(C(CC1)(C)C2)O)(C)C
MOL002005	0.4578	0.5422	0.6588	Litseae Fructus	Hinokinin	442879	FALSE	C1(C(C(=O)OC1)Cc1ccc2c(c1)OCO2)Cc1cc2c(cc1)OCO2
MOL002005	0.4578	0.5422	0.6588	Platycladi Cacumen	Hinokinin	442879	FALSE	C1(C(C(=O)OC1)Cc1ccc2c(c1)OCO2)Cc1cc2c(cc1)OCO2
MOL002007	0.9287	0.0713	0.7985	Ardisiae Japonicae Herba	myricitrin	5281673	FALSE	c1(c(cc(cc1O)c1c(OC2OC(C(C(C2O)O)O)C)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002007	0.9287	0.0713	0.7985	Polygoni Avicularis Herba	myricitrin	5281673	FALSE	c1(c(cc(cc1O)c1c(OC2OC(C(C(C2O)O)O)C)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002007	0.9287	0.0713	0.7985	Platycladi Cacumen	myricitrin	5281673	FALSE	c1(c(cc(cc1O)c1c(OC2OC(C(C(C2O)O)O)C)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Rhododendri Daurici Folium	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Portulacae Herba	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Forsythiae Fructus	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Ginkgo Folium	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Ilicis Cornutae Folium Immayuri	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Euphorbiae Helioscopiae Herba	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Hippophae Fructus	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Herbahypericiperforati	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Hoveniae Dulcis Semen	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Sedum Aizoon L.	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Potentillae Chinensis Herba	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Dioscoreaebulbiferae	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Carthami Flos	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Lysimachiae Foenigraeci Herba	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Apocyniveneti Folium	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Platycladi Cacumen	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Mori Fructus	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Polygoni Avicularis Herba	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Folium Nelumbinis	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Geranium Wilfordii Maxim.	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Choerospondiatis Fructus	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Ardisiae Japonicae Herba	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002008	0.9483	0.0517	0.9398	Astragali Cpmplanatisemen	myricetin	5281672	TRUE	c1(c(cc(cc1O)c1c(O)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL002009	0.8717	0.1283	0.7621	Ginkgo Folium	Quercitrin-2'-gallate	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1C(C(C(C(O1)C)O)O)O)C(=O)c1cc(c(c(c1)O)O)O)c1ccc(c(c1)O)O)O)O

MOL002009	0.8717	0.1283	0.7621	Houttuyniae Herba	Quercitrin-2'-gallate	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1C(C(C(C(O1)C)O)O)O)C(=O)c1cc(c(c(c1)O)O)O)c1ccc(c(c1)O)O)O)O
MOL002009	0.8717	0.1283	0.7621	Polygoni Avicularis Herba	Quercitrin-2'-gallate	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1C(C(C(C(O1)C)O)O)O)C(=O)c1cc(c(c(c1)O)O)O)c1ccc(c(c1)O)O)O)O
MOL002009	0.8717	0.1283	0.7621	Platycladi Cacumen	Quercitrin-2'-gallate	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1C(C(C(C(O1)C)O)O)O)C(=O)c1cc(c(c(c1)O)O)O)c1ccc(c(c1)O)O)O)O
MOL002009	0.8717	0.1283	0.7621	Solidaginis Herba	Quercitrin-2'-gallate	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1C(C(C(C(O1)C)O)O)O)C(=O)c1cc(c(c(c1)O)O)O)c1ccc(c(c1)O)O)O)O
MOL002011	0.9199	0.0801	0.9528	Platycladi Cacumen	Vilmorrianine C	11523	FALSE	C1CC(CCC1C)C
MOL002012	0.9448	0.0552	0.9144	Rhizome Of Whiteback Greenbrier	2-Phenylpropene	7407	FALSE	c1(ccccc1)C(=C)C
MOL002012	0.9448	0.0552	0.9144	Arisaematis Rhizoma	2-Phenylpropene	7407	FALSE	c1(ccccc1)C(=C)C
MOL002012	0.9448	0.0552	0.9144	Platycladi Cacumen	2-Phenylpropene	7407	FALSE	c1(ccccc1)C(=C)C
MOL002012	0.9448	0.0552	0.9144	Piperis Fructus	2-Phenylpropene	7407	FALSE	c1(ccccc1)C(=C)C
MOL002012	0.9448	0.0552	0.9144	Rubi Fructus	2-Phenylpropene	7407	FALSE	c1(ccccc1)C(=C)C
MOL002014	0.8318	0.1682	0.7018	Radix Salviae	SPBio_002209	6508206	FALSE	C\1=C(\C/C=C\C(C/C=C(\CC1)/C)(C)C)/C
MOL002014	0.8318	0.1682	0.7018	Borneolum Syntheticum	SPBio_002209	6508206	FALSE	C\1=C(\C/C=C\C(C/C=C(\CC1)/C)(C)C)/C
MOL002014	0.8318	0.1682	0.7018	Platycladi Cacumen	SPBio_002209	6508206	FALSE	C\1=C(\C/C=C\C(C/C=C(\CC1)/C)(C)C)/C
MOL002015	0.9041	0.0959	0.8791	Platycladi Cacumen	(E,2S)-4-[(1R)-2,6,6-trimethyl-1-cyclohex-2-enyl]but-3-en-2-ol	11063310	FALSE	CC(/C=C/C1C(=CCCC1(C)C)C)O
MOL002016	0.8418	0.1582	0.6717	Ginkgo Folium	10579-93-8	5452236	FALSE	C12CC/C(=C\CCC(=C)C1CC2(C)C)/C
MOL002016	0.8418	0.1582	0.6717	Platycladi Cacumen	10579-93-8	5452236	FALSE	C12CC/C(=C\CCC(=C)C1CC2(C)C)/C
MOL002016	0.8418	0.1582	0.6717	Et Radix Patriniae Rhizoma	10579-93-8	5452236	FALSE	C12CC/C(=C\CCC(=C)C1CC2(C)C)/C
MOL002016	0.8418	0.1582	0.6717	Scutellariae Barbatae Herba	10579-93-8	5452236	FALSE	C12CC/C(=C\CCC(=C)C1CC2(C)C)/C
MOL002016	0.8418	0.1582	0.6717	Artemisia Annua L.	10579-93-8	5452236	FALSE	C12CC/C(=C\CCC(=C)C1CC2(C)C)/C

MOL002016	0.8418	0.1582	0.6717	Moslae Herba	10579-93-8	5452236	FALSE	C12CC/C(=C\CCC(=C)C1CC2(C)C)/C
MOL002016	0.8418	0.1582	0.6717	Carthami Flos	10579-93-8	5452236	FALSE	C12CC/C(=C\CCC(=C)C1CC2(C)C)/C
MOL002016	0.8418	0.1582	0.6717	Cuscutae Semen	10579-93-8	5452236	FALSE	C12CC/C(=C\CCC(=C)C1CC2(C)C)/C
MOL002017	0.8219	0.1781	0.6920	Platycladi Cacumen	1,4,4-trimethyl-8-methylenecycloundeca-1,5-diene	21159064	FALSE	C\1(=C\CC(/C=C\CC(=C)CCC1)(C)C)/C
MOL002018	0.7664	0.2336	0.6199	Platycladi Cacumen	beta-Eudesmol	Not Available	FALSE	C1C(CCC2(CCCC(=C)C12C)C)C(O)(C)C
MOL002020	0.2907	0.7093	0.6036	Herba Selaginellae Moellendorfii	Inokiflavone	5281627	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)Oc1ccc(cc1)c1cc(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL002020	0.2907	0.7093	0.6036	Platycladi Cacumen	Inokiflavone	5281627	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)Oc1ccc(cc1)c1cc(=O)c2c(o1)cc(cc2O)O)O)c1ccc(cc1)O
MOL002021	0.9521	0.0479	0.8773	Schizonepetae Herba	4-Vinyl-m-xylene	16694	FALSE	c1(c(cc(cc1)C)C)C=C
MOL002021	0.9521	0.0479	0.8773	Folium Artemisiae Argyi	4-Vinyl-m-xylene	16694	FALSE	c1(c(cc(cc1)C)C)C=C
MOL002021	0.9521	0.0479	0.8773	Platycladi Cacumen	4-Vinyl-m-xylene	16694	FALSE	c1(c(cc(cc1)C)C)C=C
MOL002022	0.9146	0.0854	0.9101	Platycladi Cacumen	7216-56-0	5371125	FALSE	C(=C(\C=C\C=C(C)C)/C)\C
MOL002022	0.9146	0.0854	0.9101	Viticis Fructus	7216-56-0	5371125	FALSE	C(=C(\C=C\C=C(C)C)/C)\C
MOL002022	0.9146	0.0854	0.9101	Evodiae Fructus	7216-56-0	5371125	FALSE	C(=C(\C=C\C=C(C)C)/C)\C
MOL002023	0.9521	0.0479	0.8063	Paederiae Scandentis Herba	ZINC00968101	6973640	FALSE	C1(CC2CCC1(C2(C)C)C)O
MOL002023	0.9521	0.0479	0.8063	Lignum Pini Nodi	ZINC00968101	6973640	FALSE	C1(CC2CCC1(C2(C)C)C)O
MOL002023	0.9521	0.0479	0.8063	Magnolia Officinalis Rehd Et Wils.	ZINC00968101	6973640	FALSE	C1(CC2CCC1(C2(C)C)C)O
MOL002023	0.9521	0.0479	0.8063	Borneolum Syntheticum	ZINC00968101	6973640	FALSE	C1(CC2CCC1(C2(C)C)C)O
MOL002023	0.9521	0.0479	0.8063	Artemisia Annua L.	ZINC00968101	6973640	FALSE	C1(CC2CCC1(C2(C)C)C)O
MOL002023	0.9521	0.0479	0.8063	Smilacis Glabrae Rhixoma	ZINC00968101	6973640	FALSE	C1(CC2CCC1(C2(C)C)C)O
MOL002023	0.9521	0.0479	0.8063	Linderae Radix	ZINC00968101	6973640	FALSE	C1(CC2CCC1(C2(C)C)C)O
MOL002023	0.9521	0.0479	0.8063	Platycladi Cacumen	ZINC00968101	6973640	FALSE	C1(CC2CCC1(C2(C)C)C)O
MOL002024	0.9480	0.0520	0.7421	Platycladi Cacumen	(1S,4R)-1,7,7-trimethylbicyclo[2.2.1]hept-2-ene	11062489	FALSE	C12(C=CC(CC1)C2(C)C)C

MOL002024	0.9480	0.0520	0.7421	Cinnamomi Ramulus	(1S,4R)-1,7,7-trimethylbicyclo[2.2.1]hept-2-ene	11062489	FALSE	C12(C=CC(CC1)C2(C)C)C
MOL002025	0.9074	0.0926	0.9656	Pogostemon Cablin (Blanco) Benth.	Tereton	6584	FALSE	C(=O)(C)OC
MOL002025	0.9074	0.0926	0.9656	Bomboo Juice	Tereton	6584	FALSE	C(=O)(C)OC
MOL002025	0.9074	0.0926	0.9656	Maydis Seigma	Tereton	6584	FALSE	C(=O)(C)OC
MOL002025	0.9074	0.0926	0.9656	Ephedra Herba	Tereton	6584	FALSE	C(=O)(C)OC
MOL002025	0.9074	0.0926	0.9656	Platycladi Cacumen	Tereton	6584	FALSE	C(=O)(C)OC
MOL002028	0.9620	0.0380	0.9523	Platycladi Cacumen	(+)-beta-Phellandrene	442484	FALSE	CC(C1C=CC(=C)CC1)C
MOL002028	0.9620	0.0380	0.9523	Evodiae Fructus	(+)-beta-Phellandrene	442484	FALSE	CC(C1C=CC(=C)CC1)C
MOL002028	0.9620	0.0380	0.9523	Zingiberis Rhizoma	(+)-beta-Phellandrene	442484	FALSE	CC(C1C=CC(=C)CC1)C
MOL002028	0.9620	0.0380	0.9523	Aucklandiae Radix	(+)-beta-Phellandrene	442484	FALSE	CC(C1C=CC(=C)CC1)C
MOL002028	0.9620	0.0380	0.9523	Chuanxiong Rhizoma	(+)-beta-Phellandrene	442484	FALSE	CC(C1C=CC(=C)CC1)C
MOL002028	0.9620	0.0380	0.9523	Schisandrae Chinensis Fructus	(+)-beta-Phellandrene	442484	FALSE	CC(C1C=CC(=C)CC1)C
MOL002028	0.9620	0.0380	0.9523	Linderae Radix	(+)-beta-Phellandrene	442484	FALSE	CC(C1C=CC(=C)CC1)C
MOL002028	0.9620	0.0380	0.9523	Magnolia Officinalis Rehd Et Wils.	(+)-beta-Phellandrene	442484	FALSE	CC(C1C=CC(=C)CC1)C
MOL002031	0.8845	0.1155	0.9488	Perillae Fructus	toluene	1140	TRUE	c1(ccccc1)C
MOL002031	0.8845	0.1155	0.9488	Sesami Nigrum Semen	toluene	1140	TRUE	c1(ccccc1)C
MOL002031	0.8845	0.1155	0.9488	Semen Pharbitidis	toluene	1140	TRUE	c1(ccccc1)C
MOL002031	0.8845	0.1155	0.9488	Puerariae Flos	toluene	1140	TRUE	c1(ccccc1)C
MOL002031	0.8845	0.1155	0.9488	Capsici Fructus	toluene	1140	TRUE	c1(ccccc1)C
MOL002031	0.8845	0.1155	0.9488	Platycladi Cacumen	toluene	1140	TRUE	c1(ccccc1)C
MOL002031	0.8845	0.1155	0.9488	Allii Tuberosi Semen	toluene	1140	TRUE	c1(ccccc1)C
MOL002031	0.8845	0.1155	0.9488	Magnolia Officinalis Rehd Et Wils.	toluene	1140	TRUE	c1(ccccc1)C
MOL002031	0.8845	0.1155	0.9488	Ephedra Herba	toluene	1140	TRUE	c1(ccccc1)C
MOL002031	0.8845	0.1155	0.9488	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	toluene	1140	TRUE	c1(ccccc1)C
MOL002031	0.8845	0.1155	0.9488	Curculiginis Rhizome	toluene	1140	TRUE	c1(ccccc1)C
MOL002031	0.8845	0.1155	0.9488	Momordicae Fructus	toluene	1140	TRUE	c1(ccccc1)C
MOL002031	0.8845	0.1155	0.9488	Santalum Album L.	toluene	1140	TRUE	c1(ccccc1)C
MOL002031	0.8845	0.1155	0.9488	Eriobotryae Folium	toluene	1140	TRUE	c1(ccccc1)C
MOL002031	0.8845	0.1155	0.9488	Mori Fructus	toluene	1140	TRUE	c1(ccccc1)C

MOL002032	0.2695	0.7305	0.6553	Arecae Semen	DNOP	8346	FALSE	c1cc(c(cc1)C(=O)OCCCCCCCC)C(=O)OCCCCCCC
MOL002032	0.2695	0.7305	0.6553	Ginsen Radix Et Rhizoma Rubra	DNOP	8346	FALSE	c1cc(c(cc1)C(=O)OCCCCCCCC)C(=O)OCCCCCCC
MOL002032	0.2695	0.7305	0.6553	Radix Cirsii Japonici	DNOP	8346	FALSE	c1cc(c(cc1)C(=O)OCCCCCCCC)C(=O)OCCCCCCC
MOL002032	0.2695	0.7305	0.6553	Platycladi Cacumen	DNOP	8346	FALSE	c1cc(c(cc1)C(=O)OCCCCCCCC)C(=O)OCCCCCCC
MOL002034	0.4655	0.5345	0.8310	Platycladi Cacumen	(5aR,8aS,9R)-9-(3,4,5-trimethoxyphenyl)-5a,6,8a,9-tetrahydro-5H-isobenzofurano[5,6-f][1,3]benzodioxol-8-one	11711021	FALSE	O1COc2c1cc1CC3C(C(c1c2)c1cc(c(c(c1)OC)OC)OC)C(=O)OC3
MOL002035	0.8989	0.1011	0.8117	Equiseti Hiemalis Herba	3,5-dihydroxy-2-(4-hydroxyphenyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	10095180	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC1C(O)C(O)C(O)C(O1)CO)O)c1ccc(cc1)O
MOL002035	0.8989	0.1011	0.8117	Choerospondiatis Fructus	3,5-dihydroxy-2-(4-hydroxyphenyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	10095180	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC1C(O)C(O)C(O)C(O1)CO)O)c1ccc(cc1)O

MOL002035	0.8989	0.1011	0.8117	Saussureae Involucratae Herba	3,5-dihydroxy-2-(4-hydroxyphenyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	10095180	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC1C(O)C(O)C(O)C(O1)CO)O)c1ccc(cc1)O
MOL002035	0.8989	0.1011	0.8117	Daturae Flos	3,5-dihydroxy-2-(4-hydroxyphenyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	10095180	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC1C(O)C(O)C(O)C(O1)CO)O)c1ccc(cc1)O
MOL002035	0.8989	0.1011	0.8117	Paederiae Scandentis Herba	3,5-dihydroxy-2-(4-hydroxyphenyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	10095180	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC1C(O)C(O)C(O)C(O1)CO)O)c1ccc(cc1)O

MOL002035	0.8989	0.1011	0.8117	Lepidii Semen Descurainiae Semen	3,5-dihydroxy-2-(4-hydroxyphenyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	10095180	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC1C(O)C(O)C(O)C(O1)CO)O)c1ccc(cc1)O
MOL002035	0.8989	0.1011	0.8117	Platycladi Cacumen	3,5-dihydroxy-2-(4-hydroxyphenyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	10095180	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC1C(O)C(O)C(O)C(O1)CO)O)c1ccc(cc1)O
MOL002036	0.9454	0.0546	0.8813	Menthae Herba	Naphthane	7044	FALSE	C1CCCC2CCCCC12
MOL002036	0.9454	0.0546	0.8813	Aristolochiae Fructus	Naphthane	7044	FALSE	C1CCCC2CCCCC12
MOL002036	0.9454	0.0546	0.8813	Platycladi Cacumen	Naphthane	7044	FALSE	C1CCCC2CCCCC12
MOL002038	0.7705	0.2295	0.6325	Trichosanthes Kirilowii Maxim	9E,12Z-octadecadienoic acid	5282798	FALSE	C(=C\C/C=C\CCCCC)/CCCCCCCC(=O)O
MOL002038	0.7705	0.2295	0.6325	Kochiae Fructus	9E,12Z-octadecadienoic acid	5282798	FALSE	C(=C\C/C=C\CCCCC)/CCCCCCCC(=O)O
MOL002038	0.7705	0.2295	0.6325	Platycladi Cacumen	9E,12Z-octadecadienoic acid	5282798	FALSE	C(=C\C/C=C\CCCCC)/CCCCCCCC(=O)O
MOL002038	0.7705	0.2295	0.6325	Lycii Cortex	9E,12Z-octadecadienoic acid	5282798	FALSE	C(=C\C/C=C\CCCCC)/CCCCCCCC(=O)O
MOL002039	0.5602	0.4398	0.7066	Lignum Pini Nodi	Isopimaric acid	442048	FALSE	C1CC(C2C(C1)(C1C(=CC2)CC(CC1)(C=C)C)C)(C)C(=O)O
MOL002039	0.5602	0.4398	0.7066	Styrax	Isopimaric acid	442048	FALSE	C1CC(C2C(C1)(C1C(=CC2)CC(CC1)(C=C)C)C)(C)C(=O)O

MOL002039	0.5602	0.4398	0.7066	Lilii Bulbus	Isopimaric acid	442048	FALSE	C1CC(C2C(C1)(C1C(=CC2)CC(CC1)(C=C)C)C)(C)C(=O)O
MOL002039	0.5602	0.4398	0.7066	Platycladi Cacumen	Isopimaric acid	442048	FALSE	C1CC(C2C(C1)(C1C(=CC2)CC(CC1)(C=C)C)C)(C)C(=O)O
MOL002040	0.9514	0.0486	0.8109	Foeniculi Fructus	(1S,4R)-fenchone	1201521	FALSE	C12(CCC(C(C1=O)(C)C)C2)C
MOL002040	0.9514	0.0486	0.8109	Platycladi Cacumen	(1S,4R)-fenchone	1201521	FALSE	C12(CCC(C(C1=O)(C)C)C2)C
MOL002040	0.9514	0.0486	0.8109	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(1S,4R)-fenchone	1201521	FALSE	C12(CCC(C(C1=O)(C)C)C2)C
MOL002040	0.9514	0.0486	0.8109	Epimrdii Herba	(1S,4R)-fenchone	1201521	FALSE	C12(CCC(C(C1=O)(C)C)C2)C
MOL002041	0.2829	0.7171	0.6822	Platycladi Cacumen	C-Curarine	Not Available	FALSE	C123N4C=C5C6(N(C=C1C1CC7C2(c2c4cccc2)CC[N+]7(C/C/1=C\C)C)c1c(C26C4CC5/C(=C/C)/C[N+]4(CC2)C)cccc1)O3
MOL002042	0.9558	0.0442	0.9265	Lysimachiae Herba	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Acoritataninowii Rhizoma	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Platycladi Cacumen	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Zingiber Officinale Roscoe	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Eriobotryae Folium	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Moslae Herba	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Notopterygii Rhizoma Et Radix	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Agrimonia Eupatoria	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Piperis Fructus	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Lysimachiae Foenigraeci Herba	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Lonicerae Japonicae Flos	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Kaempferiae Rhizoma	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Alpiniae Officinarum Rhizome	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Forsythiae Fructus	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Perilla Frutescens	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Campsis Flos	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Coriandri Sativi Herba	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Chrysanthemi Flos	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Radix Bupleuri	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Ginkgo Folium	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Chuanxiong Rhizoma	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Fructus Carotae	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Scutellariae Barbatae Herba	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O
MOL002042	0.9558	0.0442	0.9265	Ephedra Herba	thymol	6989	FALSE	c1(c(ccc(c1)C)C(C)C)O

MOL002043	0.0349	0.9651	0.7793	Toosendan Fructus	Nimbolidin C	Not Available	FALSE	CC(=O)OC1CC(C2(C3C1(C(C(C(C3OC2)OC(=O)C(C)C)(C)C1=C(C(CC1OC(=O)C)c1cocc1)C)COC(=O)C)C)C)OC(=O)C
MOL002044	0.5526	0.4474	0.7040	Toosendan Fructus	Toosendanin	Not Available	FALSE	C1C(C2(C3C(C1)(COC2O)C1C(C(C3)O)(C23C(C(C1=O)OC(=O)C)(C(CC3O2)c1ccoc1)C)C)C)OC(=O)C
MOL002045	0.2453	0.7547	0.6914	Toosendan Fructus	Stigmasterol	Not Available	FALSE	C1C(CC2=CCC3(C(C2(C1)C)(CCC1(C3CCC1C(/C=C/C(CC)C(C)C)C)C)C)C)O
MOL002046	0.9049	0.0951	0.9633	Ilicis Purpureae Folium	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Ephedra Herba	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Lygodii Spora	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Hippophae Fructus	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Radix Cynanchi Paniculati	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Semiaquilegiae Radix	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Toosendan Fructus	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Coicis Semen	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Siphonostegiae Herba	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Achyranthis Bidentatae Radix	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Cortex Moutan	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Ginkgo Folium	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Momordicae Fructus	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Panacis Quinquefolii Radix	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Eriobotryae Folium	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Meliae Azedarach Fructus	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Codonopsis Radix	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Canarii Fructus	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Panacis Japonici Rhizoma	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Ardisiae Japonicae Herba	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Capsici Fructus	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Citri Sarcodactylis Fructus	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Ganoderma	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Carpesiumabrotanoidesl.	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Radix Clematidis	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Uncariae Ramulus Cumuncis	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Morindae Officinalis Radix	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Campsis Flos	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Radix Cynanchi	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Gossampiniflos	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Carthami Flos	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Chaenomeles Sinensis (Thouin) Koehne	hexanoic acid	8892	FALSE	CCCCCC(=O)O

MOL002046	0.9049	0.0951	0.9633	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Radix Bupleuri	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Rubi Fructus	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Cucurbitae Moschatae Semen	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002046	0.9049	0.0951	0.9633	Phyllanthi Fructus	hexanoic acid	8892	FALSE	CCCCCC(=O)O
MOL002047	0.1637	0.8363	0.7671	Toosendan Fructus	melianone	Not Available	FALSE	C1(=O)CCC2(C(CC=C3C2CCC2(C3CCC2C2CC(OC2O)C2OC2(C)C)C)C1(C)C)C
MOL002048	0.0927	0.9073	0.7072	Toosendan Fructus	Nimbolidin D	Not Available	FALSE	C(=C\C)(/C(=O)OC1CC(C2(C3C1(C(C(C(C3OC2)OC(=O)/C(=C/C)/C)(C)C1=C(C(CC1OC(=O)C)c1coccc1)C)COC(=O)C)C)C)OC(=O)C)\C
MOL002049	0.9455	0.0545	0.9301	Benzoinum	Ferulaldehyde	5280536	FALSE	c1(cc(c(cc1)O)OC)/C=C/C=O
MOL002049	0.9455	0.0545	0.9301	Viticis Fructus	Ferulaldehyde	5280536	FALSE	c1(cc(c(cc1)O)OC)/C=C/C=O
MOL002049	0.9455	0.0545	0.9301	Prinsepiae Nux	Ferulaldehyde	5280536	FALSE	c1(cc(c(cc1)O)OC)/C=C/C=O
MOL002049	0.9455	0.0545	0.9301	Hydnocarpi Anthelminticae Semen	Ferulaldehyde	5280536	FALSE	c1(cc(c(cc1)O)OC)/C=C/C=O
MOL002049	0.9455	0.0545	0.9301	Eucommiae Cortex	Ferulaldehyde	5280536	FALSE	c1(cc(c(cc1)O)OC)/C=C/C=O
MOL002049	0.9455	0.0545	0.9301	Toosendan Fructus	Ferulaldehyde	5280536	FALSE	c1(cc(c(cc1)O)OC)/C=C/C=O
MOL002049	0.9455	0.0545	0.9301	Salviae Chinensis Herba	Ferulaldehyde	5280536	FALSE	c1(cc(c(cc1)O)OC)/C=C/C=O
MOL002050	0.9391	0.0609	0.9592	Lepidii Semen Descurainiae Semen	Isovanillic acid	12575	FALSE	c1(cc(c(cc1)OC)O)C(=O)O
MOL002050	0.9391	0.0609	0.9592	Ilicis Purpureae Folium	Isovanillic acid	12575	FALSE	c1(cc(c(cc1)OC)O)C(=O)O
MOL002050	0.9391	0.0609	0.9592	Dichroae Radix	Isovanillic acid	12575	FALSE	c1(cc(c(cc1)OC)O)C(=O)O
MOL002050	0.9391	0.0609	0.9592	Toosendan Fructus	Isovanillic acid	12575	FALSE	c1(cc(c(cc1)OC)O)C(=O)O
MOL002050	0.9391	0.0609	0.9592	Polygoni Orientalis Fructus	Isovanillic acid	12575	FALSE	c1(cc(c(cc1)OC)O)C(=O)O
MOL002050	0.9391	0.0609	0.9592	Cotyledon Fimbriata Turcz.	Isovanillic acid	12575	FALSE	c1(cc(c(cc1)OC)O)C(=O)O
MOL002050	0.9391	0.0609	0.9592	Microctis Folium	Isovanillic acid	12575	FALSE	c1(cc(c(cc1)OC)O)C(=O)O
MOL002050	0.9391	0.0609	0.9592	Citrus Reticulata	Isovanillic acid	12575	FALSE	c1(cc(c(cc1)OC)O)C(=O)O
MOL002050	0.9391	0.0609	0.9592	Pine Pollen	Isovanillic acid	12575	FALSE	c1(cc(c(cc1)OC)O)C(=O)O
MOL002050	0.9391	0.0609	0.9592	Radix Clematidis	Isovanillic acid	12575	FALSE	c1(cc(c(cc1)OC)O)C(=O)O
MOL002050	0.9391	0.0609	0.9592	Dioscoreaebulbiferae	Isovanillic acid	12575	FALSE	c1(cc(c(cc1)OC)O)C(=O)O

MOL002051	0.9208	0.0792	0.8007	Toosendan Fructus	ISOQUERCITRIN	13179951	FALSE	c12c(c(cc(c1)O)O)c(=O)c(c(o2)c1cc(c(cc1)O)O)OC1OC(C(C1O)O)C(CO)O
MOL002052	0.9070	0.0930	0.8302	Toosendan Fructus	9-Octadecenoic acid	57411980	FALSE	C(=C\CCCCCCCC(=O)O)\CCC
MOL002053	0.1047	0.8953	0.7625	Toosendan Fructus	Nimbolin A	Not Available	FALSE	C1C6CC1C1C2(C(=CC1)C1(C(CC2)C2(C(CC(OC(=O)C)C3(C)COC(C1OC(=O)/C=C/c1ccccc1)C23)OC(=O)C)C)C)C
MOL002054	0.3466	0.6534	0.7571	Toosendan Fructus	Thujopsadiene	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1(O)C)C)C(=O)OC)C)C)C)(C)C)O)O
MOL002055	0.9330	0.0670	0.8531	Polygoni Cuspidati Rhizoma Et Radix	Torachrysone	5321977	FALSE	c1c(cc2c(c1O)c(c(c(c2)C)C(=O)C)O)OC
MOL002055	0.9330	0.0670	0.8531	Cassiae Semen	Torachrysone	5321977	FALSE	c1c(cc2c(c1O)c(c(c(c2)C)C(=O)C)O)OC
MOL002055	0.9330	0.0670	0.8531	Toosendan Fructus	Torachrysone	5321977	FALSE	c1c(cc2c(c1O)c(c(c(c2)C)C(=O)C)O)OC
MOL002056	0.4769	0.5231	0.7750	Toosendan Fructus	(E)-3-[(2S,3R)-2-(4-hydroxy-3-methoxy-phenyl)-7-methoxy-3-methylol-2,3-dihydrobenzofuran-5-yl]acrolein	23252258	FALSE	c1c(cc2c(c1OC)OC(C2CO)c1cc(c(cc1)O)OC)/C=C/C=O
MOL002057	0.8253	0.1747	0.8160	Toosendan Fructus	evofolin-B	46229015	FALSE	c1c(ccc(c1OC)O)C(=O)C(c1cc(c(cc1)O)OC)CO
MOL002058	0.4757	0.5243	0.7025	Solanum Nigrum Linn.	40957-99-1	181681	FALSE	c1(cc(cc(c1O)OC)C1OCC2C1COC2c1cc(c(cc1)O)OC)OC
MOL002058	0.4757	0.5243	0.7025	Eucommiae Cortex	40957-99-1	181681	FALSE	c1(cc(cc(c1O)OC)C1OCC2C1COC2c1cc(c(cc1)O)OC)OC
MOL002058	0.4757	0.5243	0.7025	Toosendan Fructus	40957-99-1	181681	FALSE	c1(cc(cc(c1O)OC)C1OCC2C1COC2c1cc(c(cc1)O)OC)OC
MOL002059	0.8499	0.1501	0.7190	Sedi Herba	7-METHYL-6-TRIDECENE	5364660	FALSE	C(CCCC)C/C(=C/CCCCC)/C
MOL002060	0.3338	0.6662	0.7380	Sedi Herba	delta-amyrone	14079468	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2(C(=C3C(CC2)(CCC(C3)(C)C)C)CC1)C)C)C)(C)C
MOL002061	0.8566	0.1434	0.6486	Sedi Herba	Epi-bicyclosesaui phellandrene	51351709	FALSE	C12C(CCC(C1=CC(=C)CC2)C(C)C)C
MOL002061	0.8566	0.1434	0.6486	Ailanthi Cortex	Epi-bicyclosesaui phellandrene	51351709	FALSE	C12C(CCC(C1=CC(=C)CC2)C(C)C)C
MOL002062	0.9479	0.0521	0.9311	Sedi Herba	Ethyl methoxycinnamate	5281783	FALSE	C(=O)(/C=C/c1ccc(cc1)OC)OCC

MOL002062	0.9479	0.0521	0.9311	Kaempferiae Rhizoma	Ethyl methoxycinnamate	5281783	FALSE	C(=O)(/C=C/c1ccc(cc1)OC)OCC
MOL002063	0.8264	0.1736	0.6799	Ardisiae Japonicae Herba	γ-selinene	Not Available	FALSE	C12(C(CC(=C(C)C)CC1)C(=C)CCC2)C
MOL002063	0.8264	0.1736	0.6799	Verbenae Herb	γ-selinene	Not Available	FALSE	C12(C(CC(=C(C)C)CC1)C(=C)CCC2)C
MOL002063	0.8264	0.1736	0.6799	Ailanthi Cortex	γ-selinene	Not Available	FALSE	C12(C(CC(=C(C)C)CC1)C(=C)CCC2)C
MOL002063	0.8264	0.1736	0.6799	Sedi Herba	γ-selinene	Not Available	FALSE	C12(C(CC(=C(C)C)CC1)C(=C)CCC2)C
MOL002064	0.9292	0.0708	0.9728	Sedi Herba	(S)-hygrine	443144	FALSE	O=C(CC1N(CCC1)C)C
MOL002065	0.9277	0.0723	0.9734	Sedi Herba	hygroline	12310695	FALSE	OC(CC1N(CCC1)C)C
MOL002067	0.7411	0.2589	0.6114	Sedi Herba	hypericin	Not Available	FALSE	c12c3c4c5c6c1c(C(=O)c1c2c(c2c3c(C(=O)c4c(cc5C)O)c(cc2O)O)c(cc1O)O)c(cc6C)O
MOL002067	0.7411	0.2589	0.6114	Forsythiae Fructus	hypericin	Not Available	FALSE	c12c3c4c5c6c1c(C(=O)c1c2c(c2c3c(C(=O)c4c(cc5C)O)c(cc2O)O)c(cc1O)O)c(cc6C)O
MOL002067	0.7411	0.2589	0.6114	Herbahypericiperforati	hypericin	Not Available	FALSE	c12c3c4c5c6c1c(C(=O)c1c2c(c2c3c(C(=O)c4c(cc5C)O)c(cc2O)O)c(cc1O)O)c(cc6C)O
MOL002067	0.7411	0.2589	0.6114	Hyperici Japonici Herber	hypericin	Not Available	FALSE	c12c3c4c5c6c1c(C(=O)c1c2c(c2c3c(C(=O)c4c(cc5C)O)c(cc2O)O)c(cc1O)O)c(cc6C)O
MOL002068	0.8671	0.1329	0.8124	Sedi Herba	isorhamnetin-3,7-diglucoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(=O)c2c(oc1c1cc(OC)c(O)cc1)cc(OC1OC(C(O)C(O)C1O)CO)cc2O)CO
MOL002069	0.8743	0.1257	0.7948	Sedi Herba	Isorhamnetin-7-O-beta-D-glucopyranoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2oc(c(O)c(=O)c2c(O)c1)c1cc(OC)c(O)cc1)CO
MOL002070	0.9134	0.0866	0.8866	Sedi Herba	isosarmentosine	Not Available	FALSE	O1C2C(OC(C1)C(CO)C#N)C(O)C(O)C(O2)CO
MOL002071	0.8835	0.1165	0.7917	Sedi Herba	limocitrin-3-glucoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2OC)c1cc(OC)c(O)cc1)CO
MOL002072	0.8618	0.1382	0.8704	Sedi Herba	3,5,7-trihydroxy-2-(4-hydroxy-3-methoxy-phenyl)-8-methoxy-chromone	5489485	FALSE	Oc1c(oc2c(c1=O)c(O)cc(O)c2OC)c1cc(OC)c(O)cc1
MOL002074	0.9134	0.0866	0.9224	Sedi Herba	(-)-Sedamine	442657	FALSE	OC(CC1N(CCCC1)C)c1ccccc1
MOL002075	0.9419	0.0581	0.9757	Sedi Herba	1-[(2S)-1-methyl-2-piperidyl]acetone	820378	FALSE	C(C(=O)C)C1N(CCCC1)C

MOL002075	0.9419	0.0581	0.9757	Sedum Aizoon L.	1-[(2S)-1-methyl-2-piperidyl]acetone	820378	FALSE	C(C(=O)C)C1N(CCCC1)C
MOL002076	0.9209	0.0791	0.9715	Sedi Herba	norhygrine	15250836	FALSE	C(C(=O)C)C1NCCC1
MOL002077	0.9412	0.0588	0.9836	Sedi Herba	1-[(2S)-2-piperidyl]acetone	10313185	FALSE	O=C(CC1NCCCC1)C
MOL002077	0.9412	0.0588	0.9836	Granati Pericarpium	1-[(2S)-2-piperidyl]acetone	10313185	FALSE	O=C(CC1NCCCC1)C
MOL002078	0.4051	0.5949	0.8100	Sedi Herba	sarmentolin	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C)(C)CC4(C3=CCC21)OO)C
MOL002079	0.9053	0.0947	0.9447	Sedi Herba	Sarmentosine	6438710	FALSE	O1C(C(O)C(O)C(O)C1OC/C=C(\CO)/C#N)CO
MOL002080	0.9296	0.0704	0.9589	Sedi Herba	sarmentosine_qt	Not Available	FALSE	OC/C=C(\CO)/C#N
MOL002081	0.7771	0.2229	0.7984	Sedi Herba	sedinone	Not Available	FALSE	C(C(=O)C)C1N(C(CCC1)CC(c1ccccc1)O)C
MOL002082	0.9337	0.0663	0.9836	Sedi Herba	Sedridine	164633	FALSE	OC(CC1NCCCC1)C
MOL002083	0.8521	0.1479	0.8928	Ephedra Herba	tricin	5281702	FALSE	c12c(oc(cc1=O)c1cc(c(c(c1)OC)O)OC)cc(cc2O)O
MOL002083	0.8521	0.1479	0.8928	Hordei Fructus Germinatus	tricin	5281702	FALSE	c12c(oc(cc1=O)c1cc(c(c(c1)OC)O)OC)cc(cc2O)O
MOL002083	0.8521	0.1479	0.8928	Trigonellae Semen	tricin	5281702	FALSE	c12c(oc(cc1=O)c1cc(c(c(c1)OC)O)OC)cc(cc2O)O
MOL002083	0.8521	0.1479	0.8928	Sedi Herba	tricin	5281702	FALSE	c12c(oc(cc1=O)c1cc(c(c(c1)OC)O)OC)cc(cc2O)O
MOL002083	0.8521	0.1479	0.8928	Phragmitis Rhizoma	tricin	5281702	FALSE	c12c(oc(cc1=O)c1cc(c(c(c1)OC)O)OC)cc(cc2O)O
MOL002083	0.8521	0.1479	0.8928	Tribulifructus	tricin	5281702	FALSE	c12c(oc(cc1=O)c1cc(c(c(c1)OC)O)OC)cc(cc2O)O
MOL002083	0.8521	0.1479	0.8928	Ginkgo Folium	tricin	5281702	FALSE	c12c(oc(cc1=O)c1cc(c(c(c1)OC)O)OC)cc(cc2O)O
MOL002083	0.8521	0.1479	0.8928	Cyperi Rhizoma	tricin	5281702	FALSE	c12c(oc(cc1=O)c1cc(c(c(c1)OC)O)OC)cc(cc2O)O
MOL002083	0.8521	0.1479	0.8928	Lonicerae Japonicae Flos	tricin	5281702	FALSE	c12c(oc(cc1=O)c1cc(c(c(c1)OC)O)OC)cc(cc2O)O
MOL002083	0.8521	0.1479	0.8928	Wikstroemiae Indicae Rasix	tricin	5281702	FALSE	c12c(oc(cc1=O)c1cc(c(c(c1)OC)O)OC)cc(cc2O)O
MOL002083	0.8521	0.1479	0.8928	Trichosanthes Kirilowii Maxim	tricin	5281702	FALSE	c12c(oc(cc1=O)c1cc(c(c(c1)OC)O)OC)cc(cc2O)O
MOL002083	0.8521	0.1479	0.8928	Epimrdii Herba	tricin	5281702	FALSE	c12c(oc(cc1=O)c1cc(c(c(c1)OC)O)OC)cc(cc2O)O
MOL002083	0.8521	0.1479	0.8928	Belamcandae Rhizome	tricin	5281702	FALSE	c12c(oc(cc1=O)c1cc(c(c(c1)OC)O)OC)cc(cc2O)O
MOL002084	0.8283	0.1717	0.7840	Sedi Herba	Tricin-7-O-beta-D-lucopyranoside	Not Available	FALSE	c1c(cc(c2c1oc(cc2=O)c1cc(c(c(c1)OC)O)OC)O)OC1C(O)C(O)C(O)C(O1)CO

MOL002086	0.3020	0.6980	0.8769	Aconiti Radix	1-[(5R,8R,9S,10S,12R,13S,14S,17S)-12-hydroxy-10,13-dimethyl-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl]ethanone	22212681	FALSE	C1CCC2(C(C1)CCC1C3CCC(C(=O)C)C3(C)C(CC21)O)C
MOL002087	0.3202	0.6798	0.8888	Aconiti Radix	delta4,16-Androstadien-3-one	92979	FALSE	C1(=O)CCC2(C(=C1)CCC1C3CC=CC3(C)CCC21)C
MOL002088	0.3806	0.6194	0.7400	Aconiti Radix	aconitine	Not Available	FALSE	C123C4C(CN(C2C(C4OC)C2(C4C1CC(C4OC(=O)C1ccccc1)(C(C2O)OC)O)OC(=O)C)CC)(C(CC3OC)O)
MOL002088	0.3806	0.6194	0.7400	Radix Aconiti Kusnezoffii	aconitine	Not Available	FALSE	C123C4C(CN(C2C(C4OC)C2(C4C1CC(C4OC(=O)C1ccccc1)(C(C2O)OC)O)OC(=O)C)CC)(C(CC3OC)O)
MOL002088	0.3806	0.6194	0.7400	Aconitum Kusnezoffii Reichb	aconitine	Not Available	FALSE	C123C4C(CN(C2C(C4OC)C2(C4C1CC(C4OC(=O)C1ccccc1)(C(C2O)OC)O)OC(=O)C)CC)(C(CC3OC)O)
MOL002089	0.4102	0.5898	0.7316	Radix Aconiti Kusnezoffii	mesaconitine	Not Available	FALSE	C123C4C(CN(C2C(C4OC)C2(C4C1CC(C4OC(=O)C1ccccc1)(C(C2O)OC)O)OC(=O)C)C)(C(CC3OC)O)C
MOL002089	0.4102	0.5898	0.7316	Aconiti Radix	mesaconitine	Not Available	FALSE	C123C4C(CN(C2C(C4OC)C2(C4C1CC(C4OC(=O)C1ccccc1)(C(C2O)OC)O)OC(=O)C)C)(C(CC3OC)O)C
MOL002089	0.4102	0.5898	0.7316	Aconitum Kusnezoffii Reichb	mesaconitine	Not Available	FALSE	C123C4C(CN(C2C(C4OC)C2(C4C1CC(C4OC(=O)C1ccccc1)(C(C2O)OC)O)OC(=O)C)C)(C(CC3OC)O)C
MOL002089	0.4102	0.5898	0.7316	Aconiti Lateralis Radix Praeparata	mesaconitine	Not Available	FALSE	C123C4C(CN(C2C(C4OC)C2(C4C1CC(C4OC(=O)C1ccccc1)(C(C2O)OC)O)OC(=O)C)C)(C(CC3OC)O)C
MOL002090	0.9589	0.0411	0.7844	Aconiti Radix	Dicyclopentadiene dioxide	Not Available	FALSE	C12C3C4C(C(C1CC1C2O1)C3)O4
MOL002091	0.9358	0.0642	0.7581	Aconiti Radix	1,7-Dimethoxynaphthalene	79197	FALSE	c12c(ccc(c2)OC)cccc1OC
MOL002092	0.9006	0.0994	0.6639	Carthami Flos	Antioxidant No. 33	7311	FALSE	c1(cc(ccc1O)C(C)(C)C)C(C)(C)C
MOL002092	0.9006	0.0994	0.6639	Sesami Nigrum Semen	Antioxidant No. 33	7311	FALSE	c1(cc(ccc1O)C(C)(C)C)C(C)(C)C

MOL002092	0.9006	0.0994	0.6639	Litchi Semen	Antioxidant No. 33	7311	FALSE	c1(cc(ccc1O)C(C)(C)C)C(C)(C)C
MOL002092	0.9006	0.0994	0.6639	Citrus Reticulata	Antioxidant No. 33	7311	FALSE	c1(cc(ccc1O)C(C)(C)C)C(C)(C)C
MOL002092	0.9006	0.0994	0.6639	Cannabis Sativa L.	Antioxidant No. 33	7311	FALSE	c1(cc(ccc1O)C(C)(C)C)C(C)(C)C
MOL002092	0.9006	0.0994	0.6639	Allii Fistulost Bulbus	Antioxidant No. 33	7311	FALSE	c1(cc(ccc1O)C(C)(C)C)C(C)(C)C
MOL002092	0.9006	0.0994	0.6639	Eriobotryae Folium	Antioxidant No. 33	7311	FALSE	c1(cc(ccc1O)C(C)(C)C)C(C)(C)C
MOL002092	0.9006	0.0994	0.6639	Equiseti Hiemalis Herba	Antioxidant No. 33	7311	FALSE	c1(cc(ccc1O)C(C)(C)C)C(C)(C)C
MOL002092	0.9006	0.0994	0.6639	Mahoniae Caulis	Antioxidant No. 33	7311	FALSE	c1(cc(ccc1O)C(C)(C)C)C(C)(C)C
MOL002092	0.9006	0.0994	0.6639	Linderae Radix	Antioxidant No. 33	7311	FALSE	c1(cc(ccc1O)C(C)(C)C)C(C)(C)C
MOL002092	0.9006	0.0994	0.6639	Lepidii Semen Descurainiae Semen	Antioxidant No. 33	7311	FALSE	c1(cc(ccc1O)C(C)(C)C)C(C)(C)C
MOL002092	0.9006	0.0994	0.6639	Radix Clematidis	Antioxidant No. 33	7311	FALSE	c1(cc(ccc1O)C(C)(C)C)C(C)(C)C
MOL002092	0.9006	0.0994	0.6639	Aconiti Radix	Antioxidant No. 33	7311	FALSE	c1(cc(ccc1O)C(C)(C)C)C(C)(C)C
MOL002092	0.9006	0.0994	0.6639	Aucklandiae Radix	Antioxidant No. 33	7311	FALSE	c1(cc(ccc1O)C(C)(C)C)C(C)(C)C
MOL002093	0.5146	0.4854	0.6907	Aconiti Radix	benzoylmesaconine	Not Available	FALSE	C123C4C(CN(C2C(C4OC)C2(C4C1CC(C4OC(=O)c1ccccc1)(C(C2O)OC)O)O)C)(C(CC3OC)O)COC
MOL002093	0.5146	0.4854	0.6907	Aconiti Lateralis Radix Praeparata	benzoylmesaconine	Not Available	FALSE	C123C4C(CN(C2C(C4OC)C2(C4C1CC(C4OC(=O)c1ccccc1)(C(C2O)OC)O)O)C)(C(CC3OC)O)COC
MOL002094	0.4430	0.5570	0.7386	Aconiti Radix	talatisamine	Not Available	FALSE	OC12C3C4N(CC5(C(C4(C4C1C(O)C(C4)C(OC)C2)C(OC)CC5)C3)COC)CC
MOL002095	0.9611	0.0389	0.8964	Aconiti Radix	DEP	6781	FALSE	c1(c(C(=O)OCC)cccc1)C(=O)OCC
MOL002095	0.9611	0.0389	0.8964	Mume Fructus	DEP	6781	FALSE	c1(c(C(=O)OCC)cccc1)C(=O)OCC
MOL002095	0.9611	0.0389	0.8964	Radix Bupleuri	DEP	6781	FALSE	c1(c(C(=O)OCC)cccc1)C(=O)OCC
MOL002095	0.9611	0.0389	0.8964	Oroxyli Semen	DEP	6781	FALSE	c1(c(C(=O)OCC)cccc1)C(=O)OCC
MOL002095	0.9611	0.0389	0.8964	Acoritataninowii Rhizoma	DEP	6781	FALSE	c1(c(C(=O)OCC)cccc1)C(=O)OCC
MOL002095	0.9611	0.0389	0.8964	Arecae Semen	DEP	6781	FALSE	c1(c(C(=O)OCC)cccc1)C(=O)OCC
MOL002095	0.9611	0.0389	0.8964	Allii Fistulost Bulbus	DEP	6781	FALSE	c1(c(C(=O)OCC)cccc1)C(=O)OCC
MOL002095	0.9611	0.0389	0.8964	Cortex Moutan	DEP	6781	FALSE	c1(c(C(=O)OCC)cccc1)C(=O)OCC
MOL002095	0.9611	0.0389	0.8964	Ephedra Herba	DEP	6781	FALSE	c1(c(C(=O)OCC)cccc1)C(=O)OCC
MOL002095	0.9611	0.0389	0.8964	Citrus Reticulata	DEP	6781	FALSE	c1(c(C(=O)OCC)cccc1)C(=O)OCC
MOL002097	0.8935	0.1065	0.9476	Chuanxiong Rhizoma	gem-Dimethylcyclopentane	15421	FALSE	C1(CCCC1)(C)C

MOL002098	0.9596	0.0404	0.9083	Angelicae Sinensis Radix	3-Butylidene-7-hydroxyphthalide	5281559	FALSE	C1(=O)O/C(=C\CCC)/c2cccc(c12)O
MOL002098	0.9596	0.0404	0.9083	Chuanxiong Rhizoma	3-Butylidene-7-hydroxyphthalide	5281559	FALSE	C1(=O)O/C(=C\CCC)/c2cccc(c12)O
MOL002099	0.9632	0.0368	0.8766	Chuanxiong Rhizoma	Senkyunolide-K	13965751	FALSE	C1(CC=CC2=C1C(OC2=O)CCCC)O
MOL002100	0.8358	0.1642	0.7643	Chuanxiong Rhizoma	(3Z,6S,7R)-3-butylidene-6-butyryl-7-hydroxy-4,5,6,7-tetrahydroisobenzofuran-1-one	11265913	FALSE	C1(C(CCC2=C1C(=O)O/C/2=C\CCC)C(=O)CCC)O
MOL002101	0.9518	0.0482	0.8822	Chuanxiong Rhizoma	Senkyunolide-N	15138552	FALSE	C1(=O)OC(C2=C1C(C(CC2)O)O)CCCC
MOL002102	0.2529	0.7471	0.8191	Chuanxiong Rhizoma	Levistolid A	Not Available	FALSE	O1/C(=C/CCC)/C23C(=CC(C4CCC5=C(C(=O)O/C/5=C\CCC)C24)CC3)C1=O
MOL002102	0.2529	0.7471	0.8191	Angelicae Sinensis Radix	Levistolid A	Not Available	FALSE	O1/C(=C/CCC)/C23C(=CC(C4CCC5=C(C(=O)O/C/5=C\CCC)C24)CC3)C1=O
MOL002103	0.2367	0.7633	0.8219	Chuanxiong Rhizoma	Senkyunolide-P	Not Available	FALSE	O1C(C23C(=CC(C4CCC5=C(C(=O)O/C/5=C/CCC)C24)CC3)C1=O)CCCC
MOL002104	0.8358	0.1642	0.7643	Chuanxiong Rhizoma	Senkyunolide-Q	Not Available	FALSE	C1(=O)O/C(=C/CCC)/C2=C1C(C(CC2)C(=O)CCC)O
MOL002105	0.9394	0.0606	0.8887	Chuanxiong Rhizoma	Senkyunolide-R	Not Available	FALSE	C1(=O)O/C(=C/C(CC)O)/C2=C1C(C(CC2)O)O
MOL002106	0.9319	0.0681	0.9503	Chuanxiong Rhizoma	1,1-Diethoxybutane	77225	FALSE	C(CCC)(OCC)OCC
MOL002107	0.9355	0.0645	0.9374	Chuanxiong Rhizoma	Valerophenone	66093	FALSE	c1(C(=O)CCCC)ccccc1
MOL002107	0.9355	0.0645	0.9374	Radix Bupleuri	Valerophenone	66093	FALSE	c1(C(=O)CCCC)ccccc1
MOL002108	0.9558	0.0442	0.7670	Chuanxiong Rhizoma	(1S,5S)-7,7-dimethyl-2-methylenebicyclo[3.1.1]hept-3-ene	21631119	FALSE	C1(C2C=CC(=C)C1C2)(C)C

MOL002109	0.2371	0.7629	0.7492	Chuanxiong Rhizoma	Z-6,8',7,3'-diligustilide	Not Available	FALSE	C1(=O)C2=C(/C(=C/CCC)/O1)CCC1C2C2(C1CCC)C1=C(C=CCC1)C(=O)O2
MOL002110	0.9146	0.0854	0.9101	Menthae Herba	Allocymene	5368821	FALSE	CC(=C/C=C/C(=C/C)/C)C
MOL002110	0.9146	0.0854	0.9101	Angelicae Sinensis Radix	Allocymene	5368821	FALSE	CC(=C/C=C/C(=C/C)/C)C
MOL002110	0.9146	0.0854	0.9101	Ephedra Herba	Allocymene	5368821	FALSE	CC(=C/C=C/C(=C/C)/C)C
MOL002110	0.9146	0.0854	0.9101	Chuanxiong Rhizoma	Allocymene	5368821	FALSE	CC(=C/C=C/C(=C/C)/C)C
MOL002110	0.9146	0.0854	0.9101	Bidentis Bipinnatae Herba	Allocymene	5368821	FALSE	CC(=C/C=C/C(=C/C)/C)C
MOL002111	0.9619	0.0381	0.8983	Ligustici Rhizoma Et Radix	BdPh	5352899	FALSE	c1ccc2c(c1)C(=O)O/C/2=C/CCC
MOL002111	0.9619	0.0381	0.8983	Chuanxiong Rhizoma	BdPh	5352899	FALSE	c1ccc2c(c1)C(=O)O/C/2=C/CCC
MOL002111	0.9619	0.0381	0.8983	Radix Bupleuri	BdPh	5352899	FALSE	c1ccc2c(c1)C(=O)O/C/2=C/CCC
MOL002111	0.9619	0.0381	0.8983	Angelicae Sinensis Radix	BdPh	5352899	FALSE	c1ccc2c(c1)C(=O)O/C/2=C/CCC
MOL002113	0.9258	0.0742	0.8489	Chuanxiong Rhizoma	1,2,3,4,4a,7-Hexahydro-l,6-dimethyl-4-(1-methylethyl)-naphthalene	Not Available	FALSE	C12C(=CCC(=C1)C)C(CCC2)C
MOL002114	0.7451	0.2549	0.7902	Chuanxiong Rhizoma	augustic-acid	15560128	FALSE	O=C(O)C12C(C3=CCC4C(C3(CC1)C)(CCC1C4(CC(O)C(O)C1(C)C)C)C)CC(CC2)(C)C
MOL002115	0.9359	0.0641	0.9069	Flos Genkwa	m-Ethyltoluene	12100	FALSE	c1(cc(ccc1)C)CC
MOL002115	0.9359	0.0641	0.9069	Oroxyli Semen	m-Ethyltoluene	12100	FALSE	c1(cc(ccc1)C)CC
MOL002115	0.9359	0.0641	0.9069	Chaenomeles Sinensis (Thouin) Koehne	m-Ethyltoluene	12100	FALSE	c1(cc(ccc1)C)CC
MOL002115	0.9359	0.0641	0.9069	Chuanxiong Rhizoma	m-Ethyltoluene	12100	FALSE	c1(cc(ccc1)C)CC
MOL002115	0.9359	0.0641	0.9069	Sojae Semen Nigrum	m-Ethyltoluene	12100	FALSE	c1(cc(ccc1)C)CC
MOL002117	0.8711	0.1289	0.7791	Chuanxiong Rhizoma	β-sesquiphellandrene	12315492	FALSE	C1=CC(CCC1=C)C(CCC=C(C)C)C
MOL002117	0.8711	0.1289	0.7791	Morindae Officinalis Radix	β-sesquiphellandrene	12315492	FALSE	C1=CC(CCC1=C)C(CCC=C(C)C)C
MOL002117	0.8711	0.1289	0.7791	Curcumae Radix	β-sesquiphellandrene	12315492	FALSE	C1=CC(CCC1=C)C(CCC=C(C)C)C
MOL002117	0.8711	0.1289	0.7791	Aucklandiae Radix	β-sesquiphellandrene	12315492	FALSE	C1=CC(CCC1=C)C(CCC=C(C)C)C

MOL002117	0.8711	0.1289	0.7791	Radix Angelicae Biseratae	β-sesquiphellandrene	12315492	FALSE	C1=CC(CCC1=C)C(CCC=C(C)C)C
MOL002117	0.8711	0.1289	0.7791	Litchi Semen	β-sesquiphellandrene	12315492	FALSE	C1=CC(CCC1=C)C(CCC=C(C)C)C
MOL002117	0.8711	0.1289	0.7791	Zingiber Officinale Roscoe	β-sesquiphellandrene	12315492	FALSE	C1=CC(CCC1=C)C(CCC=C(C)C)C
MOL002118	0.8129	0.1871	0.6579	Chuanxiong Rhizoma	(4aS,7S,8aR)-7-isopropenyl-4a-methyl-1-methylenedecalin	28237	FALSE	C1CCC(=C)C2C1(CCC(C2)C(=C)C)C
MOL002119	0.9226	0.0774	0.9046	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Artemisia triene	5320377	FALSE	C=C(/C=C/C(C=C)(C)C)C
MOL002119	0.9226	0.0774	0.9046	Chuanxiong Rhizoma	Artemisia triene	5320377	FALSE	C=C(/C=C/C(C=C)(C)C)C
MOL002121	0.8598	0.1402	0.6769	Lonicerae Japonicae Flos	(1S,4E,8E,10R)-4,8,11,11-tetramethylbicyclo[8.1.0]undeca-4,8-diene	11820258	FALSE	C\1=C(/CCC2C(/C=C(/CC1)\C)C2(C)C)\C
MOL002121	0.8598	0.1402	0.6769	Panax Ginseng C. A. Mey.	(1S,4E,8E,10R)-4,8,11,11-tetramethylbicyclo[8.1.0]undeca-4,8-diene	11820258	FALSE	C\1=C(/CCC2C(/C=C(/CC1)\C)C2(C)C)\C
MOL002121	0.8598	0.1402	0.6769	Chuanxiong Rhizoma	(1S,4E,8E,10R)-4,8,11,11-tetramethylbicyclo[8.1.0]undeca-4,8-diene	11820258	FALSE	C\1=C(/CCC2C(/C=C(/CC1)\C)C2(C)C)\C
MOL002121	0.8598	0.1402	0.6769	Bidentis Bipinnatae Herba	(1S,4E,8E,10R)-4,8,11,11-tetramethylbicyclo[8.1.0]undeca-4,8-diene	11820258	FALSE	C\1=C(/CCC2C(/C=C(/CC1)\C)C2(C)C)\C

MOL002122	0.9619	0.0381	0.8983	Chuanxiong Rhizoma	(Z)-Ligustilide	642376	FALSE	c12c(C(=O)O/C/1=C\CCC)cccc2
MOL002122	0.9619	0.0381	0.8983	Aucklandiae Radix	(Z)-Ligustilide	642376	FALSE	c12c(C(=O)O/C/1=C\CCC)cccc2
MOL002123	0.9427	0.0573	0.9323	Chuanxiong Rhizoma	Chuanxiongol	5315862	FALSE	C1(=O)CO/C(=C\CCC)/c2c1cccc2O
MOL002124	0.9590	0.0410	0.8520	Gossampiniflos	beta-asarone	5281758	FALSE	c1(c(cc(c(c1)OC)OC)OC)/C=C\C
MOL002124	0.9590	0.0410	0.8520	Acoritataninowii Rhizoma	beta-asarone	5281758	FALSE	c1(c(cc(c(c1)OC)OC)OC)/C=C\C
MOL002124	0.9590	0.0410	0.8520	Cynanchistauntonii Rhizoma Et Radix	beta-asarone	5281758	FALSE	c1(c(cc(c(c1)OC)OC)OC)/C=C\C
MOL002124	0.9590	0.0410	0.8520	Chuanxiong Rhizoma	beta-asarone	5281758	FALSE	c1(c(cc(c(c1)OC)OC)OC)/C=C\C
MOL002124	0.9590	0.0410	0.8520	Humulus Scandens (Lour.) Merr.	beta-asarone	5281758	FALSE	c1(c(cc(c(c1)OC)OC)OC)/C=C\C
MOL002125	0.9566	0.0434	0.9577	Moslae Herba	cis-Piperitol	85567	FALSE	C1(C=C(CCC1C(C)C)C)O
MOL002125	0.9566	0.0434	0.9577	Chuanxiong Rhizoma	cis-Piperitol	85567	FALSE	C1(C=C(CCC1C(C)C)C)O
MOL002126	0.9580	0.0420	0.7912	Chuanxiong Rhizoma	(1S,4R,5R)-1-isopropyl-4-methyl-4-bicyclo[3.1.0] hexanol	6326181	FALSE	C12(C(C)C)C(C2)C(CC1)(C)O
MOL002126	0.9580	0.0420	0.7912	Asari Radix Et Rhizoma	(1S,4R,5R)-1-isopropyl-4-methyl-4-bicyclo[3.1.0] hexanol	6326181	FALSE	C12(C(C)C)C(C2)C(CC1)(C)O
MOL002127	0.9475	0.0525	0.8615	Chuanxiong Rhizoma	Cnidilide	160710	FALSE	O1C(C2C(C1=O)C=CCC2)CCCC
MOL002127	0.9475	0.0525	0.8615	Cnidii Fructus	Cnidilide	160710	FALSE	O1C(C2C(C1=O)C=CCC2)CCCC
MOL002127	0.9475	0.0525	0.8615	Ligustici Rhizoma Et Radix	Cnidilide	160710	FALSE	O1C(C2C(C1=O)C=CCC2)CCCC
MOL002128	0.9534	0.0466	0.9553	Chuanxiong Rhizoma	1,3,8-p-Menthatriene	176983	FALSE	C1(=CC=C(CC1)C(=C)C)C
MOL002128	0.9534	0.0466	0.9553	Perilla Frutescens	1,3,8-p-Menthatriene	176983	FALSE	C1(=CC=C(CC1)C(=C)C)C
MOL002128	0.9534	0.0466	0.9553	Dichroae Radix	1,3,8-p-Menthatriene	176983	FALSE	C1(=CC=C(CC1)C(=C)C)C
MOL002128	0.9534	0.0466	0.9553	Evodiae Fructus	1,3,8-p-Menthatriene	176983	FALSE	C1(=CC=C(CC1)C(=C)C)C
MOL002128	0.9534	0.0466	0.9553	Panacis Japonici Rhizoma	1,3,8-p-Menthatriene	176983	FALSE	C1(=CC=C(CC1)C(=C)C)C
MOL002128	0.9534	0.0466	0.9553	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	1,3,8-p-Menthatriene	176983	FALSE	C1(=CC=C(CC1)C(=C)C)C
MOL002129	0.8702	0.1298	0.7248	Chuanxiong Rhizoma	CYCLODODECENE	637538	FALSE	C\1=C\CCCCCCCCCC1
MOL002130	0.9531	0.0469	0.9354	Chuanxiong Rhizoma	cyclohexane,1,1,2,3-tetramethyl-	57532263	FALSE	C1(C(C(CCC1)C)C)(C)C

MOL002131	0.8883	0.1117	0.7950	Chuanxiong Rhizoma	2,9-Dimethyldecane	517733	FALSE	CC(CCCCCCC(C)C)C
MOL002132	0.8159	0.1841	0.7187	Rhododendri Daurici Folium	(2R,4aR)-2-isopropenyl-4a,8-dimethyl-2,3,4,5,6,7-hexahydro-1H-naphthalene	10899741	FALSE	C1C(CCC2(CCCC(=C12)C)C)C(=C)C
MOL002132	0.8159	0.1841	0.7187	Chuanxiong Rhizoma	(2R,4aR)-2-isopropenyl-4a,8-dimethyl-2,3,4,5,6,7-hexahydro-1H-naphthalene	10899741	FALSE	C1C(CCC2(CCCC(=C12)C)C)C(=C)C
MOL002133	0.9503	0.0497	0.9447	Curcumae Radix	1,5,5-trimethyl-6-methylenecyclohexene	578237	FALSE	C1(=CCCC(C1=C)(C)C)C
MOL002133	0.9503	0.0497	0.9447	Perillae Fructus	1,5,5-trimethyl-6-methylenecyclohexene	578237	FALSE	C1(=CCCC(C1=C)(C)C)C
MOL002133	0.9503	0.0497	0.9447	Chuanxiong Rhizoma	1,5,5-trimethyl-6-methylenecyclohexene	578237	FALSE	C1(=CCCC(C1=C)(C)C)C
MOL002134	0.9479	0.0521	0.9114	Chuanxiong Rhizoma	Isobutyrophenone	69144	FALSE	c1(C(=O)C(C)C)ccccc1
MOL002136	0.9497	0.0503	0.8699	Chuanxiong Rhizoma	neocnidilide	12315453	FALSE	O1C(=O)C2=CCCCC2C1CCCC
MOL002136	0.9497	0.0503	0.8699	Panax Ginseng C. A. Mey.	neocnidilide	12315453	FALSE	O1C(=O)C2=CCCCC2C1CCCC
MOL002137	0.9286	0.0714	0.9253	Zanthoxyli Pericarpium	OCT	356	FALSE	C(CCCC)CCC
MOL002137	0.9286	0.0714	0.9253	Panax Ginseng C. A. Mey.	OCT	356	FALSE	C(CCCC)CCC
MOL002137	0.9286	0.0714	0.9253	Ginkgo Folium	OCT	356	FALSE	C(CCCC)CCC
MOL002137	0.9286	0.0714	0.9253	licorice	OCT	356	FALSE	C(CCCC)CCC
MOL002137	0.9286	0.0714	0.9253	Chuanxiong Rhizoma	OCT	356	FALSE	C(CCCC)CCC
MOL002137	0.9286	0.0714	0.9253	Semen Pharbitidis	OCT	356	FALSE	C(CCCC)CCC
MOL002137	0.9286	0.0714	0.9253	Equiseti Hiemalis Herba	OCT	356	FALSE	C(CCCC)CCC
MOL002138	0.9411	0.0589	0.9401	Coriandri Sativi Herba	p-Cymen-8-ol	14529	FALSE	C(c1ccc(cc1)C)(C)(C)O

MOL002138	0.9411	0.0589	0.9401	Curcumae Radix	p-Cymen-8-ol	14529	FALSE	C(c1ccc(cc1)C)(C)(C)O
MOL002138	0.9411	0.0589	0.9401	Cannabis Sativa L.	p-Cymen-8-ol	14529	FALSE	C(c1ccc(cc1)C)(C)(C)O
MOL002138	0.9411	0.0589	0.9401	Citrus Reticulata	p-Cymen-8-ol	14529	FALSE	C(c1ccc(cc1)C)(C)(C)O
MOL002138	0.9411	0.0589	0.9401	Piperis Fructus	p-Cymen-8-ol	14529	FALSE	C(c1ccc(cc1)C)(C)(C)O
MOL002138	0.9411	0.0589	0.9401	Ephedra Herba	p-Cymen-8-ol	14529	FALSE	C(c1ccc(cc1)C)(C)(C)O
MOL002138	0.9411	0.0589	0.9401	Aucklandiae Radix	p-Cymen-8-ol	14529	FALSE	C(c1ccc(cc1)C)(C)(C)O
MOL002138	0.9411	0.0589	0.9401	Radix Bupleuri	p-Cymen-8-ol	14529	FALSE	C(c1ccc(cc1)C)(C)(C)O
MOL002138	0.9411	0.0589	0.9401	Chuanxiong Rhizoma	p-Cymen-8-ol	14529	FALSE	C(c1ccc(cc1)C)(C)(C)O
MOL002139	0.9060	0.0940	0.9409	Chuanxiong Rhizoma	APH	8247	FALSE	c1(NNC(=O)C)ccccc1
MOL002140	0.7131	0.2869	0.7490	Hoveniae Dulcis Semen	Perlolyrine	160179	FALSE	c12c(c3c([nH]2)cccc3)ccnc1c1oc(cc1)CO
MOL002140	0.7131	0.2869	0.7490	Momordicae Fructus	Perlolyrine	160179	FALSE	c12c(c3c([nH]2)cccc3)ccnc1c1oc(cc1)CO
MOL002140	0.7131	0.2869	0.7490	Codonopsis Radix	Perlolyrine	160179	FALSE	c12c(c3c([nH]2)cccc3)ccnc1c1oc(cc1)CO
MOL002140	0.7131	0.2869	0.7490	Chuanxiong Rhizoma	Perlolyrine	160179	FALSE	c12c(c3c([nH]2)cccc3)ccnc1c1oc(cc1)CO
MOL002141	0.3749	0.6251	0.9669	Dictamni Cortex	PLO	8955	TRUE	C12C(C3C(CC2)(C(CC3)C(=O)C)C)CC=C2C1(CCC(C2)O)C
MOL002141	0.3749	0.6251	0.9669	Radix Bupleuri	PLO	8955	TRUE	C12C(C3C(CC2)(C(CC3)C(=O)C)C)CC=C2C1(CCC(C2)O)C
MOL002141	0.3749	0.6251	0.9669	Chuanxiong Rhizoma	PLO	8955	TRUE	C12C(C3C(CC2)(C(CC3)C(=O)C)C)CC=C2C1(CCC(C2)O)C
MOL002142	0.9483	0.0517	0.8905	Chuanxiong Rhizoma	sedanoic-acid	Not Available	FALSE	C1CCC=C(C1C(=O)CCCC)C(=O)O
MOL002143	0.9523	0.0477	0.9067	Chuanxiong Rhizoma	senkyunolide-C	Not Available	FALSE	C1(=O)O/C(=C/CCC)/c2cc(ccc12)O
MOL002143	0.9523	0.0477	0.9067	Angelicae Sinensis Radix	senkyunolide-C	Not Available	FALSE	C1(=O)O/C(=C/CCC)/c2cc(ccc12)O
MOL002143	0.9523	0.0477	0.9067	Ligustici Rhizoma Et Radix	senkyunolide-C	Not Available	FALSE	C1(=O)O/C(=C/CCC)/c2cc(ccc12)O
MOL002144	0.9217	0.0783	0.8550	Angelicae Sinensis Radix	senkyunolide-D	Not Available	FALSE	C1CC=CC2=C1C(OC2=O)(C(=O)CCC)O
MOL002144	0.9217	0.0783	0.8550	Chuanxiong Rhizoma	senkyunolide-D	Not Available	FALSE	C1CC=CC2=C1C(OC2=O)(C(=O)CCC)O
MOL002145	0.9533	0.0467	0.8887	Chuanxiong Rhizoma	senkyunolide-E	Not Available	FALSE	c1cccc2c1/C(=C/C(CC)O)/OC2=O
MOL002145	0.9533	0.0467	0.8887	Angelicae Sinensis Radix	senkyunolide-E	Not Available	FALSE	c1cccc2c1/C(=C/C(CC)O)/OC2=O
MOL002146	0.9518	0.0482	0.8582	Ligustici Rhizoma Et Radix	senkyunolide-F	Not Available	FALSE	C1CC=CC2=C1/C(=C\C(CC)O)/OC2=O
MOL002146	0.9518	0.0482	0.8582	Chuanxiong Rhizoma	senkyunolide-F	Not Available	FALSE	C1CC=CC2=C1/C(=C\C(CC)O)/OC2=O
MOL002147	0.9518	0.0482	0.8822	Chuanxiong Rhizoma	senkyunolide-J	Not Available	FALSE	C1CC(C(C2=C1C(OC2=O)CCCC)O)O
MOL002148	0.9221	0.0779	0.8117	Chuanxiong Rhizoma	senkyunolide-L	Not Available	FALSE	C1(C(CCC2=C1C(=O)O/C/2=C/CCC)O)Cl

MOL002149	0.9431	0.0569	0.8810	Chuanxiong Rhizoma	senkyunolide-S	Not Available	FALSE	C1CC(C(C2=C1C(CC2=O)CC(CC)O)O)O
MOL002150	0.8841	0.1159	0.8233	Chuanxiong Rhizoma	1-Acetyl-beta-carboline	638667	FALSE	c12ccccc1c1c([nH]2)c(ncc1)C(=O)C
MOL002150	0.8841	0.1159	0.8233	Arisaematis Rhizoma	1-Acetyl-beta-carboline	638667	FALSE	c12ccccc1c1c([nH]2)c(ncc1)C(=O)C
MOL002150	0.8841	0.1159	0.8233	Ailanthi Cortex	1-Acetyl-beta-carboline	638667	FALSE	c12ccccc1c1c([nH]2)c(ncc1)C(=O)C
MOL002150	0.8841	0.1159	0.8233	Momordicae Fructus	1-Acetyl-beta-carboline	638667	FALSE	c12ccccc1c1c([nH]2)c(ncc1)C(=O)C
MOL002151	0.3506	0.6494	0.7231	Chuanxiong Rhizoma	senkyunone	Not Available	FALSE	C1(=O)C(=CC(=O)C=C1C/C=C(/CC/C=C(/CCC=C(C)C)\C)\C)C
MOL002152	0.9163	0.0837	0.9076	Chuanxiong Rhizoma	sinapic acid	637775	FALSE	c1(c(c(cc(c1)/C=C/C(=O)O)OC)O)OC
MOL002152	0.9163	0.0837	0.9076	Portulacae Herba	sinapic acid	637775	FALSE	c1(c(c(cc(c1)/C=C/C(=O)O)OC)O)OC
MOL002152	0.9163	0.0837	0.9076	Hordei Fructus Germinatus	sinapic acid	637775	FALSE	c1(c(c(cc(c1)/C=C/C(=O)O)OC)O)OC
MOL002152	0.9163	0.0837	0.9076	Sinapis Semen	sinapic acid	637775	FALSE	c1(c(c(cc(c1)/C=C/C(=O)O)OC)O)OC
MOL002152	0.9163	0.0837	0.9076	Cimicifugae Rhizoma	sinapic acid	637775	FALSE	c1(c(c(cc(c1)/C=C/C(=O)O)OC)O)OC
MOL002152	0.9163	0.0837	0.9076	Drynariae Rhizoma	sinapic acid	637775	FALSE	c1(c(c(cc(c1)/C=C/C(=O)O)OC)O)OC
MOL002153	0.8895	0.1105	0.6520	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	1H-Cycloprop(e)azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, (1aR-(1aalpha,4aalpha,7beta,7abeta,7balpha))-	92231	FALSE	C1CC(C2C1C(=C)CCC1C2C1(C)C)(O)C
MOL002153	0.8895	0.1105	0.6520	Chuanxiong Rhizoma	1H-Cycloprop(e)azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, (1aR-(1aalpha,4aalpha,7beta,7abeta,7balpha))-	92231	FALSE	C1CC(C2C1C(=C)CCC1C2C1(C)C)(O)C

MOL002153	0.8895	0.1105	0.6520	Herba Clinopodii Polycephali.	1H-Cycloprop(e)azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, (1aR-(1aalpha,4aalpha,7beta,7abeta,7balpha))-	92231	FALSE	C1CC(C2C1C(=C)CCC1C2C1(C)C)(O)C
MOL002153	0.8895	0.1105	0.6520	Cinnamomi Ramulus	1H-Cycloprop(e)azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, (1aR-(1aalpha,4aalpha,7beta,7abeta,7balpha))-	92231	FALSE	C1CC(C2C1C(=C)CCC1C2C1(C)C)(O)C
MOL002153	0.8895	0.1105	0.6520	Viticis Fructus	1H-Cycloprop(e)azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, (1aR-(1aalpha,4aalpha,7beta,7abeta,7balpha))-	92231	FALSE	C1CC(C2C1C(=C)CCC1C2C1(C)C)(O)C

MOL002153	0.8895	0.1105	0.6520	Radix Salviae	1H-Cycloprop(e)azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, (1aR-(1aalpha,4aalpha,7beta,7abeta,7balpha))-	92231	FALSE	C1CC(C2C1C(=C)CCC1C2C1(C)C)(O)C
MOL002153	0.8895	0.1105	0.6520	Schisandrae Chinensis Fructus	1H-Cycloprop(e)azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, (1aR-(1aalpha,4aalpha,7beta,7abeta,7balpha))-	92231	FALSE	C1CC(C2C1C(=C)CCC1C2C1(C)C)(O)C
MOL002153	0.8895	0.1105	0.6520	Solidaginis Herba	1H-Cycloprop(e)azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, (1aR-(1aalpha,4aalpha,7beta,7abeta,7balpha))-	92231	FALSE	C1CC(C2C1C(=C)CCC1C2C1(C)C)(O)C

MOL002153	0.8895	0.1105	0.6520	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	1H-Cycloprop(e)azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, (1aR-(1aalpha,4aalpha,7beta,7abeta,7balpha))-	92231	FALSE	C1CC(C2C1C(=C)CCC1C2C1(C)C)(O)C
MOL002153	0.8895	0.1105	0.6520	Ailanthi Cortex	1H-Cycloprop(e)azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, (1aR-(1aalpha,4aalpha,7beta,7abeta,7balpha))-	92231	FALSE	C1CC(C2C1C(=C)CCC1C2C1(C)C)(O)C
MOL002154	0.9238	0.0762	0.9364	Malvae Fructus	trans-2-Nonen-1-ol	5364941	FALSE	C(C/C=C/CO)CCCC
MOL002154	0.9238	0.0762	0.9364	Chuanxiong Rhizoma	trans-2-Nonen-1-ol	5364941	FALSE	C(C/C=C/CO)CCCC
MOL002157	0.0976	0.9024	0.7062	Chuanxiong Rhizoma	wallichilide	Not Available	FALSE	O1C(=O)C2=C(/C/1=C/CCC)CCC1C3C=C(C(C21)(CC3)C(=O)CCCC)C(=O)OC
MOL002158	0.6766	0.3234	0.7510	Chuanxiong Rhizoma	xiongterpene	Not Available	FALSE	C1(C(C2C(CC1)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1)OC(=O)/C=C\c1cc(ccc1)O)C)C)C)C(=O)O)C)C
MOL002159	0.9180	0.0820	0.9284	Chuanxiong Rhizoma	1-Octanol,2,7-dimethyl-	Not Available	FALSE	C(C(CCCCC(C)C)C)O
MOL002160	0.9535	0.0465	0.9705	Ephedra Herba	1-terpineol	12443330	FALSE	C1(CC=C(CC1)C(C)C)(O)C
MOL002160	0.9535	0.0465	0.9705	Semen Pharbitidis	1-terpineol	12443330	FALSE	C1(CC=C(CC1)C(C)C)(O)C
MOL002160	0.9535	0.0465	0.9705	Chuanxiong Rhizoma	1-terpineol	12443330	FALSE	C1(CC=C(CC1)C(C)C)(O)C
MOL002160	0.9535	0.0465	0.9705	Folium Artemisiae Argyi	1-terpineol	12443330	FALSE	C1(CC=C(CC1)C(C)C)(O)C
MOL002161	0.7443	0.2557	0.7051	Chuanxiong Rhizoma	1-beta-ethylacrylate-7-aldehyde-beta-carboline	Not Available	FALSE	c1cc(cc2c1c1c(c(ncc1)/C=C/C(=O)OCC)[nH]2)C=O

MOL002162	0.8797	0.1203	0.9231	Chuanxiong Rhizoma	2-Propionylfuran	76662	FALSE	c1(C(=O)CC)ccco1
MOL002163	0.9238	0.0762	0.9190	Cinnamomi Ramulus	WLN: 2VR	7148	FALSE	c1(C(=O)CC)ccccc1
MOL002163	0.9238	0.0762	0.9190	Chuanxiong Rhizoma	WLN: 2VR	7148	FALSE	c1(C(=O)CC)ccccc1
MOL002163	0.9238	0.0762	0.9190	Sterculiae Lychnophorae Semen	WLN: 2VR	7148	FALSE	c1(C(=O)CC)ccccc1
MOL002164	0.9480	0.0520	0.9229	Chuanxiong Rhizoma	2,2,3-Trimethylcyclopent-3-ene-1-carboxaldehyde	15764610	FALSE	C1(C(C(=CC1)C)(C)C)C=O
MOL002165	0.9180	0.0820	0.9153	Chuanxiong Rhizoma	methyl 2-pentanoylbenzoate	11085323	FALSE	C(=O)(c1c(cccc1)C(=O)CCCC)OC
MOL002166	0.9291	0.0709	0.9391	Semen Pharbitidis	ISOHEPTANE	11582	FALSE	CCCCC(C)C
MOL002166	0.9291	0.0709	0.9391	Chuanxiong Rhizoma	ISOHEPTANE	11582	FALSE	CCCCC(C)C
MOL002166	0.9291	0.0709	0.9391	Perillae Fructus	ISOHEPTANE	11582	FALSE	CCCCC(C)C
MOL002166	0.9291	0.0709	0.9391	licorice	ISOHEPTANE	11582	FALSE	CCCCC(C)C
MOL002166	0.9291	0.0709	0.9391	Hippophae Fructus	ISOHEPTANE	11582	FALSE	CCCCC(C)C
MOL002167	0.8856	0.1144	0.9569	Cornus Officinalis Sieb. Et Zucc.	WLN: T5OJ BVO1	11902	FALSE	o1c(ccc1)C(=O)OC
MOL002167	0.8856	0.1144	0.9569	Momordicae Fructus	WLN: T5OJ BVO1	11902	FALSE	o1c(ccc1)C(=O)OC
MOL002167	0.8856	0.1144	0.9569	Chuanxiong Rhizoma	WLN: T5OJ BVO1	11902	FALSE	o1c(ccc1)C(=O)OC
MOL002167	0.8856	0.1144	0.9569	Ephedra Herba	WLN: T5OJ BVO1	11902	FALSE	o1c(ccc1)C(=O)OC
MOL002168	0.9440	0.0560	0.8827	Chuanxiong Rhizoma	2-Methyl-1-phenylpropene	13030	FALSE	c1(ccccc1)C=C(C)C
MOL002169	0.8947	0.1053	0.8161	Chuanxiong Rhizoma	2-methyl-5-(1-methylene)-1,3-cyclohexadiene	Not Available	FALSE	C12=C(C=CC(C1)C2)C

MOL002170	0.9566	0.0434	0.9769	Campsis Flos	(4S,6S)-cis-Carveol	443177	FALSE	C1(C(=CCC(C1)C(=C)C)C)O
MOL002170	0.9566	0.0434	0.9769	Chuanxiong Rhizoma	(4S,6S)-cis-Carveol	443177	FALSE	C1(C(=CCC(C1)C(=C)C)C)O
MOL002171	0.9347	0.0653	0.7510	Chuanxiong Rhizoma	2-Methylbenzoxazol	7225	FALSE	c12c(oc(n1)C)cccc2
MOL002172	0.9241	0.0759	0.9811	Chuanxiong Rhizoma	(5S,6R)-5,6-dimethyltetrahydropyran-2-one	11029861	FALSE	C1(=O)CCC(C(O1)C)C
MOL002173	0.9519	0.0481	0.8768	Chuanxiong Rhizoma	3(S)-3-Butyl-4,5-dihydrophthalide	14091860	FALSE	C1CCCC2=C1C(OC2=O)CCCC
MOL002174	0.9057	0.0943	0.6785	Chuanxiong Rhizoma	3,4-epoxy-2,2,7,7-tetramethyl-octane	Not Available	FALSE	CC(C1C(CCC(C)(C)C)O1)(C)C
MOL002175	0.8973	0.1027	0.9709	Chuanxiong Rhizoma	3-cyclohexen-1-ol	12532693	FALSE	C1(CCC=CC1)O
MOL002175	0.8973	0.1027	0.9709	Zingiberis Rhizoma	3-cyclohexen-1-ol	12532693	FALSE	C1(CCC=CC1)O
MOL002176	0.8669	0.1331	0.9002	Chuanxiong Rhizoma	Methyl 3-furoate	14918	FALSE	c1(ccoc1)C(=O)OC
MOL002177	0.9566	0.0434	0.9577	Chuanxiong Rhizoma	trans-Piperitol	85568	FALSE	C1(C=C(CCC1C(C)C)C)O
MOL002177	0.9566	0.0434	0.9577	Moslae Herba	trans-Piperitol	85568	FALSE	C1(C=C(CCC1C(C)C)C)O
MOL002178	0.9614	0.0386	0.8922	Chuanxiong Rhizoma	4,7-Dihydroxy-3-butylphthalide	Not Available	FALSE	c1(ccc(c2c1C(OC2=O)CCCC)O)O
MOL002180	0.9269	0.0731	0.9431	Chuanxiong Rhizoma	4-Octanone	11516	FALSE	C(=O)(CCCC)CCC
MOL002180	0.9269	0.0731	0.9431	Angelicae Sinensis Radix	4-Octanone	11516	FALSE	C(=O)(CCCC)CCC
MOL002181	0.9561	0.0439	0.9160	Chuanxiong Rhizoma	4-hydroxy-3-butylphthalide	Not Available	FALSE	c1(cccc2c1C(OC2=O)CCCC)O
MOL002182	0.8895	0.1105	0.6520	Chuanxiong Rhizoma	(-)-spathulenol	13854251	FALSE	C1(=C)C2C(C3C(CC1)C3(C)C)C(CC2)(C)O
MOL002183	0.8849	0.1151	0.9725	Chuanxiong Rhizoma	5-Propyl-2-thiouracil	3002043	FALSE	c1(c(=O)[nH]c(=S)[nH]c1)CCC
MOL002183	0.8849	0.1151	0.9725	Alpiniae Oxyphyliae Fructus	5-Propyl-2-thiouracil	3002043	FALSE	c1(c(=O)[nH]c(=S)[nH]c1)CCC

MOL002184	0.9330	0.0670	0.9248	Chuanxiong Rhizoma	(6R)-6-butylcyclohepta-1,4-diene	11804943	FALSE	C1=CCC=CC(C1)CCCC
MOL002184	0.9330	0.0670	0.9248	Angelicae Sinensis Radix	(6R)-6-butylcyclohepta-1,4-diene	11804943	FALSE	C1=CCC=CC(C1)CCCC
MOL002185	0.9636	0.0364	0.8370	Ephedra Herba	7-oxabicyclo-2.2.1-heptane,1-methyl-4-[1-methylethyl]-	10106	FALSE	C12(OC(CC1)(CC2)C)C(C)C
MOL002185	0.9636	0.0364	0.8370	Chuanxiong Rhizoma	7-oxabicyclo-2.2.1-heptane,1-methyl-4-[1-methylethyl]-	10106	FALSE	C12(OC(CC1)(CC2)C)C(C)C
MOL002185	0.9636	0.0364	0.8370	Folium Artemisiae Argyi	7-oxabicyclo-2.2.1-heptane,1-methyl-4-[1-methylethyl]-	10106	FALSE	C12(OC(CC1)(CC2)C)C(C)C
MOL002185	0.9636	0.0364	0.8370	Litseae Fructus	7-oxabicyclo-2.2.1-heptane,1-methyl-4-[1-methylethyl]-	10106	FALSE	C12(OC(CC1)(CC2)C)C(C)C
MOL002187	0.9130	0.0870	0.9121	Ligustici Rhizoma Et Radix	Amylbenzene	10864	FALSE	c1(CCCCC)ccccc1
MOL002187	0.9130	0.0870	0.9121	Chuanxiong Rhizoma	Amylbenzene	10864	FALSE	c1(CCCCC)ccccc1
MOL002187	0.9130	0.0870	0.9121	Sojae Semen Nigrum	Amylbenzene	10864	FALSE	c1(CCCCC)ccccc1
MOL002187	0.9130	0.0870	0.9121	Arisaematis Rhizoma	Amylbenzene	10864	FALSE	c1(CCCCC)ccccc1
MOL002187	0.9130	0.0870	0.9121	Radix Angelicae Biseratae	Amylbenzene	10864	FALSE	c1(CCCCC)ccccc1
MOL002187	0.9130	0.0870	0.9121	Radix Bupleuri	Amylbenzene	10864	FALSE	c1(CCCCC)ccccc1
MOL002188	0.9366	0.0634	0.9594	Chuanxiong Rhizoma	Dimethyl D-malate	11062697	FALSE	C(CC(=O)OC)(C(=O)OC)O
MOL002189	0.9525	0.0475	0.8916	Sinapis Semen	dl-3n-butylphthalide	9990075	FALSE	c12c(C(=O)OC1CCCC)cccc2
MOL002189	0.9525	0.0475	0.8916	Chuanxiong Rhizoma	dl-3n-butylphthalide	9990075	FALSE	c12c(C(=O)OC1CCCC)cccc2
MOL002191	0.8308	0.1692	0.7203	Fructus Carotae	carotol	Not Available	FALSE	C1CC(C2(CCC(=CCC12C)C)O)C(C)C
MOL002191	0.8308	0.1692	0.7203	Chuanxiong Rhizoma	carotol	Not Available	FALSE	C1CC(C2(CCC(=CCC12C)C)O)C(C)C
MOL002192	0.5731	0.4269	0.8089	Chuanxiong Rhizoma	Coniferylfcrulate	Not Available	FALSE	c1c(c(cc(c1)/C=C/C(=O)OC/C=C/c1cc(c(cc1)OC)O)OC)O

MOL002193	0.9598	0.0402	0.9580	Cinnamomi Ramulus	Cerulignol	17739	FALSE	c1(cc(ccc1O)CCC)OC
MOL002193	0.9598	0.0402	0.9580	Chuanxiong Rhizoma	Cerulignol	17739	FALSE	c1(cc(ccc1O)CCC)OC
MOL002194	0.8530	0.1470	0.6183	Chuanxiong Rhizoma	Decahydro-1,6-bis(methylene)-4-(1-methylethyl)-naphthalene	Not Available	FALSE	C1C2C(CCC1=C)C(=C)CCC2C(C)C
MOL002196	0.9072	0.0928	0.9349	Chuanxiong Rhizoma	Hexaphenone	70337	FALSE	c1(C(=O)CCCCC)ccccc1
MOL002197	0.8815	0.1185	0.8574	Chuanxiong Rhizoma	(E,E)-1,3,5-Undecatriene	5367412	FALSE	C=C/C=C/C=C/CCCCC
MOL002198	0.9300	0.0700	0.9383	Equiseti Hiemalis Herba	Heptan	8900	FALSE	C(CCC)CCC
MOL002198	0.9300	0.0700	0.9383	Notopterygii Rhizoma Et Radix	Heptan	8900	FALSE	C(CCC)CCC
MOL002198	0.9300	0.0700	0.9383	Centipedae Herba	Heptan	8900	FALSE	C(CCC)CCC
MOL002198	0.9300	0.0700	0.9383	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Heptan	8900	FALSE	C(CCC)CCC
MOL002198	0.9300	0.0700	0.9383	Notoginseng Flos	Heptan	8900	FALSE	C(CCC)CCC
MOL002198	0.9300	0.0700	0.9383	Sesami Nigrum Semen	Heptan	8900	FALSE	C(CCC)CCC
MOL002198	0.9300	0.0700	0.9383	Allium Azureum Ledeb.	Heptan	8900	FALSE	C(CCC)CCC
MOL002198	0.9300	0.0700	0.9383	Rose Rugosae Flos	Heptan	8900	FALSE	C(CCC)CCC
MOL002198	0.9300	0.0700	0.9383	licorice	Heptan	8900	FALSE	C(CCC)CCC
MOL002198	0.9300	0.0700	0.9383	Ginkgo Folium	Heptan	8900	FALSE	C(CCC)CCC
MOL002198	0.9300	0.0700	0.9383	Chuanxiong Rhizoma	Heptan	8900	FALSE	C(CCC)CCC
MOL002199	0.9261	0.0739	0.9490	Chuanxiong Rhizoma	L-valyl-L-valinc-achydride	Not Available	FALSE	CC(C)C(C(=O)CC(=O)C(C(C)C)N)N
MOL002200	0.2529	0.7471	0.8191	Chuanxiong Rhizoma	Levistolide-A	Not Available	FALSE	O1/C(=C/CCC)/C23C(=CC(C4CCC5=C(C(=O)O/C/5=C/CCC)C24)CC3)C1=O
MOL002201	0.9594	0.0406	0.8564	Radix Bupleuri	cis-ligustilide	5877292	FALSE	C12=C(C(=O)O/C/1=C/CCC)C=CCC2
MOL002201	0.9594	0.0406	0.8564	Angelicae Sinensis Radix	cis-ligustilide	5877292	FALSE	C12=C(C(=O)O/C/1=C/CCC)C=CCC2
MOL002201	0.9594	0.0406	0.8564	Chuanxiong Rhizoma	cis-ligustilide	5877292	FALSE	C12=C(C(=O)O/C/1=C/CCC)C=CCC2
MOL002201	0.9594	0.0406	0.8564	Foeniculi Fructus	cis-ligustilide	5877292	FALSE	C12=C(C(=O)O/C/1=C/CCC)C=CCC2
MOL002202	0.9446	0.0554	0.9480	Chuanxiong Rhizoma	tetramethylpyrazine	14296	FALSE	c1(c(nc(c(n1)C)C)C)C
MOL002202	0.9446	0.0554	0.9480	Ephedra Herba	tetramethylpyrazine	14296	FALSE	c1(c(nc(c(n1)C)C)C)C
MOL002202	0.9446	0.0554	0.9480	Sojae Semen Praeparatum	tetramethylpyrazine	14296	FALSE	c1(c(nc(c(n1)C)C)C)C
MOL002202	0.9446	0.0554	0.9480	Campsis Flos	tetramethylpyrazine	14296	FALSE	c1(c(nc(c(n1)C)C)C)C
MOL002202	0.9446	0.0554	0.9480	Curculiginis Rhizome	tetramethylpyrazine	14296	FALSE	c1(c(nc(c(n1)C)C)C)C

MOL002203	0.4725	0.5275	0.6118	Sojae Semen Nigrum	Exceparl M-OL	5364509	FALSE	C(CC/C=C\CCCCCCCC)CCCCC(=O)OC
MOL002203	0.4725	0.5275	0.6118	Notopterygii Rhizoma Et Radix	Exceparl M-OL	5364509	FALSE	C(CC/C=C\CCCCCCCC)CCCCC(=O)OC
MOL002203	0.4725	0.5275	0.6118	Lygodii Spora	Exceparl M-OL	5364509	FALSE	C(CC/C=C\CCCCCCCC)CCCCC(=O)OC
MOL002203	0.4725	0.5275	0.6118	Peucedani Radix	Exceparl M-OL	5364509	FALSE	C(CC/C=C\CCCCCCCC)CCCCC(=O)OC
MOL002203	0.4725	0.5275	0.6118	Peucedanidecursivi Radix	Exceparl M-OL	5364509	FALSE	C(CC/C=C\CCCCCCCC)CCCCC(=O)OC
MOL002203	0.4725	0.5275	0.6118	Chuanxiong Rhizoma	Exceparl M-OL	5364509	FALSE	C(CC/C=C\CCCCCCCC)CCCCC(=O)OC
MOL002203	0.4725	0.5275	0.6118	Cassiae Semen	Exceparl M-OL	5364509	FALSE	C(CC/C=C\CCCCCCCC)CCCCC(=O)OC
MOL002203	0.4725	0.5275	0.6118	Lepidii Semen Descurainiae Semen	Exceparl M-OL	5364509	FALSE	C(CC/C=C\CCCCCCCC)CCCCC(=O)OC
MOL002203	0.4725	0.5275	0.6118	Mori Cortex	Exceparl M-OL	5364509	FALSE	C(CC/C=C\CCCCCCCC)CCCCC(=O)OC
MOL002203	0.4725	0.5275	0.6118	Campsis Flos	Exceparl M-OL	5364509	FALSE	C(CC/C=C\CCCCCCCC)CCCCC(=O)OC
MOL002203	0.4725	0.5275	0.6118	Amygdalus Communis Vas	Exceparl M-OL	5364509	FALSE	C(CC/C=C\CCCCCCCC)CCCCC(=O)OC
MOL002203	0.4725	0.5275	0.6118	Platycladi Semen	Exceparl M-OL	5364509	FALSE	C(CC/C=C\CCCCCCCC)CCCCC(=O)OC
MOL002203	0.4725	0.5275	0.6118	Arisaematis Rhizoma	Exceparl M-OL	5364509	FALSE	C(CC/C=C\CCCCCCCC)CCCCC(=O)OC
MOL002203	0.4725	0.5275	0.6118	Sterculiae Lychnophorae Semen	Exceparl M-OL	5364509	FALSE	C(CC/C=C\CCCCCCCC)CCCCC(=O)OC
MOL002203	0.4725	0.5275	0.6118	Raphani Semen	Exceparl M-OL	5364509	FALSE	C(CC/C=C\CCCCCCCC)CCCCC(=O)OC
MOL002203	0.4725	0.5275	0.6118	Perillae Fructus	Exceparl M-OL	5364509	FALSE	C(CC/C=C\CCCCCCCC)CCCCC(=O)OC
MOL002203	0.4725	0.5275	0.6118	Ginkgo Folium	Exceparl M-OL	5364509	FALSE	C(CC/C=C\CCCCCCCC)CCCCC(=O)OC
MOL002203	0.4725	0.5275	0.6118	Cnidii Fructus	Exceparl M-OL	5364509	FALSE	C(CC/C=C\CCCCCCCC)CCCCC(=O)OC
MOL002204	0.5956	0.4044	0.6268	Chuanxiong Rhizoma	506-43-4	5365682	FALSE	C(=C\C/C=C\CCCCC)\CCCCCCCCO
MOL002205	0.5672	0.4328	0.6257	Chuanxiong Rhizoma	Octatriacontane	23599	FALSE	C(CCCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCC
MOL002206	0.9490	0.0510	0.9368	Chuanxiong Rhizoma	(2-amylphenyl)methanol	10058085	FALSE	c1(c(cccc1)CCCCC)CO

MOL002207	0.9497	0.0503	0.8699	Ephedra Herba	1(3H)-Isobenzofuranone, 3-butyl-3a,4,5,6-tetrahydro-, cis-(-)-	3083857	FALSE	C12C(=CCCC2)C(=O)OC1CCCC
MOL002207	0.9497	0.0503	0.8699	Ligustici Rhizoma Et Radix	1(3H)-Isobenzofuranone, 3-butyl-3a,4,5,6-tetrahydro-, cis-(-)-	3083857	FALSE	C12C(=CCCC2)C(=O)OC1CCCC
MOL002207	0.9497	0.0503	0.8699	Chuanxiong Rhizoma	1(3H)-Isobenzofuranone, 3-butyl-3a,4,5,6-tetrahydro-, cis-(-)-	3083857	FALSE	C12C(=CCCC2)C(=O)OC1CCCC
MOL002208	0.9526	0.0474	0.8878	Chuanxiong Rhizoma	Senkyunolide A	3085257	FALSE	C1(=O)OC(C2=C1C=CCC2)CCCC
MOL002208	0.9526	0.0474	0.8878	Farfarae Flos	Senkyunolide A	3085257	FALSE	C1(=O)OC(C2=C1C=CCC2)CCCC
MOL002208	0.9526	0.0474	0.8878	Ligustici Rhizoma Et Radix	Senkyunolide A	3085257	FALSE	C1(=O)OC(C2=C1C=CCC2)CCCC
MOL002209	0.9592	0.0408	0.8762	Ligustici Rhizoma Et Radix	Senkyunolide G	5321250	FALSE	C1C=CC2=C(C1)C(OC2=O)(O)CCCC
MOL002209	0.9592	0.0408	0.8762	Chuanxiong Rhizoma	Senkyunolide G	5321250	FALSE	C1C=CC2=C(C1)C(OC2=O)(O)CCCC
MOL002210	0.9563	0.0437	0.8701	Chuanxiong Rhizoma	(3Z,6S,7S)-3-butylidene-6,7-dihydroxy-4,5,6,7-tetrahydroisobenzofuran-1-one	11521428	FALSE	C1(C(CCC2=C1C(=O)O/C/2=C\CCC)O)O
MOL002212	0.5469	0.4531	0.6933	Tinosporae Radix	ecdysterone	5459840	FALSE	C1(C(CC2(C(C1)C(=O)C=C1C3(CCC(C(C(CCC(C)(C)O)O)(C)O)C3(C)CCC21)O)C)O)O
MOL002212	0.5469	0.4531	0.6933	Ajugae Decumbentis Herba	ecdysterone	5459840	FALSE	C1(C(CC2(C(C1)C(=O)C=C1C3(CCC(C(C(CCC(C)(C)O)O)(C)O)C3(C)CCC21)O)C)O)O
MOL002212	0.5469	0.4531	0.6933	Cyathulae Radix	ecdysterone	5459840	FALSE	C1(C(CC2(C(C1)C(=O)C=C1C3(CCC(C(C(CCC(C)(C)O)O)(C)O)C3(C)CCC21)O)C)O)O

MOL002212	0.5469	0.4531	0.6933	Kochiae Fructus	ecdysterone	5459840	FALSE	C1(C(CC2(C(C1)C(=O)C=C1C3(CCC(C(C(CCC(C)(C)O)O)(C)O)C3(C)CCC21)O)C)O)O
MOL002212	0.5469	0.4531	0.6933	Mori Follum	ecdysterone	5459840	FALSE	C1(C(CC2(C(C1)C(=O)C=C1C3(CCC(C(C(CCC(C)(C)O)O)(C)O)C3(C)CCC21)O)C)O)O
MOL002212	0.5469	0.4531	0.6933	Rhapontici Radix	ecdysterone	5459840	FALSE	C1(C(CC2(C(C1)C(=O)C=C1C3(CCC(C(C(CCC(C)(C)O)O)(C)O)C3(C)CCC21)O)C)O)O
MOL002213	0.8830	0.1170	0.8346	Hippophae Fructus	(Z)-1,3-di(phenyl)prop-2-en-1-one	5358548	FALSE	C(=O)(/C=C/c1ccccc1)c1ccccc1
MOL002213	0.8830	0.1170	0.8346	Ginkgo Folium	(Z)-1,3-di(phenyl)prop-2-en-1-one	5358548	FALSE	C(=O)(/C=C/c1ccccc1)c1ccccc1
MOL002213	0.8830	0.1170	0.8346	Cinnamomi Ramulus	(Z)-1,3-di(phenyl)prop-2-en-1-one	5358548	FALSE	C(=O)(/C=C/c1ccccc1)c1ccccc1
MOL002213	0.8830	0.1170	0.8346	Kochiae Fructus	(Z)-1,3-di(phenyl)prop-2-en-1-one	5358548	FALSE	C(=O)(/C=C/c1ccccc1)c1ccccc1
MOL002214	0.7097	0.2903	0.8370	Kochiae Fructus	96990-18-0	176596	FALSE	C1(C(C(C(OC1)OC1C(O)C(OC(C1O)OC1CCC2(C(C1(C)C)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C)C(=O)O)C)C)C(=O)O)O)O)O
MOL002215	0.7225	0.2775	0.8528	Rhododendri Daurici Folium	Oleanic acid	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(CCCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)C)C)C)O
MOL002215	0.7225	0.2775	0.8528	Boehmeriae Rhizoma Et Radix	Oleanic acid	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(CCCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)C)C)C)O
MOL002215	0.7225	0.2775	0.8528	Kochiae Fructus	Oleanic acid	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(CCCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)C)C)C)O
MOL002215	0.7225	0.2775	0.8528	Cortex Moutan	Oleanic acid	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(CCCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)C)C)C)O
MOL002215	0.7225	0.2775	0.8528	Caulis Akebiae	Oleanic acid	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(CCCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)C)C)C)O
MOL002216	0.8337	0.1663	0.6928	Lycii Cortex	9(S)-HOTrE	6439873	FALSE	C(=O)(CCCCCCCC(/C=C/C=C\C/C=C\CC)O)O
MOL002218	0.9190	0.0810	0.8272	Mori Follum	scopolin	25791637	FALSE	C1(=O)CCC2CC(C(CC2O1)OC1OC(C(C(C1O)O)O)CO)O
MOL002218	0.9190	0.0810	0.8272	Lycii Cortex	scopolin	25791637	FALSE	C1(=O)CCC2CC(C(CC2O1)OC1OC(C(C(C1O)O)O)CO)O
MOL002219	0.8849	0.1151	0.7913	Lycii Cortex	Atropine	Not Available	FALSE	c1(cc(ccc1)C1CC2(CCC(C1)N2C)CO)CC(=O)O
MOL002220	0.8405	0.1595	0.6842	Lycii Cortex	9(R)-HODE	16061059	FALSE	C(=O)(CCCCCCCC(/C=C/C=C\CCCCC)O)O
MOL002222	0.2931	0.7069	0.7743	Radix Salviae	sugiol	Not Available	FALSE	C1(CCCC2(c3cc(c(cc3C(=O)CC12)C(C)C)O)C)(C)C
MOL002222	0.2931	0.7069	0.7743	Lycii Cortex	sugiol	Not Available	FALSE	C1(CCCC2(c3cc(c(cc3C(=O)CC12)C(C)C)O)C)(C)C
MOL002222	0.2931	0.7069	0.7743	Figwort Root	sugiol	Not Available	FALSE	C1(CCCC2(c3cc(c(cc3C(=O)CC12)C(C)C)O)C)(C)C
MOL002223	0.8632	0.1368	0.8458	Thalluslaminariae	TAU	4068592	FALSE	OS(=O)(=O)CCN
MOL002223	0.8632	0.1368	0.8458	Lycii Fructus	TAU	4068592	FALSE	OS(=O)(=O)CCN
MOL002223	0.8632	0.1368	0.8458	Lycii Cortex	TAU	4068592	FALSE	OS(=O)(=O)CCN
MOL002225	0.9236	0.0764	0.9162	Cinnamomi Ramulus	Styrone	5315892	FALSE	c1cccc(c1)/C=C/CO

MOL002225	0.9236	0.0764	0.9162	Corayceps	Styrone	5315892	FALSE	c1cccc(c1)/C=C/CO
MOL002225	0.9236	0.0764	0.9162	Lycii Cortex	Styrone	5315892	FALSE	c1cccc(c1)/C=C/CO
MOL002225	0.9236	0.0764	0.9162	Mume Flos	Styrone	5315892	FALSE	c1cccc(c1)/C=C/CO
MOL002225	0.9236	0.0764	0.9162	Cinnanmomi Cortex	Styrone	5315892	FALSE	c1cccc(c1)/C=C/CO
MOL002225	0.9236	0.0764	0.9162	Styrax	Styrone	5315892	FALSE	c1cccc(c1)/C=C/CO
MOL002225	0.9236	0.0764	0.9162	Lycii Fructus	Styrone	5315892	FALSE	c1cccc(c1)/C=C/CO
MOL002226	0.5988	0.4012	0.7790	Lycii Cortex	lyciumin A	Not Available	FALSE	OCC1NC(=O)CNC(=O)C(NC(=O)C(n2cc(CC(NC1=O)C(=O)O)c1c2cccc1)NC(=O)C(NC(=O)C1N(C(=O)C2NC(=O)CC2)CCC1)Cc1ccc(cc1)O)C(C)C
MOL002227	0.5919	0.4081	0.7891	Lycii Cortex	lyciumin B	Not Available	FALSE	C1(NC(=O)CNC(=O)C(NC(=O)C(n2cc(CC(NC1=O)C(=O)O)c1c2cccc1)NC(=O)C(NC(=O)C1CCCN1C(=O)C1NC(=O)CC1)Cc1c[nH]c2c1cccc2)C(C)C)CO
MOL002228	0.2377	0.7623	0.7976	Lycii Cortex	Kulactone	Not Available	FALSE	CC(=CCCC1C(=O)OC2CC3(C(C12)(CCC1C3=CCC2C1(CCC(=O)C2(C)C)C)C)C)C
MOL002232	0.9292	0.0708	0.9136	Radix Rhei Et Rhizome	2-Cinnamoyl-glucose	11972309	FALSE	c1c(cccc1)/C=C/C(=O)OC1C(OC(C(C1O)O)CO)O
MOL002234	0.9433	0.0567	0.8512	Radix Rhei Et Rhizome	2-Methyl-5-carboxymethyl-7-hydroxychromanone	5319543	FALSE	c1(cc(c2c(c1)OC(CC2=O)C)CC(=O)O)O
MOL002235	0.8514	0.1486	0.8230	Radix Rhei Et Rhizome	EUPATIN	5317287	FALSE	COc1c(OC)c(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)OC)O
MOL002235	0.8514	0.1486	0.8230	Artemisia Annua L.	EUPATIN	5317287	FALSE	COc1c(OC)c(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)OC)O
MOL002236	0.8760	0.1240	0.7196	Radix Rhei Et Rhizome	3,5-Di-O-galloyl-4-O-digalloylquinic acid	442676	FALSE	c1c(c(c(cc1C(=O)Oc1c(c(cc(c1)C(=O)OC1C(CC(CC1OC(=O)c1cc(c(c(c1)O)O)O)(C(=O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O)O)O)O
MOL002237	0.9172	0.0828	0.9115	Radix Rhei Et Rhizome	3-Carboxy-4-hydroxy-phenoxy glucoside	10914066	FALSE	c1(ccc(c(c1)C(=O)O)O)OC1OC(C(C(C1O)O)O)CO
MOL002238	0.5979	0.4021	0.7871	Radix Rhei Et Rhizome	3-Hydroxy-25-norfriedel-3,1(10)-dien-2-one-30-oic acid	Not Available	FALSE	C1(=O)C(=C(C2(C(=C1)C1C(CC2)C2(C(CC1)(C1C(CC2)(CCC(C1)(C)C(=O)O)C)C)C)C)O
MOL002239	0.9495	0.0505	0.8604	Radix Rhei Et Rhizome	5-acetyl-7-hydroxy-2-methyl-chromone	5315891	FALSE	c1(cc(c2c(c1)oc(cc2=O)C)C(=O)C)O

MOL002240	0.9500	0.0500	0.8266	Radix Rhei Et Rhizome	5-Carboxy-7-hydroxy-2-methyl-benzopyran-gamma-one	5315688	FALSE	c1(cc(c2c(c1)oc(cc2=O)C)C(=O)O)O
MOL002241	0.9209	0.0791	0.8638	Radix Rhei Et Rhizome	Aloeemodin-omega-O-beta-D-glucopyranoside	147295	FALSE	c1ccc2c(c1O)C(=O)c1c(C2=O)cc(cc1O)COC1OC(C(C(C1O)O)O)O)CO
MOL002242	0.9280	0.0720	0.9158	Radix Rhei Et Rhizome	TPBO	637759	FALSE	c1ccc(cc1)/C=C/C(=O)C
MOL002242	0.9280	0.0720	0.9158	Campsis Flos	TPBO	637759	FALSE	c1ccc(cc1)/C=C/C(=O)C
MOL002243	0.8880	0.1120	0.8783	Polygoni Cuspidati Rhizoma Et Radix	Anthraglycoside B	Not Available	FALSE	c1(cc(c2c(c1)C(=O)c1c(C2=O)c(cc(c1)C)OC1OC(C(C(C1O)O)O)CO)O)O
MOL002243	0.8880	0.1120	0.8783	Radix Rhei Et Rhizome	Anthraglycoside B	Not Available	FALSE	c1(cc(c2c(c1)C(=O)c1c(C2=O)c(cc(c1)C)OC1OC(C(C(C1O)O)O)CO)O)O
MOL002244	0.8790	0.1210	0.8949	Radix Rhei Et Rhizome	Chrysophanol glucoside	6324923	FALSE	c1(cc(c2c(c1)C(=O)c1c(C2=O)c(ccc1)O)OC1OC(C(C(C1O)O)O)CO)C
MOL002245	0.8371	0.1629	0.7594	Polygoni Cuspidati Rhizoma Et Radix	Chrysophanol-8-O-beta-D-(6'-O-galloyl)-glucopyranoside	5315852	FALSE	c1cc(c2c(c1)C(=O)c1c(C2=O)c(cc(c1)C)O)OC1OC(C(C(C1O)O)O)COC(=O)c1cc(c(c(c1)O)O)O
MOL002245	0.8371	0.1629	0.7594	Sennae Folium	Chrysophanol-8-O-beta-D-(6'-O-galloyl)-glucopyranoside	5315852	FALSE	c1cc(c2c(c1)C(=O)c1c(C2=O)c(cc(c1)C)O)OC1OC(C(C(C1O)O)O)COC(=O)c1cc(c(c(c1)O)O)O
MOL002245	0.8371	0.1629	0.7594	Radix Rhei Et Rhizome	Chrysophanol-8-O-beta-D-(6'-O-galloyl)-glucopyranoside	5315852	FALSE	c1cc(c2c(c1)C(=O)c1c(C2=O)c(cc(c1)C)O)OC1OC(C(C(C1O)O)O)COC(=O)c1cc(c(c(c1)O)O)O
MOL002245	0.8371	0.1629	0.7594	Achyranthis Bidentatae Radix	Chrysophanol-8-O-beta-D-(6'-O-galloyl)-glucopyranoside	5315852	FALSE	c1cc(c2c(c1)C(=O)c1c(C2=O)c(cc(c1)C)O)OC1OC(C(C(C1O)O)O)COC(=O)c1cc(c(c(c1)O)O)O
MOL002247	0.9015	0.0985	0.8879	Polygoni Cuspidati Rhizoma Et Radix	Emodin-6-glucoside	5317038	FALSE	c1(cc2c(c(c1)O)C(=O)c1c(C2=O)cc(cc1O)OC1OC(C(C(C1O)O)O)CO)C
MOL002247	0.9015	0.0985	0.8879	Radix Rhei Et Rhizome	Emodin-6-glucoside	5317038	FALSE	c1(cc2c(c(c1)O)C(=O)c1c(C2=O)cc(cc1O)OC1OC(C(C(C1O)O)O)CO)C

MOL002248	0.9092	0.0908	0.8034	Radix Rhei Et Rhizome	Gallic acid-4-O-(6'-O-galloyl)-glucoside	11968477	FALSE	c1(cc(c(c(c1)O)O)O)C(=O)OCC1C(C(C(C(O1)Oc1c(cc(cc1O)C(=O)O)O)O)O)O
MOL002249	0.9495	0.0505	0.7923	Phyllanthi Fructus	gallocatechin	65084	FALSE	c1c(cc2c(c1O)CC(C(O2)c1cc(c(c(c1)O)O)O)O)O
MOL002249	0.9495	0.0505	0.7923	Tripterygii Radix	gallocatechin	65084	FALSE	c1c(cc2c(c1O)CC(C(O2)c1cc(c(c(c1)O)O)O)O)O
MOL002249	0.9495	0.0505	0.7923	Ginkgo Folium	gallocatechin	65084	FALSE	c1c(cc2c(c1O)CC(C(O2)c1cc(c(c(c1)O)O)O)O)O
MOL002249	0.9495	0.0505	0.7923	Radix Rhei Et Rhizome	gallocatechin	65084	FALSE	c1c(cc2c(c1O)CC(C(O2)c1cc(c(c(c1)O)O)O)O)O
MOL002249	0.9495	0.0505	0.7923	Hoveniae Dulcis Semen	gallocatechin	65084	FALSE	c1c(cc2c(c1O)CC(C(O2)c1cc(c(c(c1)O)O)O)O)O
MOL002250	0.8748	0.1252	0.6694	Cornus Officinalis Sieb. Et Zucc.	[(2R,3R,4S,5R,6R)-3,5-dihydroxy-2-(3,4,5-trihydroxybenzoyl)oxy-6-[(3,4,5-trihydroxybenzoyl)oxymethyl]oxan-4-yl] 3,4,5-trihydroxybenzoate	11969003	FALSE	c1(c(cc(cc1O)C(=O)OCC1C(C(C(C(O1)OC(=O)c1cc(c(c(c1)O)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O)O
MOL002250	0.8748	0.1252	0.6694	Radix Rhei Et Rhizome	[(2R,3R,4S,5R,6R)-3,5-dihydroxy-2-(3,4,5-trihydroxybenzoyl)oxy-6-[(3,4,5-trihydroxybenzoyl)oxymethyl]oxan-4-yl] 3,4,5-trihydroxybenzoate	11969003	FALSE	c1(c(cc(cc1O)C(=O)OCC1C(C(C(C(O1)OC(=O)c1cc(c(c(c1)O)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O)O
MOL002251	0.3046	0.6954	0.6314	Radix Rhei Et Rhizome	Mutatochrome	Not Available	FALSE	CC1(CCCC2(C1=CC(O2)/C(=C/C=C\C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)\C)/C)C)C
MOL002252	0.5392	0.4608	0.6453	Radix Rhei Et Rhizome	palmidin B	Not Available	FALSE	c12c(C(c3c(C1=O)c(cc(c3)C)O)C1c3c(C(=O)c4c1cc(cc4O)CO)c(ccc3)O)cccc2O
MOL002253	0.5595	0.4405	0.6557	Radix Rhei Et Rhizome	Palmidin C	44567180	FALSE	c12c(C(c3c(C1=O)c(cc(c3)C)O)C1c3c(C(=O)c4c1cc(cc4O)C)c(ccc3)O)cc(cc2O)O

MOL002256	0.7768	0.2232	0.7810	Radix Rhei Et Rhizome	1,8-dihydroxy-3-methoxy-2,6-dimethyl-9,10-anthraquinone	21770756	FALSE	c1(cc(c2c(c1)C(=O)c1c(C2=O)c(c(c(c1)OC)C)O)O)C
MOL002257	0.8903	0.1097	0.8686	Radix Rhei Et Rhizome	Physcion-8-O-beta-D-glucopyranoside	11968838	FALSE	c1cc(c2c(c1)C(=O)c1c(C2=O)c(c(c(c1O)OC)C)O)OC1OC(C(C(C1O)O)O)CO
MOL002258	0.8657	0.1343	0.7860	Radix Rhei Et Rhizome	Physcion-9-O-beta-D-glucopyranoside_qt	Not Available	FALSE	c1cc(c2c(c1)C(=O)c1c(C2=O)c(c(c(c1O)OC)C)O)O
MOL002259	0.8678	0.1322	0.8231	Polygoni Cuspidati Rhizoma Et Radix	Physciondiglucoside	442762	FALSE	c1c(cc2c(c1OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)C(=O)c1c(C2=O)cc(cc1O)C)OC
MOL002259	0.8678	0.1322	0.8231	Radix Rhei Et Rhizome	Physciondiglucoside	442762	FALSE	c1c(cc2c(c1OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)C(=O)c1c(C2=O)cc(cc1O)C)OC
MOL002259	0.8678	0.1322	0.8231	Sennae Folium	Physciondiglucoside	442762	FALSE	c1c(cc2c(c1OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)C(=O)c1c(C2=O)cc(cc1O)C)OC
MOL002260	0.6984	0.3016	0.7613	Radix Rhei Et Rhizome	Procyanidin B-5,3'-O-gallate	Not Available	FALSE	c1c(c2c(cc1O)OC(C(C2c1c(c2c(cc1O)OC(C(C2)OC(=O)c1cc(c(c(c1)O)O)O)c1ccc(c(c1)O)O)O)O)c1cc(c(cc1)O)O)O
MOL002261	0.3247	0.6753	0.9535	Radix Rhei Et Rhizome	ZINC04081604	11876100	FALSE	C1C(=O)C=C2C(C1)(C1C(CC2)C2C(CC1)(C(CC2)C(=O)C)C)C
MOL002262	0.8629	0.1371	0.8819	Radix Rhei Et Rhizome	5-[(Z)-2-(3-hydroxy-4-methoxy-phenyl)vinyl]resorcinol	10879760	FALSE	c1(cc(cc(c1)/C=C\c1cc(c(cc1)OC)O)O)O
MOL002263	0.5641	0.4359	0.7174	Radix Rhei Et Rhizome	1-Cinnamoyl-3-hydroxy-11-methoxymeliacarpinin	Not Available	FALSE	C1C(C2(C3C4(C1OC(=O)/C=C/c1ccccc1)C(C1(C(C3OC2)OC2(C1(C1CC2C2(C(O1)OC=C2)O)O)C)C)C(OC4)(C(=O)OC)OC)C)O
MOL002264	0.6401	0.3599	0.7128	Radix Rhei Et Rhizome	Rhapontisterone	Not Available	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1O)(C(CC2)C(C(CC(C(C)C)O)O)(O)C)C)O)C)O)O
MOL002265	0.6398	0.3602	0.6339	Radix Rhei Et Rhizome	Rheidin B	Not Available	FALSE	c12c(C(c3c(C1=O)c(cc(c3)C)O)C1c3c(C(=O)c4c1cc(cc4O)C(=O)O)c(ccc3)O)cccc2O
MOL002266	0.5960	0.4040	0.6406	Radix Rhei Et Rhizome	Rheidin C	Not Available	FALSE	c12c(C(c3c(C1=O)c(cc(c3)C)O)C1c3c(C(=O)c4c1cc(cc4O)C(=O)O)c(ccc3)O)cc(cc2O)OC
MOL002267	0.8610	0.1390	0.7800	Radix Rhei Et Rhizome	Rhein diglucoside	Not Available	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3OC1C(C(C(C(O1)CO)O)O)O)O)C(=O)O)c(ccc2)OC1C(C(C(C(O1)CO)O)O)O

MOL002267	0.8610	0.1390	0.7800	Polygoni Cuspidati Rhizoma Et Radix	Rhein diglucoside	Not Available	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3OC1C(C(C(C(O1)CO)O)O)O)C(=O)O)c(ccc2)OC1C(C(C(C(O1)CO)O)O)O
MOL002267	0.8610	0.1390	0.7800	Sennae Folium	Rhein diglucoside	Not Available	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3OC1C(C(C(C(O1)CO)O)O)O)C(=O)O)c(ccc2)OC1C(C(C(C(O1)CO)O)O)O
MOL002268	0.9251	0.0749	0.7737	Sennae Folium	rhein	10168	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C(=O)O)c(ccc2)O
MOL002268	0.9251	0.0749	0.7737	Hippophae Fructus	rhein	10168	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C(=O)O)c(ccc2)O
MOL002268	0.9251	0.0749	0.7737	Cassiae Semen	rhein	10168	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C(=O)O)c(ccc2)O
MOL002268	0.9251	0.0749	0.7737	Radix Rhei Et Rhizome	rhein	10168	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C(=O)O)c(ccc2)O
MOL002268	0.9251	0.0749	0.7737	Hemerocallis Radix	rhein	10168	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C(=O)O)c(ccc2)O
MOL002268	0.9251	0.0749	0.7737	Semen Pharbitidis	rhein	10168	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C(=O)O)c(ccc2)O
MOL002268	0.9251	0.0749	0.7737	Polygoni Cuspidati Rhizoma Et Radix	rhein	10168	FALSE	c12c(C(=O)c3c(C1=O)cc(cc3O)C(=O)O)c(ccc2)O
MOL002269	0.8596	0.1404	0.8052	Radix Rhei Et Rhizome	Rheinoside A	13888124	FALSE	c12c(C(=O)c3c(C1(O)C1C(C(C(C(O1)CO)O)O)O)cc(cc3O)C(=O)O)c(ccc2)OC1C(C(C(C(O1)CO)O)O)O
MOL002270	0.8841	0.1159	0.8455	Radix Rhei Et Rhizome	Rheinoside A_qt	Not Available	FALSE	c12c(C(=O)c3c(C1(O)C1C(C(C(C(O1)CO)O)O)O)cc(cc3O)C(=O)O)c(ccc2)O
MOL002271	0.9318	0.0682	0.7978	Radix Rhei Et Rhizome	Rheumin	Not Available	FALSE	C1=C(CC(C(=O)O1)C(=O)/C=C\c1cc(cc(c1)O)O)O
MOL002272	0.6855	0.3145	0.6238	Radix Rhei Et Rhizome	Sennidin C	Not Available	FALSE	c12c(c(ccc1)O)C(=O)c1c(C2C2c3c(C(=O)c4c2cc(cc4O)C(=O)O)c(ccc3)O)cc(cc1O)CO
MOL002274	0.7421	0.2579	0.6094	Radix Rhei Et Rhizome	(9S)-9-[(9R)-2-carboxy-4,5-dihydroxy-10-oxo-9H-anthracen-9-yl]-4,5-dihydroxy-10-oxo-9H-anthracene-2-carboxylic acid	10459879	FALSE	c12c(c(ccc1)O)C(=O)c1c(C2C2c3c(C(=O)c4c2cc(cc4O)C(=O)O)c(ccc3)O)cc(cc1O)C(=O)O
MOL002274	0.7421	0.2579	0.6094	Sennae Folium	(9S)-9-[(9R)-2-carboxy-4,5-dihydroxy-10-oxo-9H-anthracen-9-yl]-4,5-dihydroxy-10-oxo-9H-anthracene-2-carboxylic acid	10459879	FALSE	c12c(c(ccc1)O)C(=O)c1c(C2C2c3c(C(=O)c4c2cc(cc4O)C(=O)O)c(ccc3)O)cc(cc1O)C(=O)O

MOL002275	0.7802	0.2198	0.7787	Sennae Folium	Sennoside C	Not Available	FALSE	c12c(c(ccc1)OC1OC(C(C(C1O)O)O)CO)C(=O)c1c(C2C2c3c(C(=O)c4c2cc(cc4O)CO)c(ccc3)OC2OC(C(C(C2O)O)O)CO)cc(cc1O)C(=O)O
MOL002275	0.7802	0.2198	0.7787	Chebulae Fructus	Sennoside C	Not Available	FALSE	c12c(c(ccc1)OC1OC(C(C(C1O)O)O)CO)C(=O)c1c(C2C2c3c(C(=O)c4c2cc(cc4O)CO)c(ccc3)OC2OC(C(C(C2O)O)O)CO)cc(cc1O)C(=O)O
MOL002275	0.7802	0.2198	0.7787	Radix Rhei Et Rhizome	Sennoside C	Not Available	FALSE	c12c(c(ccc1)OC1OC(C(C(C1O)O)O)CO)C(=O)c1c(C2C2c3c(C(=O)c4c2cc(cc4O)CO)c(ccc3)OC2OC(C(C(C2O)O)O)CO)cc(cc1O)C(=O)O
MOL002276	0.6855	0.3145	0.6238	Radix Rhei Et Rhizome	Sennoside E_qt	Not Available	FALSE	c12c(c(ccc1)O)C(=O)c1c(C2C2c3c(C(=O)c4c2cc(cc4O)CO)c(ccc3)O)cc(cc1O)C(=O)O
MOL002276	0.6855	0.3145	0.6238	Chebulae Fructus	Sennoside E_qt	Not Available	FALSE	c12c(c(ccc1)O)C(=O)c1c(C2C2c3c(C(=O)c4c2cc(cc4O)CO)c(ccc3)O)cc(cc1O)C(=O)O
MOL002276	0.6855	0.3145	0.6238	Sennae Folium	Sennoside E_qt	Not Available	FALSE	c12c(c(ccc1)O)C(=O)c1c(C2C2c3c(C(=O)c4c2cc(cc4O)CO)c(ccc3)O)cc(cc1O)C(=O)O
MOL002278	0.7550	0.2450	0.7767	Sennae Folium	Sennoside E	Not Available	FALSE	c12c(c(ccc1)OC1OC(C(C(C1O)O)O)CO)C(=O)c1c(C2C2c3c(C(=O)c4c2cc(cc4O)CO)c(ccc3)OC2OC(C(C(C2O)O)O)COC(=O)C(=O)O)cc(cc1O)C(=O)O
MOL002278	0.7550	0.2450	0.7767	Radix Rhei Et Rhizome	Sennoside E	Not Available	FALSE	c12c(c(ccc1)OC1OC(C(C(C1O)O)O)CO)C(=O)c1c(C2C2c3c(C(=O)c4c2cc(cc4O)CO)c(ccc3)OC2OC(C(C(C2O)O)O)COC(=O)C(=O)O)cc(cc1O)C(=O)O
MOL002279	0.9379	0.0621	0.9148	Hippophae Fructus	Serotonin	5202	FALSE	c12c(cc(cc1)O)c(c[nH]2)CCN
MOL002279	0.9379	0.0621	0.9148	Radix Rhei Et Rhizome	Serotonin	5202	FALSE	c12c(cc(cc1)O)c(c[nH]2)CCN
MOL002280	0.8541	0.1459	0.6852	Radix Rhei Et Rhizome	Torachrysone-8-O-beta-D-(6'-oxayl)-glucoside	Not Available	FALSE	c1c(cc2c(c1OC1OC(C(C(C1O)O)O)COC(=O)C(=O)O)c(c(c2)C)C(=O)C)O)OC
MOL002280	0.8541	0.1459	0.6852	Polygoni Cuspidati Rhizoma Et Radix	Torachrysone-8-O-beta-D-(6'-oxayl)-glucoside	Not Available	FALSE	c1c(cc2c(c1OC1OC(C(C(C1O)O)O)COC(=O)C(=O)O)c(c(c2)C)C(=O)C)O)OC
MOL002281	0.9032	0.0968	0.8270	Eriocauli Flos	Toralactone	5321980	FALSE	c1c(cc2c(c1O)c(c1c(c2)cc(oc1=O)C)O)OC
MOL002281	0.9032	0.0968	0.8270	Radix Rhei Et Rhizome	Toralactone	5321980	FALSE	c1c(cc2c(c1O)c(c1c(c2)cc(oc1=O)C)O)OC
MOL002281	0.9032	0.0968	0.8270	Cassiae Semen	Toralactone	5321980	FALSE	c1c(cc2c(c1O)c(c1c(c2)cc(oc1=O)C)O)OC
MOL002282	0.7631	0.2369	0.6156	Radix Rhei Et Rhizome	[Epicatechin-(48)]5-epicatechin	Not Available	FALSE	c1c(cc(c2c1OC(c1cc(c(cc1)O)O)C(C2c1c(cc(c2c1OC(C(C2c1c(cc(c2c1CC(C(C2c1c(cc(c2c1OC(c1cc(c(cc1)O)O)C(C2c1c(cc(c2c1OC(C(C2c1c(cc(c2c1CC(C(C2)O)c1cc(c(cc1)O)O)O)O)O)c1cc(c(cc1)O)O)O)O)O)O)c1cc(c(cc1)O)O)O)O)c1cc(c((cc1)O)O)O)O)O)O

MOL002282	0.7631	0.2369	0.6156	Ginkgo Folium	[Epicatechin-(48)]5-epicatechin	Not Available	FALSE	c1c(cc(c2c1OC(c1cc(c(cc1)O)O)C(C2c1c(cc(c2c1OC(C(C2c1c(cc(c2c1CC(C(C2c1c(cc(c2c1OC(c1cc(c(cc1)O)O)C(C2c1c(cc(c2c1OC(C(C2c1c(cc(c2c1CC(C(C2)O)c1cc(c(cc1)O)O)O)O)c1cc(c(cc1)O)O)O)O)O)O)c1cc(c(cc1)O)O)O)O)c1cc(c(cc1)O)O)O)O)O)O)O
MOL002283	0.6298	0.3702	0.6044	Radix Rhei Et Rhizome	[(2R,3S,4S,5R,6S)-6-[4-[(Z)-2-(3,5-dihydroxyphenyl)ethenyl]phenoxy]-3,4,5-trihydroxyoxan-2-yl]methyl 3,4,5-trihydroxybenzoate	11800639	FALSE	c1(c(cc(cc1O)C(=O)OCC1C(C(C(C(O1)Oc1ccc(cc1)/C=C\c1cc(cc(c1)O)O)O)O)O)O)O
MOL002284	0.9180	0.0820	0.8493	Radix Rhei Et Rhizome	PIT	667639	FALSE	c1(cc(c(cc1)O)O)/C=C/c1cc(cc(c1)O)O
MOL002285	0.9235	0.0765	0.9204	Radix Rhei Et Rhizome	1-O-Galloyl-glycerol	51543739	FALSE	c1(c(cc(cc1O)C(=O)OCC(CO)O)O)O
MOL002285	0.9235	0.0765	0.9204	Chebulae Fructus	1-O-Galloyl-glycerol	51543739	FALSE	c1(c(cc(cc1O)C(=O)OCC(CO)O)O)O
MOL002286	0.9121	0.0879	0.7288	Radix Rhei Et Rhizome	laccaic acid D	Not Available	FALSE	c1(c(cc2c(c1)C(=O)c1c(c2=O)c(cc(c1)O)O)C(=O)O)O
MOL002287	0.9508	0.0492	0.8971	Radix Rhei Et Rhizome	Rheosmin	21648	FALSE	c1(ccc(cc1)O)CCC(=O)C
MOL002288	0.8632	0.1368	0.8717	Sennae Folium	Emodin-1-O-beta-D-glucopyranoside	11968447	FALSE	c12c(cc(cc1OC1C(C(C(C(O1)CO)O)O)O)O)C(=O)c1c(C2=O)c(cc(c1)C)O
MOL002288	0.8632	0.1368	0.8717	Radix Rhei Et Rhizome	Emodin-1-O-beta-D-glucopyranoside	11968447	FALSE	c12c(cc(cc1OC1C(C(C(C(O1)CO)O)O)O)O)C(=O)c1c(C2=O)c(cc(c1)C)O
MOL002289	0.8721	0.1279	0.8162	Radix Rhei Et Rhizome	physcione	71413104	FALSE	c1c(cc2c(c1O)C(=O)c1c(C2=O)cc(cc1O)CO)C
MOL002290	0.7716	0.2284	0.7710	Sennae Folium	Sennoside B	91440	FALSE	O(C1OC(C(O)C(O)C1O)CO)c1c2c(C(C3c4c(C(=O)c5c3cc(cc5O)C(=O)O)c(OC3OC(C(O)C(O)C3O)CO)ccc4)c3c(C2=O)c(O)cc(c3)C(=O)O)ccc1
MOL002290	0.7716	0.2284	0.7710	Radix Rhei Et Rhizome	Sennoside B	91440	FALSE	O(C1OC(C(O)C(O)C1O)CO)c1c2c(C(C3c4c(C(=O)c5c3cc(cc5O)C(=O)O)c(OC3OC(C(O)C(O)C3O)CO)ccc4)c3c(C2=O)c(O)cc(c3)C(=O)O)ccc1
MOL002291	0.6278	0.3722	0.7258	Radix Rhei Et Rhizome	1-O-Galloylpedunculagin	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC1C(C3C(C(O1)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1c(c(c(c(c1)O)O)O)c1c(cc(c(c1O)O)O)C(=O)O3)OC(=O)c1c2c(c(c(c1)O)O)O)O

MOL002292	0.7802	0.2198	0.7769	Radix Rhei Et Rhizome	Sennoside D	46173829	FALSE	O(C1OC(C(O)C(O)C1O)CO)c1c2c(C(C3c4c(C(=O)c5c3cc(cc5O)C(=O)O)c(OC3OC(C(O)C(O)C3O)CO)ccc4)c3c(C2=O)c(O)cc(c3)CO)ccc1
MOL002292	0.7802	0.2198	0.7769	Sennae Folium	Sennoside D	46173829	FALSE	O(C1OC(C(O)C(O)C1O)CO)c1c2c(C(C3c4c(C(=O)c5c3cc(cc5O)C(=O)O)c(OC3OC(C(O)C(O)C3O)CO)ccc4)c3c(C2=O)c(O)cc(c3)CO)ccc1
MOL002293	0.6855	0.3145	0.6238	Sennae Folium	Sennoside D_qt	Not Available	FALSE	Oc1c2c(C(C3c4c(C(=O)c5c3cc(cc5O)C(=O)O)c(O)ccc4)c3c(C2=O)c(O)cc(c3)CO)ccc1
MOL002293	0.6855	0.3145	0.6238	Radix Rhei Et Rhizome	Sennoside D_qt	Not Available	FALSE	Oc1c2c(C(C3c4c(C(=O)c5c3cc(cc5O)C(=O)O)c(O)ccc4)c3c(C2=O)c(O)cc(c3)CO)ccc1
MOL002295	0.9278	0.0722	0.9110	Scutellariae Barbatae Herba	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002295	0.9278	0.0722	0.9110	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002295	0.9278	0.0722	0.9110	Radix Rhei Et Rhizome	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002295	0.9278	0.0722	0.9110	Figwort Root	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002295	0.9278	0.0722	0.9110	Semen Pharbitidis	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002295	0.9278	0.0722	0.9110	Campsis Flos	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002295	0.9278	0.0722	0.9110	Boschniakia Rossica Herba	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002295	0.9278	0.0722	0.9110	Aloe	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002295	0.9278	0.0722	0.9110	Meliae Azedarach Fructus	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002295	0.9278	0.0722	0.9110	Selaginella Doederleinii Hieron	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002295	0.9278	0.0722	0.9110	Benzoinum	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002295	0.9278	0.0722	0.9110	Solidaginis Herba	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002295	0.9278	0.0722	0.9110	Cinnanmomi Cortex	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002295	0.9278	0.0722	0.9110	Typhonii Rhizoma	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002295	0.9278	0.0722	0.9110	Plantaginis Herba	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002295	0.9278	0.0722	0.9110	Fritiliariae Irrhosae Bulbus	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002295	0.9278	0.0722	0.9110	Styrax	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002295	0.9278	0.0722	0.9110	Chaenomeles Sinensis (Thouin) Koehne	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002295	0.9278	0.0722	0.9110	Drynariae Rhizoma	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002295	0.9278	0.0722	0.9110	Cinnamomi Ramulus	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002295	0.9278	0.0722	0.9110	Ephedra Herba	cinnamic acid	444539	FALSE	c1c(cccc1)/C=C/C(=O)O
MOL002298	0.8924	0.1076	0.7604	Sennae Folium	aloeemodin	Not Available	FALSE	C12C(C=CC=C1O)C(=O)c1c(C2=O)c(cc(c1)CO)O
MOL002298	0.8924	0.1076	0.7604	Radix Rhei Et Rhizome	aloeemodin	Not Available	FALSE	C12C(C=CC=C1O)C(=O)c1c(C2=O)c(cc(c1)CO)O
MOL002299	0.8998	0.1002	0.9695	Radix Rhei Et Rhizome	DMR	92824	FALSE	OC(=O)C(CC(=O)O)O
MOL002299	0.8998	0.1002	0.9695	Stemonae Radix	DMR	92824	FALSE	OC(=O)C(CC(=O)O)O
MOL002299	0.8998	0.1002	0.9695	Hippophae Fructus	DMR	92824	FALSE	OC(=O)C(CC(=O)O)O

MOL002300	0.5201	0.4799	0.7448	Radix Rhei Et Rhizome	10beta-Hydroxy-6beta-isobutyrylfuranoeremophilane	442377	FALSE	C1CC(C2(C(C1)(Cc1c(C2OC(=O)C(C)C)c(co1)C)O)C)C
MOL002301	0.8939	0.1061	0.9621	Maydis Seigma	DLA	61503	FALSE	CC(O)C(=O)O
MOL002301	0.8939	0.1061	0.9621	Radix Rhei Et Rhizome	DLA	61503	FALSE	CC(O)C(=O)O
MOL002301	0.8939	0.1061	0.9621	Pollen Typhae	DLA	61503	FALSE	CC(O)C(=O)O
MOL002302	0.8838	0.1162	0.7751	Radix Rhei Et Rhizome	RHAPONTIN	Not Available	FALSE	C1(C(C(OC(C1O)Oc1cc(cc(c1)/C=C/c1cc(c(cc1)OC)O)O)O)O)O
MOL002303	0.5863	0.4137	0.6493	Radix Rhei Et Rhizome	palmidin A	Not Available	FALSE	c12c(cc(cc1O)CO)C(c1c(C2=O)c(ccc1)O)C1c2c(c(cc(c2)O)O)C(=O)c2c1cc(cc2O)C
MOL002304	0.7483	0.2517	0.6857	Radix Rhei Et Rhizome	Glycerite	Not Available	FALSE	c1(c(cc(cc1O)C(=O)Oc1cc(cc(c1O)O)C(=O)OCC1OC(C(C(C1OC(=O)c1cc(c(c(c1)OC(=O)c1cc(c(c(c1)O)O)O)O)O)OC(=O)c1cc(c(c(c1)OC(=O)c1cc(c(c(c1)O)O)O)O)O)OC(=O)c1cc(c(c(c1)OC(=O)c1cc(c(c(c1)O)O)O)O)O)OC(=C)c1cc(c(c(c1)OC(=C)c1cc(c(c(c1)O)O)O)O)O)O
MOL002305	0.9244	0.0756	0.7967	Radix Rhei Et Rhizome	2,3-Digalloylglucose	471118	FALSE	C1(C(C(C(C(O1)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)CO
MOL002306	0.8841	0.1159	0.8704	Isatidis Folium	(1R,4S)-bicyclo[2.2.1]hept-2-ene	638051	FALSE	C12CC(CC1)C=C2
MOL002307	0.2016	0.7984	0.6741	Polygoni Tinctorii Foliu	20-Hexadecanoylingenol	Not Available	FALSE	C123C(=O)C(C4C(CC1C)C4(C)C)C=C(COC(=O)CCCCCCCCCCCCCCC)C(C2(C(C(=C3)C)O)O)O
MOL002307	0.2016	0.7984	0.6741	Houttuyniae Herba	20-Hexadecanoylingenol	Not Available	FALSE	C123C(=O)C(C4C(CC1C)C4(C)C)C=C(COC(=O)CCCCCCCCCCCCCCC)C(C2(C(C(=C3)C)O)O)O
MOL002307	0.2016	0.7984	0.6741	Radix Bupleuri	20-Hexadecanoylingenol	Not Available	FALSE	C123C(=O)C(C4C(CC1C)C4(C)C)C=C(COC(=O)CCCCCCCCCCCCCCC)C(C2(C(C(=C3)C)O)O)O
MOL002307	0.2016	0.7984	0.6741	Codonopsis Radix	20-Hexadecanoylingenol	Not Available	FALSE	C123C(=O)C(C4C(CC1C)C4(C)C)C=C(COC(=O)CCCCCCCCCCCCCCC)C(C2(C(C(=C3)C)O)O)O
MOL002307	0.2016	0.7984	0.6741	Jujubae Fructus	20-Hexadecanoylingenol	Not Available	FALSE	C123C(=O)C(C4C(CC1C)C4(C)C)C=C(COC(=O)CCCCCCCCCCCCCCC)C(C2(C(C(=C3)C)O)O)O
MOL002307	0.2016	0.7984	0.6741	Epimrdii Herba	20-Hexadecanoylingenol	Not Available	FALSE	C123C(=O)C(C4C(CC1C)C4(C)C)C=C(COC(=O)CCCCCCCCCCCCCCC)C(C2(C(C(=C3)C)O)O)O

MOL002307	0.2016	0.7984	0.6741	Isatidis Folium	20-Hexadecanoyl ingenol	Not Available	FALSE	C123C(=O)C(C4C(CC1C)C4(C)C)C=C(COC(=O)CCCCCCCCCCCCCCC)C(C2(C(C(=C3)C)O)O)O
MOL002307	0.2016	0.7984	0.6741	Semen Euphorbiae	20-Hexadecanoyl ingenol	Not Available	FALSE	C123C(=O)C(C4C(CC1C)C4(C)C)C=C(COC(=O)CCCCCCCCCCCCCCC)C(C2(C(C(=C3)C)O)O)O
MOL002307	0.2016	0.7984	0.6741	Cornus Officinalis Sieb. Et Zucc.	20-Hexadecanoyl ingenol	Not Available	FALSE	C123C(=O)C(C4C(CC1C)C4(C)C)C=C(COC(=O)CCCCCCCCCCCCCCC)C(C2(C(C(=C3)C)O)O)O
MOL002307	0.2016	0.7984	0.6741	Panax Ginseng C. A. Mey.	20-Hexadecanoyl ingenol	Not Available	FALSE	C123C(=O)C(C4C(CC1C)C4(C)C)C=C(COC(=O)CCCCCCCCCCCCCCC)C(C2(C(C(=C3)C)O)O)O
MOL002307	0.2016	0.7984	0.6741	Corayceps	20-Hexadecanoyl ingenol	Not Available	FALSE	C123C(=O)C(C4C(CC1C)C4(C)C)C=C(COC(=O)CCCCCCCCCCCCCCC)C(C2(C(C(=C3)C)O)O)O
MOL002308	0.9321	0.0679	0.7260	Isatidis Folium	Indicaxanthin	Not Available	FALSE	C1C/[N+](=C/C=C\2/CC(NC(=C2)C(=O)O)C(=O)O)/C(C1)C(=O)O
MOL002308	0.9321	0.0679	0.7260	Polygoni Tinctorii Foliu	Indicaxanthin	Not Available	FALSE	C1C/[N+](=C/C=C\2/CC(NC(=C2)C(=O)O)C(=O)O)/C(C1)C(=O)O
MOL002309	0.8181	0.1819	0.7480	Indigo Naturalis	indirubin	5359405	FALSE	c1ccc2c(c1)C(=O)/C(=C/1\C(=O)Nc3c1cccc3)/N2
MOL002309	0.8181	0.1819	0.7480	Isatidis Folium	indirubin	5359405	FALSE	c1ccc2c(c1)C(=O)/C(=C/1\C(=O)Nc3c1cccc3)/N2
MOL002310	0.8561	0.1439	0.6762	Isatidis Folium	Isatidine	Not Available	FALSE	C12C3CC[N+]1(CC=C2COC(=O)C(C(C/C(=C\C)/C(=O)O3)C)(O)CO)O
MOL002310	0.8561	0.1439	0.6762	Polygoni Tinctorii Foliu	Isatidine	Not Available	FALSE	C12C3CC[N+]1(CC=C2COC(=O)C(C(C/C(=C\C)/C(=O)O3)C)(O)CO)O
MOL002311	0.6859	0.3141	0.7518	Isatidis Folium	Glycyrol	5320083	FALSE	C(−CCC1(OC)c2(cc1O)oC(−O)c1c20c2c1ccc(c2)O)(C)C
MOL002311	0.6859	0.3141	0.7518	Polygoni Tinctorii Foliu	Glycyrol	5320083	FALSE	C(−CCC1(OC)c2(cc1O)oC(−O)c1c20c2c1ccc(c2)O)(C)C
MOL002311	0.6859	0.3141	0.7518	licorice	Glycyrol	5320083	FALSE	C(−CCC1(OC)c2(cc1O)oC(−O)c1c20c2c1ccc(c2)O)(C)C

MOL002312	0.8289	0.1711	0.7193	Polygoni Tinctorii Foliu	[(3S,4R,5R)-5-[[(2R,3S,4S,5R,6S)-6-(2-acetyl-5-methoxyphenoxy)-3,4,5-trihydroxyoxan-2-yl]methoxy]-3,4-dihydroxyoxolan-3-yl]methyl 3,4,5-trihydroxybenzoate	9986231	FALSE	c1(c(c(cc(c1)C(=O)OCC1(C(C(OC1)OCC1C(C(C(C(O1)Oc1c(ccc(c1)OC)C(=O)C)O)O)O)O)O)O)O)O
MOL002312	0.8289	0.1711	0.7193	Panax Ginseng C. A. Mey.	[(3S,4R,5R)-5-[[(2R,3S,4S,5R,6S)-6-(2-acetyl-5-methoxyphenoxy)-3,4,5-trihydroxyoxan-2-yl]methoxy]-3,4-dihydroxyoxolan-3-yl]methyl 3,4,5-trihydroxybenzoate	9986231	FALSE	c1(c(c(cc(c1)C(=O)OCC1(C(C(OC1)OCC1C(C(C(C(O1)Oc1c(ccc(c1)OC)C(=O)C)O)O)O)O)O)O)O)O

MOL002312	0.8289	0.1711	0.7193	Pyrrosiae Folium	[(3S,4R,5R)-5-[[(2R,3S,4S,5R,6S)-6-(2-acetyl-5-methoxyphenoxy)-3,4,5-trihydroxyoxan-2-yl]methoxy]-3,4-dihydroxyoxolan-3-yl]methyl 3,4,5-trihydroxybenzoate	9986231	FALSE	c1(c(c(cc(c1)C(=O)OCC1(C(C(OC1)OCC1C(C(C(C(O1)Oc1c(ccc(c1)OC)C(=O)C)O)O)O)O)O)O)O)O
MOL002312	0.8289	0.1711	0.7193	Isatidis Folium	[(3S,4R,5R)-5-[[(2R,3S,4S,5R,6S)-6-(2-acetyl-5-methoxyphenoxy)-3,4,5-trihydroxyoxan-2-yl]methoxy]-3,4-dihydroxyoxolan-3-yl]methyl 3,4,5-trihydroxybenzoate	9986231	FALSE	c1(c(c(cc(c1)C(=O)OCC1(C(C(OC1)OCC1C(C(C(C(O1)Oc1c(ccc(c1)OC)C(=O)C)O)O)O)O)O)O)O)O
MOL002313	0.6259	0.3741	0.8215	Lycii Fructus	TR-saponin A	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2O)O)(C(C(C(C1)(C)C)OC(=O)/C(=C\C)/C)OC(=O)/C(=C\C)/C)CO)C)C)(C)C(=O)OC)OC1OC(C(C(C1O)OC1OCC(C(C1O)O)O)O)C(=O)OC
MOL002313	0.6259	0.3741	0.8215	Isatidis Folium	TR-saponin A	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2O)O)(C(C(C(C1)(C)C)OC(=O)/C(=C\C)/C)OC(=O)/C(=C\C)/C)CO)C)C)(C)C(=O)OC)OC1OC(C(C(C1O)OC1OCC(C(C1O)O)O)O)C(=O)OC

MOL002313	0.6259	0.3741	0.8215	Polygoni Tinctorii Foliu	TR-saponin A	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2O)O)(C(C(C(C1)(C)C)OC(=O)/C(=C\C)/C)OC(=O)/C(=C\C)/C)CO)C)C)C)(C)C(=O)OC)OC1OC(C(C(C1O)OC1OCC(C(C1O)O)O)O)C(=O)OC
MOL002314	0.4365	0.5635	0.7464	Isatidis Folium	TR-saponin A_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2O)O)(C(C(C(C1)(C)C)OC(=O)/C(=C\C)/C)OC(=O)/C(=C\C)/C)CO)C)C)C)(C)C(=O)OC)O
MOL002314	0.4365	0.5635	0.7464	Lycii Fructus	TR-saponin A_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2O)O)(C(C(C(C1)(C)C)OC(=O)/C(=C\C)/C)OC(=O)/C(=C\C)/C)CO)C)C)C)(C)C(=O)OC)O
MOL002315	0.7002	0.2998	0.7771	Isatidis Folium	Thladioside H1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(O1)C)OC1C(C(C(CO1)O)OC1C(C(C(CO1)O)O)O)O)O)O)C)C)(C)C=O)OC1C(C(C(C(O1)C(=O)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)O
MOL002315	0.7002	0.2998	0.7771	Polygoni Tinctorii Foliu	Thladioside H1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(O1)C)OC1C(C(C(CO1)O)OC1C(C(C(CO1)O)O)O)O)O)O)C)C)(C)C=O)OC1C(C(C(C(O1)C(=O)O)O)O)OC1C(C(C(C(O1)CO)O)O)O
MOL002316	0.7411	0.2589	0.8610	Polygoni Tinctorii Foliu	Thladioside H1_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)O)C)C)(C)C=O)O
MOL002316	0.7411	0.2589	0.8610	Isatidis Folium	Thladioside H1_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)O)C)C)(C)C=O)O
MOL002317	0.9183	0.0817	0.9362	Isatidis Folium	vitamin L1	3734162	FALSE	c1(c(cccc1)N)C(=O)O
MOL002319	0.8582	0.1418	0.8449	Isatidis Folium	Isoscoparin	442611	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c2c(oc(cc2=O)c2cc(OC)c(O)cc2)cc1O
MOL002321	0.9099	0.0901	0.9655	Indigo Naturalis	Pca	7405	FALSE	C1(NC(=O)CC1)C(=O)O
MOL002321	0.9099	0.0901	0.9655	Isatidis Folium	Pca	7405	FALSE	C1(NC(=O)CC1)C(=O)O
MOL002321	0.9099	0.0901	0.9655	Rehmanniae Radix Praeparata	Pca	7405	FALSE	C1(NC(=O)CC1)C(=O)O
MOL002322	0.8621	0.1379	0.8440	Herba Patriniae	isovitexin	162350	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1O
MOL002322	0.8621	0.1379	0.8440	Trigonellae Semen	isovitexin	162350	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1O
MOL002322	0.8621	0.1379	0.8440	Microctis Folium	isovitexin	162350	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1O
MOL002322	0.8621	0.1379	0.8440	Hordei Fructus Germinatus	isovitexin	162350	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1O
MOL002322	0.8621	0.1379	0.8440	Gentianae Radix Et Rhozima	isovitexin	162350	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1O
MOL002322	0.8621	0.1379	0.8440	Belamcandae Rhizome	isovitexin	162350	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1O

MOL002322	0.8621	0.1379	0.8440	Isatdis Radix	isovitexin	162350	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1O
MOL002322	0.8621	0.1379	0.8440	Indigo Naturalis	isovitexin	162350	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1O
MOL002322	0.8621	0.1379	0.8440	Santalum Album L.	isovitexin	162350	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1O
MOL002322	0.8621	0.1379	0.8440	Vaccariae Semen	isovitexin	162350	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1O
MOL002322	0.8621	0.1379	0.8440	Isatidis Folium	isovitexin	162350	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1O
MOL002323	0.9273	0.0727	0.9000	Isatidis Folium	L-Adenosine	448374	FALSE	n1cnc2c(c1N)ncn2C1C(C(C(O1)CO)O)O
MOL002323	0.9273	0.0727	0.9000	Panax Ginseng C. A. Mey.	L-Adenosine	448374	FALSE	n1cnc2c(c1N)ncn2C1C(C(C(O1)CO)O)O
MOL002324	0.7499	0.2501	0.6019	Isatidis Folium	3-[2-sulfooxyimino-2-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]sulfanylethyl]indole-1-sulfonic acid	6602379	FALSE	S(/C(=N\OS(=O)(=O)O)/Cc1cn(c2c1cccc2)S(=O)(=O)O)C1OC(C(C(C1O)O)O)CO
MOL002326	0.9249	0.0751	0.8843	Stephaniae Tetrandrae Radix	2,2,2-triethoxyethanol	5322034	FALSE	CCOC(CO)(OCC)OCC
MOL002327	0.2264	0.7736	0.6791	Stephaniae Tetrandrae Radix	Fenfangjine D	Not Available	FALSE	c1c2c3c(c(c1OC)O)Oc1c(cc4c(c1)C(N(CC4)C)Cc1ccc(cc1)Oc1c(ccc(Cc3[n+](cc2)C)c1)OC)OC
MOL002328	0.8320	0.1680	0.7093	Aloe	Feralolide	5317333	FALSE	c1(cc(c2c(c1)CC(OC2=O)Cc1cc(cc(c1C(=O)C)O)O)O)O
MOL002328	0.8320	0.1680	0.7093	Stephaniae Tetrandrae Radix	Feralolide	5317333	FALSE	c1(cc(c2c(c1)CC(OC2=O)Cc1cc(cc(c1C(=O)C)O)O)O)O
MOL002330	0.2190	0.7810	0.7258	Radix Stephaniae Cepharanthae.	TNP00326	Not Available	FALSE	c1c2c3c(c(c1OC)OC)Oc1c(cc4c(c1)C(N(CC4)C)Cc1ccc(Oc4c(ccc(CC3N(CC2)C)c4)OC)cc1)OC
MOL002330	0.2190	0.7810	0.7258	Stephaniae Tetrandrae Radix	TNP00326	Not Available	FALSE	c1c2c3c(c(c1OC)OC)Oc1c(cc4c(c1)C(N(CC4)C)Cc1ccc(Oc4c(ccc(CC3N(CC2)C)c4)OC)cc1)OC
MOL002331	0.6508	0.3492	0.8644	Stephaniae Tetrandrae Radix	N-Methylflindersine	72819	FALSE	c12c(n(c(=O)c3c1OC(C=C3)(C)C)C)cccc2
MOL002331	0.6508	0.3492	0.8644	Phellodendri Amurensis Cortex	N-Methylflindersine	72819	FALSE	c12c(n(c(=O)c3c1OC(C=C3)(C)C)C)cccc2
MOL002332	0.6284	0.3716	0.8021	Stephaniae Tetrandrae Radix	STOCK1N-53032	Not Available	FALSE	c1(c(c2c3c(c1)CCNC3CC12C=CC(=O)C=C1)OC)OC

MOL002333	0.7438	0.2562	0.7049	Stephaniae Tetrandrae Radix	Tetraneurin A	174868	FALSE	C12(C(C3C(CCC1COC(=O)C)C(=C)C(=O)O3)(C(=O)CC2)C)O
MOL002334	0.9469	0.0531	0.9644	Magnolia Officinalis Rehd Et Wils.	Homocresol	62465	FALSE	c1(cc(ccc1O)CC)OC
MOL002334	0.9469	0.0531	0.9644	Benzoinum	Homocresol	62465	FALSE	c1(cc(ccc1O)CC)OC
MOL002334	0.9469	0.0531	0.9644	Stephaniae Tetrandrae Radix	Homocresol	62465	FALSE	c1(cc(ccc1O)CC)OC
MOL002334	0.9469	0.0531	0.9644	Alpiniae Officinarum Rhizome	Homocresol	62465	FALSE	c1(cc(ccc1O)CC)OC
MOL002334	0.9469	0.0531	0.9644	Radix Cynanchi Paniculati	Homocresol	62465	FALSE	c1(cc(ccc1O)CC)OC
MOL002337	0.8531	0.1469	0.7307	Stephaniae Tetrandrae Radix	longipinocarvone	Not Available	FALSE	O=C1CC2C3(C(C2C(CCC3)(C)C)C1=C)C
MOL002338	0.8895	0.1105	0.6520	Pogostemon Cablin (Blanco) Benth.	136458-42-9	178323	FALSE	OC1(C2C3C(C3CCC(=C)C2CC1)(C)C)C
MOL002338	0.8895	0.1105	0.6520	Schizonepetae Spica	136458-42-9	178323	FALSE	OC1(C2C3C(C3CCC(=C)C2CC1)(C)C)C
MOL002338	0.8895	0.1105	0.6520	Farfarae Flos	136458-42-9	178323	FALSE	OC1(C2C3C(C3CCC(=C)C2CC1)(C)C)C
MOL002338	0.8895	0.1105	0.6520	Tamaricis Cacumen	136458-42-9	178323	FALSE	OC1(C2C3C(C3CCC(=C)C2CC1)(C)C)C
MOL002338	0.8895	0.1105	0.6520	Curcumae Radix	136458-42-9	178323	FALSE	OC1(C2C3C(C3CCC(=C)C2CC1)(C)C)C
MOL002338	0.8895	0.1105	0.6520	Verbenae Herb	136458-42-9	178323	FALSE	OC1(C2C3C(C3CCC(=C)C2CC1)(C)C)C
MOL002338	0.8895	0.1105	0.6520	Stephaniae Tetrandrae Radix	136458-42-9	178323	FALSE	OC1(C2C3C(C3CCC(=C)C2CC1)(C)C)C
MOL002338	0.8895	0.1105	0.6520	Bidentis Bipinnatae Herba	136458-42-9	178323	FALSE	OC1(C2C3C(C3CCC(=C)C2CC1)(C)C)C
MOL002338	0.8895	0.1105	0.6520	Anisi Stellati Fructus	136458-42-9	178323	FALSE	OC1(C2C3C(C3CCC(=C)C2CC1)(C)C)C
MOL002339	0.8893	0.1107	0.8513	Stephaniae Tetrandrae Radix	9-Oxofarnesol	5320326	FALSE	C(C(=O)C=C(C)C)/C(=C\CC/C(=C/CO)/C)/C
MOL002341	0.9131	0.0869	0.9366	Stephaniae Tetrandrae Radix	Hesperetin	72281	FALSE	Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1
MOL002341	0.9131	0.0869	0.9366	Gossampiniflos	Hesperetin	72281	FALSE	Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1
MOL002341	0.9131	0.0869	0.9366	Aurantii Fructus	Hesperetin	72281	FALSE	Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1
MOL002341	0.9131	0.0869	0.9366	Schizonepetae Spica	Hesperetin	72281	FALSE	Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1
MOL002341	0.9131	0.0869	0.9366	Citri Fructus	Hesperetin	72281	FALSE	Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1
MOL002341	0.9131	0.0869	0.9366	Lobeliae Chinensis Herba	Hesperetin	72281	FALSE	Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1
MOL002341	0.9131	0.0869	0.9366	Allium Azureum Ledeb.	Hesperetin	72281	FALSE	Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1
MOL002341	0.9131	0.0869	0.9366	Echinopsis Radix	Hesperetin	72281	FALSE	Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1
MOL002341	0.9131	0.0869	0.9366	Lysimachiae Herba	Hesperetin	72281	FALSE	Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1
MOL002342	0.2116	0.7884	0.6959	Polygoni Cuspidati Rhizoma Et Radix	(+)-Limacine	Not Available	FALSE	c12c3Oc4cc5c(cc4OC)CCN(C5Cc4ccc(Oc5cc(CC1N(CCc2cc(c3O)OC)C)ccc5OC)cc4)C
MOL002342	0.2116	0.7884	0.6959	Stephaniae Tetrandrae Radix	(+)-Limacine	Not Available	FALSE	c12c3Oc4cc5c(cc4OC)CCN(C5Cc4ccc(Oc5cc(CC1N(CCc2cc(c3O)OC)C)ccc5OC)cc4)C
MOL002343	0.2190	0.7810	0.7258	Radix Stephaniae Cepharanthae.	tetrandrine	Not Available	FALSE	O1c2c3C(N(CCc3cc(OC)c2OC)C)Cc2cc(Oc3ccc(CC4N(CCc5c4cc1c(OC)c5)C)cc3)c(OC)cc2
MOL002343	0.2190	0.7810	0.7258	Menispermi Rhizoma	tetrandrine	Not Available	FALSE	O1c2c3C(N(CCc3cc(OC)c2OC)C)Cc2cc(Oc3ccc(CC4N(CCc5c4cc1c(OC)c5)C)cc3)c(OC)cc2

MOL002343	0.2190	0.7810	0.7258	Cornus Officinalis Sieb. Et Zucc.	tetrandrine	Not Available	FALSE	O1c2c3C(N(CCc3cc(OC)c2OC)C)Cc2cc(Oc3ccc(CC4N(CCc5c4cc1c(OC)c5)C)cc3)c(OC)cc2
MOL002343	0.2190	0.7810	0.7258	Stephaniae Tetrandrae Radix	tetrandrine	Not Available	FALSE	O1c2c3C(N(CCc3cc(OC)c2OC)C)Cc2cc(Oc3ccc(CC4N(CCc5c4cc1c(OC)c5)C)cc3)c(OC)cc2
MOL002344	0.5546	0.4454	0.7244	Tinosporae Radix	cyclanoline	3082134	FALSE	c12c(CC[N+]3(Cc4c(CC13)ccc(c4O)OC)C)cc(c(c2)O)OC
MOL002344	0.5546	0.4454	0.7244	Stephaniae Tetrandrae Radix	cyclanoline	3082134	FALSE	c12c(CC[N+]3(Cc4c(CC13)ccc(c4O)OC)C)cc(c(c2)O)OC
MOL002345	0.8497	0.1503	0.7869	Stephaniae Tetrandrae Radix	Aristololactum	Not Available	FALSE	[nH]1c(=O)c2c3c(c4c(cc13)c(ccc4)OC)c1OCOc1c2
MOL002345	0.8497	0.1503	0.7869	Rhizoma Seu Herba Aristolochiae Mollissimae	Aristololactum	Not Available	FALSE	[nH]1c(=O)c2c3c(c4c(cc13)c(ccc4)OC)c1OCOc1c2
MOL002345	0.8497	0.1503	0.7869	Aristolochiae Fructus	Aristololactum	Not Available	FALSE	[nH]1c(=O)c2c3c(c4c(cc13)c(ccc4)OC)c1OCOc1c2
MOL002346	0.9017	0.0983	0.6542	Stephaniae Tetrandrae Radix	Betaine	2236	FALSE	c1cc(c2c(c1)c1c(c(c2)[N+](=O)O)c(cc2c1OCO2)C(=O)O)OC
MOL002346	0.9017	0.0983	0.6542	Aristolochiae Fructus	Betaine	2236	FALSE	c1cc(c2c(c1)c1c(c(c2)[N+](=O)O)c(cc2c1OCO2)C(=O)O)OC
MOL002346	0.9017	0.0983	0.6542	Rhizoma Seu Herba Aristolochiae Mollissimae	Betaine	2236	FALSE	c1cc(c2c(c1)c1c(c(c2)[N+](=O)O)c(cc2c1OCO2)C(=O)O)OC
MOL002347	0.8952	0.1048	0.8793	Radix Puerariae	(R)-Allantoin	439713	FALSE	O=C1NC(=O)C(N1)NC(=O)N
MOL002347	0.8952	0.1048	0.8793	Bolbostemae Paniculati Bulbus	(R)-Allantoin	439713	FALSE	O=C1NC(=O)C(N1)NC(=O)N
MOL002347	0.8952	0.1048	0.8793	Aristolochiae Fructus	(R)-Allantoin	439713	FALSE	O=C1NC(=O)C(N1)NC(=O)N
MOL002347	0.8952	0.1048	0.8793	Rhizoma Seu Herba Aristolochiae Mollissimae	(R)-Allantoin	439713	FALSE	O=C1NC(=O)C(N1)NC(=O)N
MOL002347	0.8952	0.1048	0.8793	Achyranthis Bidentatae Radix	(R)-Allantoin	439713	FALSE	O=C1NC(=O)C(N1)NC(=O)N
MOL002347	0.8952	0.1048	0.8793	Stephaniae Tetrandrae Radix	(R)-Allantoin	439713	FALSE	O=C1NC(=O)C(N1)NC(=O)N
MOL002347	0.8952	0.1048	0.8793	Maydis Seigma	(R)-Allantoin	439713	FALSE	O=C1NC(=O)C(N1)NC(=O)N
MOL002347	0.8952	0.1048	0.8793	Puerariae Flos	(R)-Allantoin	439713	FALSE	O=C1NC(=O)C(N1)NC(=O)N
MOL002348	0.8470	0.1530	0.6094	Styrax	aristolene	Not Available	FALSE	C12C(C1CC=C1C2(C(CCC1)C)C)(C)C
MOL002348	0.8470	0.1530	0.6094	Linderae Radix	aristolene	Not Available	FALSE	C12C(C1CC=C1C2(C(CCC1)C)C)(C)C
MOL002348	0.8470	0.1530	0.6094	Nardostachyos Radix Et Rhizoma	aristolene	Not Available	FALSE	C12C(C1CC=C1C2(C(CCC1)C)C)(C)C
MOL002348	0.8470	0.1530	0.6094	Stephaniae Tetrandrae Radix	aristolene	Not Available	FALSE	C12C(C1CC=C1C2(C(CCC1)C)C)(C)C
MOL002349	0.8057	0.1943	0.7686	Alpiniae Oxyphyliae Fructus	ZINC05225089	7567181	FALSE	C12(C(=CC(=O)CC2C)CCC(C1)C(=C)C)C
MOL002349	0.8057	0.1943	0.7686	Stephaniae Tetrandrae Radix	ZINC05225089	7567181	FALSE	C12(C(=CC(=O)CC2C)CCC(C1)C(=C)C)C
MOL002349	0.8057	0.1943	0.7686	Linderae Radix	ZINC05225089	7567181	FALSE	C12(C(=CC(=O)CC2C)CCC(C1)C(=C)C)C

MOL002351	0.9244	0.0756	0.9493	Stephaniae Tetrandrae Radix	3-Hexenol	5281167	FALSE	C(=C\CC)\CCO
MOL002351	0.9244	0.0756	0.9493	Folium Artemisiae Argyi	3-Hexenol	5281167	FALSE	C(=C\CC)\CCO
MOL002351	0.9244	0.0756	0.9493	Dianthi Herba	3-Hexenol	5281167	FALSE	C(=C\CC)\CCO
MOL002351	0.9244	0.0756	0.9493	Eucommiae Folium	3-Hexenol	5281167	FALSE	C(=C\CC)\CCO
MOL002351	0.9244	0.0756	0.9493	Apocyniveneti Folium	3-Hexenol	5281167	FALSE	C(=C\CC)\CCO
MOL002351	0.9244	0.0756	0.9493	Rhododendri Daurici Folium	3-Hexenol	5281167	FALSE	C(=C\CC)\CCO
MOL002351	0.9244	0.0756	0.9493	Folium Nelumbinis	3-Hexenol	5281167	FALSE	C(=C\CC)\CCO
MOL002351	0.9244	0.0756	0.9493	Mume Fructus	3-Hexenol	5281167	FALSE	C(=C\CC)\CCO
MOL002351	0.9244	0.0756	0.9493	Ginkgo Folium	3-Hexenol	5281167	FALSE	C(=C\CC)\CCO
MOL002351	0.9244	0.0756	0.9493	Citrus Aurantium	3-Hexenol	5281167	FALSE	C(=C\CC)\CCO
MOL002351	0.9244	0.0756	0.9493	Campsis Flos	3-Hexenol	5281167	FALSE	C(=C\CC)\CCO
MOL002351	0.9244	0.0756	0.9493	Eriobotryae Folium	3-Hexenol	5281167	FALSE	C(=C\CC)\CCO
MOL002351	0.9244	0.0756	0.9493	Capsellae Herba	3-Hexenol	5281167	FALSE	C(=C\CC)\CCO
MOL002351	0.9244	0.0756	0.9493	Ephedra Herba	3-Hexenol	5281167	FALSE	C(=C\CC)\CCO
MOL002351	0.9244	0.0756	0.9493	Dichroae Radix	3-Hexenol	5281167	FALSE	C(=C\CC)\CCO
MOL002351	0.9244	0.0756	0.9493	Lonicerae Japonicae Flos	3-Hexenol	5281167	FALSE	C(=C\CC)\CCO
MOL002352	0.2098	0.7902	0.7029	Thalictri Glandulosissimi Et	Berbamine	Not Available	FALSE	O1c2c3C(N(CCc3cc(OC)c2OC)C)Cc2cc(Oc3ccc(CC4N(CCc5c4cc1c(OC)c5)C)cc3)c(O)cc2
MOL002352	0.2098	0.7902	0.7029	Mahoniae Caulis	Berbamine	Not Available	FALSE	O1c2c3C(N(CCc3cc(OC)c2OC)C)Cc2cc(Oc3ccc(CC4N(CCc5c4cc1c(OC)c5)C)cc3)c(O)cc2
MOL002352	0.2098	0.7902	0.7029	Stephaniae Tetrandrae Radix	Berbamine	Not Available	FALSE	O1c2c3C(N(CCc3cc(OC)c2OC)C)Cc2cc(Oc3ccc(CC4N(CCc5c4cc1c(OC)c5)C)cc3)c(O)cc2
MOL002352	0.2098	0.7902	0.7029	Mahoniae Eadix	Berbamine	Not Available	FALSE	O1c2c3C(N(CCc3cc(OC)c2OC)C)Cc2cc(Oc3ccc(CC4N(CCc5c4cc1c(OC)c5)C)cc3)c(O)cc2
MOL002353	0.2323	0.7677	0.6811	Stephaniae Tetrandrae Radix	Curine	Not Available	FALSE	O1c2c3C(N(CCc3cc(OC)c2O)C)Cc2cc(Oc3cc4C(N(CCc4cc3OC)C)Cc3ccc1cc3)c(O)cc2
MOL002354	0.1937	0.8063	0.6845	Stephaniae Tetrandrae Radix	Cissampareine	Not Available	FALSE	C1c2c3C(N(C1)C)Cc1ccc(COc4c(cc5CCN=C(Cc6ccc(cc6)Oc3c(c(c2)OC)OC)c5c4O)OC)cc1
MOL002355	0.2267	0.7733	0.7144	Stephaniae Tetrandrae Radix	Cycleaneonine	Not Available	FALSE	c1c2c3c(c(c1OC)OC)Oc1ccc(cc1)CC1c4c(cc(c(OCc5ccc(CC3N(CC2)C)cc5)c4O)OC)CCN1C
MOL002356	0.7876	0.2124	0.7486	Stephaniae Tetrandrae Radix	Dichotomitin	5316653	FALSE	c12c(c(c3c(c1)occ(c3=O)c1cc(c(c(c1)O)OC)OC)O)OCO2
MOL002356	0.7876	0.2124	0.7486	Belamcandae Rhizome	Dichotomitin	5316653	FALSE	c12c(c(c3c(c1)occ(c3=O)c1cc(c(c(c1)O)OC)OC)O)OCO2
MOL002357	0.8683	0.1317	0.6011	Stephaniae Tetrandrae Radix	ZINC04568391	Not Available	FALSE	OC1(C2C(C3C(C2)(C(CC3)C)CC1)(C)C)C
MOL002358	0.4114	0.5886	0.7226	Stephaniae Tetrandrae Radix	Faradiol	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C1C(CC2)(CC=C(C1)C)C)C)C)(C)C)O
MOL002359	0.9215	0.0785	0.8505	Sennae Folium	6-Hydroxy-musizin-8-O-beta-D-glucoside	100753	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(cc(c(c2O)C(=O)C)C)cc(O)c1)CO

MOL002360	0.8775	0.1225	0.8957	Sennae Folium	Pulmatin	442731	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(C(=O)c3c(C2=O)c(O)cc(c3)C)ccc1)CO
MOL002361	0.9566	0.0434	0.9402	Foeniculi Fructus	Terragon	8815	FALSE	c1(ccc(cc1)OC)CC=C
MOL002361	0.9566	0.0434	0.9402	Epimrdii Herba	Terragon	8815	FALSE	c1(ccc(cc1)OC)CC=C
MOL002361	0.9566	0.0434	0.9402	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Terragon	8815	FALSE	c1(ccc(cc1)OC)CC=C
MOL002361	0.9566	0.0434	0.9402	Cinnamomi Ramulus	Terragon	8815	FALSE	c1(ccc(cc1)OC)CC=C
MOL002361	0.9566	0.0434	0.9402	Eriobotryae Folium	Terragon	8815	FALSE	c1(ccc(cc1)OC)CC=C
MOL002361	0.9566	0.0434	0.9402	Mume Flos	Terragon	8815	FALSE	c1(ccc(cc1)OC)CC=C
MOL002361	0.9566	0.0434	0.9402	Semen Euphorbiae	Terragon	8815	FALSE	c1(ccc(cc1)OC)CC=C
MOL002361	0.9566	0.0434	0.9402	Zingiberis Rhizoma	Terragon	8815	FALSE	c1(ccc(cc1)OC)CC=C
MOL002361	0.9566	0.0434	0.9402	Citrus Aurantium	Terragon	8815	FALSE	c1(ccc(cc1)OC)CC=C
MOL002361	0.9566	0.0434	0.9402	Sennae Folium	Terragon	8815	FALSE	c1(ccc(cc1)OC)CC=C
MOL002361	0.9566	0.0434	0.9402	Asari Radix Et Rhizoma	Terragon	8815	FALSE	c1(ccc(cc1)OC)CC=C
MOL002361	0.9566	0.0434	0.9402	Chaenomeles Sinensis (Thouin) Koehne	Terragon	8815	FALSE	c1(ccc(cc1)OC)CC=C
MOL002361	0.9566	0.0434	0.9402	Magnoliae Flos	Terragon	8815	FALSE	c1(ccc(cc1)OC)CC=C
MOL002361	0.9566	0.0434	0.9402	Anisi Stellati Fructus	Terragon	8815	FALSE	c1(ccc(cc1)OC)CC=C
MOL002361	0.9566	0.0434	0.9402	Piperis Fructus	Terragon	8815	FALSE	c1(ccc(cc1)OC)CC=C
MOL002361	0.9566	0.0434	0.9402	Caryophylliflos	Terragon	8815	FALSE	c1(ccc(cc1)OC)CC=C
MOL002361	0.9566	0.0434	0.9402	Acoritataninowii Rhizoma	Terragon	8815	FALSE	c1(ccc(cc1)OC)CC=C
MOL002361	0.9566	0.0434	0.9402	Aucklandiae Radix	Terragon	8815	FALSE	c1(ccc(cc1)OC)CC=C
MOL002361	0.9566	0.0434	0.9402	Zanthoxyli Pericarpium	Terragon	8815	FALSE	c1(ccc(cc1)OC)CC=C
MOL002362	0.9296	0.0704	0.9472	Sennae Folium	Isogeraniol	5362876	FALSE	OCC/C(=C\CC=C(C)C)/C
MOL002363	0.9203	0.0797	0.8908	Aucklandiae Radix	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Lysimachiae Foenigraeci Herba	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Sennae Folium	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Lysimachiae Herba	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Dianthi Herba	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Mume Flos	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Campsis Flos	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Hippophae Fructus	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Thalluslaminariae	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Lycii Fructus	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Capsici Fructus	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Ephedra Herba	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Nardostachyos Radix Et Rhizoma	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Bidentis Bipinnatae Herba	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Celastri Orbiculati Fructus	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Perilla Frutescens	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Ginkgo Folium	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C

MOL002363	0.9203	0.0797	0.8908	Herba Taxilli	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Lygodii Spora	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Carthami Flos	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Croci Stigma	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Humulus Scandens (Lour.) Merr.	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Junci Medulla	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Amygdalus Communis Vas	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002363	0.9203	0.0797	0.8908	Eriobotryae Folium	beta-Ionone	638014	FALSE	C1C(=C(C(CC1)(C)C)/C=C/C(=O)C)C
MOL002364	0.9543	0.0457	0.9542	Sennae Folium	D-Isomenthol	45056	FALSE	C1CC(C(CC1C)O)C(C)C
MOL002365	0.9587	0.0413	0.9777	Coriandri Sativi Herba	(s)-carvone	16724	FALSE	C1(=CCC(CC1=O)C(=C)C)C
MOL002365	0.9587	0.0413	0.9777	Radix Bupleuri	(s)-carvone	16724	FALSE	C1(=CCC(CC1=O)C(=C)C)C
MOL002365	0.9587	0.0413	0.9777	Ardisiae Japonicae Herba	(s)-carvone	16724	FALSE	C1(=CCC(CC1=O)C(=C)C)C
MOL002365	0.9587	0.0413	0.9777	Schizonepetae Herba	(s)-carvone	16724	FALSE	C1(=CCC(CC1=O)C(=C)C)C
MOL002365	0.9587	0.0413	0.9777	Eriobotryae Folium	(s)-carvone	16724	FALSE	C1(=CCC(CC1=O)C(=C)C)C
MOL002365	0.9587	0.0413	0.9777	Schizonepetae Spica	(s)-carvone	16724	FALSE	C1(=CCC(CC1=O)C(=C)C)C
MOL002365	0.9587	0.0413	0.9777	Phellodendri Chinrnsis Cortex	(s)-carvone	16724	FALSE	C1(=CCC(CC1=O)C(=C)C)C
MOL002365	0.9587	0.0413	0.9777	Aristolochiae Fructus	(s)-carvone	16724	FALSE	C1(=CCC(CC1=O)C(=C)C)C
MOL002365	0.9587	0.0413	0.9777	Ganoderma	(s)-carvone	16724	FALSE	C1(=CCC(CC1=O)C(=C)C)C
MOL002365	0.9587	0.0413	0.9777	Sennae Folium	(s)-carvone	16724	FALSE	C1(=CCC(CC1=O)C(=C)C)C
MOL002366	0.8607	0.1393	0.8825	Sennae Folium	Rheochrysin	168938	FALSE	c1c(cc2c(c1OC1C(C(C(C(O1)CO)O)O)O)C(=O)c1c(C2=O)cc(cc1O)C)OC
MOL002366	0.8607	0.1393	0.8825	Radix Rhei Et Rhizome	Rheochrysin	168938	FALSE	c1c(cc2c(c1OC1C(C(C(C(O1)CO)O)O)O)C(=O)c1c(C2=O)cc(cc1O)C)OC
MOL002367	0.8888	0.1112	0.8503	Sennae Folium	4,5-dihydroxy-9,10-dioxo-8-[(2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]anthracene-2-carboxylic acid	3087148	FALSE	c1(cc(c2c(c1)C(=O)c1c(C2=O)c(ccc1C1C(C(C(C(O1)CO)O)O)O)O)O)C(=O)O
MOL002368	0.7716	0.2284	0.7723	Sennae Folium	Sennoside A	73111	FALSE	O(C1OC(C(O)C(O)C1O)CO)c1c2c(C(C3c4c(C(=O)c5c3cc(cc5O)C(=O)O)c(OC3OC(C(O)C(O)C3O)CO)ccc4)c3c(C2=O)c(O)cc(c3)C(=O)O)ccc1

MOL002368	0.7716	0.2284	0.7723	Radix Rhei Et Rhizome	Sennoside A	73111	FALSE	O(C1OC(C(O)C(O)C1O)CO)c1c2c(C(C3c4c(C(=O)c5c3cc(cc5O)C(=O)O)c(OC3OC(C(O)C(O)C3O)CO)ccc4)c3c(C2=O)c(O)cc(c3)C(=O)O)ccc1
MOL002369	0.7421	0.2579	0.6094	Sennae Folium	Dihydroxydianthrone	92826	FALSE	Oc1c2c(C(C3c4c(C(=O)c5c3cc(cc5O)C(=O)O)c(O)ccc4)c3c(C2=O)c(O)cc(c3)C(=O)O)ccc1
MOL002370	0.9038	0.0962	0.8962	Sennae Folium	Pseudoionone	Not Available	FALSE	C=CCC/C(=C/C=C/C(=O)C)/C
MOL002371	0.9355	0.0645	0.9489	Sennae Folium	D-3-O-methylinostiol	440079	FALSE	O(C1C(O)C(O)C(O)C(O)C1O)C
MOL002374	0.9543	0.0457	0.9542	Sennae Folium	()-Neomenthol	439263	FALSE	C1C(CCC(C1O)C(C)C)C
MOL002374	0.9543	0.0457	0.9542	Schizonepetae Herba	()-Neomenthol	439263	FALSE	C1C(CCC(C1O)C(C)C)C
MOL002375	0.9586	0.0414	0.9571	Radix Bupleuri	(-)-isomenthone	6432469	FALSE	C1C(CCC(C1=O)C(C)C)C
MOL002375	0.9586	0.0414	0.9571	Glechomae Herba	(-)-isomenthone	6432469	FALSE	C1C(CCC(C1=O)C(C)C)C
MOL002375	0.9586	0.0414	0.9571	Sennae Folium	(-)-isomenthone	6432469	FALSE	C1C(CCC(C1=O)C(C)C)C
MOL002375	0.9586	0.0414	0.9571	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	(-)-isomenthone	6432469	FALSE	C1C(CCC(C1=O)C(C)C)C
MOL002375	0.9586	0.0414	0.9571	Geranium Wilfordii Maxim.	(-)-isomenthone	6432469	FALSE	C1C(CCC(C1=O)C(C)C)C
MOL002375	0.9586	0.0414	0.9571	Gynostemmae Pentaphylli Herba	(-)-isomenthone	6432469	FALSE	C1C(CCC(C1=O)C(C)C)C
MOL002375	0.9586	0.0414	0.9571	Schizonepetae Herba	(-)-isomenthone	6432469	FALSE	C1C(CCC(C1=O)C(C)C)C
MOL002377	0.8953	0.1047	0.8185	Inulae Flos	Kaempferol-3-arabofuranoside	Not Available	FALSE	c1c(cc2c(c1O)c(=O)c(c(o2)c1ccc(cc1)O)OC1OC(C(C1O)O)CO)O
MOL002377	0.8953	0.1047	0.8185	Lunulatae Herba	Kaempferol-3-arabofuranoside	Not Available	FALSE	c1c(cc2c(c1O)c(=O)c(c(o2)c1ccc(cc1)O)OC1OC(C(C1O)O)CO)O
MOL002377	0.8953	0.1047	0.8185	Panax Ginseng C. A. Mey.	Kaempferol-3-arabofuranoside	Not Available	FALSE	c1c(cc2c(c1O)c(=O)c(c(o2)c1ccc(cc1)O)OC1OC(C(C1O)O)CO)O

MOL002377	0.8953	0.1047	0.8185	Sennae Folium	Kaempferol-3-arabofuranoside	Not Available	FALSE	c1c(cc2c(c1O)c(=O)c(c(o2)c1ccc(cc1)O)OC1OC(C(C1O)O)CO)O
MOL002377	0.8953	0.1047	0.8185	Ginkgo Semen	Kaempferol-3-arabofuranoside	Not Available	FALSE	c1c(cc2c(c1O)c(=O)c(c(o2)c1ccc(cc1)O)OC1OC(C(C1O)O)CO)O
MOL002377	0.8953	0.1047	0.8185	Pyrrosiae Folium	Kaempferol-3-arabofuranoside	Not Available	FALSE	c1c(cc2c(c1O)c(=O)c(c(o2)c1ccc(cc1)O)OC1OC(C(C1O)O)CO)O
MOL002378	0.8912	0.1088	0.8467	Radix Angelicae Biseratae	UND	14257	FALSE	CCCCCCCCCCC
MOL002378	0.8912	0.1088	0.8467	Farfarae Flos	UND	14257	FALSE	CCCCCCCCCCC
MOL002378	0.8912	0.1088	0.8467	Peucedanidecursivi Radix	UND	14257	FALSE	CCCCCCCCCCC
MOL002378	0.8912	0.1088	0.8467	Rose Rugosae Flos	UND	14257	FALSE	CCCCCCCCCCC
MOL002378	0.8912	0.1088	0.8467	Peucedani Radix	UND	14257	FALSE	CCCCCCCCCCC
MOL002378	0.8912	0.1088	0.8467	Panacis Quinquefolii Radix	UND	14257	FALSE	CCCCCCCCCCC
MOL002378	0.8912	0.1088	0.8467	Lepidii Semen Descurainiae Semen	UND	14257	FALSE	CCCCCCCCCCC
MOL002378	0.8912	0.1088	0.8467	Perillae Fructus	UND	14257	FALSE	CCCCCCCCCCC
MOL002378	0.8912	0.1088	0.8467	Sojae Semen Nigrum	UND	14257	FALSE	CCCCCCCCCCC
MOL002378	0.8912	0.1088	0.8467	Cnidii Fructus	UND	14257	FALSE	CCCCCCCCCCC
MOL002378	0.8912	0.1088	0.8467	Sennae Folium	UND	14257	FALSE	CCCCCCCCCCC
MOL002378	0.8912	0.1088	0.8467	Arisaematis Rhizoma	UND	14257	FALSE	CCCCCCCCCCC
MOL002378	0.8912	0.1088	0.8467	Herbahypericiperforati	UND	14257	FALSE	CCCCCCCCCCC
MOL002378	0.8912	0.1088	0.8467	Radix Bupleuri	UND	14257	FALSE	CCCCCCCCCCC
MOL002378	0.8912	0.1088	0.8467	Broussonetiae Fructus	UND	14257	FALSE	CCCCCCCCCCC
MOL002378	0.8912	0.1088	0.8467	Hyperici Japonici Herber	UND	14257	FALSE	CCCCCCCCCCC
MOL002378	0.8912	0.1088	0.8467	Platycodon Grandiforus	UND	14257	FALSE	CCCCCCCCCCC
MOL002379	0.9303	0.0697	0.9689	Bombyx Mori L.	PTL	8063	FALSE	C(CC=O)CC
MOL002379	0.9303	0.0697	0.9689	Evodiae Fructus	PTL	8063	FALSE	C(CC=O)CC
MOL002379	0.9303	0.0697	0.9689	Radix Bupleuri	PTL	8063	FALSE	C(CC=O)CC
MOL002379	0.9303	0.0697	0.9689	Lunulatae Herba	PTL	8063	FALSE	C(CC=O)CC
MOL002379	0.9303	0.0697	0.9689	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	PTL	8063	FALSE	C(CC=O)CC
MOL002379	0.9303	0.0697	0.9689	Sennae Folium	PTL	8063	FALSE	C(CC=O)CC
MOL002379	0.9303	0.0697	0.9689	Lonicerae Japonicae Flos	PTL	8063	FALSE	C(CC=O)CC
MOL002379	0.9303	0.0697	0.9689	Achyranthis Bidentatae Radix	PTL	8063	FALSE	C(CC=O)CC
MOL002379	0.9303	0.0697	0.9689	Campsis Flos	PTL	8063	FALSE	C(CC=O)CC
MOL002380	0.9568	0.0432	0.9300	Sennae Folium	cis-Anethol	1549040	FALSE	c1(ccc(cc1)OC)/C=C/C

MOL002380	0.9568	0.0432	0.9300	Zanthoxyli Pericarpium	cis-Anethol	1549040	FALSE	c1(ccc(cc1)OC)/C=C/C
MOL002380	0.9568	0.0432	0.9300	Lilii Bulbus	cis-Anethol	1549040	FALSE	c1(ccc(cc1)OC)/C=C/C
MOL002381	0.9215	0.0785	0.8505	Sennae Folium	Tinnevellin glucoside	5318296	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(cc(c(c2O)C(=O)C)C)cc(O)c1)CO
MOL002382	0.9447	0.0553	0.7752	Sennae Folium	1-(1,6,8-trihydroxy-3-methyl-2-naphthyl)ethanone	23643241	FALSE	Oc1c2c(cc(c(c2O)C(=O)C)C)cc(O)c1
MOL002384	0.3921	0.6079	0.7543	Aconiti Lateralis Radix Praeparata	14-Deoxy-11,12-didehydroandrographolide	Not Available	FALSE	O1C=CC(C1=O)/C=C\C1C2(C(CCC1=C)C(C(CC2)O)(C)CO)C
MOL002385	0.5548	0.4452	0.6321	Aconiti Lateralis Radix Praeparata	Delcorine	Not Available	FALSE	C1CC2(C3C4(C1OC)C1C5C6(C(C3O)(OCO6)C4N(C2)CC)CC(C(C5OC)C1)OC)COC
MOL002386	0.7236	0.2764	0.7773	Aconiti Lateralis Radix Praeparata	Delphamine	Not Available	FALSE	C1CC2(C3C4(C1O)C1C5C(C(C3OC)(C4N(C2)CC)O)(O)CC(C(C5O)C1)OC)COC
MOL002389	0.3571	0.6429	0.6995	Aconiti Lateralis Radix Praeparata	Delsemine B	Not Available	FALSE	C1CC2(C3C4(C1OC)C1C5C(C(C3OC)(C4N(C2)CC)O)(CC(C(C5OC)C1)OC)O)COC(=O)c1ccccc1NC(=O)CC(C(=O)N)C
MOL002390	0.6574	0.3426	0.8752	Aconiti Lateralis Radix Praeparata	Delsoline	Not Available	FALSE	C1CC2(C3C4(C1O)C1C5C(C(C3OC)(C4N(C2)CC)O)(O)CC(C(C5OC)C1)OC)COC
MOL002391	0.6781	0.3219	0.7544	Aconiti Lateralis Radix Praeparata	Deltamine	Not Available	FALSE	C1CC2(C3C4(C1OC)C(N(C2)CC)C1(C2(C5C4(CC(C5OC)C(C2)OC)O)OCO1)C3O)C
MOL002392	0.3752	0.6248	0.6972	Aconiti Lateralis Radix Praeparata	Deltoin	Not Available	FALSE	CC(=O)/C(=C\OC(C1Oc2c(C1)cc1c(c2)oc(=O)cc1)(C)C)/C
MOL002393	0.4981	0.5019	0.6831	Aconiti Lateralis Radix Praeparata	Demethyldelavaine A	Not Available	FALSE	C1CC2(C3C4(C1OC)C1C5C(C(C3OC)(C4N(C2)CC)O)(CC(C(C5OC)C1)OC)O)COC(=O)c1ccccc1NC(=O)C(CC(=O)O)C
MOL002394	0.4992	0.5008	0.6825	Aconiti Lateralis Radix Praeparata	Demethyldelavaine B	Not Available	FALSE	C1CC2(C3C4(C1OC)C1C5C(C(C3OC)(C4N(C2)CC)O)(CC(C(C5OC)C1)OC)O)COC(=O)c1ccccc1NC(=O)CC(C(=O)O)C
MOL002395	0.3638	0.6362	0.7185	Aconiti Lateralis Radix Praeparata	Deoxyandrographolide	15922991	FALSE	C(C1=CCOC1=O)CC1C(=C)CCC2C1(CCC(C2(C)CO)O)C
MOL002396	0.3504	0.6496	0.6813	Aconiti Lateralis Radix Praeparata	14-acetyltalatisamine	Not Available	FALSE	OC12C3C4N(CC5(C(C4(C4C1C(OC(=O)C)C(C4)C(OC)C2)C(OC)CC5)C3)COC)CC
MOL002397	0.6923	0.3077	0.8477	Aconitum Kusnezoffii Reichb	karakoline	Not Available	FALSE	C123C4C(CC2C(CN4CC)(CCC3O)C)C2(C3C1CC(C3O)C(C2)OC)O
MOL002397	0.6923	0.3077	0.8477	Aconiti Lateralis Radix Praeparata	karakoline	Not Available	FALSE	C123C4C(CC2C(CN4CC)(CCC3O)C)C2(C3C1CC(C3O)C(C2)OC)O
MOL002398	0.5443	0.4557	0.8464	Aconiti Lateralis Radix Praeparata	Karanjin	100633	FALSE	c12ccc3c(c1cco2)oc(c(c3=O)OC)c1ccccc1

MOL002399	0.9581	0.0419	0.9173	Myristicae Semen	TMPEA	4076	FALSE	c1(cc(cc(c1OC)OC)CCN)OC
MOL002399	0.9581	0.0419	0.9173	Aconiti Lateralis Radix Praeparata	TMPEA	4076	FALSE	c1(cc(cc(c1OC)OC)CCN)OC
MOL002400	0.2624	0.7376	0.6669	Aconiti Lateralis Radix Praeparata	Neojiangyouaconitine	Not Available	FALSE	O=C(OC1C2(O)C(OC)C(C3(C1C(C2)C12C4C3C(C2C(CN4CC)(CCC1OC)COC)OC)OC)O)c1ccccc1
MOL002401	0.5207	0.4793	0.7136	Aconiti Lateralis Radix Praeparata	Neokadsuranic acid B	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=C(CC2)C2(C(C1)C(=C)C(CC2)C(CC/C=C(\C(=O)O)/C)C)C)C)(C)C
MOL002402	0.7314	0.2686	0.7784	Aconiti Lateralis Radix Praeparata	Senbusine A	Not Available	FALSE	OC12C3C4N(CC5(C(C4(C4C1C(O)C(C4)C(OC)C2)C(O)CC5)C3O)COC)CC
MOL002403	0.7299	0.2701	0.7801	Aconiti Lateralis Radix Praeparata	Senbusine B	Not Available	FALSE	OC12C3C4N(CC5(C(C4(C4C1C(O)C(C4)C(OC)C2O)C(O)CC5)C3)COC)CC
MOL002404	0.6892	0.3108	0.7510	Aconiti Lateralis Radix Praeparata	Senbusine C	Not Available	FALSE	OC12C3C4N(CC5(C(C4(C4C1C(O)C(C4)C(OC)C2O)C(O)CC5)C3OC)COC)CC
MOL002406	0.1213	0.8787	0.8642	Aconiti Lateralis Radix Praeparata	2,7-Dideacetyl-2,7-dibenzoyl-taxayunnanine F	Not Available	FALSE	C1(C(C2=C(C(CC2(C(C2C1(C(CC1C2(CO1)OC(=O)C)OC(=O)c1ccccc1)C)OC(=O)c1ccccc1)C(C)(O)C)OC(=O)C)C)OC(=O)C)OC(=O)C
MOL002407	0.4759	0.5241	0.6753	Aconiti Lateralis Radix Praeparata	beiwutine	Not Available	FALSE	C123C4(C5C(C6C2N(CC(C1C6OC)(C(CC3OC)O)C)C)(C(C(C4)(C5OC(=O)c1ccccc1)O)OC)O)OC
MOL002407	0.4759	0.5241	0.6753	Radix Aconiti Kusnezoffii	beiwutine	Not Available	FALSE	C123C4(C5C(C6C2N(CC(C1C6OC)(C(CC3OC)O)C)C)(C(C(C4)(C5OC(=O)c1ccccc1)O)OC)O)OC
MOL002407	0.4759	0.5241	0.6753	Aconitum Kusnezoffii Reichb	beiwutine	Not Available	FALSE	C123C4(C5C(C6C2N(CC(C1C6OC)(C(CC3OC)O)C)C)(C(C(C4)(C5OC(=O)c1ccccc1)O)OC)O)OC
MOL002408	0.4937	0.5063	0.7141	Aconiti Lateralis Radix Praeparata	benzoylaconine	Not Available	FALSE	C123C4C(CN(C1C(C4OC)C1(C4C2CC(C4OC(=O)c2ccccc2)(C(C1O)OC)O)O)CC)(C(CC3OC)O)COC
MOL002408	0.4937	0.5063	0.7141	Aconitum Kusnezoffii Reichb	benzoylaconine	Not Available	FALSE	C123C4C(CN(C1C(C4OC)C1(C4C2CC(C4OC(=O)c2ccccc2)(C(C1O)OC)O)O)CC)(C(CC3OC)O)COC
MOL002408	0.4937	0.5063	0.7141	Radix Aconiti Kusnezoffii	benzoylaconine	Not Available	FALSE	C123C4C(CN(C1C(C4OC)C1(C4C2CC(C4OC(=O)c2ccccc2)(C(C1O)OC)O)O)CC)(C(CC3OC)O)COC
MOL002409	0.4388	0.5612	0.7346	Aconiti Lateralis Radix Praeparata	benzoylhypaconine	Not Available	FALSE	OC12C3C4N(CC5(C(C4(C4C1C(OC(=O)c1ccccc1)C(O)(C4)C(OC)C2O)C(OC)CC5)C3OC)COC)C
MOL002410	0.3628	0.6372	0.6676	Aconiti Lateralis Radix Praeparata	benzoylnapelline	Not Available	FALSE	O(C1C23C4C5(C6C2N(CC(C3C6)(CC1)C)CC)CC(C(O)C4)C(=C)C5O)C(=O)c1ccccc1
MOL002411	0.1925	0.8075	0.6842	Aconiti Lateralis Radix Praeparata	chasmaconitine	Not Available	FALSE	O(C12C3C4N(CC5(C(C4(C4C1C(OC(=O)c1ccccc1)C(O)(C4)C(OC)C2)C(OC)CC5)C3OC)COC)CC)C(=O)C
MOL002412	0.4580	0.5420	0.7195	Aconiti Lateralis Radix Praeparata	chasmanine	Not Available	FALSE	C123C4C(CN(C1C(C4OC)C1(C4C2CC(C4O)C(C1)OC)O)CC)(CCC3OC)COC
MOL002413	0.9607	0.0393	0.8974	Aconiti Lateralis Radix Praeparata	coryneine	165581	FALSE	[N+](CCc1cc(c(cc1)O)O)(C)(C)C
MOL002414	0.5045	0.4955	0.8424	Aconiti Lateralis Radix Praeparata	denudatine	Not Available	FALSE	OC1C2C34C5N(CC(C3CC5C32CCC1C(=C)C3O)(CCC4)C)CC

MOL002415	0.7276	0.2724	0.7836	Aconiti Lateralis Radix Praeparata	6-Demethyldesoline	Not Available	FALSE	C1CC2(C3C4(C1O)C1C5C(C(C3O)(C4N(C2)CC)O)(CC(C(C5OC)C1)OC)O)COC
MOL002416	0.2774	0.7226	0.7376	Aconiti Lateralis Radix Praeparata	deoxyaconitine	Not Available	FALSE	O(C12C3C4N(CC5(C(C4(C4C1C(OC(=O)c1ccccc1)C(O)(C4)C(OC)C2O)C(OC)CC5)C3OC)COC)CC)C(=O)C
MOL002417	0.6489	0.3511	0.6788	Aconiti Lateralis Radix Praeparata	fuzitine	Not Available	FALSE	[N+]1(CCc2c3c(c4c(CC13)ccc(c4O)O)c(c(c2)OC)OC)(C)C
MOL002418	0.7897	0.2103	0.8269	Aconiti Lateralis Radix Praeparata	hetisine	Not Available	FALSE	OC1C2C34C5N6C(C3C(C6)(CC(O)C4)C)CC32C5C(O)C1C(=C)C3
MOL002419	0.8933	0.1067	0.8147	Nelumbinis Plumula	(R)-Norcoclaurine	440988	FALSE	c12C(Cc3ccc(cc3)O)NCCc1cc(c(c2)O)O
MOL002419	0.8933	0.1067	0.8147	Aconiti Lateralis Radix Praeparata	(R)-Norcoclaurine	440988	FALSE	c12C(Cc3ccc(cc3)O)NCCc1cc(c(c2)O)O
MOL002420	0.3887	0.6113	0.7280	Aconiti Lateralis Radix Praeparata	hokbusine A	Not Available	FALSE	O(C12C3C4N(CC5(C(C4(C4C1C(OC(=O)c1ccccc1)C(O)(C4)C(OC)C2O)C(OC)CC5O)C3OC)COC)C)C
MOL002421	0.6307	0.3693	0.7080	Aconiti Lateralis Radix Praeparata	ignavine	Not Available	FALSE	C123C4(C56C(C1N1C(C2C(C1)(C(C(C3)OC(=O)c1ccccc1)O)C)C5)CC(C4)C(=C)C6O)O
MOL002422	0.6343	0.3657	0.7951	Aconiti Lateralis Radix Praeparata	isotalatizidine	Not Available	FALSE	O(C1C2C(O)C3C(C1)(O)C1C4C5(C3C2)C(O)CCC(C5C1)(CN4CC)COC)C
MOL002423	0.3795	0.6205	0.7229	Aconiti Lateralis Radix Praeparata	jesaconitine	Not Available	FALSE	C123C4C(CN(C2C(C4OC)C2(C4C1CC(C4OC(=O)c1ccc(cc1)OC)(C(C2O)OC)O)OC(=O)C)CC)(C(CC3OC)O)COC
MOL002424	0.3806	0.6194	0.7400	Aconiti Lateralis Radix Praeparata	Aconitine	Not Available	FALSE	C1C(C2(C3C4(C1OC)C1C5C(C(C3OC)C4N(CC)C2)(OC(=O)C)C(C(C(C5OC(=O)c2ccccc2)(C1)O)OC)O)COC)O
MOL002425	0.9001	0.0999	0.9348	Aconiti Lateralis Radix Praeparata	Zoba EG	11568	FALSE	c1(cccc(c1)N)O
MOL002426	0.6086	0.3914	0.7641	Aconiti Lateralis Radix Praeparata	neoline	Not Available	FALSE	OC12C3C4N(CC5(C(C4(C4C1C(O)C(C4)C(OC)C2)C(O)CC5)C3OC)COC)CC
MOL002427	0.8941	0.1059	0.9333	Aconiti Lateralis Radix Praeparata	Zoba 3GA	5801	FALSE	c1ccc(c(c1)O)N
MOL002428	0.9011	0.0989	0.9335	Aconiti Lateralis Radix Praeparata	UNAL	403	FALSE	c1cc(ccc1N)O
MOL002428	0.9011	0.0989	0.9335	Sojae Semen Nigrum	UNAL	403	FALSE	c1cc(ccc1N)O
MOL002429	0.9389	0.0611	0.8991	Aconiti Lateralis Radix Praeparata	Pyrrolezanthine	636825	FALSE	OCc1n(CCc2ccc(O)cc2)c(cc1)C=O
MOL002430	0.9543	0.0457	0.9472	Aconiti Lateralis Radix Praeparata	Salsolinol	91588	TRUE	Oc1cc2C(NCCc2cc1O)C
MOL002431	0.6469	0.3531	0.8898	Aconiti Lateralis Radix Praeparata	songorine	Not Available	FALSE	C123C4C5(C6C1N(CC(C2C6)(CCC3O)C)CC)CC(C(=O)C4)C(=C)C5O
MOL002431	0.6469	0.3531	0.8898	Aconitum Kusnezoffii Reichb	songorine	Not Available	FALSE	C123C4C5(C6C1N(CC(C2C6)(CCC3O)C)CC)CC(C(=O)C4)C(=C)C5O
MOL002432	0.4430	0.5570	0.7386	Aconiti Lateralis Radix Praeparata	talatizamine	Not Available	FALSE	C123C4C(CN(C1C(C4)C1(C4C2CC(C4O)C(C1)OC)O)CC)(CCC3OC)COC

MOL002433	0.7081	0.2919	0.8094	Aconiti Lateralis Radix Praeparata	(3R,8S,9R,10R,13R,14S,17R)-3-hydroxy-4,4,9,13,14-pentamethyl-17-[(E,2R)-6-methyl-7-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxan-2-yl]oxyhept-5-en-2-yl]-1,2,3,7,8,10,12,15,16,17-decahydr	6324887	FALSE	C1C(C(C2=CCC3C(C2C1)(C(=O)CC1(C3(CCC1C(CC/C=C(/COC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)\C)C)C)C)(C)C)O
MOL002434	0.2078	0.7922	0.7471	Aconiti Lateralis Radix Praeparata	Carnosifloside I_qt	Not Available	FALSE	C1C(C(C2=CCC3C(C2C1)(C(=O)CC1(C3(CCC1C(CC/C=C(/CO)\C)C)C)C)C)(C)C)O
MOL002435	0.7102	0.2898	0.6291	Aconiti Lateralis Radix Praeparata	STOCK1N-53073	Not Available	FALSE	C123C4C(CN(C1C(C4OC)C1(C4C2CC(C4O)(C(C1O)OC)O)O)CC)(C(CC3OC)O)COC
MOL002436	0.3308	0.6692	0.6748	Aconiti Lateralis Radix Praeparata	Delavaconitine	Not Available	FALSE	C1CC2C3C4(C1OC)C1C5C(C(C3)C4N(C2)CC)(CC(C(C5OC(=O)c2ccccc2)(C1)O)OC)O
MOL002437	0.5580	0.4420	0.6210	Aconiti Lateralis Radix Praeparata	Delbruline	Not Available	FALSE	C1CC2(C3C4(C1OC)C1C5C6(C(C3OC)(OCO6)C4N(C2)CC)CC(C(C5O)C1)OC)COC
MOL002439	0.1830	0.8170	0.8102	Calyx Cucumis	Elatine	Not Available	FALSE	O1C23C4N(CC5(C(C4(C4C6C2(OC1)CC(OC)C(C4)C6OC)C(OC)CC5)C3OC)COC(=O)c1c(N2C(=O)C(CC2=O)C)cccc1)CC
MOL002440	0.2518	0.7482	0.7169	Trichosanthis Radix	cucurbitacin b	5281316	FALSE	OC1C(C2(C(C3C(C4C(=CC3)C(C(=O)C(O)C4)(C)C)(C(=O)C2)C)(C1)C)C)C(O)(C)C(=O)/C=C/C(OC(=O)C)(C)C
MOL002440	0.2518	0.7482	0.7169	Picrorhizae Rhizoma	cucurbitacin b	5281316	FALSE	OC1C(C2(C(C3C(C4C(=CC3)C(C(=O)C(O)C4)(C)C)(C(=O)C2)C)(C1)C)C)C(O)(C)C(=O)/C=C/C(OC(=O)C)(C)C
MOL002440	0.2518	0.7482	0.7169	Bolbostemae Paniculati Bulbus	cucurbitacin b	5281316	FALSE	OC1C(C2(C(C3C(C4C(=CC3)C(C(=O)C(O)C4)(C)C)(C(=O)C2)C)(C1)C)C)C(O)(C)C(=O)/C=C/C(OC(=O)C)(C)C
MOL002440	0.2518	0.7482	0.7169	Calyx Cucumis	cucurbitacin b	5281316	FALSE	OC1C(C2(C(C3C(C4C(=CC3)C(C(=O)C(O)C4)(C)C)(C(=O)C2)C)(C1)C)C)C(O)(C)C(=O)/C=C/C(OC(=O)C)(C)C

MOL002441	0.6746	0.3254	0.8605	Smilax China	Dioscin	Not Available	FALSE	C12(C3C(CC1C1C(CC2)C2(C(=CC1)CC(CC2)OC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)C)O)O)O)O)OC1C(C(C(C(O1)C)O)O)O)C)OC1(C3C)CCC(CO1)C)C
MOL002441	0.6746	0.3254	0.8605	Smilacis Glabrae Rhixoma	Dioscin	Not Available	FALSE	C12(C3C(CC1C1C(CC2)C2(C(=CC1)CC(CC2)OC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)C)O)O)O)O)OC1C(C(C(C(O1)C)O)O)O)C)OC1(C3C)CCC(CO1)C)C
MOL002441	0.6746	0.3254	0.8605	Calyx Cucumis	Dioscin	Not Available	FALSE	C12(C3C(CC1C1C(CC2)C2(C(=CC1)CC(CC2)OC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)C)O)O)O)O)OC1C(C(C(C(O1)C)O)O)O)C)OC1(C3C)CCC(CO1)C)C
MOL002443	0.3066	0.6934	0.7355	Calyx Cucumis	Cucurbitacin C	5281317	FALSE	C1C(C(C2=CCC3C(C2C1)(C(=O)CC1(C3(CC(C1C(C(=O)/C=C/C(C)(OC(=O)C)C)(C)O)O)C)C)CO)(C)
MOL002444	0.2371	0.7629	0.7256	Bolbostemae Paniculati Bulbus	Cucurbitacin E	5281319	FALSE	OC1C(C2(C(C3C(C(=O)C2)(C2C(=CC3)C(C(=O)C(=C2)O)(C)C)C)(C1)C)C)C(O)(C)C(=O)/C=C/C(OC(=O)C)(C)C
MOL002444	0.2371	0.7629	0.7256	Calyx Cucumis	Cucurbitacin E	5281319	FALSE	OC1C(C2(C(C3C(C(=O)C2)(C2C(=CC3)C(C(=O)C(=C2)O)(C)C)C)(C1)C)C)C(O)(C)C(=O)/C=C/C(OC(=O)C)(C)C
MOL002445	0.4113	0.5887	0.7156	Calyx Cucumis	Cucurbitacin F	Not Available	FALSE	C1(C(C(C2=CCC3C(C2C1)(C(=O)CC1(C3(C)CC(C1C(C(=O)/C=C/C(C)(C)O)(O)C)O)C)C)C)(C)C)O
MOL002447	0.3987	0.6013	0.7453	Calyx Cucumis	Cucurbitacin D	Not Available	FALSE	C12(C(C(C(C2)O)C(C(=O)/C=C/C(C)(C)O)(C)O)(CC(=O)C2(C1CC=C1C2CC(C(=O)C1(C)C)O)C)C
MOL002448	0.6934	0.3066	0.8593	Calyx Cucumis	Ginsenoside Rg3	Not Available	FALSE	OC1C2(C(C3C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)CC4)(C)C)C)C1)(CCC2C(O)(CCC=C(C)C)C)C
MOL002448	0.6934	0.3066	0.8593	Notoginseng Flos	Ginsenoside Rg3	Not Available	FALSE	OC1C2(C(C3C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)CC4)(C)C)C)C1)(CCC2C(O)(CCC=C(C)C)C)C
MOL002449	0.2576	0.7424	0.7291	Calyx Cucumis	Ginsenoside Rg3_qt	Not Available	FALSE	OC1C2(C(C3C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)(CCC2C(O)(CCC=C(C)C)C)C
MOL002449	0.2576	0.7424	0.7291	Notoginseng Flos	Ginsenoside Rg3_qt	Not Available	FALSE	OC1C2(C(C3C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)(CCC2C(O)(CCC=C(C)C)C)C
MOL002450	0.9095	0.0905	0.7572	Zingiberis Rhizoma	(+)-1,5-Epoxy-nor-ketoguaia-11-ene	Not Available	FALSE	C123C(CCC1C)(C(=O)CCC(C2)C(=C)C)O3
MOL002451	0.8858	0.1142	0.7969	Humulus Scandens (Lour.) Merr.	β-humulene	25229928	FALSE	C1(C/C=C(/CCC(=C)C/C=C/1)\C)(C)C
MOL002451	0.8858	0.1142	0.7969	Folium Nelumbinis	β-humulene	25229928	FALSE	C1(C/C=C(/CCC(=C)C/C=C/1)\C)(C)C
MOL002451	0.8858	0.1142	0.7969	Zingiberis Rhizoma	β-humulene	25229928	FALSE	C1(C/C=C(/CCC(=C)C/C=C/1)\C)(C)C
MOL002452	0.8711	0.1289	0.7791	Eriobotryae Folium	β-sesquiphellandrene	12315493	FALSE	C1(C(CCC=C(C)C)C)CCC(=C)C=C1
MOL002452	0.8711	0.1289	0.7791	Zingiberis Rhizoma	β-sesquiphellandrene	12315493	FALSE	C1(C(CCC=C(C)C)C)CCC(=C)C=C1

MOL002453	0.9479	0.0521	0.7669	Eriobotryae Folium	(-)-Comphene	440966	FALSE	C12C(C)(C)C(=C)C(CC1)C2
MOL002453	0.9479	0.0521	0.7669	Folium Artemisiae Argyi	(-)-Comphene	440966	FALSE	C12C(C)(C)C(=C)C(CC1)C2
MOL002453	0.9479	0.0521	0.7669	Schisandrae Chinensis Fructus	(-)-Comphene	440966	FALSE	C12C(C)(C)C(=C)C(CC1)C2
MOL002453	0.9479	0.0521	0.7669	Rhododendri Daurici Folium	(-)-Comphene	440966	FALSE	C12C(C)(C)C(=C)C(CC1)C2
MOL002453	0.9479	0.0521	0.7669	Citri Fructus	(-)-Comphene	440966	FALSE	C12C(C)(C)C(=C)C(CC1)C2
MOL002453	0.9479	0.0521	0.7669	Styrax	(-)-Comphene	440966	FALSE	C12C(C)(C)C(=C)C(CC1)C2
MOL002453	0.9479	0.0521	0.7669	Canarii Fructus	(-)-Comphene	440966	FALSE	C12C(C)(C)C(=C)C(CC1)C2
MOL002453	0.9479	0.0521	0.7669	Zanthoxyli Pericarpium	(-)-Comphene	440966	FALSE	C12C(C)(C)C(=C)C(CC1)C2
MOL002453	0.9479	0.0521	0.7669	Zingiberis Rhizoma	(-)-Comphene	440966	FALSE	C12C(C)(C)C(=C)C(CC1)C2
MOL002453	0.9479	0.0521	0.7669	Houttuyniae Herba	(-)-Comphene	440966	FALSE	C12C(C)(C)C(=C)C(CC1)C2
MOL002454	0.4356	0.5644	0.7773	Zingiberis Rhizoma	10-Gingerdione	Not Available	FALSE	C(c1cc(c(cc1)O)OC)CC(=O)/C=C(\O)/CCCCCCCC
MOL002455	0.9198	0.0802	0.9211	Zingiberis Rhizoma	[(3S)-3,7-dimethyloct-6-enyl] acetate	6999975	FALSE	C(CCC=C(C)C)(CCOC(=O)C)C
MOL002455	0.9198	0.0802	0.9211	Evodiae Fructus	[(3S)-3,7-dimethyloct-6-enyl] acetate	6999975	FALSE	C(CCC=C(C)C)(CCOC(=O)C)C
MOL002455	0.9198	0.0802	0.9211	Zanthoxyli Pericarpium	[(3S)-3,7-dimethyloct-6-enyl] acetate	6999975	FALSE	C(CCC=C(C)C)(CCOC(=O)C)C
MOL002455	0.9198	0.0802	0.9211	Schisandrae Chinensis Fructus	[(3S)-3,7-dimethyloct-6-enyl] acetate	6999975	FALSE	C(CCC=C(C)C)(CCOC(=O)C)C
MOL002455	0.9198	0.0802	0.9211	Rose Rugosae Flos	[(3S)-3,7-dimethyloct-6-enyl] acetate	6999975	FALSE	C(CCC=C(C)C)(CCOC(=O)C)C
MOL002455	0.9198	0.0802	0.9211	Ligustici Rhizoma Et Radix	[(3S)-3,7-dimethyloct-6-enyl] acetate	6999975	FALSE	C(CCC=C(C)C)(CCOC(=O)C)C
MOL002456	0.8857	0.1143	0.8592	Zingiberis Rhizoma	[(3R)-3,7-dimethyloct-6-enyl] butanoate	23616651	FALSE	C(CCOC(=O)CCC)(CCC=C(C)C)C

MOL002456	0.8857	0.1143	0.8592	Citrus Reticulata	[(3R)-3,7-dimethyloct-6-enyl] butanoate	23616651	FALSE	C(CCOC(=O)CCC)(CCC=C(C)C)C
MOL002456	0.8857	0.1143	0.8592	Rose Rugosae Flos	[(3R)-3,7-dimethyloct-6-enyl] butanoate	23616651	FALSE	C(CCOC(=O)CCC)(CCC=C(C)C)C
MOL002457	0.8934	0.1066	0.7862	Zingiberis Rhizoma	Cyclopropyl ketone	70721	FALSE	C(=O)(C1CC1)C1CC1
MOL002458	0.9487	0.0513	0.8045	Cnidii Fructus	ZINC01850974	6973643	FALSE	C12(C(C(C(C1)CC2)(C)C)O)C
MOL002458	0.9487	0.0513	0.8045	Citrus Aurantium	ZINC01850974	6973643	FALSE	C12(C(C(C(C1)CC2)(C)C)O)C
MOL002458	0.9487	0.0513	0.8045	Cinnanmomi Cortex	ZINC01850974	6973643	FALSE	C12(C(C(C(C1)CC2)(C)C)O)C
MOL002458	0.9487	0.0513	0.8045	Zingiberis Rhizoma	ZINC01850974	6973643	FALSE	C12(C(C(C(C1)CC2)(C)C)O)C
MOL002458	0.9487	0.0513	0.8045	Lignum Pini Nodi	ZINC01850974	6973643	FALSE	C12(C(C(C(C1)CC2)(C)C)O)C
MOL002458	0.9487	0.0513	0.8045	Magnolia Officinalis Rehd Et Wils.	ZINC01850974	6973643	FALSE	C12(C(C(C(C1)CC2)(C)C)O)C
MOL002458	0.9487	0.0513	0.8045	Alpiniae Officinarum Rhizome	ZINC01850974	6973643	FALSE	C12(C(C(C(C1)CC2)(C)C)O)C
MOL002458	0.9487	0.0513	0.8045	Rhododendri Daurici Folium	ZINC01850974	6973643	FALSE	C12(C(C(C(C1)CC2)(C)C)O)C
MOL002459	0.4574	0.5426	0.7432	Zingiberis Rhizoma	(S)-5-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)-3-tetradecanone	168115	FALSE	c1(cc(c(cc1)O)OC)CCC(=O)CC(CCCCCCCCC)O
MOL002460	0.7557	0.2443	0.6143	Zingiberis Rhizoma	12,13-Di-acetoxyl-1,4,6,11-eudesmanetetol	Not Available	FALSE	C1CC(C2(C(C1O)(CCC(C2O)C(O)(COC(=O)C)OC(=O)C)C)C)(C)O
MOL002461	0.4624	0.5376	0.6293	Zingiberis Rhizoma	Gingerglycolipid A	6450152	FALSE	O1C(C(O)C(OC(=O)CCCCCCC/C=C\C/C=C\C/C=C\CC)(O)C(O)(O)C1OCCC)COC1OC(C(O)C(O)C1O)CO

MOL002463	0.5375	0.4625	0.6526	Zingiberis Rhizoma	[(2S)-2-hydroxy-3-[(2R,3R,4S,5R,6R)-3,4,5-trihydroxy-6-[[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydropyran-2-yl]oxymethyl]tetrahydropyran-2-yl]oxymethyl]tetrahydropyran-2-yl]oxy-propyl] (9Z,12Z)-octadeca-9,12-dienoate	10009754	FALSE	O1C(C(O)C(O)C(O)C1OCC(O)COC(=O)CCCCCCC/C=C\C/C=C\CCCCC)COC1OC(C(O)C(O)C1O)CO
MOL002465	0.4520	0.5480	0.6105	Zingiber Officinale Roscoe	9-Octadecenoic acid (Z)-, 3-((6-O-alpha-D-galactopyranosyl-beta-D-galactopyranosyl)oxy)-2-hydroxypropyl ester, (S)-	6450013	FALSE	O1C(C(O)C(OC(=O)CCCCCCC/C=C\CCCCCCCC)(O)C(O)(O)C1OCCC)COC1OC(C(O)C(O)C1O)CO
MOL002465	0.4520	0.5480	0.6105	Zingiberis Rhizoma	9-Octadecenoic acid (Z)-, 3-((6-O-alpha-D-galactopyranosyl-beta-D-galactopyranosyl)oxy)-2-hydroxypropyl ester, (S)-	6450013	FALSE	O1C(C(O)C(OC(=O)CCCCCCC/C=C\CCCCCCCC)(O)C(O)(O)C1OCCC)COC1OC(C(O)C(O)C1O)CO
MOL002467	0.8218	0.1782	0.8422	Zingiberis Rhizoma	6-gingerol	442793	FALSE	C(CC(=O)CC(CCCCC)O)c1cc(c(cc1)O)OC
MOL002467	0.8218	0.1782	0.8422	Zingiber Officinale Roscoe	6-gingerol	442793	FALSE	C(CC(=O)CC(CCCCC)O)c1cc(c(cc1)O)OC

MOL002468	0.5692	0.4308	0.7444	Zingiberis Rhizoma	hexahydrocurcumin	13347318	FALSE	OC(CCc1cc(OC)c(O)cc1)CC(=O)CCc1cc(OC)c(O)cc1
MOL002468	0.5692	0.4308	0.7444	Alpiniae Officinarum Rhizome	hexahydrocurcumin	13347318	FALSE	OC(CCc1cc(OC)c(O)cc1)CC(=O)CCc1cc(OC)c(O)cc1
MOL002469	0.3368	0.6632	0.6462	Zingiberis Rhizoma	12-Gingerol	Not Available	FALSE	C(c1cc(c(cc1)O)OC)CC(=O)CC(O)CCCCCCCCCCC
MOL002470	0.3501	0.6499	0.8000	Zingiberis Rhizoma	Isogingerenone-B	5318568	FALSE	C(CC(=O)/C=C/CCc1cc(c(cc1)O)OC)c1cc(c(c(c1)OC)O)OC
MOL002471	0.8921	0.1079	0.8732	Menthae Herba	[(1R,2R,5R)-2-isopropyl-5-methyl-cyclohexyl] acetate	88692	FALSE	C(=O)(C)OC1C(CCC(C1)C)C(C)C
MOL002471	0.8921	0.1079	0.8732	Zingiberis Rhizoma	[(1R,2R,5R)-2-isopropyl-5-methyl-cyclohexyl] acetate	88692	FALSE	C(=O)(C)OC1C(CCC(C1)C)C(C)C
MOL002472	0.9117	0.0883	0.8972	Zingiberis Rhizoma	Neryl propionate	5365982	FALSE	C(=C\COC(=O)CC)(\CCC=C(C)C)/C
MOL002473	0.3412	0.6588	0.7549	Zingiberis Rhizoma	ZINC04081584	7092657	FALSE	C12C(C3(C(CC2)CC(=O)C=C3)C)CCC2(C1CCC2(C)O)C
MOL002474	0.9410	0.0590	0.9674	Evodiae Fructus	p-mentha-1,5-dien-8-ol	13965283	FALSE	CC(C)(O)C1C=CC(=CC1)C
MOL002474	0.9410	0.0590	0.9674	Zingiberis Rhizoma	p-mentha-1,5-dien-8-ol	13965283	FALSE	CC(C)(O)C1C=CC(=CC1)C
MOL002475	0.8302	0.1698	0.7293	Curcumae Radix	himachalene	11586487	FALSE	C12C(=C(CCCC1(C)C)C)CCC(=C2)C
MOL002475	0.8302	0.1698	0.7293	Ligustici Rhizoma Et Radix	himachalene	11586487	FALSE	C12C(=C(CCCC1(C)C)C)CCC(=C2)C
MOL002475	0.8302	0.1698	0.7293	Zingiberis Rhizoma	himachalene	11586487	FALSE	C12C(=C(CCCC1(C)C)C)CCC(=C2)C
MOL002477	0.9239	0.0761	0.9418	Zingiberis Rhizoma	(2R)-2,6-dimethylhept-5-enal	6997374	FALSE	C(CCC=C(C)C)(C=O)C
MOL002477	0.9239	0.0761	0.9418	Campsis Flos	(2R)-2,6-dimethylhept-5-enal	6997374	FALSE	C(CCC=C(C)C)(C=O)C
MOL002478	0.9343	0.0657	0.9527	Rubi Fructus	(2R)-heptan-2-ol	6992611	FALSE	C(CCCC)C(C)O
MOL002478	0.9343	0.0657	0.9527	Momordicae Fructus	(2R)-heptan-2-ol	6992611	FALSE	C(CCCC)C(C)O
MOL002478	0.9343	0.0657	0.9527	Zingiberis Rhizoma	(2R)-heptan-2-ol	6992611	FALSE	C(CCCC)C(C)O
MOL002478	0.9343	0.0657	0.9527	Caryophylliflos	(2R)-heptan-2-ol	6992611	FALSE	C(CCCC)C(C)O

MOL002479	0.9337	0.0663	0.9590	Capsici Fructus	(2S)-2-methylpentanal	6999050	FALSE	C(CCC)(C=O)C
MOL002479	0.9337	0.0663	0.9590	Zingiberis Rhizoma	(2S)-2-methylpentanal	6999050	FALSE	C(CCC)(C=O)C
MOL002480	0.9141	0.0859	0.9670	Angelicae Sinensis Radix	Methylbutenol	8257	FALSE	C(C=C)(C)(C)O
MOL002480	0.9141	0.0859	0.9670	Zingiberis Rhizoma	Methylbutenol	8257	FALSE	C(C=C)(C)(C)O
MOL002481	0.9203	0.0797	0.9277	Zingiberis Rhizoma	2-Methylhept-2-ene	12330	FALSE	C(=C(C)C)CCCC
MOL002482	0.9209	0.0791	0.9183	Zingiberis Rhizoma	()-beta-Citronellene	10887985	FALSE	C(CCC=C(C)C)(C=C)C
MOL002483	0.7544	0.2456	0.8948	Zingiber Officinale Roscoe	1-(4-Hydroxy-3-methoxyphenyl)decan-5-one	21117016	FALSE	C(CCCC(=O)CCCCC)c1cc(c(cc1)O)OC
MOL002483	0.7544	0.2456	0.8948	Zingiberis Rhizoma	1-(4-Hydroxy-3-methoxyphenyl)decan-5-one	21117016	FALSE	C(CCCC(=O)CCCCC)c1cc(c(cc1)O)OC
MOL002484	0.9154	0.0846	0.9673	Santalum Album L.	Isovaleral	11552	FALSE	C(C(C)C)C=O
MOL002484	0.9154	0.0846	0.9673	Bombyx Mori L.	Isovaleral	11552	FALSE	C(C(C)C)C=O
MOL002484	0.9154	0.0846	0.9673	Rubi Fructus	Isovaleral	11552	FALSE	C(C(C)C)C=O
MOL002484	0.9154	0.0846	0.9673	Sesami Nigrum Semen	Isovaleral	11552	FALSE	C(C(C)C)C=O
MOL002484	0.9154	0.0846	0.9673	Campsis Flos	Isovaleral	11552	FALSE	C(C(C)C)C=O
MOL002484	0.9154	0.0846	0.9673	Zingiberis Rhizoma	Isovaleral	11552	FALSE	C(C(C)C)C=O
MOL002485	0.9284	0.0716	0.8904	Zingiberis Rhizoma	4-(1,5-Dimethylhex-4-enyl)cyclohex-2-enone	Not Available	FALSE	C1(=O)C=CC(CC1)C(CCC=C(C)C)C
MOL002486	0.9164	0.0836	0.9087	Zingiberis Rhizoma	4-Gingerol	46901319	FALSE	C(CC(=O)CC(CCC)O)c1cc(c(cc1)O)OC

MOL002487	0.6670	0.3330	0.6922	Zingiberis Rhizoma	5-hydroxy-7-(4-hydroxyphenyl)-1-(4-hydroxy-3-methoxyphenyl)-3-heptanone	44575993	FALSE	C(CC(=O)CC(CCc1ccc(cc1)O)O)c1cc(c(cc1)O)OC
MOL002488	0.7750	0.2250	0.8433	Zingiberis Rhizoma	6-Gingerdione	Not Available	FALSE	C(c1cc(c(cc1)O)OC)CC(=O)/C=C(\O)/CCCCC
MOL002489	0.9146	0.0854	0.9124	Zingiberis Rhizoma	[(3S)-3,7-dimethyloct-7-enyl] acetate	23616650	FALSE	C(CCCC(=C)C)(CCOC(=O)C)C
MOL002490	0.4241	0.5759	0.8156	Zingiberis Rhizoma	6-gingediacetate	Not Available	FALSE	c1(c(cc(cc1)CCC(CC(CCCCC)OC(=O)C)OC(=O)C)OC)O
MOL002491	0.6859	0.3141	0.8464	Zingiberis Rhizoma	6-gingediol-3-acetate	Not Available	FALSE	c1(c(cc(cc1)CCC(CC(CCCCC)O)OC(=O)C)OC)O
MOL002492	0.6371	0.3629	0.8021	Zingiberis Rhizoma	6-gingediol-5-acetate	Not Available	FALSE	c1(c(cc(cc1)CCC(CC(CCCCC)OC(=O)C)O)OC)O
MOL002493	0.8290	0.1710	0.8180	Zingiberis Rhizoma	6-gingediol	Not Available	FALSE	C(CC(CC(CCCCC)O)O)c1cc(c(cc1)O)OC
MOL002495	0.7595	0.2405	0.8134	Zingiber Officinale Roscoe	6-shogaol	5281794	FALSE	c1(cc(c(cc1)O)OC)CCC(=O)/C=C/CCCCC
MOL002495	0.7595	0.2405	0.8134	Zingiberis Rhizoma	6-shogaol	5281794	FALSE	c1(cc(c(cc1)O)OC)CCC(=O)/C=C/CCCCC
MOL002495	0.7595	0.2405	0.8134	Arum Ternatum Thunb.	6-shogaol	5281794	FALSE	c1(cc(c(cc1)O)OC)CCC(=O)/C=C/CCCCC
MOL002496	0.9225	0.0775	0.9467	Alpiniae Officinarum Rhizome	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C
MOL002496	0.9225	0.0775	0.9467	Apocyniveneti Folium	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C
MOL002496	0.9225	0.0775	0.9467	Benzoinum	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C
MOL002496	0.9225	0.0775	0.9467	Ganoderma	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C
MOL002496	0.9225	0.0775	0.9467	Eriobotryae Folium	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C
MOL002496	0.9225	0.0775	0.9467	Rose Rugosae Flos	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C
MOL002496	0.9225	0.0775	0.9467	Lonicerae Japonicae Flos	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C
MOL002496	0.9225	0.0775	0.9467	Morindae Officinalis Radix	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C
MOL002496	0.9225	0.0775	0.9467	Zingiber Officinale Roscoe	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C
MOL002496	0.9225	0.0775	0.9467	Cinnamomi Ramulus	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C
MOL002496	0.9225	0.0775	0.9467	Hippophae Fructus	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C
MOL002496	0.9225	0.0775	0.9467	Litseae Fructus	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C
MOL002496	0.9225	0.0775	0.9467	Capsici Fructus	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C
MOL002496	0.9225	0.0775	0.9467	Bombyx Mori L.	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C
MOL002496	0.9225	0.0775	0.9467	Cinnanmomi Cortex	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C
MOL002496	0.9225	0.0775	0.9467	Campsis Flos	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C
MOL002496	0.9225	0.0775	0.9467	Ginkgo Folium	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C
MOL002496	0.9225	0.0775	0.9467	Mume Flos	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C
MOL002496	0.9225	0.0775	0.9467	Ephedra Herba	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C

MOL002496	0.9225	0.0775	0.9467	Lysimachiae Foenigraeci Herba	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C
MOL002496	0.9225	0.0775	0.9467	Zingiberis Rhizoma	Sulcatone	9862	FALSE	C(=CCCC(=O)C)(C)C
MOL002497	0.6456	0.3544	0.7936	Uncariae Ramulus Cumuncis	(8)-Gingerol	168114	FALSE	c1(cc(c(cc1)O)OC)CCC(=O)CC(CCCCCCC)O
MOL002497	0.6456	0.3544	0.7936	Zingiberis Rhizoma	(8)-Gingerol	168114	FALSE	c1(cc(c(cc1)O)OC)CCC(=O)CC(CCCCCCC)O
MOL002498	0.9319	0.0681	0.9640	Citri Sarcodactylis Fructus	PGR	259994	FALSE	C(C(C)O)O
MOL002498	0.9319	0.0681	0.9640	Hordei Fructus Germinatus	PGR	259994	FALSE	C(C(C)O)O
MOL002498	0.9319	0.0681	0.9640	Zingiberis Rhizoma	PGR	259994	FALSE	C(C(C)O)O
MOL002499	0.9619	0.0381	0.7507	Zingiberis Rhizoma	Bicyclo[3. 1. 0]hex-2-ene,4-methyl-1-(1-methylethyl)-	12444328	FALSE	C12(C=CC(C1C2)C)C(C)C
MOL002500	0.8438	0.1562	0.6497	Schizonepetae Herba	Campherenol	Not Available	FALSE	C1CC2(C(CC1C2(CCC=C(C)C)C)O)C
MOL002500	0.8438	0.1562	0.6497	Zingiberis Rhizoma	Campherenol	Not Available	FALSE	C1CC2(C(CC1C2(CCC=C(C)C)C)O)C
MOL002500	0.8438	0.1562	0.6497	Forsythiae Fructus	Campherenol	Not Available	FALSE	C1CC2(C(CC1C2(CCC=C(C)C)C)O)C
MOL002500	0.8438	0.1562	0.6497	Houttuyniae Herba	Campherenol	Not Available	FALSE	C1CC2(C(CC1C2(CCC=C(C)C)C)O)C
MOL002500	0.8438	0.1562	0.6497	Asari Radix Et Rhizoma	Campherenol	Not Available	FALSE	C1CC2(C(CC1C2(CCC=C(C)C)C)O)C
MOL002501	0.3048	0.6952	0.6695	Asari Radix Et Rhizoma	[(1S)-3-[(E)-but-2-enyl]-2-methyl-4-oxo-1-cyclopent-2-enyl] (1R,3R)-3-[(E)-3-methoxy-2-methyl-3-oxoprop-1-enyl]-2,2-dimethylcyclopropane-1-carboxylate	5315890	FALSE	C/C(=C\C1C(C1(C)C)C(=O)OC1C(=C(C(=O)C1)C/C=C/C)C)/C(=O)OC

MOL002501	0.3048	0.6952	0.6695	Zingiberis Rhizoma	[(1S)-3-[(E)-but-2-enyl]-2-methyl-4-oxo-1-cyclopent-2-enyl] (1R,3R)-3-[(E)-3-methoxy-2-methyl-3-oxoprop-1-enyl]-2,2-dimethylcyclopropane-1-carboxylate	5315890	FALSE	C/C(=C\C1C(C1(C)C)C(=O)OC1C(=C(C(=O)C1)C/C=C/C)C)/C(=O)OC
MOL002503	0.5085	0.4915	0.7690	Asari Radix Et Rhizoma	Cynanuriculoside A	Not Available	FALSE	C1(CC2=CCC3(C(C2(CC1)C)CC(C1(C3(O)CCC1O)CC(=O)C)OC(=O)/C=C(/C(C)C)\C)O)OC1OC(C(C(C1)OC)OC1OC(C(C(C1)OC)OC1OC(C(C(C1)OC)OC1OC(C(C(C1O)O)O)CO)C)C)C
MOL002503	0.5085	0.4915	0.7690	Forsythiae Fructus	Cynanuriculoside A	Not Available	FALSE	C1(CC2=CCC3(C(C2(CC1)C)CC(C1(C3(O)CCC1O)CC(=O)C)OC(=O)/C=C(/C(C)C)\C)O)OC1OC(C(C(C1)OC)OC1OC(C(C(C1)OC)OC1OC(C(C(C1)OC)OC1OC(C(C(C1O)O)O)CO)C)C)C
MOL002503	0.5085	0.4915	0.7690	Schizonepetae Herba	Cynanuriculoside A	Not Available	FALSE	C1(CC2=CCC3(C(C2(CC1)C)CC(C1(C3(O)CCC1O)CC(=O)C)OC(=O)/C=C(/C(C)C)\C)O)OC1OC(C(C(C1)OC)OC1OC(C(C(C1)OC)OC1OC(C(C(C1)OC)OC1OC(C(C(C1O)O)O)CO)C)C)C
MOL002503	0.5085	0.4915	0.7690	Zingiberis Rhizoma	Cynanuriculoside A	Not Available	FALSE	C1(CC2=CCC3(C(C2(CC1)C)CC(C1(C3(O)CCC1O)CC(=O)C)OC(=O)/C=C(/C(C)C)\C)O)OC1OC(C(C(C1)OC)OC1OC(C(C(C1)OC)OC1OC(C(C(C1)OC)OC1OC(C(C(C1O)O)O)CO)C)C)C
MOL002504	0.8642	0.1358	0.7920	A. Dahurica (Fisch.) Benth. Et Hook	Peruviol	5356544	FALSE	C(C)(C=C)(CC/C=C(/C)\CCC=C(C)C)O
MOL002504	0.8642	0.1358	0.7920	Ephedra Herba	Peruviol	5356544	FALSE	C(C)(C=C)(CC/C=C(/C)\CCC=C(C)C)O
MOL002504	0.8642	0.1358	0.7920	Aucklandiae Radix	Peruviol	5356544	FALSE	C(C)(C=C)(CC/C=C(/C)\CCC=C(C)C)O
MOL002504	0.8642	0.1358	0.7920	Dalbergiae Odoriferae Lignum	Peruviol	5356544	FALSE	C(C)(C=C)(CC/C=C(/C)\CCC=C(C)C)O
MOL002504	0.8642	0.1358	0.7920	Eriobotryae Folium	Peruviol	5356544	FALSE	C(C)(C=C)(CC/C=C(/C)\CCC=C(C)C)O
MOL002504	0.8642	0.1358	0.7920	Zingiberis Rhizoma	Peruviol	5356544	FALSE	C(C)(C=C)(CC/C=C(/C)\CCC=C(C)C)O
MOL002504	0.8642	0.1358	0.7920	Cnidii Fructus	Peruviol	5356544	FALSE	C(C)(C=C)(CC/C=C(/C)\CCC=C(C)C)O
MOL002504	0.8642	0.1358	0.7920	Magnolia Officinalis Rehd Et Wils.	Peruviol	5356544	FALSE	C(C)(C=C)(CC/C=C(/C)\CCC=C(C)C)O

MOL002505	0.6274	0.3726	0.7443	Zingiberis Rhizoma	C10230	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC1OC(OC(=O)c3cc(c(c(c3)O)O)O)C3C(C1OC(=O)C1=CC(=O)C4(C(C1c1c(C(=O)O3)cc(c(c1O4)O)O)(O)O)O)OC(=O)c1c2c(c(c(c1)
MOL002505	0.6274	0.3726	0.7443	Euphorbiae Helioscopiae Herba	C10230	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC1OC(OC(=O)c3cc(c(c(c3)O)O)O)C3C(C1OC(=O)C1=CC(=O)C4(C(C1c1c(C(=O)O3)cc(c(c1O4)O)O)(O)O)O)OC(=O)c1c2c(c(c(c1)
MOL002505	0.6274	0.3726	0.7443	Forsythiae Fructus	C10230	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC1OC(OC(=O)c3cc(c(c(c3)O)O)O)C3C(C1OC(=O)C1=CC(=O)C4(C(C1c1c(C(=O)O3)cc(c(c1O4)O)O)(O)O)O)OC(=O)c1c2c(c(c(c1)
MOL002505	0.6274	0.3726	0.7443	Geranium Wilfordii Maxim.	C10230	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC1OC(OC(=O)c3cc(c(c(c3)O)O)O)C3C(C1OC(=O)C1=CC(=O)C4(C(C1c1c(C(=O)O3)cc(c(c1O4)O)O)(O)O)O)OC(=O)c1c2c(c(c(c1)
MOL002505	0.6274	0.3726	0.7443	Phyllanthi Fructus	C10230	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC1OC(OC(=O)c3cc(c(c(c3)O)O)O)C3C(C1OC(=O)C1=CC(=O)C4(C(C1c1c(C(=O)O3)cc(c(c1O4)O)O)(O)O)O)OC(=O)c1c2c(c(c(c1)
MOL002506	0.4368	0.5632	0.8218	Zingiberis Rhizoma	Gingerenone A	5281775	FALSE	C(c1cc(c(cc1)O)OC)CC(=O)/C=C/CCc1cc(c(cc1)O)OC
MOL002507	0.3492	0.6508	0.8002	Zingiberis Rhizoma	Gingerenone B	5317592	FALSE	c1(c(ccc(c1)CCC(=O)/C=C/CCc1cc(c(c(c1)OC)O)OC)O)OC
MOL002508	0.5026	0.4974	0.7539	Zingiberis Rhizoma	Gingerenone-C	5317593	FALSE	c1(c(ccc(c1)CCC(=O)/C=C/CCc1ccc(cc1)O)O)OC
MOL002509	0.2858	0.7142	0.6314	Ginkgo Folium	Ginkgetin	5271805	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)c1c(cc(c2c1oc(cc2=O)c1ccc(cc1)O)O)O)O)OC
MOL002509	0.2858	0.7142	0.6314	Epimrdii Herba	Ginkgetin	5271805	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)c1c(cc(c2c1oc(cc2=O)c1ccc(cc1)O)O)O)O)OC
MOL002509	0.2858	0.7142	0.6314	Zingiberis Rhizoma	Ginkgetin	5271805	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)c1c(cc(c2c1oc(cc2=O)c1ccc(cc1)O)O)O)O)OC
MOL002509	0.2858	0.7142	0.6314	Ginkgo Semen	Ginkgetin	5271805	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)c1c(cc(c2c1oc(cc2=O)c1ccc(cc1)O)O)O)O)OC
MOL002510	0.7246	0.2754	0.7315	Zingiberis Rhizoma	Heptaphylline	5318015	FALSE	O=Cc1c(O)c(c2c(c1)c1c([nH]2)cccc1)CC=C(C)C
MOL002511	0.2163	0.7837	0.6312	Ginkgo Folium	Isoginkgetin	5318569	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)c1c2oc(cc(=O)c2c(cc1O)O)c1ccc(cc1)OC)O)O
MOL002511	0.2163	0.7837	0.6312	Epimrdii Herba	Isoginkgetin	5318569	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)c1c2oc(cc(=O)c2c(cc1O)O)c1ccc(cc1)OC)O)O
MOL002511	0.2163	0.7837	0.6312	Ranunculi Ternati Radix	Isoginkgetin	5318569	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)c1c2oc(cc(=O)c2c(cc1O)O)c1ccc(cc1)OC)O)O
MOL002511	0.2163	0.7837	0.6312	Zingiberis Rhizoma	Isoginkgetin	5318569	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)c1c2oc(cc(=O)c2c(cc1O)O)c1ccc(cc1)OC)O)O
MOL002512	0.9242	0.0758	0.9644	Zingiberis Rhizoma	Mesotrihydroxypiperidine	445612	FALSE	C1(CNCC(C1O)O)O
MOL002513	0.9244	0.0756	0.8145	Myrrha	Xanthorrhizol	93135	FALSE	c1(cc(c(cc1)C)O)C(CCC=C(C)C)C
MOL002513	0.9244	0.0756	0.8145	Litchi Semen	Xanthorrhizol	93135	FALSE	c1(cc(c(cc1)C)O)C(CCC=C(C)C)C
MOL002513	0.9244	0.0756	0.8145	Zingiberis Rhizoma	Xanthorrhizol	93135	FALSE	c1(cc(c(cc1)C)O)C(CCC=C(C)C)C

MOL002513	0.9244	0.0756	0.8145	Curcumae Radix	Xanthorrhizol	93135	FALSE	c1(cc(c(cc1)C)O)C(CCC=C(C)C)C
MOL002514	0.8770	0.1230	0.8715	Zingiberis Rhizoma	Sexangulareti	5281698	FALSE	c12c(c(c(cc1O)O)OC)oc(c(c2=O)O)c1ccc(cc1)O
MOL002514	0.8770	0.1230	0.8715	Mori Cortex	Sexangulareti	5281698	FALSE	c12c(c(c(cc1O)O)OC)oc(c(c2=O)O)c1ccc(cc1)O
MOL002515	0.8705	0.1295	0.6791	Zingiberis Rhizoma	Shyobunone	5321293	FALSE	C1(C(C(=O)C(CC1)C(C)C)C(=C)C)(C=C)C
MOL002516	0.9535	0.0465	0.9398	Alpiniae Officinarum Rhizome	zingerone	31211	FALSE	c1(cc(c(cc1)O)OC)CCC(=O)C
MOL002516	0.9535	0.0465	0.9398	Zingiberis Rhizoma	zingerone	31211	FALSE	c1(cc(c(cc1)O)OC)CCC(=O)C
MOL002516	0.9535	0.0465	0.9398	Schisandrae Chinensis Fructus	zingerone	31211	FALSE	c1(cc(c(cc1)O)OC)CCC(=O)C
MOL002516	0.9535	0.0465	0.9398	Zingiber Officinale Roscoe	zingerone	31211	FALSE	c1(cc(c(cc1)O)OC)CCC(=O)C
MOL002517	0.6877	0.3123	0.8595	Zingiberis Rhizoma	Zingiberoside A3	Not Available	FALSE	O1C2(CCC(C1)C)OC1C(C2C)C2(C(C1)C1C(CC2)C2(C(=CC1)CC(CC2)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)OC1OC(C(C(C1O)O)O)CO)CO)C)C
MOL002518	0.2872	0.7128	0.7586	Zingiberis Rhizoma	Zingiberoside A3_qt	Not Available	FALSE	O1C2(CCC(C1)C)OC1C(C2C)C2(C(C1)C1C(CC2)C2(C(=CC1)CC(CC2)O)C)C
MOL002519	0.9249	0.0751	0.9326	Zingiberis Rhizoma	Decamethylenediol	37153	FALSE	C(CCCCCO)CCCCO
MOL002520	0.9561	0.0439	0.7701	Alpiniae Officinarum Rhizome	.beta.-Fenchyl acetate, exo-	156660	FALSE	C12(C(C(C(C1)CC2)(C)C)OC(=O)C)C
MOL002520	0.9561	0.0439	0.7701	Zingiberis Rhizoma	.beta.-Fenchyl acetate, exo-	156660	FALSE	C12(C(C(C(C1)CC2)(C)C)OC(=O)C)C
MOL002521	0.8712	0.1288	0.8185	Codonopsis Radix	beta-Curcumene	Not Available	FALSE	C1=C(CC=C(C1)C(CCCC(=C)C)C)C
MOL002521	0.8712	0.1288	0.8185	Zingiberis Rhizoma	beta-Curcumene	Not Available	FALSE	C1=C(CC=C(C1)C(CCCC(=C)C)C)C
MOL002521	0.8712	0.1288	0.8185	Panacis Quinquefolii Radix	beta-Curcumene	Not Available	FALSE	C1=C(CC=C(C1)C(CCCC(=C)C)C)C
MOL002522	0.9310	0.0690	0.9422	Zingiber Officinale Roscoe	beta-Rhodinol	7793	FALSE	C(CCC=C(C)C)(CCO)C
MOL002522	0.9310	0.0690	0.9422	Campsis Flos	beta-Rhodinol	7793	FALSE	C(CCC=C(C)C)(CCO)C
MOL002522	0.9310	0.0690	0.9422	Zingiberis Rhizoma	beta-Rhodinol	7793	FALSE	C(CCC=C(C)C)(CCO)C
MOL002522	0.9310	0.0690	0.9422	Curcumae Radix	beta-Rhodinol	7793	FALSE	C(CCC=C(C)C)(CCO)C
MOL002522	0.9310	0.0690	0.9422	Coriandri Sativi Herba	beta-Rhodinol	7793	FALSE	C(CCC=C(C)C)(CCO)C
MOL002522	0.9310	0.0690	0.9422	Rose Rugosae Flos	beta-Rhodinol	7793	FALSE	C(CCC=C(C)C)(CCO)C
MOL002522	0.9310	0.0690	0.9422	Mori Cortex	beta-Rhodinol	7793	FALSE	C(CCC=C(C)C)(CCO)C
MOL002522	0.9310	0.0690	0.9422	Alpiniae Officinarum Rhizome	beta-Rhodinol	7793	FALSE	C(CCC=C(C)C)(CCO)C
MOL002522	0.9310	0.0690	0.9422	Citri Fructus	beta-Rhodinol	7793	FALSE	C(CCC=C(C)C)(CCO)C
MOL002522	0.9310	0.0690	0.9422	Lonicerae Japonicae Flos	beta-Rhodinol	7793	FALSE	C(CCC=C(C)C)(CCO)C
MOL002524	0.8619	0.1381	0.6520	Evodiae Fructus	(-)-cis-beta-Elemene	641756	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C)C=C
MOL002524	0.8619	0.1381	0.6520	Alpiniae Officinarum Rhizome	(-)-cis-beta-Elemene	641756	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C)C=C

MOL002524	0.8619	0.1381	0.6520	Pogostemon Cablin (Blanco) Benth.	(-)-cis-beta-Elemene	641756	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C)C=C
MOL002525	0.9490	0.0510	0.9697	Alpiniae Officinarum Rhizome	Vasodil	5504	FALSE	c1(CC2=NCCN2)ccccc1
MOL002526	0.8478	0.1522	0.7174	Ligustici Rhizoma Et Radix	3691-11-0	94275	FALSE	C1CC(=C2C(CC1C(=C)C)C(CC2)C)C
MOL002526	0.8478	0.1522	0.7174	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	3691-11-0	94275	FALSE	C1CC(=C2C(CC1C(=C)C)C(CC2)C)C
MOL002526	0.8478	0.1522	0.7174	Codonopsis Radix	3691-11-0	94275	FALSE	C1CC(=C2C(CC1C(=C)C)C(CC2)C)C
MOL002526	0.8478	0.1522	0.7174	Linderae Radix	3691-11-0	94275	FALSE	C1CC(=C2C(CC1C(=C)C)C(CC2)C)C
MOL002526	0.8478	0.1522	0.7174	Alpiniae Officinarum Rhizome	3691-11-0	94275	FALSE	C1CC(=C2C(CC1C(=C)C)C(CC2)C)C
MOL002526	0.8478	0.1522	0.7174	Pogostemon Cablin (Blanco) Benth.	3691-11-0	94275	FALSE	C1CC(=C2C(CC1C(=C)C)C(CC2)C)C
MOL002526	0.8478	0.1522	0.7174	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	3691-11-0	94275	FALSE	C1CC(=C2C(CC1C(=C)C)C(CC2)C)C
MOL002526	0.8478	0.1522	0.7174	Evodiae Fructus	3691-11-0	94275	FALSE	C1CC(=C2C(CC1C(=C)C)C(CC2)C)C
MOL002526	0.8478	0.1522	0.7174	Echinopsis Radix	3691-11-0	94275	FALSE	C1CC(=C2C(CC1C(=C)C)C(CC2)C)C
MOL002526	0.8478	0.1522	0.7174	Cinnanmomi Cortex	3691-11-0	94275	FALSE	C1CC(=C2C(CC1C(=C)C)C(CC2)C)C
MOL002526	0.8478	0.1522	0.7174	Panax Ginseng C. A. Mey.	3691-11-0	94275	FALSE	C1CC(=C2C(CC1C(=C)C)C(CC2)C)C
MOL002527	0.5470	0.4530	0.7508	Alpiniae Officinarum Rhizome	1,2-Dihydrocurcumin	5372374	FALSE	O(c1cc(CCC(=O)/C=C(\O)/C=C/c2cc(OC)c(O)cc2)ccc1O)C
MOL002527	0.5470	0.4530	0.7508	Curcumae Radix	1,2-Dihydrocurcumin	5372374	FALSE	O(c1cc(CCC(=O)/C=C(\O)/C=C/c2cc(OC)c(O)cc2)ccc1O)C
MOL002528	0.9332	0.0668	0.9132	Alpiniae Officinarum Rhizome	2,5-Dibutylfuran	586437	FALSE	o1c(ccc1CCCC)CCCC
MOL002529	0.8976	0.1024	0.8722	Alpiniae Officinarum Rhizome	Geranyl butyrate	5355856	FALSE	C(=C\COC(=O)CCC)(/CCC=C(C)C)\C
MOL002530	0.9518	0.0482	0.9350	Ephedra Herba	Isobutyl benzoate	61048	FALSE	c1(C(=O)OCC(C)C)ccccc1
MOL002530	0.9518	0.0482	0.9350	Alpiniae Officinarum Rhizome	Isobutyl benzoate	61048	FALSE	c1(C(=O)OCC(C)C)ccccc1
MOL002531	0.8989	0.1011	0.9103	Alpiniae Officinarum Rhizome	Phenethyl isobutyrate	7655	FALSE	c1(CCOC(=O)C(C)C)ccccc1
MOL002532	0.9204	0.0796	0.8808	Alpiniae Officinarum Rhizome	khusilic acid	Not Available	FALSE	C1=C(CCC2C(=C)CCC(C12)C=C)C(=O)O

MOL002533	0.7275	0.2725	0.7729	Alpiniae Officinarum Rhizome	2-(Acetoxymethyl)-3-(methoxycarbonyl)biphenylene	610255	FALSE	c1c(c(cc2c3ccccc3c12)C(=O)OC)COC(=O)C
MOL002534	0.8477	0.1523	0.6782	Evodiae Fructus	1,6-dimethyl-4-isopropyl-1,2,3,4,4a,7-hexahydronaphthalene	Not Available	FALSE	C1(CCC(C2C=C(CC=C12)C)C(C)C)C
MOL002534	0.8477	0.1523	0.6782	Ailanthi Cortex	1,6-dimethyl-4-isopropyl-1,2,3,4,4a,7-hexahydronaphthalene	Not Available	FALSE	C1(CCC(C2C=C(CC=C12)C)C(C)C)C
MOL002534	0.8477	0.1523	0.6782	Cornus Officinalis Sieb. Et Zucc.	1,6-dimethyl-4-isopropyl-1,2,3,4,4a,7-hexahydronaphthalene	Not Available	FALSE	C1(CCC(C2C=C(CC=C12)C)C(C)C)C
MOL002534	0.8477	0.1523	0.6782	Rhododendri Daurici Folium	1,6-dimethyl-4-isopropyl-1,2,3,4,4a,7-hexahydronaphthalene	Not Available	FALSE	C1(CCC(C2C=C(CC=C12)C)C(C)C)C
MOL002534	0.8477	0.1523	0.6782	Alpiniae Officinarum Rhizome	1,6-dimethyl-4-isopropyl-1,2,3,4,4a,7-hexahydronaphthalene	Not Available	FALSE	C1(CCC(C2C=C(CC=C12)C)C(C)C)C
MOL002535	0.5862	0.4138	0.7215	Alpiniae Officinarum Rhizome	(3R,5R)-1,7-bis(4-hydroxy-3-methoxyphenyl)heptane-3,5-diol	10883331	FALSE	OC(CC(O)CCc1cc(OC)c(O)cc1)CCc1cc(OC)c(O)cc1
MOL002535	0.5862	0.4138	0.7215	Curcumae Radix	(3R,5R)-1,7-bis(4-hydroxy-3-methoxyphenyl)heptane-3,5-diol	10883331	FALSE	OC(CC(O)CCc1cc(OC)c(O)cc1)CCc1cc(OC)c(O)cc1

MOL002536	0.8366	0.1634	0.8516	Alpiniae Officinarum Rhizome	Phenethyl octanoate	229888	FALSE	c1(CCOC(=O)CCCCCCC)ccccc1
MOL002537	0.9516	0.0484	0.9559	Alpiniae Officinarum Rhizome	trans-p-mentha-1(7),8-diene	68140	FALSE	C1(=C)CCC(CC1)C(=C)C
MOL002538	0.9380	0.0620	0.9530	Rhododendri Daurici Folium	Benzylacetone	17355	FALSE	c1(CCC(=O)C)ccccc1
MOL002538	0.9380	0.0620	0.9530	Linderae Radix	Benzylacetone	17355	FALSE	c1(CCC(=O)C)ccccc1
MOL002538	0.9380	0.0620	0.9530	Alpiniae Officinarum Rhizome	Benzylacetone	17355	FALSE	c1(CCC(=O)C)ccccc1
MOL002538	0.9380	0.0620	0.9530	Gossampiniflos	Benzylacetone	17355	FALSE	c1(CCC(=O)C)ccccc1
MOL002539	0.9329	0.0671	0.9574	Benzoinum	Phlorol	6997	FALSE	c1(c(cccc1)O)CC
MOL002539	0.9329	0.0671	0.9574	Alpiniae Officinarum Rhizome	Phlorol	6997	FALSE	c1(c(cccc1)O)CC
MOL002539	0.9329	0.0671	0.9574	Styrax	Phlorol	6997	FALSE	c1(c(cccc1)O)CC
MOL002540	0.9296	0.0704	0.9483	Alpiniae Officinarum Rhizome	2-octen-4-ol	Not Available	FALSE	C(CCCC)(/C=C/C)O
MOL002541	0.9141	0.0859	0.9373	Benzoinum	WLN: VH2R	7707	FALSE	c1(ccccc1)CCC=O
MOL002541	0.9141	0.0859	0.9373	Cinnamomi Ramulus	WLN: VH2R	7707	FALSE	c1(ccccc1)CCC=O
MOL002541	0.9141	0.0859	0.9373	Cinnanmomi Cortex	WLN: VH2R	7707	FALSE	c1(ccccc1)CCC=O
MOL002541	0.9141	0.0859	0.9373	Styrax	WLN: VH2R	7707	FALSE	c1(ccccc1)CCC=O
MOL002541	0.9141	0.0859	0.9373	Alpiniae Officinarum Rhizome	WLN: VH2R	7707	FALSE	c1(ccccc1)CCC=O
MOL002541	0.9141	0.0859	0.9373	Saussureae Involucratae Herba	WLN: VH2R	7707	FALSE	c1(ccccc1)CCC=O
MOL002542	0.9312	0.0688	0.9657	Alpiniae Officinarum Rhizome	Pentanone	7895	FALSE	C(C(=O)C)CC
MOL002542	0.9312	0.0688	0.9657	Ginkgo Folium	Pentanone	7895	FALSE	C(C(=O)C)CC
MOL002543	0.6626	0.3374	0.8223	Alpiniae Officinarum Rhizome	(2S,3R)-2-(3,4-dimethoxyphenyl)-5,7-dimethoxychroman-3-ol	6576809	FALSE	C1(C(Cc2c(O1)cc(cc2OC)OC)O)c1cc(c(cc1)OC)OC
MOL002544	0.5781	0.4219	0.7140	Alpiniae Officinarum Rhizome	1,7-diphenyl-5-hydroxy-3-heptanone	46213118	FALSE	C(CC(=O)CC(CCc1ccccc1)O)c1ccccc1
MOL002545	0.9394	0.0606	0.9521	Alpiniae Officinarum Rhizome	Phenethyl isovalerate	8792	FALSE	c1(CCOC(=O)CC(C)C)ccccc1
MOL002546	0.9309	0.0691	0.9646	Alpiniae Officinarum Rhizome	ZINC02031653	6999724	FALSE	C(C(C)O)C=C

MOL002547	0.9546	0.0454	0.7471	licorice	21987_FLUKA	16211586	FALSE	C12C(C1(C)C)CC(C=C2)C
MOL002547	0.9546	0.0454	0.7471	Alpiniae Officinarum Rhizome	21987_FLUKA	16211586	FALSE	C12C(C1(C)C)CC(C=C2)C
MOL002547	0.9546	0.0454	0.7471	Moslae Herba	21987_FLUKA	16211586	FALSE	C12C(C1(C)C)CC(C=C2)C
MOL002547	0.9546	0.0454	0.7471	Piperis Fructus	21987_FLUKA	16211586	FALSE	C12C(C1(C)C)CC(C=C2)C
MOL002547	0.9546	0.0454	0.7471	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	21987_FLUKA	16211586	FALSE	C12C(C1(C)C)CC(C=C2)C
MOL002548	0.9244	0.0756	0.9531	Alpiniae Officinarum Rhizome	Acetyl isobutyryl	24115	FALSE	C(=O)(C(C)C)C(=O)C
MOL002550	0.5148	0.4852	0.7281	Alpiniae Officinarum Rhizome	(5R)-5-hydroxy-7-(4-hydroxy-3-methoxyphenyl)-1-phenylheptan-3-one	155165	FALSE	C(CC(=O)CC(CCc1cc(c(cc1)O)OC)O)c1ccccc1
MOL002551	0.5363	0.4637	0.7674	Alpiniae Officinarum Rhizome	5-Methoxy-7-(4'-hydroxyphenyl)-1-phenyl-3-heptanone	Not Available	FALSE	c1cccc(c1)CCC(=O)CC(CCc1ccc(cc1)O)OC
MOL002552	0.8719	0.1281	0.7606	Alpiniae Officinarum Rhizome	8-Hydroxybergapten	3083726	FALSE	c1(=O)ccc2c(o1)c(c1c(c2OC)cco1)O
MOL002552	0.8719	0.1281	0.7606	A. Dahurica (Fisch.) Benth. Et Hook	8-Hydroxybergapten	3083726	FALSE	c1(=O)ccc2c(o1)c(c1c(c2OC)cco1)O
MOL002553	0.6453	0.3547	0.6316	Alpiniae Officinarum Rhizome	(5R)-5-hydroxy-7-(4-hydroxyphenyl)-1-phenylheptan-3-one	10086048	FALSE	C(CC(=O)CC(CCc1ccc(cc1)O)O)c1ccccc1
MOL002554	0.5007	0.4993	0.7793	Alpiniae Officinarum Rhizome	5-methoxy-1,7-diphenyl-3-heptanone	26437441	FALSE	C(CC(=O)CC(CCc1ccccc1)OC)c1ccccc1

MOL002555	0.9473	0.0527	0.7748	Alpiniae Officinarum Rhizome	7-Hydroxy-2-(2-hydroxy)propyl-5-methyl-benzopyran-gamma-one	Not Available	FALSE	c1c(c2c(cc1O)oc(cc2=O)CC(C)O)C
MOL002556	0.7662	0.2338	0.7921	Alpiniae Officinarum Rhizome	7-Methoxy-8-(2'-ethoxy-3'-hydroxy-3'-methybutyl)coumarin	Not Available	FALSE	c1c(c(c2c(c1)ccc(=O)o2)CC(C(C)(O)C)OCC)OC
MOL002557	0.9292	0.0708	0.9568	Alpiniae Officinarum Rhizome	1,2-dimethylcycloheptene	519742	FALSE	C1(=C(CCCCC1)C)C
MOL002558	0.9383	0.0617	0.8429	Calendula Officinalis	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Citri Exocarpium Rubrum	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Mori Cortex	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Flos Genkwa	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Herbahypericiperforati	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Alpiniae Officinarum Rhizome	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Radix Angelicae Biseratae	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Actinidia Chinensis Planch	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	A. Dahurica (Fisch.) Benth. Et Hook	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Wikstroemiae Indicae Rasix	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Citri Grandis Exocarpium	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Folium Artemisiae Argyi	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Eucommiae Cortex	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Dichroae Radix	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Foeniculi Fructus	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Euphorbiae Humifusae Herba	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Peucedanidecursivi Radix	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Prunellae Spica	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Rhododendri Daurici Folium	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Bombyx Mori L.	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Radix Euphorbiae Pekinensis	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Coriandri Sativi Herba	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Zanthoxyli Pericarpium	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2

MOL002558	0.9383	0.0617	0.8429	Siphonostegiae Herba	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002558	0.9383	0.0617	0.8429	Peucedani Radix	Skimmetin	5281426	TRUE	c12c(cc(cc1)O)oc(=O)cc2
MOL002559	0.9194	0.0806	0.8004	Alpiniae Officinarum Rhizome	9-ethoxy-10-oxatricyclo[7.2.1.0(1,6)]dodecan-11-one	Not Available	FALSE	C123CCCCC1CCC(OC2=O)(C3)OCC
MOL002560	0.9247	0.0753	0.9430	Alpiniae Oxyphyliae Fructus	chrysin	5281607	TRUE	c12c(oc(cc1=O)c1ccccc1)cc(cc2O)O
MOL002560	0.9247	0.0753	0.9430	Oroxyli Semen	chrysin	5281607	TRUE	c12c(oc(cc1=O)c1ccccc1)cc(cc2O)O
MOL002560	0.9247	0.0753	0.9430	Alpiniae Officinarum Rhizome	chrysin	5281607	TRUE	c12c(oc(cc1=O)c1ccccc1)cc(cc2O)O
MOL002560	0.9247	0.0753	0.9430	Phellodendri Amurensis Cortex	chrysin	5281607	TRUE	c12c(oc(cc1=O)c1ccccc1)cc(cc2O)O
MOL002560	0.9247	0.0753	0.9430	Scutellariae Radix	chrysin	5281607	TRUE	c12c(oc(cc1=O)c1ccccc1)cc(cc2O)O
MOL002560	0.9247	0.0753	0.9430	Cassiae Semen	chrysin	5281607	TRUE	c12c(oc(cc1=O)c1ccccc1)cc(cc2O)O
MOL002561	0.8392	0.1608	0.8490	Alpiniae Officinarum Rhizome	(2S,3R)-2,3-dihydroxy-1,3-di(phenyl)propan-1-one	11413813	FALSE	c1cccc(c1)C(C(O)C(=O)c1ccccc1)O
MOL002562	0.6209	0.3791	0.7712	Alpiniae Officinarum Rhizome	(R)-N-Methylcoclaurine	440595	FALSE	c1cc(ccc1O)CC1N(CCc2c1cc(c(c2)OC)O)C
MOL002562	0.6209	0.3791	0.7712	Folium Nelumbinis	(R)-N-Methylcoclaurine	440595	FALSE	c1cc(ccc1O)CC1N(CCc2c1cc(c(c2)OC)O)C
MOL002563	0.9351	0.0649	0.9259	Alpiniae Officinarum Rhizome	galangin	5281616	TRUE	c12c(oc(c(c1=O)O)c1ccccc1)cc(cc2O)O
MOL002563	0.9351	0.0649	0.9259	Asteris Radix Et Rhizoma	galangin	5281616	TRUE	c12c(oc(c(c1=O)O)c1ccccc1)cc(cc2O)O
MOL002564	0.2204	0.7796	0.6450	Alpiniae Officinarum Rhizome	(3Z)-3-[2-[(1R,2S,4aS,8aS)-5,5,8a-trimethylspiro[decalin-2,2'-oxirane]-1-yl]ethylidene]tetrahydrofuran-2-one	10064490	FALSE	C1CC(C2C(C1)(C(C1(CC2)OC1)C/C=C\1/CCOC1=O)C)(C)C
MOL002565	0.8402	0.1598	0.7410	Alpiniae Officinarum Rhizome	Medicarpin	336327	FALSE	c1cc2c(cc1O)OCC1C2Oc2c1ccc(c2)OC
MOL002565	0.8402	0.1598	0.7410	Dalbergiae Odoriferae Lignum	Medicarpin	336327	FALSE	c1cc2c(cc1O)OCC1C2Oc2c1ccc(c2)OC
MOL002565	0.8402	0.1598	0.7410	licorice	Medicarpin	336327	FALSE	c1cc2c(cc1O)OCC1C2Oc2c1ccc(c2)OC

MOL002566	0.8986	0.1014	0.9053	Artemisia Annua L.	3-O-Methylquercetin	5280681	FALSE	c1(c(OC)c(=O)c2c(O)cc(O)cc2o1)c1cc(O)c(O)cc1
MOL002566	0.8986	0.1014	0.9053	Lonicerae Japonicae Flos	3-O-Methylquercetin	5280681	FALSE	c1(c(OC)c(=O)c2c(O)cc(O)cc2o1)c1cc(O)c(O)cc1
MOL002566	0.8986	0.1014	0.9053	Alpiniae Officinarum Rhizome	3-O-Methylquercetin	5280681	FALSE	c1(c(OC)c(=O)c2c(O)cc(O)cc2o1)c1cc(O)c(O)cc1
MOL002566	0.8986	0.1014	0.9053	Centipedae Herba	3-O-Methylquercetin	5280681	FALSE	c1(c(OC)c(=O)c2c(O)cc(O)cc2o1)c1cc(O)c(O)cc1
MOL002566	0.8986	0.1014	0.9053	Capsellae Herba	3-O-Methylquercetin	5280681	FALSE	c1(c(OC)c(=O)c2c(O)cc(O)cc2o1)c1cc(O)c(O)cc1
MOL002567	0.9229	0.0771	0.9473	Alpiniae Officinarum Rhizome	AllOAc	11584	FALSE	O(C(=O)C)CC=C
MOL002568	0.4965	0.5035	0.7488	Alpiniae Officinarum Rhizome	DAH-3-Keto-4-en	5316932	FALSE	O=C(CCc1ccccc1)/C=C/CCc1ccccc1
MOL002569	0.9600	0.0400	0.9503	Alpiniae Officinarum Rhizome	p-Ethylphenetole	74107	FALSE	c1(ccc(cc1)CC)OCC
MOL002570	0.9443	0.0557	0.8288	Alpiniae Officinarum Rhizome	cyclobutylbenzene	138219	FALSE	c1(ccccc1)C1CCC1
MOL002571	0.9323	0.0677	0.9188	Alpiniae Officinarum Rhizome	[(2R)-pentan-2-yl]benzene	11744785	FALSE	c1(C(CCC)C)ccccc1
MOL002572	0.9258	0.0742	0.9697	Alpiniae Officinarum Rhizome	1-hydroxypentan-2-one	522131	FALSE	C(C(=O)CCC)O
MOL002574	0.9292	0.0708	0.9562	Alpiniae Officinarum Rhizome	VINYLBUTYRATE	31247	FALSE	C(=O)(CCC)OC=C
MOL002575	0.3687	0.6313	0.8994	Alpiniae Officinarum Rhizome	butyl-2-ethylhexyl phthalate	Not Available	FALSE	c1(c(cccc1)C(=O)OCCCC)C(=O)OC(CCCCC)CC
MOL002576	0.8990	0.1010	0.8990	Bomboo Juice	GBL	7302	FALSE	C1(=O)CCCO1
MOL002576	0.8990	0.1010	0.8990	Ephedra Herba	GBL	7302	FALSE	C1(=O)CCCO1
MOL002576	0.8990	0.1010	0.8990	Alpiniae Officinarum Rhizome	GBL	7302	FALSE	C1(=O)CCCO1
MOL002576	0.8990	0.1010	0.8990	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	GBL	7302	FALSE	C1(=O)CCCO1
MOL002577	0.9451	0.0549	0.7641	Alpiniae Officinarum Rhizome	1-Naphthylmethanol	20908	FALSE	c12c(cccc1CO)cccc2

MOL002579	0.8208	0.1792	0.7781	Alpiniae Officinarum Rhizome	capsaicin	1548943	FALSE	c1(cc(c(cc1)O)OC)CNC(=O)CCCC/C=C/C(C)C
MOL002579	0.8208	0.1792	0.7781	Capsici Fructus	capsaicin	1548943	FALSE	c1(cc(c(cc1)O)OC)CNC(=O)CCCC/C=C/C(C)C
MOL002579	0.8208	0.1792	0.7781	Ginkgo Semen	capsaicin	1548943	FALSE	c1(cc(c(cc1)O)OC)CNC(=O)CCCC/C=C/C(C)C
MOL002579	0.8208	0.1792	0.7781	Codonopsis Radix	capsaicin	1548943	FALSE	c1(cc(c(cc1)O)OC)CNC(=O)CCCC/C=C/C(C)C
MOL002579	0.8208	0.1792	0.7781	Radix Bupleuri	capsaicin	1548943	FALSE	c1(cc(c(cc1)O)OC)CNC(=O)CCCC/C=C/C(C)C
MOL002579	0.8208	0.1792	0.7781	Panacis Quinquefolii Radix	capsaicin	1548943	FALSE	c1(cc(c(cc1)O)OC)CNC(=O)CCCC/C=C/C(C)C
MOL002580	0.2044	0.7956	0.6592	Scutellariae Barbatae Herba	cholesta-6,22,24-trien,4,4-dimethyl	Not Available	FALSE	C1CCC2(C(C1(C)C)C=CC1C3CCC(C(/C=C/C=C(C)C)C)C3(C)CCC21)C
MOL002580	0.2044	0.7956	0.6592	Alpiniae Officinarum Rhizome	cholesta-6,22,24-trien,4,4-dimethyl	Not Available	FALSE	C1CCC2(C(C1(C)C)C=CC1C3CCC(C(/C=C/C=C(C)C)C)C3(C)CCC21)C
MOL002581	0.5271	0.4729	0.7282	Curcumae Radix	curcumin	24884282	FALSE	c1(cc(c(cc1)O)OC)/C=C/C(=O)CC(=O)/C=C\c1cc(c(cc1)O)OC
MOL002581	0.5271	0.4729	0.7282	Alpiniae Officinarum Rhizome	curcumin	24884282	FALSE	c1(cc(c(cc1)O)OC)/C=C/C(=O)CC(=O)/C=C\c1cc(c(cc1)O)OC
MOL002581	0.5271	0.4729	0.7282	Momordicae Fructus	curcumin	24884282	FALSE	c1(cc(c(cc1)O)OC)/C=C/C(=O)CC(=O)/C=C\c1cc(c(cc1)O)OC
MOL002582	0.1535	0.8465	0.6928	Kansui Radix	20-O-(2,3-dimethylbutanoyl)-13-O-dodecanoylingenol	Not Available	FALSE	C1(=CC23C(C1O)(C(C(=CC(C2=O)C1C(CC3C)(C1(C)C)OC(=O)CCCCCCCCCCC)COC(=O)C(C)C(C)C)O)O)C
MOL002583	0.1772	0.8228	0.6909	Kansui Radix	3-O-Benzoyl-20-deoxyingenol	Not Available	FALSE	C1(=CC23C(C1OC(=O)c1ccccc1)(C(C(=CC(C2=O)C1C(CC3C)C1(C)C)C)O)O)C
MOL002584	0.1923	0.8077	0.7305	Kansui Radix	3-O-benzoyl-13-O-dodecanoylingenol	Not Available	FALSE	C1(=CC23C(C1OC(=O)c1ccccc1)(C(C(=CC(C2=O)C1C(CC3C)(C1(C)C)OC(=O)CCCCCCCCCCC)CO)O)O)C
MOL002585	0.1765	0.8235	0.6832	Kansui Radix	5-O-Benzoyl-20-deoxyingenol	Not Available	FALSE	C1(=CC23C(C1O)(C(C(=CC(C2=O)C1C(CC3C)C1(C)C)C)OC(=O)c1ccccc1)O)C
MOL002586	0.9515	0.0485	0.8576	Kansui Radix	[(1S,2R,5S,6R)-6-methyl-2-methylol-norpinan-6-yl]methanol	21631096	FALSE	C1C(C2C(C(C1)C2)(CO)C)CO
MOL002587	0.8418	0.1582	0.7713	Kansui Radix	Euphorbetin	5317297	FALSE	c1(c(c(c2c(c1)oc(=O)cc2)c1c2c(cc(c1O)O)oc(=O)cc2)O)O

MOL002587	0.8418	0.1582	0.7713	Semen Aesculi	Euphorbetin	5317297	FALSE	c1(c(c(c2c(c1)oc(=O)cc2)c1c2c(cc(c1O)O)oc(=O)cc2)O)O
MOL002587	0.8418	0.1582	0.7713	Semen Euphorbiae	Euphorbetin	5317297	FALSE	c1(c(c(c2c(c1)oc(=O)cc2)c1c2c(cc(c1O)O)oc(=O)cc2)O)O
MOL002588	0.2510	0.7490	0.6702	Kansui Radix	(3S,5R,10S,13R,14R,17R)-17-[(1R)-1,5-dimethyl-4-methylenehexyl]-4,4,10,13,14-pentamethyl-2,3,5,6,7,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-3-ol	9803310	FALSE	OC1C(C2C(C3=C(C4(C(C(CC4)C(CCC(=C)C(C)C)C)(CC3)C)C)CC2)(CC1)C)(C)C
MOL002588	0.2510	0.7490	0.6702	Hippophae Fructus	(3S,5R,10S,13R,14R,17R)-17-[(1R)-1,5-dimethyl-4-methylenehexyl]-4,4,10,13,14-pentamethyl-2,3,5,6,7,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-3-ol	9803310	FALSE	OC1C(C2C(C3=C(C4(C(C(CC4)C(CCC(=C)C(C)C)C)(CC3)C)C)CC2)(CC1)C)(C)C
MOL002590	0.7750	0.2250	0.8372	Kansui Radix	Karacolidine	Not Available	FALSE	C1CC2(C3C4(C1O)C1(C5C(C(C3)C4N(CC)C2)(CC(C(C1)C5O)OC)O)O)C
MOL002591	0.2057	0.7943	0.7275	Kansui Radix	20-O-Benzoyl-13-O-dodeeanoyl ingenol	Not Available	FALSE	C1(=CC23C(C1O)(C(C(=CC(C2=O)C1C(CC3C)(C1(C)C)OC(=O)CCCCCCCCCCC)COC(=O)c1ccccc1)O)O)C

MOL002592	0.6776	0.3224	0.6908	Kansui Radix	(1S,4aS,10aR)-7-isopropyl-1,4a-dimethyl-5,8-dioxo-2,3,4,9,10,10a-hexahydrophenanthrene-1-carboxylic acid	10381980	FALSE	OC(=O)C1(C2C(CCC1)(C1=C(CC2)C(=O)C(=CC1=O)C(C)C)C)C
MOL002593	0.0682	0.9318	0.8351	Kansui Radix	kansuinin A	Not Available	FALSE	O1C2(O)C3(OC(=O)C)C(C(OC(=O)C)C(C3)C)C(OC(=O)C)C(=C)C(OC(=O)C)C(OC(=O)c3ccccc3)C(OC(=O)C)C(C1C(=O)C2C)(C)C
MOL002596	0.2068	0.7932	0.7271	Kansui Radix	NSC 403164	101257	FALSE	OC1C(C2C(C3=C(C4(C(C(CC4)C(CCC=C(C)C)C)(CC3)C)C)CC2)(CC1)C)(C)C
MOL002596	0.2068	0.7932	0.7271	Radix Euphorbiae Pekinensis	NSC 403164	101257	FALSE	OC1C(C2C(C3=C(C4(C(C(CC4)C(CCC=C(C)C)C)(CC3)C)C)CC2)(CC1)C)(C)C
MOL002596	0.2068	0.7932	0.7271	Omphalia	NSC 403164	101257	FALSE	OC1C(C2C(C3=C(C4(C(C(CC4)C(CCC=C(C)C)C)(CC3)C)C)CC2)(CC1)C)(C)C
MOL002597	0.2068	0.7932	0.7271	Radix Euphorbiae Pekinensis	Euphol	441678	FALSE	OC1C(C2C(C3=C(C4(C(C(CC4)C(CCC=C(C)C)C)(CC3)C)C)CC2)(CC1)C)(C)C
MOL002597	0.2068	0.7932	0.7271	Semen Euphorbiae	Euphol	441678	FALSE	OC1C(C2C(C3=C(C4(C(C(CC4)C(CCC=C(C)C)C)(CC3)C)C)CC2)(CC1)C)(C)C
MOL002597	0.2068	0.7932	0.7271	Kansui Radix	Euphol	441678	FALSE	OC1C(C2C(C3=C(C4(C(C(CC4)C(CCC=C(C)C)C)(CC3)C)C)CC2)(CC1)C)(C)C
MOL002597	0.2068	0.7932	0.7271	Lunulatae Herba	Euphol	441678	FALSE	OC1C(C2C(C3=C(C4(C(C(CC4)C(CCC=C(C)C)C)(CC3)C)C)CC2)(CC1)C)(C)C
MOL002598	0.1906	0.8094	0.7410	Kansui Radix	20-OD-ingenol Z	Not Available	FALSE	C1(=CC23C(C1O)(C(C(=CC(C2=O)C1C(CC3C)C1(C)C)COC(=O)/C=C/C=C\CCCCC)O)O)C
MOL002599	0.2411	0.7589	0.6831	Kansui Radix	Kanziol	Not Available	FALSE	C1C(C(C2C(C1)(C1=C(CC2)C2(C(CC1)(C(CC2)(C(CCC=C(C)C)C)C)C)C)(C)C)O
MOL002600	0.7554	0.2446	0.7321	Kansui Radix	Glycerite	Not Available	FALSE	c1(cc(cc(c1O)O)C(=O)Cc1cc(cc(c1O)O)C(=O)OCC1C(C(C(C(O1)OC(=O)c1cc(c(c(c1)OC(=O)c1cc(c(c(c1)O)O)O)O)O)O)OC(=O)c1cc(c(c(c1)OC(=O)c1cc(c(c(c1)O)O)O)O)O)OC(=O)c1cc(c(c(c1)OC(=O)c1cc(c(c(c1)O)O)O)O)O)OC(=O)c1cc(c(c(c1)OC(=O)c1cc(c(c(c1)O)O)O)O)O
MOL002601	0.1324	0.8676	0.7244	Kansui Radix	3-O-(2,3-Dimethylbutanoyl)-13-O-decanoyl ingenol	Not Available	FALSE	C1(=CC23C(C1OC(=O)C(C)C(C)C)(C(C(=CC(C2=O)C1C(CC3C)(C1(C)C)OC(=O)CCCCCCCCC)CO)O)O)C

MOL002602	0.1754	0.8246	0.6863	Kansui Radix	3-O-(2,3-Dimethylbutanoyl)-13-O-dodecanoyl-20-O-acetylingenol	Not Available	FALSE	C1(=CC23C(C1OC(=O)C(C)C(C)C)(C(C(=CC(C2=O)C1C(CC3C)(C1(C)C)OC(=O)CCCCCCCCCCC)COC(=O)C)O)O)C
MOL002603	0.1313	0.8687	0.6934	Kansui Radix	3-O-(2,3-Dimethylbutanoyl)-13-O-dodecanoyl-20-deoxyingenol	Not Available	FALSE	C1(=CC23C(C1OC(=O)C(C)C(C)C)(C(C(=CC(C2=O)C1C(CC3C)(C1(C)C)OC(=O)CCCCCCCCCCC)C)O)O)C
MOL002604	0.1415	0.8585	0.7123	Kansui Radix	3-O-(2,3-dimethyl-butanoyl)-13-dodecanoylingenol	Not Available	FALSE	C1(=CC23C(C1OC(=O)C(C)C(C)C)(C(C(=CC(C2=O)C1C(CC3C)(C1(C)C)OC(=O)CCCCCCCCCCC)CO)O)O)C
MOL002605	0.4113	0.5887	0.6305	Fortunes Bossfern Rhizome	11-Hydroxynumantenine	Not Available	FALSE	c1c(cc2c(c1)C1(C(=O)N2OC)C2CC3/C(=C/C)/CN(C(C3CO2)C1)C)O
MOL002606	0.4099	0.5901	0.6955	Fortunes Bossfern Rhizome	Hopene	92155	FALSE	C1CC(C2C(C1)(C1C(CC2)(C2(C(CC1)C1(C(CC2)C(CC1)C(=C)C)C)C)C)C)(C)C
MOL002606	0.4099	0.5901	0.6955	Pyrrosiae Folium	Hopene	92155	FALSE	C1CC(C2C(C1)(C1C(CC2)(C2(C(CC1)C1(C(CC2)C(CC1)C(=C)C)C)C)C)C)(C)C
MOL002606	0.4099	0.5901	0.6955	Prinsepiae Nux	Hopene	92155	FALSE	C1CC(C2C(C1)(C1C(CC2)(C2(C(CC1)C1(C(CC2)C(CC1)C(=C)C)C)C)C)C)(C)C
MOL002606	0.4099	0.5901	0.6955	Drynariae Rhizoma	Hopene	92155	FALSE	C1CC(C2C(C1)(C1C(CC2)(C2(C(CC1)C1(C(CC2)C(CC1)C(=C)C)C)C)C)C)(C)C
MOL002608	0.9468	0.0532	0.8508	Fortunes Bossfern Rhizome	Aspidinol	122841	FALSE	c1c(c(c(c(c1OC)C)O)C(=O)CCC)O
MOL002608	0.9468	0.0532	0.8508	Cassiae Semen	Aspidinol	122841	FALSE	c1c(c(c(c(c1OC)C)O)C(=O)CCC)O
MOL002609	0.0935	0.9065	0.8712	Fortunes Bossfern Rhizome	Harmonyl	8550	FALSE	c12c(C3N(CC1)CC1C(C3)C(C(C(C1)OC(=O)c1cc(c(c(c1)OC)OC)OC)OC)C(=O)OC)[nH]c1c2cccc1
MOL002610	0.8533	0.1467	0.7552	Fortunes Bossfern Rhizome	ZINC00035529	673467	FALSE	c1ccc2c(c1)c(c1c(n2)OC(C1)C(C)(CO)O)OC
MOL002611	0.9039	0.0961	0.9671	Fortunes Bossfern Rhizome	filicinic acid	550690	FALSE	C1(=CC(=O)C=C(C1(C)C)O)O
MOL002614	0.8698	0.1302	0.7984	Fortunes Bossfern Rhizome	Flavidin	Not Available	FALSE	c12cc(cc3c1c1c(CC2)cc(cc1CO3)O)O
MOL002615	0.3764	0.6236	0.6572	Pyrrosiae Folium	Neohop-13(18)ene solution	12310619	FALSE	C1CC(C2C(C1)(C1C(CC2)(C2(C(=C3C(CC2)(C(CC3)C(C)C)C)CC1)C)C)C)(C)C

MOL002615	0.3764	0.6236	0.6572	Fortunes Bossfern Rhizome	Neohop-13(18)ene solution	12310619	FALSE	C1CC(C2C(C1)(C1C(CC2)(C2(C(=C3C(CC2)(C(CC3)C(C)C)C)CC1)C)C)C)(C)C
MOL002617	0.4094	0.5906	0.7278	Drynariae Rhizoma	Diplopterol	164874	FALSE	C1CC(C2C(C1)(C1C(CC2)(C2(C(CC1)C1(C(CC2)C(CC1)C(O)(C)C)C)C)C)C)(C)C
MOL002617	0.4094	0.5906	0.7278	Fortunes Bossfern Rhizome	Diplopterol	164874	FALSE	C1CC(C2C(C1)(C1C(CC2)(C2(C(CC1)C1(C(CC2)C(CC1)C(O)(C)C)C)C)C)C)(C)C
MOL002620	0.4622	0.5378	0.6340	Fortunes Bossfern Rhizome	Dryocrassin	3082025	FALSE	C1(=C(C(=C(C(=O)C1(C)C)C(=O)C)O)Cc1c(c(c(c(c1O)Cc1c(c(c(c(c1O)C(=O)CCC)O)CC1=C(C(C(=O)C(=C1O)C(=O)C)(C)C)O)O)O)C(=O)CCC)O)O
MOL002624	0.7823	0.2177	0.8107	Fortunes Bossfern Rhizome	Paradol	94378	FALSE	c1(c(ccc(c1)CCC(=O)CCCCCCC)O)OC
MOL002625	0.8468	0.1532	0.8032	Fortunes Bossfern Rhizome	Kaempfe-rol-3,7-dirhamnoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)C)OC1C(O)C(O)C(O)C(O1)C)c1ccc(O)cc1
MOL002626	0.3590	0.6410	0.7004	Fortunes Bossfern Rhizome	Adlantone	15558363	FALSE	C1CC(C2C(C1)(C1C(CC2)(C2(C(CC1)C1(C(CC2)C(CC1)C(=O)C)C)C)C)C)(C)C
MOL002627	0.4080	0.5920	0.6691	Fortunes Bossfern Rhizome	Filicene	12309888	FALSE	C1C=C(C2(C(C1)C1(C(CC2)C2(C(CC1)(C1C(CC2)(C(CC1)C(C)C)C)C)C)C)C)C
MOL002628	0.9427	0.0573	0.7583	Fortunes Bossfern Rhizome	isopentenyladenosine	40532341	FALSE	c12c(ncnc1NCC=C(C)C)n(cn2)C1OC(C(C1O)O)CO
MOL002629	0.4002	0.5998	0.6645	Fortunes Bossfern Rhizome	7-Fernene	13857703	FALSE	C1CC(C2C(C1)(C1C(=CC2)C2(C(CC1)(C1C(CC2)(C(CC1)C(C)C)C)C)C)C)(C)C
MOL002630	0.4001	0.5999	0.6642	Fortunes Bossfern Rhizome	9-(11)-Fernene	Not Available	FALSE	C1CC(C2C(C1)(C1=CCC3(C(C1CC2)(CCC1(C3CCC1C(C)C)C)C)C)C)(C)C
MOL002631	0.3822	0.6178	0.6651	Fortunes Bossfern Rhizome	9-(11)-Fernene	Not Available	FALSE	C1CC(C2C(C1)(C1=CCC3(C(C1CC2)(C)CCC1C3CCC1C(C)C)C)C)(C)C
MOL002632	0.3590	0.6410	0.7004	Fortunes Bossfern Rhizome	Adiantone	Not Available	FALSE	C1CC(C2C(C1)(C1C(CC2)(C2(C(CC1)C1(C(CC2)C(CC1)C(=O)C)C)C)C)C)(C)C
MOL002635	0.6541	0.3459	0.6802	Phellodendri Chinrnsis Cortex	(±)-lyoniresinol	Not Available	FALSE	C1(C(C(Cc2cc(c(c(c12)OC)O)OC)CO)CO)c1cc(c(c(c1)OC)O)OC
MOL002636	0.1268	0.8732	0.7297	Phellodendri Chinrnsis Cortex	Kihadalactone A	Not Available	FALSE	O(C1C2(C(C3(C(C1)C(OC(=O)CC3OC(=O)C)(C)C)C)CCC1(C2=CCC1c1ccoc1)C)C)C(=O)C
MOL002637	0.6017	0.3983	0.6781	Dictamni Cortex	Obacunoic acid	Not Available	FALSE	c1cc(co1)C1C2(C3(C(C(=O)O1)O3)C1(C(CC2)C(C(CC1=O)C(O)(C)C)(/C=C/C(=O)O)C)C)C
MOL002637	0.6017	0.3983	0.6781	Phellodendri Amurensis Cortex	Obacunoic acid	Not Available	FALSE	c1cc(co1)C1C2(C3(C(C(=O)O1)O3)C1(C(CC2)C(C(CC1=O)C(O)(C)C)(/C=C/C(=O)O)C)C)C
MOL002637	0.6017	0.3983	0.6781	Coptidis Rhizoma	Obacunoic acid	Not Available	FALSE	c1cc(co1)C1C2(C3(C(C(=O)O1)O3)C1(C(CC2)C(C(CC1=O)C(O)(C)C)(/C=C/C(=O)O)C)C)C
MOL002637	0.6017	0.3983	0.6781	Phellodendri Chinrnsis Cortex	Obacunoic acid	Not Available	FALSE	c1cc(co1)C1C2(C3(C(C(=O)O1)O3)C1(C(CC2)C(C(CC1=O)C(O)(C)C)(/C=C/C(=O)O)C)C)C
MOL002637	0.6017	0.3983	0.6781	Evodiae Fructus	Obacunoic acid	Not Available	FALSE	c1cc(co1)C1C2(C3(C(C(=O)O1)O3)C1(C(CC2)C(C(CC1=O)C(O)(C)C)(/C=C/C(=O)O)C)C)C

MOL002639	0.2313	0.7687	0.6768	Phellodendri Chinrnsis Cortex	Obamegine	Not Available	FALSE	C1CN(C2c3c1cc(c(c3Oc1c(OC)cc3c(c1)C(N(CC3)C)Cc1ccc(Oc3c(ccc(C2)c3)O)cc1)O)OC)C
MOL002639	0.2313	0.7687	0.6768	Evodiae Fructus	Obamegine	Not Available	FALSE	C1CN(C2c3c1cc(c(c3Oc1c(OC)cc3c(c1)C(N(CC3)C)Cc1ccc(Oc3c(ccc(C2)c3)O)cc1)O)OC)C
MOL002639	0.2313	0.7687	0.6768	Coptidis Rhizoma	Obamegine	Not Available	FALSE	C1CN(C2c3c1cc(c(c3Oc1c(OC)cc3c(c1)C(N(CC3)C)Cc1ccc(Oc3c(ccc(C2)c3)O)cc1)O)OC)C
MOL002640	0.8058	0.1942	0.7861	Phellodendri Amurensis Cortex	phellavin	Not Available	FALSE	c1(c(cc2c(c1O)C(=O)C(C(O2)c1ccc(cc1)O)O)OC1OC(C(C(C1O)O)O)CO)CCC(O)(C)C
MOL002640	0.8058	0.1942	0.7861	Phellodendri Chinrnsis Cortex	phellavin	Not Available	FALSE	c1(c(cc2c(c1O)C(=O)C(C(O2)c1ccc(cc1)O)O)OC1OC(C(C(C1O)O)O)CO)CCC(O)(C)C
MOL002641	0.7545	0.2455	0.7910	Phellodendri Chinrnsis Cortex	Phellavin_qt	Not Available	FALSE	c1(c(cc2c(c1O)C(=O)C(C(O2)c1ccc(cc1)O)O)O)CCC(O)(C)C
MOL002642	0.5545	0.4455	0.7206	Phellodendri Amurensis Cortex	phellodendrine	3081405	FALSE	c1c(c(cc2c1CC[N+]1(C2Cc2c(C1)cc(c(c2)O)OC)C)O)OC
MOL002642	0.5545	0.4455	0.7206	Phellodendri Chinrnsis Cortex	phellodendrine	3081405	FALSE	c1c(c(cc2c1CC[N+]1(C2Cc2c(C1)cc(c(c2)O)OC)C)O)OC
MOL002643	0.2400	0.7600	0.6133	Phellodendri Chinrnsis Cortex	delta 7-stigmastenol	12315385	FALSE	OC1CC2C(C3C(=CC2)C2C(C(CC2)C(CCC(C(C)C)CC)C)(CC3)C)(CC1)C
MOL002643	0.2400	0.7600	0.6133	Achyranthis Bidentatae Radix	delta 7-stigmastenol	12315385	FALSE	OC1CC2C(C3C(=CC2)C2C(C(CC2)C(CCC(C(C)C)CC)C)(CC3)C)(CC1)C
MOL002644	0.7034	0.2966	0.8354	Phellodendri Chinrnsis Cortex	Phellopterin	98608	FALSE	c12c(c(c3c(c1OC)ccc(=O)o3)OCC=C(C)C)occ2
MOL002644	0.7034	0.2966	0.8354	Saposhnikoviae Radix	Phellopterin	98608	FALSE	c12c(c(c3c(c1OC)ccc(=O)o3)OCC=C(C)C)occ2
MOL002644	0.7034	0.2966	0.8354	Zanthoxylum Nitidum	Phellopterin	98608	FALSE	c12c(c(c3c(c1OC)ccc(=O)o3)OCC=C(C)C)occ2
MOL002644	0.7034	0.2966	0.8354	Peucedani Radix	Phellopterin	98608	FALSE	c12c(c(c3c(c1OC)ccc(=O)o3)OCC=C(C)C)occ2
MOL002645	0.9532	0.0468	0.9492	Phellodendri Chinrnsis Cortex	PEA	1001	TRUE	c1cccc(c1)CCN
MOL002646	0.9335	0.0665	0.9003	Phellodendri Chinrnsis Cortex	Vanilloloside	Not Available	FALSE	OCC1OC(Oc2ccc(CO)cc2OC)C(O)C(O)C1O
MOL002647	0.9189	0.0811	0.9645	Coriolus	Vanillyl alcohol	62348	FALSE	Oc1ccc(CO)cc1OC
MOL002647	0.9189	0.0811	0.9645	Mori Fructus	Vanillyl alcohol	62348	FALSE	Oc1ccc(CO)cc1OC
MOL002647	0.9189	0.0811	0.9645	Phellodendri Chinrnsis Cortex	Vanillyl alcohol	62348	FALSE	Oc1ccc(CO)cc1OC
MOL002647	0.9189	0.0811	0.9645	Phellodendri Amurensis Cortex	Vanillyl alcohol	62348	FALSE	Oc1ccc(CO)cc1OC
MOL002648	0.9626	0.0374	0.8817	Lysimachiae Foenigraeci Herba	(4R)-limonene 1beta,2beta-epoxide	6857487	FALSE	C12(C(O1)CC(CC2)C(=C)C)C

MOL002648	0.9626	0.0374	0.8817	Phellodendri Chinrnsis Cortex	(4R)-limonene 1beta,2beta-epoxide	6857487	FALSE	C12(C(O1)CC(CC2)C(=C)C)C
MOL002649	0.9284	0.0716	0.8681	Phellodendri Chinrnsis Cortex	Coniferin	5280372	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(OC)cc(cc1)/C=C/CO)CO
MOL002649	0.9284	0.0716	0.8681	Asparagi Radix	Coniferin	5280372	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(OC)cc(cc1)/C=C/CO)CO
MOL002649	0.9284	0.0716	0.8681	Picrorhizae Rhizoma	Coniferin	5280372	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(OC)cc(cc1)/C=C/CO)CO
MOL002649	0.9284	0.0716	0.8681	Eucommiae Cortex	Coniferin	5280372	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(OC)cc(cc1)/C=C/CO)CO
MOL002649	0.9284	0.0716	0.8681	Aurantii Fructus Immaturus	Coniferin	5280372	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(OC)cc(cc1)/C=C/CO)CO
MOL002649	0.9284	0.0716	0.8681	Fructus Ligustri Lucidi	Coniferin	5280372	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(OC)cc(cc1)/C=C/CO)CO
MOL002649	0.9284	0.0716	0.8681	Phellodendri Amurensis Cortex	Coniferin	5280372	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(OC)cc(cc1)/C=C/CO)CO
MOL002649	0.9284	0.0716	0.8681	Ailanthi Cortex	Coniferin	5280372	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(OC)cc(cc1)/C=C/CO)CO
MOL002650	0.9365	0.0635	0.9245	Ligustici Rhizoma Et Radix	Coniferol	1549095	FALSE	Oc1c(OC)cc(cc1)/C=C/CO
MOL002650	0.9365	0.0635	0.9245	Fructus Ligustri Lucidi	Coniferol	1549095	FALSE	Oc1c(OC)cc(cc1)/C=C/CO
MOL002650	0.9365	0.0635	0.9245	Asparagi Radix	Coniferol	1549095	FALSE	Oc1c(OC)cc(cc1)/C=C/CO
MOL002650	0.9365	0.0635	0.9245	Mori Fructus	Coniferol	1549095	FALSE	Oc1c(OC)cc(cc1)/C=C/CO
MOL002650	0.9365	0.0635	0.9245	Aurantii Fructus Immaturus	Coniferol	1549095	FALSE	Oc1c(OC)cc(cc1)/C=C/CO
MOL002650	0.9365	0.0635	0.9245	Picrorhizae Rhizoma	Coniferol	1549095	FALSE	Oc1c(OC)cc(cc1)/C=C/CO
MOL002650	0.9365	0.0635	0.9245	Phellodendri Amurensis Cortex	Coniferol	1549095	FALSE	Oc1c(OC)cc(cc1)/C=C/CO
MOL002650	0.9365	0.0635	0.9245	Eucommiae Cortex	Coniferol	1549095	FALSE	Oc1c(OC)cc(cc1)/C=C/CO
MOL002650	0.9365	0.0635	0.9245	Phellodendri Chinrnsis Cortex	Coniferol	1549095	FALSE	Oc1c(OC)cc(cc1)/C=C/CO
MOL002651	0.6574	0.3426	0.8175	Radix Salviae	Dehydrotanshinone II A	128994	FALSE	c12c(ccc3c1C(=O)C(=O)c1c3occ1C)C(CC=C2)(C)C
MOL002651	0.6574	0.3426	0.8175	Phellodendri Chinrnsis Cortex	Dehydrotanshinone II A	128994	FALSE	c12c(ccc3c1C(=O)C(=O)c1c3occ1C)C(CC=C2)(C)C
MOL002653	0.8866	0.1134	0.7755	Phellodendri Chinrnsis Cortex	Dictamine	68085	FALSE	c12c(c3c(nc1occ2)cccc3)OC
MOL002653	0.8866	0.1134	0.7755	Dichroae Radix	Dictamine	68085	FALSE	c12c(c3c(nc1occ2)cccc3)OC
MOL002653	0.8866	0.1134	0.7755	Dictamni Cortex	Dictamine	68085	FALSE	c12c(c3c(nc1occ2)cccc3)OC
MOL002653	0.8866	0.1134	0.7755	Zanthoxylum Nitidum	Dictamine	68085	FALSE	c12c(c3c(nc1occ2)cccc3)OC
MOL002654	0.8218	0.1782	0.7904	Phellodendri Amurensis Cortex	Amurensin	5318156	FALSE	C1(C(C(C(C(O1)Oc1c(c2c(c(c1)O)c(=O)c(c(o2)c1ccc(cc1)O)O)CCC(C)(C)O)O)O)O)CO
MOL002654	0.8218	0.1782	0.7904	Phellodendri Chinrnsis Cortex	Amurensin	5318156	FALSE	C1(C(C(C(C(O1)Oc1c(c2c(c(c1)O)c(=O)c(c(o2)c1ccc(cc1)O)O)CCC(C)(C)O)O)O)O)CO
MOL002656	0.2022	0.7978	0.7354	Phellodendri Chinrnsis Cortex	dihydronilotic in	Not Available	FALSE	OC1C(C2C(C3C(=CC2)C2(C(C(CC2)C(CC(O)C2OC2(C)C)C)(CC3)C)C)(CC1)C)(C)C

MOL002657	0.2871	0.7129	0.6045	Phellodendri Chinrnsis Cortex	hispidol B	Not Available	FALSE	C1(C2C(CCC1O)(C1C(=CC2)C2(C(C(CC2)C(CC(O)C(O)C(O)(C)C)C)(CC1)C)C)(C)C
MOL002658	0.1225	0.8775	0.7344	Phellodendri Chinrnsis Cortex	kihadalactone B	Not Available	FALSE	O(C1C2(C(C3(C(C1)C(OC(=O)CC3OC(=O)C)(C)C)C)CCC1(C2=CCC1C1CC(=O)OC1)C)C)C(=O)C
MOL002659	0.6745	0.3255	0.7296	Phellodendri Chinrnsis Cortex	kihadanin A	Not Available	FALSE	O1C23C4(C(C5(C(CC4=O)C(OC(=O)C=C5)(C)C)C)CCC2(C(OC(=O)C13)C1=CC(=O)OC1O)C)C
MOL002660	0.1883	0.8117	0.7529	Phellodendri Chinrnsis Cortex	niloticin	44559946	FALSE	O1C(C(O)CC(C2C3(C(C4=CCC5C(C4CC3)(CCC(=O)C5(C)C)C)(CC2)C)C)C)C1(C)C
MOL002660	0.1883	0.8117	0.7529	Phellodendri Amurensis Cortex	niloticin	44559946	FALSE	O1C(C(O)CC(C2C3(C(C4=CCC5C(C4CC3)(CCC(=O)C5(C)C)C)(CC2)C)C)C)C1(C)C
MOL002661	0.4469	0.5531	0.7423	Phellodendri Chinrnsis Cortex	nomilin	Not Available	FALSE	C123C4(C(C5(C(CC4=O)C(OC(=O)CC5OC(=O)C)(C)C)C)CCC1(C(c1ccoc1)OC(=O)C2O3)C)C
MOL002661	0.4469	0.5531	0.7423	Aurantii Fructus Immaturus	nomilin	Not Available	FALSE	C123C4(C(C5(C(CC4=O)C(OC(=O)CC5OC(=O)C)(C)C)C)CCC1(C(c1ccoc1)OC(=O)C2O3)C)C
MOL002662	0.8282	0.1718	0.7367	Phellodendri Chinrnsis Cortex	rutaecarpine	Not Available	FALSE	O=c1n2CCc3c([nH]c4c3cccc4)c2nc2c1cccc2
MOL002662	0.8282	0.1718	0.7367	Evodiae Fructus	rutaecarpine	Not Available	FALSE	O=c1n2CCc3c([nH]c4c3cccc4)c2nc2c1cccc2
MOL002663	0.8865	0.1135	0.8877	Phellodendri Chinrnsis Cortex	Skimmianin	6760	TRUE	o1c2nc3c(c(OC)c2cc1)ccc(OC)c3OC
MOL002663	0.8865	0.1135	0.8877	Dictamni Cortex	Skimmianin	6760	TRUE	o1c2nc3c(c(OC)c2cc1)ccc(OC)c3OC
MOL002663	0.8865	0.1135	0.8877	Dichroae Radix	Skimmianin	6760	TRUE	o1c2nc3c(c(OC)c2cc1)ccc(OC)c3OC
MOL002663	0.8865	0.1135	0.8877	Zanthoxyli Pericarpium	Skimmianin	6760	TRUE	o1c2nc3c(c(OC)c2cc1)ccc(OC)c3OC
MOL002663	0.8865	0.1135	0.8877	Zanthoxylum Nitidum	Skimmianin	6760	TRUE	o1c2nc3c(c(OC)c2cc1)ccc(OC)c3OC
MOL002664	0.8774	0.1226	0.8329	Dictamni Cortex	Fagarine	107936	FALSE	o1c2nc3c(c(OC)c2cc1)cccc3OC
MOL002664	0.8774	0.1226	0.8329	Phellodendri Chinrnsis Cortex	Fagarine	107936	FALSE	o1c2nc3c(c(OC)c2cc1)cccc3OC
MOL002664	0.8774	0.1226	0.8329	Coptidis Rhizoma	Fagarine	107936	FALSE	o1c2nc3c(c(OC)c2cc1)cccc3OC
MOL002665	0.9506	0.0494	0.9260	Phellodendri Chinrnsis Cortex	Ferulic Acid	Not Available	FALSE	c1(cc(c(cc1)O)OC)/C=C/C(=C)O
MOL002666	0.6320	0.3680	0.7473	Phellodendri Chinrnsis Cortex	Chelerythrine	Not Available	FALSE	c12c(cc3c(c1)ccc1c3ccc3c1ccc(c3OC)OC)OCO2
MOL002668	0.8196	0.1804	0.7856	Phellodendri Chinrnsis Cortex	Worenine	Not Available	FALSE	O1c2cc3c4[n+](CCc3cc2OC1)cc1c(c4C)cc2OCOc2c1
MOL002670	0.4658	0.5342	0.8083	Phellodendri Chinrnsis Cortex	Cavidine	Not Available	FALSE	O1c2c3CN4C(C(c3ccc2OC1)C)c1c(CC4)cc(OC)c(OC)c1
MOL002670	0.4658	0.5342	0.8083	Arum Ternatum Thunb.	Cavidine	Not Available	FALSE	O1c2c3CN4C(C(c3ccc2OC1)C)c1c(CC4)cc(OC)c(OC)c1
MOL002670	0.4658	0.5342	0.8083	Corydalis Rhizoma	Cavidine	Not Available	FALSE	O1c2c3CN4C(C(c3ccc2OC1)C)c1c(CC4)cc(OC)c(OC)c1
MOL002671	0.1345	0.8655	0.7371	Phellodendri Chinrnsis Cortex	Candletoxin A	Not Available	FALSE	C1(C2(C(C3C(C1)(C3(C)C)O)C(=O)C(C)CC)OC(=O)Cc1ccccc1)C=C(CC1(C2C=C(C1=O)C)O)COC(=O)C)O)C
MOL002672	0.0621	0.9379	0.7869	Phellodendri Chinrnsis Cortex	Hericenone H	Not Available	FALSE	C(=CC(=O)CC1(C)CCc2c(O1)c(c(cc2OC)OC(=O)CCCCCCC/C=C\C/C=C\CCCCC)C=O)(C)C
MOL002673	0.2337	0.7663	0.6737	Phellodendri Chinrnsis Cortex	Hispidone	Not Available	FALSE	O1C(C(C(CC(C1)C1C2(CCC3C4(C(CC=C3C2(CC1)C)C(C(=O)CC4)(C)C)C)C)O)O)(C)C

MOL002674	0.8350	0.1650	0.7485	Carthami Flos	(E)-1,3-Tridecadiene-5,7,9,11-tetrayne	5352699	FALSE	C(=C\C#CC#CC#CC)/C=C
MOL002675	0.9259	0.0741	0.9508	Eriobotryae Folium	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Meliae Azedarach Fructus	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Lonicerae Japonicae Flos	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Celastri Orbiculati Fructus	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Eucommiae Folium	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Bombyx Mori L.	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Capsici Fructus	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Evodiae Fructus	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Scutellariae Barbatae Herba	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Folium Nelumbinis	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Benincasae Exocarpium	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Ginkgo Folium	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Dichroae Radix	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Rhododendri Daurici Folium	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Viticis Negundo Folium	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Bidentis Bipinnatae Herba	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Lysimachiae Foenigraeci Herba	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Carthami Flos	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Thalluslaminariae	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Polygonati Odorati Rhizoma	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Folium Artemisiae Argyi	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Amygdalus Communis Vas	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002675	0.9259	0.0741	0.9508	Pogostemon Cablin (Blanco) Benth.	Hexenal	5281168	FALSE	O=C/C=C/CCC
MOL002678	0.9345	0.0655	0.9378	Rubi Fructus	EB	7500	FALSE	c1(ccccc1)CC
MOL002678	0.9345	0.0655	0.9378	Eriobotryae Folium	EB	7500	FALSE	c1(ccccc1)CC
MOL002678	0.9345	0.0655	0.9378	Chaenomeles Sinensis (Thouin) Koehne	EB	7500	FALSE	c1(ccccc1)CC
MOL002678	0.9345	0.0655	0.9378	Carthami Flos	EB	7500	FALSE	c1(ccccc1)CC
MOL002678	0.9345	0.0655	0.9378	licorice	EB	7500	FALSE	c1(ccccc1)CC
MOL002678	0.9345	0.0655	0.9378	Perillae Fructus	EB	7500	FALSE	c1(ccccc1)CC
MOL002678	0.9345	0.0655	0.9378	Sterculiae Lychnophorae Semen	EB	7500	FALSE	c1(ccccc1)CC

MOL002678	0.9345	0.0655	0.9378	Arisaematis Rhizoma	EB	7500	FALSE	c1(ccccc1)CC
MOL002678	0.9345	0.0655	0.9378	Mori Fructus	EB	7500	FALSE	c1(ccccc1)CC
MOL002678	0.9345	0.0655	0.9378	Radix Cynanchi Paniculati	EB	7500	FALSE	c1(ccccc1)CC
MOL002679	0.9231	0.0769	0.9466	Carthami Flos	Ethone	31214	FALSE	C(OCC)(OCC)OCC
MOL002682	0.9461	0.0539	0.9688	Carthami Flos	aldehydo-D-galactose	3037556	FALSE	O=CC(O)C(O)C(O)C(O)CO
MOL002682	0.9461	0.0539	0.9688	Trichosanthes Kirilowii Maxim	aldehydo-D-galactose	3037556	FALSE	O=CC(O)C(O)C(O)C(O)CO
MOL002682	0.9461	0.0539	0.9688	Stachyurimedulla Helwingiaemedulla	aldehydo-D-galactose	3037556	FALSE	O=CC(O)C(O)C(O)C(O)CO
MOL002682	0.9461	0.0539	0.9688	Tetrapanacis Medulla	aldehydo-D-galactose	3037556	FALSE	O=CC(O)C(O)C(O)C(O)CO
MOL002683	0.7663	0.2337	0.6490	Cannabis Sativa L.	Ligla	5280933	FALSE	C(=C\CCCCC(=O)O)\C/C=C\C/C=C\CCCCC
MOL002683	0.7663	0.2337	0.6490	Carthami Flos	Ligla	5280933	FALSE	C(=C\CCCCC(=O)O)\C/C=C\C/C=C\CCCCC
MOL002683	0.7663	0.2337	0.6490	Sojae Semen Nigrum	Ligla	5280933	FALSE	C(=C\CCCCC(=O)O)\C/C=C\C/C=C\CCCCC
MOL002683	0.7663	0.2337	0.6490	Thalluslaminariae	Ligla	5280933	FALSE	C(=C\CCCCC(=O)O)\C/C=C\C/C=C\CCCCC
MOL002683	0.7663	0.2337	0.6490	Ginkgo Folium	Ligla	5280933	FALSE	C(=C\CCCCC(=O)O)\C/C=C\C/C=C\CCCCC
MOL002685	0.9096	0.0904	0.9013	Carthami Flos	[(2S)-2,3-dihydroxypropyl] octanoate	3085369	FALSE	O(C(=O)CCCCCCC)CC(O)CO
MOL002686	0.8459	0.1541	0.8603	Carthami Flos	GLV	760	FALSE	C(=O)(C=O)O
MOL002687	0.8910	0.1090	0.8303	Fritiliariae Irrhosae Bulbus	guanosine	12219153	FALSE	c12n(C3OC(C(C3O)O)CO)cnc1c(=O)[nH]c(n2)N
MOL002687	0.8910	0.1090	0.8303	Carthami Flos	guanosine	12219153	FALSE	c12n(C3OC(C(C3O)O)CO)cnc1c(=O)[nH]c(n2)N
MOL002689	0.9645	0.0355	0.8867	Asari Radix Et Rhizoma	3,4,5-Trimethoxytoluene	80922	FALSE	c1(c(cc(cc1OC)C)OC)OC
MOL002689	0.9645	0.0355	0.8867	Curculiginis Rhizome	3,4,5-Trimethoxytoluene	80922	FALSE	c1(c(cc(cc1OC)C)OC)OC
MOL002689	0.9645	0.0355	0.8867	Epimrdii Herba	3,4,5-Trimethoxytoluene	80922	FALSE	c1(c(cc(cc1OC)C)OC)OC
MOL002689	0.9645	0.0355	0.8867	Carthami Flos	3,4,5-Trimethoxytoluene	80922	FALSE	c1(c(cc(cc1OC)C)OC)OC
MOL002690	0.8792	0.1208	0.7631	Carthami Flos	hydroxysafflor-yellow-A	Not Available	FALSE	O1C(C2(O)C(=O)C(=C(O)/C(=C(\O)/C=C/c3cc(O)cc3)/C2=O)C2OC(C(O)C(O)C2O)CO)C(O)C(O)C(O)C1CO
MOL002691	0.9034	0.0966	0.9708	A. Dahurica (Fisch.) Benth. Et Hook	Iva	10430	FALSE	C(CC(=O)O)(C)C
MOL002691	0.9034	0.0966	0.9708	Capsici Fructus	Iva	10430	FALSE	C(CC(=O)O)(C)C
MOL002691	0.9034	0.0966	0.9708	Panacis Japonici Rhizoma	Iva	10430	FALSE	C(CC(=O)O)(C)C

MOL002691	0.9034	0.0966	0.9708	Et Radix Patriniae Rhizoma	Iva	10430	FALSE	C(CC(=O)O)(C)C
MOL002691	0.9034	0.0966	0.9708	Nardostachyos Radix Et Rhizoma	Iva	10430	FALSE	C(CC(=O)O)(C)C
MOL002691	0.9034	0.0966	0.9708	Mume Fructus	Iva	10430	FALSE	C(CC(=O)O)(C)C
MOL002691	0.9034	0.0966	0.9708	Sojae Semen Nigrum	Iva	10430	FALSE	C(CC(=O)O)(C)C
MOL002691	0.9034	0.0966	0.9708	Carthami Flos	Iva	10430	FALSE	C(CC(=O)O)(C)C
MOL002691	0.9034	0.0966	0.9708	Lithospermum Erythrorhizon	Iva	10430	FALSE	C(CC(=O)O)(C)C
MOL002691	0.9034	0.0966	0.9708	Campsis Flos	Iva	10430	FALSE	C(CC(=O)O)(C)C
MOL002692	0.9140	0.0860	0.8280	Mori Cortex	Amoenin A3	5742687	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)CO
MOL002692	0.9140	0.0860	0.8280	Carthami Flos	Amoenin A3	5742687	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)CO
MOL002693	0.8807	0.1193	0.8493	Geranium Wilfordii Maxim.	nicotiflorin	5318767	FALSE	c1(c(c2ccc(cc2)O)oc2c(c1=O)c(cc(c2)O)O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL002693	0.8807	0.1193	0.8493	Ginkgo Folium	nicotiflorin	5318767	FALSE	c1(c(c2ccc(cc2)O)oc2c(c1=O)c(cc(c2)O)O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL002693	0.8807	0.1193	0.8493	Lysimachiae Herba	nicotiflorin	5318767	FALSE	c1(c(c2ccc(cc2)O)oc2c(c1=O)c(cc(c2)O)O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL002693	0.8807	0.1193	0.8493	Rubi Fructus	nicotiflorin	5318767	FALSE	c1(c(c2ccc(cc2)O)oc2c(c1=O)c(cc(c2)O)O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL002693	0.8807	0.1193	0.8493	Puerariae Flos	nicotiflorin	5318767	FALSE	c1(c(c2ccc(cc2)O)oc2c(c1=O)c(cc(c2)O)O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL002693	0.8807	0.1193	0.8493	Acoritataninowii Rhizoma	nicotiflorin	5318767	FALSE	c1(c(c2ccc(cc2)O)oc2c(c1=O)c(cc(c2)O)O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL002693	0.8807	0.1193	0.8493	Solidaginis Herba	nicotiflorin	5318767	FALSE	c1(c(c2ccc(cc2)O)oc2c(c1=O)c(cc(c2)O)O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL002693	0.8807	0.1193	0.8493	Asari Radix Et Rhizoma	nicotiflorin	5318767	FALSE	c1(c(c2ccc(cc2)O)oc2c(c1=O)c(cc(c2)O)O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL002693	0.8807	0.1193	0.8493	Carthami Flos	nicotiflorin	5318767	FALSE	c1(c(c2ccc(cc2)O)oc2c(c1=O)c(cc(c2)O)O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL002693	0.8807	0.1193	0.8493	Sophora Japonica L.	nicotiflorin	5318767	FALSE	c1(c(c2ccc(cc2)O)oc2c(c1=O)c(cc(c2)O)O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL002693	0.8807	0.1193	0.8493	licorice	nicotiflorin	5318767	FALSE	c1(c(c2ccc(cc2)O)oc2c(c1=O)c(cc(c2)O)O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O

MOL002694	0.7624	0.2376	0.8178	Carthami Flos	4-[(E)-4-(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)but-2-enylidene]-2,6-dimethoxycyclohexa-2,5-dien-1-one	10237057	FALSE	C1(=C/C(=C\C=C\C=C/2\C=C(C(=O)C(=C2)OC)OC)/C=C(C1=O)OC)OC
MOL002696	0.6038	0.3962	0.6502	Carthami Flos	lirioresinol-A	Not Available	FALSE	c1(c(cc(cc1OC)C1C2C(CO1)C(OC2)c1cc(c(c(c1)OC)O)OC)O)O
MOL002698	0.5853	0.4147	0.6415	Carthami Flos	lupeol-palmitate	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C(=C)C)C4C3CCC21)C)OC(=O)CCCCCCCCCCCCCCCC
MOL002700	0.8784	0.1216	0.8152	Carthami Flos	luteolin-7-O-B-D-glucoside	Not Available	FALSE	O(C1C(O)C(O)C(OC1Oc1cc2oc(cc(=O)c2c(O)c1)c1cc(O)c(O)cc1)CO)C1OCC(O)(C1O)CO
MOL002701	0.9060	0.0940	0.8014	Carthami Flos	neocarthamin	46173973	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(OC(CC2=O)c2ccc(O)cc2)cc(O)c1O)CO
MOL002704	0.9201	0.0799	0.9504	Carthami Flos	D-Phenylalanine	6919011	FALSE	OC(=O)C(N)Cc1ccccc1
MOL002706	0.5498	0.4502	0.7078	Carthami Flos	Phytoene	5280784	FALSE	C(C/C=C(/CCC=C(C)C)\C)/C(=C/CC/C(=C/C=C/C=C(/CC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C)\C)/C)/C
MOL002707	0.5345	0.4655	0.6867	Lonicerae Japonicae Flos	phytofluene	Not Available	FALSE	C(C/C=C(/CCC=C(C)C)\C)/C(=C/CC/C(=C/C=C/C=C(/C=C/C=C(/CC/C=C(/CCC=C(C)C)\C)\C)\C)/C)/C
MOL002707	0.5345	0.4655	0.6867	Citri Fructus	phytofluene	Not Available	FALSE	C(C/C=C(/CCC=C(C)C)\C)/C(=C/CC/C(=C/C=C/C=C(/C=C/C=C(/CC/C=C(/CCC=C(C)C)\C)\C)\C)/C)/C
MOL002707	0.5345	0.4655	0.6867	Carthami Flos	phytofluene	Not Available	FALSE	C(C/C=C(/CCC=C(C)C)\C)/C(=C/CC/C(=C/C=C/C=C(/C=C/C=C(/CC/C=C(/CCC=C(C)C)\C)\C)\C)/C)/C
MOL002708	0.8153	0.1847	0.7311	Carthami Flos	precarthamin	Not Available	FALSE	C1(C(C(OC(C1O)OCCc1c(c(cc1O)O)C(/C=C\c1ccc(cc1)O)C)O)O)O)O
MOL002709	0.9032	0.0968	0.8827	Carthami Flos	propanetriol-a-arabinofuranosyl(1→4)	Not Available	FALSE	C1(C(C(OC1C1C(OC(C(C1O)O)OCC(CO)O)O)O)O)O)O
MOL002710	0.2436	0.7564	0.6486	Carthami Flos	Pyrethrin II	5281555	FALSE	C1(C(C1(C)C)C(=O)OC1C(=C(C(=O)C1)C/C=C\C=C)C)/C=C(/C(=O)OC)\C
MOL002711	0.9291	0.0709	0.9678	Eriobotryae Folium	ZINC01692449	6994331	FALSE	C(CC)(C=C)O
MOL002711	0.9291	0.0709	0.9678	Carthami Flos	ZINC01692449	6994331	FALSE	C(CC)(C=C)O

MOL002712	0.9438	0.0562	0.9050	Carthami Flos	6-Hydroxykaempferol	5281638	FALSE	c1(c(c(c2c(c1)oc(c(c2=O)O)c1ccc(cc1)O)O)O)O
MOL002713	0.8627	0.1373	0.8005	Carthami Flos	qt_Kaempferol-3-O-rutinoside-7-O-galactoside	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OCC1OC(C(C(C1O)O)O)O)OCC(C(C(C(C=O)O)O)O)O)c1ccc(cc1)O)O)OC
MOL002714	0.9170	0.0830	0.8375	Polygonati Rhizoma	baicalein	5281605	FALSE	c12c(c(c(c(c2)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002714	0.9170	0.0830	0.8375	Carthami Flos	baicalein	5281605	FALSE	c12c(c(c(c(c2)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002714	0.9170	0.0830	0.8375	Radix Paeoniae Rubra	baicalein	5281605	FALSE	c12c(c(c(c(c2)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002714	0.9170	0.0830	0.8375	Oroxyli Semen	baicalein	5281605	FALSE	c12c(c(c(c(c2)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002714	0.9170	0.0830	0.8375	Arum Ternatum Thunb.	baicalein	5281605	FALSE	c12c(c(c(c(c2)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002714	0.9170	0.0830	0.8375	Achyranthis Bidentatae Radix	baicalein	5281605	FALSE	c12c(c(c(c(c2)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002714	0.9170	0.0830	0.8375	Fructussophorae	baicalein	5281605	FALSE	c12c(c(c(c(c2)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002714	0.9170	0.0830	0.8375	Plantaginis Herba	baicalein	5281605	FALSE	c12c(c(c(c(c2)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002714	0.9170	0.0830	0.8375	Scutellariae Barbatae Herba	baicalein	5281605	FALSE	c12c(c(c(c(c2)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002714	0.9170	0.0830	0.8375	Scutellariae Radix	baicalein	5281605	FALSE	c12c(c(c(c(c2)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002714	0.9170	0.0830	0.8375	Phellodendri Amurensis Cortex	baicalein	5281605	FALSE	c12c(c(c(c(c2)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002715	0.5816	0.4184	0.6208	Carthami Flos	qt_carthamin-precursor	Not Available	FALSE	c1(ccc(cc1)/C=C\C(=O)C1=C(C(C(=C(C1=O)C(C1=C(C(C(=C(C1=O)C(=O)/C=C\c1ccc(cc1)O)O)(C)O)O)C(=O)O)O)(O)C)O)O
MOL002716	0.6962	0.3038	0.6343	Carthami Flos	qt_carthamin	Not Available	FALSE	C1(CC2=C(C(C(=C(C2=O)C(=O)/C=C/c2ccc(cc2)O)O)(O)O)O)C(=O)C(C(=C(C1=O)C(=O)/C=C\c1ccc(cc1)O)O)(O)O
MOL002717	0.9135	0.0865	0.7545	Carthami Flos	qt_carthamone	Not Available	FALSE	OC1=C(C(=CC(=O)C1=O)O)C(=O)/C=C/c1ccc(O)cc1
MOL002718	0.9191	0.0809	0.8684	Carthami Flos	qt_hydroxysaflor-yellow-A	Not Available	FALSE	OC1C(=O)C=C(O)/C(=C(\O)/C=C/c2ccc(O)cc2)/C1=O
MOL002719	0.9417	0.0583	0.8922	Scutellariae Barbatae Herba	6-Hydroxynaringenin	188308	FALSE	Oc1c2c(OC(CC2=O)c2ccc(O)cc2)cc(O)c1O
MOL002719	0.9417	0.0583	0.8922	Carthami Flos	6-Hydroxynaringenin	188308	FALSE	Oc1c2c(OC(CC2=O)c2ccc(O)cc2)cc(O)c1O
MOL002720	0.7459	0.2541	0.7277	Carthami Flos	qt_precarthamin	Not Available	FALSE	OCCc1c(c(c(cc1O)O)C(/C=C\c1ccc(cc1)O)C)O
MOL002721	0.9457	0.0543	0.8960	Inulae Herba	quercetagetin	5281680	FALSE	c1(c(O)c(=O)c2c(O)c(c(O)cc2o1)O)c1cc(O)c(O)cc1
MOL002721	0.9457	0.0543	0.8960	Carthami Flos	quercetagetin	5281680	FALSE	c1(c(O)c(=O)c2c(O)c(c(O)cc2o1)O)c1cc(O)c(O)cc1
MOL002721	0.9457	0.0543	0.8960	Eriocauli Flos	quercetagetin	5281680	FALSE	c1(c(O)c(=O)c2c(O)c(c(O)cc2o1)O)c1cc(O)c(O)cc1
MOL002722	0.8828	0.1172	0.7871	Strychni Semen	Vomifoliol	5280462	FALSE	OC1(C(CC(=O)C=C1C)(C)C)/C=C/C(O)C
MOL002722	0.8828	0.1172	0.7871	Daturae Flos	Vomifoliol	5280462	FALSE	OC1(C(CC(=O)C=C1C)(C)C)/C=C/C(O)C

MOL002722	0.8828	0.1172	0.7871	Carthami Flos	Vomifoliol	5280462	FALSE	OC1(C(CC(=O)C=C1C)(C)C)/C=C/C(O)C
MOL002722	0.8828	0.1172	0.7871	Bombyx Mori L.	Vomifoliol	5280462	FALSE	OC1(C(CC(=O)C=C1C)(C)C)/C=C/C(O)C
MOL002722	0.8828	0.1172	0.7871	Jujubae Fructus	Vomifoliol	5280462	FALSE	OC1(C(CC(=O)C=C1C)(C)C)/C=C/C(O)C
MOL002722	0.8828	0.1172	0.7871	Fructus Ligustri Lucidi	Vomifoliol	5280462	FALSE	OC1(C(CC(=O)C=C1C)(C)C)/C=C/C(O)C
MOL002722	0.8828	0.1172	0.7871	Eriobotryae Folium	Vomifoliol	5280462	FALSE	OC1(C(CC(=O)C=C1C)(C)C)/C=C/C(O)C
MOL002723	0.9191	0.0809	0.8684	Carthami Flos	qt_safflomin-A	Not Available	FALSE	OC1C(=O)C=C(O)/C(=C(\O)/C=C/c2ccc(O)cc2)/C1=O
MOL002724	0.8106	0.1894	0.6693	Carthami Flos	qt_safflomin-C	Not Available	FALSE	OC1C(=O)C(=C(O)/C(=C(\O)/C=C/c2ccc(O)cc2)/C1=O)C(CC(=O)O)c1ccc(O)cc1
MOL002725	0.9036	0.0964	0.8025	Carthami Flos	qt_safflow-yellow-A	Not Available	FALSE	C12=C(C(C(=C(C2=O)C(=O)/C=C\c2ccc(cc2)O)O)(O)O)OC2C1OC(C(C2O)O)CO
MOL002726	0.6448	0.3552	0.6488	Carthami Flos	qt_safflower-yellow-B	Not Available	FALSE	c1(ccc(cc1)/C=C\C(=O)C1=C(C(C(=C(C1=O)C(C(O)C(O)C(O)C(O)CO)C1=C(C(C(=C(C1=O)C(=O)/C=C\c1ccc(cc1)O)O)(C)O)O)O)(O)C)O)O
MOL002727	0.8373	0.1627	0.7503	Carthami Flos	C08464	441552	FALSE	C=CC#CC#CC#CC#CC#CC
MOL002728	0.8885	0.1115	0.8070	Carthami Flos	sesquiterpene	13345443	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(=O)c2c(oc1c1cc(O)c(O)cc1)cc(OC1OC(C(O)C(O)C1O)CO)cc2O)CO
MOL002729	0.9164	0.0836	0.7815	Carthami Flos	quercetin-6-glucoside	Not Available	FALSE	c1(c(O)c(=O)c2c(O)c(c(O)cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL002730	0.8784	0.1216	0.6346	Raphani Semen	Vitamin- G	493570	FALSE	n1(c2c(nc3c1nc(=O)[nH]c3=O)cc(c(c2)C)C)CC(C(C(CO)O)O)O
MOL002730	0.8784	0.1216	0.6346	Vigna Radiata	Vitamin- G	493570	FALSE	n1(c2c(nc3c1nc(=O)[nH]c3=O)cc(c(c2)C)C)CC(C(C(CO)O)O)O
MOL002730	0.8784	0.1216	0.6346	Euryales Semen	Vitamin- G	493570	FALSE	n1(c2c(nc3c1nc(=O)[nH]c3=O)cc(c(c2)C)C)CC(C(C(CO)O)O)O
MOL002730	0.8784	0.1216	0.6346	Hippophae Fructus	Vitamin- G	493570	FALSE	n1(c2c(nc3c1nc(=O)[nH]c3=O)cc(c(c2)C)C)CC(C(C(CO)O)O)O
MOL002730	0.8784	0.1216	0.6346	Jujubae Fructus	Vitamin- G	493570	FALSE	n1(c2c(nc3c1nc(=O)[nH]c3=O)cc(c(c2)C)C)CC(C(C(CO)O)O)O
MOL002730	0.8784	0.1216	0.6346	Corayceps	Vitamin- G	493570	FALSE	n1(c2c(nc3c1nc(=O)[nH]c3=O)cc(c(c2)C)C)CC(C(C(CO)O)O)O
MOL002730	0.8784	0.1216	0.6346	Carthami Flos	Vitamin- G	493570	FALSE	n1(c2c(nc3c1nc(=O)[nH]c3=O)cc(c(c2)C)C)CC(C(C(CO)O)O)O
MOL002730	0.8784	0.1216	0.6346	Rosae Laevigatae Fructus	Vitamin- G	493570	FALSE	n1(c2c(nc3c1nc(=O)[nH]c3=O)cc(c(c2)C)C)CC(C(C(CO)O)O)O
MOL002730	0.8784	0.1216	0.6346	Crataegi Folium	Vitamin- G	493570	FALSE	n1(c2c(nc3c1nc(=O)[nH]c3=O)cc(c(c2)C)C)CC(C(C(CO)O)O)O
MOL002730	0.8784	0.1216	0.6346	Humulus Scandens (Lour.) Merr.	Vitamin- G	493570	FALSE	n1(c2c(nc3c1nc(=O)[nH]c3=O)cc(c(c2)C)C)CC(C(C(CO)O)O)O

MOL002731	0.8706	0.1294	0.7857	Jujubae Fructus	(4S)-4-hydroxy-3,5,5-trimethyl-4-[(E,3R)-3-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydropyran-2-yl]oxybut-1-enyl]cyclohex-2-en-1-one	9930064	FALSE	O1C(OC(/C=C/C2(O)C(CC(=O)C=C2C)(C)C)C)C(O)C(O)C(O)C1CO
MOL002731	0.8706	0.1294	0.7857	Daturae Flos	(4S)-4-hydroxy-3,5,5-trimethyl-4-[(E,3R)-3-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydropyran-2-yl]oxybut-1-enyl]cyclohex-2-en-1-one	9930064	FALSE	O1C(OC(/C=C/C2(O)C(CC(=O)C=C2C)(C)C)C)C(O)C(O)C(O)C1CO
MOL002731	0.8706	0.1294	0.7857	Fructus Ligustri Lucidi	(4S)-4-hydroxy-3,5,5-trimethyl-4-[(E,3R)-3-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydropyran-2-yl]oxybut-1-enyl]cyclohex-2-en-1-one	9930064	FALSE	O1C(OC(/C=C/C2(O)C(CC(=O)C=C2C)(C)C)C)C(O)C(O)C(O)C1CO

MOL002731	0.8706	0.1294	0.7857	Eriobotryae Folium	(4S)-4-hydroxy-3,5,5-trimethyl-4-[(E,3R)-3-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydropyran-2-yl]oxybut-1-enyl]cyclohex-2-en-1-one	9930064	FALSE	O1C(OC(/C=C/C2(O)C(CC(=O)C=C2C)(C)C)C)C(O)C(O)C(O)C1CO
MOL002731	0.8706	0.1294	0.7857	Carthami Flos	(4S)-4-hydroxy-3,5,5-trimethyl-4-[(E,3R)-3-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydropyran-2-yl]oxybut-1-enyl]cyclohex-2-en-1-one	9930064	FALSE	O1C(OC(/C=C/C2(O)C(CC(=O)C=C2C)(C)C)C)C(O)C(O)C(O)C1CO
MOL002732	0.8327	0.1673	0.7453	Carthami Flos	7-Chloro-2,4-quinolinedicarboxylic acid	5322029	FALSE	CC#CC#CC#C/C=C/C=C/C=C
MOL002733	0.8792	0.1208	0.7631	Carthami Flos	safflomin-A	Not Available	FALSE	O1C(C2(O)C(=O)C(=C(O)/C(=C(\O)/C=C/c3ccc(O)cc3)/C2=O)C2OC(C(O)C(O)C2O)CO)C(O)C(O)C(O)C1CO
MOL002734	0.7917	0.2083	0.7052	Carthami Flos	safflomin-C	Not Available	FALSE	O1C(C(O)C(O)C(O)C1CO)C1(O)C(=O)C(=C(O)/C(=C(\O)/C=C/c2ccc(O)cc2)/C1=O)C(CC(=O)O)c1ccc(O)cc1
MOL002735	0.8674	0.1326	0.8028	Carthami Flos	safflow-yellow-A	Not Available	FALSE	C12=C(C(C(=C(C2=O)C(=O)/C=C\c2ccc(cc2)O)O)OC2OC(C(C(C2O)O)O)CO)O)OC2C1OC(C(C2O)O)CO
MOL002736	0.7640	0.2360	0.7275	Carthami Flos	safflower-yellow-B	Not Available	FALSE	C1(C(C(C(OC1CO)CC1(C(=C(C(=O)C(=C1O)C(C1=C(C(C(=C(C(=O)/C=C/c2ccc(cc2)O)C1=O)O)(O)C C1OC(C(C(C1O)O)O)CO)O)C(O)C(O)C(O)C(O)CO)C(=O)/C=C\c1ccc(cc1)O)O)O)O)O)O
MOL002737	0.9238	0.0762	0.8771	Carthami Flos	scutellarein	5281697	FALSE	c12c(c(=O)cc(o1)c1ccc(cc1)O)c(c(c(c2)O)O)O
MOL002737	0.9238	0.0762	0.8771	Oroxyli Semen	scutellarein	5281697	FALSE	c12c(c(=O)cc(o1)c1ccc(cc1)O)c(c(c(c2)O)O)O

MOL002737	0.9238	0.0762	0.8771	Perilla Frutescens	scutellarein	5281697	FALSE	c12c(c(=O)cc(o1)c1ccc(cc1)O)c(c(c(c2)O)O)O
MOL002737	0.9238	0.0762	0.8771	Scutellariae Barbatae Herba	scutellarein	5281697	FALSE	c12c(c(=O)cc(o1)c1ccc(cc1)O)c(c(c(c2)O)O)O
MOL002737	0.9238	0.0762	0.8771	Plantaginis Herba	scutellarein	5281697	FALSE	c12c(c(=O)cc(o1)c1ccc(cc1)O)c(c(c(c2)O)O)O
MOL002737	0.9238	0.0762	0.8771	Scutellariae Radix	scutellarein	5281697	FALSE	c12c(c(=O)cc(o1)c1ccc(cc1)O)c(c(c(c2)O)O)O
MOL002738	0.8026	0.1974	0.7732	Carthami Flos	Diamylphenol	34303	FALSE	c1(cc(ccc1O)CCCCC)CCCCC
MOL002739	0.9298	0.0702	0.7664	Carthami Flos	tagetiin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)c(O)c(O)c2)c1cc(O)c(O)cc1)CO
MOL002740	0.7963	0.2037	0.6512	Carthami Flos	thymopentin	Not Available	FALSE	O=C(NC(C(=O)NC(C(C)C)C(=O)NC(Cc1ccc(O)cc1)C(=O)O)CC(=O)O)C(NC(=O)C(N)CCCN=C(N)N)CCCN
MOL002741	0.8701	0.1299	0.7387	Carthami Flos	tinctorimine	Not Available	FALSE	C1(C(C(OC(C1O)O)C1(O)C(=C(C(=O)C(=C1O)C(=O)/C=C\c1ccc(cc1)O)O)/C(=C\1/NC(C(C1O)O)O)O)O)CO
MOL002743	0.9344	0.0656	0.9609	Menthae Herba	ZINC01666986	6993810	FALSE	C(C(C)O)CCC
MOL002743	0.9344	0.0656	0.9609	Carthami Flos	ZINC01666986	6993810	FALSE	C(C(C)O)CCC
MOL002744	0.9000	0.1000	0.9670	Carthami Flos	(R)-2-methylbutyric acid	6950479	FALSE	C(C(=O)O)(CC)C
MOL002744	0.9000	0.1000	0.9670	Eriobotryae Folium	(R)-2-methylbutyric acid	6950479	FALSE	C(C(=O)O)(CC)C
MOL002745	0.9326	0.0674	0.9636	Carthami Flos	ZINC01690417	6994293	FALSE	C(CCC)(CC)O
MOL002746	0.9316	0.0684	0.8559	Carthami Flos	L-2-Amino-3-(5-hydroxyindolyl)propionic acid	6971044	FALSE	C(=O)(C(N)Cc1c[nH]c2ccc(cc12)O)O
MOL002747	0.9329	0.0671	0.9549	Carthami Flos	(2R)-5-methylhexan-2-ol	6999721	FALSE	C(CCC(C)O)(C)C
MOL002749	0.8777	0.1223	0.7758	Carthami Flos	6-hydroxykaempferol-3,6,7-tri-O-beta-D-glucoside	Not Available	FALSE	c1(c(c(c2c(c1)oc(c(c2=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)O)OC1OC(C(C(C1O)O)O)CO)OC1OC(C(C(C1O)O)O)CO
MOL002750	0.8308	0.1692	0.7376	Carthami Flos	2,4-Dichloro-5-([(E)-(4-chlorophenyl)methylidene]amino)benzoic acid	5352698	FALSE	C(=C\C=C)/C=C/C#CC#C/C=C/C

MOL002751	0.9262	0.0738	0.7905	Carthami Flos	6-hydroxykaempferol-3-O-beta-D-glucoside	Not Available	FALSE	c1(c(c(c2c(c1)oc(c(c2=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)O)O)O
MOL002752	0.8693	0.1307	0.7571	Carthami Flos	6-hydroxykaempferol-3-O-beta-d-Rutoside-6-O-beta-d-glucoside	Not Available	FALSE	c1(c(c(c2c(c1)oc(c(c2=O)OCC1OC(C(C(C1O)O)O)OCC(C(C(C(C(=O)O)O)O)O)O)c1ccc(cc1)O)O)OC1OC(C(C(C1O)O)O)CO)O
MOL002753	0.9262	0.0738	0.7905	Carthami Flos	6-hydroxykaempferol-3-O-glucoside	25017112	FALSE	c1(c(c(=O)c2c(O)c(c(O)cc2o1)O)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL002754	0.8747	0.1253	0.7907	Carthami Flos	6-hydroxykaempferol-3,6-di-O-beta-D-glucoside	Not Available	FALSE	c1(c(c(c2c(c1)oc(c(c2=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)O)OC1OC(C(C(C1O)O)O)CO)O
MOL002755	0.8779	0.1221	0.8025	Carthami Flos	6-hydroxykaempferol-6,7-di-O-beta-D-glucoside	Not Available	FALSE	c1(c(c(c2c(c1)oc(c(c2=O)O)c1ccc(cc1)O)O)OC1OC(C(C(C1O)O)O)CO)OC1OC(C(C(C1O)O)O)CO
MOL002756	0.9228	0.0772	0.7881	Carthami Flos	6-Hydroxykaempferol-7-O-glucoside	5318240	FALSE	c1(c(O)c(=O)c2c(O)c(c(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)O)c1ccc(O)cc1
MOL002757	0.8947	0.1053	0.6814	Carthami Flos	7,8-dimethyl-1H-pyrimido[5,6-g]quinoxaline-2,4-dione	21786815	FALSE	[nH]1c(=O)[nH]c(=O)c2cc3c(cc12)nc(c(n3)C)C
MOL002758	0.7909	0.2091	0.7424	Carthami Flos	(E,Z)-2,8-Decadien-4,6-diyn-1-yl 3-methylbutanoate	5352701	FALSE	C(CC(=O)OC/C=C/C#CC#C/C=C\C)(C)C
MOL002759	0.5543	0.4457	0.6250	Carthami Flos	Glyceryl pps	6438900	FALSE	O(C(=O)CCCCCCCCCCCCCCC)CC(OC(=O)/C=C/C=C/C)COC(=O)CCCCCCCCCCCCCCC

MOL002761	0.8763	0.1237	0.8257	Carthami Flos	Sophoraflavonoloside	5282155	FALSE	c1(c(c2ccc(cc2)O)oc2c(c1=O)c(cc(c2)O)O)OC1C(OC2OC(C(C(C2O)O)O)CO)C(C(C(O1)CO)O)O
MOL002761	0.8763	0.1237	0.8257	Allii Fistulost Bulbus	Sophoraflavonoloside	5282155	FALSE	c1(c(c2ccc(cc2)O)oc2c(c1=O)c(cc(c2)O)O)OC1C(OC2OC(C(C(C2O)O)O)CO)C(C(C(O1)CO)O)O
MOL002761	0.8763	0.1237	0.8257	Fructussophorae	Sophoraflavonoloside	5282155	FALSE	c1(c(c2ccc(cc2)O)oc2c(c1=O)c(cc(c2)O)O)OC1C(OC2OC(C(C(C2O)O)O)CO)C(C(C(O1)CO)O)O
MOL002761	0.8763	0.1237	0.8257	Mori Cortex	Sophoraflavonoloside	5282155	FALSE	c1(c(c2ccc(cc2)O)oc2c(c1=O)c(cc(c2)O)O)OC1C(OC2OC(C(C(C2O)O)O)CO)C(C(C(O1)CO)O)O
MOL002761	0.8763	0.1237	0.8257	Sophorae Tonkinensis Radix Et Rhizome	Sophoraflavonoloside	5282155	FALSE	c1(c(c2ccc(cc2)O)oc2c(c1=O)c(cc(c2)O)O)OC1C(OC2OC(C(C(C2O)O)O)CO)C(C(C(O1)CO)O)O
MOL002762	0.8797	0.1203	0.7994	Carthami Flos	Kaempferol-3-O-beta-d-rutinoside	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OCC1OC(C(C(C1O)O)O)O)OCC(C(C(C(C=O)O)O)O)O)c1ccc(cc1)O)O)O
MOL002763	0.8652	0.1348	0.7475	Carthami Flos	Kaempferol-3-O-rutinoside-7-O-galactoside	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OCC1OC(C(C(C1O)O)O)O)OCC(C(C(C(C=O)O)O)O)O)c1ccc(cc1)O)O)OCC1C(C(C(C(O1)O)O)O)O
MOL002766	0.8884	0.1116	0.8046	Carthami Flos	Quercetin-3,7-di-O-beta-d-glucoside	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1OC(C(C(C1O)O)O)O)CO)c1ccc(c(c1)O)O)O)OC1OC(C(C(C1O)O)O)O)CO
MOL002767	0.8354	0.1646	0.7481	Carthami Flos	1,11(Z)-Tridecadien-3,5,7,9-tetrayne	5352703	FALSE	C/C=C\C#CC#CC#CC#CC=C
MOL002769	0.8943	0.1057	0.7320	Carthami Flos	(Z)-2-methyl-5-[(1R,2S,4S)-2-methyl-3-methylene-2-norbornanyl]pent-2-en-1-ol	20055019	FALSE	C(/C(=C\CCC1(C2CCC(C1=C)C2)C)/C)O
MOL002772	0.7805	0.2195	0.7367	Carthami Flos	[(Z)-dec-8-en-4,6-diynyl] 3-methylbutanoate	5352705	FALSE	C(=O)(CC(C)C)OCCCC#CC#C/C=C\C
MOL002773	0.3628	0.6372	0.6146	Mori Follum	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Solanum Nigrum Linn.	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Verbenae Herb	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Citri Fructus	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)

MOL002773	0.3628	0.6372	0.6146	Aloe	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Vigna Radiata	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Spirodelae Herba	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Lonicerae Japonicae Flos	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Jujubae Fructus	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Ginkgo Semen	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Broussonetiae Fructus	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Perillae Fructus	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Hydnocarpi Anthelminticae Semen	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Semen Pini Koraiensis	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Benincasae Exocarpium	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Bombyx Mori L.	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Portulacae Herba	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Perilla Frutescens	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Lablab Semen Album	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Mori Fructus	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Rose Rugosae Flos	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Capsici Fructus	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Carthami Flos	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Euryales Semen	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)
MOL002773	0.3628	0.6372	0.6146	Hippophae Fructus	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)

MOL002773	0.3628	0.6372	0.6146	Capsellae Herba	beta-carotene	5280489	FALSE	C1(CCCC(=C1/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)(C)C
MOL002776	0.8928	0.1072	0.8274	Achyranthis Bidentatae Radix	Baicalin	64982	FALSE	c12c(c(c(c(c2)OC2OC(C(C(C2O)O)O)C(=O)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002776	0.8928	0.1072	0.8274	Scutellariae Barbatae Herba	Baicalin	64982	FALSE	c12c(c(c(c(c2)OC2OC(C(C(C2O)O)O)C(=O)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002776	0.8928	0.1072	0.8274	Arum Ternatum Thunb.	Baicalin	64982	FALSE	c12c(c(c(c(c2)OC2OC(C(C(C2O)O)O)C(=O)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002776	0.8928	0.1072	0.8274	Thalictri Glandulosissimi Et	Baicalin	64982	FALSE	c12c(c(c(c(c2)OC2OC(C(C(C2O)O)O)C(=O)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002776	0.8928	0.1072	0.8274	Plantaginis Herba	Baicalin	64982	FALSE	c12c(c(c(c(c2)OC2OC(C(C(C2O)O)O)C(=O)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002776	0.8928	0.1072	0.8274	Oroxyli Semen	Baicalin	64982	FALSE	c12c(c(c(c(c2)OC2OC(C(C(C2O)O)O)C(=O)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002776	0.8928	0.1072	0.8274	Carthami Flos	Baicalin	64982	FALSE	c12c(c(c(c(c2)OC2OC(C(C(C2O)O)O)C(=O)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002776	0.8928	0.1072	0.8274	Fructussophorae	Baicalin	64982	FALSE	c12c(c(c(c(c2)OC2OC(C(C(C2O)O)O)C(=O)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002776	0.8928	0.1072	0.8274	Radix Salviae	Baicalin	64982	FALSE	c12c(c(c(c(c2)OC2OC(C(C(C2O)O)O)C(=O)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002776	0.8928	0.1072	0.8274	Radix Bupleuri	Baicalin	64982	FALSE	c12c(c(c(c(c2)OC2OC(C(C(C2O)O)O)C(=O)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002776	0.8928	0.1072	0.8274	Radix Paeoniae Rubra	Baicalin	64982	FALSE	c12c(c(c(c(c2)OC2OC(C(C(C2O)O)O)C(=O)O)O)O)c(=O)cc(o1)c1ccccc1
MOL002777	0.8332	0.1668	0.7416	Carthami Flos	124604-44-0	5352706	FALSE	C/C=C/C#CC#CC#C/C=C\C=C
MOL002778	0.9083	0.0917	0.8469	Carthami Flos	THZ	7222	FALSE	c12c(scn1)cccc2
MOL002778	0.9083	0.0917	0.8469	Platycodon Grandiforus	THZ	7222	FALSE	c12c(scn1)cccc2
MOL002778	0.9083	0.0917	0.8469	Dalbergiae Odoriferae Lignum	THZ	7222	FALSE	c12c(scn1)cccc2
MOL002778	0.9083	0.0917	0.8469	Typhonii Rhizoma	THZ	7222	FALSE	c12c(scn1)cccc2
MOL002778	0.9083	0.0917	0.8469	Cornus Officinalis Sieb. Et Zucc.	THZ	7222	FALSE	c12c(scn1)cccc2
MOL002778	0.9083	0.0917	0.8469	Momordicae Fructus	THZ	7222	FALSE	c12c(scn1)cccc2
MOL002778	0.9083	0.0917	0.8469	Ginseng Folium	THZ	7222	FALSE	c12c(scn1)cccc2
MOL002779	0.7568	0.2432	0.7440	Carthami Flos	carthamin-precursor	Not Available	FALSE	C1(C(C(C(OC1CO)CC1(C(=C(C(=O)C(=C1O)C(C1=C(C(C(=C(C(=O)/C=C/c2ccc(cc2)O)C1=O)O)(O)CC1OC(C(C(C1O)O)O)CO)O)C(=O)O)C(=O)/C=C\c1ccc(cc1)O)O)O)O)O)O
MOL002780	0.7394	0.2606	0.7430	Carthami Flos	carthamin	Not Available	FALSE	C1(CC2=C(C(C(=C(C2=O)C(=O)/C=C\c2ccc(cc2)O)O)(OC2OC(C(C(C2O)O)O)CO)O)O)C(=O)C(C(=C(C1=O)C(=O)/C=C/c1ccc(cc1)O)O)(OC1OC(C(C(C1O)O)O)CO)O
MOL002781	0.9062	0.0938	0.7569	Carthami Flos	carthamone	Not Available	FALSE	O1C(C(O)C(O)C(O)C1OC1=C(C(=CC(=O)C1=O)O)C(=O)/C=C/c1ccc(O)cc1)CO

MOL002783	0.9223	0.0777	0.9720	Carthami Flos	Cumalic acid	68141	FALSE	c1(C(=O)O)ccc(=O)oc1
MOL002783	0.9223	0.0777	0.9720	Herbahypericiperforati	Cumalic acid	68141	FALSE	c1(C(=O)O)ccc(=O)oc1
MOL002783	0.9223	0.0777	0.9720	Lycii Fructus	Cumalic acid	68141	FALSE	c1(C(=O)O)ccc(=O)oc1
MOL002783	0.9223	0.0777	0.9720	Notopterygii Rhizoma Et Radix	Cumalic acid	68141	FALSE	c1(C(=O)O)ccc(=O)oc1
MOL002783	0.9223	0.0777	0.9720	Paederiae Scandentis Herba	Cumalic acid	68141	FALSE	c1(C(=O)O)ccc(=O)oc1
MOL002783	0.9223	0.0777	0.9720	Siegesbeckiae Herba	Cumalic acid	68141	FALSE	c1(C(=O)O)ccc(=O)oc1
MOL002784	0.8959	0.1041	0.7771	A. Dahurica (Fisch.) Benth. Et Hook	CYCLODODECANOL	15595	FALSE	C1CCCCCCC(CCCC1)O
MOL002784	0.8959	0.1041	0.7771	Carthami Flos	CYCLODODECANOL	15595	FALSE	C1CCCCCCC(CCCC1)O
MOL002785	0.7727	0.2273	0.7256	Carthami Flos	deca-4,6-diynyl 3-methylbutanoate	528753	FALSE	CC(CC(=O)OCCCC#CC#CCCC)C
MOL002786	0.9394	0.0606	0.9600	Cortex Moutan	Apocynin	2214	FALSE	c1(cc(ccc1O)C(=O)C)OC
MOL002786	0.9394	0.0606	0.9600	Picrorhizae Rhizoma	Apocynin	2214	FALSE	c1(cc(ccc1O)C(=O)C)OC
MOL002786	0.9394	0.0606	0.9600	Violsse Herba	Apocynin	2214	FALSE	c1(cc(ccc1O)C(=O)C)OC
MOL002786	0.9394	0.0606	0.9600	Radix Cynanchi	Apocynin	2214	FALSE	c1(cc(ccc1O)C(=O)C)OC
MOL002786	0.9394	0.0606	0.9600	Gypsophila Licentiana Hand.-Mazz.	Apocynin	2214	FALSE	c1(cc(ccc1O)C(=O)C)OC
MOL002786	0.9394	0.0606	0.9600	Radix Bupleuri	Apocynin	2214	FALSE	c1(cc(ccc1O)C(=O)C)OC
MOL002786	0.9394	0.0606	0.9600	Iridis Tectori Rhizoma	Apocynin	2214	FALSE	c1(cc(ccc1O)C(=O)C)OC
MOL002786	0.9394	0.0606	0.9600	Belamcandae Rhizome	Apocynin	2214	FALSE	c1(cc(ccc1O)C(=O)C)OC
MOL002786	0.9394	0.0606	0.9600	Radix Cynanchi Paniculati	Apocynin	2214	FALSE	c1(cc(ccc1O)C(=O)C)OC
MOL002786	0.9394	0.0606	0.9600	Apocyniveneti Folium	Apocynin	2214	FALSE	c1(cc(ccc1O)C(=O)C)OC
MOL002787	0.8285	0.1715	0.7708	Picrorhizae Rhizoma	6-Feruloylcatalpol	Not Available	FALSE	c1(c(ccc(c1)/C=C\C(=O)OC1C2C(C3C1C=COC3OC1OC(C(C(C1O)O)O)CO)(O2)CO)O)OC
MOL002788	0.6998	0.3002	0.7518	Picrorhizae Rhizoma	6-Feruloylcatalpol_qt	Not Available	FALSE	c1(c(ccc(c1)/C=C/C(=O)OC1C2C(C3C1C=COC3O)(O2)CO)O)OC
MOL002789	0.6249	0.3751	0.6889	Picrorhizae Rhizoma	hemiphroside A	Not Available	FALSE	O(C1C(O)C(OC2C(O)C(O)C(O)C(O2)CO)C(C(O1)CO)OC(=O)/C=C\c1cc(c(cc1)O)OC)CCc1cc(c(cc1)OC)O
MOL002790	0.5141	0.4859	0.6476	Picrorhizae Rhizoma	hemiphroside A_qt	Not Available	FALSE	O(C1C(O)C(O)C(C(O1)CO)OC(=O)/C=C\c1cc(c(cc1)O)OC)CCc1cc(c(cc1)OC)O
MOL002791	0.8993	0.1007	0.7049	Picrorhizae Rhizoma	pikuroside	Not Available	FALSE	O1C2OCC3(C(C(C(C3O)OC(=O)c3cc(c(cc3)O)OC)C2)C1OC1OC(C(C(C1O)O)O)CO)O
MOL002792	0.8970	0.1030	0.7257	Picrorhizae Rhizoma	pikuroside_qt	Not Available	FALSE	O1C2OCC3(C(C(C(C3O)OC(=O)c3cc(c(cc3)O)OC)C2)C1O)O
MOL002795	0.7184	0.2816	0.7004	Picrorhizae Rhizoma	scrophuloside A	Not Available	FALSE	O1C(OC2OC(C(O)C(O)C2O)CO)C2C(CC(OC(=O)/C=C\c3ccc(OC)cc3)C2C)C(=C1)C(=O)O

MOL002797	0.7913	0.2087	0.7520	Picrorhizae Rhizoma	specioside	Not Available	FALSE	O1C(=O)C=C(C(Cc2c1cc(cc2)O)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)O
MOL002799	0.8735	0.1265	0.8038	Picrorhizae Rhizoma	verminoside	Not Available	FALSE	O1C2(C1C(OC(=O)/C=C/c1cc(O)c(O)cc1)C1C2C(OC=C1)OC1OC(C(O)C(O)C1O)CO)CO
MOL002800	0.8136	0.1864	0.8039	Picrorhizae Rhizoma	verminoside_qt	Not Available	FALSE	O1C2(C1C(OC(=O)/C=C/c1cc(O)c(O)cc1)C1C2C(OC=C1)O)CO
MOL002801	0.9304	0.0696	0.8540	Picrorhizae Rhizoma	1-[3-methoxy-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]ethanone	20055279	FALSE	C(=O)(C)c1cc(c(cc1)OC1C(O)C(O)C(O)C(O1)CO)OC
MOL002803	0.5173	0.4827	0.8500	Picrorhizae Rhizoma	Arvenin I	6441104	FALSE	C1(=O)C(CC2C(=CCC3C4(C)CC(C(C(C(=O)/C=C/C(C)(C)OC(=O)C)(C)O)C4(C)CC(=O)C23C)O)C1(C)C)OC1C(O)C(O)C(O)C(O1)CO
MOL002804	0.5555	0.4445	0.8481	Picrorhizae Rhizoma	MEGxp0_000823	21579640	FALSE	C1(=O)C(CC2C(=CCC3C4(C)CC(C(C(C(=O)/C=C/C(C)(C)O)(C)O)C4(C)CC(=O)C23C)O)C1(C)C)OC1C(O)C(O)C(O)C(O1)CO
MOL002805	0.3987	0.6013	0.7453	Picrorhizae Rhizoma	Elatericin A	5281318	FALSE	C1(=O)C(CC2C(=CCC3C4(C)CC(C(C(C(=O)/C=C/C(C)(C)O)(C)O)C4(C)CC(=O)C23C)O)C1(C)C)O
MOL002805	0.3987	0.6013	0.7453	Trichosanthis Radix	Elatericin A	5281318	FALSE	C1(=O)C(CC2C(=CCC3C4(C)CC(C(C(C(=O)/C=C/C(C)(C)O)(C)O)C4(C)CC(=O)C23C)O)C1(C)C)O
MOL002806	0.3788	0.6212	0.7664	Picrorhizae Rhizoma	CUCURBITACIN I	Not Available	FALSE	C12(C(C(C(C2)O)C(C(=O)/C=C/C(C)(C)O)(C)O)(CC(=O)C2(C1CC=C1C2C=C(C(=O)C1(C)C)O)C)C)C
MOL002807	0.7404	0.2596	0.7562	Picrorhizae Rhizoma	Picroside I	Not Available	FALSE	c1ccc(cc1)/C=C\C(=O)OCC12OC1C(C1C2C(OC=C1)OC1C(C(C(C(O1)CO)O)O)O)O
MOL002808	0.6107	0.3893	0.6374	Picrorhizae Rhizoma	Picroside I_qt	Not Available	FALSE	c1ccc(cc1)/C=C\C(=O)OCC12OC1C(C1C2C(OC=C1)O)O
MOL002809	0.8596	0.1404	0.7435	Picrorhizae Rhizoma	Picroside II	Not Available	FALSE	c1(c(cc(cc1)C(=O)OC1C2C(C3(C1O3)CO)C(OC=C2)OC1C(C(C(C(O1)CO)O)O)O)OC)O
MOL002810	0.8268	0.1732	0.7304	Picrorhizae Rhizoma	Picroside II_qt	Not Available	FALSE	c1(c(cc(cc1)C(=O)OC1C2C(C3(C1O3)CO)C(OC=C2)O)OC)O
MOL002811	0.7785	0.2215	0.7523	Picrorhizae Rhizoma	Picroside III	Not Available	FALSE	C1=CC2C(C(O1)OC1(C(O)C(C(C(O1)COC(=O)/C=C\c1cc(c(cc1)O)OC)O)O)C)C1(C(C2O)O1)CO
MOL002812	0.6766	0.3234	0.7829	Picrorhizae Rhizoma	PICROSIDE I	Not Available	FALSE	C1=CC2C(C(O1)OC1OC(C(C(C1O)O)O)O)CCC(=O)/C=C\c1ccccc1)C1(C(C2O)O1)CO
MOL002813	0.9292	0.0708	0.8745	Picrorhizae Rhizoma	Aucubin	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)(CO)O)C1C2C(C=CO1)CC=C2CO
MOL002814	0.9576	0.0424	0.8822	Picrorhizae Rhizoma	Aucubin_qt	Not Available	FALSE	OC1C2C(C=CO1)CC=C2CO
MOL002815	0.9336	0.0664	0.9400	Picrorhizae Rhizoma	Arbutin	Not Available	FALSE	c1(ccc(cc1)OC1OC(C(C(C1O)O)O)O)CO)O
MOL002816	0.9099	0.0901	0.9288	Peucedani Radix	Bergenin	66065	FALSE	C1(c(cc2c(c1O)OC1C(OC2=O)C(C(C(O1)CO)O)O)O)OC

MOL002816	0.9099	0.0901	0.9288	Picrorhizae Rhizoma	Bergenin	66065	FALSE	C1(C(CC2(C1O)C1C(OC2=O)C(C(C(O1)CO)O)O)O)O
MOL002816	0.9099	0.0901	0.9288	Ardisiae Japonicae Herba	Bergenin	66065	FALSE	C1(C(CC2(C1O)C1C(OC2=O)C(C(C(O1)CO)O)O)O)O
MOL002816	0.9099	0.0901	0.9288	Saxifraga Stolonifera	Bergenin	66065	FALSE	C1(C(CC2(C1O)C1C(OC2=O)C(C(C(O1)CO)O)O)O)O
MOL002817	0.9252	0.0748	0.8663	Ephedra Herba	Picein	92123	FALSE	C(=O)(C)c1ccc(cc1)OC1C(O)C(O)C(O)C(O1)CO
MOL002817	0.9252	0.0748	0.8663	Picrorhizae Rhizoma	Picein	92123	FALSE	C(=O)(C)c1ccc(cc1)OC1C(O)C(O)C(O)C(O1)CO
MOL002817	0.9252	0.0748	0.8663	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	Picein	92123	FALSE	C(=O)(C)c1ccc(cc1)OC1C(O)C(O)C(O)C(O1)CO
MOL002818	0.9410	0.0590	0.9619	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	Piceol	7469	FALSE	C(=O)(C)c1ccc(cc1)O
MOL002818	0.9410	0.0590	0.9619	Belamcandae Rhizome	Piceol	7469	FALSE	C(=O)(C)c1ccc(cc1)O
MOL002818	0.9410	0.0590	0.9619	Daturae Flos	Piceol	7469	FALSE	C(=O)(C)c1ccc(cc1)O
MOL002818	0.9410	0.0590	0.9619	Radix Cynanchi	Piceol	7469	FALSE	C(=O)(C)c1ccc(cc1)O
MOL002818	0.9410	0.0590	0.9619	Artemisiae Scopariae Herba	Piceol	7469	FALSE	C(=O)(C)c1ccc(cc1)O
MOL002818	0.9410	0.0590	0.9619	Ephedra Herba	Piceol	7469	FALSE	C(=O)(C)c1ccc(cc1)O
MOL002818	0.9410	0.0590	0.9619	Picrorhizae Rhizoma	Piceol	7469	FALSE	C(=O)(C)c1ccc(cc1)O
MOL002818	0.9410	0.0590	0.9619	Rhododendri Daurici Folium	Piceol	7469	FALSE	C(=O)(C)c1ccc(cc1)O
MOL002818	0.9410	0.0590	0.9619	Saxifraga Stolonifera	Piceol	7469	FALSE	C(=O)(C)c1ccc(cc1)O
MOL002818	0.9410	0.0590	0.9619	Trollius Chinensis	Piceol	7469	FALSE	C(=O)(C)c1ccc(cc1)O
MOL002818	0.9410	0.0590	0.9619	Apocyniveneti Folium	Piceol	7469	FALSE	C(=O)(C)c1ccc(cc1)O
MOL002818	0.9410	0.0590	0.9619	Radix Cynanchi Paniculati	Piceol	7469	FALSE	C(=O)(C)c1ccc(cc1)O
MOL002819	0.9229	0.0771	0.8448	Plantaginis Semen	catalpol	91520	FALSE	C1=CC2C(C(O1)OC1C(O)C(C(C(O1)CO)O)O)C1(C(C2O)O1)CO
MOL002819	0.9229	0.0771	0.8448	Picrorhizae Rhizoma	catalpol	91520	FALSE	C1=CC2C(C(O1)OC1C(O)C(C(C(O1)CO)O)O)C1(C(C2O)O1)CO
MOL002819	0.9229	0.0771	0.8448	Buddlejae Flos	catalpol	91520	FALSE	C1=CC2C(C(O1)OC1C(O)C(C(C(O1)CO)O)O)C1(C(C2O)O1)CO
MOL002819	0.9229	0.0771	0.8448	Rehmanniae Radix Praeparata	catalpol	91520	FALSE	C1=CC2C(C(O1)OC1C(O)C(C(C(O1)CO)O)O)C1(C(C2O)O1)CO
MOL002820	0.9188	0.0812	0.7906	Picrorhizae Rhizoma	catapol_qt	Not Available	FALSE	C1=CC2C(C(O1)O)C1(C(C2O)O1)CO
MOL002820	0.9188	0.0812	0.7906	Buddlejae Flos	catapol_qt	Not Available	FALSE	C1=CC2C(C(O1)O)C1(C(C2O)O1)CO
MOL002820	0.9188	0.0812	0.7906	Figwort Root	catapol_qt	Not Available	FALSE	C1=CC2C(C(O1)O)C1(C(C2O)O1)CO
MOL002820	0.9188	0.0812	0.7906	Rehmanniae Radix Praeparata	catapol_qt	Not Available	FALSE	C1=CC2C(C(O1)O)C1(C(C2O)O1)CO
MOL002821	0.9325	0.0675	0.9424	Picrorhizae Rhizoma	D-Mannoheptulose	Not Available	FALSE	OCC(O)C(C(O)C(C(=O)CO)O)O
MOL002821	0.9325	0.0675	0.9424	Capsellae Herba	D-Mannoheptulose	Not Available	FALSE	OCC(O)C(C(O)C(C(=O)CO)O)O

MOL002821	0.9325	0.0675	0.9424	Corayceps	D-Mannoheptulose	Not Available	FALSE	OCC(O)C(C(O)C(C(=O)CO)O)O
MOL002821	0.9325	0.0675	0.9424	Fructus Ligustri Lucidi	D-Mannoheptulose	Not Available	FALSE	OCC(O)C(C(O)C(C(=O)CO)O)O
MOL002822	0.9046	0.0954	0.8078	Picrorhizae Rhizoma	Mingjinianuronide A	Not Available	FALSE	C1(C(C(C(OC1C(=O)O)Oc1cc(c2c(c1O)oc(c(c2=O)O)c1ccc(cc1)O)O)O)O)O
MOL002823	0.9299	0.0701	0.9084	Cotyledon Fimbriata Turcz.	Herbacetin	5280544	FALSE	c1(cc(c2c(c1O)oc(c(c2=O)O)c1ccc(cc1)O)O)O
MOL002823	0.9299	0.0701	0.9084	Picrorhizae Rhizoma	Herbacetin	5280544	FALSE	c1(cc(c2c(c1O)oc(c(c2=O)O)c1ccc(cc1)O)O)O
MOL002823	0.9299	0.0701	0.9084	Ephedra Herba	Herbacetin	5280544	FALSE	c1(cc(c2c(c1O)oc(c(c2=O)O)c1ccc(cc1)O)O)O
MOL002823	0.9299	0.0701	0.9084	Equiseti Hiemalis Herba	Herbacetin	5280544	FALSE	c1(cc(c2c(c1O)oc(c(c2=O)O)c1ccc(cc1)O)O)O
MOL002824	0.8596	0.1404	0.7435	Picrorhizae Rhizoma	Picroside II	Not Available	FALSE	C1=CC2C(C(O1)OC1OC(C(C(C1O)O)O)CO)C1(C(C2OC(=O)c2cc(c(cc2)O)OC)O1)CO
MOL002825	0.8268	0.1732	0.7304	Picrorhizae Rhizoma	Picroside II_qt	Not Available	FALSE	C1=CC2C(C(O1)O)C1(C(C2OC(=O)c2cc(c(cc2)O)OC)O1)CO
MOL002826	0.8981	0.1019	0.7798	Picrorhizae Rhizoma	Picrotin	Not Available	FALSE	C12(C3C(C(C4(C1(C1(C(=O)O2)C(C4)O1)C)O)C(=O)O3)C(C)(C)O)C
MOL002827	0.9541	0.0459	0.7681	Piperis Fructus	(1S)-(+)-3-Carene	Not Available	FALSE	C12CC(=CCC1C2(C)C)C
MOL002827	0.9541	0.0459	0.7681	Caryophylliflos	(1S)-(+)-3-Carene	Not Available	FALSE	C12CC(=CCC1C2(C)C)C
MOL002828	0.9630	0.0370	0.9740	Piperis Fructus	1(7),2-p-Menthadien-6-ol	Not Available	FALSE	C1(CC(C=CC1=C)C(C)C)O
MOL002829	0.9598	0.0402	0.9671	Piperis Fructus	trans-p-2-Menthen-1-ol	5319367	FALSE	C1(CCC(C=C1)C(C)C)(C)O
MOL002830	0.8927	0.1073	0.9559	Angelicae Sinensis Radix	PCR	2879	FALSE	c1(ccc(cc1)O)C
MOL002830	0.8927	0.1073	0.9559	Junci Medulla	PCR	2879	FALSE	c1(ccc(cc1)O)C
MOL002830	0.8927	0.1073	0.9559	Piperis Fructus	PCR	2879	FALSE	c1(ccc(cc1)O)C
MOL002830	0.8927	0.1073	0.9559	Mori Follum	PCR	2879	FALSE	c1(ccc(cc1)O)C
MOL002830	0.8927	0.1073	0.9559	Bomboo Juice	PCR	2879	FALSE	c1(ccc(cc1)O)C
MOL002830	0.8927	0.1073	0.9559	Capsici Fructus	PCR	2879	FALSE	c1(ccc(cc1)O)C
MOL002830	0.8927	0.1073	0.9559	Radix Angelicae Biseratae	PCR	2879	FALSE	c1(ccc(cc1)O)C
MOL002830	0.8927	0.1073	0.9559	Ephedra Herba	PCR	2879	FALSE	c1(ccc(cc1)O)C
MOL002830	0.8927	0.1073	0.9559	Mume Flos	PCR	2879	FALSE	c1(ccc(cc1)O)C
MOL002830	0.8927	0.1073	0.9559	Radix Bupleuri	PCR	2879	FALSE	c1(ccc(cc1)O)C
MOL002831	0.9540	0.0460	0.9704	Piperis Fructus	(1R)-4-isopropenyl-1-methyl-1-cyclohex-3-enol	5319364	FALSE	C1CC(=CCC1(O)C)C(=C)C

MOL002832	0.9069	0.0931	0.9730	Piperis Fructus	3-Cyclohexene-1-methanol	12299191	FALSE	C1(CCC=CC1)CO
MOL002833	0.9504	0.0496	0.9750	Piperis Fructus	1-(4-methylenecyclohexyl)ethenol	5319362	FALSE	C1CC(CCC1=C)C(=C)O
MOL002834	0.9352	0.0648	0.9211	Kaempferiae Rhizoma	Ethylcinnamate	637758	FALSE	c1(/C=C/C(=O)OCC)ccccc1
MOL002834	0.9352	0.0648	0.9211	Benzoinum	Ethylcinnamate	637758	FALSE	c1(/C=C/C(=O)OCC)ccccc1
MOL002834	0.9352	0.0648	0.9211	Piperis Fructus	Ethylcinnamate	637758	FALSE	c1(/C=C/C(=O)OCC)ccccc1
MOL002835	0.8526	0.1474	0.6851	Evodiae Fructus	δ-cadinol	12306055	FALSE	C1(CCC(=C2CCC(=CC12)C)C)C(C)C
MOL002835	0.8526	0.1474	0.6851	Ardisiae Japonicae Herba	δ-cadinol	12306055	FALSE	C1(CCC(=C2CCC(=CC12)C)C)C(C)C
MOL002835	0.8526	0.1474	0.6851	Piperis Fructus	δ-cadinol	12306055	FALSE	C1(CCC(=C2CCC(=CC12)C)C)C(C)C
MOL002835	0.8526	0.1474	0.6851	Aristolochiae Fructus	δ-cadinol	12306055	FALSE	C1(CCC(=C2CCC(=CC12)C)C)C(C)C
MOL002835	0.8526	0.1474	0.6851	Pogostemon Cablin (Blanco) Benth.	δ-cadinol	12306055	FALSE	C1(CCC(=C2CCC(=CC12)C)C)C(C)C
MOL002835	0.8526	0.1474	0.6851	Radix Salviae	δ-cadinol	12306055	FALSE	C1(CCC(=C2CCC(=CC12)C)C)C(C)C
MOL002835	0.8526	0.1474	0.6851	Rhododendri Daurici Folium	δ-cadinol	12306055	FALSE	C1(CCC(=C2CCC(=CC12)C)C)C(C)C
MOL002835	0.8526	0.1474	0.6851	Moslae Herba	δ-cadinol	12306055	FALSE	C1(CCC(=C2CCC(=CC12)C)C)C(C)C
MOL002836	0.9426	0.0574	0.9653	Cinnanmomi Cortex	anisaldehyde	31244	FALSE	c1(ccc(cc1)OC)C=O
MOL002836	0.9426	0.0574	0.9653	Cinnamomi Ramulus	anisaldehyde	31244	FALSE	c1(ccc(cc1)OC)C=O
MOL002836	0.9426	0.0574	0.9653	Piperis Fructus	anisaldehyde	31244	FALSE	c1(ccc(cc1)OC)C=O
MOL002836	0.9426	0.0574	0.9653	Kaempferiae Rhizoma	anisaldehyde	31244	FALSE	c1(ccc(cc1)OC)C=O
MOL002836	0.9426	0.0574	0.9653	Siphonostegiae Herba	anisaldehyde	31244	FALSE	c1(ccc(cc1)OC)C=O
MOL002836	0.9426	0.0574	0.9653	Eriobotryae Folium	anisaldehyde	31244	FALSE	c1(ccc(cc1)OC)C=O
MOL002836	0.9426	0.0574	0.9653	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	anisaldehyde	31244	FALSE	c1(ccc(cc1)OC)C=O
MOL002836	0.9426	0.0574	0.9653	Foeniculi Fructus	anisaldehyde	31244	FALSE	c1(ccc(cc1)OC)C=O
MOL002836	0.9426	0.0574	0.9653	Anisi Stellati Fructus	anisaldehyde	31244	FALSE	c1(ccc(cc1)OC)C=O
MOL002837	0.7217	0.2783	0.6166	Piperis Fructus	5,10(15)-cadiene-4-ol	Not Available	FALSE	C12=CC(CCC1C(=C)CCC2C(C)C)(C)C
MOL002838	0.9274	0.0726	0.9471	Piperis Fructus	6-Methylheptan-2-one	13572	FALSE	C(CCCC(=O)C)(C)C
MOL002838	0.9274	0.0726	0.9471	Ephedra Herba	6-Methylheptan-2-one	13572	FALSE	C(CCCC(=O)C)(C)C
MOL002839	0.9462	0.0538	0.9372	Piperis Fructus	chavicol	68148	FALSE	c1c(ccc(c1)O)CC=C
MOL002839	0.9462	0.0538	0.9372	Ginkgo Folium	chavicol	68148	FALSE	c1c(ccc(c1)O)CC=C

MOL002839	0.9462	0.0538	0.9372	Caryophylliflos	chavicol	68148	FALSE	c1c(ccc(c1)O)CC=C
MOL002839	0.9462	0.0538	0.9372	Magnolia Officinalis Rehd Et Wils.	chavicol	68148	FALSE	c1c(ccc(c1)O)CC=C
MOL002839	0.9462	0.0538	0.9372	Mume Flos	chavicol	68148	FALSE	c1c(ccc(c1)O)CC=C
MOL002840	0.5790	0.4210	0.7048	Piperis Fructus	Cryptopimaric acid	221580	FALSE	C1CC(C2C(C1)(C1C(=CC(CC1)(C=C)C)CC2)C)(C(=O)O)C
MOL002841	0.9514	0.0486	0.8109	Artemisia Annua L.	l-alpha-Fenchone	82229	FALSE	C12(C(=O)C(C(C1)CC2)(C)C)C
MOL002841	0.9514	0.0486	0.8109	Prunellae Spica	l-alpha-Fenchone	82229	FALSE	C12(C(=O)C(C(C1)CC2)(C)C)C
MOL002841	0.9514	0.0486	0.8109	Piperis Fructus	l-alpha-Fenchone	82229	FALSE	C12(C(=O)C(C(C1)CC2)(C)C)C
MOL002841	0.9514	0.0486	0.8109	Cinnanmomi Cortex	l-alpha-Fenchone	82229	FALSE	C12(C(=O)C(C(C1)CC2)(C)C)C
MOL002842	0.9294	0.0706	0.9777	Piperis Fructus	NFP	17429	FALSE	N1(CCCCC1)C=O
MOL002844	0.9121	0.0879	0.9154	licorice	Pinocembrin	68071	FALSE	c1c(c2c(cc1O)OC(CC2=O)c1ccccc1)O
MOL002844	0.9121	0.0879	0.9154	Piperis Fructus	Pinocembrin	68071	FALSE	c1c(c2c(cc1O)OC(CC2=O)c1ccccc1)O
MOL002845	0.9533	0.0467	0.9684	Piperis Fructus	2-[(1R)-4-methyl-1-cyclohex-3-enyl]prop-2-enyl acetate	11333027	FALSE	C1C(=CCC(C1)C(=C)COC(=O)C)C
MOL002847	0.1422	0.8578	0.8287	Piperis Fructus	Piperolein B	Not Available	FALSE	N1(CCCCC1)C(=O)CCCCCC/C=C\c1cc2OCOc2cc1
MOL002848	0.9115	0.0885	0.7937	Piperis Fructus	cis-Piplartine	643764	FALSE	C1=CCCN(C1=O)C(=O)/C=C\c1cc(c(c(c1)OC)OC)O C
MOL002849	0.8537	0.1463	0.8216	Piperis Fructus	Pyrrolidine, 1-((2E,4E)-1-oxo-2,4-decadienyl)-	6440616	FALSE	N1(CCCC1)C(=O)/C=C/C=C/CCCCC
MOL002850	0.8881	0.1119	0.6017	Santalum Album L.	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002850	0.8881	0.1119	0.6017	Piperis Fructus	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002850	0.8881	0.1119	0.6017	Lysimachiae Foenigraeci Herba	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002850	0.8881	0.1119	0.6017	Aucklandiae Radix	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002850	0.8881	0.1119	0.6017	Cornus Officinalis Sieb. Et Zucc.	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C

MOL002850	0.8881	0.1119	0.6017	Ginseng Folium	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002850	0.8881	0.1119	0.6017	Morindae Officinalis Radix	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002850	0.8881	0.1119	0.6017	Gypsophila Licentiana Hand.-Mazz.	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002850	0.8881	0.1119	0.6017	Amygdalus Communis Vas	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002850	0.8881	0.1119	0.6017	Sesami Nigrum Semen	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002850	0.8881	0.1119	0.6017	Chebulae Fructus	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002850	0.8881	0.1119	0.6017	Mori Fructus	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002850	0.8881	0.1119	0.6017	Litchi Semen	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002850	0.8881	0.1119	0.6017	Linderae Radix	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002850	0.8881	0.1119	0.6017	Celastri Orbiculati Fructus	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002850	0.8881	0.1119	0.6017	Hippophae Fructus	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002850	0.8881	0.1119	0.6017	Capsellae Herba	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002850	0.8881	0.1119	0.6017	licorice	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002850	0.8881	0.1119	0.6017	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C

MOL002850	0.8881	0.1119	0.6017	Humulus Scandens (Lour.) Merr.	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002850	0.8881	0.1119	0.6017	Pogostemon Cablin (Blanco) Benth.	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002850	0.8881	0.1119	0.6017	Allii Fistulost Bulbus	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002850	0.8881	0.1119	0.6017	Arecae Semen	butylated hydroxytoluene	31404	FALSE	c1(c(c(C(C)(C)C)cc(c1)C)O)C(C)(C)C
MOL002851	0.8035	0.1965	0.6474	Citri Sarcodactylis Fructus	ZINC05224268	Not Available	FALSE	O1C2(C1CCC(=C)C1C(C(C1)(C)C)CC2)C
MOL002851	0.8035	0.1965	0.6474	Piperis Fructus	ZINC05224268	Not Available	FALSE	O1C2(C1CCC(=C)C1C(C(C1)(C)C)CC2)C
MOL002851	0.8035	0.1965	0.6474	Rubi Fructus	ZINC05224268	Not Available	FALSE	O1C2(C1CCC(=C)C1C(C(C1)(C)C)CC2)C
MOL002851	0.8035	0.1965	0.6474	Aurantii Fructus	ZINC05224268	Not Available	FALSE	O1C2(C1CCC(=C)C1C(C(C1)(C)C)CC2)C
MOL002851	0.8035	0.1965	0.6474	Mahoniae Folum	ZINC05224268	Not Available	FALSE	O1C2(C1CCC(=C)C1C(C(C1)(C)C)CC2)C
MOL002851	0.8035	0.1965	0.6474	Ailanthi Cortex	ZINC05224268	Not Available	FALSE	O1C2(C1CCC(=C)C1C(C(C1)(C)C)CC2)C
MOL002851	0.8035	0.1965	0.6474	Campsis Flos	ZINC05224268	Not Available	FALSE	O1C2(C1CCC(=C)C1C(C(C1)(C)C)CC2)C
MOL002851	0.8035	0.1965	0.6474	Dichroae Radix	ZINC05224268	Not Available	FALSE	O1C2(C1CCC(=C)C1C(C(C1)(C)C)CC2)C
MOL002851	0.8035	0.1965	0.6474	Echinopsis Radix	ZINC05224268	Not Available	FALSE	O1C2(C1CCC(=C)C1C(C(C1)(C)C)CC2)C
MOL002851	0.8035	0.1965	0.6474	Ginkgo Folium	ZINC05224268	Not Available	FALSE	O1C2(C1CCC(=C)C1C(C(C1)(C)C)CC2)C
MOL002851	0.8035	0.1965	0.6474	Mahoniae Caulis	ZINC05224268	Not Available	FALSE	O1C2(C1CCC(=C)C1C(C(C1)(C)C)CC2)C
MOL002851	0.8035	0.1965	0.6474	Polygoni Orientalis Fructus	ZINC05224268	Not Available	FALSE	O1C2(C1CCC(=C)C1C(C(C1)(C)C)CC2)C
MOL002851	0.8035	0.1965	0.6474	Aristolochiae Fructus	ZINC05224268	Not Available	FALSE	O1C2(C1CCC(=C)C1C(C(C1)(C)C)CC2)C
MOL002852	0.8602	0.1398	0.8976	Piperis Fructus	coumaperine	Not Available	FALSE	C(=O)(/C=C/C=C\c1ccc(cc1)O)N1CCCCC1
MOL002853	0.9376	0.0624	0.7069	Caryophylliflos	cyclofenchene	Not Available	FALSE	C12(C3C(C(CC13)C2)(C)C)C
MOL002853	0.9376	0.0624	0.7069	Rhizome Of Whiteback Greenbrier	cyclofenchene	Not Available	FALSE	C12(C3C(C(CC13)C2)(C)C)C
MOL002853	0.9376	0.0624	0.7069	Piperis Fructus	cyclofenchene	Not Available	FALSE	C12(C3C(C(CC13)C2)(C)C)C

MOL002853	0.9376	0.0624	0.7069	Lilii Bulbus	cyclofenchene	Not Available	FALSE	C12(C3C(C(CC13)C2)(C)C)C
MOL002853	0.9376	0.0624	0.7069	Hippophae Fructus	cyclofenchene	Not Available	FALSE	C12(C3C(C(CC13)C2)(C)C)C
MOL002854	0.9570	0.0430	0.9744	Lonicerae Japonicae Flos	(1R,2R,4R)-Dihydrocarveol	443163	FALSE	C1(CC(C(CC1)C)O)C(=C)C
MOL002854	0.9570	0.0430	0.9744	Piperis Fructus	(1R,2R,4R)-Dihydrocarveol	443163	FALSE	C1(CC(C(CC1)C)O)C(=C)C
MOL002854	0.9570	0.0430	0.9744	Ephedra Herba	(1R,2R,4R)-Dihydrocarveol	443163	FALSE	C1(CC(C(CC1)C)O)C(=C)C
MOL002854	0.9570	0.0430	0.9744	Ecliptae Herba	(1R,2R,4R)-Dihydrocarveol	443163	FALSE	C1(CC(C(CC1)C)O)C(=C)C
MOL002855	0.7908	0.2092	0.9312	Piperis Fructus	5-(4-hydroxy-3-methoxy-phenyl)-1-piperidino-penta-2,4-dien-1-one	6290038	FALSE	N1(CCCCC1)C(=O)/C=C/C=C/c1cc(c(cc1)O)OC
MOL002856	0.8257	0.1743	0.6972	Piperis Fructus	1,8,8-trimethyl-5-methylenecycloundeca-1,6-diene	5846461	FALSE	C1(/C=C\C(=C)CC/C=C(\CCC1)/C)(C)C
MOL002857	0.1939	0.8061	0.6545	Piperis Fructus	55038-30-7	6442405	FALSE	O1c2cc(/C=C/CCCCCC/C=C/C=C/C(=O)NCC(C)C)ccc2OC1
MOL002858	0.9646	0.0354	0.9307	Piperis Fructus	1-(2-methoxypropan-2-yl)-4-methylbenzene	14121774	FALSE	Cc1ccc(cc1)C(C)(C)OC
MOL002859	0.9505	0.0495	0.9595	Piperis Fructus	(1S,6R)-6-isopropyl-3-methyl-1-cyclohex-3-enol	21604552	FALSE	C1(CC(=CCC1C(C)C)C)O
MOL002860	0.9559	0.0441	0.8307	Cyperi Rhizoma	(1S,3R,5S)-6,6-dimethyl-2-methylene-3-norpinanol	1201530	FALSE	OC1CC2C(C(C2)C1=C)(C)C

MOL002860	0.9559	0.0441	0.8307	Piperis Fructus	(1S,3R,5S)-6,6-dimethyl-2-methylene-3-norpinanol	1201530	FALSE	OC1CC2C(C(C2)C1=C)(C)C
MOL002861	0.6743	0.3257	0.8671	Piperis Longi Fructus	Piperanine	5320618	FALSE	C(=O)(/C=C/CCc1cc2OCOc2cc1)N1CCCCC1
MOL002861	0.6743	0.3257	0.8671	Piperis Fructus	Piperanine	5320618	FALSE	C(=O)(/C=C/CCc1cc2OCOc2cc1)N1CCCCC1
MOL002862	0.1900	0.8100	0.6938	Piperis Fructus	pipercide	Not Available	FALSE	C(=O)(/C=C/C=C/C=C/CC/C=C\c1cc2OCOc2cc1)NCC(C)C
MOL002863	0.4660	0.5340	0.8363	Piperis Fructus	(E)-7-(1,3-benzodioxol-5-yl)-1-piperidino-hept-6-en-1-one	11141599	FALSE	O=C(N1CCCCC1)CCCC/C=C/c1cc2OCOc2cc1
MOL002864	0.7530	0.2470	0.8510	Piperis Fructus	(2E,4Z)-5-(1,3-benzodioxol-5-yl)-1-piperidino-penta-2,4-dien-1-one	1548914	FALSE	C(=O)(/C=C/C=C\c1cc2OCOc2cc1)N1CCCCC1
MOL002865	0.8345	0.1655	0.8248	Piperis Fructus	Trichostachine	636537	FALSE	C(=O)(/C=C/C=C/c1ccc2OCOc2c1)N1CCCC1
MOL002866	0.2546	0.7454	0.7766	Piperis Fructus	(2E,4E,8E)-9-(1,3-benzodioxol-5-yl)-N-isobutylnona-2,4,8-trienamide	11012859	FALSE	O1c2c(OC1)ccc(c2)/C=C/CC/C=C/C=C/C(=O)NCC(C)C
MOL002868	0.8850	0.1150	0.8805	Lygodii Spora	1-Undecyne	75249	FALSE	C#CCCCCCCCCC
MOL002868	0.8850	0.1150	0.8805	Citrus Reticulata	1-Undecyne	75249	FALSE	C#CCCCCCCCCC
MOL002869	0.7906	0.2094	0.7117	Lygodii Spora	5,9-Tetradecadiyne	142832	FALSE	CCCCC#CCCC#CCCCC
MOL002870	0.9326	0.0674	0.9536	Lygodii Spora	Isoheptan-1-ol	12331	FALSE	C(CCCC(C)C)O
MOL002871	0.9334	0.0666	0.9558	Pogostemon Cablin (Blanco) Benth.	MIAK	8034	FALSE	CC(=O)CCC(C)C
MOL002871	0.9334	0.0666	0.9558	Lygodii Spora	MIAK	8034	FALSE	CC(=O)CCC(C)C
MOL002872	0.9222	0.0778	0.9221	Lygodii Spora	1-OCTYNE	12370	FALSE	C#CCCCCCC
MOL002873	0.9278	0.0722	0.9324	Lygodii Spora	ZINC02017307	1712076	FALSE	CC(CCCC(C=C)C)(O)C

MOL002875	0.4725	0.5275	0.6118	Coicis Semen	Methyl oleate	5280590	FALSE	C(=O)(CCCCCCC/C=C/CCCCCCCC)OC
MOL002875	0.4725	0.5275	0.6118	Lygodii Spora	Methyl oleate	5280590	FALSE	C(=O)(CCCCCCC/C=C/CCCCCCCC)OC
MOL002875	0.4725	0.5275	0.6118	Broussonetiae Fructus	Methyl oleate	5280590	FALSE	C(=O)(CCCCCCC/C=C/CCCCCCCC)OC
MOL002875	0.4725	0.5275	0.6118	Echinopsis Radix	Methyl oleate	5280590	FALSE	C(=O)(CCCCCCC/C=C/CCCCCCCC)OC
MOL002875	0.4725	0.5275	0.6118	Canarii Fructus	Methyl oleate	5280590	FALSE	C(=O)(CCCCCCC/C=C/CCCCCCCC)OC
MOL002876	0.9075	0.0925	0.9540	Lygodii Spora	2-HEXENOIC ACID	5282707	FALSE	C(=O)(/C=C/CCC)O
MOL002876	0.9075	0.0925	0.9540	Eriobotryae Folium	2-HEXENOIC ACID	5282707	FALSE	C(=O)(/C=C/CCC)O
MOL002877	0.9248	0.0752	0.7974	Lygodii Spora	2,4-Dimethylpentane-2,4-diol	141153	FALSE	CC(CC(C)(O)C)(O)C
MOL002878	0.9016	0.0984	0.9625	Lygodii Spora	WLN: L8VTJ	10403	FALSE	C1(=O)CCCCCCC1
MOL002879	0.2560	0.7440	0.6844	Capsici Fructus	Diop	33934	FALSE	c1(c(cccc1)C(=O)OCCCCCC(C)C)C(=O)OCCCCCC(C)C
MOL002879	0.2560	0.7440	0.6844	Morindae Officinalis Radix	Diop	33934	FALSE	c1(c(cccc1)C(=O)OCCCCCC(C)C)C(=O)OCCCCCC(C)C
MOL002879	0.2560	0.7440	0.6844	Lygodii Spora	Diop	33934	FALSE	c1(c(cccc1)C(=O)OCCCCCC(C)C)C(=O)OCCCCCC(C)C
MOL002879	0.2560	0.7440	0.6844	Radix Cirsii Japonici	Diop	33934	FALSE	c1(c(cccc1)C(=O)OCCCCCC(C)C)C(=O)OCCCCCC(C)C
MOL002879	0.2560	0.7440	0.6844	Pogostemon Cablin (Blanco) Benth.	Diop	33934	FALSE	c1(c(cccc1)C(=O)OCCCCCC(C)C)C(=O)OCCCCCC(C)C
MOL002879	0.2560	0.7440	0.6844	Cornus Officinalis Sieb. Et Zucc.	Diop	33934	FALSE	c1(c(cccc1)C(=O)OCCCCCC(C)C)C(=O)OCCCCCC(C)C
MOL002879	0.2560	0.7440	0.6844	Codonopsis Radix	Diop	33934	FALSE	c1(c(cccc1)C(=O)OCCCCCC(C)C)C(=O)OCCCCCC(C)C
MOL002879	0.2560	0.7440	0.6844	Ardisiae Japonicae Herba	Diop	33934	FALSE	c1(c(cccc1)C(=O)OCCCCCC(C)C)C(=O)OCCCCCC(C)C
MOL002879	0.2560	0.7440	0.6844	Panax Ginseng C. A. Mey.	Diop	33934	FALSE	c1(c(cccc1)C(=O)OCCCCCC(C)C)C(=O)OCCCCCC(C)C
MOL002879	0.2560	0.7440	0.6844	Capsellae Herba	Diop	33934	FALSE	c1(c(cccc1)C(=O)OCCCCCC(C)C)C(=O)OCCCCCC(C)C
MOL002879	0.2560	0.7440	0.6844	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	Diop	33934	FALSE	c1(c(cccc1)C(=O)OCCCCCC(C)C)C(=O)OCCCCCC(C)C
MOL002879	0.2560	0.7440	0.6844	Viticis Negundo Folium	Diop	33934	FALSE	c1(c(cccc1)C(=O)OCCCCCC(C)C)C(=O)OCCCCCC(C)C
MOL002881	0.8945	0.1055	0.9374	Zanthoxyli Pericarpium	Diosmetin	5281612	TRUE	Oc1cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)O)O
MOL002881	0.8945	0.1055	0.9374	Citri Sarcodactylis Fructus	Diosmetin	5281612	TRUE	Oc1cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)O)O
MOL002881	0.8945	0.1055	0.9374	Verbenae Herb	Diosmetin	5281612	TRUE	Oc1cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)O)O
MOL002881	0.8945	0.1055	0.9374	Schizonepetae Herba	Diosmetin	5281612	TRUE	Oc1cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)O)O
MOL002881	0.8945	0.1055	0.9374	Cnidii Fructus	Diosmetin	5281612	TRUE	Oc1cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)O)O
MOL002881	0.8945	0.1055	0.9374	Menthae Herba	Diosmetin	5281612	TRUE	Oc1cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)O)O
MOL002881	0.8945	0.1055	0.9374	Lobeliae Chinensis Herba	Diosmetin	5281612	TRUE	Oc1cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)O)O
MOL002881	0.8945	0.1055	0.9374	Trichosanthes Kirilowii Maxim	Diosmetin	5281612	TRUE	Oc1cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)O)O
MOL002881	0.8945	0.1055	0.9374	Lygodii Spora	Diosmetin	5281612	TRUE	Oc1cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)O)O
MOL002881	0.8945	0.1055	0.9374	Ginkgo Folium	Diosmetin	5281612	TRUE	Oc1cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)O)O
MOL002881	0.8945	0.1055	0.9374	Capsellae Herba	Diosmetin	5281612	TRUE	Oc1cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)O)O
MOL002881	0.8945	0.1055	0.9374	Zanthoxylum Nitidum	Diosmetin	5281612	TRUE	Oc1cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)O)O

MOL002884	0.9259	0.0741	0.9595	Lygodii Spora	2-amino-4-methoxyphenol	1419108	FALSE	c1(c(cc(cc1)OC)N)O
MOL002885	0.9015	0.0985	0.9680	Mume Fructus	WLN: QV4	7991	FALSE	C(=O)(CCCC)O
MOL002885	0.9015	0.0985	0.9680	Capsici Fructus	WLN: QV4	7991	FALSE	C(=O)(CCCC)O
MOL002885	0.9015	0.0985	0.9680	Ranunculi Ternati Radix	WLN: QV4	7991	FALSE	C(=O)(CCCC)O
MOL002885	0.9015	0.0985	0.9680	Campsis Flos	WLN: QV4	7991	FALSE	C(=O)(CCCC)O
MOL002885	0.9015	0.0985	0.9680	Eriobotryae Folium	WLN: QV4	7991	FALSE	C(=O)(CCCC)O
MOL002885	0.9015	0.0985	0.9680	Citrus Aurantium	WLN: QV4	7991	FALSE	C(=O)(CCCC)O
MOL002885	0.9015	0.0985	0.9680	Radix Bupleuri	WLN: QV4	7991	FALSE	C(=O)(CCCC)O
MOL002885	0.9015	0.0985	0.9680	Bomboo Juice	WLN: QV4	7991	FALSE	C(=O)(CCCC)O
MOL002885	0.9015	0.0985	0.9680	Lygodii Spora	WLN: QV4	7991	FALSE	C(=O)(CCCC)O
MOL002885	0.9015	0.0985	0.9680	Semen Pharbitidis	WLN: QV4	7991	FALSE	C(=O)(CCCC)O
MOL002886	0.8776	0.1224	0.9026	Lygodii Spora	2-Hexynoic acid	324380	FALSE	C(=O)(C#CCCC)O
MOL002887	0.9257	0.0743	0.9634	Lygodii Spora	ZINC01592387	1549701	FALSE	C=C(C(CC)O)C
MOL002888	0.9303	0.0697	0.9430	Solidaginis Herba	o-Anisaldehyde	8658	FALSE	C(=O)c1c(cccc1)OC
MOL002888	0.9303	0.0697	0.9430	Lygodii Spora	o-Anisaldehyde	8658	FALSE	C(=O)c1c(cccc1)OC
MOL002888	0.9303	0.0697	0.9430	Cinnamomi Ramulus	o-Anisaldehyde	8658	FALSE	C(=O)c1c(cccc1)OC
MOL002889	0.9310	0.0690	0.9658	Lygodii Spora	(3R)-3-methylpentan-1-ol	6999792	FALSE	C(CC(CC)C)O
MOL002890	0.7854	0.2146	0.7932	Coptidis Rhizoma	2-Carboxymethyl-3-prenyl-2,3-epoxy-1,4-naphthoquinone	Not Available	FALSE	c1ccc2c(c1)C(=O)C1(C(C2=O)(CC=C(C)C)O1)C(=O)OC
MOL002891	0.6627	0.3373	0.7711	Zanthoxylum Nitidum	magnoflorine	73337	FALSE	Oc1c2c3C([N+](CCc3cc1OC)(C)C)Cc1c2c(O)c(OC)cc1
MOL002891	0.6627	0.3373	0.7711	Mahoniae Caulis	magnoflorine	73337	FALSE	Oc1c2c3C([N+](CCc3cc1OC)(C)C)Cc1c2c(O)c(OC)cc1
MOL002891	0.6627	0.3373	0.7711	Phellodendri Amurensis Cortex	magnoflorine	73337	FALSE	Oc1c2c3C([N+](CCc3cc1OC)(C)C)Cc1c2c(O)c(OC)cc1
MOL002891	0.6627	0.3373	0.7711	Coptidis Rhizoma	magnoflorine	73337	FALSE	Oc1c2c3C([N+](CCc3cc1OC)(C)C)Cc1c2c(O)c(OC)cc1
MOL002891	0.6627	0.3373	0.7711	Tinosporae Radix	magnoflorine	73337	FALSE	Oc1c2c3C([N+](CCc3cc1OC)(C)C)Cc1c2c(O)c(OC)cc1
MOL002891	0.6627	0.3373	0.7711	Menispermi Rhizoma	magnoflorine	73337	FALSE	Oc1c2c3C([N+](CCc3cc1OC)(C)C)Cc1c2c(O)c(OC)cc1
MOL002891	0.6627	0.3373	0.7711	Semiaquilegiae Radix	magnoflorine	73337	FALSE	Oc1c2c3C([N+](CCc3cc1OC)(C)C)Cc1c2c(O)c(OC)cc1
MOL002891	0.6627	0.3373	0.7711	Epimrdii Herba	magnoflorine	73337	FALSE	Oc1c2c3C([N+](CCc3cc1OC)(C)C)Cc1c2c(O)c(OC)cc1
MOL002891	0.6627	0.3373	0.7711	Mahoniae Folum	magnoflorine	73337	FALSE	Oc1c2c3C([N+](CCc3cc1OC)(C)C)Cc1c2c(O)c(OC)cc1

MOL002894	0.7879	0.2121	0.7691	Coptidis Rhizoma	berberrubine	Not Available	FALSE	O1c2cc3CC[n+]4c(c3cc2OC1)cc1c(c4)c(O)c(OC)cc1
MOL002894	0.7879	0.2121	0.7691	Phellodendri Amurensis Cortex	berberrubine	Not Available	FALSE	O1c2cc3CC[n+]4c(c3cc2OC1)cc1c(c4)c(O)c(OC)cc1
MOL002894	0.7879	0.2121	0.7691	Semiaquilegiae Radix	berberrubine	Not Available	FALSE	O1c2cc3CC[n+]4c(c3cc2OC1)cc1c(c4)c(O)c(OC)cc1
MOL002895	0.7126	0.2874	0.8114	Linderae Radix	DPEC	129670	FALSE	c1c(c2c(c(c1)O)oc(cc2=O)CCc1ccccc1)O
MOL002895	0.7126	0.2874	0.8114	Coptidis Rhizoma	DPEC	129670	FALSE	c1c(c2c(c(c1)O)oc(cc2=O)CCc1ccccc1)O
MOL002896	0.9444	0.0556	0.9054	Coptidis Rhizoma	Corydaldine	610097	FALSE	c12c(cc(c(c1)OC)OC)C(=O)NCC2
MOL002897	0.7582	0.2418	0.8211	Achyranthis Bidentatae Radix	epiberberine	Not Available	FALSE	O1c2c3c[n+]4CCc5c(c4cc3ccc2OC1)cc(OC)c(OC)c5
MOL002897	0.7582	0.2418	0.8211	Coptidis Rhizoma	epiberberine	Not Available	FALSE	O1c2c3c[n+]4CCc5c(c4cc3ccc2OC1)cc(OC)c(OC)c5
MOL002898	0.7912	0.2088	0.7822	Coptidis Rhizoma	groenlandicin e	Not Available	FALSE	c12c(CC[n+]3cc4c(cc13)ccc1OCOc41)cc(c(c2)OC)O
MOL002898	0.7912	0.2088	0.7822	Thalictri Glandulosissimi Et	groenlandicin e	Not Available	FALSE	c12c(CC[n+]3cc4c(cc13)ccc1OCOc41)cc(c(c2)OC)O
MOL002898	0.7912	0.2088	0.7822	Corydalis Bungeanae Herba	groenlandicin e	Not Available	FALSE	c12c(CC[n+]3cc4c(cc13)ccc1OCOc41)cc(c(c2)OC)O
MOL002900	0.9139	0.0861	0.8053	Coptidis Rhizoma	Noroxyhydrastinine	89047	FALSE	c12c(cc3c(c1)OCO3)CCNC2=O
MOL002900	0.9139	0.0861	0.8053	Thalictri Glandulosissimi Et	Noroxyhydrastinine	89047	FALSE	c12c(cc3c(c1)OCO3)CCNC2=O
MOL002900	0.9139	0.0861	0.8053	Corydalis Rhizoma	Noroxyhydrastinine	89047	FALSE	c12c(cc3c(c1)OCO3)CCNC2=O
MOL002901	0.5545	0.4455	0.7206	Coptidis Rhizoma	phellodendrine	Not Available	FALSE	c12c(cc(c(c1)O)OC)C[N+]1(C(C2)c2c(CC1)cc(c(c2)O)OC)C
MOL002902	0.9350	0.0650	0.9409	Plantaginis Herba	Ethyl caffeate	5317238	FALSE	c1(cc(c(cc1)O)O)/C=C/C(=O)OCC
MOL002902	0.9350	0.0650	0.9409	Cortex Periplocae Radicis	Ethyl caffeate	5317238	FALSE	c1(cc(c(cc1)O)O)/C=C/C(=O)OCC
MOL002902	0.9350	0.0650	0.9409	Prunellae Spica	Ethyl caffeate	5317238	FALSE	c1(cc(c(cc1)O)O)/C=C/C(=O)OCC
MOL002902	0.9350	0.0650	0.9409	Coptidis Rhizoma	Ethyl caffeate	5317238	FALSE	c1(cc(c(cc1)O)O)/C=C/C(=O)OCC
MOL002902	0.9350	0.0650	0.9409	Solanum Melongena L	Ethyl caffeate	5317238	FALSE	c1(cc(c(cc1)O)O)/C=C/C(=O)OCC
MOL002903	0.7381	0.2619	0.9085	Corydalis Rhizoma	(R)-Canadine	Not Available	FALSE	c12c(c(cc1)OC)OC)CN1C(C2)c2c(CC1)cc1c(c2)OCO1
MOL002903	0.7381	0.2619	0.9085	Coptidis Rhizoma	(R)-Canadine	Not Available	FALSE	c12c(c(cc1)OC)OC)CN1C(C2)c2c(CC1)cc1c(c2)OCO1
MOL002904	0.7527	0.2473	0.8182	Thalictri Glandulosissimi Et	Berlambine	Not Available	FALSE	c12c3c(cc4c(c3)OCO4)CCn1c(=O)c1c(c2)ccc(c1OC)OC
MOL002904	0.7527	0.2473	0.8182	Coptidis Rhizoma	Berlambine	Not Available	FALSE	c12c3c(cc4c(c3)OCO4)CCn1c(=O)c1c(c2)ccc(c1OC)OC
MOL002905	0.3852	0.6148	0.7526	Coptidis Rhizoma	Zosimin	6436246	FALSE	c1c2c(c3c(c1)ccc(=O)o3)CC(O2)C(OC(=O)/C(=C\C)/C)(C)C
MOL002905	0.3852	0.6148	0.7526	Peucedani Radix	Zosimin	6436246	FALSE	c1c2c(c3c(c1)ccc(=O)o3)CC(O2)C(OC(=O)/C(=C\C)/C)(C)C
MOL002905	0.3852	0.6148	0.7526	Cnidii Fructus	Zosimin	6436246	FALSE	c1c2c(c3c(c1)ccc(=O)o3)CC(O2)C(OC(=O)/C(=C\C)/C)(C)C
MOL002905	0.3852	0.6148	0.7526	Radix Angelicae Biseratae	Zosimin	6436246	FALSE	c1c2c(c3c(c1)ccc(=O)o3)CC(O2)C(OC(=O)/C(=C\C)/C)(C)C
MOL002905	0.3852	0.6148	0.7526	Peucedanidecursivi Radix	Zosimin	6436246	FALSE	c1c2c(c3c(c1)ccc(=O)o3)CC(O2)C(OC(=O)/C(=C\C)/C)(C)C

MOL002906	0.5157	0.4843	0.7078	Coptidis Rhizoma	Corchoroside A	Not Available	FALSE	C1C(CC2(C(C1)(C1C(CC2)C2(C(CC1)(C(CC2)C1=CC(=O)OC1)C)O)C=O)O)OC1OC(C(C(C1)O)O)C
MOL002907	0.6450	0.3550	0.7872	Coptidis Rhizoma	Corchoroside A_qt	Not Available	FALSE	C1C(CC2(C(C1)(C1C(CC2)C2(C(CC1)(C(CC2)C1=CC(=O)OC1)C)O)C=O)O)O
MOL002908	0.8459	0.1541	0.8900	Scutellariae Radix	5,8,2'-Trihydroxy-7-methoxyflavone	156992	FALSE	c1(cc(=O)c2c(cc(c(c2o1)O)OC)O)c1c(cccc1)O
MOL002909	0.8661	0.1339	0.8094	Scutellariae Radix	5,7,2,5-tetrahydroxy-8,6-dimethoxyflavone	44258628	FALSE	c1(c(c(c2c(c1OC)oc(cc2=O)c1c(c(ccc1O)O)OC)O)OC)O
MOL002910	0.9417	0.0583	0.8922	Scutellariae Radix	Carthamidin	Not Available	FALSE	c12c(C(=O)CC(O1)c1ccc(cc1)O)c(c(c(c2)O)O)O
MOL002911	0.8775	0.1225	0.7041	Scutellariae Radix	2,6,2',4'-tetrahydroxy-6'-methoxychalcone	Not Available	FALSE	C(=C\c1c(cccc1O)O)\C(=O)c1c(cc(cc1OC)O)O
MOL002912	0.8865	0.1135	0.8409	Scutellariae Radix	Dihydrobaicalin	Not Available	FALSE	O1C(Oc2cc3OC(CC(=O)c3c(O)c2O)c2ccccc2)C(O)C(O)C(O)C1C(=O)O
MOL002913	0.9364	0.0636	0.8382	Scutellariae Radix	Dihydrobaicalin_qt	14135323	FALSE	Oc1cc2OC(CC(=O)c2c(O)c1O)c1ccccc1
MOL002914	0.9326	0.0674	0.9041	Rhododendri Daurici Folium	Eriodyctiol (flavanone)	373261	FALSE	c12c(C(=O)CC(O1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL002914	0.9326	0.0674	0.9041	Gleditsiae Spina	Eriodyctiol (flavanone)	373261	FALSE	c12c(C(=O)CC(O1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL002914	0.9326	0.0674	0.9041	Catechu	Eriodyctiol (flavanone)	373261	FALSE	c12c(C(=O)CC(O1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL002914	0.9326	0.0674	0.9041	Dalbergiae Odoriferae Lignum	Eriodyctiol (flavanone)	373261	FALSE	c12c(C(=O)CC(O1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL002914	0.9326	0.0674	0.9041	Drynariae Rhizoma	Eriodyctiol (flavanone)	373261	FALSE	c12c(C(=O)CC(O1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL002914	0.9326	0.0674	0.9041	Peanut Skin	Eriodyctiol (flavanone)	373261	FALSE	c12c(C(=O)CC(O1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL002914	0.9326	0.0674	0.9041	Lonicerae Japonicae Flos	Eriodyctiol (flavanone)	373261	FALSE	c12c(C(=O)CC(O1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL002914	0.9326	0.0674	0.9041	Scutellariae Radix	Eriodyctiol (flavanone)	373261	FALSE	c12c(C(=O)CC(O1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL002914	0.9326	0.0674	0.9041	Rhizoma Fagopyri Cymosi	Eriodyctiol (flavanone)	373261	FALSE	c12c(C(=O)CC(O1)c1cc(c(cc1)O)O)c(cc(c2)O)O

MOL002914	0.9326	0.0674	0.9041	Aurantii Fructus Immaturus	Eriodyctiol (flavanone)	373261	FALSE	c12c(C(=O)CC(O1)c1cc(c(cc1)O)O)c(cc(c2)O)O
MOL002915	0.7341	0.2659	0.9323	Scutellariae Radix	Salvigenin	161271	FALSE	c12c(c(c(c(c2)OC)OC)O)c(=O)cc(o1)c1ccc(cc1)OC
MOL002915	0.7341	0.2659	0.9323	Scutellariae Barbatae Herba	Salvigenin	161271	FALSE	c12c(c(c(c(c2)OC)OC)O)c(=O)cc(o1)c1ccc(cc1)OC
MOL002916	0.9129	0.0871	0.7309	Scutellariae Radix	2-(2,6-dihydroxyphenyl)-3,5,7-trihydroxy-chromone	5320471	FALSE	o1c(c2c(O)cccc2O)c(O)c(=O)c2c1cc(O)cc2O
MOL002917	0.8843	0.1157	0.7090	Scutellariae Radix	5,2',6'-Trihydroxy-7,8-dimethoxyflavone	5322059	FALSE	o1c2c(c(=O)cc1c1c(O)cccc1O)c(O)cc(OC)c2OC
MOL002917	0.8843	0.1157	0.7090	Citri Sarcodactylis Fructus	5,2',6'-Trihydroxy-7,8-dimethoxyflavone	5322059	FALSE	o1c2c(c(=O)cc1c1c(O)cccc1O)c(O)cc(OC)c2OC
MOL002918	0.8375	0.1625	0.8323	Scutellariae Radix	Gallinulagenin	5271991	FALSE	c1(cc(=O)c2c(cc(c(c2o1)OC)O)O)c1c(c(ccc1O)O)OC
MOL002919	0.8509	0.1491	0.8610	Scutellariae Radix	Viscidulin III	44259518	FALSE	o1c(c2c(OC)c(O)c(OC)cc2)c(O)c(=O)c2c1cc(O)cc2O
MOL002921	0.8828	0.1172	0.7341	Scutellariae Radix	(2S,3R,4R,5R,6S)-2-[(2R,3R,4S,5R,6R)-3,5-dihydroxy-2-[2-(3-hydroxy-4-methoxy-phenyl)ethoxy]-6-methylol-tetrahydropyran-4-yl]oxy-6-methyl-tetrahydropyran-3,4,5-triol	21668724	FALSE	O(C1C(O)C(OC(OCCc2cc(O)c(OC)cc2)C1O)CO)C1OC(C(O)C(O)C1O)C
MOL002922	0.9497	0.0503	0.9709	Semiaquilegiae Radix	5-(2-hydroxyethyl)-2-methoxyphenol	10034991	FALSE	OCCc1cc(O)c(OC)cc1

MOL002922	0.9497	0.0503	0.9709	Figwort Root	5-(2-hydroxyethyl)-2-methoxyphenol	10034991	FALSE	OCCc1cc(O)c(OC)cc1
MOL002922	0.9497	0.0503	0.9709	Scutellariae Radix	5-(2-hydroxyethyl)-2-methoxyphenol	10034991	FALSE	OCCc1cc(O)c(OC)cc1
MOL002923	0.9058	0.0942	0.7392	Scutellariae Radix	darendoside B	Not Available	FALSE	O(C1C(O)(C(OC(C1O)CO)OCC)c1cc(O)c(OC)cc1)C1OC(C(O)C(O)C1O)C
MOL002924	0.9285	0.0715	0.7985	Scutellariae Radix	darendoside B_qt	Not Available	FALSE	OC1C(O)(C(OC(C1O)CO)OCC)c1cc(O)c(OC)cc1
MOL002925	0.9026	0.0974	0.7418	Scutellariae Radix	5,7,2',6'-Tetrahydroxyflavone	5321865	FALSE	c1(cc(=O)c2c(cc(cc2o1)O)O)c1c(cccc1O)O
MOL002926	0.7876	0.2124	0.9245	Scutellariae Radix	dihydrooroxylin A	Not Available	FALSE	c1(cc(c2c(c1O)C(=O)CC(O2)c1ccccc1)O)OC
MOL002927	0.7288	0.2712	0.6916	Scutellariae Radix	Skullcapflavone II	124211	FALSE	c12c(c(c(c(c1OC)OC)OC)O)c(=O)cc(o2)c1c(cccc1O)OC
MOL002928	0.7791	0.2209	0.9489	Oroxyli Semen	oroxylin a	5320315	FALSE	c12c(oc(cc2=O)c2ccccc2)cc(c(c1O)OC)O
MOL002928	0.7791	0.2209	0.9489	Andrographis Herba	oroxylin a	5320315	FALSE	c12c(oc(cc2=O)c2ccccc2)cc(c(c1O)OC)O
MOL002928	0.7791	0.2209	0.9489	Scutellariae Radix	oroxylin a	5320315	FALSE	c12c(oc(cc2=O)c2ccccc2)cc(c(c1O)OC)O
MOL002929	0.9339	0.0661	0.8942	Sargentodoxae Caulis	salidroside	Not Available	FALSE	C1(OC(C(C(C1O)O)O)CO)OCCc1ccc(cc1)O
MOL002929	0.9339	0.0661	0.8942	Scutellariae Radix	salidroside	Not Available	FALSE	C1(OC(C(C(C1O)O)O)CO)OCCc1ccc(cc1)O
MOL002929	0.9339	0.0661	0.8942	Epimrdii Herba	salidroside	Not Available	FALSE	C1(OC(C(C(C1O)O)O)CO)OCCc1ccc(cc1)O
MOL002929	0.9339	0.0661	0.8942	Sedum Aizoon L.	salidroside	Not Available	FALSE	C1(OC(C(C(C1O)O)O)CO)OCCc1ccc(cc1)O
MOL002930	0.9415	0.0585	0.9712	Catechu	Tyrosol	10393	FALSE	OCCc1ccc(cc1)O
MOL002930	0.9415	0.0585	0.9712	Forsythiae Fructus	Tyrosol	10393	FALSE	OCCc1ccc(cc1)O
MOL002930	0.9415	0.0585	0.9712	Fraxini Cortex	Tyrosol	10393	FALSE	OCCc1ccc(cc1)O
MOL002930	0.9415	0.0585	0.9712	Cistanches Herba	Tyrosol	10393	FALSE	OCCc1ccc(cc1)O
MOL002930	0.9415	0.0585	0.9712	Daturae Flos	Tyrosol	10393	FALSE	OCCc1ccc(cc1)O
MOL002930	0.9415	0.0585	0.9712	Fructus Ligustri Lucidi	Tyrosol	10393	FALSE	OCCc1ccc(cc1)O
MOL002930	0.9415	0.0585	0.9712	Sedum Aizoon L.	Tyrosol	10393	FALSE	OCCc1ccc(cc1)O
MOL002930	0.9415	0.0585	0.9712	Epimrdii Herba	Tyrosol	10393	FALSE	OCCc1ccc(cc1)O
MOL002930	0.9415	0.0585	0.9712	Scutellariae Radix	Tyrosol	10393	FALSE	OCCc1ccc(cc1)O
MOL002930	0.9415	0.0585	0.9712	Oroxyli Semen	Tyrosol	10393	FALSE	OCCc1ccc(cc1)O
MOL002930	0.9415	0.0585	0.9712	Capsellae Herba	Tyrosol	10393	FALSE	OCCc1ccc(cc1)O
MOL002930	0.9415	0.0585	0.9712	Polygoni Orientalis Fructus	Tyrosol	10393	FALSE	OCCc1ccc(cc1)O
MOL002930	0.9415	0.0585	0.9712	Semiaquilegiae Radix	Tyrosol	10393	FALSE	OCCc1ccc(cc1)O
MOL002930	0.9415	0.0585	0.9712	Plantaginis Herba	Tyrosol	10393	FALSE	OCCc1ccc(cc1)O

MOL002930	0.9415	0.0585	0.9712	Pseudobulbus Cremastrae Seu Pleiones	Tyrosol	10393	FALSE	OCCc1ccc(cc1)O
MOL002930	0.9415	0.0585	0.9712	Sargentodoxae Caulis	Tyrosol	10393	FALSE	OCCc1ccc(cc1)O
MOL002931	0.9011	0.0989	0.8150	Perilla Frutescens	scutellarin	185617	FALSE	c12c(oc(cc1=O)c1ccc(cc1)O)cc(c(c2O)O)OC1OC(C(C(C1O)O)O)C(=O)O
MOL002931	0.9011	0.0989	0.8150	Scutellariae Radix	scutellarin	185617	FALSE	c12c(oc(cc1=O)c1ccc(cc1)O)cc(c(c2O)O)OC1OC(C(C(C1O)O)O)C(=O)O
MOL002931	0.9011	0.0989	0.8150	Scutellariae Barbatae Herba	scutellarin	185617	FALSE	c12c(oc(cc1=O)c1ccc(cc1)O)cc(c(c2O)O)OC1OC(C(C(C1O)O)O)C(=O)O
MOL002931	0.9011	0.0989	0.8150	Oroxyli Semen	scutellarin	185617	FALSE	c12c(oc(cc1=O)c1ccc(cc1)O)cc(c(c2O)O)OC1OC(C(C(C1O)O)O)C(=O)O
MOL002932	0.8558	0.1442	0.7488	Scutellariae Radix	Panicolin	5320399	FALSE	o1c2c(c(O)cc(OC)c2OC)c(=O)cc1c1c(O)cccc1
MOL002932	0.8558	0.1442	0.7488	Andrographis Herba	Panicolin	5320399	FALSE	o1c2c(c(O)cc(OC)c2OC)c(=O)cc1c1c(O)cccc1
MOL002933	0.8491	0.1509	0.8940	Scutellariae Radix	5,7,4'-Trihydroxy-8-methoxyflavone	5322078	FALSE	c1(cc(=O)c2c(cc(c(c2o1)OC)O)O)c1ccc(cc1)O
MOL002933	0.8491	0.1509	0.8940	Verbenae Herb	5,7,4'-Trihydroxy-8-methoxyflavone	5322078	FALSE	c1(cc(=O)c2c(cc(c(c2o1)OC)O)O)c1ccc(cc1)O
MOL002934	0.7270	0.2730	0.7128	Scutellariae Radix	NEOBAICALEIN	Not Available	FALSE	c1(c(c(c2c(c1OC)oc(cc2=O)c1cc(ccc1O)OC)O)OC)OC
MOL002935	0.8751	0.1249	0.8394	Scutellariae Radix	Baicalin	Not Available	FALSE	C1(C(C(C(C(O1)Oc1cc2c(c(c1O)O)c(=O)cc(o2)c1ccccc1)O)O)O)(C(=O)O)C
MOL002936	0.7721	0.2279	0.9147	Radix Bupleuri	5,8-Dihydroxy-6,7-dimethoxyflavone	153441	FALSE	c1(cc(=O)c2c(c(c(c(c2o1)O)OC)OC)O)c1ccccc1
MOL002936	0.7721	0.2279	0.9147	Scutellariae Radix	5,8-Dihydroxy-6,7-dimethoxyflavone	153441	FALSE	c1(cc(=O)c2c(c(c(c(c2o1)O)OC)OC)O)c1ccccc1
MOL002937	0.8021	0.1979	0.9141	Scutellariae Radix	DIHYDROOROXYLIN	25721350	FALSE	c1(c(c(c2c(c1)OC(CC2=O)c1ccccc1)O)OC)O
MOL002937	0.8021	0.1979	0.9141	Moslae Herba	DIHYDROOROXYLIN	25721350	FALSE	c1(c(c(c2c(c1)OC(CC2=O)c1ccccc1)O)OC)O

MOL002938	0.8956	0.1044	0.8960	Dalbergiae Odoriferae Lignum	(3R)-4'-Methoxy-2',3,7-trihydroxyisoflavanone	5319494	FALSE	C1(C(=O)c2ccc(cc2OC1)O)(c1c(cc(cc1)OC)O)O
MOL002939	0.8640	0.1360	0.8988	Dalbergiae Odoriferae Lignum	(3R)-5'-Methoxyvestitol	5319496	FALSE	c1c2c(ccc1O)CC(CO2)c1c(cc(c(c1)OC)OC)O
MOL002940	0.9248	0.0752	0.8531	Dalbergiae Odoriferae Lignum	(3R)-3-(2,3-dihydroxy-4-methoxyphenyl)-7-hydroxychroman-4-one	14353662	FALSE	C1C(C(=O)c2ccc(cc2O1)O)c1c(c(c(cc1)OC)O)O
MOL002941	0.9245	0.0755	0.8675	Dalbergiae Odoriferae Lignum	(3R)-3-(2,3-dihydroxy-4-methoxyphenyl)chroman-7,8-diol	14353660	FALSE	C1C(Cc2ccc(c(c2O1)O)O)c1c(c(c(cc1)OC)O)O
MOL002942	0.9352	0.0648	0.9501	Dalbergiae Odoriferae Lignum	(1S,2S,4R)-1,2,4-trimethylcyclohexane	12536912	FALSE	C1(C(CCC(C1)C)C)C
MOL002943	0.9336	0.0664	0.9647	Campsis Flos	BuOH	263	FALSE	C(CC)CO
MOL002943	0.9336	0.0664	0.9647	Dalbergiae Odoriferae Lignum	BuOH	263	FALSE	C(CC)CO
MOL002943	0.9336	0.0664	0.9647	Semiaquilegiae Radix	BuOH	263	FALSE	C(CC)CO
MOL002943	0.9336	0.0664	0.9647	Ginkgo Folium	BuOH	263	FALSE	C(CC)CO
MOL002943	0.9336	0.0664	0.9647	Codonopsis Radix	BuOH	263	FALSE	C(CC)CO
MOL002943	0.9336	0.0664	0.9647	Mori Cortex	BuOH	263	FALSE	C(CC)CO
MOL002943	0.9336	0.0664	0.9647	Lobeliae Chinensis Herba	BuOH	263	FALSE	C(CC)CO
MOL002943	0.9336	0.0664	0.9647	licorice	BuOH	263	FALSE	C(CC)CO
MOL002944	0.9356	0.0644	0.9480	Ardisiae Japonicae Herba	(E)-Linalol pyranoxide	6428300	FALSE	O1C(C(CCC1(C=C)C)O)(C)C
MOL002944	0.9356	0.0644	0.9480	Citrus Reticulata	(E)-Linalol pyranoxide	6428300	FALSE	O1C(C(CCC1(C=C)C)O)(C)C
MOL002944	0.9356	0.0644	0.9480	Dalbergiae Odoriferae Lignum	(E)-Linalol pyranoxide	6428300	FALSE	O1C(C(CCC1(C=C)C)O)(C)C

MOL002945	0.1948	0.8052	0.6008	Dalbergiae Odoriferae Lignum	2,3-didehydro-2',7-dihydroxy-4'-methoxy-3(2',7-dihydroxy-4'-methoxyisoflavan-5'-yl)flavan	Not Available	FALSE	c1(cc2c(cc1)CC(CO2)c1cc(c(cc1O)OC)C1=C(c2c(cc(cc2)OC)O)Oc2c(C1)ccc(c2)O)O
MOL002946	0.2331	0.7669	0.6067	Dalbergiae Odoriferae Lignum	2,3-didehydro-2',7-dihydroxy-4'-methoxy-3-(2',7-dihydroxy-4'-methoxyisoflavan-5'-yl)flavone	Not Available	FALSE	c1(cc2c(cc1)CC(CO2)c1cc(c(cc1O)OC)c1c(=O)c2c(oc1c1c(cc(cc1)OC)O)cc(cc2)O)O
MOL002948	0.8974	0.1026	0.8962	Dalbergiae Odoriferae Lignum	2,4-dihydroxy-5-methoxybenzophenone	Not Available	FALSE	C(=O)(c1c(cc(c(c1)OC)O)O)c1ccccc1
MOL002949	0.9249	0.0751	0.9541	Dalbergiae Odoriferae Lignum	ST5437276	11194554	FALSE	C(=O)c1c(cc(c(c1)OC)O)O
MOL002950	0.8532	0.1468	0.8730	Dalbergiae Odoriferae Lignum	(3R)-7,2',3'-trihydroxy-4-methoxyisoflavan	Not Available	FALSE	C1(C(c2ccc(cc2OC1)O)OC)c1c(c(ccc1)O)O
MOL002951	0.9122	0.0878	0.8859	Ardisiae Japonicae Herba	2,4-Dimethyl-2,4-heptadienal	5370090	FALSE	C(=O)/C(=C/C(=C/CC)/C)/C
MOL002951	0.9122	0.0878	0.8859	Dalbergiae Odoriferae Lignum	2,4-Dimethyl-2,4-heptadienal	5370090	FALSE	C(=O)/C(=C/C(=C/CC)/C)/C
MOL002952	0.9057	0.0943	0.8876	Dalbergiae Odoriferae Lignum	ZINC02539267	7017921	FALSE	C(=O)/C(=C/C(CC=C)C)/C
MOL002953	0.9263	0.0737	0.6847	Hedysari Radix	2-(2-hydroxy-4-methoxyphenyl)-6-benzofuranol	641806	FALSE	c1c(c(ccc1OC)c1cc2c(o1)cc(cc2)O)O

MOL002953	0.9263	0.0737	0.6847	Dalbergiae Odoriferae Lignum	2-(2-hydroxy-4-methoxyphenyl)-6-benzofuranol	641806	FALSE	c1c(c(ccc1OC)c1cc2c(o1)cc(cc2)O)O
MOL002954	0.9525	0.0475	0.7927	Dalbergiae Odoriferae Lignum	2-methylquinolin-6-ol	594395	FALSE	n1c(ccc2cc(ccc12)O)C
MOL002955	0.8954	0.1046	0.7663	Acoritataninowii Rhizoma	2'-O-Methylisoliquiritigenin	5319688	FALSE	O(c1c(ccc(O)c1)C(=O)/C=C/c1ccc(O)cc1)C
MOL002955	0.8954	0.1046	0.7663	Dalbergiae Odoriferae Lignum	2'-O-Methylisoliquiritigenin	5319688	FALSE	O(c1c(ccc(O)c1)C(=O)/C=C/c1ccc(O)cc1)C
MOL002956	0.8916	0.1084	0.8537	Dalbergiae Odoriferae Lignum	7,3',4'-Trihydroxyflavone	5322065	FALSE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)O)ccc(c2)O
MOL002957	0.8631	0.1369	0.7741	Dalbergiae Odoriferae Lignum	9-O-Methylcoumestrol	5319565	FALSE	c12c(c3c(o2)cc(cc3)OC)c(=O)oc2c1ccc(c2)O
MOL002958	0.8676	0.1324	0.8023	Dalbergiae Odoriferae Lignum	3'-Hydroxymelanettin	5318262	FALSE	c12c(cc(c(c1)OC)O)c(cc(=O)o2)c1cc(c(cc1)O)O
MOL002959	0.8325	0.1675	0.9172	Polygonati Rhizoma	3'-Methoxydaidzein	5319422	FALSE	c1c(c(=O)c2ccc(cc2o1)O)c1cc(c(cc1)O)OC
MOL002959	0.8325	0.1675	0.9172	Dalbergiae Odoriferae Lignum	3'-Methoxydaidzein	5319422	FALSE	c1c(c(=O)c2ccc(cc2o1)O)c1cc(c(cc1)O)OC
MOL002959	0.8325	0.1675	0.9172	Radix Puerariae	3'-Methoxydaidzein	5319422	FALSE	c1c(c(=O)c2ccc(cc2o1)O)c1cc(c(cc1)O)OC
MOL002960	0.8741	0.1259	0.9509	Dalbergiae Odoriferae Lignum	3-methoxypyridazine	292493	FALSE	c1(cccnn1)OC
MOL002961	0.9005	0.0995	0.8992	Dalbergiae Odoriferae Lignum	(-)-Vestitol	182259	FALSE	C1C(Cc2ccc(cc2O1)O)c1ccc(cc1O)OC
MOL002962	0.7740	0.2260	0.9393	Dalbergiae Odoriferae Lignum	(3S)-7-hydroxy-3-(2,3,4-trimethoxyphenyl)chroman-4-one	10019512	FALSE	C1(C(=O)c2ccc(cc2OC1)O)c1c(c(c(cc1)OC)OC)OC

MOL002962	0.7740	0.2260	0.9393	Asari Radix Et Rhizoma	(3S)-7-hydroxy-3-(2,3,4-trimethoxyphenyl)chroman-4-one	10019512	FALSE	C1(C(=O)c2ccc(cc2OC1)O)c1c(c(c(cc1)OC)OC)OC
MOL002963	0.5718	0.4282	0.7691	Dalbergiae Odoriferae Lignum	4',5',7-trimethyl-3-methoxyflavone	Not Available	FALSE	c1(c(c(=O)c2ccc(cc2o1)C)OC)c1ccc(c(c1)C)C
MOL002964	0.8624	0.1376	0.9140	Dalbergiae Odoriferae Lignum	(R)-4-Methoxydalbergione	442809	FALSE	C1(=O)C(=CC(=O)C(=C1)C(C=C)c1ccccc1)OC
MOL002965	0.9057	0.0943	0.9725	Dalbergiae Odoriferae Lignum	4-Hydroxy-4-methylcyclohexanone	28539	FALSE	C1C(=O)CCC(C1)(O)C
MOL002966	0.7659	0.2341	0.9030	Dalbergiae Odoriferae Lignum	Dalbergin	442768	FALSE	o1c2c(c(c3ccccc3)cc1=O)cc(O)c(OC)c2
MOL002967	0.1465	0.8535	0.6960	Dalbergiae Odoriferae Lignum	7-hydroxy-4'-methoxy-2',5'-dioxo-4-[(3R)-2',7-dihydroxy-4'-methoxyisoflavan-5'-yl]isoflavane	Not Available	FALSE	c1(cc2c(cc1)CC(CO2)c1cc(c(cc1O)OC)C1=C(C(=O)C=C(C1=O)C1Cc2c(OC1)cc(cc2)O)OC)O
MOL002968	0.8915	0.1085	0.8132	Dalbergiae Odoriferae Lignum	9-Oxonerolidol	Not Available	FALSE	C(=C)C(CCCCCC(=O)C=C(C)C)(O)C
MOL002969	0.2103	0.7897	0.7403	Dalbergiae Odoriferae Lignum	(3R,4R)-2',3',7-trihydroxy-4'-methoxy-4-[(3R)-2',7-dihydroxy-4'-methoxyisoflavan-5'-yl]-isoflavan	Not Available	FALSE	C1(C(c2ccc(cc2OC1)O)c1c(cc(c(C2Cc3ccc(cc3OC2)O)c1)O)OC)c1c(c(c(cc1)OC)O)O
MOL002970	0.8951	0.1049	0.8139	Dalbergiae Odoriferae Lignum	BZF	9223	FALSE	c12c(occ1)cccc2
MOL002971	0.8912	0.1088	0.9710	Dalbergiae Odoriferae Lignum	(R)-5-methylfuran-2(5H)-one	9548741	FALSE	O1C(C=CC1=O)C

MOL002972	0.8659	0.1341	0.8062	Ardisiae Japonicae Herba	(4S)-1-methyl-4-(6-methylhepta-1,5-dien-2-yl)cyclohexene	10104370	FALSE	C1(C(=C)CCC=C(C)C)CC=C(CC1)C
MOL002972	0.8659	0.1341	0.8062	Ganoderma	(4S)-1-methyl-4-(6-methylhepta-1,5-dien-2-yl)cyclohexene	10104370	FALSE	C1(C(=C)CCC=C(C)C)CC=C(CC1)C
MOL002972	0.8659	0.1341	0.8062	Rubi Fructus	(4S)-1-methyl-4-(6-methylhepta-1,5-dien-2-yl)cyclohexene	10104370	FALSE	C1(C(=C)CCC=C(C)C)CC=C(CC1)C
MOL002972	0.8659	0.1341	0.8062	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(4S)-1-methyl-4-(6-methylhepta-1,5-dien-2-yl)cyclohexene	10104370	FALSE	C1(C(=C)CCC=C(C)C)CC=C(CC1)C
MOL002972	0.8659	0.1341	0.8062	Zingiber Officinale Roscoe	(4S)-1-methyl-4-(6-methylhepta-1,5-dien-2-yl)cyclohexene	10104370	FALSE	C1(C(=C)CCC=C(C)C)CC=C(CC1)C
MOL002972	0.8659	0.1341	0.8062	Benzoinum	(4S)-1-methyl-4-(6-methylhepta-1,5-dien-2-yl)cyclohexene	10104370	FALSE	C1(C(=C)CCC=C(C)C)CC=C(CC1)C
MOL002972	0.8659	0.1341	0.8062	Farfarae Flos	(4S)-1-methyl-4-(6-methylhepta-1,5-dien-2-yl)cyclohexene	10104370	FALSE	C1(C(=C)CCC=C(C)C)CC=C(CC1)C

MOL002972	0.8659	0.1341	0.8062	Sesami Nigrum Semen	(4S)-1-methyl-4-(6-methylhepta-1,5-dien-2-yl)cyclohexene	10104370	FALSE	C1(C(=C)CCC=C(C)C)CC=C(CC1)C
MOL002972	0.8659	0.1341	0.8062	Cinnanmomi Cortex	(4S)-1-methyl-4-(6-methylhepta-1,5-dien-2-yl)cyclohexene	10104370	FALSE	C1(C(=C)CCC=C(C)C)CC=C(CC1)C
MOL002972	0.8659	0.1341	0.8062	Eriobotryae Folium	(4S)-1-methyl-4-(6-methylhepta-1,5-dien-2-yl)cyclohexene	10104370	FALSE	C1(C(=C)CCC=C(C)C)CC=C(CC1)C
MOL002972	0.8659	0.1341	0.8062	Angelicae Sinensis Radix	(4S)-1-methyl-4-(6-methylhepta-1,5-dien-2-yl)cyclohexene	10104370	FALSE	C1(C(=C)CCC=C(C)C)CC=C(CC1)C
MOL002972	0.8659	0.1341	0.8062	Broussonetiae Fructus	(4S)-1-methyl-4-(6-methylhepta-1,5-dien-2-yl)cyclohexene	10104370	FALSE	C1(C(=C)CCC=C(C)C)CC=C(CC1)C
MOL002972	0.8659	0.1341	0.8062	Panacis Quinquefolii Radix	(4S)-1-methyl-4-(6-methylhepta-1,5-dien-2-yl)cyclohexene	10104370	FALSE	C1(C(=C)CCC=C(C)C)CC=C(CC1)C
MOL002972	0.8659	0.1341	0.8062	Radix Bupleuri	(4S)-1-methyl-4-(6-methylhepta-1,5-dien-2-yl)cyclohexene	10104370	FALSE	C1(C(=C)CCC=C(C)C)CC=C(CC1)C

MOL002972	0.8659	0.1341	0.8062	Echinopsis Radix	(4S)-1-methyl-4-(6-methylhepta-1,5-dien-2-yl)cyclohexene	10104370	FALSE	C1(C(=C)CCC=C(C)C)CC=C(CC1)C
MOL002972	0.8659	0.1341	0.8062	Dalbergiae Odoriferae Lignum	(4S)-1-methyl-4-(6-methylhepta-1,5-dien-2-yl)cyclohexene	10104370	FALSE	C1(C(=C)CCC=C(C)C)CC=C(CC1)C
MOL002973	0.9281	0.0719	0.8964	Dalbergiae Odoriferae Lignum	Bowdichione	5281705	FALSE	C1(=O)C(=CC(=O)C(=C1)OC)c1coc2c(c1=O)ccc(c2)O
MOL002974	0.9253	0.0747	0.8705	Dalbergiae Odoriferae Lignum	Butein	5281222	FALSE	c1(c(cc(cc1)O)O)C(=O)/C=C/c1cc(c(cc1)O)O
MOL002975	0.9069	0.0931	0.8628	Dalbergiae Odoriferae Lignum	butin	28125525	FALSE	c12c(C(=O)CC(O1)c1cc(c(cc1)O)O)ccc(c2)O
MOL002975	0.9069	0.0931	0.8628	Ecliptae Herba	butin	28125525	FALSE	c12c(C(=O)CC(O1)c1cc(c(cc1)O)O)ccc(c2)O
MOL002975	0.9069	0.0931	0.8628	Abri Herba	butin	28125525	FALSE	c12c(C(=O)CC(O1)c1cc(c(cc1)O)O)ccc(c2)O
MOL002976	0.1149	0.8851	0.7249	Dalbergiae Odoriferae Lignum	(3R,4R)-2',7-dihydroxy-4',5'-dimethoxy-4-[(3R)-2',7-dihydroxy-4'-methoxyisoflavan-5'-yl]isoflavan	Not Available	FALSE	C1(C(c2ccc(cc2OC1)O)c1c(cc(c(C2Cc3ccc(cc3OC2)O)c1)O)OC)c1c(cc(c(c1)OC)OC)O
MOL002977	0.9051	0.0949	0.8927	Dalbergiae Odoriferae Lignum	(2,5-dihydroxy-4-methoxyphenyl)-phenylmethanone	3938139	FALSE	C(=O)(c1c(cc(c(c1)O)OC)O)c1ccccc1
MOL002978	0.8830	0.1170	0.8346	Dalbergiae Odoriferae Lignum	Chalkone	637760	TRUE	C(=C\c1ccccc1)/C(=O)c1ccccc1
MOL002979	0.9023	0.0977	0.8497	Dalbergiae Odoriferae Lignum	3R-Claussequinone	332771	FALSE	C1(=O)C(=CC(=O)C(=C1)OC)C1COc2c(C1)ccc(c2)O
MOL002980	0.9294	0.0706	0.9332	Dalbergiae Odoriferae Lignum	dihydrolinalool	Not Available	FALSE	C(CCCC(C)C)(C=C)(C)O

MOL002981	0.7762	0.2238	0.8312	Dalbergiae Odoriferae Lignum	Duartin	127790	FALSE	C1C(Cc2c(O1)c(c(cc2)O)OC)c1c(c(c(cc1)OC)O)OC
MOL002982	0.4040	0.5960	0.7303	Dalbergiae Odoriferae Lignum	(3R,4R)-3',7-dihydroxy-2',4'-dimethoxy-4-[(2S)-4',5,7-trihydroxyflavanone-6-yl]isoflavan	14777423	FALSE	C1(C(c2ccc(cc2OC1)O)c1c(c2C(=O)CC(Oc2cc1O)c1ccc(cc1)O)O)c1c(c(c(cc1)OC)O)OC
MOL002983	0.9142	0.0858	0.9647	Phragmitis Rhizoma	Guasol	460	FALSE	c1(c(cccc1)O)OC
MOL002983	0.9142	0.0858	0.9647	Gynostemmae Pentaphylli Herba	Guasol	460	FALSE	c1(c(cccc1)O)OC
MOL002983	0.9142	0.0858	0.9647	Angelicae Sinensis Radix	Guasol	460	FALSE	c1(c(cccc1)O)OC
MOL002983	0.9142	0.0858	0.9647	Mume Fructus	Guasol	460	FALSE	c1(c(cccc1)O)OC
MOL002983	0.9142	0.0858	0.9647	Radix Clematidis	Guasol	460	FALSE	c1(c(cccc1)O)OC
MOL002983	0.9142	0.0858	0.9647	Daturae Flos	Guasol	460	FALSE	c1(c(cccc1)O)OC
MOL002983	0.9142	0.0858	0.9647	Ginkgo Folium	Guasol	460	FALSE	c1(c(cccc1)O)OC
MOL002983	0.9142	0.0858	0.9647	Mume Flos	Guasol	460	FALSE	c1(c(cccc1)O)OC
MOL002983	0.9142	0.0858	0.9647	Radix Bupleuri	Guasol	460	FALSE	c1(c(cccc1)O)OC
MOL002983	0.9142	0.0858	0.9647	Magnolia Officinalis Rehd Et Wils.	Guasol	460	FALSE	c1(c(cccc1)O)OC
MOL002983	0.9142	0.0858	0.9647	Campsis Flos	Guasol	460	FALSE	c1(c(cccc1)O)OC
MOL002983	0.9142	0.0858	0.9647	Bomboo Juice	Guasol	460	FALSE	c1(c(cccc1)O)OC
MOL002983	0.9142	0.0858	0.9647	Ardisiae Japonicae Herba	Guasol	460	FALSE	c1(c(cccc1)O)OC
MOL002983	0.9142	0.0858	0.9647	Momordicae Fructus	Guasol	460	FALSE	c1(c(cccc1)O)OC
MOL002983	0.9142	0.0858	0.9647	Dalbergiae Odoriferae Lignum	Guasol	460	FALSE	c1(c(cccc1)O)OC
MOL002983	0.9142	0.0858	0.9647	Sojae Semen Nigrum	Guasol	460	FALSE	c1(c(cccc1)O)OC
MOL002984	0.8212	0.1788	0.7598	Dalbergiae Odoriferae Lignum	3-methoxy-4-[(E)-3-phenylprop-2-enyl]pyrocatechol	11777169	FALSE	c1ccc(cc1)/C=C/Cc1c(c(c(cc1)O)O)OC
MOL002985	0.7776	0.2224	0.7945	Dalbergiae Odoriferae Lignum	isoduartin	Not Available	FALSE	c1(ccc2c(c1OC)OCC(C2)c1ccc(c(c1O)OC)OC)O
MOL002986	0.7386	0.2614	0.8409	Dalbergiae Odoriferae Lignum	2,6-dimethoxy-3-[(E)-3-phenylprop-2-enyl]phenol	10423261	FALSE	c1(c(c(ccc1OC)C/C=C/c1ccccc1)OC)O

MOL002987	0.9208	0.0792	0.8480	Dalbergiae Odoriferae Lignum	Koparin	5318834	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1c(c(c(cc1)OC)O)O
MOL002988	0.1587	0.8413	0.7481	Dalbergiae Odoriferae Lignum	(3R,4R)-3',7-dihydroxy-2',4'-dimethoxy-4-[(3R)-2',7-dihydroxy-4'-methoxyisoflavan-5'-yl]isoflavan	Not Available	FALSE	c1c(cc2c(c1)CC(CO2)c1cc(c(cc1O)OC)C1c2c(OCC1c1c(c(c(cc1)OC)O)OC)cc(cc2)O)O
MOL002989	0.7277	0.2723	0.7319	Dalbergiae Odoriferae Lignum	4-Hydroxyhomopterocarpin	442792	FALSE	C1C2C(c3c(O1)c(c(cc3)OC)O)Oc1c2ccc(c1)OC
MOL002990	0.7833	0.2167	0.6756	Dalbergiae Odoriferae Lignum	(6aR,11aR)-3,9,10-trimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-4-ol	23259932	FALSE	c12c(ccc(c1OC)OC)C1C(O2)c2c(OC1)c(c(cc2)OC)O
MOL002991	0.8321	0.1679	0.7412	Dalbergiae Odoriferae Lignum	(6aR,11aR)-3,9-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromene-4,10-diol	23259933	FALSE	C1C2C(c3ccc(c(c3O1)O)OC)Oc1c2ccc(c1O)OC
MOL002992	0.9247	0.0753	0.8843	Dalbergiae Odoriferae Lignum	methyl 2-hydroxy-3,4-dimethoxybenzoate	5319678	FALSE	C(=O)(c1c(c(c(cc1)OC)OC)O)OC
MOL002994	0.9121	0.0879	0.9163	Dalbergiae Odoriferae Lignum	55282-90-1	5363302	FALSE	CC(=O)/C=C/CCCC=C
MOL002995	0.8559	0.1441	0.8734	Dalbergiae Odoriferae Lignum	3-methoxy-4-[(E)-3-phenylprop-2-enyl]phenol	6450240	FALSE	c1(cc(c(cc1)C/C=C/c1ccccc1)OC)O
MOL002996	0.7813	0.2187	0.6809	Dalbergiae Odoriferae Lignum	odoricarpin	Not Available	FALSE	C1C2C(c3ccc(c(c3O1)OC)OC)Oc1c2ccc(c1O)OC

MOL002997	0.8142	0.1858	0.8901	Dalbergiae Odoriferae Lignum	3-(2-hydroxy-3,4-dimethoxyphenyl)-2H-chromen-7-ol	11779541	FALSE	C1(=Cc2ccc(cc2OC1)O)c1c(c(c(cc1)OC)OC)O
MOL002998	0.8914	0.1086	0.9612	Paederiae Scandentis Herba	IPH	20488062	TRUE	c1(ccccc1)O
MOL002998	0.8914	0.1086	0.9612	Viticis Fructus	IPH	20488062	TRUE	c1(ccccc1)O
MOL002998	0.8914	0.1086	0.9612	Platycodon Grandiforus	IPH	20488062	TRUE	c1(ccccc1)O
MOL002998	0.8914	0.1086	0.9612	Cyathulae Radix	IPH	20488062	TRUE	c1(ccccc1)O
MOL002998	0.8914	0.1086	0.9612	Bomboo Juice	IPH	20488062	TRUE	c1(ccccc1)O
MOL002998	0.8914	0.1086	0.9612	Sojae Semen Nigrum	IPH	20488062	TRUE	c1(ccccc1)O
MOL002998	0.8914	0.1086	0.9612	Dalbergiae Odoriferae Lignum	IPH	20488062	TRUE	c1(ccccc1)O
MOL002998	0.8914	0.1086	0.9612	Hippophae Fructus	IPH	20488062	TRUE	c1(ccccc1)O
MOL002998	0.8914	0.1086	0.9612	Radix Bupleuri	IPH	20488062	TRUE	c1(ccccc1)O
MOL002998	0.8914	0.1086	0.9612	Chaenomeles Sinensis (Thouin) Koehne	IPH	20488062	TRUE	c1(ccccc1)O
MOL002998	0.8914	0.1086	0.9612	Viticis Negundo Folium	IPH	20488062	TRUE	c1(ccccc1)O
MOL002998	0.8914	0.1086	0.9612	Junci Medulla	IPH	20488062	TRUE	c1(ccccc1)O
MOL002998	0.8914	0.1086	0.9612	Panacis Quinquefolii Radix	IPH	20488062	TRUE	c1(ccccc1)O
MOL002998	0.8914	0.1086	0.9612	Campsis Flos	IPH	20488062	TRUE	c1(ccccc1)O
MOL002998	0.8914	0.1086	0.9612	Radix Cynanchi Paniculati	IPH	20488062	TRUE	c1(ccccc1)O
MOL002998	0.8914	0.1086	0.9612	Capsici Fructus	IPH	20488062	TRUE	c1(ccccc1)O
MOL002998	0.8914	0.1086	0.9612	Catechu	IPH	20488062	TRUE	c1(ccccc1)O
MOL002998	0.8914	0.1086	0.9612	Ginkgo Folium	IPH	20488062	TRUE	c1(ccccc1)O
MOL002998	0.8914	0.1086	0.9612	Angelicae Sinensis Radix	IPH	20488062	TRUE	c1(ccccc1)O
MOL002999	0.8315	0.1685	0.9482	Dalbergiae Odoriferae Lignum	Sativanone	5321142	FALSE	C1C(C(=O)c2c(O1)cc(cc2)O)c1c(cc(cc1)OC)OC
MOL003000	0.7782	0.2218	0.7997	Dalbergiae Odoriferae Lignum	Stevein	5321501	FALSE	c1(c(cc2c(c1)oc(=O)cc2c1cc(ccc1)O)O)OC
MOL003001	0.9205	0.0795	0.8856	Dalbergiae Odoriferae Lignum	Vestitone	44446897	FALSE	C1C(C(=O)c2c(O1)cc(cc2)O)c1c(cc(cc1)OC)O
MOL003002	0.7676	0.2324	0.9138	Dalbergiae Odoriferae Lignum	violanone	44446884	FALSE	C1(C(=O)c2ccc(cc2OC1)O)c1c(c(c(cc1)OC)O)OC
MOL003003	0.9169	0.0831	0.9368	Dalbergiae Odoriferae Lignum	Xenognosin B	5280551	FALSE	c1(ccc2c(c1)occ(c2=O)c1c(cc(cc1)OC)O)O

MOL003004	0.8566	0.1434	0.6486	Lonicerae Japonicae Flos	(1R,4S,4aR)-1-isopropyl-4-methyl-7-methylene-2,3,4,4a,5,6-hexahydro-1H-naphthalene	10750739	FALSE	C1(CCC(C2CCC(=C)C=C12)C)C(C)C
MOL003004	0.8566	0.1434	0.6486	Farfarae Flos	(1R,4S,4aR)-1-isopropyl-4-methyl-7-methylene-2,3,4,4a,5,6-hexahydro-1H-naphthalene	10750739	FALSE	C1(CCC(C2CCC(=C)C=C12)C)C(C)C
MOL003004	0.8566	0.1434	0.6486	Bidentis Bipinnatae Herba	(1R,4S,4aR)-1-isopropyl-4-methyl-7-methylene-2,3,4,4a,5,6-hexahydro-1H-naphthalene	10750739	FALSE	C1(CCC(C2CCC(=C)C=C12)C)C(C)C
MOL003006	0.8820	0.1180	0.6575	Lonicerae Japonicae Flos	(-)-(3R,8S,9R,9aS,10aS)-9-ethenyl-8-(beta-D-glucopyranosyloxy)-2,3,9,9a,10,10a-hexahydro-5-oxo-5H,8H-pyrano[4,3-d]oxazolo[3,2-a]pyridine-3-carboxylic acid_qt	Not Available	FALSE	C12CC3C(=COC(C3C=C)O)C(=O)N1C(CO2)C(=O)O
MOL003008	0.7502	0.2498	0.7360	Lonicerae Japonicae Flos	madreselvin B	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1)COC1OC(C(O)C(O)C1O)COC(=O)/C=C/c1cc(O)c(O)cc1

MOL003010	0.9072	0.0928	0.8001	Lonicerae Japonicae Flos	quercetin-3-o-beta-D-glu	Not Available	FALSE	O1C(Oc2c(oc3c(c2=O)c(O)cc(O)c3)c2cc(O)c(O)cc2)C(O)C(O)C(O)C1C(=O)O
MOL003010	0.9072	0.0928	0.8001	Cornus Officinalis Sieb. Et Zucc.	quercetin-3-o-beta-D-glu	Not Available	FALSE	O1C(Oc2c(oc3c(c2=O)c(O)cc(O)c3)c2cc(O)c(O)cc2)C(O)C(O)C(O)C1C(=O)O
MOL003011	0.9353	0.0647	0.8040	Lonicerae Japonicae Flos	Secologanate	439612	FALSE	C1(C(C(C(=CO1)C(=O)O)CC=O)C=C)OC1C(O)C(O)C(O)C(O1)CO
MOL003012	0.9230	0.0770	0.8900	Lonicerae Japonicae Flos	secologanic acid_qt	Not Available	FALSE	C1(C(C(C(=CO1)C(=O)O)CC=O)C=C)O
MOL003014	0.4903	0.5097	0.6869	Lonicerae Japonicae Flos	secologanic dibutylacetal_qt	Not Available	FALSE	C1(C(C(C(=CO1)C(=O)OC)CC(OCCCCC)OCCCCC)C=C)O
MOL003016	0.9227	0.0773	0.8349	Lonicerae Japonicae Flos	secologanin dimethylacetal_qt	Not Available	FALSE	C1(C(C(C(=CO1)C(=O)OC)CC(OC)OC)C=C)O
MOL003017	0.9466	0.0534	0.8938	Lonicerae Japonicae Flos	Desaspidinol-A	24135	FALSE	c1(c(cc(cc1O)OC)O)C(=O)C
MOL003018	0.9108	0.0892	0.7042	Lonicerae Japonicae Flos	SCG	161276	FALSE	C1(C(C(C(=CO1)C(=O)OC)CC=O)C=C)OC1C(O)C(O)C(O)C(O1)CO
MOL003019	0.9436	0.0564	0.8631	Strychni Semen	secologanin_qt	Not Available	FALSE	C1(C(C(C(=CO1)C(=O)OC)CC=O)C=C)O
MOL003019	0.9436	0.0564	0.8631	Lonicerae Japonicae Flos	secologanin_qt	Not Available	FALSE	C1(C(C(C(=CO1)C(=O)OC)CC=O)C=C)O
MOL003020	0.9294	0.0706	0.7997	Lonicerae Japonicae Flos	secologanoside 7-methylester	Not Available	FALSE	C1(C(C(OC=C1C(=O)O)OOC1C(O)C(O)C(O)C(O1)CO)C=C)CC(=O)OC
MOL003021	0.9343	0.0657	0.8866	Lonicerae Japonicae Flos	secologanoside 7-methylester_qt	Not Available	FALSE	C1(C(C(OC=C1C(=O)O)OO)C=C)CC(=O)OC
MOL003022	0.9321	0.0679	0.7298	Lonicerae Japonicae Flos	Secoxyloganin	162868	FALSE	C1(C(C(C(=CO1)C(=O)OC)CC(=O)O)C=C)OC1C(O)C(O)C(O)C(O1)CO
MOL003023	0.9393	0.0607	0.8492	Lonicerae Japonicae Flos	secoxyloganin_qt	Not Available	FALSE	C1(C(C(C(=CO1)C(=O)OC)CC(=O)O)C=C)O
MOL003024	0.9341	0.0659	0.9274	Lonicerae Japonicae Flos	loganic	Not Available	FALSE	C1(C(CCCC1)(O)O)(C(=O)O)O
MOL003025	0.8955	0.1045	0.6826	Lonicerae Japonicae Flos	vogeloside	Not Available	FALSE	C1(=O)C2=COC(C(C2CC(O1)OC)C=C)OC1C(O)C(O)C(O)C(O1)CO

MOL003026	0.9498	0.0502	0.8265	Lonicerae Japonicae Flos	(3R,4aS,5R,6R)-6-hydroxy-3-methoxy-5-vinyl-4,4a,5,6-tetrahydro-3H-pyrano[5,4-c]pyran-1-one	10823100	FALSE	C1(=O)C2=COC(C(C2CC(O1)OC)C=C)O
MOL003027	0.8418	0.1582	0.6717	Lonicerae Japonicae Flos	9-epi-(E)-caryophyllene	6429274	FALSE	C12CC/C(=C/CCC(=C)C1CC2(C)C)/C
MOL003028	0.8128	0.1872	0.6826	Lonicerae Japonicae Flos	Eudesmol	Not Available	FALSE	C1(CCC(C)C2CC(C(C)C)CCC12C)O
MOL003028	0.8128	0.1872	0.6826	Rhododendri Daurici Folium	Eudesmol	Not Available	FALSE	C1(CCC(C)C2CC(C(C)C)CCC12C)O
MOL003028	0.8128	0.1872	0.6826	Curcumae Radix	Eudesmol	Not Available	FALSE	C1(CCC(C)C2CC(C(C)C)CCC12C)O
MOL003028	0.8128	0.1872	0.6826	Belamcandae Rhizome	Eudesmol	Not Available	FALSE	C1(CCC(C)C2CC(C(C)C)CCC12C)O
MOL003028	0.8128	0.1872	0.6826	Aucklandiae Radix	Eudesmol	Not Available	FALSE	C1(CCC(C)C2CC(C(C)C)CCC12C)O
MOL003031	0.9274	0.0726	0.9509	Capsici Fructus	Propyl vinyl ketone	15395	FALSE	C(=O)(CCC)C=C
MOL003031	0.9274	0.0726	0.9509	Lonicerae Japonicae Flos	Propyl vinyl ketone	15395	FALSE	C(=O)(CCC)C=C
MOL003032	0.8791	0.1209	0.9190	Lonicerae Japonicae Flos	BZM	2345	FALSE	c1(C(=O)OCc2ccccc2)ccccc1
MOL003032	0.8791	0.1209	0.9190	Linderae Radix	BZM	2345	FALSE	c1(C(=O)OCc2ccccc2)ccccc1
MOL003032	0.8791	0.1209	0.9190	Eriobotryae Folium	BZM	2345	FALSE	c1(C(=O)OCc2ccccc2)ccccc1
MOL003032	0.8791	0.1209	0.9190	Dianthi Herba	BZM	2345	FALSE	c1(C(=O)OCc2ccccc2)ccccc1
MOL003032	0.8791	0.1209	0.9190	Notopterygii Rhizoma Et Radix	BZM	2345	FALSE	c1(C(=O)OCc2ccccc2)ccccc1
MOL003032	0.8791	0.1209	0.9190	Cinnanmomi Cortex	BZM	2345	FALSE	c1(C(=O)OCc2ccccc2)ccccc1
MOL003032	0.8791	0.1209	0.9190	Evodiae Fructus	BZM	2345	FALSE	c1(C(=O)OCc2ccccc2)ccccc1
MOL003032	0.8791	0.1209	0.9190	Sinapis Semen	BZM	2345	FALSE	c1(C(=O)OCc2ccccc2)ccccc1
MOL003032	0.8791	0.1209	0.9190	Mume Flos	BZM	2345	FALSE	c1(C(=O)OCc2ccccc2)ccccc1
MOL003032	0.8791	0.1209	0.9190	Cinnamomi Ramulus	BZM	2345	FALSE	c1(C(=O)OCc2ccccc2)ccccc1
MOL003032	0.8791	0.1209	0.9190	Benzoinum	BZM	2345	FALSE	c1(C(=O)OCc2ccccc2)ccccc1
MOL003032	0.8791	0.1209	0.9190	Adenophprae Ae Radix	BZM	2345	FALSE	c1(C(=O)OCc2ccccc2)ccccc1
MOL003032	0.8791	0.1209	0.9190	Acoritataninowii Rhizoma	BZM	2345	FALSE	c1(C(=O)OCc2ccccc2)ccccc1
MOL003033	0.9275	0.0725	0.9477	Lonicerae Japonicae Flos	Hexene	11597	FALSE	C(CC=C)CC
MOL003033	0.9275	0.0725	0.9477	Rubi Fructus	Hexene	11597	FALSE	C(CC=C)CC
MOL003034	0.7765	0.2235	0.8032	Lonicerae Japonicae Flos	disacoside B	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)COC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1OC1OC(C(O)C(O)C1O)C

MOL003037	0.3343	0.6657	0.8408	Lonicerae Japonicae Flos	hydnocarpinhydnocarpinhydnocarpin	Not Available	FALSE	O1C(C(Oc2c1ccc(c2)c1oc2c(c(=O)c1)c(O)cc(O)c2)CO)c1cc(OC)c(O)cc1
MOL003038	0.7622	0.2378	0.7972	Lonicerae Japonicae Flos	fulvotomentoside A	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(OC4OC(C(O)C(O)C4O)CO)C(O)C3O)CO)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(OC2OCC(O)C(O)C2O)C1OC1OC(C(O)C(O)C1O)C
MOL003040	0.9309	0.0691	0.9692	Lonicerae Japonicae Flos	Amylol	6276	FALSE	C(CCCC)O
MOL003040	0.9309	0.0691	0.9692	Rose Rugosae Flos	Amylol	6276	FALSE	C(CCCC)O
MOL003040	0.9309	0.0691	0.9692	Ephedra Herba	Amylol	6276	FALSE	C(CCCC)O
MOL003040	0.9309	0.0691	0.9692	Sesami Nigrum Semen	Amylol	6276	FALSE	C(CCCC)O
MOL003040	0.9309	0.0691	0.9692	Achyranthis Bidentatae Radix	Amylol	6276	FALSE	C(CCCC)O
MOL003040	0.9309	0.0691	0.9692	Radix Bupleuri	Amylol	6276	FALSE	C(CCCC)O
MOL003040	0.9309	0.0691	0.9692	Campsis Flos	Amylol	6276	FALSE	C(CCCC)O
MOL003041	0.7736	0.2264	0.7868	Lonicerae Japonicae Flos	macranthoidin A	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)COC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1OC1OC(C(O)C(OC2OC(C(O)C(O)C2O)CO)C1O)C
MOL003041	0.7736	0.2264	0.7868	Dipsaci Radix	macranthoidin A	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)COC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1OC1OC(C(O)C(OC2OC(C(O)C(O)C2O)CO)C1O)C
MOL003042	0.7847	0.2153	0.7837	Lonicerae Japonicae Flos	macranthoidin B	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)COC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(CO)C)C1OCC(OC2OC(C(O)C(O)C2O)CO)C(OC2OC(C(O)C(O)C2O)CO)C1OC1OC(C(O)C(O)C1O)C
MOL003043	0.5569	0.4431	0.6604	Rose Rugosae Flos	(5Z,9Z)-6,10,14-trimethylpentadeca-5,9,13-trien-2-one	1711942	FALSE	CC(=O)CC/C=C(/C)\CC/C=C(\CCC=C(C)C)/C
MOL003043	0.5569	0.4431	0.6604	Tamaricis Cacumen	(5Z,9Z)-6,10,14-trimethylpentadeca-5,9,13-trien-2-one	1711942	FALSE	CC(=O)CC/C=C(/C)\CC/C=C(\CCC=C(C)C)/C
MOL003043	0.5569	0.4431	0.6604	Lonicerae Japonicae Flos	(5Z,9Z)-6,10,14-trimethylpentadeca-5,9,13-trien-2-one	1711942	FALSE	CC(=O)CC/C=C(/C)\CC/C=C(\CCC=C(C)C)/C

MOL003044	0.8907	0.1093	0.8941	Oroxyli Semen	Chryseriol	5280666	FALSE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)OC)c(cc(c2)O)O
MOL003044	0.8907	0.1093	0.8941	Hydnocarpi Anthelminticae Semen	Chryseriol	5280666	FALSE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)OC)c(cc(c2)O)O
MOL003044	0.8907	0.1093	0.8941	Cyperi Rhizoma	Chryseriol	5280666	FALSE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)OC)c(cc(c2)O)O
MOL003044	0.8907	0.1093	0.8941	Inulae Flos	Chryseriol	5280666	FALSE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)OC)c(cc(c2)O)O
MOL003044	0.8907	0.1093	0.8941	Maydis Seigma	Chryseriol	5280666	FALSE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)OC)c(cc(c2)O)O
MOL003044	0.8907	0.1093	0.8941	Moslae Herba	Chryseriol	5280666	FALSE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)OC)c(cc(c2)O)O
MOL003044	0.8907	0.1093	0.8941	Polygoni Orientalis Fructus	Chryseriol	5280666	FALSE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)OC)c(cc(c2)O)O
MOL003044	0.8907	0.1093	0.8941	Ginkgo Folium	Chryseriol	5280666	FALSE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)OC)c(cc(c2)O)O
MOL003044	0.8907	0.1093	0.8941	Lonicerae Japonicae Flos	Chryseriol	5280666	FALSE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)OC)c(cc(c2)O)O
MOL003044	0.8907	0.1093	0.8941	Peanut Skin	Chryseriol	5280666	FALSE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)OC)c(cc(c2)O)O
MOL003044	0.8907	0.1093	0.8941	Epimrdii Herba	Chryseriol	5280666	FALSE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)OC)c(cc(c2)O)O
MOL003044	0.8907	0.1093	0.8941	Lobeliae Chinensis Herba	Chryseriol	5280666	FALSE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)OC)c(cc(c2)O)O
MOL003044	0.8907	0.1093	0.8941	Chrysanthemi Flos	Chryseriol	5280666	FALSE	c12c(c(=O)cc(o1)c1cc(c(cc1)O)OC)c(cc(c2)O)O
MOL003047	0.9521	0.0479	0.8063	Radix Salviae	[(1S)-endo]-(-)-Borneol	1201518	FALSE	C12(CCC(CC1O)C2(C)C)C
MOL003047	0.9521	0.0479	0.8063	Cinnanmomi Cortex	[(1S)-endo]-(-)-Borneol	1201518	FALSE	C12(CCC(CC1O)C2(C)C)C
MOL003047	0.9521	0.0479	0.8063	Morindae Officinalis Radix	[(1S)-endo]-(-)-Borneol	1201518	FALSE	C12(CCC(CC1O)C2(C)C)C
MOL003047	0.9521	0.0479	0.8063	Campsis Flos	[(1S)-endo]-(-)-Borneol	1201518	FALSE	C12(CCC(CC1O)C2(C)C)C
MOL003047	0.9521	0.0479	0.8063	Folium Artemisiae Argyi	[(1S)-endo]-(-)-Borneol	1201518	FALSE	C12(CCC(CC1O)C2(C)C)C
MOL003047	0.9521	0.0479	0.8063	Curcumae Radix	[(1S)-endo]-(-)-Borneol	1201518	FALSE	C12(CCC(CC1O)C2(C)C)C
MOL003047	0.9521	0.0479	0.8063	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	[(1S)-endo]-(-)-Borneol	1201518	FALSE	C12(CCC(CC1O)C2(C)C)C
MOL003047	0.9521	0.0479	0.8063	Polygonati Odorati Rhizoma	[(1S)-endo]-(-)-Borneol	1201518	FALSE	C12(CCC(CC1O)C2(C)C)C
MOL003047	0.9521	0.0479	0.8063	Lonicerae Japonicae Flos	[(1S)-endo]-(-)-Borneol	1201518	FALSE	C12(CCC(CC1O)C2(C)C)C
MOL003047	0.9521	0.0479	0.8063	Schisandrae Chinensis Fructus	[(1S)-endo]-(-)-Borneol	1201518	FALSE	C12(CCC(CC1O)C2(C)C)C
MOL003047	0.9521	0.0479	0.8063	Magnolia Officinalis Rehd Et Wils.	[(1S)-endo]-(-)-Borneol	1201518	FALSE	C12(CCC(CC1O)C2(C)C)C
MOL003047	0.9521	0.0479	0.8063	Acoritataninowii Rhizoma	[(1S)-endo]-(-)-Borneol	1201518	FALSE	C12(CCC(CC1O)C2(C)C)C
MOL003047	0.9521	0.0479	0.8063	Mori Cortex	[(1S)-endo]-(-)-Borneol	1201518	FALSE	C12(CCC(CC1O)C2(C)C)C
MOL003047	0.9521	0.0479	0.8063	Forsythiae Fructus	[(1S)-endo]-(-)-Borneol	1201518	FALSE	C12(CCC(CC1O)C2(C)C)C

MOL003047	0.9521	0.0479	0.8063	Cinnamomi Ramulus	[(1S)-endo]-(-)-Borneol	1201518	FALSE	C12(CCC(CC1O)C2(C)C)C
MOL003048	0.9012	0.0988	0.8749	Lonicerae Japonicae Flos	methyl chlorogenate	71720841	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)OC)C(=O)/C=C\c1cc(O)c(O)cc1
MOL003049	0.7446	0.2554	0.8458	Sapindi Mukorossi Semen	Olean-12-en-28-oic acid, 23-hydroxy-3-((O-beta-D-xylopyranosyl-(1-3)-O-6-deoxy-alpha-L-mannopyranosyl-(1-2)-alpha-L-arabinopyranosyl)oxy)-, (3beta,4alpha)-	161686	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1OC1OC(C(O)C(OC2OCC(O)C(O)C2O)C1O)C
MOL003049	0.7446	0.2554	0.8458	Sapindi Mukorossiperic Arpium	Olean-12-en-28-oic acid, 23-hydroxy-3-((O-beta-D-xylopyranosyl-(1-3)-O-6-deoxy-alpha-L-mannopyranosyl-(1-2)-alpha-L-arabinopyranosyl)oxy)-, (3beta,4alpha)-	161686	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1OC1OC(C(O)C(OC2OCC(O)C(O)C2O)C1O)C

MOL003049	0.7446	0.2554	0.8458	Lonicerae Japonicae Flos	Olean-12-en-28-oic acid, 23-hydroxy-3-((O-beta-D-xylopyranosyl-(1-3)-O-6-deoxy-alpha-L-mannopyranosyl-(1-2)-alpha-L-arabinopyranosyl)oxy)-, (3beta,4alpha)-	161686	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1OC1OC(C(O)C(OC2OCC(O)C(O)C2O)C1O)C
MOL003050	0.9264	0.0736	0.9463	Panacis Quinquefolii Radix	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Rose Rugosae Flos	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Lysimachiae Foenigraeci Herba	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Campsis Flos	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Folium Ilicis Cornutae	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Eriobotryae Folium	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Trichosanthes Kirilowii Maxim	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Ganoderma	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Mori Fructus	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Paederiae Scandentis Herba	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Humulus Scandens (Lour.) Merr.	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Lonicerae Japonicae Flos	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Portulacae Herba	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Ephedra Herba	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Meliae Azedarach Fructus	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	A. Dahurica (Fisch.) Benth. Et Hook	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Codonopsis Radix	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Broussonetiae Fructus	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Radix Bupleuri	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Chaenomeles Sinensis (Thouin) Koehne	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Gossampiniflos	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Citri Grandis Exocarpium	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O

MOL003050	0.9264	0.0736	0.9463	Polygoni Orientalis Fructus	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Arisaematis Rhizoma	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Mori Cortex	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Coicis Semen	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Malvae Fructus	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Momordicae Fructus	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Semiaquilegiae Radix	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003050	0.9264	0.0736	0.9463	Morindae Officinalis Radix	nonanoic acid	8158	FALSE	C(CCCCC)CCC(=O)O
MOL003051	0.8826	0.1174	0.8734	Saussureae Involucratae Herba	Scolymoside	5282152	FALSE	O(C1C(O)C(O)C(OC1Oc1cc2oc(cc(=O)c2c(O)c1)c1cc(O)c(O)cc1)CO)C1OC(C(O)C(O)C1O)C
MOL003051	0.8826	0.1174	0.8734	Buddlejae Flos	Scolymoside	5282152	FALSE	O(C1C(O)C(O)C(OC1Oc1cc2oc(cc(=O)c2c(O)c1)c1cc(O)c(O)cc1)CO)C1OC(C(O)C(O)C1O)C
MOL003051	0.8826	0.1174	0.8734	Lonicerae Japonicae Flos	Scolymoside	5282152	FALSE	O(C1C(O)C(O)C(OC1Oc1cc2oc(cc(=O)c2c(O)c1)c1cc(O)c(O)cc1)CO)C1OC(C(O)C(O)C1O)C
MOL003051	0.8826	0.1174	0.8734	Verbenae Herb	Scolymoside	5282152	FALSE	O(C1C(O)C(O)C(OC1Oc1cc2oc(cc(=O)c2c(O)c1)c1cc(O)c(O)cc1)CO)C1OC(C(O)C(O)C1O)C
MOL003051	0.8826	0.1174	0.8734	Aurantii Fructus Immaturus	Scolymoside	5282152	FALSE	O(C1C(O)C(O)C(OC1Oc1cc2oc(cc(=O)c2c(O)c1)c1cc(O)c(O)cc1)CO)C1OC(C(O)C(O)C1O)C
MOL003052	0.9172	0.0828	0.9150	Lonicerae Japonicae Flos	Isothiazole, trimethyl-	581460	FALSE	s1nc(c(c1C)C)C
MOL003053	0.8021	0.1979	0.7475	Lonicerae Japonicae Flos	Methyl isomyristate	21204	FALSE	C(=O)(CCCCCCCCCCC(C)C)OC
MOL003053	0.8021	0.1979	0.7475	Perillae Fructus	Methyl isomyristate	21204	FALSE	C(=O)(CCCCCCCCCCC(C)C)OC
MOL003054	0.8981	0.1019	0.8052	Lonicerae Japonicae Flos	eriodictyol-7-o-glucoside	Not Available	FALSE	c12c(OC(CC1=O)c1cc(c(cc1)O)O)cc(cc2O)OC1OC(C(C(C1O)O)O)CO
MOL003056	0.9277	0.0723	0.8386	Lonicerae Japonicae Flos	BNL	7094	FALSE	C1(C2CCCCC2)CCCCC1
MOL003056	0.9277	0.0723	0.8386	Raphani Semen	BNL	7094	FALSE	C1(C2CCCCC2)CCCCC1
MOL003057	0.9588	0.0412	0.9673	Eucommiae Folium	3-Methyl-2-pent-2-enyl-cyclopent-2-enone	1549019	FALSE	C1(=O)C(=C(CC1)C)C/C=C/CC
MOL003057	0.9588	0.0412	0.9673	Lonicerae Japonicae Flos	3-Methyl-2-pent-2-enyl-cyclopent-2-enone	1549019	FALSE	C1(=O)C(=C(CC1)C)C/C=C/CC
MOL003058	0.8835	0.1165	0.9672	Lonicerae Japonicae Flos	2,3-DIMETHYLPYRAZINE	22201	FALSE	c1(c(nccn1)C)C
MOL003060	0.9142	0.0858	0.9348	Dichroae Radix	Hexadienal	637564	FALSE	C(=O)/C=C/C=C/C
MOL003060	0.9142	0.0858	0.9348	Lonicerae Japonicae Flos	Hexadienal	637564	FALSE	C(=O)/C=C/C=C/C

MOL003062	0.2549	0.7451	0.6481	Lonicerae Japonicae Flos	4,5'-Retro-.beta.,.beta.-Carotene-3,3'-dione, 4',5'-didehydro-	5380108	FALSE	O=C1CC(/C(=C/C=C(\C)/C=C/C=C(/C=C/C=C/C(=C/C=C/C(=C/C=C\2/C(CC(=O)C=C2C)(C)C)/C)/C)\C)/C(=C1)C)(C)C
MOL003064	0.9366	0.0634	0.7413	Lonicerae Japonicae Flos	Leukol	7047	FALSE	n1cccc2ccccc12
MOL003065	0.9409	0.0591	0.9203	Lonicerae Japonicae Flos	4-caffeoylquinic acid	Not Available	FALSE	O(C(=O)/C=C\c1ccc(c(c1)O)O)C1C(CC(CC1O)(O)C(=O)O)O
MOL003066	0.9497	0.0503	0.9440	Boehmeriae Rhizoma Et Radix	Neochlorogenic acid	Not Available	FALSE	C1C(C(C(CC1(O)C(=O)O)OC(=O)/C=C\c1ccc(c(c1)O)O)O)O
MOL003066	0.9497	0.0503	0.9440	Houttuyniae Herba	Neochlorogenic acid	Not Available	FALSE	C1C(C(C(CC1(O)C(=O)O)OC(=O)/C=C\c1ccc(c(c1)O)O)O)O
MOL003066	0.9497	0.0503	0.9440	Lonicerae Japonicae Flos	Neochlorogenic acid	Not Available	FALSE	C1C(C(C(CC1(O)C(=O)O)OC(=O)/C=C\c1ccc(c(c1)O)O)O)O
MOL003067	0.8343	0.1657	0.7250	Lonicerae Japonicae Flos	3,4-Dicaffeoylquinic acid	Not Available	FALSE	C1(CC(C(C(C1)O)OC(=O)/C=C/c1cc(cc(c1)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)(C(=O)O)O
MOL003068	0.8368	0.1632	0.7310	Lonicerae Japonicae Flos	4,5-Dicaffeoylquinic acid	Not Available	FALSE	C1(CC(C(C(C1)O)OC(=O)/C=C/c1cc(c(cc1)O)O)OC(=O)/C=C\c1cc(c(cc1)O)O)(C(=O)O)O
MOL003069	0.9313	0.0687	0.9526	Ginkgo Semen	quinic acid	6508	FALSE	C1(C(=O)O)(CC(C(C(C1)O)O)O)O
MOL003069	0.9313	0.0687	0.9526	Schisandrae Chinensis Fructus	quinic acid	6508	FALSE	C1(C(=O)O)(CC(C(C(C1)O)O)O)O
MOL003069	0.9313	0.0687	0.9526	Ginkgo Folium	quinic acid	6508	FALSE	C1(C(=O)O)(CC(C(C(C1)O)O)O)O
MOL003069	0.9313	0.0687	0.9526	Chaenomeles Sinensis (Thouin) Koehne	quinic acid	6508	FALSE	C1(C(=O)O)(CC(C(C(C1)O)O)O)O
MOL003069	0.9313	0.0687	0.9526	Chebulae Fructus	quinic acid	6508	FALSE	C1(C(=O)O)(CC(C(C(C1)O)O)O)O
MOL003069	0.9313	0.0687	0.9526	Rose Rugosae Flos	quinic acid	6508	FALSE	C1(C(=O)O)(CC(C(C(C1)O)O)O)O
MOL003069	0.9313	0.0687	0.9526	Lonicerae Japonicae Flos	quinic acid	6508	FALSE	C1(C(=O)O)(CC(C(C(C1)O)O)O)O
MOL003071	0.9355	0.0645	0.8092	Lonicerae Japonicae Flos	secologanoside	Not Available	FALSE	O1C(C(C(O)C(O)C1OC1C(C(C(=CO1)C(=O)O)CC(=O)O)C=C)O)CO
MOL003072	0.9311	0.0689	0.8714	Lonicerae Japonicae Flos	secologanoside_qt	Not Available	FALSE	OC1C(C(C(=CO1)C(=O)O)CC(=O)O)C=C
MOL003073	0.9130	0.0870	0.8362	Lonicerae Japonicae Flos	8-epiloganin	Not Available	FALSE	O1C(C(C(C(C1CO)O)O)O)OC1C2C(C(=CO1)C(=O)OC)CC(C2C)O
MOL003074	0.9569	0.0431	0.8722	Lonicerae Japonicae Flos	8-epiloganin_qt	49775368	FALSE	OC1C2C(C(=CO1)C(=O)OC)CC(C2C)O
MOL003075	0.5635	0.4365	0.6741	Lonicerae Japonicae Flos	3,4-di-O-caffeoylquinic acid methyl ester	Not Available	FALSE	C1(CC(C(C(C1)O)OC(=O)/C=C\c1cc(cc(c1)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)(C(=O)OC)O

MOL003076	0.6880	0.3120	0.6986	Lonicerae Japonicae Flos	3,5-di-O-caffeoylquinic acid methyl ester	Not Available	FALSE	C1(C(C(CC(C1)(C(=O)OC)O)OC(=O)/C=C/c1cc(c(cc1)O)O)O)OC(=O)/C=C\c1cc(c(cc1)O)O
MOL003077	0.6789	0.3211	0.6950	Lonicerae Japonicae Flos	4,5-di-O-caffeoylquinic acid methyl ester	Not Available	FALSE	C1(CC(C(C(C1)O)OC(=O)/C=C/c1cc(c(cc1)O)O)OC(=O)/C=C\c1cc(c(cc1)O)O)(C(=O)OC)O
MOL003078	0.9234	0.0766	0.9360	Lonicerae Japonicae Flos	WLN: NCR B1	10721	FALSE	c1(c(cccc1)C)C#N
MOL003079	0.6911	0.3089	0.6322	Lonicerae Japonicae Flos	(1alpha,3R,4alpha,5R)-3,4,5-Tris[[(2E)-3-(3,4-dihydroxyphenyl)-1-oxo-2-propen-1-yl]oxy]-1-hydroxycyclohexanecarboxylic acid	Not Available	FALSE	C1(CC(C(C(C1)OC(=O)/C=C\c1cc(c(cc1)O)O)OC(=O)/C=C\c1cc(c(cc1)O)O)OC(=O)/C=C\c1cc(c(cc1)O)O)(C(=O)O)O
MOL003081	0.9250	0.0750	0.9644	Lonicerae Japonicae Flos	CIS-2-PENTENOL	5364919	FALSE	C(=C\CO)\CC
MOL003082	0.9155	0.0845	0.9243	Lonicerae Japonicae Flos	Isobutyl tiglate	5367806	FALSE	C(=O)(/C(=C/C)/C)OCC(C)C
MOL003083	0.8881	0.1119	0.9565	Lonicerae Japonicae Flos	ETHYL FURAN	18554	FALSE	o1c(ccc1)CC
MOL003083	0.8881	0.1119	0.9565	Dichroae Radix	ETHYL FURAN	18554	FALSE	o1c(ccc1)CC
MOL003083	0.8881	0.1119	0.9565	Humulus Scandens (Lour.) Merr.	ETHYL FURAN	18554	FALSE	o1c(ccc1)CC
MOL003083	0.8881	0.1119	0.9565	Pogostemon Cablin (Blanco) Benth.	ETHYL FURAN	18554	FALSE	o1c(ccc1)CC
MOL003084	0.9333	0.0667	0.9494	Lonicerae Japonicae Flos	2-isopropenyl-5-methylhex-4-enal	Not Available	FALSE	O=CC(CC=C(C)C)C(=C)C
MOL003085	0.9216	0.0784	0.8766	Lonicerae Japonicae Flos	(S)-phenethyl 2-bromopropanoate	Not Available	FALSE	C(=O)(C(C)Br)OCCc1ccccc1

MOL003086	0.8096	0.1904	0.6250	Lonicerae Japonicae Flos	2-bromododecane	Not Available	FALSE	CC(CCCCCCCCCC)Br
MOL003087	0.9316	0.0684	0.9614	Lonicerae Japonicae Flos	3,4-Dimethyl-2-hexanone	Not Available	FALSE	CCC(C(C(=O)C)C)C
MOL003088	0.9474	0.0526	0.9457	Eucommiae Cortex	HYKOP	348154	FALSE	c1(cc(c(cc1)O)O)CCC(=O)O
MOL003088	0.9474	0.0526	0.9457	Eucommiae Folium	HYKOP	348154	FALSE	c1(cc(c(cc1)O)O)CCC(=O)O
MOL003088	0.9474	0.0526	0.9457	Lonicerae Japonicae Flos	HYKOP	348154	FALSE	c1(cc(c(cc1)O)O)CCC(=O)O
MOL003089	0.9304	0.0696	0.9666	Lonicerae Japonicae Flos	Methional	18635	FALSE	C(=O)CCSC
MOL003089	0.9304	0.0696	0.9666	Paederiae Scandentis Herba	Methional	18635	FALSE	C(=O)CCSC
MOL003090	0.9083	0.0917	0.9664	Dichroae Radix	Prenal	61020	FALSE	C(=O)C=C(C)C
MOL003090	0.9083	0.0917	0.9664	Lonicerae Japonicae Flos	Prenal	61020	FALSE	C(=O)C=C(C)C
MOL003091	0.9286	0.0714	0.9582	Eriobotryae Folium	pent-3-en-2-one	637920	FALSE	CC(=O)/C=C/C
MOL003091	0.9286	0.0714	0.9582	Ginkgo Folium	pent-3-en-2-one	637920	FALSE	CC(=O)/C=C/C
MOL003091	0.9286	0.0714	0.9582	Achyranthis Bidentatae Radix	pent-3-en-2-one	637920	FALSE	CC(=O)/C=C/C
MOL003091	0.9286	0.0714	0.9582	Lonicerae Japonicae Flos	pent-3-en-2-one	637920	FALSE	CC(=O)/C=C/C
MOL003093	0.8172	0.1828	0.7679	Lonicerae Japonicae Flos	5-O-Caffeoyl quinic acid butyl ester	Not Available	FALSE	C(=O)(/C=C/c1cc(c(cc1)O)O)OC1(CC(C(C(C1)O)O)O)C(=O)OCCCC
MOL003094	0.4352	0.5648	0.6112	Lonicerae Japonicae Flos	(E,E,E)-3,7-11,16-tetramethyl hexadeca-2,6,10,14-tetraen-1-ol	21159986	FALSE	C(/C=C(/CC/C=C(/CC/C=C(/CC/C=C/CC)\C)\C)\C)O
MOL003095	0.7848	0.2152	0.9405	Lonicerae Japonicae Flos	5-hydroxy-7-methoxy-2-(3,4,5-trimethoxyphenyl)chromone	10970376	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1cc(c(c(c1)OC)OC)OC)O)OC
MOL003096	0.8226	0.1774	0.9491	Lonicerae Japonicae Flos	2-(3,4-dimethoxyphenyl)-5-hydroxy-7-methoxy-chromone	5272653	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)OC)O)OC
MOL003097	0.8289	0.1711	0.9588	Tamaricis Cacumen	Flavone der.	5281601	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1ccc(cc1)OC)O)OC
MOL003097	0.8289	0.1711	0.9588	Lonicerae Japonicae Flos	Flavone der.	5281601	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1ccc(cc1)OC)O)OC

MOL003097	0.8289	0.1711	0.9588	Scutellariae Barbatae Herba	Flavone der.	5281601	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1ccc(cc1)OC)O)OC
MOL003097	0.8289	0.1711	0.9588	Andrographis Herba	Flavone der.	5281601	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1ccc(cc1)OC)O)OC
MOL003097	0.8289	0.1711	0.9588	Wikstroemiae Indicae Rasix	Flavone der.	5281601	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1ccc(cc1)OC)O)OC
MOL003097	0.8289	0.1711	0.9588	Epimrdii Herba	Flavone der.	5281601	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1ccc(cc1)OC)O)OC
MOL003098	0.8095	0.1905	0.9180	Lonicerae Japonicae Flos	2-(2,4-dimethoxyphenyl)-3-hydroxy-7-methoxy-chromone	688717	FALSE	c1(c2oc3c(c(=O)c2O)ccc(c3)OC)c(cc(cc1)OC)OC
MOL003099	0.9130	0.0870	0.8362	Lonicerae Japonicae Flos	7-epi-Loganin	7160355	FALSE	C1C2C(C(C1O)C)C(OC1C(C(C(C(O1)CO)O)O)O)OC=C2C(=O)OC
MOL003100	0.9569	0.0431	0.8722	Lonicerae Japonicae Flos	7-epi-Loganin_qt	Not Available	FALSE	C1C2C(C(C1O)C)C(O)OC=C2C(=O)OC
MOL003101	0.8916	0.1084	0.7233	Lonicerae Japonicae Flos	7-epi-Vogeloside	Not Available	FALSE	C1(CC2(C(=COC(C2(C)C=C)OOC2C(O)C(O)C(O)C(O2)CO)C(=O)O1)C)OC
MOL003102	0.9225	0.0775	0.8460	Lonicerae Japonicae Flos	7-epi-Vogeloside_qt	Not Available	FALSE	C1(CC2(C(=COC(C2(C)C=C)OO)C(=O)O1)C)OC
MOL003103	0.4768	0.5232	0.6405	Sojae Semen Nigrum	Methyl octadeca-8,11-dienoate	5319737	FALSE	CCCCCC/C=C/C/C=C/CCCCCCC(=O)OC
MOL003103	0.4768	0.5232	0.6405	Lonicerae Japonicae Flos	Methyl octadeca-8,11-dienoate	5319737	FALSE	CCCCCC/C=C/C/C=C/CCCCCCC(=O)OC
MOL003104	0.8635	0.1365	0.8063	Ginkgo Folium	(Z,E)-farnesol	1549108	FALSE	OC/C=C(\CC/C=C(/CCC=C(C)C)\C)/C
MOL003104	0.8635	0.1365	0.8063	Lonicerae Japonicae Flos	(Z,E)-farnesol	1549108	FALSE	OC/C=C(\CC/C=C(/CCC=C(C)C)\C)/C
MOL003104	0.8635	0.1365	0.8063	Eriobotryae Folium	(Z,E)-farnesol	1549108	FALSE	OC/C=C(\CC/C=C(/CCC=C(C)C)\C)/C
MOL003105	0.7610	0.2390	0.6645	Lonicerae Japonicae Flos	methyl-9-methyl tetradecanoate	Not Available	FALSE	C(=O)(CCCCCCCC(CCCCC)C)OC
MOL003106	0.7700	0.2300	0.8290	Lonicerae Japonicae Flos	Akebiasaponin D	Not Available	FALSE	C1(C(COC(C1O)OC1CCC2(C(C1(C)CO)CCC1(C2C=C2C1(CCC1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(C(O1)COC1OC(C(C(C1O)O)O)CO)O)O)O)C)C)C)O)O
MOL003106	0.7700	0.2300	0.8290	Dipsaci Radix	Akebiasaponin D	Not Available	FALSE	C1(C(COC(C1O)OC1CCC2(C(C1(C)CO)CCC1(C2C=C2C1(CCC1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(C(O1)COC1OC(C(C(C1O)O)O)CO)O)O)O)C)C)C)O)O
MOL003107	0.7613	0.2387	0.8412	Sapindi Mukorossi Semen	Akebiasaponin D_qt	Not Available	FALSE	OC1CCC2(C(C1(C)CO)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C)C(=O)O)C)C)C
MOL003107	0.7613	0.2387	0.8412	Dipsaci Radix	Akebiasaponin D_qt	Not Available	FALSE	OC1CCC2(C(C1(C)CO)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C)C(=O)O)C)C)C

MOL003107	0.7613	0.2387	0.8412	Sapindi Mukorossiperic Arpium	Akebiasaponin D_qt	Not Available	FALSE	OC1CCC2(C(C1(C)CO)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C)C(=O)O)C)C)C
MOL003107	0.7613	0.2387	0.8412	Lonicerae Japonicae Flos	Akebiasaponin D_qt	Not Available	FALSE	OC1CCC2(C(C1(C)CO)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C)C(=O)O)C)C)C
MOL003109	0.8910	0.1090	0.6437	Lonicerae Japonicae Flos	Caeruloside C_qt	Not Available	FALSE	O=CC(O)C(O)C1OC(OCC1O)CC1C(C(OC=C1C(=O)OC)O)C=C
MOL003112	0.8635	0.1365	0.8063	Lonicerae Japonicae Flos	(E,Z)-farnesol	1549109	FALSE	OC/C=C(/CC/C=C(\CCC=C(C)C)/C)\C
MOL003113	0.8885	0.1115	0.6842	Lonicerae Japonicae Flos	Dehydroxymorroniside	Not Available	FALSE	O(C1C(O)C(C(O)C(O1)CO)O)C1C2C(OC=CC2C(=CO1)C(=O)OC)C
MOL003114	0.9516	0.0484	0.8160	Lonicerae Japonicae Flos	Dehydroxymorroniside_qt	Not Available	FALSE	OC1C2C(OC=CC2C(=CO1)C(=O)OC)C
MOL003116	0.8288	0.1712	0.6543	Lonicerae Japonicae Flos	Ioniceracetalides B	Not Available	FALSE	C1(C(C(OC=C1C(=O)OC)OOC1C(O)C(O)C(O)C(O1)CO)C=C)CC1OC(C(O1)C)C
MOL003117	0.9544	0.0456	0.7914	Lonicerae Japonicae Flos	Ioniceracetalides B_qt	Not Available	FALSE	C1(C(C(OC=C1C(=O)OC)OO)C=C)CC1OC(C(O1)C)C
MOL003118	0.8368	0.1632	0.7310	Lonicerae Japonicae Flos	Isochlorogenic acid C	Not Available	FALSE	O(C1C(OC(=O)/C=C\c2cc(O)c(O)cc2)C(O)CC(O)(C1)C(=O)O)C(=O)/C=C\c1cc(O)c(O)cc1
MOL003120	0.9377	0.0623	0.7975	Lonicerae Japonicae Flos	Loniceracetalide A_qt	Not Available	FALSE	OC1OC=C(C(C1C=C)CC1OC(C(O1)C)C)C(=O)OC
MOL003122	0.9377	0.0623	0.7975	Lonicerae Japonicae Flos	Loniceracetalide B_qt	Not Available	FALSE	OC1OC=C(C(C1C=C)CC1OC(C(O1)C)C)C(=O)OC
MOL003123	0.8755	0.1245	0.9625	Lonicerae Japonicae Flos	WLN: QR BQ DQ	10787	FALSE	c1(c(ccc(c1)O)O)O
MOL003125	0.9045	0.0955	0.6809	Lonicerae Japonicae Flos	XYLOSTOSIDINE_qt	Not Available	FALSE	S1C2N(C(=O)C3=COC(O)C(C3C2)C=C)CC1
MOL003126	0.8553	0.1447	0.6426	Acoritataninowii Rhizoma	alpha cadinene	12306049	FALSE	C1(CC=C(C2CCC(=CC12)C)C)C(C)C
MOL003126	0.8553	0.1447	0.6426	Bidentis Bipinnatae Herba	alpha cadinene	12306049	FALSE	C1(CC=C(C2CCC(=CC12)C)C)C(C)C
MOL003126	0.8553	0.1447	0.6426	Moslae Herba	alpha cadinene	12306049	FALSE	C1(CC=C(C2CCC(=CC12)C)C)C(C)C
MOL003126	0.8553	0.1447	0.6426	Morindae Officinalis Radix	alpha cadinene	12306049	FALSE	C1(CC=C(C2CCC(=CC12)C)C)C(C)C
MOL003126	0.8553	0.1447	0.6426	Cnidii Fructus	alpha cadinene	12306049	FALSE	C1(CC=C(C2CCC(=CC12)C)C)C(C)C
MOL003126	0.8553	0.1447	0.6426	Lycii Fructus	alpha cadinene	12306049	FALSE	C1(CC=C(C2CCC(=CC12)C)C)C(C)C
MOL003126	0.8553	0.1447	0.6426	Lonicerae Japonicae Flos	alpha cadinene	12306049	FALSE	C1(CC=C(C2CCC(=CC12)C)C)C(C)C
MOL003127	0.8344	0.1656	0.7950	Ailanthi Cortex	Germacrene D	5317570	FALSE	C\1(=C/CCC(=C)/C=C/C(CC1)C(C)C)/C
MOL003127	0.8344	0.1656	0.7950	Curcumae Rhizoma	Germacrene D	5317570	FALSE	C\1(=C/CCC(=C)/C=C/C(CC1)C(C)C)/C
MOL003127	0.8344	0.1656	0.7950	Scutellariae Radix	Germacrene D	5317570	FALSE	C\1(=C/CCC(=C)/C=C/C(CC1)C(C)C)/C
MOL003127	0.8344	0.1656	0.7950	Radix Salviae	Germacrene D	5317570	FALSE	C\1(=C/CCC(=C)/C=C/C(CC1)C(C)C)/C

MOL003127	0.8344	0.1656	0.7950	Platycladi Cacumen	Germacrene D	5317570	FALSE	C\1(=C/CCC(=C)/C=C/C(CC1)C(C)C)/C
MOL003127	0.8344	0.1656	0.7950	Coriandri Sativi Herba	Germacrene D	5317570	FALSE	C\1(=C/CCC(=C)/C=C/C(CC1)C(C)C)/C
MOL003127	0.8344	0.1656	0.7950	Myrrha	Germacrene D	5317570	FALSE	C\1(=C/CCC(=C)/C=C/C(CC1)C(C)C)/C
MOL003127	0.8344	0.1656	0.7950	Lonicerae Japonicae Flos	Germacrene D	5317570	FALSE	C\1(=C/CCC(=C)/C=C/C(CC1)C(C)C)/C
MOL003127	0.8344	0.1656	0.7950	Dichroae Radix	Germacrene D	5317570	FALSE	C\1(=C/CCC(=C)/C=C/C(CC1)C(C)C)/C
MOL003127	0.8344	0.1656	0.7950	Rubi Fructus	Germacrene D	5317570	FALSE	C\1(=C/CCC(=C)/C=C/C(CC1)C(C)C)/C
MOL003127	0.8344	0.1656	0.7950	Perillae Fructus	Germacrene D	5317570	FALSE	C\1(=C/CCC(=C)/C=C/C(CC1)C(C)C)/C
MOL003127	0.8344	0.1656	0.7950	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	Germacrene D	5317570	FALSE	C\1(=C/CCC(=C)/C=C/C(CC1)C(C)C)/C
MOL003127	0.8344	0.1656	0.7950	Chuanxiong Rhizoma	Germacrene D	5317570	FALSE	C\1(=C/CCC(=C)/C=C/C(CC1)C(C)C)/C
MOL003127	0.8344	0.1656	0.7950	Farfarae Flos	Germacrene D	5317570	FALSE	C\1(=C/CCC(=C)/C=C/C(CC1)C(C)C)/C
MOL003128	0.8919	0.1081	0.7410	Lonicerae Japonicae Flos	dinethylsecologanoside	Not Available	FALSE	C1(C(C(OC=C1C(=O)OC)OOC1C(O)C(O)C(O)C(O1)CO)C=C)CC(=O)OC
MOL003129	0.9373	0.0627	0.8616	Lonicerae Japonicae Flos	dinethylsecologanoside_qt	Not Available	FALSE	C1(C(C(OC=C1C(=O)OC)OO)C=C)CC(=O)OC
MOL003130	0.8847	0.1153	0.8461	Lonicerae Japonicae Flos	madreselvin A	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2oc(c(OC)c(=O)c2c(O)c1)c1cc(O)c(O)cc1)COC1OC(C(O)C(O)C1O)CO
MOL003131	0.4106	0.5894	0.6895	Gentianae Radix Et Rhozima	17beta,21beta-Epoxyhopan-3-one	Not Available	FALSE	O1C23C(C4C(C5(C(C6(C(CC5)C(C(=O)CC6)(C)C)C)CC4)C)(CC3)C)(CCC12C(C)C)C
MOL003133	0.9569	0.0431	0.8722	Gentianae Radix Et Rhozima	Loganin_qt	Not Available	FALSE	OC1C2C(C(=CO1)C(=O)OC)CC(C2C)O
MOL003134	0.9076	0.0924	0.8423	Gentianae Radix Et Rhozima	Rishitin	108064	FALSE	C1(C(C(C2=C(C1)CCC(C2)C(=C)C)C)O)O
MOL003135	0.9210	0.0790	0.8818	Gentianae Radix Et Rhozima	Scandoside	Not Available	FALSE	C1(OC=C(C2C1C(=CC2O)CO)C(=O)O)OC1OC(C(C(C1O)O)O)CO
MOL003136	0.9468	0.0532	0.8480	Gentianae Radix Et Rhozima	Scandoside_qt	Not Available	FALSE	C1(OC=C(C2C1C(=CC2O)CO)C(=O)O)O
MOL003137	0.8563	0.1437	0.8220	Swertiae Mileensis Herba	Leucanthoside	442659	FALSE	C1(C(C(OC(C1O)CO)c1c(c2c(cc1OC)oc(cc2=O)c1ccc(c(c1)O)O)O)O)O
MOL003137	0.8563	0.1437	0.8220	Cornus Officinalis Sieb. Et Zucc.	Leucanthoside	442659	FALSE	C1(C(C(OC(C1O)CO)c1c(c2c(cc1OC)oc(cc2=O)c1ccc(c(c1)O)O)O)O)O
MOL003137	0.8563	0.1437	0.8220	Gentianae Radix Et Rhozima	Leucanthoside	442659	FALSE	C1(C(C(OC(C1O)CO)c1c(c2c(cc1OC)oc(cc2=O)c1ccc(c(c1)O)O)O)O)O
MOL003138	0.9202	0.0798	0.8028	Gentianae Radix Et Rhozima	Swertianin	5281661	FALSE	c1(c(c2c(cc1)oc1c(c2=O)c(cc(c1)OC)O)O)O
MOL003140	0.8248	0.1752	0.7864	Gentianae Radix Et Rhozima	Amarogentin	Not Available	FALSE	C1CC2C(=COC(C2O)OC2OC(C(C(C2OC(=O)c2c(O)cc(cc2c2cc(ccc2)O)O)O)O)O)CO)C(=O)O1
MOL003141	0.4476	0.5524	0.7011	Gentianae Radix Et Rhozima	chiratenol	Not Available	FALSE	C1C2(C(C(C(C1)C)(C)C)CCC1(C2CCC2C1(CC=C1C2(CCC(C1)(C)C)C)C)C)C

MOL003142	0.9603	0.0397	0.8704	Gentianae Radix Et Rhozima	gentianal	Not Available	FALSE	O1C(c2c(CC1)c(c(=O)[nH]c2)C=O)C
MOL003143	0.5892	0.4108	0.6842	Gentianae Radix Et Rhozima	gentirigenic acid	44423055	FALSE	O1C(C2C3C(C4(C(C5(C(CC4)C(C(O)CC5)(CO)C)C)CC3)C)(CC2)C)(CC(O)C(O)C1(C)C)C(=O)O
MOL003144	0.7373	0.2627	0.7885	Gentianae Radix Et Rhozima	Amaroswerin	Not Available	FALSE	C1CC2(C(=COC(C2C=C)OC2OC(C(C(C2OC(=O)c2c(O)cc(cc2c2cc(ccc2)O)O)O)O)O)CO)C(=O)O1)O
MOL003145	0.6192	0.3808	0.7994	Gentianae Radix Et Rhozima	gentirigeoside A	44422964	FALSE	O1C(C2C3C(C4(C(C5(C(CC4)C(C(OC4OC(C(O)C(O)C4O)CO)CC5)(CO)C)C)CC3)C)(CC2)C)(CC(O)C(O)C1(C)C)C(=O)O
MOL003146	0.6883	0.3117	0.8499	Gentianae Radix Et Rhozima	gentirigeoside B	44422965	FALSE	O1C(C2C3C(C4(C(C5(C(CC4)C(C(OC4OC(C(O)C(O)C4OC4OC(C(O)C(O)C4O)CO)CO)CC5)(CO)C)C)CC3)C)(CC2)C)(CC(O)C(O)C1(C)C)C(=O)O
MOL003147	0.6835	0.3165	0.7447	Gentianae Radix Et Rhozima	gentirigeoside C	44422966	FALSE	O1C(C2C3C(C4(C(C5(C(CC4)C(C(OC4OC(C(O)C(O)C4O)CO)CC5)(COC4OC(C(O)C(O)C4O)CO)C)C)CC3)C)(CC2)C)(CC(O)C(O)C1(C)C)C(=O)O
MOL003148	0.6478	0.3522	0.7939	Gentianae Radix Et Rhozima	gentirigeoside D	44422967	FALSE	O1C(C2C3C(C4(C(C5(C(CC4)C(C(OC4OC(C(O)C(O)C4O)CO)CC5)(CO)C)C)CC3)C)(CC2)C)(CC(O)C(O)C1(CO)C)C(=O)O
MOL003149	0.6013	0.3987	0.6661	Gentianae Radix Et Rhozima	gentirigeoside D_qt	Not Available	FALSE	O1C(C2C3C(C4(C(C5(C(CC4)C(C(O)CC5)(CO)C)C)CC3)C)(CC2)C)(CC(O)C(O)C1(CO)C)C(=O)O
MOL003150	0.6852	0.3148	0.8605	Gentianae Radix Et Rhozima	gentirigeoside E	44422968	FALSE	O1C(C2C3C(C4(C(C5(C(CC4)C(C(OC4OC(C(O)C(O)C4OC4OC(C(O)C(O)C4O)CO)CO)CC5)(C)C)C)CC3)C)(CC2)C)(CC(O)C(O)C1(C)C)C(=O)O
MOL003151	0.5711	0.4289	0.6772	Gentianae Radix Et Rhozima	gentirigeoside E_qt	Not Available	FALSE	O1C(C2C3C(C4(C(C5(C(CC4)C(C(O)CC5)(C)C)C)CC3)C)(CC2)C)(CC(O)C(O)C1(C)C)C(=O)O
MOL003152	0.9282	0.0718	0.8286	Gentianae Radix Et Rhozima	Gentisin	5281636	FALSE	c12c(oc3c(c1=O)cc(cc3)O)cc(cc2O)OC
MOL003152	0.9282	0.0718	0.8286	Dipsaci Radix	Gentisin	5281636	FALSE	c12c(oc3c(c1=O)cc(cc3)O)cc(cc2O)OC
MOL003153	0.8684	0.1316	0.7121	Gentianae Radix Et Rhozima	isosaponarin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c2c(oc(cc2=O)c2ccc(OC3OC(C(O)C(O)C3O)CO)cc2)cc1O
MOL003153	0.8684	0.1316	0.7121	Vaccariae Semen	isosaponarin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c2c(oc(cc2=O)c2ccc(OC3OC(C(O)C(O)C3O)CO)cc2)cc1O
MOL003155	0.5600	0.4400	0.9186	Gentianae Radix Et Rhozima	pranferin	Not Available	FALSE	c1(ccc2c(c1CC1OC(OC1(C)C)(C)C)oc(=O)cc2)OC
MOL003156	0.4023	0.5977	0.7041	Gentianae Radix Et Rhozima	pseudotaraxasterol	Not Available	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CC=C(C5C)C)C)CC3)C)(CC2)C)(CC1)C)(C)C

MOL003158	0.8655	0.1345	0.7058	Gentianae Radix Et Rhozima	(5R,6S)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)-2-tetrahydropyranyl]oxymethyl]-2-tetrahydropyranyl]oxymethyl]-2-tetrahydropyranyl]oxy]-5-vinyl-5,6-dihydro-3H-pyran	11388341	FALSE	C1(C(C(C(C(O1)OC1C(C2=CCOC(=O)C2=CO1)C=C)O)O)O)COC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO

MOL003159	0.8634	0.1366	0.7076	Gentianae Radix Et Rhozima	(5R,6S)-6-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)-2-tetrahydropyranyl]oxymethyl]-2-tetrahydropyranyl]oxymethyl]-2-tetrahydropyr	11216673	FALSE	C1(C(C(C(C(O1)OC1C(C2=CCOC(=O)C2=CO1)C=C)O)O)O)COC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO
MOL003160	0.8446	0.1554	0.7213	Gentianae Radix Et Rhozima	scabrans G5	Not Available	FALSE	C1(C(C(C(C(O1)OC1C(C2=CCOC(=O)C2=CO1)C=C)O)O)O)COC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO
MOL003161	0.4385	0.5615	0.6590	Gentianae Radix Et Rhozima	scabraside	Not Available	FALSE	O1C(OC2OC=C3C(C2C=C)CCOC3=O)C(OC(=O)c2ccccc2)C(OC(=O)C)C(OC(=O)c2c(O)c(OC3OC(C(O)C(O)C3O)CO)ccc2)C1COC(=O)C
MOL003163	0.8940	0.1060	0.6807	Gentianae Radix Et Rhozima	(5R,6S,8R)-5-ethenyl-8-methoxy-6-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4,5,6,8-tetrahydro-3H-pyrano[3,4-c]pyran-1-one	11361225	FALSE	C1(C(C(C(C(O1)OC1C(C2=C(C(O1)OC)C(=O)OCC2)C=C)O)O)O)CO

MOL003164	0.9504	0.0496	0.7598	Gentianae Radix Et Rhozima	swertiajaposide A_qt	Not Available	FALSE	OC1C(C2=C(C(O1)OC)C(=O)OCC2)C=C
MOL003165	0.9588	0.0412	0.8567	Gentianae Radix Et Rhozima	Gentianol	Not Available	FALSE	O1C(C2=C(CC1)C(C(=O)N=C2)C=O)C
MOL003165	0.9588	0.0412	0.8567	Trigonellae Semen	Gentianol	Not Available	FALSE	O1C(C2=C(CC1)C(C(=O)N=C2)C=O)C
MOL003166	0.9055	0.0945	0.8208	Euphorbiae Helioscopiae Herba	Swertiamarin	442435	FALSE	C12=COC(C(C1(CCOC2=O)O)C=C)OC1C(C(C(C(O1)CO)O)O)O
MOL003166	0.9055	0.0945	0.8208	Gentianae Radix Et Rhozima	Swertiamarin	442435	FALSE	C12=COC(C(C1(CCOC2=O)O)C=C)OC1C(C(C(C(O1)CO)O)O)O
MOL003166	0.9055	0.0945	0.8208	Swertiae Mileensis Herba	Swertiamarin	442435	FALSE	C12=COC(C(C1(CCOC2=O)O)C=C)OC1C(C(C(C(O1)CO)O)O)O
MOL003166	0.9055	0.0945	0.8208	Gentiana Macrophylla Pall	Swertiamarin	442435	FALSE	C12=COC(C(C1(CCOC2=O)O)C=C)OC1C(C(C(C(O1)CO)O)O)O
MOL003166	0.9055	0.0945	0.8208	Cornus Officinalis Sieb. Et Zucc.	Swertiamarin	442435	FALSE	C12=COC(C(C1(CCOC2=O)O)C=C)OC1C(C(C(C(O1)CO)O)O)O
MOL003167	0.6262	0.3738	0.6108	Gentianae Radix Et Rhozima	trifloroside	Not Available	FALSE	C1(=O)C2=COC(C(C2CCO1)C=C)OC1C(OC(=O)C)C(OC(=O)C)C(OC(=O)c2c(c(ccc2)OC2C(O)C(O)C(O)C(O2)CO)O)C(O1)COC(=O)C
MOL003170	0.9419	0.0581	0.7861	Gentianae Radix Et Rhozima	Gentisein	5281635	FALSE	c1(cc(c2c(c1)oc1c(c2=O)cc(cc1)O)O)O
MOL003171	0.9329	0.0671	0.9514	Phragmitis Rhizoma	2,5-Dimethoxybenzoquinone	101405	FALSE	C1=C(C(=O)C=C(C1=O)OC)OC
MOL003171	0.9329	0.0671	0.9514	Tripterygii Radix	2,5-Dimethoxybenzoquinone	101405	FALSE	C1=C(C(=O)C=C(C1=O)OC)OC
MOL003171	0.9329	0.0671	0.9514	Fritillariae Thunbrgii Bulbus	2,5-Dimethoxybenzoquinone	101405	FALSE	C1=C(C(=O)C=C(C1=O)OC)OC
MOL003171	0.9329	0.0671	0.9514	Acoritataninowii Rhizoma	2,5-Dimethoxybenzoquinone	101405	FALSE	C1=C(C(=O)C=C(C1=O)OC)OC
MOL003172	0.9038	0.0962	0.6794	Phragmitis Rhizoma	7-chloroarctinone B	44511380	FALSE	c1(ccc(s1)C(=O)CCl)c1ccc(s1)C#CC
MOL003173	0.8322	0.1678	0.7576	Phragmitis Rhizoma	Thiarubrine A	72386	FALSE	S1SC(=CC=C1C#CC)C#CC#CC=C
MOL003173	0.8322	0.1678	0.7576	Trigonellae Semen	Thiarubrine A	72386	FALSE	S1SC(=CC=C1C#CC)C#CC#CC=C
MOL003175	0.9004	0.0996	0.7180	Phragmitis Rhizoma	arctinal	13779265	FALSE	c1(ccc(s1)C=O)c1ccc(s1)C#CC
MOL003175	0.9004	0.0996	0.7180	Rhapontici Radix	arctinal	13779265	FALSE	c1(ccc(s1)C=O)c1ccc(s1)C#CC
MOL003176	0.4906	0.5094	0.7033	Phragmitis Rhizoma	b-AMYRIN	Not Available	FALSE	C1(C2(C(CCC1C)(C1(C(CC2)C2(C(=CC1)C1(C(CC2)(CCC(C1)(C)C)C)C)C)C)C)(C)C
MOL003177	0.9350	0.0650	0.9504	Evodiae Fructus	Syringaldehyde	8655	FALSE	c1(c(c(cc(c1)C=O)OC)O)OC

MOL003177	0.9350	0.0650	0.9504	Codonopsis Radix	Syringaldehyde	8655	FALSE	c1(c(c(cc(c1)C=O)OC)O)OC
MOL003177	0.9350	0.0650	0.9504	Flos Genkwa	Syringaldehyde	8655	FALSE	c1(c(c(cc(c1)C=O)OC)O)OC
MOL003177	0.9350	0.0650	0.9504	Choerospondiatis Fructus	Syringaldehyde	8655	FALSE	c1(c(c(cc(c1)C=O)OC)O)OC
MOL003177	0.9350	0.0650	0.9504	Santalum Album L.	Syringaldehyde	8655	FALSE	c1(c(c(cc(c1)C=O)OC)O)OC
MOL003177	0.9350	0.0650	0.9504	Phragmitis Rhizoma	Syringaldehyde	8655	FALSE	c1(c(c(cc(c1)C=O)OC)O)OC
MOL003177	0.9350	0.0650	0.9504	Salviae Chinensis Herba	Syringaldehyde	8655	FALSE	c1(c(c(cc(c1)C=O)OC)O)OC
MOL003177	0.9350	0.0650	0.9504	Fraxini Cortex	Syringaldehyde	8655	FALSE	c1(c(c(cc(c1)C=O)OC)O)OC
MOL003177	0.9350	0.0650	0.9504	Radix Angelicae Biseratae	Syringaldehyde	8655	FALSE	c1(c(c(cc(c1)C=O)OC)O)OC
MOL003177	0.9350	0.0650	0.9504	Lepidii Semen Descurainiae Semen	Syringaldehyde	8655	FALSE	c1(c(c(cc(c1)C=O)OC)O)OC
MOL003178	0.9197	0.0803	0.9463	Calendula Officinalis	GENOP	3469	FALSE	c1(c(cc(cc1)O)C(=O)O)O
MOL003178	0.9197	0.0803	0.9463	Ilicis Purpureae Folium	GENOP	3469	FALSE	c1(c(cc(cc1)O)C(=O)O)O
MOL003178	0.9197	0.0803	0.9463	Herbahypericiperforati	GENOP	3469	FALSE	c1(c(cc(cc1)O)C(=O)O)O
MOL003178	0.9197	0.0803	0.9463	Plantaginis Herba	GENOP	3469	FALSE	c1(c(cc(cc1)O)C(=O)O)O
MOL003178	0.9197	0.0803	0.9463	Ampelopsis Japonica	GENOP	3469	FALSE	c1(c(cc(cc1)O)C(=O)O)O
MOL003178	0.9197	0.0803	0.9463	Phragmitis Rhizoma	GENOP	3469	FALSE	c1(c(cc(cc1)O)C(=O)O)O
MOL003179	0.9455	0.0545	0.9301	Santalum Album L.	4'-Hydroxy-3'-methoxycinnamaldehyde	5352904	FALSE	c1(ccc(c(c1)OC)O)/C=C\C=O
MOL003179	0.9455	0.0545	0.9301	Swertiae Mileensis Herba	4'-Hydroxy-3'-methoxycinnamaldehyde	5352904	FALSE	c1(ccc(c(c1)OC)O)/C=C\C=O
MOL003179	0.9455	0.0545	0.9301	Phragmitis Rhizoma	4'-Hydroxy-3'-methoxycinnamaldehyde	5352904	FALSE	c1(ccc(c(c1)OC)O)/C=C\C=O

MOL003181	0.5840	0.4160	0.6755	Tripterygii Radix	(2S,3R,4S,5S,6R)-2-[4-[(1S,3aR,4S,6aR)-4-[3-methoxy-4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]-1,3,3a,4,6,6a-hexahydrofuro[4,3-c]furan-1-yl]-2,6-dimethoxyphenoxy]-6-(hydroxymethyl)oxane-3,4,5-triol	13991184	FALSE	C1(C(C(C(OC1CO)Oc1ccc(cc1OC)C1OCC2C1COC2c1cc(c(c(c1)OC)OC1C(C(C(C(O1)CO)O)O)O)OC)O)O)O
MOL003182	0.4757	0.5243	0.7025	Tripterygii Radix	(+)-Medioresinol di-O-beta-D-glucopyranoside_qt	Not Available	FALSE	Oc1ccc(cc1OC)C1OCC2C1COC2c1cc(c(c(c1)OC)O)OC
MOL003183	0.7156	0.2844	0.8163	Tripterygii Radix	TRIPTOTRITERPENIC ACID B	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)C(CC(C)(C(=O)O)CC4C3=CCC21)O)C)O
MOL003184	0.3964	0.6036	0.7739	Tripterygii Radix	81827-74-9	133766	FALSE	O1CC2=C(C1=O)CCC1(c3c(cc(c(c3CCC21)OC)C(C)C)O)C

MOL003185	0.3123	0.6877	0.7103	Tripterygii Radix	(1R,4aR,10aS)-5-hydroxy-1-(hydroxymethyl)-7-isopropyl-8-methoxy-1,4a-dimethyl-4,9,10,10a-tetrahydro-3H-phenanthren-2-one	159330	FALSE	O=C1C(C2C(CC1)(c1c(CC2)c(OC)c(cc1O)C(C)C)C)(CO)C
MOL003186	0.5804	0.4196	0.7775	Tripterygii Radix	tripterine	122724	FALSE	C1(=O)C(=C(C2=CC=C3C(C2=C1)(CCC1(C3(CCC2(C1CC(CC2)(C)C(=O)O)C)C)C)C)O
MOL003186	0.5804	0.4196	0.7775	Celastri Orbiculati Fructus	tripterine	122724	FALSE	C1(=O)C(=C(C2=CC=C3C(C2=C1)(CCC1(C3(CCC2(C1CC(CC2)(C)C(=O)O)C)C)C)C)O
MOL003187	0.8386	0.1614	0.7990	Tripterygii Radix	triptolide	Not Available	FALSE	C12C(C(C34C5(C1O5)C1(C(CC3O4)C3=C(CC1)C(=O)OC3)C)O)(C(C)C)O2
MOL003188	0.8327	0.1673	0.7638	Tripterygii Radix	Tripchlorolide	Not Available	FALSE	O1C(=O)C2=C(C1)C1C(CC2)(C23C4(C(C1)O4)C(C(C(C2O3)Cl)(C(C)C)O)O)C
MOL003189	0.3118	0.6882	0.8002	Tripterygii Radix	WILFORLIDE A	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)C(CC(C)(C(=O)OC)CC4C3=CCC21)O)C)O
MOL003190	0.4537	0.5463	0.7931	Tripterygii Radix	WILFORLIDE B	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)C(CC5(C)C(=O)OCC4(C5)C3=CCC21)O)C
MOL003191	0.8856	0.1144	0.7618	Tripterygii Radix	Tripdiolide	Not Available	FALSE	C1(C2=C(C3C4(C1)C1(C5(C(C3)O5)C(C3(C(C1C)O3)C(C)C)O)O4)COC2=O)O
MOL003192	0.8459	0.1541	0.7370	Tripterygii Radix	Triptonide	Not Available	FALSE	C12C(C(=O)C34C5(C1O5)C1C(CC3O4)C3=C(CC1)C(=O)OC3)(C(C)C)O2
MOL003193	0.7611	0.2389	0.8429	Tripterygii Radix	TRIPTOTRITERPENIC ACID C	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)C(CC(C(=O)O)C(C)C4C3=CCC21)O)C)O
MOL003194	0.7121	0.2879	0.8745	Tripterygii Radix	3-epikatonic acid	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C)(C(=O)O)CC4C3=CCC21)C)O
MOL003195	0.5979	0.4021	0.7871	Tripterygii Radix	tripterygone	Not Available	FALSE	C1(=O)C(=C(C2(C(=C1)C1C(CC2)C2(C(CC1)(C1C(CC2)(CCC(C1)(C)C(=O)O)C)C)C)C)O
MOL003196	0.4593	0.5407	0.8481	Tripterygii Radix	Tryptophenolide	173273	FALSE	O1CC2=C(C1=O)CCC1(c3ccc(c(c3CCC21)O)C(C)C)C
MOL003197	0.7135	0.2865	0.7407	Tripterygii Radix	orthosphenic acid	Not Available	FALSE	O1C2(O)C(C3(C(C4(C(C5(C(C6C(CC5)(CCC(C6)(C)C(=O)O)C)(CC4)C)C)CC3)C)CC2O)C1)C

MOL003198	0.0779	0.9221	0.6713	Tripterygii Radix	5 alpha-Benzoyl-4 alpha-hydroxy-1 beta,8 alpha-dinicotinoyl-dihydro-agarofuran	Not Available	FALSE	C1C2C(C3(C(C1OC(=O)c1cnccc1)(C(CCC3(O)C)OC(=O)c1cccnc1)C)OC2(C)C)OC(=O)c1ccccc1
MOL003199	0.6809	0.3191	0.7530	Tripterygii Radix	5,8-Dihydroxy-7-(4-hydroxy-5-methyl-coumarin-3)-coumarin	54714258	FALSE	c1cc(c2c(c1)oc(=O)c(c2O)c1c(O)c2c(c(c1)O)ccc(=O)o2)C
MOL003200	0.9316	0.0684	0.8559	Tripterygii Radix	HRP	6971055	FALSE	c1(ccc2c(c1)c(c[nH]2)CC(C(=O)O)N)O
MOL003202	0.9352	0.0648	0.8855	Rehmanniae Radix Praeparata	8-epi-Loganic acid	158144	FALSE	C12C(CC(C1C)O)C(=COC2OC1OC(C(C(C1O)O)O)CO)C(=O)O
MOL003202	0.9352	0.0648	0.8855	Tripterygii Radix	8-epi-Loganic acid	158144	FALSE	C12C(CC(C1C)O)C(=COC2OC1OC(C(C(C1O)O)O)CO)C(=O)O
MOL003202	0.9352	0.0648	0.8855	Cistanches Herba	8-epi-Loganic acid	158144	FALSE	C12C(CC(C1C)O)C(=COC2OC1OC(C(C(C1O)O)O)CO)C(=O)O
MOL003203	0.9508	0.0492	0.8563	Tripterygii Radix	8-Epilpganic acid_qt	49775370	FALSE	C12C(CC(C1C)O)C(=COC2O)C(=O)O
MOL003203	0.9508	0.0492	0.8563	Cistanches Herba	8-Epilpganic acid_qt	49775370	FALSE	C12C(CC(C1C)O)C(=COC2O)C(=O)O
MOL003204	0.7156	0.2844	0.8163	Tripterygii Radix	(2S,4S,4aR,6aR,6aS,6bR,8aR,10S,12aR,14bS)-4,10-dihydroxy-2,4a,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-2-carboxylic acid	21594203	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(CC(C1)(C)C(=O)O)O)C)C)C)(C)C)O
MOL003205	0.4044	0.5956	0.8078	Tripterygii Radix	Wilforlide A	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C2CC(C1)(C)C(=O)O2)C)C)C)(C)C)O

MOL003206	0.8868	0.1132	0.7974	Tripterygii Radix	Canin	Not Available	FALSE	C123C(C4C(CCC1(O)C)C(=C)C(=O)O4)C1(C(C2O3)O1)C
MOL003211	0.3272	0.6728	0.6057	Tripterygii Radix	Celaxanthin	Not Available	FALSE	C1C=CC(=C(C1(C)C)/C=C/C(=C\C=C/C(=C/C=C/C=C(/C=C\C=C(/C=C/C1=C(CC(CC1(C)C)O)C)\C)\C)/C)/C
MOL003212	0.3495	0.6505	0.7876	Tripterygii Radix	142182-52-3	126634	FALSE	C1C(C(=C)C2C(C1)(c1c(C(=O)C2)c(c(c(c1O)OC)C(=C)C)O)C)C
MOL003213	0.3027	0.6973	0.6912	Tripterygii Radix	Deoxygomisin A	Not Available	FALSE	c12c(cc3c(c1OC)OCO3)CC(C(Cc1c2c(OC)c(c(c1)OC)OC)C)C
MOL003213	0.3027	0.6973	0.6912	Kadsurae Coccineae Radix Et Caulis	Deoxygomisin A	Not Available	FALSE	c12c(cc3c(c1OC)OCO3)CC(C(Cc1c2c(OC)c(c(c1)OC)OC)C)C
MOL003214	0.9105	0.0895	0.7763	Tripterygii Radix	Dunnisinin	Not Available	FALSE	C12C3C(OCC1C(=O)OC)OCC3(C=C2)O
MOL003214	0.9105	0.0895	0.7763	Eucommiae Cortex	Dunnisinin	Not Available	FALSE	C12C3C(OCC1C(=O)OC)OCC3(C=C2)O
MOL003215	0.8959	0.1041	0.8808	Tripterygii Radix	(2,5-Dioxo-4-imidazolidinyl)carbamic acid	Not Available	FALSE	C1(=O)C(NC(=O)N1)NC(=O)O
MOL003216	0.9665	0.0335	0.8994	Tripterygii Radix	trans-Nepetalactone	442430	FALSE	C12C(C(=COC1=O)C)CCC2C
MOL003217	0.2766	0.7234	0.6475	Radix Euphorbiae Pekinensis	Isoxanthohumol	Not Available	FALSE	c1c(c(c2c(c1OC)C(=O)CC(O2)c1ccc(cc1)O)CC=C(C)C)O
MOL003217	0.2766	0.7234	0.6475	Tripterygii Radix	Isoxanthohumol	Not Available	FALSE	c1c(c(c2c(c1OC)C(=O)CC(O2)c1ccc(cc1)O)CC=C(C)C)O
MOL003218	0.6357	0.3643	0.6862	Tripterygii Radix	Neouralenol	5320118	FALSE	c1(cc2c(cc1O)oc(c(c2=O)O)c1c(CC=C(C)C)c(c(cc1)O)O)O
MOL003218	0.6357	0.3643	0.6862	licorice	Neouralenol	5320118	FALSE	c1(cc2c(cc1O)oc(c(c2=O)O)c1c(CC=C(C)C)c(c(cc1)O)O)O
MOL003221	0.3228	0.6772	0.8061	Tripterygii Radix	Regelindiol A	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(CC(C1C)C(=O)OC)O)C)C)C)(C)C)O
MOL003222	0.9179	0.0821	0.6408	Tripterygii Radix	Salazinic acid	Not Available	FALSE	c1(c(cc(c2c1Oc1c(c(c(c3c1C(OC3=O)O)O)CO)OC2=O)C)O)C(=O)C
MOL003223	0.3316	0.6684	0.7394	Tripterygii Radix	Tingenone	441687	FALSE	C1C2C(CC(=O)C1C)(CCC1(C2(CCC2(C1=CC=C1C2=CC(=O)C(=C1C)O)C)C)C)C
MOL003223	0.3316	0.6684	0.7394	Anemarrhenae Rhizoma	Tingenone	441687	FALSE	C1C2C(CC(=O)C1C)(CCC1(C2(CCC2(C1=CC=C1C2=CC(=O)C(=C1C)O)C)C)C)C
MOL003224	0.8362	0.1638	0.8229	Tripterygii Radix	Tripdiotolnide	Not Available	FALSE	C1C2=C(C3C(C1)(C1=C(C(=O)C3)C(C3(C(C1O)O3)C(C)C)O)C)COC2=O
MOL003225	0.4729	0.5271	0.9296	Tripterygii Radix	Hypodiolide A	Not Available	FALSE	C1CC2(C3C(C1)(C1C4(CC3)CC(CC1)C(C4)(O)C)COC2=O)C
MOL003226	0.2071	0.7929	0.6435	Tripterygii Radix	(24Z)-27-Hydroxy-3-oxo-7,24-tirucalladien-21-al	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(=CC2)C2(C(CC1)(C(CC2)C(C=O)CC/C=C(/C)\CO)C)C)C)(C)C

MOL003227	0.9318	0.0682	0.8386	Tripterygii Radix	Tripteroside	5281664	FALSE	C1(C(C(C(OC1CO)Oc1c(cc2c(c1)oc1c(c2=O)c(cc(c1)O)O)O)O)O)O
MOL003228	0.8967	0.1033	0.8388	Tripterygii Radix	Norathyriol	5281656	FALSE	Oc1c(cc2c(c1)oc1c(c2=O)c(cc(c1)O)O)O
MOL003228	0.8967	0.1033	0.8388	Ilicis Cornutae Folium Immayuri	Norathyriol	5281656	FALSE	Oc1c(cc2c(c1)oc1c(c2=O)c(cc(c1)O)O)O
MOL003228	0.8967	0.1033	0.8388	Gossampiniflos	Norathyriol	5281656	FALSE	Oc1c(cc2c(c1)oc1c(c2=O)c(cc(c1)O)O)O
MOL003228	0.8967	0.1033	0.8388	Hypericii Japonici Herber	Norathyriol	5281656	FALSE	Oc1c(cc2c(c1)oc1c(c2=O)c(cc(c1)O)O)O
MOL003229	0.6395	0.3605	0.7914	Tripterygii Radix	Triptinin B	Not Available	FALSE	C(=O)(C1=C(C)C2C(CC1)(c1c(CC2)c(c(cc1)C(C)C)O)C)O
MOL003230	0.3062	0.6938	0.8043	Tripterygii Radix	Triptodihydroxy acid methyl ester	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(CO)C(=O)OC)C)C)C)(C)C)O
MOL003231	0.5643	0.4357	0.7286	Tripterygii Radix	Triptoditerpenic acid B	Not Available	FALSE	C(=O)(O)C1=C(C)C2C(CC1)(c1c(CC2)c(c(cc1)C(C)C)OC)C
MOL003233	0.0578	0.9422	0.7186	Tripterygii Radix	Triptofordin B2	Not Available	FALSE	c1cc(ccc1)C(=O)OC1C(C2C(C3(C1(C(C(=O)CC3(C)O)OC(=O)C)C)OC2(C)C)OC(=O)C)OC(=O)c1ccccc1
MOL003234	0.1019	0.8981	0.6725	Tripterygii Radix	Triptofordin C2	Not Available	FALSE	c1cc(ccc1)C(=O)OC1C(C2C(C3(C1(C(C(CC3(O)C)O)OC(=O)C)C)OC2(C)C)OC(=O)C)OC(=O)c1ccccc1
MOL003235	0.0347	0.9653	0.8031	Tripterygii Radix	Triptofordin D1	Not Available	FALSE	c1(OC2C(=O)C3C(C4(C2(C(CCC4(O)C)OC(=O)/C=C\c2ccccc2)COC(=O)C)OC3(C)C)OC(=O)C)ccccc1
MOL003236	0.0272	0.9728	0.8595	Tripterygii Radix	Triptofordin D2	Not Available	FALSE	c1(OC2C(C3C(C4(C2(C(CCC4(O)C)OC(=O)/C=C\c2ccccc2)COC(=O)C)OC3(C)C)OC(=O)C)OC(=O)C)ccccc1
MOL003238	0.0919	0.9081	0.8312	Tripterygii Radix	Triptofordin F1	Not Available	FALSE	C(=O)(OC1C(C2C(C3(C1(C(C(CC3(O)C)OC(=O)C)OC(=O)/C=C\c1ccccc1)COC(=O)C)OC2(C)C)O)OC(=O)C)c1ccccc1
MOL003239	0.0984	0.9016	0.7362	Tripterygii Radix	Triptofordin F2	Not Available	FALSE	C(=O)(OC1C(C2C(C3(C1(C(C(CC3(O)C)OC(=O)C)OC(=O)C)COC(=O)C)OC2(C)C)O)OC(=O)c1ccccc1)c1ccccc1
MOL003240	0.0555	0.9445	0.8942	Tripterygii Radix	Triptofordin F3	Not Available	FALSE	C(=O)(OC1C(C2C(C3(C1(C(C(CC3(O)C)OC(=O)C)OC(=O)c1ccccc1)COC(=O)C)OC2(C)C)OC(=O)C)OC(=O)C)c1ccccc1
MOL003241	0.1350	0.8650	0.6815	Tripterygii Radix	Triptofordin F4	Not Available	FALSE	C(=O)(OC1C(C2C(C3(C1(C(C(CC3(O)C)OC(=O)C)OC(=O)/C=C\c1ccccc1)COC(=O)C)OC2(C)C)O)O)c1ccccc1
MOL003242	0.0766	0.9234	0.8206	Tripterygii Radix	Triptofordinine A2	Not Available	FALSE	C(=O)(OC1C(C2C(C3(C1(C(CCC3(O)C)OC(=O)/C=C\c1ccccc1)COC(=O)C)OC2(C)C)OC(=O)C)OC(=O)c1cnccc1)c1ccccc1
MOL003243	0.8634	0.1366	0.7737	Tripterygii Radix	Triptolidenol	Not Available	FALSE	C1(=O)OCC2=C1CCC1(C2CC2C3(C41C(C1C(C3O)(C(C)(C)O)O1)O4)O2)C
MOL003244	0.8475	0.1525	0.7661	Tripterygii Radix	Triptonide	Not Available	FALSE	C1(=O)OCC2=C1CCC1(C2CC2C3(C41C(C1C(C3=O)(C(C)C)O1)O4)O2)C
MOL003245	0.6001	0.3999	0.7736	Tripterygii Radix	Triptonoditerpenic acid	Not Available	FALSE	C1C(=C(C2C(C1)(c1c(CC2)c(c(c(c1)OC)C(C)C)O)C)C(=O)O

MOL003247	0.2225	0.7775	0.7631	Tripterygii Radix	Triptonoterpene methyl ether	Not Available	FALSE	O=C1C(C2C(CC1)(c1c(CC2)c(c(cc1O)C(C)C)OC)C)(C)C
MOL003248	0.3564	0.6436	0.6578	Tripterygii Radix	Triptonoterpene	Not Available	FALSE	O=C1C(C2C(CC1)(c1c(CC2)c(c(cc1)C(C)C)O)C)(C)C
MOL003249	0.7404	0.2596	0.7552	Tripterygii Radix	Triptoriterpenic acid A	Not Available	FALSE	OC1C(C2C(CC1O)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(=O)O)CCC(C1(C)O)C)C)C)(C)C
MOL003250	0.7315	0.2685	0.8478	Tripterygii Radix	Triptotin	Not Available	FALSE	OC1C(C23C(CC1)C1(C(CC2O3)C2(C(CC1)(C1C(CC2)(CCC(C1)(C(=O)O)C)C)C)C)(C)C
MOL003251	0.7156	0.2844	0.8163	Tripterygii Radix	Triptotriterpenic acid A	Not Available	FALSE	OC1C(C2C(CC1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(CC(C1)(C(=O)O)C)O)C)C)C)(C)C
MOL003252	0.7156	0.2844	0.8163	Tripterygii Radix	Triptotriterpenic acid B	Not Available	FALSE	OC1C(C2C(CC1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(CC(C1)(C(=O)O)C)O)C)C)C)(C)C
MOL003253	0.7611	0.2389	0.8429	Tripterygii Radix	Triptotriterpenic acid C	Not Available	FALSE	OC1C(C2C(CC1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(CC(C1C)C(=O)O)O)C)C)C)(C)C
MOL003254	0.4198	0.5802	0.7686	Tripterygii Radix	Triptotriterpenoidel lactone A	Not Available	FALSE	OC1C(C2C(CC1)(C1C(CC2)(C2(C(=CC1)C1C3(CC2CC3=O)CCC(C1)(C)C)C)C)(C)C
MOL003255	0.4531	0.5469	0.6624	Tripterygii Radix	WILFORNINE A	Not Available	FALSE	O1C23C4(C(OC(=O)C)C(OC(=O)C)C(C2OC(=O)C)C1(COC(=O)c1c(nccc1)CCC(OC(=O)c1ccccc1)(C(=O)OC(C3(O)C)C(OC(=O)C)C4OC(=O)C)C)COC(=O)C
MOL003256	0.4658	0.5342	0.6652	Tripterygii Radix	WILFORNINE B	Not Available	FALSE	O1C23C4(C(OC(=O)C)C(OC(=O)C)C(C2O)C1(COC(=O)c1c(nccc1)CCC(OC(=O)c1ccccc1)(C(=O)OC(C3(O)C)C(OC(=O)C)C4OC(=O)C)C)COC(=O)C
MOL003257	0.4749	0.5251	0.6965	Tripterygii Radix	WILFORNINE C	Not Available	FALSE	O1C23C4(C(OC(=O)C)C(OC(=O)C)C(C2OC(=O)c2ccccc2)C1(COC(=O)c1c(nccc1)CCC(OC(=O)c1ccccc1)(C(=O)OC(C3(O)C)C(OC(=O)C)C4OC(=O)C)C)COC(=O)C
MOL003258	0.4621	0.5379	0.6286	Tripterygii Radix	WILFORNINE D	Not Available	FALSE	O1C23C4(C(OC(=O)C)C(OC(=O)C)C(C2OC(=O)C)C1(COC(=O)c1c(nccc1)CCC(OC(=O)c1occc1)(C(=O)OC(C3(O)C)C(OC(=O)C)C4OC(=O)C)C)COC(=O)C
MOL003260	0.3810	0.6190	0.6833	Tripterygii Radix	WILFORNINE F	Not Available	FALSE	O1C23C4(C(OC(=O)C)C(OC(=O)C)C(C2OC(=O)c2ccccc2)C1(COC(=O)c1c(nccc1)C(C(C(=O)OC(C3(O)C)C(O)C4OC(=O)C)C)C)COC(=O)C
MOL003261	0.4533	0.5467	0.7069	Tripterygii Radix	WILFORNINE I	Not Available	FALSE	O1C23C4(C(OC(=O)C)C(OC(=O)C)C(C2OC(=O)c2ccccc2)C1(COC(=O)c1c(C(C(O)(C(=O)OC(C3(O)C)C(OC(=O)c2ccccc2)C4OC(=O)C)C)C)ccnc1)C)COC(=O)C
MOL003263	0.9160	0.0840	0.8001	Tripterygii Radix	Wilfordic acid	Not Available	FALSE	c1ccnc(c1C(=O)O)CC(CC(=O)O)C
MOL003264	0.3963	0.6037	0.6821	Tripterygii Radix	Wilfordside	Not Available	FALSE	C1(C2C(C34C(C1OC(=O)C)(C(C(C(C3(O)C)OC(=O)C(C(c1c(C(=O)OCC2(O4)C)cncc1)C)(C)O)OC(=O)c1ccccc1)OC(=O)C)COC(=O)C)OC(=O)C)OC(=O)C
MOL003265	0.3496	0.6504	0.7920	Tripterygii Radix	Wilforlide B	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C2CC(C1)(C(=O)O2)C)C)C)C)(C)C

MOL003266	0.3495	0.6505	0.7271	Tripterygii Radix	21-Hydroxy-30-norhopan-22-one	Not Available	FALSE	C1CC(C2C(C1)(C1C(CC2)(C2(C(CC1)C1(C(CC2)C(CC1)(C(=O)C)O)C)C)C)(C)C
MOL003268	0.5286	0.4714	0.6669	Tripterygii Radix	Wilfornine	Not Available	FALSE	C1(C2C3C45C(C1OC(=O)C)(C(C(C(C4(C)O)OC(=O)C(C)CCc1c(C(=O)OCC(C5)(C)C23OC(=O)C)cccn1)OC(=O)c1cnccc1)OC(=O)C)COC(=O)C)OC(=O)C
MOL003269	0.9084	0.0916	0.8392	Tripterygii Radix	104331-87-5	190797	FALSE	C1C2=C(C3C(C1)(CC(=O)CC3)C)COC2=O
MOL003270	0.4626	0.5374	0.6599	Tripterygii Radix	Wilforzine	Not Available	FALSE	C1(C2C(C34C(C1O)(C(C(C(C3OC(=O)C)C(O4)(COC(=O)c1c(CCC(C(=O)O2)C)nccc1)C)OC(=O)C)OC(=O)C)COC(=O)C)(C)O)OC(=O)c1ccccc1
MOL003271	0.4886	0.5114	0.6019	Tripterygii Radix	Wilfotrine	Not Available	FALSE	C1(C2C(C34C(C1OC(=O)C)(C(C(C(C3OC(=O)C)C(O4)(COC(=O)c1c(CCC(C(=O)O2)(O)C)nccc1)C)OC(=O)C)OC(=O)C)COC(=O)C)(C)O)OC(=O)c1ccoc1
MOL003272	0.5098	0.4902	0.8195	Tripterygii Radix	Wilsonine	Not Available	FALSE	c1(cc2c(cc1OC)CCCN1C32C2(C(C1)O2)C=CC(C3)OC)OC
MOL003274	0.4024	0.5976	0.6371	Tripterygii Radix	neowilforine	Not Available	FALSE	c12cccnc1CCC(C(=O)OC1C(C34C(C(C(COC2=O)(C)C)C4)C(C(C3(C(C1OC(=O)c1ccccc1)OC(=O)C)COC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C)C
MOL003275	0.4186	0.5814	0.6697	Tripterygii Radix	wilfordine	Not Available	FALSE	C1(C2C(C34C(C1OC(=O)C)(C(C(C(C3(O)C)OC(=O)C(C)(O)CCc1c(C(=O)OCC2(O4)C)cccn1)OC(=O)c1ccccc1)OC(=O)C)COC(=O)C)OC(=O)C)OC(=O)C
MOL003276	0.4222	0.5778	0.6709	Tripterygii Radix	wilforine	Not Available	FALSE	C1(C2C(C34C(C1OC(=O)C)(C(C(C(C3OC(=O)C)C(O4)(COC(=O)c1c(CCC(C(=O)O2)C)nccc1)C)OC(=O)C)OC(=O)C)COC(=O)C)(O)C)OC(=O)c1ccccc1
MOL003277	0.4887	0.5113	0.6016	Tripterygii Radix	wilfortrine	Not Available	FALSE	O1C23C4(C(OC(=O)C)C(OC(=O)C)C(C2OC(=O)C)C1(COC(=O)c1c(nccc1)CCC(O)(C(=O)OC(C3(O)C)C(OC(=O)c1ccoc1)C4OC(=O)C)C)C)COC(=O)C
MOL003278	0.7315	0.2685	0.8508	Tripterygii Radix	salaspermic acid	Not Available	FALSE	C1C2(C(C3(C(C1)C1(C(CC3)C3(C(CC1)(C1C(CC3)(CCC(C1)(C)C(=O)O)C)C)C)CO2)C)O
MOL003279	0.8634	0.1366	0.7737	Tripterygii Radix	99694-86-7	Not Available	FALSE	O1C23C4(OC4CC4C3(CCC3=C4COC3=O)C)C(O)C3(OC3C12)C(O)(C)C
MOL003280	0.6153	0.3847	0.8180	Tripterygii Radix	TRIPTONOLIDE	46176013	FALSE	O1CC2=C(C1=O)CCC1(c3ccc(c(c3C(=O)CC21)O)C(C)C)C
MOL003281	0.1836	0.8164	0.7220	Forsythiae Fructus	20(S)-dammar-24-ene-3β,20-diol-3-acetate	Not Available	FALSE	C1CC(C(C2C1(C1C(CC2)(C2(C(CC1)C(CC2)C(O)(C)CCC=C(C)C)C)C)(C)C)OC(=O)C
MOL003282	0.2968	0.7032	0.7383	Forsythiae Fructus	iso-Baurenylacetate	Not Available	FALSE	C1CC(C(C2C1(C1=C(CC2)C2(C(CC1)(C1C(CC2)(C)CCC(C1C)C)C)C)C)(C)C)OC(=O)C

MOL003283	0.6905	0.3095	0.7091	Ailanthi Altissimae Fructus	(2R,3R,4S)-4-(4-hydroxy-3-methoxy-phenyl)-7-methoxy-2,3-dimethylol-tetralin-6-ol	160521	FALSE	c1(ccc(c(c1)OC)O)C1C(C(Cc2c1cc(c(c2)OC)O)CO)CO
MOL003283	0.6905	0.3095	0.7091	Ampelopsis Japonica	(2R,3R,4S)-4-(4-hydroxy-3-methoxy-phenyl)-7-methoxy-2,3-dimethylol-tetralin-6-ol	160521	FALSE	c1(ccc(c(c1)OC)O)C1C(C(Cc2c1cc(c(c2)OC)O)CO)CO
MOL003283	0.6905	0.3095	0.7091	Rubia Cordifolia	(2R,3R,4S)-4-(4-hydroxy-3-methoxy-phenyl)-7-methoxy-2,3-dimethylol-tetralin-6-ol	160521	FALSE	c1(ccc(c(c1)OC)O)C1C(C(Cc2c1cc(c(c2)OC)O)CO)CO
MOL003283	0.6905	0.3095	0.7091	Daturae Flos	(2R,3R,4S)-4-(4-hydroxy-3-methoxy-phenyl)-7-methoxy-2,3-dimethylol-tetralin-6-ol	160521	FALSE	c1(ccc(c(c1)OC)O)C1C(C(Cc2c1cc(c(c2)OC)O)CO)CO
MOL003283	0.6905	0.3095	0.7091	Forsythiae Fructus	(2R,3R,4S)-4-(4-hydroxy-3-methoxy-phenyl)-7-methoxy-2,3-dimethylol-tetralin-6-ol	160521	FALSE	c1(ccc(c(c1)OC)O)C1C(C(Cc2c1cc(c(c2)OC)O)CO)CO
MOL003284	0.7728	0.2272	0.7308	Forsythiae Fructus	caleolarioside A	Not Available	FALSE	c1(c(cc(cc1)CCOC1OC(C(C(C1O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)CO)O)O

MOL003285	0.4510	0.5490	0.6146	Forsythiae Fructus	(2S,3R,4S,5S,6R)-2-[4-[(1R,3aS,4R,6aS)-4-(4-hydroxy-3-methoxyphenyl)-1,3,3a,4,6,6a-hexahydrofuro[4,3-c]furan-1-yl]-2-methoxyphenoxy]-6-(hydroxymethyl)oxane-3,4,5-triol	11168362	FALSE	O1C(C2C(C1)C(OC2)c1cc(c(cc1)OC1C(O)C(O)C(O)C(O1)CO)OC)c1cc(c(cc1)O)OC
MOL003287	0.6711	0.3289	0.7842	Forsythiae Fructus	(2S,3R)-2-(4-hydroxy-3-methoxy-phenyl)-5-(3-hydroxypropyl)-3-methylol-2,3-dihydrobenzofuran-7-ol	11210164	FALSE	c1c(c(cc(c1)C1Oc2c(C1CO)cc(cc2O)CCCO)OC)O
MOL003288	0.9334	0.0666	0.9253	Forsythiae Fructus	Cornoside	3084796	FALSE	O1C(C(O)C(O)C(O)C1OCCC1(O)C=CC(=O)C=C1)CO
MOL003289	0.9416	0.0584	0.9639	Forsythiae Fructus	cornoside_qt	Not Available	FALSE	OCCC1(O)C=CC(=O)C=C1
MOL003290	0.3500	0.6500	0.6985	Forsythiae Fructus	(3R,4R)-3,4-bis[(3,4-dimethoxyphenyl)methyl]oxolan-2-one	384877	FALSE	O1CC(C(Cc2cc(OC)c(OC)cc2)C1=O)Cc1cc(OC)c(OC)cc1
MOL003291	0.5480	0.4520	0.8204	Forsythiae Fructus	EGENINE	Not Available	FALSE	c12c(cc3c(c1)CCN(C3C1c3c(c4c(cc3)OCO4)C(O1)OC)C)OCO2
MOL003292	0.4510	0.5490	0.6146	Forsythiae Fructus	(+)-epipinoresinol-4'-O-D-glucoside	Not Available	FALSE	O1C(C2C(C1)C(OC2)c1cc(c(cc1)OC1C(O)C(O)C(O)C(O1)CO)OC)c1cc(c(cc1)O)OC
MOL003294	0.9416	0.0584	0.9625	Forsythiae Fructus	Threitol	169019	FALSE	C(C(CO)O)(CO)O
MOL003295	0.3551	0.6449	0.7108	Forsythiae Fructus	(+)-pinoresinol monomethyl ether	Not Available	FALSE	O1C(C2C(C1)C(OC2)c1cc(c(cc1)OC)OC)c1cc(c(cc1)O)OC

MOL003296	0.7490	0.2510	0.7529	Forsythiae Fructus	[(2R,3S,4S,5R,6R)-3,4,5-trihydroxy-6-[2-(1-hydroxy-4-oxo-1-cyclohexa-2,5-dienyl)ethoxy]oxan-2-yl]methyl 2-(4-hydroxyphenyl)acetate	11797786	FALSE	C1(C=CC(=O)C=C1)(CCOC1C(O)C(O)C(O)C(O1)COC(=O)Cc1ccc(cc1)O)O
MOL003297	0.8234	0.1766	0.7508	Forsythiae Fructus	[(2R,3S,4S,5R,6R)-3,4,5-trihydroxy-6-[2-(1-hydroxy-4-oxo-1-cyclohexa-2,5-dienyl)ethoxy]oxan-2-yl]methyl 2-(1-hydroxy-4-oxo-1-cyclohexa-2,5-dienyl)acetate	10576163	FALSE	C1(C=CC(=O)C=C1)(CCOC1C(O)C(O)C(O)C(O1)COC(=O)CC1(C=CC(=O)C=C1)O)O
MOL003299	0.9229	0.0771	0.8811	Forsythiae Fructus	forsythide	Not Available	FALSE	C12C(C(OC=C1C(=O)O)OC1OC(C(C(C1O)O)O)CO)C(CC2)C(=O)O
MOL003300	0.9471	0.0529	0.8443	Forsythiae Fructus	forsythide_qt	Not Available	FALSE	C12C(C(OC=C1C(=O)O)O)C(CC2)C(=O)O
MOL003301	0.9147	0.0853	0.8264	Forsythiae Fructus	forsythidmethylester	Not Available	FALSE	C12C(C(OC=C1C(=O)O)OC1OC(C(C(C1O)O)O)CO)C(CC2)OC(=O)C
MOL003302	0.9402	0.0598	0.7685	Forsythiae Fructus	forsythidmethylester_qt	Not Available	FALSE	C12C(C(OC=C1C(=O)O)O)C(CC2)OC(=O)C
MOL003306	0.3551	0.6449	0.7108	Forsythiae Fructus	ACon1_001697	21722915	FALSE	C12C(C(OC1)c1cc(c(cc1)O)OC)COC2c1cc(c(cc1)OC)OC

MOL003308	0.3680	0.6320	0.7887	Forsythiae Fructus	(+)-pinoresinol monomethyl ether-4-D-beta-glucoside_qt	Not Available	FALSE	O1C(C2C(C1)C(OC2)c1cc(c(cc1OC)O)c1cc(c(cc1)OC)OC
MOL003309	0.7679	0.2321	0.7312	Forsythiae Fructus	plantainoside A	Not Available	FALSE	c1(cc(c(cc1)O)O)/C=C\C(=O)OC1C(C(OCCc2cc(c(cc2)O)O)OC(C1O)CO)O
MOL003310	0.9570	0.0430	0.8256	Forsythiae Fructus	3-ethyl-7hydroxyphthalide	Not Available	FALSE	O=C1OC(c2cccc(c12)O)CC
MOL003311	0.9324	0.0676	0.9558	Forsythiae Fructus	suspenol	Not Available	FALSE	C1(C(CCC(C1)O)(O)CCO)O
MOL003312	0.9440	0.0560	0.9497	Forsythiae Fructus	suspenolic acid	Not Available	FALSE	C(=O)(/C=C\1/CCC(CC1)OC(=O)C)O
MOL003313	0.8072	0.1928	0.7542	Forsythiae Fructus	suspensaside A	Not Available	FALSE	c1(c(ccc(c1)C1OC2C(C(OC(=O)/C=C/c3cc(c(cc3)O)O)C(OC2OC1)COC1C(C(C(C(O1)C)O)O)O)O)O)O
MOL003314	0.5651	0.4349	0.6840	Forsythiae Fructus	suspensaside B	Not Available	FALSE	C(=O)(/C=C/c1cc(c(cc1)O)O)OC1C(C(C(OC1COC1C(C(C(C(O1)C)O)O)O)O)OCC(OCCCC)c1ccc(c(c1)O)O)O)O
MOL003315	0.1741	0.8259	0.6958	Forsythiae Fructus	3beta-Acetyl-20,25-epoxydammarane-24alpha-ol	Not Available	FALSE	C1CC(C(C2C1(C1C(CC2)(C2(C(CC1)C(CC2)C1(OC(C(CC1)O)(C)C)C)C)C)C)C)OC(=O)C
MOL003316	0.8227	0.1773	0.7426	Forsythiae Fructus	β-hydroxyacteoside	Not Available	FALSE	C1(C(C(C(C(O1)OCC(O)c1ccc(c(c1)O)O)O)OC1OC(C(C(C1O)O)O)C)OC(=O)/C=C\c1cc(c(cc1)O)O)CO
MOL003318	0.1741	0.8259	0.6958	Forsythiae Fructus	3beta-Acetyl-20,25-epoxydammarane-24beta-ol	Not Available	FALSE	C1CC(C(C2C1(C1C(CC2)(C2(C(CC1)C(CC2)C1(OC(C(CC1)O)(C)C)C)C)C)C)C)OC(=O)C
MOL003319	0.9518	0.0482	0.9626	Inulae Herba	4-Carboxymethylphenol	127	FALSE	c1(ccc(cc1)CC(=O)O)O
MOL003319	0.9518	0.0482	0.9626	Forsythiae Fructus	4-Carboxymethylphenol	127	FALSE	c1(ccc(cc1)CC(=O)O)O
MOL003320	0.8013	0.1987	0.7010	Forsythiae Fructus	(-)-Olivir	5273570	FALSE	C1(c(cc(c1)C1OCC(C1CO)(Cc1cc(c(cc1)O)OC)O)O
MOL003320	0.8013	0.1987	0.7010	Eucommiae Cortex	(-)-Olivir	5273570	FALSE	C1(c(cc(c1)C1OCC(C1CO)(Cc1cc(c(cc1)O)OC)O)O
MOL003320	0.8013	0.1987	0.7010	Fructus Ligustri Lucidi	(-)-Olivir	5273570	FALSE	C1(c(cc(c1)C1OCC(C1CO)(Cc1cc(c(cc1)O)OC)O)O
MOL003322	0.4163	0.5837	0.6817	Forsythiae Fructus	FORSYTHINOL	Not Available	FALSE	C12C(C(OC2)c2cc(c(cc2)OC)OC)COC1c1c(cc(cc1)O)OC

MOL003323	0.9376	0.0624	0.9675	Forsythiae Fructus	4-hydroxy-4-(2-hydroxyethyl) cyclohexan-1-one	184824	FALSE	C1(CCC(=O)CC1)(CCO)O
MOL003324	0.9264	0.0736	0.9071	Forsythiae Fructus	rengyoside A	Not Available	FALSE	C1C(CCC(C1)O)(O)CCOC1C(O)C(O)C(O)C(O1)CO
MOL003325	0.9365	0.0635	0.9711	Oroxyli Semen	rengyol	Not Available	FALSE	C1C(CCC(C1)O)(O)CCO
MOL003325	0.9365	0.0635	0.9711	Forsythiae Fructus	rengyol	Not Available	FALSE	C1C(CCC(C1)O)(O)CCO
MOL003326	0.9243	0.0757	0.9124	Forsythiae Fructus	4-hydroxy-4-[2-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyethyl]cyclohexan-1-one	11045420	FALSE	C1(CCC(=O)CC1)(CCOC1C(O)C(O)C(O)C(O1)CO)O
MOL003327	0.7529	0.2471	0.7257	Forsythiae Fructus	rengyoside C	Not Available	FALSE	C1C(CCC(C1)O)(O)CCOC1C(O)C(O)C(O)C(O1)COC(=O)Cc1ccc(cc1)O
MOL003328	0.9434	0.0566	0.9536	Forsythiae Fructus	rengyolone	Not Available	FALSE	C1(CCC(CC1)O)(CC(=O)O)O
MOL003329	0.9334	0.0666	0.9253	Forsythiae Fructus	4-hydroxy-4-[2-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyethyl]cyclohexa-2,5-dien-1-one	11809239	FALSE	C1(C=CC(=O)C=C1)(CCOC1C(O)C(O)C(O)C(O1)CO)O
MOL003330	0.3551	0.6449	0.7108	Forsythiae Fructus	(-)-Phillygenin	Not Available	FALSE	c1cc(c(cc1C1OCC2C1COC2c1cc(c(cc1)O)OC)OC)OC
MOL003331	0.7754	0.2246	0.7047	Rehmanniae Radix Praeparata	Forsythiaside	5281773	FALSE	C1(C(OC(C(C1O)O)C)OCC1OC(C(C(C1OC(=O)/C=C/c1cc(c(cc1)O)O)O)O)OCCc1ccc(c(c1)O)O)O
MOL003331	0.7754	0.2246	0.7047	Forsythiae Fructus	Forsythiaside	5281773	FALSE	C1(C(OC(C(C1O)O)C)OCC1OC(C(C(C1OC(=O)/C=C/c1cc(c(cc1)O)O)O)O)OCCc1ccc(c(c1)O)O)O
MOL003332	0.8343	0.1657	0.7213	Forsythiae Fructus	Forsythoside C	Not Available	FALSE	O(C1C(O)C(O)C(C(O1)COC1C(O)C(O)C(O)C(O1)C)OC(=O)/C=C\c1cc(c(cc1)O)O)CC(O)c1cc(c(cc1)O)O
MOL003333	0.7807	0.2193	0.7348	Buddlejae Flos	acteoside	5281800	FALSE	c1(c(cc(cc1)/C=C/C(=O)OC1C(C(C(OC1CO)OCCc1cc(c(cc1)O)O)O)OC1OC(C(C(C1O)O)O)C)O)O
MOL003333	0.7807	0.2193	0.7348	Verbenae Herb	acteoside	5281800	FALSE	c1(c(cc(cc1)/C=C/C(=O)OC1C(C(C(OC1CO)OCCc1cc(c(cc1)O)O)O)OC1OC(C(C(C1O)O)O)C)O)O

MOL003333	0.7807	0.2193	0.7348	Cistanches Herba	acteoside	5281800	FALSE	c1(c(cc(cc1)/C=C/C(=O)OC1C(C(C(OC1CO)OCCc1cc(c(cc1)O)O)O)OC1OC(C(C(C1O)O)O)C)O)O
MOL003333	0.7807	0.2193	0.7348	Plantaginis Herba	acteoside	5281800	FALSE	c1(c(cc(cc1)/C=C/C(=O)OC1C(C(C(OC1CO)OCCc1cc(c(cc1)O)O)O)OC1OC(C(C(C1O)O)O)C)O)O
MOL003333	0.7807	0.2193	0.7348	Oroxyli Semen	acteoside	5281800	FALSE	c1(c(cc(cc1)/C=C/C(=O)OC1C(C(C(OC1CO)OCCc1cc(c(cc1)O)O)O)OC1OC(C(C(C1O)O)O)C)O)O
MOL003333	0.7807	0.2193	0.7348	Fructus Ligustri Lucidi	acteoside	5281800	FALSE	c1(c(cc(cc1)/C=C/C(=O)OC1C(C(C(OC1CO)OCCc1cc(c(cc1)O)O)O)OC1OC(C(C(C1O)O)O)C)O)O
MOL003333	0.7807	0.2193	0.7348	Forsythiae Fructus	acteoside	5281800	FALSE	c1(c(cc(cc1)/C=C/C(=O)OC1C(C(C(OC1CO)OCCc1cc(c(cc1)O)O)O)OC1OC(C(C(C1O)O)O)C)O)O
MOL003333	0.7807	0.2193	0.7348	Clerodendrum Trichotomum Thunb	acteoside	5281800	FALSE	c1(c(cc(cc1)/C=C/C(=O)OC1C(C(C(OC1CO)OCCc1cc(c(cc1)O)O)O)OC1OC(C(C(C1O)O)O)C)O)O
MOL003333	0.7807	0.2193	0.7348	Rehmanniae Radix Praeparata	acteoside	5281800	FALSE	c1(c(cc(cc1)/C=C/C(=O)OC1C(C(C(OC1CO)OCCc1cc(c(cc1)O)O)O)OC1OC(C(C(C1O)O)O)C)O)O
MOL003333	0.7807	0.2193	0.7348	Pogostemon Cablin (Blanco) Benth.	acteoside	5281800	FALSE	c1(c(cc(cc1)/C=C/C(=O)OC1C(C(C(OC1CO)OCCc1cc(c(cc1)O)O)O)OC1OC(C(C(C1O)O)O)C)O)O
MOL003333	0.7807	0.2193	0.7348	Figwort Root	acteoside	5281800	FALSE	c1(c(cc(cc1)/C=C/C(=O)OC1C(C(C(OC1CO)OCCc1cc(c(cc1)O)O)O)OC1OC(C(C(C1O)O)O)C)O)O
MOL003333	0.7807	0.2193	0.7348	Campsis Flos	acteoside	5281800	FALSE	c1(c(cc(cc1)/C=C/C(=O)OC1C(C(C(OC1CO)OCCc1cc(c(cc1)O)O)O)OC1OC(C(C(C1O)O)O)C)O)O
MOL003334	0.9029	0.0971	0.7933	Forsythiae Fructus	Forsythoside D	Not Available	FALSE	c1(c(cc(cc1)C(O)COC1OC(C(C(C1O)O)O)O)COC1OC(C(C(C1O)O)O)C)O)O
MOL003335	0.9314	0.0686	0.9613	Forsythiae Fructus	ZINC00402871	6951097	FALSE	c1(c(cc(cc1)C(O)CO)O)O
MOL003336	0.9020	0.0980	0.7900	Forsythiae Fructus	Forsythoside E	Not Available	FALSE	c1(c(cc(cc1)CCOC1OC(C(C(C1O)O)O)O)COC1OC(C(C(C1O)O)O)C)O)O
MOL003337	0.7150	0.2850	0.7285	Forsythiae Fructus	Forsythoside F	Not Available	FALSE	C1(C(C(C(OC1COC1OCC(C(C1O)O)O)O)OCCc1ccc(c(c1)O)O)O)OC1C(C(C(C(O1)C)O)O)O)OC(=O)/C=C/c1ccc(c(c1)O)O
MOL003338	0.6007	0.3993	0.7017	Forsythiae Fructus	Forsythoside G	Not Available	FALSE	c1cc(c(cc1CCOC1C(C(C(C(O1)COC1OCC(C1OC)(CO)O)OC(=O)/C=C\c1cc(c(cc1)O)O)OC1OC(C(C(C1O)O)O)C)O)O)O
MOL003339	0.9339	0.0661	0.8857	Forsythiae Fructus	Adoxosidic acid	13892717	FALSE	C12C(C(OC=C1C(=O)O)OC1OC(C(C(C1O)O)O)CO)C(CC2)CO
MOL003340	0.9509	0.0491	0.8601	Forsythiae Fructus	Adoxosidic acid_qt	Not Available	FALSE	C12C(C(OC=C1C(=O)O)O)C(CC2)CO
MOL003341	0.9339	0.0661	0.8942	Oroxyli Semen	salidroside	159278	FALSE	O1C(C(O)C(O)C(O)C1OCCc1ccc(O)cc1)CO
MOL003341	0.9339	0.0661	0.8942	Sargentodoxae Caulis	salidroside	159278	FALSE	O1C(C(O)C(O)C(O)C1OCCc1ccc(O)cc1)CO
MOL003341	0.9339	0.0661	0.8942	Semiaquilegiae Radix	salidroside	159278	FALSE	O1C(C(O)C(O)C(O)C1OCCc1ccc(O)cc1)CO
MOL003341	0.9339	0.0661	0.8942	Cistanches Herba	salidroside	159278	FALSE	O1C(C(O)C(O)C(O)C1OCCc1ccc(O)cc1)CO
MOL003341	0.9339	0.0661	0.8942	Fructus Ligustri Lucidi	salidroside	159278	FALSE	O1C(C(O)C(O)C(O)C1OCCc1ccc(O)cc1)CO
MOL003341	0.9339	0.0661	0.8942	Forsythiae Fructus	salidroside	159278	FALSE	O1C(C(O)C(O)C(O)C1OCCc1ccc(O)cc1)CO
MOL003342	0.9365	0.0635	0.9711	Oroxyli Semen	isorengyol	363707	FALSE	C1CC(CCC1(CCO)O)O

MOL003342	0.9365	0.0635	0.9711	Forsythiae Fructus	isorengyol	363707	FALSE	C1CC(CCC1(CCO)O)O
MOL003343	0.9357	0.0643	0.8727	Forsythiae Fructus	rengyoxide	14353410	FALSE	C1CC2(CCC1(CCO)O2)O
MOL003344	0.3289	0.6711	0.7461	Forsythiae Fructus	β-amyrin acetate	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C)C)(CC2)C)(CC1)C)(C)C)C(=O)C
MOL003344	0.3289	0.6711	0.7461	Radix Cirsii Japonici	β-amyrin acetate	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C)C)(CC2)C)(CC1)C)(C)C)C(=O)C
MOL003345	0.9133	0.0867	0.8176	Forsythiae Fructus	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-chromone	5320854	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1)C
MOL003346	0.7435	0.2565	0.6279	Forsythiae Fructus	Psuedohypericin	Not Available	FALSE	O=C1c2c3c4c5c6c(c3c(cc2O)CO)c(cc(O)c6C(=O)c2c5c(c3c4c1c(O)cc3O)c(O)cc2O)C
MOL003346	0.7435	0.2565	0.6279	Panax Ginseng C. A. Mey.	Psuedohypericin	Not Available	FALSE	O=C1c2c3c4c5c6c(c3c(cc2O)CO)c(cc(O)c6C(=O)c2c5c(c3c4c1c(O)cc3O)c(O)cc2O)C
MOL003349	0.7485	0.2515	0.6302	Forsythiae Fructus	Protopseudohypericin	Not Available	FALSE	Oc1c2c3c(c4c5c2c(O)cc(O)c5C(=O)c2c4cc(cc2O)C)c2c(C(=O)c3c(O)c1)c(O)cc(c2)CO
MOL003350	0.7503	0.2497	0.6244	Forsythiae Fructus	Protohypericin	Not Available	FALSE	Oc1c2c3c(c4c5c2c(O)cc(O)c5C(=O)c2c4cc(cc2O)C)c2c(C(=O)c3c(O)c1)c(O)cc(c2)C
MOL003351	0.7357	0.2643	0.6945	Forsythiae Fructus	cyclopseudo-hypericin	Not Available	FALSE	Ic1c(O)c2c3c4c5c6c7c8c4c4c(c3c1O)c(O)cc(O)c4C(=O)c8c(O)cc7ccc6cc(O)c5C2=O
MOL003352	0.6985	0.3015	0.7534	Forsythiae Fructus	Procyanidin	Not Available	FALSE	O(C1(Oc2c(C(O)C1O)c(O)cc(O)c2)c1cc(O)c(O)cc1)C1C(Oc2c(C1)c(O)cc(O)c2)c1cc(O)c(O)cc1
MOL003353	0.8992	0.1008	0.7540	Forsythiae Fructus	Emodinanthrone	122635	FALSE	O=C1c2c(Cc3c1c(O)cc(O)c3)cc(cc2O)C
MOL003353	0.8992	0.1008	0.7540	Lilii Bulbus	Emodinanthrone	122635	FALSE	O=C1c2c(Cc3c1c(O)cc(O)c3)cc(cc2O)C
MOL003353	0.8992	0.1008	0.7540	Polygoni Cuspidati Rhizoma Et Radix	Emodinanthrone	122635	FALSE	O=C1c2c(Cc3c1c(O)cc(O)c3)cc(cc2O)C
MOL003353	0.8992	0.1008	0.7540	Radix Rhei Et Rhizome	Emodinanthrone	122635	FALSE	O=C1c2c(Cc3c1c(O)cc(O)c3)cc(cc2O)C
MOL003354	0.9461	0.0539	0.8873	Forsythiae Fructus	(2R,3R,4R)-2-(3,4-dihydroxyphenyl)chroman-3,4,5,7-tetrol	11208959	FALSE	O1C(C(O)C(O)c2c1cc(O)cc2O)c1cc(O)c(O)cc1

MOL003355	0.8013	0.1987	0.7010	Forsythiae Fructus	olivil	44566587	FALSE	O1C(C(C(O)(C1)Cc1cc(OC)c(O)cc1)CO)c1cc(OC)c(O)cc1
MOL003356	0.6387	0.3613	0.7732	Forsythiae Fructus	8-hydroxypinoresinol	Not Available	FALSE	O1CC2C(C1c1cc(c(cc1)OC)O)(COC2c1cc(c(cc1)O)OC)O
MOL003357	0.6446	0.3554	0.7544	Forsythiae Fructus	(1R,3aR,4R,6aS)-1,4-bis(4-hydroxy-3-methoxyphenyl)-3,3a,4,6-tetrahydro-1H-furo[3,4-c]furan-6a-ol	21632947	FALSE	O1CC2C(C1c1cc(c(cc1)O)OC)(COC2c1cc(c(cc1)O)OC)O
MOL003358	0.9380	0.0620	0.8173	Forsythiae Fructus	Euxanthone	5281631	FALSE	c12c(c(=O)c3c(o1)ccc(c3)O)c(ccc2)O
MOL003359	0.9267	0.0733	0.9323	Forsythiae Fructus	Myrcenol	10975	FALSE	C(CCCC(=C)C=C)(C)(C)O
MOL003360	0.8869	0.1131	0.8979	Forsythiae Fructus	Norlapachol	231114	FALSE	OC1=C(C(=O)C(=O)c2c1cccc2)C=C(C)C
MOL003361	0.9372	0.0628	0.8058	Forsythiae Fructus	(1S,6R)-3,7,7-trimethylbicyclo[4.1.0]hept-3-ene-2,5-dione	10057860	FALSE	C1(=CC(=O)C2C(C1=O)C2(C)C)C
MOL003362	0.4739	0.5261	0.6624	Forsythiae Fructus	Cynanuriculoside A_qt	Not Available	FALSE	C1(CC2=CCC3(C(C2(CC1)C)CC(C1(C3(O)CCC1O)CC(=O)C)OC(=O)/C=C(/C(C)C)\C)O)O
MOL003363	0.7111	0.2889	0.7186	Forsythiae Fructus	Forsythoside B	Not Available	FALSE	c1(c(cc(cc1)/C=C/C(=O)OC1C(C(C(OC1COC1OCC(C1O)(CO)O)OCCc1ccc(c(c1)O)O)O)OC1OC(C(C(C1O)O)O)C)O)O
MOL003364	0.4034	0.5966	0.7008	Forsythiae Fructus	gamma-Camphorene	Not Available	FALSE	C1(=CCCC(C1)C(=C)CCC=C(C)C)CCC=C(C)C
MOL003365	0.2290	0.7710	0.6491	Forsythiae Fructus	Lactucasterol	Not Available	FALSE	C1C(C(=O)C2=CCC3C(C2(C1)C)CCC1(C3CCC1C(CC1C(C1C(C)C)C)C)C)O
MOL003366	0.9495	0.0505	0.9144	Forsythiae Fructus	Matatabiether	Not Available	FALSE	C1CCC2C(=C)C1(OCC2C)C
MOL003367	0.3576	0.6424	0.7664	Schisandrae Chinensis Fructus	Myricadiol	Not Available	FALSE	C1CC(C(C2C1(C1C(CC2)(C2=CCC3(C(C2(CC1)C)CC(CC3)(C)C)CO)C)C)(C)C)O
MOL003367	0.3576	0.6424	0.7664	Houttuyniae Herba	Myricadiol	Not Available	FALSE	C1CC(C(C2C1(C1C(CC2)(C2=CCC3(C(C2(CC1)C)CC(CC3)(C)C)CO)C)C)(C)C)O
MOL003367	0.3576	0.6424	0.7664	Radix Bupleuri	Myricadiol	Not Available	FALSE	C1CC(C(C2C1(C1C(CC2)(C2=CCC3(C(C2(CC1)C)CC(CC3)(C)C)CO)C)C)(C)C)O
MOL003367	0.3576	0.6424	0.7664	Forsythiae Fructus	Myricadiol	Not Available	FALSE	C1CC(C(C2C1(C1C(CC2)(C2=CCC3(C(C2(CC1)C)CC(CC3)(C)C)CO)C)C)(C)C)O
MOL003367	0.3576	0.6424	0.7664	Asari Radix Et Rhizoma	Myricadiol	Not Available	FALSE	C1CC(C(C2C1(C1C(CC2)(C2=CCC3(C(C2(CC1)C)CC(CC3)(C)C)CO)C)C)(C)C)O

MOL003369	0.7150	0.2850	0.7681	Forsythiae Fructus	Onjisaponin G	Not Available	FALSE	O1CC(C(C1OC1C(C(OC(C1OC1OCC(C(C1O)O)O)C)OC1C(OC(C(C1O)OC(=O)/C=C/c1cc(c(c(c1)OC)OC)OC)C)OC(=O)C12CCC3(C4(CCC5C(C(C(CC5(C4CC=C3C1CC(CC2)(C)C)C)O)OC1OC(C(C(C1O)O)O)CO)(C(=O)O)C)C)CO)O)O)(O)CO
MOL003370	0.8102	0.1898	0.7548	Forsythiae Fructus	Onjixanthone I	5320290	FALSE	c1c(ccc2c1c(=O)c1c(o2)cc(c(c1OC)OC)OC)O
MOL003371	0.8219	0.1781	0.7798	Asari Radix Et Rhizoma	Safynol	5281155	FALSE	C/C=C/C#CC#CC#C/C=C/C(CO)O
MOL003371	0.8219	0.1781	0.7798	Forsythiae Fructus	Safynol	5281155	FALSE	C/C=C/C#CC#CC#C/C=C/C(CO)O
MOL003372	0.9469	0.0531	0.7835	Forsythiae Fructus	Scopine	Not Available	FALSE	C1C2N(C(CC1O)C1C2O1)C
MOL003373	0.2376	0.7624	0.7297	Forsythiae Fructus	Sutchuenensine IV	Not Available	FALSE	c12c3cc(c(c1)OC)Oc1ccc(cc1OC)CC1c4c(c(c(cc4CCN1C)OC)OC)Oc1ccc(CC3N(CC2)C)cc1
MOL003375	0.8640	0.1360	0.6322	Ecliptae Herba	.alpha.-T COOH deriv.	159047	FALSE	c1ccc(s1)c1ccc(s1)c1ccc(s1)C(=O)O
MOL003376	0.8996	0.1004	0.6983	Ecliptae Herba	2-(Buta-1,3-diynyl)-5-(4-chloro-3-hydroxybut-1-ynyl) thiophene	Not Available	FALSE	C(C#Cc1sc(cc1)C#CC#C)(CCl)O
MOL003377	0.9047	0.0953	0.7835	Ecliptae Herba	Demethylwedelolactone-7-glucoside	6325048	FALSE	c1c(cc2c(c1O)c1c(c(=O)o2)c2c(o1)cc(c(c2)O)O)OC1OC(C(C(C1O)O)O)CO
MOL003378	0.9183	0.0817	0.8256	Ecliptae Herba	1,3,8,9-tetrahydroxybenzofurano[3,2-c]chromen-6-one	5489605	FALSE	c1c(cc2c(c1O)c1c(c(=O)o2)c2c(o1)cc(c(c2)O)O)O
MOL003379	0.7411	0.2589	0.8158	Ecliptae Herba	Demissine	Not Available	FALSE	C1C2N(CC(C1)C)C1C(C2C)C2(C(C1)C1C(CC2)C2(C(CC1)CC(CC2)OC1OC(C(C(C1O)O)O)O)COC1OC(C(C(C1OC1OC(C(C(C1O)O)O)O)CO)OC1OCC(C(C1O)O)O)O)CO)C)C
MOL003380	0.4334	0.5666	0.6486	Ecliptae Herba	Demissine_qt	Not Available	FALSE	C1C2N(CC(C1)C)C1C(C2C)C2(C(C1)C1C(CC2)C2(C(CC1)CC(CC2)O)C)C
MOL003381	0.7585	0.2415	0.8326	Ecliptae Herba	Ecliptasaponin B	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)OC1OC(C(C(C1O)O)O)CO)C)C)(C)C)OC1OC(C(C(C1O)O)OC1OC(C(C(C1O)O)O)CO)CO
MOL003382	0.7626	0.2374	0.8354	Ecliptae Herba	Ecliptasaponin B_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O
MOL003383	0.7297	0.2703	0.7284	Ecliptae Herba	Ecliptasaponin D	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CC(C4(C(=O)O)CCC(C)(C)CC4C3=CCC21)O)C)OC1C(O)C(O)C(O)C(O1)CO
MOL003384	0.7626	0.2374	0.8354	Ecliptae Herba	Ecliptasaponin D_qt	29927648	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CC(C4(C(=O)O)CCC(C)(C)CC4C3=CCC21)O)C)O

MOL003385	0.7297	0.2703	0.7284	Ecliptae Herba	Ecliptasaponin	44584168	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CC(C4(C(=O)O)CCC(C)(C)CC4C3=CCC21)O)C)OC1C(O)C(O)C(O)C(O1)CO
MOL003386	0.7626	0.2374	0.8354	Ecliptae Herba	Ecliptasaponin_qt	476486	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CC(C4(C(=O)O)CCC(C)(C)CC4C3=CCC21)O)C)O
MOL003387	0.8417	0.1583	0.7521	Ecliptae Herba	3-[(2S)-2,3-dihydroxy-3-methyl-butyl]-4-methoxy-1-methyl-carbostyril	10902387	FALSE	c1ccc2c(c1)c(c(c(=O)n2C)CC(O)C(C)(O)C)OC
MOL003389	0.9181	0.0819	0.8772	Ecliptae Herba	3'-O-Methylorobol	5319744	FALSE	c12c(cc(cc2O)O)occ(c1=O)c1cc(c(cc1)O)OC
MOL003393	0.8597	0.1403	0.6921	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	(1S,4S)-7-isopropylidene-1,4-dimethyl-2,3,4,5,6,8-hexahydro-1H-azulene	15560252	FALSE	C12=C(C(CC2)C)CC(=C(C)C)CCC1C
MOL003393	0.8597	0.1403	0.6921	Ecliptae Herba	(1S,4S)-7-isopropylidene-1,4-dimethyl-2,3,4,5,6,8-hexahydro-1H-azulene	15560252	FALSE	C12=C(C(CC2)C)CC(=C(C)C)CCC1C
MOL003393	0.8597	0.1403	0.6921	Solidaginis Herba	(1S,4S)-7-isopropylidene-1,4-dimethyl-2,3,4,5,6,8-hexahydro-1H-azulene	15560252	FALSE	C12=C(C(CC2)C)CC(=C(C)C)CCC1C
MOL003394	0.8018	0.1982	0.7152	Ecliptae Herba	Benzofurano(3',2':3,4)coumarin	638309	FALSE	c1(=O)c2c(c3c(o1)cccc3)oc1c2cccc1
MOL003396	0.7626	0.2374	0.8354	Gleditsiae Fructus	echinocystic acid	73309	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O
MOL003396	0.7626	0.2374	0.8354	Asteris Radix Et Rhizoma	echinocystic acid	73309	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O
MOL003396	0.7626	0.2374	0.8354	Gleditsiae Spina	echinocystic acid	73309	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O

MOL003396	0.7626	0.2374	0.8354	Ecliptae Herba	echinocystic acid	73309	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O
MOL003396	0.7626	0.2374	0.8354	Gleditsiae Fructus Abnormalis	echinocystic acid	73309	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O
MOL003398	0.9129	0.0871	0.8534	Peanut Skin	Pratensein	5281803	FALSE	o1c2c(c(=O)c(c3cc(O)c(OC)cc3)c1)c(O)cc(O)c2
MOL003398	0.9129	0.0871	0.8534	Inulae Flos	Pratensein	5281803	FALSE	o1c2c(c(=O)c(c3cc(O)c(OC)cc3)c1)c(O)cc(O)c2
MOL003398	0.9129	0.0871	0.8534	Ecliptae Herba	Pratensein	5281803	FALSE	o1c2c(c(=O)c(c3cc(O)c(OC)cc3)c1)c(O)cc(O)c2
MOL003399	0.7471	0.2529	0.7872	Ecliptae Herba	Caulophyllogenin	104361	FALSE	C1CC(C(C2C1(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)O)C)C)(C)CO)O
MOL003400	0.7297	0.2703	0.7284	Ecliptae Herba	Ecliptasaponin A	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CC(C4(C(=O)O)CCC(C)(C)CC4C3=CCC21)O)C)OC1C(O)C(O)C(O)C(O1)CO
MOL003401	0.7626	0.2374	0.8354	Ecliptae Herba	Ecliptasaponin A_qt	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CC(C4(C(=O)O)CCC(C)(C)CC4C3=CCC21)O)C)O
MOL003402	0.9331	0.0669	0.8261	Ecliptae Herba	demethylwedelolactone	Not Available	FALSE	c1(c(cc2c(c1)c1c(o2)C2C(OC1=O)C=C(C=C2O)O)O)O
MOL003403	0.9673	0.0327	0.8769	Bombyx Mori L.	nicotine	89594	FALSE	c1c(cccn1)C1CCCN1C
MOL003403	0.9673	0.0327	0.8769	Equiseti Hiemalis Herba	nicotine	89594	FALSE	c1c(cccn1)C1CCCN1C
MOL003403	0.9673	0.0327	0.8769	Ecliptae Herba	nicotine	89594	FALSE	c1c(cccn1)C1CCCN1C
MOL003403	0.9673	0.0327	0.8769	Momordicae Fructus	nicotine	89594	FALSE	c1c(cccn1)C1CCCN1C
MOL003404	0.9064	0.0936	0.8027	Ecliptae Herba	wedelolactone	5281813	FALSE	c1(c(cc2c(c1)c1c(o2)c2c(oc1=O)cc(cc2O)OC)O)O
MOL003405	0.7462	0.2538	0.7832	Ecliptae Herba	Chloromaloside	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C2C(C(=O)C1)(C1C(C2)OC(C1C)(CCC(COC1OC(C(C(C1O)O)O)CO)C)O)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)OC1OC(C(C(C1OC1OCC(C(C1O)O)O)OC1OCC(C(C1O)O)O)O)CO)CO
MOL003406	0.3786	0.6214	0.6871	Ecliptae Herba	Chloromaloside_qt	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C2C(C(=O)C1)(C1C(C2)OC(C1C)(CCC(CO)C)O)C)C)O
MOL003407	0.6845	0.3155	0.6877	Strychni Semen	(-)-5'-Methoxyisolariciresinol	70697973	FALSE	c12c(C(C(C(C1)CO)CO)c1cc(c(c(c1)OC)O)OC)cc(c(c2)OC)O
MOL003409	0.5512	0.4488	0.8087	Strychni Semen	Colubrinoside	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C23C(CC1)C1C(OC2)(OC(CC1(O)C)C=C(C)C)C3)C)(C)C)OC1OCC(C(C1OC(=O)C)OC1OC(C(C(C1O)OC1OCC(C(C1O)O)O)O)OC(=O)C)CO)O
MOL003410	0.3975	0.6025	0.7953	Strychni Semen	Ziziphin_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C23C(CC1)C1C(OC2)(OC(CC1(O)C)C=C(C)C)C3)C)(C)C)O
MOL003410	0.3975	0.6025	0.7953	Jujubae Fructus	Ziziphin_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C23C(CC1)C1C(OC2)(OC(CC1(O)C)C=C(C)C)C3)C)(C)C)O
MOL003412	0.6188	0.3812	0.6487	Strychni Semen	Isobrucine N-oxide	Not Available	FALSE	c1(c(cc2c(c1)C13C4N2C(=O)CC=C4C2CC1[N+](C/C/2=C\CO)(CC3)O)OC)OC
MOL003413	0.6809	0.3191	0.7294	Strychni Semen	Isostrychnine N-oxide (I)	Not Available	FALSE	c1ccc2c(c1)C13C4N2C(=O)CCC4C2CC1[N+](C/C/2=C\CO)(CC3)O
MOL003414	0.6695	0.3305	0.7197	Strychni Semen	Isostrychnine N-oxide (II)	Not Available	FALSE	c1ccc2c(c1)C13C4N2C(=O)CC=C4C2CC1[N+](C/C/2=C\CO)(CC3)O

MOL003415	0.8743	0.1257	0.8173	Strychni Semen	CCRIS 1712	73687	FALSE	C1CC(C2C(C1)(C(C(=CC2)C=O)C=O)C)(C)C
MOL003416	0.9047	0.0953	0.8833	Sesami Nigrum Semen	Isobutyral	6561	FALSE	CC(C=O)C
MOL003416	0.9047	0.0953	0.8833	Strychni Semen	Isobutyral	6561	FALSE	CC(C=O)C
MOL003416	0.9047	0.0953	0.8833	Ephedra Herba	Isobutyral	6561	FALSE	CC(C=O)C
MOL003416	0.9047	0.0953	0.8833	Capsici Fructus	Isobutyral	6561	FALSE	CC(C=O)C
MOL003417	0.6417	0.3583	0.6830	Strychni Semen	Lokundjoside	441865	FALSE	C1(C(C(C(OC1C)OC1CC2(C(CC1)(C1C(CC2)C2(C(CC1O)(C(CC2)C1=CC(=O)OC1)C)O)C)O)O)O)O
MOL003418	0.6708	0.3292	0.7631	Strychni Semen	Lokundjoside_qt	Not Available	FALSE	OC1CC2(C(CC1)(C1C(CC2)C2(C(CC1O)(C(CC2)C1=CC(=O)OC1)C)O)C)O
MOL003419	0.8068	0.1932	0.7668	Strychni Semen	16beta-Hydroxy-19S-vindolinine N-oxide	Not Available	FALSE	[N+]12(C3C4(C=CC1)CC(C1(C3(c3c(N1)cccc3)CC2)C4C)(C(=O)OC)O)O
MOL003420	0.2396	0.7604	0.7007	Strychni Semen	Maytanbutacine	Not Available	FALSE	C12(C(/C=C/C=C(/C(c3cc(c(c(c3)OC)Cl)N(C)CC(=O)CC(C3(C(C(C(OC(=O)N1)C2)C)O3)C)OC(=O)C(C)C)OC(=O)C)\C)OC)O
MOL003421	0.2109	0.7891	0.6894	Strychni Semen	Normenisarine	Not Available	FALSE	c1(cc2c3c4c1Oc1c(O4)c(c4c(c1)CCN=C4Cc1ccc(c(c1)Oc1ccc(CC3NCC2)cc1)OC)OC)OC
MOL003423	0.5498	0.4502	0.6662	Strychni Semen	Protoveratrine A	Not Available	FALSE	C1N2C(CCC1C)C(C1C(C2)C2C(C(C1O)OC(=O)C(CC)C)(C1C3(C4(C(C(C1OC(=O)C)OC(=O)C)C(C(CC4)OC(=O)C(CC)(C)O)(O)O3)C)C2)O)(C)O
MOL003425	0.7269	0.2731	0.6675	Strychni Semen	Pseudostrychnine	Not Available	FALSE	O1C2C3C4N(c5c(C64C4N(CC6O)CC(=CC1)C3C4)cccc5)C(=O)C2
MOL003426	0.8839	0.1161	0.8451	Strychni Semen	Salipurposide	Not Available	FALSE	c1(cc(c2c(c1)OC(CC2=O)c1ccc(cc1)O)OC1OC(C(C(C1O)O)O)CO)O
MOL003427	0.8132	0.1868	0.8044	Strychni Semen	2-Hydroxymethylanthraquinone	87014	FALSE	c1cc2c(cc1)C(=O)c1c(C2=O)ccc(c1)CO
MOL003429	0.6264	0.3736	0.6818	Strychni Semen	COLUBRINE, BETA	251890	FALSE	c1(ccc2c(c1)C13C4N2C(=O)CC2C4C4CC3N(CC1)CC4=CCO2)OC
MOL003430	0.5164	0.4836	0.7280	Strychni Semen	α-Colubrine	Not Available	FALSE	c1(cc2c(cc1)C13C4N2C(=O)CC2C4C(CC1CCC3)C(=CO2)CCCN)OC
MOL003431	0.5181	0.4819	0.7293	Strychni Semen	beta-Colubrine	Not Available	FALSE	c1cc2c(cc1OC)C13C4N2C(=O)CC2C4C(CC1CCC3)C(=CO2)CCCN
MOL003433	0.7038	0.2962	0.6071	Strychni Semen	brucine-N-oxide	Not Available	FALSE	O[N+]12C3C4(C5N(c6c4cc(OC)c(OC)c6)C(=O)CC4OCC=C(C(C54)C3)C2)CC1
MOL003434	0.6540	0.3460	0.7165	Strychni Semen	4-Hydroxy-3-methoxystrychnine	Not Available	FALSE	c1(c(c2c(cc1)C13C4N2C(=O)CC=C4C2CC1N(C/C/2=C\CO)CC3)O)OC
MOL003435	0.5802	0.4198	0.6637	Strychni Semen	brucine	442021	FALSE	O1C2C3C4N(c5c(C64C4N(CC6)CC(=CC1)C3C4)cc(OC)c(OC)c5)C(=O)C2

MOL003435	0.5802	0.4198	0.6637	Bruceae Fructus	brucine	442021	FALSE	O1C2C3C4N(c5c(C64C4N(CC6)CC(=CC1)C3C4)cc(OC)c(OC)c5)C(=O)C2
MOL003436	0.4763	0.5237	0.7421	Strychni Semen	Isobrucine	Not Available	FALSE	O=C1N2C3C4(C5N(CC4)C/C(=C/CO)/C(C5)C3=CC1)c1c2cccc1
MOL003437	0.4620	0.5380	0.6810	Strychni Semen	Isobrucine	Not Available	FALSE	O=C1N2C3C4(C5N(CC4)C/C(=C/CO)/C(C5)C3=CC1)c1c2cc(OC)c(OC)c1
MOL003438	0.7553	0.2447	0.6799	Strychni Semen	4-hydroxystrychnine	21680048	FALSE	O1C2C3C4N(c5c(C64C4N(CC6)CC(=CC1)C3C4)cccc5O)C(=O)C2
MOL003439	0.3036	0.6964	0.6023	Strychni Semen	7alpha-Hydroxyconessine	Not Available	FALSE	C1C(CC2=CC(C3C(C2(C1)C)CCC12C3CC(C1C(N(C2)C)C)C)O)C(C)C
MOL003440	0.7038	0.2962	0.6071	Strychni Semen	Brucine N-oxide	Not Available	FALSE	c1(c(cc2c(c1)C13C4N2C(=O)CC2C4C4CC3[N+](CC1)(CC4=CCO2)O)OC)OC
MOL003441	0.2717	0.7283	0.7474	Polygoni Avicularis Herba	Chlorogenin	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2O)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)C
MOL003441	0.2717	0.7283	0.7474	Pyrrosiae Folium	Chlorogenin	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2O)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)C
MOL003441	0.2717	0.7283	0.7474	Strychni Semen	Chlorogenin	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2O)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)C
MOL003441	0.2717	0.7283	0.7474	Houttuyniae Herba	Chlorogenin	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2O)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)C
MOL003441	0.2717	0.7283	0.7474	Inulae Flos	Chlorogenin	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2O)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)C
MOL003442	0.8652	0.1348	0.6488	Adenophprae Ae Radix	(+)-Octahydro-4,8,8,9-tetramethyl-1,4-methanoazulen-7(1H)-one	Not Available	FALSE	O=C1C(C2C3C(C(C2CC3)C)(CC1)C)(C)C
MOL003443	0.9212	0.0788	0.9178	Adenophprae Ae Radix	2-Decenal	5354834	FALSE	O=C/C=C\CCCCCCC
MOL003444	0.8587	0.1413	0.7525	Adenophprae Ae Radix	1-(1,5-Dimethyl-4-hexenyl)-4-methyl benzene	Not Available	FALSE	CC(CCC=C(C)C)Cc1ccccc1
MOL003445	0.9046	0.0954	0.8890	Adenophprae Ae Radix	1,1-Diethoxyheptane	69644	FALSE	O(C(OCC)CCCCCC)CC
MOL003446	0.9128	0.0872	0.9144	Adenophprae Ae Radix	1,1-Diethoxyhexane	77224	FALSE	O(C(OCC)CCCCC)CC

MOL003447	0.8710	0.1290	0.8228	Adenophprae Ae Radix	1,1-Diethoxynonane	108625	FALSE	O(C(OCC)CCCCCCCC)CC
MOL003448	0.8687	0.1313	0.8530	Adenophprae Ae Radix	1,1-Diethoxyoctane	101364	FALSE	O(C(OCC)CCCCCCC)CC
MOL003449	0.6969	0.3031	0.6084	Adenophprae Ae Radix	(2S)-2-myristyloxirane	10900762	FALSE	O1C(CCCCCCCCCCCCCC)C1
MOL003450	0.8867	0.1133	0.8672	Coriandri Sativi Herba	dodec-2-enal	5283361	FALSE	C(=O)/C=C/CCCCCCCCC
MOL003450	0.8867	0.1133	0.8672	Citrus Reticulata	dodec-2-enal	5283361	FALSE	C(=O)/C=C/CCCCCCCCC
MOL003450	0.8867	0.1133	0.8672	Adenophprae Ae Radix	dodec-2-enal	5283361	FALSE	C(=O)/C=C/CCCCCCCCC
MOL003452	0.9243	0.0757	0.7370	Adenophprae Ae Radix	1-Ethylidene-1H-indene	Not Available	FALSE	C1=Cc2c(/C/1=C\C)cccc2
MOL003453	0.9321	0.0679	0.9386	Farfarae Flos	ZINC02571348	7021340	FALSE	OC(CCCCCC)C=C
MOL003453	0.9321	0.0679	0.9386	Viticis Negundo Folium	ZINC02571348	7021340	FALSE	OC(CCCCCC)C=C
MOL003453	0.9321	0.0679	0.9386	Adenophprae Ae Radix	ZINC02571348	7021340	FALSE	OC(CCCCCC)C=C
MOL003454	0.9600	0.0400	0.9535	Adenophprae Ae Radix	2-(1,2-Diethoxyethyl)-furan	Not Available	FALSE	o1c(ccc1)C(COCC)OCC
MOL003455	0.9424	0.0576	0.8043	Adenophprae Ae Radix	2,2-Dimethyl-3-(4-methyl-4-pentenyl)-cyclopropanecarboxylic acid	Not Available	FALSE	C1(C(C1CCCC(=C)C)(C)C)C(=O)O
MOL003456	0.8930	0.1070	0.8478	Adenophprae Ae Radix	2,5,5-Trimethyl-3-phenyl-cyclohexanone	Not Available	FALSE	C1(=O)C(C(CC(C1)(C)C)c1ccccc1)C
MOL003459	0.8869	0.1131	0.7132	Adenophprae Ae Radix	2,6,8-Trimethyl-decane	Not Available	FALSE	CC(CCCC(CC(CC)C)C)C
MOL003460	0.9071	0.0929	0.8814	Adenophprae Ae Radix	2-Butyl-2,7-octadien-1-ol	5362707	FALSE	OC/C(=C/CCCC=C)/CCCC
MOL003461	0.9262	0.0738	0.9274	Adenophprae Ae Radix	l-2-Hydroxydecanoic acid	5312797	FALSE	C(C(C(=O)O)O)CCCCCCC

MOL003462	0.8457	0.1543	0.7052	Adenophprae Ae Radix	2-Methylene-6,8,8-trimethyl-tricyclo-[5.2.2.0(1,6)] undecan-3-ol	Not Available	FALSE	C123C(=C)C(CCC1(C(C(C2)(C)C)CC3)C)O
MOL003463	0.9026	0.0974	0.8758	Adenophprae Ae Radix	Undeca-3,4-diene-2,10-dione	538547	FALSE	CC(=O)C=C=CCCCCC(=O)C
MOL003465	0.9280	0.0720	0.9606	Adenophprae Ae Radix	3-Methyl-4-methylene-2-hexanone	Not Available	FALSE	CC(=O)C(C(=C)CC)C
MOL003466	0.9284	0.0716	0.9298	Adenophprae Ae Radix	Methyl 3-nonenoate	5366844	FALSE	C(=C\CC(=O)OC)/CCCCC
MOL003468	0.9332	0.0668	0.9772	Adenophprae Ae Radix	4-Ethylcyclohexanol	78293	FALSE	OC1CCC(CC1)CC
MOL003469	0.9269	0.0731	0.7814	Adenophprae Ae Radix	(E)-4-[(4R)-4-hydroxy-2,6,6-trimethyl-1-cyclohexenyl] but-3-en-2-one	11127505	FALSE	OC1CC(C(=C(C1)C)/C=C/C(=O)C)(C)C
MOL003469	0.9269	0.0731	0.7814	Ginkgo Folium	(E)-4-[(4R)-4-hydroxy-2,6,6-trimethyl-1-cyclohexenyl] but-3-en-2-one	11127505	FALSE	OC1CC(C(=C(C1)C)/C=C/C(=O)C)(C)C
MOL003470	0.5659	0.4341	0.6742	Adenophprae Ae Radix	Methyl 5,8,11-heptadecatriynoate	582271	FALSE	O(C(=O)CCCC#CCC#CCC#CCCCCC)C
MOL003472	0.7259	0.2741	0.6301	Adenophprae Ae Radix	8-Hexadecanol	Not Available	FALSE	OC(CCCCCCCC)CCCCCCC
MOL003473	0.8790	0.1210	0.7429	Adenophprae Ae Radix	Acridone	2015	FALSE	O=c1c2c([nH]c3c1cccc3)cccc2
MOL003474	0.9256	0.0744	0.9276	Adenophprae Ae Radix	4-nonenal	5283337	FALSE	C(=O)CC/C=C/CCCC
MOL003475	0.8799	0.1201	0.6163	Adenophprae Ae Radix	9-Cedranone	Not Available	FALSE	O=C1CC23C(C(C(C2)C1C)(C)C)CCC3C
MOL003476	0.8686	0.1314	0.7095	Adenophprae Ae Radix	Tolan	10390	FALSE	c1(ccccc1)C#Cc1ccccc1

MOL003477	0.6587	0.3413	0.6414	Momordicae Fructus	Butyric acid 2-tridecyl ester	Not Available	FALSE	C(=O)(CCC)OC(C)CCCCCCCCCCC
MOL003477	0.6587	0.3413	0.6414	Adenophprae Ae Radix	Butyric acid 2-tridecyl ester	Not Available	FALSE	C(=O)(CCC)OC(C)CCCCCCCCCCC
MOL003479	0.2872	0.7128	0.7151	Adenophprae Ae Radix	cycloartenol acetate	Not Available	FALSE	O(C1C(C2C3(C4(C(C5(C(C(CC5)C(CCC=C(C)C)C)(CC4)C)C)CC2)C3)CC1)(C)C)C(=O)C
MOL003481	0.9463	0.0537	0.9663	Adenophprae Ae Radix	Lilac aldehyde D	71587756	FALSE	O1C(CCC1(C)C=C)C(C)C=O
MOL003482	0.8967	0.1033	0.8982	Adenophprae Ae Radix	Nona-3,5-dien-2-one	5368916	FALSE	O=C(/C=C/C=C/CCC)C
MOL003483	0.9248	0.0752	0.9227	Adenophprae Ae Radix	Ethyl octoate	7799	FALSE	O(C(=O)CCCCCCC)CC
MOL003483	0.9248	0.0752	0.9227	Chaenomeles Sinensis (Thouin) Koehne	Ethyl octoate	7799	FALSE	O(C(=O)CCCCCCC)CC
MOL003483	0.9248	0.0752	0.9227	Saxifraga Stolonifera	Ethyl octoate	7799	FALSE	O(C(=O)CCCCCCC)CC
MOL003483	0.9248	0.0752	0.9227	Litchi Semen	Ethyl octoate	7799	FALSE	O(C(=O)CCCCCCC)CC
MOL003483	0.9248	0.0752	0.9227	Notoginseng Flos	Ethyl octoate	7799	FALSE	O(C(=O)CCCCCCC)CC
MOL003485	0.2482	0.7518	0.7082	Adenophprae Ae Radix	Phthalic acid, isobutyl undecyl ester	6423494	FALSE	O(C(=O)c1c(C(=O)OCCCCCCCCCCC)cccc1)CC(C)C
MOL003486	0.3190	0.6810	0.7975	Adenophprae Ae Radix	Praeruptorin A	38347612	FALSE	O1C(C(OC(=O)/C(=C\C)/C)C(OC(=O)C)c2c1ccc1c2oc(=O)cc1)(C)C
MOL003487	0.3252	0.6748	0.7338	Cichorii Radix	D-Friedoolean-14-en-3-one	92785	FALSE	O=C1C(C2C(C3C(C4=CCC5(C(C4(CC3)C)CC(CC5)(C)C)C)(CC2)C)(CC1)C)(C)C
MOL003487	0.3252	0.6748	0.7338	Codonopsis Radix	D-Friedoolean-14-en-3-one	92785	FALSE	O=C1C(C2C(C3C(C4=CCC5(C(C4(CC3)C)CC(CC5)(C)C)C)(CC2)C)(CC1)C)(C)C
MOL003487	0.3252	0.6748	0.7338	Ailanthi Cortex	D-Friedoolean-14-en-3-one	92785	FALSE	O=C1C(C2C(C3C(C4=CCC5(C(C4(CC3)C)CC(CC5)(C)C)C)(CC2)C)(CC1)C)(C)C
MOL003487	0.3252	0.6748	0.7338	Adenophprae Ae Radix	D-Friedoolean-14-en-3-one	92785	FALSE	O=C1C(C2C(C3C(C4=CCC5(C(C4(CC3)C)CC(CC5)(C)C)C)(CC2)C)(CC1)C)(C)C
MOL003487	0.3252	0.6748	0.7338	Ailanthi Altissimae Fructus	D-Friedoolean-14-en-3-one	92785	FALSE	O=C1C(C2C(C3C(C4=CCC5(C(C4(CC3)C)CC(CC5)(C)C)C)(CC2)C)(CC1)C)(C)C
MOL003488	0.8890	0.1110	0.8676	Adenophprae Ae Radix	(E)-dodec-5-enal	5362688	FALSE	O=CCCC/C=C/CCCCCC
MOL003489	0.5783	0.4217	0.6114	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(E)-13-Octadecenal	5367670	FALSE	C(=O)CCCCCCCCCCC/C=C/CCCC

MOL003489	0.5783	0.4217	0.6114	Celastri Orbiculati Fructus	(E)-13-Octadecenal	5367670	FALSE	C(=O)CCCCCCCCCCC/C=C/CCCC
MOL003490	0.9033	0.0967	0.8904	Celastri Orbiculati Fructus	5-UNDECEN-4-ONE	5371437	FALSE	CCCC(=O)/C=C/CCCCC
MOL003491	0.9298	0.0702	0.9396	Celastri Orbiculati Fructus	AllOCOPen	31266	FALSE	C(C(=O)OCC=C)CCCC
MOL003492	0.7987	0.2013	0.6238	Celastri Orbiculati Fructus	Lauryl bromide	8919	FALSE	C(CCCCCC)CCCCCBr
MOL003493	0.9283	0.0717	0.7419	Benzoinum	naphthalene	931	FALSE	c12c(cccc1)cccc2
MOL003493	0.9283	0.0717	0.7419	Ginkgo Folium	naphthalene	931	FALSE	c12c(cccc1)cccc2
MOL003493	0.9283	0.0717	0.7419	Rhododendri Daurici Folium	naphthalene	931	FALSE	c12c(cccc1)cccc2
MOL003493	0.9283	0.0717	0.7419	Ranunculi Ternati Radix	naphthalene	931	FALSE	c12c(cccc1)cccc2
MOL003493	0.9283	0.0717	0.7419	Rhizome Of Whiteback Greenbrier	naphthalene	931	FALSE	c12c(cccc1)cccc2
MOL003493	0.9283	0.0717	0.7419	Achyranthis Asperae Herba	naphthalene	931	FALSE	c12c(cccc1)cccc2
MOL003493	0.9283	0.0717	0.7419	Ephedra Herba	naphthalene	931	FALSE	c12c(cccc1)cccc2
MOL003493	0.9283	0.0717	0.7419	Magnoliae Flos	naphthalene	931	FALSE	c12c(cccc1)cccc2
MOL003493	0.9283	0.0717	0.7419	Ginseng Folium	naphthalene	931	FALSE	c12c(cccc1)cccc2
MOL003493	0.9283	0.0717	0.7419	Asari Radix Et Rhizoma	naphthalene	931	FALSE	c12c(cccc1)cccc2
MOL003493	0.9283	0.0717	0.7419	Celastri Orbiculati Fructus	naphthalene	931	FALSE	c12c(cccc1)cccc2
MOL003493	0.9283	0.0717	0.7419	Caryophylliflos	naphthalene	931	FALSE	c12c(cccc1)cccc2
MOL003493	0.9283	0.0717	0.7419	Rhizoma Fagopyri Cymosi	naphthalene	931	FALSE	c12c(cccc1)cccc2
MOL003493	0.9283	0.0717	0.7419	Mori Fructus	naphthalene	931	FALSE	c12c(cccc1)cccc2
MOL003493	0.9283	0.0717	0.7419	Radix Bupleuri	naphthalene	931	FALSE	c12c(cccc1)cccc2
MOL003497	0.3008	0.6992	0.6993	Celastri Orbiculati Fructus	Pristimerin	159516	FALSE	C12(C(C3C(CC2)(CCC(C3)(C(=O)OC)C)C)(CCC2(C1=CC=C1C2=CC(=O)C(=C1C)O)C)C)C
MOL003498	0.9309	0.0691	0.9669	Celastri Orbiculati Fructus	1-ETHYLCYCLOHEXNE	73937	FALSE	C1(=CCCCC1)CC
MOL003499	0.9326	0.0674	0.9662	Celastri Orbiculati Fructus	(6R)-2,2,6-trimethylcyclohexan-1-one	6999893	FALSE	C1(=O)C(CCCC1C)(C)C
MOL003500	0.9375	0.0625	0.9025	Celastri Orbiculati Fructus	Homocyclocitral, beta-	61124	FALSE	C1(=C(CCCC1(C)C)C)CC=O
MOL003501	0.9349	0.0651	0.8038	Lycii Fructus	(2R,4aS,6S,8aR)-2,6-dimethyldecalin	21718045	FALSE	C1C(CCC2CC(CCC12)C)C
MOL003501	0.9349	0.0651	0.8038	Celastri Orbiculati Fructus	(2R,4aS,6S,8aR)-2,6-dimethyldecalin	21718045	FALSE	C1C(CCC2CC(CCC12)C)C

MOL003502	0.8534	0.1466	0.8261	Caryophylliflos	(3R,4S)-3-(4-hydroxy-3-methoxy-benzyl)chroman-3,4,7-triol	13846639	FALSE	c1(ccc2c(c1)OCC(C2O)(Cc1ccc(c(c1)OC)O)O)O
MOL003502	0.8534	0.1466	0.8261	Dianthi Herba	(3R,4S)-3-(4-hydroxy-3-methoxy-benzyl)chroman-3,4,7-triol	13846639	FALSE	c1(ccc2c(c1)OCC(C2O)(Cc1ccc(c(c1)OC)O)O)O
MOL003502	0.8534	0.1466	0.8261	Mori Follum	(3R,4S)-3-(4-hydroxy-3-methoxy-benzyl)chroman-3,4,7-triol	13846639	FALSE	c1(ccc2c(c1)OCC(C2O)(Cc1ccc(c(c1)OC)O)O)O
MOL003503	0.9267	0.0733	0.9498	Ranunculi Ternati Radix	Methyl protocatechuate	287064	FALSE	C(=O)(c1cc(c(cc1)O)O)OC
MOL003503	0.9267	0.0733	0.9498	Trollius Chinensis	Methyl protocatechuate	287064	FALSE	C(=O)(c1cc(c(cc1)O)O)OC
MOL003503	0.9267	0.0733	0.9498	Rhizoma Fagopyri Cymosi	Methyl protocatechuate	287064	FALSE	C(=O)(c1cc(c(cc1)O)O)OC
MOL003503	0.9267	0.0733	0.9498	Dianthi Herba	Methyl protocatechuate	287064	FALSE	C(=O)(c1cc(c(cc1)O)O)OC
MOL003503	0.9267	0.0733	0.9498	Perilla Frutescens	Methyl protocatechuate	287064	FALSE	C(=O)(c1cc(c(cc1)O)O)OC
MOL003504	0.9427	0.0573	0.9519	Dianthi Herba	Tolualdehyde	7725	FALSE	c1(ccc(cc1)C)C=O
MOL003504	0.9427	0.0573	0.9519	Radix Clematidis	Tolualdehyde	7725	FALSE	c1(ccc(cc1)C)C=O
MOL003505	0.9007	0.0993	0.9384	Dianthi Herba	Panosorb	643460	FALSE	C(=O)(/C=C/C=C/C)O
MOL003505	0.9007	0.0993	0.9384	Arecae Semen	Panosorb	643460	FALSE	C(=O)(/C=C/C=C/C)O
MOL003505	0.9007	0.0993	0.9384	Mori Fructus	Panosorb	643460	FALSE	C(=O)(/C=C/C=C/C)O
MOL003506	0.8875	0.1125	0.9471	Eriobotryae Folium	WLN: QR BVO1R	8363	FALSE	C(=O)(c1c(O)cccc1)OCc1ccccc1
MOL003506	0.8875	0.1125	0.9471	Dianthi Herba	WLN: QR BVO1R	8363	FALSE	C(=O)(c1c(O)cccc1)OCc1ccccc1
MOL003507	0.9361	0.0639	0.9534	Rose Rugosae Flos	Heptanol	8129	FALSE	C(CCCCCC)O
MOL003507	0.9361	0.0639	0.9534	Allii Tuberosi Semen	Heptanol	8129	FALSE	C(CCCCCC)O
MOL003507	0.9361	0.0639	0.9534	Ephedra Herba	Heptanol	8129	FALSE	C(CCCCCC)O
MOL003507	0.9361	0.0639	0.9534	Radix Bupleuri	Heptanol	8129	FALSE	C(CCCCCC)O

MOL003507	0.9361	0.0639	0.9534	Dianthi Herba	Heptanol	8129	FALSE	C(CCCCCC)O
MOL003507	0.9361	0.0639	0.9534	Achyranthis Bidentatae Radix	Heptanol	8129	FALSE	C(CCCCCC)O
MOL003508	0.9202	0.0798	0.9218	A. Dahurica (Fisch.) Benth. Et Hook	Antak	8174	FALSE	C(CCCCCCCCC)O
MOL003508	0.9202	0.0798	0.9218	Citrus Reticulata	Antak	8174	FALSE	C(CCCCCCCCC)O
MOL003508	0.9202	0.0798	0.9218	Dianthi Herba	Antak	8174	FALSE	C(CCCCCCCCC)O
MOL003508	0.9202	0.0798	0.9218	Hippophae Fructus	Antak	8174	FALSE	C(CCCCCCCCC)O
MOL003509	0.9325	0.0675	0.9380	Codonopsis Radix	Nonanol	8914	FALSE	C(CCCCCCCC)O
MOL003509	0.9325	0.0675	0.9380	Ginseng Folium	Nonanol	8914	FALSE	C(CCCCCCCC)O
MOL003509	0.9325	0.0675	0.9380	Chaenomeles Sinensis (Thouin) Koehne	Nonanol	8914	FALSE	C(CCCCCCCC)O
MOL003509	0.9325	0.0675	0.9380	Ganoderma	Nonanol	8914	FALSE	C(CCCCCCCC)O
MOL003509	0.9325	0.0675	0.9380	Meliae Azedarach Fructus	Nonanol	8914	FALSE	C(CCCCCCCC)O
MOL003509	0.9325	0.0675	0.9380	Radix Bupleuri	Nonanol	8914	FALSE	C(CCCCCCCC)O
MOL003509	0.9325	0.0675	0.9380	Panacis Quinquefolii Radix	Nonanol	8914	FALSE	C(CCCCCCCC)O
MOL003509	0.9325	0.0675	0.9380	Dianthi Herba	Nonanol	8914	FALSE	C(CCCCCCCC)O
MOL003510	0.7444	0.2556	0.8294	Dianthi Herba	dianoside A	Not Available	FALSE	C1(C(C(C(OC1CO)OC1CCC2(C(C1(C)C(=O)O)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C)C(=O)OC1C(O)C(C(C(O1)CO)O)O)C)C)O)O)O
MOL003511	0.7344	0.2656	0.8125	Dianthi Herba	dianoside A_qt	71719485	FALSE	OC1CCC2(C(C1(C)C(=O)O)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C)C(=O)O)C)C
MOL003512	0.7564	0.2436	0.8140	Dianthi Herba	dianoside E	Not Available	FALSE	C1(C(C(C(OC1CO)OC1CCC2(C(C1(C)C(=O)O)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(CO)C)C(=O)OC1OC(C(C(C1O)O)O)COC1C(O)C(C(C(O1)CC)C)O)C)C)O)O)O
MOL003513	0.7203	0.2797	0.7576	Dianthi Herba	dianoside E_qt	Not Available	FALSE	OC1CCC2(C(C1(C)C(=O)O)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(CO)C)C(=O)O)C)C
MOL003514	0.7569	0.2431	0.8274	Dianthi Herba	dianoside G	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1OC(C(C(C1O)OC1OC(C(C(C1O)O)O)CO)O)COC1C(O)C(C(C(O1)CO)O)O)C)C)C)(C)C(=O)O)O

MOL003515	0.7344	0.2656	0.8125	Dianthi Herba	(3S,4S,4aR,6aR,6bS,8aS,12aS,14aR,14bR)-3-hydroxy-4,6a,6b,11,11,14b-hexamethyl-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydropicene-4,8a-dicarboxylic acid	15560324	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C(=O)O)O
MOL003516	0.9219	0.0781	0.9483	Dianthi Herba	ZINC00896812	6971127	FALSE	CC(CCC=C(C)C)O
MOL003516	0.9219	0.0781	0.9483	Ardisiae Japonicae Herba	ZINC00896812	6971127	FALSE	CC(CCC=C(C)C)O
MOL003517	0.9193	0.0807	0.8984	Drynariae Rhizoma	Dianthoside	5316639	FALSE	c1(c(c(=O)cco1)OC1C(O)C(O)C(O)C(O1)CO)C
MOL003517	0.9193	0.0807	0.8984	Dianthi Herba	Dianthoside	5316639	FALSE	c1(c(c(=O)cco1)OC1C(O)C(O)C(O)C(O1)CO)C
MOL003518	0.9092	0.0908	0.9748	Epimrdii Herba	Vetol	8369	FALSE	c1(c(c(=O)cco1)O)C
MOL003518	0.9092	0.0908	0.9748	Drynariae Rhizoma	Vetol	8369	FALSE	c1(c(c(=O)cco1)O)C
MOL003518	0.9092	0.0908	0.9748	Fructussophorae	Vetol	8369	FALSE	c1(c(c(=O)cco1)O)C
MOL003518	0.9092	0.0908	0.9748	Bolbostemae Paniculati Bulbus	Vetol	8369	FALSE	c1(c(c(=O)cco1)O)C
MOL003518	0.9092	0.0908	0.9748	Sophorae Tonkinensis Radix Et Rhizome	Vetol	8369	FALSE	c1(c(c(=O)cco1)O)C
MOL003518	0.9092	0.0908	0.9748	Ginsen Radix Et Rhizoma Rubra	Vetol	8369	FALSE	c1(c(c(=O)cco1)O)C
MOL003518	0.9092	0.0908	0.9748	Dianthi Herba	Vetol	8369	FALSE	c1(c(c(=O)cco1)O)C
MOL003519	0.9220	0.0780	0.9333	Schisandrae Chinensis Fructus	(E)-oct-2-en-4-one	5365891	FALSE	C(=C\C(=O)CCCC)/C
MOL003519	0.9220	0.0780	0.9333	Ephedra Herba	(E)-oct-2-en-4-one	5365891	FALSE	C(=C\C(=O)CCCC)/C
MOL003519	0.9220	0.0780	0.9333	Dianthi Herba	(E)-oct-2-en-4-one	5365891	FALSE	C(=C\C(=O)CCCC)/C
MOL003520	0.9315	0.0685	0.7970	Mahoniae Folum	Damascenone	5366074	FALSE	C1(=C(C=CCC1(C)C)C)C(=O)/C=C/C
MOL003520	0.9315	0.0685	0.7970	Campsis Flos	Damascenone	5366074	FALSE	C1(=C(C=CCC1(C)C)C)C(=O)/C=C/C
MOL003520	0.9315	0.0685	0.7970	Lysimachiae Foenigraeci Herba	Damascenone	5366074	FALSE	C1(=C(C=CCC1(C)C)C)C(=O)/C=C/C
MOL003520	0.9315	0.0685	0.7970	Eucommiae Folium	Damascenone	5366074	FALSE	C1(=C(C=CCC1(C)C)C)C(=O)/C=C/C
MOL003520	0.9315	0.0685	0.7970	Radix Cynanchi Paniculati	Damascenone	5366074	FALSE	C1(=C(C=CCC1(C)C)C)C(=O)/C=C/C
MOL003520	0.9315	0.0685	0.7970	Dianthi Herba	Damascenone	5366074	FALSE	C1(=C(C=CCC1(C)C)C)C(=O)/C=C/C

MOL003520	0.9315	0.0685	0.7970	Fructus Ligustri Lucidi	Damascenone	5366074	FALSE	C1(=C(C=CCC1(C)C)C)C(=O)/C=C/C
MOL003520	0.9315	0.0685	0.7970	Ephedra Herba	Damascenone	5366074	FALSE	C1(=C(C=CCC1(C)C)C)C(=O)/C=C/C
MOL003520	0.9315	0.0685	0.7970	Apocyniveneti Folium	Damascenone	5366074	FALSE	C1(=C(C=CCC1(C)C)C)C(=O)/C=C/C
MOL003520	0.9315	0.0685	0.7970	Epimrdii Herba	Damascenone	5366074	FALSE	C1(=C(C=CCC1(C)C)C)C(=O)/C=C/C
MOL003521	0.9651	0.0349	0.9300	Folium Artemisiae Argyi	Isohomogenol	637776	FALSE	c1(c(ccc(c1)/C=C/C)OC)OC
MOL003521	0.9651	0.0349	0.9300	Cinnanmomi Cortex	Isohomogenol	637776	FALSE	c1(c(ccc(c1)/C=C/C)OC)OC
MOL003521	0.9651	0.0349	0.9300	Gossampiniflos	Isohomogenol	637776	FALSE	c1(c(ccc(c1)/C=C/C)OC)OC
MOL003521	0.9651	0.0349	0.9300	Myristicae Semen	Isohomogenol	637776	FALSE	c1(c(ccc(c1)/C=C/C)OC)OC
MOL003521	0.9651	0.0349	0.9300	Rhizome Of Whiteback Greenbrier	Isohomogenol	637776	FALSE	c1(c(ccc(c1)/C=C/C)OC)OC
MOL003521	0.9651	0.0349	0.9300	Acoritataninowii Rhizoma	Isohomogenol	637776	FALSE	c1(c(ccc(c1)/C=C/C)OC)OC
MOL003523	0.7114	0.2886	0.6528	Cinnanmomi Cortex	hexadec-11-enal	5283376	FALSE	C(=O)CCCCCCCCC/C=C/CCCC
MOL003524	0.9291	0.0709	0.9466	Cinnanmomi Cortex	Benzenepropanol	31234	FALSE	c1(ccccc1)CCCO
MOL003525	0.9460	0.0540	0.9170	Ephedra Herba	Pyruvophenone	11363	FALSE	c1(C(=O)C(=O)C)ccccc1
MOL003525	0.9460	0.0540	0.9170	Cinnamomi Ramulus	Pyruvophenone	11363	FALSE	c1(C(=O)C(=O)C)ccccc1
MOL003525	0.9460	0.0540	0.9170	Benzoinum	Pyruvophenone	11363	FALSE	c1(C(=O)C(=O)C)ccccc1
MOL003525	0.9460	0.0540	0.9170	Cinnanmomi Cortex	Pyruvophenone	11363	FALSE	c1(C(=O)C(=O)C)ccccc1
MOL003526	0.9287	0.0713	0.9216	Mume Flos	Cinnamyl acetate	5282110	FALSE	c1(/C=C/COC(=O)C)ccccc1
MOL003526	0.9287	0.0713	0.9216	Cinnamomi Ramulus	Cinnamyl acetate	5282110	FALSE	c1(/C=C/COC(=O)C)ccccc1
MOL003526	0.9287	0.0713	0.9216	Cinnanmomi Cortex	Cinnamyl acetate	5282110	FALSE	c1(/C=C/COC(=O)C)ccccc1
MOL003526	0.9287	0.0713	0.9216	Styrax	Cinnamyl acetate	5282110	FALSE	c1(/C=C/COC(=O)C)ccccc1
MOL003526	0.9287	0.0713	0.9216	Magnolia Officinalis Rehd Et Wils.	Cinnamyl acetate	5282110	FALSE	c1(/C=C/COC(=O)C)ccccc1
MOL003527	0.9225	0.0775	0.9438	Litchi Semen	Tyranton	31256	FALSE	C(CC(=O)C)(C)(C)O
MOL003527	0.9225	0.0775	0.9438	Chaenomeles Sinensis (Thouin) Koehne	Tyranton	31256	FALSE	C(CC(=O)C)(C)(C)O
MOL003527	0.9225	0.0775	0.9438	Cornus Officinalis Sieb. Et Zucc.	Tyranton	31256	FALSE	C(CC(=O)C)(C)(C)O
MOL003527	0.9225	0.0775	0.9438	Cinnanmomi Cortex	Tyranton	31256	FALSE	C(CC(=O)C)(C)(C)O
MOL003527	0.9225	0.0775	0.9438	Raphani Semen	Tyranton	31256	FALSE	C(CC(=O)C)(C)(C)O
MOL003528	0.9566	0.0434	0.7422	Eucommiae Folium	METHYLBENZOFURAN	20263	FALSE	c12c(oc(c1)C)cccc2

MOL003528	0.9566	0.0434	0.7422	Arisaematis Rhizoma	METHYLBENZOFURAN	20263	FALSE	c12c(oc(c1)C)cccc2
MOL003528	0.9566	0.0434	0.7422	Morindae Officinalis Radix	METHYLBENZOFURAN	20263	FALSE	c12c(oc(c1)C)cccc2
MOL003528	0.9566	0.0434	0.7422	Cinnanmomi Cortex	METHYLBENZOFURAN	20263	FALSE	c12c(oc(c1)C)cccc2
MOL003529	0.9379	0.0621	0.9214	Ephedra Herba	m-Methylacetophenone	11455	FALSE	c1(cc(ccc1)C)C(=O)C
MOL003529	0.9379	0.0621	0.9214	Cinnanmomi Cortex	m-Methylacetophenone	11455	FALSE	c1(cc(ccc1)C)C(=O)C
MOL003529	0.9379	0.0621	0.9214	Ginkgo Folium	m-Methylacetophenone	11455	FALSE	c1(cc(ccc1)C)C(=O)C
MOL003530	0.9598	0.0402	0.9334	Cinnamomi Ramulus	O-METHOXYCINNAMALDEHYDE	641298	FALSE	c1(c(cccc1)OC)/C=C/C=O
MOL003530	0.9598	0.0402	0.9334	Cinnanmomi Cortex	O-METHOXYCINNAMALDEHYDE	641298	FALSE	c1(c(cccc1)OC)/C=C/C=O
MOL003531	0.9660	0.0340	0.9405	Cinnanmomi Cortex	3-methoxycinnamaldehyde	20979959	FALSE	c1(cccc(c1)/C=C\C=O)OC
MOL003532	0.9597	0.0403	0.9566	Cinnanmomi Cortex	(1R)-1-(4-methylphenyl)ethanol	6999807	FALSE	c1(C(C)O)ccc(cc1)C
MOL003532	0.9597	0.0403	0.9566	Curcumae Radix	(1R)-1-(4-methylphenyl)ethanol	6999807	FALSE	c1(C(C)O)ccc(cc1)C
MOL003533	0.8520	0.1480	0.6840	Cinnanmomi Cortex	Bicyclo[4.4.0]dec-1-ene,2-isopropy-5-methyl-9-methylene-	Not Available	FALSE	C12=C(CCC(C1CCC(=C)C2)C)C(C)C
MOL003533	0.8520	0.1480	0.6840	Perillae Fructus	Bicyclo[4.4.0]dec-1-ene,2-isopropy-5-methyl-9-methylene-	Not Available	FALSE	C12=C(CCC(C1CCC(=C)C2)C)C(C)C
MOL003534	0.8568	0.1432	0.6274	Citri Grandis Exocarpium	CADINENE	10657	FALSE	C12C(C(=CCC1C(C)C)C)CC=C(C2)C

MOL003534	0.8568	0.1432	0.6274	Cinnanmomi Cortex	CADINENE	10657	FALSE	C12C(C(=CCC1C(C)C)C)CC=C(C2)C
MOL003534	0.8568	0.1432	0.6274	Alpiniae Officinarum Rhizome	CADINENE	10657	FALSE	C12C(C(=CCC1C(C)C)C)CC=C(C2)C
MOL003534	0.8568	0.1432	0.6274	Ligustici Rhizoma Et Radix	CADINENE	10657	FALSE	C12C(C(=CCC1C(C)C)C)CC=C(C2)C
MOL003534	0.8568	0.1432	0.6274	Acoritataninowii Rhizoma	CADINENE	10657	FALSE	C12C(C(=CCC1C(C)C)C)CC=C(C2)C
MOL003534	0.8568	0.1432	0.6274	Litseae Fructus	CADINENE	10657	FALSE	C12C(C(=CCC1C(C)C)C)CC=C(C2)C
MOL003534	0.8568	0.1432	0.6274	Cyperi Rhizoma	CADINENE	10657	FALSE	C12C(C(=CCC1C(C)C)C)CC=C(C2)C
MOL003534	0.8568	0.1432	0.6274	Curcumae Radix	CADINENE	10657	FALSE	C12C(C(=CCC1C(C)C)C)CC=C(C2)C
MOL003534	0.8568	0.1432	0.6274	Zanthoxyli Pericarpium	CADINENE	10657	FALSE	C12C(C(=CCC1C(C)C)C)CC=C(C2)C
MOL003534	0.8568	0.1432	0.6274	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	CADINENE	10657	FALSE	C12C(C(=CCC1C(C)C)C)CC=C(C2)C
MOL003534	0.8568	0.1432	0.6274	Angelicae Sinensis Radix	CADINENE	10657	FALSE	C12C(C(=CCC1C(C)C)C)CC=C(C2)C
MOL003534	0.8568	0.1432	0.6274	Eriobotryae Folium	CADINENE	10657	FALSE	C12C(C(=CCC1C(C)C)C)CC=C(C2)C
MOL003534	0.8568	0.1432	0.6274	Solidaginis Herba	CADINENE	10657	FALSE	C12C(C(=CCC1C(C)C)C)CC=C(C2)C
MOL003534	0.8568	0.1432	0.6274	Schizonepetae Spica	CADINENE	10657	FALSE	C12C(C(=CCC1C(C)C)C)CC=C(C2)C
MOL003535	0.9159	0.0841	0.7128	Magnolia Officinalis Rehd Et Wils.	1,1,6-trimethyl-2H-naphthalene	121677	FALSE	C1=Cc2c(C(C1)(C)C)ccc(c2)C
MOL003535	0.9159	0.0841	0.7128	Cinnanmomi Cortex	1,1,6-trimethyl-2H-naphthalene	121677	FALSE	C1=Cc2c(C(C1)(C)C)ccc(c2)C
MOL003535	0.9159	0.0841	0.7128	Lycii Fructus	1,1,6-trimethyl-2H-naphthalene	121677	FALSE	C1=Cc2c(C(C1)(C)C)ccc(c2)C
MOL003535	0.9159	0.0841	0.7128	Lysimachiae Foenigraeci Herba	1,1,6-trimethyl-2H-naphthalene	121677	FALSE	C1=Cc2c(C(C1)(C)C)ccc(c2)C
MOL003536	0.8265	0.1735	0.6775	Bidentis Bipinnatae Herba	T-Cadinol	160799	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C
MOL003536	0.8265	0.1735	0.6775	Cinnanmomi Cortex	T-Cadinol	160799	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C
MOL003536	0.8265	0.1735	0.6775	Dichroae Radix	T-Cadinol	160799	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C
MOL003536	0.8265	0.1735	0.6775	Tamaricis Cacumen	T-Cadinol	160799	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C
MOL003537	0.8265	0.1735	0.6775	Zanthoxyli Pericarpium	T-Muurolol	3084331	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C
MOL003537	0.8265	0.1735	0.6775	Schisandrae Chinensis Fructus	T-Muurolol	3084331	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C
MOL003537	0.8265	0.1735	0.6775	Cinnamomi Ramulus	T-Muurolol	3084331	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C
MOL003537	0.8265	0.1735	0.6775	Viticis Fructus	T-Muurolol	3084331	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C
MOL003537	0.8265	0.1735	0.6775	Solidaginis Herba	T-Muurolol	3084331	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C
MOL003537	0.8265	0.1735	0.6775	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	T-Muurolol	3084331	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C
MOL003537	0.8265	0.1735	0.6775	Ailanthi Cortex	T-Muurolol	3084331	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C
MOL003537	0.8265	0.1735	0.6775	Momordicae Fructus	T-Muurolol	3084331	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C

MOL003537	0.8265	0.1735	0.6775	Cynanchistauntonii Rhizoma Et Radix	T-Muurolol	3084331	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C
MOL003537	0.8265	0.1735	0.6775	Notoginseng Flos	T-Muurolol	3084331	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C
MOL003537	0.8265	0.1735	0.6775	Bidentis Bipinnatae Herba	T-Muurolol	3084331	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C
MOL003537	0.8265	0.1735	0.6775	Cinnanmomi Cortex	T-Muurolol	3084331	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C
MOL003537	0.8265	0.1735	0.6775	Cayratiae Japonicae Herba	T-Muurolol	3084331	FALSE	C1(CCC(C2C=C(CCC12)C)C(C)C)(O)C
MOL003539	0.9137	0.0863	0.9593	Acoritataninowii Rhizoma	(E)-2-propenoic acid,3-(3-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl),methyl ester	Not Available	FALSE	OC1CCC(C(=C1C)/C=C/C(=O)OC)(C)C
MOL003540	0.9283	0.0717	0.7807	Acoritataninowii Rhizoma	(1R)-Camphor-10-sulfonic acid	5771688	FALSE	C12(C(C(CC1=O)CC2)(C)C)CS(=O)(=O)O
MOL003541	0.8318	0.1682	0.6026	Cinnamomi Ramulus	()-alpha-Longipinene	Not Available	FALSE	C12C3C(C1(CCCC3(C)C)C)CC=C2C
MOL003541	0.8318	0.1682	0.6026	Capsici Fructus	()-alpha-Longipinene	Not Available	FALSE	C12C3C(C1(CCCC3(C)C)C)CC=C2C
MOL003541	0.8318	0.1682	0.6026	Magnolia Officinalis Rehd Et Wils.	()-alpha-Longipinene	Not Available	FALSE	C12C3C(C1(CCCC3(C)C)C)CC=C2C
MOL003541	0.8318	0.1682	0.6026	Cnidii Fructus	()-alpha-Longipinene	Not Available	FALSE	C12C3C(C1(CCCC3(C)C)C)CC=C2C
MOL003541	0.8318	0.1682	0.6026	Aucklandiae Radix	()-alpha-Longipinene	Not Available	FALSE	C12C3C(C1(CCCC3(C)C)C)CC=C2C
MOL003541	0.8318	0.1682	0.6026	Acoritataninowii Rhizoma	()-alpha-Longipinene	Not Available	FALSE	C12C3C(C1(CCCC3(C)C)C)CC=C2C
MOL003541	0.8318	0.1682	0.6026	Schisandrae Chinensis Fructus	()-alpha-Longipinene	Not Available	FALSE	C12C3C(C1(CCCC3(C)C)C)CC=C2C
MOL003542	0.5621	0.4379	0.6387	Radix Euphorbiae Pekinensis	8-Isopentenyl-kaempferol	5318624	FALSE	c1(c(O)c(=O)c2c(O)cc(O)c(c2o1)CC=C(C)C)c1ccc(O)cc1
MOL003542	0.5621	0.4379	0.6387	Acoritataninowii Rhizoma	8-Isopentenyl-kaempferol	5318624	FALSE	c1(c(O)c(=O)c2c(O)cc(O)c(c2o1)CC=C(C)C)c1ccc(O)cc1
MOL003542	0.5621	0.4379	0.6387	Semen Pharbitidis	8-Isopentenyl-kaempferol	5318624	FALSE	c1(c(O)c(=O)c2c(O)cc(O)c(c2o1)CC=C(C)C)c1ccc(O)cc1

MOL003542	0.5621	0.4379	0.6387	Epimrdii Herba	8-Isopentenyl-kaempferol	5318624	FALSE	c1(c(O)c(=O)c2c(O)cc(O)c(c2o1)CC=C(C)C)c1ccc(O)cc1
MOL003542	0.5621	0.4379	0.6387	Sophorae Flavescentis Radix	8-Isopentenyl-kaempferol	5318624	FALSE	c1(c(O)c(=O)c2c(O)cc(O)c(c2o1)CC=C(C)C)c1ccc(O)cc1
MOL003542	0.5621	0.4379	0.6387	Cyperi Rhizoma	8-Isopentenyl-kaempferol	5318624	FALSE	c1(c(O)c(=O)c2c(O)cc(O)c(c2o1)CC=C(C)C)c1ccc(O)cc1
MOL003543	0.8782	0.1218	0.7591	Acoritataninowii Rhizoma	Aminacrin	7019	FALSE	c12c(c(c3c(n1)cccc3)N)cccc2
MOL003544	0.9630	0.0370	0.8512	Acoritataninowii Rhizoma	Acoramone	3083746	FALSE	O(c1c(CC(=O)C)cc(OC)c(OC)c1)C
MOL003545	0.8470	0.1530	0.6094	Aristolochiae Fructus	aristolene	12309878	FALSE	C12C(C1CC=C1C2(C(CCC1)C)C)(C)C
MOL003545	0.8470	0.1530	0.6094	Peucedanidecursivi Radix	aristolene	12309878	FALSE	C12C(C1CC=C1C2(C(CCC1)C)C)(C)C
MOL003545	0.8470	0.1530	0.6094	Acoritataninowii Rhizoma	aristolene	12309878	FALSE	C12C(C1CC=C1C2(C(CCC1)C)C)(C)C
MOL003545	0.8470	0.1530	0.6094	Peucedani Radix	aristolene	12309878	FALSE	C12C(C1CC=C1C2(C(CCC1)C)C)(C)C
MOL003546	0.8698	0.1302	0.7281	Aristolochiae Fructus	Aristolone	165536	FALSE	O=C1C2C(C2(C)C)C2(C(CCCC2=C1)C)C
MOL003546	0.8698	0.1302	0.7281	Cornus Officinalis Sieb. Et Zucc.	Aristolone	165536	FALSE	O=C1C2C(C2(C)C)C2(C(CCCC2=C1)C)C
MOL003546	0.8698	0.1302	0.7281	Schisandrae Chinensis Fructus	Aristolone	165536	FALSE	O=C1C2C(C2(C)C)C2(C(CCCC2=C1)C)C
MOL003546	0.8698	0.1302	0.7281	Pogostemon Cablin (Blanco) Benth.	Aristolone	165536	FALSE	O=C1C2C(C2(C)C)C2(C(CCCC2=C1)C)C
MOL003546	0.8698	0.1302	0.7281	Achyranthis Asperae Herba	Aristolone	165536	FALSE	O=C1C2C(C2(C)C)C2(C(CCCC2=C1)C)C
MOL003546	0.8698	0.1302	0.7281	Cyperi Rhizoma	Aristolone	165536	FALSE	O=C1C2C(C2(C)C)C2(C(CCCC2=C1)C)C
MOL003546	0.8698	0.1302	0.7281	A. Dahurica (Fisch.) Benth. Et Hook	Aristolone	165536	FALSE	O=C1C2C(C2(C)C)C2(C(CCCC2=C1)C)C
MOL003546	0.8698	0.1302	0.7281	Acoritataninowii Rhizoma	Aristolone	165536	FALSE	O=C1C2C(C2(C)C)C2(C(CCCC2=C1)C)C
MOL003547	0.9590	0.0410	0.8520	Dichroae Radix	Azaron	636822	FALSE	c1(c(cc(c(c1)/C=C/C)OC)OC)OC
MOL003547	0.9590	0.0410	0.8520	Gossampiniflos	Azaron	636822	FALSE	c1(c(cc(c(c1)/C=C/C)OC)OC)OC
MOL003547	0.9590	0.0410	0.8520	Magnoliae Flos	Azaron	636822	FALSE	c1(c(cc(c(c1)/C=C/C)OC)OC)OC
MOL003547	0.9590	0.0410	0.8520	Arisaematis Rhizoma	Azaron	636822	FALSE	c1(c(cc(c(c1)/C=C/C)OC)OC)OC
MOL003547	0.9590	0.0410	0.8520	Alpiniae Oxyphyliae Fructus	Azaron	636822	FALSE	c1(c(cc(c(c1)/C=C/C)OC)OC)OC
MOL003547	0.9590	0.0410	0.8520	Cornus Officinalis Sieb. Et Zucc.	Azaron	636822	FALSE	c1(c(cc(c(c1)/C=C/C)OC)OC)OC
MOL003547	0.9590	0.0410	0.8520	Asari Radix Et Rhizoma	Azaron	636822	FALSE	c1(c(cc(c(c1)/C=C/C)OC)OC)OC
MOL003547	0.9590	0.0410	0.8520	Acoritataninowii Rhizoma	Azaron	636822	FALSE	c1(c(cc(c(c1)/C=C/C)OC)OC)OC
MOL003547	0.9590	0.0410	0.8520	Fructus Carotae	Azaron	636822	FALSE	c1(c(cc(c(c1)/C=C/C)OC)OC)OC
MOL003547	0.9590	0.0410	0.8520	Epimrdii Herba	Azaron	636822	FALSE	c1(c(cc(c(c1)/C=C/C)OC)OC)OC
MOL003547	0.9590	0.0410	0.8520	Lycii Fructus	Azaron	636822	FALSE	c1(c(cc(c(c1)/C=C/C)OC)OC)OC
MOL003549	0.9599	0.0401	0.8599	Acoritataninowii Rhizoma	gamma-Asarone	636750	FALSE	c1(c(cc(c(c1)OC)CC=C)OC)OC

MOL003549	0.9599	0.0401	0.8599	Gossampiniflos	gamma-Asarone	636750	FALSE	c1(c(cc(c(c1)OC)CC=C)OC)OC
MOL003550	0.9416	0.0584	0.9606	Acoritataninowii Rhizoma	WLN: G1R	7503	FALSE	c1(ccccc1)CCl
MOL003552	0.9484	0.0516	0.9618	Acoritataninowii Rhizoma	Cyclite	7498	FALSE	c1(ccccc1)CBr
MOL003553	0.9111	0.0889	0.7617	Acoritataninowii Rhizoma	Calamendiol	Not Available	FALSE	OC12C(C(O)(CC=C1C(C)C)C)CCC(=C)C2
MOL003554	0.9573	0.0427	0.8981	Litseae Fructus	Gazarin	20525	FALSE	C(=O)c1c(cc(c(c1)OC)OC)OC
MOL003554	0.9573	0.0427	0.8981	Fructus Carotae	Gazarin	20525	FALSE	C(=O)c1c(cc(c(c1)OC)OC)OC
MOL003554	0.9573	0.0427	0.8981	Acoritataninowii Rhizoma	Gazarin	20525	FALSE	C(=O)c1c(cc(c(c1)OC)OC)OC
MOL003555	0.9651	0.0349	0.9300	Acoritataninowii Rhizoma	Methyl isoeugenol	1549045	FALSE	O(c1c(OC)ccc(c1)/C=C\C)C
MOL003556	0.8526	0.1474	0.6851	Acoritataninowii Rhizoma	δ-cadinene	12306059	FALSE	C1(C2C(=C(CC1)C)CCC(=C2)C)C(C)C
MOL003557	0.8009	0.1991	0.6810	Cyperi Rhizoma	()-Valencene	11160025	FALSE	C12(C(CCC=C2CCC(C1)C(=C)C)C)C
MOL003557	0.8009	0.1991	0.6810	Acoritataninowii Rhizoma	()-Valencene	11160025	FALSE	C12(C(CCC=C2CCC(C1)C(=C)C)C)C
MOL003557	0.8009	0.1991	0.6810	Santalum Album L.	()-Valencene	11160025	FALSE	C12(C(CCC=C2CCC(C1)C(=C)C)C)C
MOL003557	0.8009	0.1991	0.6810	Ailanthi Cortex	()-Valencene	11160025	FALSE	C12(C(CCC=C2CCC(C1)C(=C)C)C)C
MOL003558	0.9356	0.0644	0.8759	Acoritataninowii Rhizoma	Asaronic acid	10276	FALSE	c1(c(cc(c(c1)OC)OC)OC)C(=O)O
MOL003559	0.8297	0.1703	0.7702	Acoritataninowii Rhizoma	gramenone	Not Available	FALSE	C1(=O)C(=CCC2(CCC(CC12)C)C)C(C)C
MOL003560	0.8720	0.1280	0.7298	Acoritataninowii Rhizoma	Isocalamendiol	Not Available	FALSE	OC12C(C(O)(CCC1C(C)C)C)CCC(=C)C2
MOL003561	0.8969	0.1031	0.7556	Selaginella Doederleinii Hieron	isopimpinellin	68079	FALSE	c12c(c(c3c(c1OC)occ3)OC)ccc(=O)o2
MOL003561	0.8969	0.1031	0.7556	Radix Angelicae Biseratae	isopimpinellin	68079	FALSE	c12c(c(c3c(c1OC)occ3)OC)ccc(=O)o2
MOL003561	0.8969	0.1031	0.7556	Zanthoxylum Nitidum	isopimpinellin	68079	FALSE	c12c(c(c3c(c1OC)occ3)OC)ccc(=O)o2
MOL003561	0.8969	0.1031	0.7556	Saussureae Involucratae Herba	isopimpinellin	68079	FALSE	c12c(c(c3c(c1OC)occ3)OC)ccc(=O)o2
MOL003561	0.8969	0.1031	0.7556	Acoritataninowii Rhizoma	isopimpinellin	68079	FALSE	c12c(c(c3c(c1OC)occ3)OC)ccc(=O)o2
MOL003561	0.8969	0.1031	0.7556	Peucedani Radix	isopimpinellin	68079	FALSE	c12c(c(c3c(c1OC)occ3)OC)ccc(=O)o2
MOL003561	0.8969	0.1031	0.7556	Aurantii Fructus Immaturus	isopimpinellin	68079	FALSE	c12c(c(c3c(c1OC)occ3)OC)ccc(=O)o2
MOL003561	0.8969	0.1031	0.7556	Portulacae Herba	isopimpinellin	68079	FALSE	c12c(c(c3c(c1OC)occ3)OC)ccc(=O)o2
MOL003563	0.8765	0.1235	0.6884	Acoritataninowii Rhizoma	Isoshyobunone	5318673	FALSE	C1(=O)C(=C(C)C)C(CCC1C(C)C)(C)C=C
MOL003564	0.9430	0.0570	0.8934	Acoritataninowii Rhizoma	(E)-3-(2,4-dimethylphenyl)acrylic acid	13809865	FALSE	c1(c(cc(cc1)C)C)/C=C/C(=O)O
MOL003566	0.8759	0.1241	0.7500	Acoritataninowii Rhizoma	Murolan-3,9(11)-diene-10-peroxy	Not Available	FALSE	O(O)C1C2C(C(C=CC2C(C)C)C)CCC1=C
MOL003567	0.9468	0.0532	0.9447	Acoritataninowii Rhizoma	Diethylbenzylamine	61211	FALSE	c1(CN(CC)CC)ccccc1

MOL003569	0.9075	0.0925	0.8096	Acoritataninowii Rhizoma	3,5,8-trihydroxy-2-(4-hydroxyphenyl)-7-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-chromone	21626477	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(O)c2oc(c(O)c(=O)c2c(O)c1)c1ccc(O)cc1)C
MOL003570	0.8705	0.1295	0.6791	Acoritataninowii Rhizoma	Epishyobunone	5317120	FALSE	O=C1C(CCC(C1C(=C)C)(C)C=C)C(C)C
MOL003571	0.8895	0.1105	0.6520	Zanthoxyli Pericarpium	spathulenol	13854256	FALSE	OC1(C2C3C(C3CCC(=C)C2CC1)(C)C)C
MOL003571	0.8895	0.1105	0.6520	Acoritataninowii Rhizoma	spathulenol	13854256	FALSE	OC1(C2C3C(C3CCC(=C)C2CC1)(C)C)C
MOL003571	0.8895	0.1105	0.6520	Humulus Scandens (Lour.) Merr.	spathulenol	13854256	FALSE	OC1(C2C3C(C3CCC(=C)C2CC1)(C)C)C
MOL003571	0.8895	0.1105	0.6520	Rhododendri Daurici Folium	spathulenol	13854256	FALSE	OC1(C2C3C(C3CCC(=C)C2CC1)(C)C)C
MOL003571	0.8895	0.1105	0.6520	Ginsen Radix Et Rhizoma Rubra	spathulenol	13854256	FALSE	OC1(C2C3C(C3CCC(=C)C2CC1)(C)C)C
MOL003571	0.8895	0.1105	0.6520	Ginkgo Folium	spathulenol	13854256	FALSE	OC1(C2C3C(C3CCC(=C)C2CC1)(C)C)C
MOL003572	0.8905	0.1095	0.8395	Acoritataninowii Rhizoma	ZINC01849758	1616126	FALSE	OC(C1CCC(=CC1)C)(CCC=C(C)C)C
MOL003572	0.8905	0.1095	0.8395	Citri Sarcodactylis Fructus	ZINC01849758	1616126	FALSE	OC(C1CCC(=CC1)C)(CCC=C(C)C)C
MOL003573	0.8621	0.1379	0.6441	Curcumae Radix	calacorene	12302243	FALSE	C1(C(C)C)CC=C(c2c1cc(cc2)C)C
MOL003573	0.8621	0.1379	0.6441	Ephedra Herba	calacorene	12302243	FALSE	C1(C(C)C)CC=C(c2c1cc(cc2)C)C
MOL003573	0.8621	0.1379	0.6441	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	calacorene	12302243	FALSE	C1(C(C)C)CC=C(c2c1cc(cc2)C)C
MOL003573	0.8621	0.1379	0.6441	Acoritataninowii Rhizoma	calacorene	12302243	FALSE	C1(C(C)C)CC=C(c2c1cc(cc2)C)C
MOL003573	0.8621	0.1379	0.6441	Ailanthi Cortex	calacorene	12302243	FALSE	C1(C(C)C)CC=C(c2c1cc(cc2)C)C
MOL003573	0.8621	0.1379	0.6441	Radix Bupleuri	calacorene	12302243	FALSE	C1(C(C)C)CC=C(c2c1cc(cc2)C)C
MOL003573	0.8621	0.1379	0.6441	Cornus Officinalis Sieb. Et Zucc.	calacorene	12302243	FALSE	C1(C(C)C)CC=C(c2c1cc(cc2)C)C
MOL003573	0.8621	0.1379	0.6441	Mahoniae Caulis	calacorene	12302243	FALSE	C1(C(C)C)CC=C(c2c1cc(cc2)C)C
MOL003573	0.8621	0.1379	0.6441	Ardisiae Japonicae Herba	calacorene	12302243	FALSE	C1(C(C)C)CC=C(c2c1cc(cc2)C)C

MOL003576	0.2663	0.7337	0.6910	Acoritataninowii Rhizoma	(1R,3aS,4R,6aS)-1,4-bis(3,4-dimethoxyphenyl)-1,3,3a,4,6,6a-hexahydrofuro[4,3-c]furan	325601	FALSE	C12C(C(OC2)c2cc(c(cc2)OC)OC)COC1c1cc(c(cc1)OC)OC
MOL003578	0.3361	0.6639	0.7070	Millettiae Speciosae Radix	Cycloartenol	Not Available	FALSE	C123C4(C2)C(C(C(CC4)O)(C)C)CCC1C1(C(CC3)(C(CC1)C(CCC=C(C)C)C)C)C
MOL003578	0.3361	0.6639	0.7070	Semen Lini	Cycloartenol	Not Available	FALSE	C123C4(C2)C(C(C(CC4)O)(C)C)CCC1C1(C(CC3)(C(CC1)C(CCC=C(C)C)C)C)C
MOL003578	0.3361	0.6639	0.7070	Broussonetiae Fructus	Cycloartenol	Not Available	FALSE	C123C4(C2)C(C(C(CC4)O)(C)C)CCC1C1(C(CC3)(C(CC1)C(CCC=C(C)C)C)C)C
MOL003578	0.3361	0.6639	0.7070	Lycii Fructus	Cycloartenol	Not Available	FALSE	C123C4(C2)C(C(C(CC4)O)(C)C)CCC1C1(C(CC3)(C(CC1)C(CCC=C(C)C)C)C)C
MOL003578	0.3361	0.6639	0.7070	Curculiginis Rhizome	Cycloartenol	Not Available	FALSE	C123C4(C2)C(C(C(CC4)O)(C)C)CCC1C1(C(CC3)(C(CC1)C(CCC=C(C)C)C)C)C
MOL003578	0.3361	0.6639	0.7070	Abrus Precatorius L.	Cycloartenol	Not Available	FALSE	C123C4(C2)C(C(C(CC4)O)(C)C)CCC1C1(C(CC3)(C(CC1)C(CCC=C(C)C)C)C)C
MOL003578	0.3361	0.6639	0.7070	Folium Nelumbinis	Cycloartenol	Not Available	FALSE	C123C4(C2)C(C(C(CC4)O)(C)C)CCC1C1(C(CC3)(C(CC1)C(CCC=C(C)C)C)C)C
MOL003578	0.3361	0.6639	0.7070	Portulacae Herba	Cycloartenol	Not Available	FALSE	C123C4(C2)C(C(C(CC4)O)(C)C)CCC1C1(C(CC3)(C(CC1)C(CCC=C(C)C)C)C)C
MOL003578	0.3361	0.6639	0.7070	Acoritataninowii Rhizoma	Cycloartenol	Not Available	FALSE	C123C4(C2)C(C(C(CC4)O)(C)C)CCC1C1(C(CC3)(C(CC1)C(CCC=C(C)C)C)C)C
MOL003578	0.3361	0.6639	0.7070	Calyx Seu Fructus Physalis	Cycloartenol	Not Available	FALSE	C123C4(C2)C(C(C(CC4)O)(C)C)CCC1C1(C(CC3)(C(CC1)C(CCC=C(C)C)C)C)C
MOL003578	0.3361	0.6639	0.7070	Arum Ternatum Thunb.	Cycloartenol	Not Available	FALSE	C123C4(C2)C(C(C(CC4)O)(C)C)CCC1C1(C(CC3)(C(CC1)C(CCC=C(C)C)C)C)C
MOL003579	0.9158	0.0842	0.9560	Asteris Radix Et Rhizoma	Anizol	7519	FALSE	c1(ccccc1)OC
MOL003579	0.9158	0.0842	0.9560	Zanthoxyli Pericarpium	Anizol	7519	FALSE	c1(ccccc1)OC
MOL003579	0.9158	0.0842	0.9560	Acoritataninowii Rhizoma	Anizol	7519	FALSE	c1(ccccc1)OC
MOL003579	0.9158	0.0842	0.9560	Cannabis Sativa L.	Anizol	7519	FALSE	c1(ccccc1)OC
MOL003581	0.9332	0.0668	0.9540	Chaenomeles Sinensis (Thouin) Koehne	[(2R)-2,3-dihydroxypropyl] acetate	6999061	FALSE	C(COC(=O)C)(CO)O
MOL003581	0.9332	0.0668	0.9540	Cnidii Fructus	[(2R)-2,3-dihydroxypropyl] acetate	6999061	FALSE	C(COC(=O)C)(CO)O
MOL003582	0.9276	0.0724	0.9684	Cnidii Fructus	Prenol	11173	FALSE	C(=C(C)C)CO
MOL003582	0.9276	0.0724	0.9684	Ardisiae Japonicae Herba	Prenol	11173	FALSE	C(=C(C)C)CO

MOL003583	0.9534	0.0466	0.9682	Cnidii Fructus	[(4S)-4-isopropenyl-1-cyclohexenyl] methyl acetate	5325829	FALSE	C1(CCC(=CC1)COC(=O)C)C(=C)C
MOL003584	0.7227	0.2773	0.9061	Cnidii Fructus	Xanthoxylin N	66548	FALSE	c1(=O)ccc2c(o1)cc1c(c2OC)C=CC(O1)(C)C
MOL003585	0.9535	0.0465	0.8640	Cnidii Fructus	7-Methoxy-4-methylcoumarin	390807	FALSE	o1c2c(c(cc1=O)C)ccc(OC)c2
MOL003586	0.9607	0.0393	0.8079	Cnidii Fructus	7-methoxy-2-oxochromene-8-carbaldehyde	11275724	FALSE	o1c(=O)ccc2ccc(c(c12)C=O)OC
MOL003588	0.6617	0.3383	0.8666	Cnidii Fructus	Prangenidin	69502	FALSE	c12c(c(c3c(c1CC=C(C)C)ccc(=O)o3)O)occ2
MOL003589	0.9239	0.0761	0.9546	Cnidii Fructus	1,2-propanediol,2-acetate	Not Available	FALSE	C(C(C)OC(=O)C)O
MOL003590	0.9457	0.0543	0.7156	Peucedani Radix	angelicin	10658	TRUE	c12c3c(ccc1ccc(=O)o2)occ3
MOL003590	0.9457	0.0543	0.7156	Cnidii Fructus	angelicin	10658	TRUE	c12c3c(ccc1ccc(=O)o2)occ3
MOL003590	0.9457	0.0543	0.7156	A. Dahurica (Fisch.) Benth. Et Hook	angelicin	10658	TRUE	c12c3c(ccc1ccc(=O)o2)occ3
MOL003590	0.9457	0.0543	0.7156	Radix Bupleuri	angelicin	10658	TRUE	c12c3c(ccc1ccc(=O)o2)occ3
MOL003590	0.9457	0.0543	0.7156	Radix Angelicae Biserratae	angelicin	10658	TRUE	c12c3c(ccc1ccc(=O)o2)occ3
MOL003590	0.9457	0.0543	0.7156	Nardostachyos Radix Et Rhizoma	angelicin	10658	TRUE	c12c3c(ccc1ccc(=O)o2)occ3
MOL003592	0.9151	0.0849	0.9251	Cnidii Fructus	auraptenol	13343541	FALSE	c1(=O)ccc2c(o1)c(c(cc2)OC)CC(C(=C)C)O
MOL003593	0.9201	0.0799	0.8192	Cnidii Fructus	2'-Acetylangelicin	5315489	FALSE	c1c2c(c3c(c1)ccc(=O)o3)cc(o2)C(=O)C
MOL003594	0.9319	0.0681	0.9293	Cnidii Fructus	l-Carvyl acetate	102024	FALSE	O(C1CC(CC=C1C)C(=C)C)C(=O)C
MOL003595	0.9596	0.0404	0.9673	Cnidii Fructus	cis-p-2,8-Menthadien-1-ol	5319363	FALSE	C1=CC(CCC1C(=C)C)(O)C
MOL003596	0.9433	0.0567	0.7952	Cnidii Fructus	cnideol B	15199342	FALSE	o1ccc2c1c(c(c(c2)CCC(=O)O)O)OC
MOL003597	0.4841	0.5159	0.8687	Cnidii Fructus	cnidiadin	Not Available	FALSE	O1C(C(OC(=O)C(C)C)(C)C)Cc2c1ccc1c2oc(=O)cc1

MOL003598	0.5071	0.4929	0.7207	Cnidii Fructus	9-hydroxy-4-[(7-methoxy-2-oxochromen-8-yl)methyl]furo[3,2-g]chromen-7-one	10715412	FALSE	c1cc(=O)oc2c1ccc(c2Cc1c2c(c(c3c1ccc(=O)o3)O)occ2)OC
MOL003599	0.8834	0.1166	0.8595	Cnidii Fructus	cnidimol A	Not Available	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)C/C=C(\CO)/C)O)C
MOL003600	0.9120	0.0880	0.8734	Cnidii Fructus	cnidimol B	Not Available	FALSE	c1(cc(=O)c2c(o1)cc1c(c2O)CC(O1)C(CO)(C)O)C
MOL003601	0.9327	0.0673	0.7846	Cnidii Fructus	cnidimol C	70697378	FALSE	c1(cc(=O)c2c(o1)cc(cc2O)O)CO
MOL003602	0.9240	0.0760	0.8199	Cnidii Fructus	cnidimol D	70682746	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)C/C=C(\CO)/C)O)CO
MOL003603	0.9224	0.0776	0.8330	Cnidii Fructus	cnidimol E	Not Available	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)CC(C(=C)C)O)O)CO
MOL003604	0.8555	0.1445	0.7925	Cnidii Fructus	cnidimol F	Not Available	FALSE	O1CC(C=Cc2c1cc1c(c2O)c(=O)cc(o1)CO)(C)O
MOL003605	0.2089	0.7911	0.8039	Cnidii Fructus	(E)-2,3-bis(2-keto-7-methoxy-chromen-8-yl)acrolein	10597338	FALSE	c1c2c(oc(=O)c1)c(c(cc2)OC)/C(=C\c1c(ccc2c1oc(=O)cc2)OC)/C=O
MOL003606	0.3299	0.6701	0.7858	Cnidii Fructus	cniforin A	15553295	FALSE	C(=O)(C(C)C)OC1c2c3c(ccc(=O)o3)ccc2OC1C(C)(C)OC(=O)C
MOL003607	0.1105	0.8895	0.6513	Cnidii Fructus	cniforin B	58488745	FALSE	C(=O)(/C(=C\C)/C)OC(C)(C)C1Oc2c(c3c(ccc(=O)o3)cc2)C1OC(=O)C(C)C
MOL003608	0.7301	0.2699	0.8787	Cnidii Fructus	O-Acetylcolumbianetin	161409	FALSE	c1c2c(c3c(c1)ccc(=O)o3)CC(O2)C(C)(C)OC(=O)C
MOL003608	0.7301	0.2699	0.8787	Radix Angelicae Biseratae	O-Acetylcolumbianetin	161409	FALSE	c1c2c(c3c(c1)ccc(=O)o3)CC(O2)C(C)(C)OC(=O)C
MOL003609	0.8460	0.1540	0.8447	Cnidii Fructus	(8S)-8-(2-hydroxypropan-2-yl)-8,9-dihydrofuro[2,3-h]chromen-2-one	92201	FALSE	c1(=O)ccc2c(o1)c1c(cc2)OC(C1)C(C)(C)O
MOL003609	0.8460	0.1540	0.8447	Notopterygii Rhizoma Et Radix	(8S)-8-(2-hydroxypropan-2-yl)-8,9-dihydrofuro[2,3-h]chromen-2-one	92201	FALSE	c1(=O)ccc2c(o1)c1c(cc2)OC(C1)C(C)(C)O

MOL003609	0.8460	0.1540	0.8447	Radix Angelicae Biseratae	(8S)-8-(2-hydroxypropan-2-yl)-8,9-dihydrofuro[2,3-h]chromen-2-one	92201	FALSE	c1(=O)ccc2c(o1)c1c(cc2)OC(C1)C(C)(C)O
MOL003610	0.6613	0.3387	0.8237	Tinosporae Radix	Columbin	Not Available	FALSE	C1=CC2(C3(C(C1OC2=O)C1(C(CC3)C(=O)OC(C1)c1cocc1)C)C)O
MOL003610	0.6613	0.3387	0.8237	Cnidii Fructus	Columbin	Not Available	FALSE	C1=CC2(C3(C(C1OC2=O)C1(C(CC3)C(=O)OC(C1)c1cocc1)C)C)O
MOL003611	0.9376	0.0624	0.7069	Cnidii Fructus	cyclofenchene	Not Available	FALSE	C12(C3C1CC(C3(C)C)C2)C
MOL003612	0.3412	0.6588	0.6769	Cnidii Fructus	Edultin	5317013	FALSE	O1C(C(OC(=O)C)(C)C)C(OC(=O)/C(=C\C)/C)c2c1ccc1c2oc(=O)cc1
MOL003612	0.3412	0.6588	0.6769	Saussureae Involucratae Herba	Edultin	5317013	FALSE	O1C(C(OC(=O)C)(C)C)C(OC(=O)/C(=C\C)/C)c2c1ccc1c2oc(=O)cc1
MOL003613	0.8804	0.1196	0.9674	Cnidii Fructus	Silvan	10797	FALSE	c1(ccco1)C
MOL003614	0.9561	0.0439	0.7701	Cnidii Fructus	Fenchylacetate	14019266	FALSE	O(C1C2(CC(C1(C)C)CC2)C)C(=O)C
MOL003614	0.9561	0.0439	0.7701	Foeniculi Fructus	Fenchylacetate	14019266	FALSE	O(C1C2(CC(C1(C)C)CC2)C)C(=O)C
MOL003615	0.9006	0.0994	0.8533	Cnidii Fructus	2-octen-1-ol,7-[(tetrahydro-2H-pyran-2-yl)oxy]	Not Available	FALSE	O(C1OCCCC1)C(CCC/C=C/CO)C
MOL003617	0.7892	0.2108	0.7006	Cnidii Fructus	isogosferol	Not Available	FALSE	c1(=O)ccc2c(o1)c(c1c(c2)cco1)OCC(C(=C)C)O
MOL003618	0.9612	0.0388	0.8272	Glechomae Herba	Isopinocamphone	6427105	FALSE	C12CC(CC(=O)C1C)C2(C)C
MOL003618	0.9612	0.0388	0.8272	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Isopinocamphone	6427105	FALSE	C12CC(CC(=O)C1C)C2(C)C
MOL003618	0.9612	0.0388	0.8272	Cnidii Fructus	Isopinocamphone	6427105	FALSE	C12CC(CC(=O)C1C)C2(C)C
MOL003620	0.6721	0.3279	0.6750	Cnidii Fructus	Karenin	6440661	FALSE	O[C@H]1[C@@H]2[C@@]3([C@]4([C@@H](C=CC3)C3[C@@]([C@@H]4CC3)(C)C)COC(=O)/C=C\c3ccc(O)cc3)C(=O)O)(CC2)C)(CC1)C)(C)C
MOL003621	0.9195	0.0805	0.8367	Cnidii Fructus	meranzin hydrate	821434	FALSE	c1(=O)ccc2c(o1)c(c(cc2)OC)CC(C(C)(C)O)O
MOL003622	0.9212	0.0788	0.9400	Cnidii Fructus	Methyl geranate	5365910	FALSE	C(=C\C(=O)OC)(/CCC=C(C)C)\C
MOL003622	0.9212	0.0788	0.9400	Perillae Fructus	Methyl geranate	5365910	FALSE	C(=C\C(=O)OC)(/CCC=C(C)C)\C
MOL003622	0.9212	0.0788	0.9400	Aristolochiae Fructus	Methyl geranate	5365910	FALSE	C(=C\C(=O)OC)(/CCC=C(C)C)\C

MOL003622	0.9212	0.0788	0.9400	Perilla Frutescens	Methyl geranate	5365910	FALSE	C(=C\C(=O)OC)(/CCC=C(C)C)\C
MOL003623	0.8669	0.1331	0.8201	Cnidii Fructus	2-TRIDECENAL	5283363	FALSE	C(CCC/C=C/C=O)CCCCCC
MOL003624	0.4112	0.5888	0.8125	Cnidii Fructus	o-Isovalerylcolum bianetin	51522494	FALSE	C(C)(CC(=O)OC(C)(C)C1Oc2c(C1)c1c(cc2)ccc(=O)o1)C
MOL003625	0.8266	0.1734	0.8674	Cnidii Fructus	Kvannin	74477	FALSE	c12c3c(ccc1oc(c2)C(=C)C)ccc(=O)o3
MOL003626	0.4640	0.5360	0.7953	Cnidii Fructus	Ostruthin	5281420	FALSE	C(=CCC/C(=C/Cc1cc2c(cc1O)oc(=O)cc2)/C)(C)C
MOL003628	0.8778	0.1222	0.6737	Sophorae Tonkinensis Radix Et Rhizome	1,2,3-Tri-O-galloyl-beta-D-glucose	11969001	FALSE	c1(c(c(cc(c1)C(=O)OC1C(C(OC(C1OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)CO)O)O)O)O
MOL003630	0.8644	0.1356	0.8471	Sojae Semen Nigrum	Genistein 8-C-glucoside	5281757	FALSE	c1(coc2c(c1=O)c(cc(c2C1OC(C(C(C1O)O)O)CO)O)O)c1ccc(cc1)O
MOL003630	0.8644	0.1356	0.8471	Sophorae Tonkinensis Radix Et Rhizome	Genistein 8-C-glucoside	5281757	FALSE	c1(coc2c(c1=O)c(cc(c2C1OC(C(C(C1O)O)O)CO)O)O)c1ccc(cc1)O
MOL003631	0.3780	0.6220	0.8190	Sophorae Tonkinensis Radix Et Rhizome	Matsukazelactone	5319307	FALSE	c12c(ccc(=O)o1)cc(c(c2)OC)c1c2oc(=O)ccc2ccc1OC
MOL003632	0.9091	0.0909	0.6745	Sophorae Tonkinensis Radix Et Rhizome	N-methylcytisine	Not Available	FALSE	O=c1n2CC3CC(CN(C3)C)c2ccc1
MOL003634	0.8402	0.1598	0.7016	Sophorae Tonkinensis Radix Et Rhizome	Pterocarpol	Not Available	FALSE	C1(CC(=C)C2C(C1)(CCC(C2)C(C)(O)C)C)O
MOL003635	0.7322	0.2678	0.8613	Sophorae Tonkinensis Radix Et Rhizome	8-O-methylretusin	Not Available	FALSE	c12c(CC(CO2)c2ccc(cc2)OC)ccc(c1OC)O
MOL003636	0.0452	0.9548	0.6323	Sophorae Tonkinensis Radix Et Rhizome	Sophoradochromene	5321394	FALSE	c1(c(c(CC=C(C)C)c(cc1)O)O)C(=O)/C=C/c1cc2c(OC(C=C2)(C)C)c(c1)CC=C(C)C
MOL003637	0.8341	0.1659	0.6842	Sophorae Tonkinensis Radix Et Rhizome	Sophoricoside	5321398	FALSE	c1(coc2c(c1=O)c(cc(c2)O)O)c1ccc(cc1)OC1OC(C(C(C1O)O)O)CO
MOL003637	0.8341	0.1659	0.6842	Fructussophorae	Sophoricoside	5321398	FALSE	c1(coc2c(c1=O)c(cc(c2)O)O)c1ccc(cc1)OC1OC(C(C(C1O)O)O)CO
MOL003639	0.7618	0.2382	0.7899	Sojae Semen Nigrum	Soyasaponin A4	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(C(C(C1)(C)C)O)OC1OCC(C(C1O)OC1OCC(C(C1O)O)O)O)C)C)C)(CO)C)OC1OC(C(C(C1OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)O)CO)O)O)CO)O)O)C(=O)O
MOL003639	0.7618	0.2382	0.7899	Sophorae Tonkinensis Radix Et Rhizome	Soyasaponin A4	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(C(C(C1)(C)C)O)OC1OCC(C(C1O)OC1OCC(C(C1O)O)O)O)C)C)C)(CO)C)OC1OC(C(C(C1OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)O)CO)O)O)CO)O)O)C(=O)O
MOL003640	0.4800	0.5200	0.7116	Sojae Semen Nigrum	Soyasaponin A6_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(C(C(C1)(C)C)O)O)C)C)C)C)(CO)C)O

MOL003640	0.4800	0.5200	0.7116	Sophorae Tonkinensis Radix Et Rhizome	Soyasaponin A6_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(C(C(C1)(C)C)O)O)C)C)C)(CO)C)O
MOL003641	0.4261	0.5739	0.7644	Sophorae Tonkinensis Radix Et Rhizome	Soyasapogenol B	115012	FALSE	C12C(C3(C(=CC2)C2C(CC3)(C(CC(C2)(C)C)O)C)C)(CCC2C1(CCC(C2(CO)C)O)C)C
MOL003641	0.4261	0.5739	0.7644	Peanut Skin	Soyasapogenol B	115012	FALSE	C12C(C3(C(=CC2)C2C(CC3)(C(CC(C2)(C)C)O)C)C)(CCC2C1(CCC(C2(CO)C)O)C)C
MOL003641	0.4261	0.5739	0.7644	Abri Herba	Soyasapogenol B	115012	FALSE	C12C(C3(C(=CC2)C2C(CC3)(C(CC(C2)(C)C)O)C)C)(CCC2C1(CCC(C2(CO)C)O)C)C
MOL003641	0.4261	0.5739	0.7644	Radix Puerariae	Soyasapogenol B	115012	FALSE	C12C(C3(C(=CC2)C2C(CC3)(C(CC(C2)(C)C)O)C)C)(CCC2C1(CCC(C2(CO)C)O)C)C
MOL003641	0.4261	0.5739	0.7644	Trigonellae Semen	Soyasapogenol B	115012	FALSE	C12C(C3(C(=CC2)C2C(CC3)(C(CC(C2)(C)C)O)C)C)(CCC2C1(CCC(C2(CO)C)O)C)C
MOL003641	0.4261	0.5739	0.7644	Sophora Japonica L.	Soyasapogenol B	115012	FALSE	C12C(C3(C(=CC2)C2C(CC3)(C(CC(C2)(C)C)O)C)C)(CCC2C1(CCC(C2(CO)C)O)C)C
MOL003641	0.4261	0.5739	0.7644	Sojae Semen Nigrum	Soyasapogenol B	115012	FALSE	C12C(C3(C(=CC2)C2C(CC3)(C(CC(C2)(C)C)O)C)C)(CCC2C1(CCC(C2(CO)C)O)C)C
MOL003641	0.4261	0.5739	0.7644	Sophorae Flavescentis Radix	Soyasapogenol B	115012	FALSE	C12C(C3(C(=CC2)C2C(CC3)(C(CC(C2)(C)C)O)C)C)(CCC2C1(CCC(C2(CO)C)O)C)C
MOL003642	0.7596	0.2404	0.8448	Sophorae Tonkinensis Radix Et Rhizome	Soyasaponin II	443614	FALSE	C12C(C3(C(=CC2)C2C(CC3)(C(CC(C2)(C)C)O)C)C)(CCC2C1(CCC(C2(CO)C)OC1C(OC2C(OC3C(C(C(C(O3)C)O)O)O)C(C(CO2)O)O)C(C(C(O1)C(=O)O)O)O)C)C

MOL003643	0.7368	0.2632	0.8516	Sophorae Tonkinensis Radix Et Rhizome	(2S,3S,4S,5R,6R)-6-[[(3S,4S,4aR,6aR,6bS,8aR,9R,12aS,14aR,14bR)-9-hydroxy-4-(hydroxymethyl)-4,6a,6b,8a,11,11,14b-heptamethyl-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydropicen-3-yl]oxy]-3,4-dihydroxy-5-[[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymet	21607811	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)OC1C(OC2OC(C(C(C2O)O)O)CO)C(C(C(O1)C(=O)O)O)O)(CO)C)C)C1C(CC3)(C(CC(C1)(C)C)O)C)C)C
MOL003644	0.3372	0.6628	0.7791	Sophorae Tonkinensis Radix Et Rhizome	Witha ferine	Not Available	FALSE	C1=CC(C23C(C1=O)(C1C(CC2O3)C2C(CC1)(C(CC2)C(C1OC(=O)C(=C(C1)C)CO)C)C)C)O
MOL003644	0.3372	0.6628	0.7791	Daturae Flos	Witha ferine	Not Available	FALSE	C1=CC(C23C(C1=O)(C1C(CC2O3)C2C(CC1)(C(CC2)C(C1OC(=O)C(=C(C1)C)CO)C)C)C)O
MOL003645	0.3842	0.6158	0.8194	Sophorae Tonkinensis Radix Et Rhizome	abrisapogenol H	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)C(=O)CC(C)(CO)CC4C3=CCC21)C)O
MOL003646	0.4676	0.5324	0.7208	Sophorae Tonkinensis Radix Et Rhizome	Abrisapogenol C	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(C(C(C1)(C)CO)O)O)C)C)C)(C)C)O
MOL003646	0.4676	0.5324	0.7208	Abri Herba	Abrisapogenol C	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(C(C(C1)(C)CO)O)O)C)C)C)(C)C)O
MOL003647	0.8866	0.1134	0.6191	Sophorae Tonkinensis Radix Et Rhizome	Sophojaponicin	Not Available	FALSE	c12c(OCO1)cc1c(c2)C2C(O1)c1c(OC2)cc(cc1)OC1OC(C(C(C1O)O)O)CO
MOL003648	0.9187	0.0813	0.7311	Panax Ginseng C. A. Mey.	Inermin	Not Available	FALSE	c12c(OCO1)cc1c(c2)C2C(O1)c1c(OC2)cc(cc1)O
MOL003648	0.9187	0.0813	0.7311	Sophorae Tonkinensis Radix Et Rhizome	Inermin	Not Available	FALSE	c12c(OCO1)cc1c(c2)C2C(O1)c1c(OC2)cc(cc1)O
MOL003648	0.9187	0.0813	0.7311	Sophorae Flavescentis Radix	Inermin	Not Available	FALSE	c12c(OCO1)cc1c(c2)C2C(O1)c1c(OC2)cc(cc1)O
MOL003648	0.9187	0.0813	0.7311	Pyrrosiae Folium	Inermin	Not Available	FALSE	c12c(OCO1)cc1c(c2)C2C(O1)c1c(OC2)cc(cc1)O

MOL003649	0.8193	0.1807	0.8537	Sophorae Tonkinensis Radix Et Rhizome	7-hydroxy-2-(4-hydroxyphenyl)-8-[(2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]chromone	21721991	FALSE	c1(cc(=O)c2c(o1)c(c(cc2)O)C1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)O
MOL003650	0.7576	0.2424	0.8374	Sophorae Tonkinensis Radix Et Rhizome	C13837	656760	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(=O)CC(C3)(C)C)C)C)(CC2)C)(CC1)C)(CO)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)CO)C(=O)O
MOL003650	0.7576	0.2424	0.8374	Abri Herba	C13837	656760	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(=O)CC(C3)(C)C)C)C)(CC2)C)(CC1)C)(CO)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)CO)C(=O)O
MOL003651	0.3950	0.6050	0.7969	Abri Herba	(4aR,6aR,6aS,6bR,8aR,9S,10S,12aR,14bS)-10-hydroxy-2,2,4a,6a,6b,9,12a-heptamethyl-9-methylol-3,5,6,6a,7,8,8a,10,11,12,13,14b-dodecahydro-1H-picen-4-one	13632872	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(=O)CC(C3)(C)C)C)C)(CC2)C)(CC1)C)(CO)C

MOL003651	0.3950	0.6050	0.7969	Sophorae Tonkinensis Radix Et Rhizome	(4aR,6aR,6aS,6bR,8aR,9S,10S,12aR,14bS)-10-hydroxy-2,2,4a,6a,6b,9,12a-heptamethyl-9-methylol-3,5,6,6a,7,8,8a,10,11,12,13,14b-dodecahydro-1H-picen-4-one	13632872	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(=O)CC(C3)(C)C)C)C)(CC2)C)(CC1)C)(CO)C
MOL003652	0.9017	0.0983	0.9262	Sophorae Tonkinensis Radix Et Rhizome	gamma-Dodecalactone	12237820	FALSE	CCCCCCCCC1OC(=O)CC1
MOL003653	0.7667	0.2333	0.8416	Abri Herba	kaikasaponinIII	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(O)CC(C3)(C)C)C)C)(CC2)C)(CC1)C)(C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)C)CO)C(=O)O
MOL003653	0.7667	0.2333	0.8416	Sophora Japonica L.	kaikasaponinIII	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(O)CC(C3)(C)C)C)C)(CC2)C)(CC1)C)(C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)C)CO)C(=O)O
MOL003653	0.7667	0.2333	0.8416	Sophorae Tonkinensis Radix Et Rhizome	kaikasaponinIII	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(O)CC(C3)(C)C)C)C)(CC2)C)(CC1)C)(C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)C)CO)C(=O)O
MOL003654	0.4108	0.5892	0.7532	Sophorae Tonkinensis Radix Et Rhizome	kaikasaponinIII_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(O)CC(C3)(C)C)C)C)(CC2)C)(CC1)C)(C)C
MOL003655	0.5481	0.4519	0.6969	Sophorae Tonkinensis Radix Et Rhizome	kudzusapogenol A	Not Available	FALSE	C1(CCC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C)C(C(C(C)(CO)CC4C3=CCC21O)O)O)C)O
MOL003655	0.5481	0.4519	0.6969	Abri Herba	kudzusapogenol A	Not Available	FALSE	C1(CCC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C)C(C(C(C)(CO)CC4C3=CCC21O)O)O)C)O
MOL003656	0.5136	0.4864	0.7521	Sophorae Tonkinensis Radix Et Rhizome	Lupiwighteone	5317480	FALSE	c12c(=O)c(coc1c(c(cc2O)O)CC=C(C)C)c1ccc(cc1)O
MOL003656	0.5136	0.4864	0.7521	licorice	Lupiwighteone	5317480	FALSE	c12c(=O)c(coc1c(c(cc2O)O)CC=C(C)C)c1ccc(cc1)O
MOL003657	0.4158	0.5842	0.7795	Sophorae Tonkinensis Radix Et Rhizome	Abrisapogenol D	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(CC(C1)(CO)C)O)C)C)C)(C)C)O
MOL003657	0.4158	0.5842	0.7795	Abri Herba	Abrisapogenol D	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(CC(C1)(CO)C)O)C)C)C)(C)C)O
MOL003658	0.4108	0.5892	0.7532	Sophorae Tonkinensis Radix Et Rhizome	sophoradiol	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(O)CC(C3)(C)C)C)C)(CC2)C)(CC1)C)(C)C

MOL003659	0.8408	0.1592	0.8223	Sophorae Tonkinensis Radix Et Rhizome	sophoraflavone A	Not Available	FALSE	O(C1C(O)C(O)C(OC1c1c2oc(cc(=O)c2ccc1O)c1ccc(O)cc1)CO)C1OC(C(O)C(O)C1O)C
MOL003660	0.8193	0.1807	0.8537	Sophorae Tonkinensis Radix Et Rhizome	sophoraflavone A_qt	Not Available	FALSE	o1c2c(c(O)ccc2c(=O)cc1c1ccc(O)cc1)C1OC(C(O)C(O)C1O)CO
MOL003661	0.7603	0.2397	0.6567	Sophorae Tonkinensis Radix Et Rhizome	7-hydroxy-2-[4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]oxyphenyl] chromone	5491513	FALSE	O1C(C(O)C(O)C(O)C1Oc1ccc(cc1)c1oc2c(c(=O)c1)ccc(O)c2)CO
MOL003662	0.9211	0.0789	0.7774	licorice	7,4'-Dihydroxyflavone	5282073	FALSE	Oc1ccc(cc1)c1oc2c(c(=O)c1)ccc(O)c2
MOL003662	0.9211	0.0789	0.7774	Sophorae Tonkinensis Radix Et Rhizome	7,4'-Dihydroxyflavone	5282073	FALSE	Oc1ccc(cc1)c1oc2c(c(=O)c1)ccc(O)c2
MOL003665	0.4800	0.5200	0.7116	Sophorae Tonkinensis Radix Et Rhizome	soyasapogenol A	Not Available	FALSE	C1C(C(C(C2(CCC3(C4(CCC5C(C(CCC5(C4CC=C3C12)C)O)(C)CO)C)C)C)O)O)(C)C
MOL003666	0.4212	0.5788	0.7579	Sophorae Tonkinensis Radix Et Rhizome	subprogenin A	Not Available	FALSE	C1(CCC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C)C(=O)CC(C)(CO)CC4C3=CCC21)C)O
MOL003667	0.4921	0.5079	0.7234	Sophorae Tonkinensis Radix Et Rhizome	subprogenin B	Not Available	FALSE	C1(CCC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C)C(=O)CC(CO)(CO)CC4C3=CCC21)C)O
MOL003668	0.4605	0.5395	0.7456	Abri Herba	Abrisapogenol E	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(CC(C1)(CO)C)O)C)C)C)(CO)C)O
MOL003668	0.4605	0.5395	0.7456	Sophorae Tonkinensis Radix Et Rhizome	Abrisapogenol E	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(CC(C1)(CO)C)O)C)C)C)(CO)C)O
MOL003669	0.7209	0.2791	0.8380	Sophorae Tonkinensis Radix Et Rhizome	subprogenin C	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)C(=O)CC(C)(C(=O)O)CC4C3=CCC21)C)O
MOL003670	0.7209	0.2791	0.8380	Sophorae Tonkinensis Radix Et Rhizome	subprogenin D	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)C(=O)CC(C)(C(=O)O)CC4C3=CCC21)C)O

MOL003671	0.1715	0.8285	0.6528	Sophorae Tonkinensis Radix Et Rhizome	3,5-dihydroxy-2-(4-hydroxyphenyl)-8,8-dimethyl-10-(3-methylbut-2-enyl)pyrano[5,6-g]chromen-4-one	16215899	FALSE	c12c(c(c3c(c1CC=C(C)C)oc(c(c3=O)O)c1ccc(cc1)O)O)C=CC(O2)(C)C
MOL003673	0.5280	0.4720	0.7152	Sophorae Flavescentis Radix	Wighteone	5281814	FALSE	c1c(c(=O)c2c(o1)cc(c(c2O)CC=C(C)C)O)c1ccc(cc1)O
MOL003673	0.5280	0.4720	0.7152	Sophorae Tonkinensis Radix Et Rhizome	Wighteone	5281814	FALSE	c1c(c(=O)c2c(o1)cc(c(c2O)CC=C(C)C)O)c1ccc(cc1)O
MOL003674	0.4212	0.5788	0.7579	Sophorae Tonkinensis Radix Et Rhizome	wistariasapogenol A	Not Available	FALSE	C1(CCC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C)C(=O)CC(C)(CO)CC4C3=CCC21)C)O
MOL003678	0.7635	0.2365	0.8291	Sophorae Tonkinensis Radix Et Rhizome	Abrisaponin 1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(=O)CC(C1)(C(=O)O)C)C)C)C)(CO)C)OC1OC(C(C(C1OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO)O)O)C(=O)O
MOL003679	0.7158	0.2842	0.7748	Sophorae Tonkinensis Radix Et Rhizome	Abrisaponin 1_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(=O)CC(C1)(C(=O)O)C)C)C)C)(CO)C)O
MOL003681	0.8623	0.1377	0.8231	Sophorae Tonkinensis Radix Et Rhizome	N-methylcytisine	Not Available	FALSE	C1(CC2Cn3c(C(C1)C2)cccc3=O)C
MOL003682	0.9556	0.0444	0.7242	Sophorae Tonkinensis Radix Et Rhizome	BB_NC-0046	Not Available	FALSE	N1CC2Cn3c(C(C1)C2)cccc3=O
MOL003686	0.8764	0.1236	0.8492	Ginkgo Folium	Narcissoside	5481663	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(OC)c(O)cc1)COC1OC(C(O)C(O)C1O)C
MOL003686	0.8764	0.1236	0.8492	Microctis Folium	Narcissoside	5481663	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(OC)c(O)cc1)COC1OC(C(O)C(O)C1O)C
MOL003686	0.8764	0.1236	0.8492	licorice	Narcissoside	5481663	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(OC)c(O)cc1)COC1OC(C(O)C(O)C1O)C
MOL003686	0.8764	0.1236	0.8492	Radix Bupleuri	Narcissoside	5481663	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(OC)c(O)cc1)COC1OC(C(O)C(O)C1O)C
MOL003686	0.8764	0.1236	0.8492	Sophorae Tonkinensis Radix Et Rhizome	Narcissoside	5481663	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(OC)c(O)cc1)COC1OC(C(O)C(O)C1O)C
MOL003688	0.4550	0.5450	0.6446	Rehmanniae Radix Praeparata	2-(4-hydroxyphenyl)ethyl hexacosanoate	481679	FALSE	O(C(=O)CCCCCCCCCCCCCCCCCCCCCCCCC)CCc1ccc(O)cc1

MOL003689	0.9307	0.0693	0.8105	Rehmanniae Radix Praeparata	aeginetic acid	Not Available	FALSE	OC1(C(CCCC1(O)C)(C)C)/C=C/C(=C/C(=O)O)/C
MOL003690	0.9273	0.0727	0.8712	Rehmanniae Radix Praeparata	Ajugol	Not Available	FALSE	O(C1OC=CC2C1C(O)(CC2)C)C1OC(O)(C(O)C(O)C1O)CO
MOL003691	0.9075	0.0925	0.7741	Rehmanniae Radix Praeparata	Ajugoside	Not Available	FALSE	O(C1(C2C(CC1)C=COC2OC1OC(O)(C(O)C(O)C1O)CO)C)C(=O)C
MOL003692	0.9609	0.0391	0.8480	Rehmanniae Radix Praeparata	Ajugoside_qt	Not Available	FALSE	O(C1(C2C(CC1)C=COC2O)C)C(=O)C
MOL003694	0.9128	0.0872	0.9371	Arisaematis Rhizoma	Cerebrosid	Not Available	FALSE	C(=O)(C(N)CO)NC1C(O)C(O)C(O)C(O1)CO
MOL003694	0.9128	0.0872	0.9371	Rehmanniae Radix Praeparata	Cerebrosid	Not Available	FALSE	C(=O)(C(N)CO)NC1C(O)C(O)C(O)C(O1)CO
MOL003695	0.6308	0.3692	0.7190	Rehmanniae Radix Praeparata	Cistanoside A	Not Available	FALSE	C1(C(C(C(C(O1)OCCc1cc(c(cc1)O)OC)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)COC1C(C(OC2C(C(C(C(O2)C)O)O)O)O)C(C(O1)CO)O)O
MOL003696	0.8862	0.1138	0.7477	Rehmanniae Radix Praeparata	Cistanoside F	Not Available	FALSE	O1C(C(C(C(C1C)O)O)O)OC1C(C(OC(C1O)O)CO)OC(=O)/C=C\c1cc(c(cc1)O)O
MOL003697	0.5447	0.4553	0.7013	Sojae Semen Nigrum	methyl 9,10-methylene-hexadecanoate	12159685	FALSE	O(C(=O)CCCCCCCC1C(C1)CCCCCC)C
MOL003697	0.5447	0.4553	0.7013	Rehmanniae Radix Praeparata	methyl 9,10-methylene-hexadecanoate	12159685	FALSE	O(C(=O)CCCCCCCC1C(C1)CCCCCC)C
MOL003698	0.9348	0.0652	0.8767	Rehmanniae Radix Praeparata	(2S,3R,4R,5S,6R)-2-[[(1S,4aS,5R,7aR)-4a,5-dihydroxy-7-methylol-5,7a-dihydro-1H-cyclopenta[c]pyran-1-yl]oxy]-6-methylol-tetrahydropyran-3,4,5-triol	21550273	FALSE	O(C1OC=CC2(O)C1C(=CC2O)CO)C1OC(C(O)C(O)C1O)CO
MOL003699	0.9255	0.0745	0.8521	Rehmanniae Radix Praeparata	melittoside_qt	Not Available	FALSE	OC1OC=CC2(O)C1C(=CC2O)CO
MOL003700	0.9215	0.0785	0.8297	Rehmanniae Radix Praeparata	Dihydrocatalpol	5705531	FALSE	O1C2(C1C(O)C1C2C(OCC1)OC1OC(C(O)C(O)C1O)CO)CO

MOL003701	0.9323	0.0677	0.8667	Rehmanniae Radix Praeparata	geniposide	29927666	FALSE	C1(=COC(OC2C(C(C(C(O2)CO)O)O)O)C2C1CC=C2CO)C(=O)CO
MOL003702	0.9480	0.0520	0.8832	Rehmanniae Radix Praeparata	geniposide_qt	Not Available	FALSE	C1(=COC(O)C2C1CC=C2CO)C(=O)CO
MOL003702	0.9480	0.0520	0.8832	Achyranthis Bidentatae Radix	geniposide_qt	Not Available	FALSE	C1(=COC(O)C2C1CC=C2CO)C(=O)CO
MOL003703	0.8950	0.1050	0.7989	Rehmanniae Radix Praeparata	glutinoside	Not Available	FALSE	O1C2OCC3(C(C(C(C3Cl)O)C2)C1OC1OC(C(C(C1O)O)O)CO)O
MOL003704	0.9370	0.0630	0.8651	Rehmanniae Radix Praeparata	Jiofuran	5318702	FALSE	OC1C(c2c(C1O)coc2)CCO
MOL003705	0.9065	0.0935	0.7765	Rehmanniae Radix Praeparata	jioglutin A	Not Available	FALSE	ClC1C2(O)C3C(C1O)CC(OC3OC2)OC
MOL003706	0.9065	0.0935	0.7765	Rehmanniae Radix Praeparata	jioglutin B	Not Available	FALSE	ClC1C2(O)C3C(C1O)CC(OC3OC2)OC
MOL003707	0.9326	0.0674	0.7827	Rehmanniae Radix Praeparata	jioglutin C	Not Available	FALSE	O1C2OC(OC)CC3C2C(O)(C(O)C3O)C1
MOL003708	0.9166	0.0834	0.7642	Rehmanniae Radix Praeparata	jioglutin D	Not Available	FALSE	O1C2(C1C(O)C1C2C(OC(OC)C1)OC)CO
MOL003709	0.9470	0.0530	0.8196	Rehmanniae Radix Praeparata	jioglutin E	Not Available	FALSE	O1C(OC)C2C(C(O)CC2(O)C)CC1OC
MOL003710	0.9416	0.0584	0.8485	Rehmanniae Radix Praeparata	jioglutolide	Not Available	FALSE	OC1(C2C(C(O)C1)CC(=O)OC2)C
MOL003711	0.9268	0.0732	0.8476	Rehmanniae Radix Praeparata	Jioglutoside A	Not Available	FALSE	O1C2(C1C(O)C1C2C(OC=C1)OC1OC(C(O)C(O)C1O)C)CO

MOL003712	0.8427	0.1573	0.6982	Rehmanniae Radix Praeparata	methyl (1S,4aS,7aS)-7-methylene-1-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[[(2R,3R,4R,5S,6R)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxymethyl]tetrahydropyran-2-yl]oxy-4a,5,6,7a-tetrahydro-1H-cyclopenta[d]pyran-4-carboxylate	21550422	FALSE	O(C1OC=C(C2C1C(=C)CC2)C(=O)OC)C1OC(C(O)C(O)C1O)COC1OC(C(O)C(O)C1O)C
MOL003713	0.9609	0.0391	0.9047	Rehmanniae Radix Praeparata	Jioglutoside B_qt	15102018	FALSE	OC1OC=C(C2C1C(=C)CC2)C(=O)OC
MOL003714	0.6149	0.3851	0.7182	Rehmanniae Radix Praeparata	Jionoside A	Not Available	FALSE	O(C1C(OC(=O)/C=C\c2cc(OC)c(O)cc2)C(OC(OCCc2cc(O)c(O)cc2)C1O)COC1OC(C(O)C(O)C1O)CO)C1OC(C(O)C(O)C1O)C
MOL003715	0.5550	0.4450	0.7074	Rehmanniae Radix Praeparata	Jionoside B	Not Available	FALSE	O(C1C(OC(=O)/C=C\c2cc(OC)c(O)cc2)C(OC(OCCc2cc(O)c(OC)cc2)C1O)COC1OC(C(O)C(O)C1O)CO)C1OC(C(O)C(O)C1O)C
MOL003716	0.8956	0.1044	0.7725	Rehmanniae Radix Praeparata	Melittoside	11968737	FALSE	O(C12C(C(OC3OC(C(O)C(O)C3O)CO)OC=C2)C(=CC1O)CO)C1OC(C(O)C(O)C1O)CO
MOL003717	0.6603	0.3397	0.6582	Perillae Fructus	METHYL PALMITOLEATE	643801	FALSE	O(C(=O)CCCCCCC/C=C\CCCCCC)C
MOL003717	0.6603	0.3397	0.6582	Polygoni Orientalis Fructus	METHYL PALMITOLEATE	643801	FALSE	O(C(=O)CCCCCCC/C=C\CCCCCC)C
MOL003717	0.6603	0.3397	0.6582	Sojae Semen Nigrum	METHYL PALMITOLEATE	643801	FALSE	O(C(=O)CCCCCCC/C=C\CCCCCC)C

MOL003717	0.6603	0.3397	0.6582	Impatientis Semen	METHYL PALMITOLEATE	643801	FALSE	O(C(=O)CCCCCCC/C=C\CCCCCC)C
MOL003717	0.6603	0.3397	0.6582	Broussonetiae Fructus	METHYL PALMITOLEATE	643801	FALSE	O(C(=O)CCCCCCC/C=C\CCCCCC)C
MOL003717	0.6603	0.3397	0.6582	Rehmanniae Radix Praeparata	METHYL PALMITOLEATE	643801	FALSE	O(C(=O)CCCCCCC/C=C\CCCCCC)C
MOL003717	0.6603	0.3397	0.6582	Sterculiae Lychnophorae Semen	METHYL PALMITOLEATE	643801	FALSE	O(C(=O)CCCCCCC/C=C\CCCCCC)C
MOL003718	0.7535	0.2465	0.7103	Rehmanniae Radix Praeparata	6-O-p-coumaroylajugol	Not Available	FALSE	OC1(C2C(C(OC(=O)/C=C\c3cc(OC)c(O)cc3)C1)C=COC2OC1OC(C(O)C(O)C1O)CO)C
MOL003719	0.8162	0.1838	0.6227	Rehmanniae Radix Praeparata	methyl-2,6,10-trimethyltridecanoate	Not Available	FALSE	C(=O)(C(CCCC(CCCC(CCC)C)C)(C)C)O
MOL003720	0.7264	0.2736	0.7281	Rehmanniae Radix Praeparata	Purpureaside C	Not Available	FALSE	O(C1C(OC(=O)/C=C\c2cc(O)c(O)cc2)C(OC(OCCc2cc(O)c(O)cc2)C1O)COC1OC(C(O)C(O)C1O)CO)C1OC(C(O)C(O)C1O)C
MOL003721	0.9030	0.0970	0.7826	Rehmanniae Radix Praeparata	Rehmaglutin B	Not Available	FALSE	O1C2OCC3(C2C(C(C3Cl)O)CC1O)O
MOL003722	0.9222	0.0778	0.8138	Rehmanniae Radix Praeparata	(3aS,4R,6aS)-4-hydroxy-6,6a-dimethylol-3a,4-dihydro-3H-cyclopenta[d]furan-2-one	21637649	FALSE	O1C(=O)CC2C(C=C(C12CO)CO)O

MOL003723	0.8723	0.1277	0.7977	Rehmanniae Radix Praeparata	(2S,3R,4S,5S,6R)-2-[(1R,2R)-2-hydroxy-2-[(E,3S)-3-hydroxybut-1-enyl]-1,3,3-trimethylcyclohexoxy]-6-(hydroxymethyl)tetrahydropyran-3,4,5-triol	10023290	FALSE	O(C1(C(O)(C(CCC1)(C)C)/C=C/C(O)C)C)C1OC(C(O)C(O)C1O)CO
MOL003724	0.8723	0.1277	0.7977	Rehmanniae Radix Praeparata	(2S,3R,4S,5S,6R)-2-[(1R,2R)-2-hydroxy-2-[(E,3R)-3-hydroxybut-1-enyl]-1,3,3-trimethylcyclohexoxy]-6-(hydroxymethyl)tetrahydropyran-3,4,5-triol	10430488	FALSE	O(C1(C(O)(C(CCC1)(C)C)/C=C/C(O)C)C)C1OC(C(O)C(O)C1O)CO
MOL003725	0.8609	0.1391	0.8026	Rehmanniae Radix Praeparata	Rehmaionoside C	11740990	FALSE	O(C1(C(O)(C(CCC1)(C)C)/C=C/C(=O)C)C)C1OC(C(O)C(O)C1O)CO
MOL003726	0.9018	0.0982	0.7488	Rehmanniae Radix Praeparata	rehmannioside B	Not Available	FALSE	O1C2(C1C(OC1OC(C(O)C(O)C1O)CO)C1C2C(OC=C1)OC1OC(C(O)C(O)C1O)CO)CO
MOL003727	0.9083	0.0917	0.7378	Rehmanniae Radix Praeparata	rehmannioside C	Not Available	FALSE	O(C1C2C(C(O)(C1)C)C(OC=C2)OC1OC(C(O)C(O)C1O)CO)C1OC(C(O)C(O)C1O)CO
MOL003728	0.8202	0.1798	0.7460	Rehmanniae Radix Praeparata	6-O-p-hydroxybenzoylajugol	14396661	FALSE	OC1(C2C(C(OC(=O)c3ccc(O)cc3)C1)C=COC2OC1OC(C(O)C(O)C1O)CO)C

MOL003729	0.9452	0.0548	0.8867	Rehmanniae Radix Praeparata	(3R)-2,6,6-trimethyl-3-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxycyclohexene-1-carboxylic acid	21637711	FALSE	O1C(C(C(C(C1CO)O)O)O)OC1CCC(C(=C1C)C(=O)O)(C)C
MOL003730	0.8972	0.1028	0.7516	Rehmanniae Radix Praeparata	Rehmannioside A	6325881	FALSE	C1(C(C(C(C(O1)COC1OC(C(C(C1O)O)O)CO)O)O)O)OC1OC=CC2C1C1(CO)C(C2O)O1
MOL003731	0.9221	0.0779	0.7875	Rehmanniae Radix Praeparata	Rehmaglutin A	Not Available	FALSE	O1CC2(C3C(CCOC13)C(C2O)O)O
MOL003731	0.9221	0.0779	0.7875	Picrorhizae Rhizoma	Rehmaglutin A	Not Available	FALSE	O1CC2(C3C(CCOC13)C(C2O)O)O
MOL003732	0.9245	0.0755	0.7981	Rehmanniae Radix Praeparata	Rehmaglutin D	Not Available	FALSE	O1CC2(C3C(CCOC13)C(C2Cl)O)O
MOL003732	0.9245	0.0755	0.7981	Picrorhizae Rhizoma	Rehmaglutin D	Not Available	FALSE	O1CC2(C3C(CCOC13)C(C2Cl)O)O
MOL003733	0.8518	0.1482	0.7352	Rehmanniae Radix Praeparata	6-O-vanilloylajugol	Not Available	FALSE	c1(c(ccc(c1)C(=O)OC1CC(C2C1C=COC2OC1OC(C(C(C1O)O)O)O)(O)C)O)OC
MOL003734	0.7264	0.2736	0.7281	Rehmanniae Radix Praeparata	echinacoside	Not Available	FALSE	C1(C(C(C(OC1COC1OC(C(C(C1O)O)O)CO)OCCc1ccc(c(cc1O)O)O)O)OC1C(C(C(C(O1)C)O)O)O)OC(=O)/C=C\c1cc(c(cc1)O)O
MOL003735	0.9364	0.0636	0.8850	Plantaginis Semen	aucubin	91458	FALSE	C12C(OC3OC(C(C(C3O)O)O)CO)OC=CC1C(C=C2
MOL003735	0.9364	0.0636	0.8850	Eucommiae Cortex	aucubin	91458	FALSE	C12C(OC3OC(C(C(C3O)O)O)CO)OC=CC1C(C=C2
MOL003735	0.9364	0.0636	0.8850	Figwort Root	aucubin	91458	FALSE	C12C(OC3OC(C(C(C3O)O)O)CO)OC=CC1C(C=C2
MOL003735	0.9364	0.0636	0.8850	Eucommiae Folium	aucubin	91458	FALSE	C12C(OC3OC(C(C(C3O)O)O)CO)OC=CC1C(C=C2
MOL003735	0.9364	0.0636	0.8850	Verbenae Herb	aucubin	91458	FALSE	C12C(OC3OC(C(C(C3O)O)O)CO)OC=CC1C(C=C2
MOL003735	0.9364	0.0636	0.8850	Plantaginis Herba	aucubin	91458	FALSE	C12C(OC3OC(C(C(C3O)O)O)CO)OC=CC1C(C=C2CO)O
MOL003735	0.9364	0.0636	0.8850	Rehmanniae Radix Praeparata	aucubin	91458	FALSE	C12C(OC3OC(C(C(C3O)O)O)CO)OC=CC1C(C=C2CO)O
MOL003735	0.9364	0.0636	0.8850	Buddlejae Flos	aucubin	91458	FALSE	C12C(OC3OC(C(C(C3O)O)O)CO)OC=CC1C(C=C2CO)O
MOL003736	0.9091	0.0909	0.7892	Rehmanniae Radix Praeparata	Acetylcatalpol	Not Available	FALSE	OC1C2C(C2)(C2C1C=COC2OC1OC(C(O)C(O)C1O)CO)COC(=O)C
MOL003737	0.9654	0.0346	0.8961	Belamcandae Rhizome	(+)-iridodial lactol	442438	FALSE	C12C(C(OC=C1C)O)C(CC2)C
MOL003738	0.8700	0.1300	0.9632	Folium Ilicis Cornutae	Quinone	4650	FALSE	C1(=O)C=CC(=O)C=C1
MOL003738	0.8700	0.1300	0.9632	Meliae Cortex	Quinone	4650	FALSE	C1(=O)C=CC(=O)C=C1
MOL003738	0.8700	0.1300	0.9632	Belamcandae Rhizome	Quinone	4650	FALSE	C1(=O)C=CC(=O)C=C1

MOL003739	0.8865	0.1135	0.7466	Belamcandae Rhizome	Tectoruside	5321783	FALSE	c1(ccc(cc1OC)C(=O)C)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO
MOL003740	0.9304	0.0696	0.8540	Picrorhizae Rhizoma	Androsin	164648	FALSE	c1(c(cc(cc1)C(=O)C)OC)OC1OC(C(C(C1O)O)O)CO
MOL003740	0.9304	0.0696	0.8540	Belamcandae Rhizome	Androsin	164648	FALSE	c1(c(cc(cc1)C(=O)C)OC)OC1OC(C(C(C1O)O)O)CO
MOL003740	0.9304	0.0696	0.8540	Iridis Tectori Rhizoma	Androsin	164648	FALSE	c1(c(cc(cc1)C(=O)C)OC)OC1OC(C(C(C1O)O)O)CO
MOL003742	0.3856	0.6144	0.7603	Belamcandae Rhizome	ardisianone A	Not Available	FALSE	O=C1C(=CC(=O)C=C1)C(CCCCC)CC/C=C/CCCC(OC)C
MOL003745	0.2955	0.7045	0.6408	Belamcandae Rhizome	Belamcandol A	5321906	FALSE	c1(c(cc(cc1CCCCCCCCC/C=C\CCCC)OC)OC)O
MOL003745	0.2955	0.7045	0.6408	Ardisiae Japonicae Herba	Belamcandol A	5321906	FALSE	c1(c(cc(cc1CCCCCCCCC/C=C\CCCC)OC)OC)O
MOL003749	0.7423	0.2577	0.7744	Belamcandae Rhizome	belamcandin	15290942	FALSE	O1C2C(C(=O)C(C3CC(OC)C(OC)CC3)C1C(O)C(OC)C(OC)c2
MOL003750	0.3332	0.6668	0.6527	Belamcandae Rhizome	3-methoxy-5-[(Z)-pentadec-10-enyl]phenol	10969651	FALSE	O(c1cc(CCCCCCCCC/C=C\CCCC)cc(O)c1)C
MOL003750	0.3332	0.6668	0.6527	Ardisiae Japonicae Herba	3-methoxy-5-[(Z)-pentadec-10-enyl]phenol	10969651	FALSE	O(c1cc(CCCCCCCCC/C=C\CCCC)cc(O)c1)C
MOL003751	0.7268	0.2732	0.8951	Belamcandae Rhizome	HTMF	152430	FALSE	C1(CC(=O)C2C(C(C(CC2O1)OC)OC)O)C1CC(C(CC1)OC)OC
MOL003752	0.3501	0.6499	0.6987	Calyx Seu Fructus Physalis	cycloartanol	Not Available	FALSE	C123C4(C1)C(C(C(CC4)O)(C)C)CCC2C1(C(C(CC1)C(CCCC(C)C)C)(CC3)C)C
MOL003752	0.3501	0.6499	0.6987	Perillae Fructus	cycloartanol	Not Available	FALSE	C123C4(C1)C(C(C(CC4)O)(C)C)CCC2C1(C(C(CC1)C(CCCC(C)C)C)(CC3)C)C
MOL003752	0.3501	0.6499	0.6987	Belamcandae Rhizome	cycloartanol	Not Available	FALSE	C123C4(C1)C(C(C(CC4)O)(C)C)CCC2C1(C(C(CC1)C(CCCC(C)C)C)(CC3)C)C
MOL003753	0.8976	0.1024	0.8970	Belamcandae Rhizome	dihydrokaempferide	Not Available	FALSE	O1C(C(O)C(=O)c2c1cc(O)cc2O)c1ccc(OC)cc1
MOL003755	0.8790	0.1210	0.8299	Iridis Tectori Rhizoma	irigenin	5464170	FALSE	o1c2c(c(=O)c(c3cc(OC)c(OC)c(O)c3)c1)c(O)c(OC)c(O)c2
MOL003755	0.8790	0.1210	0.8299	Belamcandae Rhizome	irigenin	5464170	FALSE	o1c2c(c(=O)c(c3cc(OC)c(OC)c(O)c3)c1)c(O)c(OC)c(O)c2
MOL003756	0.6823	0.3177	0.7330	Iridis Tectori Rhizoma	Irisflorentin	170569	FALSE	c12c(c3c(cc1occ(c2=O)c1cc(c(c(c1)OC)OC)OC)OCO3)OC
MOL003756	0.6823	0.3177	0.7330	Belamcandae Rhizome	Irisflorentin	170569	FALSE	c12c(c3c(cc1occ(c2=O)c1cc(c(c(c1)OC)OC)OC)OCO3)OC
MOL003757	0.4195	0.5805	0.6062	Belamcandae Rhizome	iristectorene B	Not Available	FALSE	OC1(C(C(/C(=C(\C)/C=O)/CC1)CCCOC(=O)CCCCCCCCCC)(CC/C=C(/C(O)C/C=C(/CCC=C(C)C)\C)\C)C
MOL003758	0.8997	0.1003	0.8662	Mori Cortex	Iristectorigenin (9CI)	5488781	FALSE	o1c2c(c(=O)c(c3cc(O)c(OC)cc3)c1)c(O)c(OC)c(O)c2
MOL003758	0.8997	0.1003	0.8662	Belamcandae Rhizome	Iristectorigenin (9CI)	5488781	FALSE	o1c2c(c(=O)c(c3cc(O)c(OC)cc3)c1)c(O)c(OC)c(O)c2

MOL003758	0.8997	0.1003	0.8662	Iridis Tectori Rhizoma	Iristectorigenin (9CI)	5488781	FALSE	o1c2c(c(=O)c(c3cc(O)c(OC)cc3)c1)c(O)c(OC)c(O)c2
MOL003759	0.9074	0.0926	0.8436	Belamcandae Rhizome	Iristectorigenin A	5491637	FALSE	o1c2c(c(=O)c(c3cc(OC)c(O)cc3)c1)c(O)c(OC)c(O)c2
MOL003759	0.9074	0.0926	0.8436	Iridis Tectori Rhizoma	Iristectorigenin A	5491637	FALSE	o1c2c(c(=O)c(c3cc(OC)c(O)cc3)c1)c(O)c(OC)c(O)c2
MOL003760	0.8431	0.1569	0.7729	Iridis Tectori Rhizoma	Iristectorin A	11968629	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(OC)c(O)c2c(occ(c2=O)c2cc(O)c(OC)cc2)c1)CO
MOL003760	0.8431	0.1569	0.7729	Belamcandae Rhizome	Iristectorin A	11968629	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(OC)c(O)c2c(occ(c2=O)c2cc(O)c(OC)cc2)c1)CO
MOL003761	0.8347	0.1653	0.7686	Belamcandae Rhizome	Iristectorin B	5318487	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(OC)c(O)c2c(occ(c2=O)c2cc(OC)c(O)cc2)c1)CO
MOL003763	0.8576	0.1424	0.8883	Belamcandae Rhizome	5-[(Z)-2-(4-hydroxy-3-methoxy-phenyl)vinyl]resorcinol	21681009	FALSE	c1c(cc(c(c1)O)OC)/C=C\c1cc(cc(c1)O)O
MOL003764	0.7404	0.2596	0.9427	Belamcandae Rhizome	6-hydroxy-3-(4-hydroxyphenyl)-5,7-dimethoxy-chromone	252471	FALSE	c1c(c(=O)c2c(c(c(cc2o1)OC)O)OC)c1ccc(cc1)O
MOL003765	0.7271	0.2729	0.6641	Belamcandae Rhizome	noririsflorentin	44133422	FALSE	c1c(c(=O)c2c(o1)cc1c(c2O)OCO1)c1cc(c(c(c1)OC)OC)OC
MOL003766	0.8492	0.1508	0.8262	Belamcandae Rhizome	Shekanin	5281810	FALSE	c12c(c(=O)c(co2)c2ccc(cc2)O)c(c(c(c1)OC1OC(C(C(C1O)O)O)CO)OC)O
MOL003766	0.8492	0.1508	0.8262	Codonopsis Radix	Shekanin	5281810	FALSE	c12c(c(=O)c(co2)c2ccc(cc2)O)c(c(c(c1)OC1OC(C(C(C1O)O)O)CO)OC)O
MOL003766	0.8492	0.1508	0.8262	Iridis Tectori Rhizoma	Shekanin	5281810	FALSE	c12c(c(=O)c(co2)c2ccc(cc2)O)c(c(c(c1)OC1OC(C(C(C1O)O)O)CO)OC)O
MOL003766	0.8492	0.1508	0.8262	Puerariae Flos	Shekanin	5281810	FALSE	c12c(c(=O)c(co2)c2ccc(cc2)O)c(c(c(c1)OC1OC(C(C(C1O)O)O)CO)OC)O
MOL003767	0.8899	0.1101	0.9148	Belamcandae Rhizome	tectorigenin	5281811	FALSE	c12c(c(=O)c(co2)c2ccc(cc2)O)c(c(c(c1)O)OC)O
MOL003767	0.8899	0.1101	0.9148	Codonopsis Radix	tectorigenin	5281811	FALSE	c12c(c(=O)c(co2)c2ccc(cc2)O)c(c(c(c1)O)OC)O
MOL003767	0.8899	0.1101	0.9148	Mori Cortex	tectorigenin	5281811	FALSE	c12c(c(=O)c(co2)c2ccc(cc2)O)c(c(c(c1)O)OC)O
MOL003767	0.8899	0.1101	0.9148	Puerariae Flos	tectorigenin	5281811	FALSE	c12c(c(=O)c(co2)c2ccc(cc2)O)c(c(c(c1)O)OC)O
MOL003767	0.8899	0.1101	0.9148	Iridis Tectori Rhizoma	tectorigenin	5281811	FALSE	c12c(c(=O)c(co2)c2ccc(cc2)O)c(c(c(c1)O)OC)O
MOL003769	0.8374	0.1626	0.8380	Belamcandae Rhizome	Irolone	5281779	FALSE	c1(ccc(cc1)c1coc2c(c1=O)c(c1c(c2)OCO1)O)O
MOL003769	0.8374	0.1626	0.8380	Trigonellae Semen	Irolone	5281779	FALSE	c1(ccc(cc1)c1coc2c(c1=O)c(c1c(c2)OCO1)O)O
MOL003773	0.6612	0.3388	0.7615	Anemarrhenae Rhizoma	Mangiferolic acid	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2C(CC1)(C(CC2)C(CC/C=C(\C)/C(=O)O)C)C)C3)(C)C)O

MOL003773	0.6612	0.3388	0.7615	Pyrrosiae Folium	Mangiferolic acid	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2C(CC1)(C(CC2)C(CC/C=C(\C)/C(=O)O)C)C)C3)(C)C)O
MOL003773	0.6612	0.3388	0.7615	Belamcandae Rhizome	Mangiferolic acid	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2C(CC1)(C(CC2)C(CC/C=C(\C)/C(=O)O)C)C)C3)(C)C)O
MOL003774	0.9230	0.0770	0.9021	Styrax	Propyl cinnamate	5270647	FALSE	O(CCC)C(=O)/C=C/c1ccccc1
MOL003775	0.9412	0.0588	0.8381	Styrax	musk ambrette	6753	FALSE	c1(c(c(c(cc1C(C)(C)C)[N+](=O)O)C)[N+](=O)O)OC
MOL003776	0.7297	0.2703	0.8856	Styrax	oleanonic acid	12313704	FALSE	O=C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(C)C
MOL003776	0.7297	0.2703	0.8856	Jujubae Fructus	oleanonic acid	12313704	FALSE	O=C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(C)C
MOL003777	0.1726	0.8274	0.6886	Styrax	Hydroabietyl alcohol	Not Available	FALSE	C12C3(C(C(CCC3)(CO)C)CCC1=CC(CC2)C(C)C)C
MOL003778	0.7553	0.2447	0.9079	Styrax	pjs-1_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)C)(C)C)O
MOL003778	0.7553	0.2447	0.9079	Achyranthis Bidentatae Radix	pjs-1_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)C)(C)C)O
MOL003779	0.7619	0.2381	0.8395	Styrax	3-Epi-oleanolic acid-28-O-alpha-L-rhamno-pyranosyl-(1-B58666)-beta-D-glucopyranoside qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)OC1OC(C(C(C1O)O)O)C)CO)C)C)C)(C)C)O
MOL003780	0.2264	0.7736	0.7321	Styrax	(2S,4aR,4bS,7S)-7-isopropyl-1,1,4a-trimethyl-2,4b,5,6,7,8-hexahydrophenanthren-2-ol	21142297	FALSE	C12(C3C(=CC=C1C(C(C=C2)O)(C)C)CC(CC3)C(C)C)C
MOL003781	0.6081	0.3919	0.7154	Styrax	Styracin	1550890	FALSE	O(C/C=C/c1ccccc1)C(=O)/C=C/c1ccccc1
MOL003781	0.6081	0.3919	0.7154	Benzoinum	Styracin	1550890	FALSE	O(C/C=C/c1ccccc1)C(=O)/C=C/c1ccccc1
MOL003782	0.5997	0.4003	0.7164	Styrax	dehydroabietic acid	6552012	FALSE	C12C(c3c(CC2)cc(cc3)C(C)C)(CCCC1(C(=O)O)C)C

MOL003783	0.8799	0.1201	0.6163	Styrax	(3R,3aR,6R,7S,8aS)-3,6,8,8-tetramethylhexahydro-1H-3a,7-methanoazulen-5(4H)-one	Not Available	FALSE	C1CC(C23CC(=O)C(C(C(C12)(C)C)C3)C)C
MOL003784	0.9481	0.0519	0.9595	Styrax	Propyl phenylacetate	221641	FALSE	c1(CC(=O)OCCC)ccccc1
MOL003785	0.9409	0.0591	0.9700	Paederiae Scandentis Herba	Benzyl acetate	8785	FALSE	c1(COC(=O)C)ccccc1
MOL003785	0.9409	0.0591	0.9700	Mume Flos	Benzyl acetate	8785	FALSE	c1(COC(=O)C)ccccc1
MOL003785	0.9409	0.0591	0.9700	Styrax	Benzyl acetate	8785	FALSE	c1(COC(=O)C)ccccc1
MOL003785	0.9409	0.0591	0.9700	Caryophylliflos	Benzyl acetate	8785	FALSE	c1(COC(=O)C)ccccc1
MOL003787	0.8576	0.1424	0.8872	Styrax	Isolapachol	Not Available	FALSE	OC1=C(/C=C\C(C)C)C(=O)C(=O)c2c1cccc2
MOL003788	0.8489	0.1511	0.8435	Evodiae Fructus	Cinnamein	5273469	FALSE	c1(/C=C/C(=O)OCc2ccccc2)ccccc1
MOL003788	0.8489	0.1511	0.8435	Cornus Officinalis Sieb. Et Zucc.	Cinnamein	5273469	FALSE	c1(/C=C/C(=O)OCc2ccccc2)ccccc1
MOL003788	0.8489	0.1511	0.8435	Benzoinum	Cinnamein	5273469	FALSE	c1(/C=C/C(=O)OCc2ccccc2)ccccc1
MOL003788	0.8489	0.1511	0.8435	Styrax	Cinnamein	5273469	FALSE	c1(/C=C/C(=O)OCc2ccccc2)ccccc1
MOL003789	0.9079	0.0921	0.8948	Trollius Chinensis	Coumaran	10329	FALSE	c12c(OCC1)cccc2
MOL003789	0.9079	0.0921	0.8948	Campsis Flos	Coumaran	10329	FALSE	c12c(OCC1)cccc2
MOL003789	0.9079	0.0921	0.8948	Styrax	Coumaran	10329	FALSE	c12c(OCC1)cccc2
MOL003789	0.9079	0.0921	0.8948	Cornus Officinalis Sieb. Et Zucc.	Coumaran	10329	FALSE	c12c(OCC1)cccc2
MOL003789	0.9079	0.0921	0.8948	Cannabis Sativa L.	Coumaran	10329	FALSE	c12c(OCC1)cccc2
MOL003789	0.9079	0.0921	0.8948	Ginsen Radix Et Rhizoma Rubra	Coumaran	10329	FALSE	c12c(OCC1)cccc2
MOL003789	0.9079	0.0921	0.8948	Evodiae Fructus	Coumaran	10329	FALSE	c12c(OCC1)cccc2
MOL003789	0.9079	0.0921	0.8948	Bomboo Juice	Coumaran	10329	FALSE	c12c(OCC1)cccc2
MOL003789	0.9079	0.0921	0.8948	Scutellariae Barbatae Herba	Coumaran	10329	FALSE	c12c(OCC1)cccc2
MOL003789	0.9079	0.0921	0.8948	Eriobotryae Folium	Coumaran	10329	FALSE	c12c(OCC1)cccc2
MOL003789	0.9079	0.0921	0.8948	Siphonostegiae Herba	Coumaran	10329	FALSE	c12c(OCC1)cccc2
MOL003789	0.9079	0.0921	0.8948	Microctis Folium	Coumaran	10329	FALSE	c12c(OCC1)cccc2
MOL003790	0.2455	0.7545	0.6085	Styrax	Androstane	94144	FALSE	C12C(C3(C(CC2)CCCC3)C)CCC2(C1CCC2)C
MOL003791	0.4292	0.5708	0.6686	Phytolaccae Radix	Linolein, 2-mono-	5365676	FALSE	OCC(OC(=O)CCCCCCC/C=C\C/C=C\CCCCC)CO

MOL003792	0.7415	0.2585	0.8040	Phytolaccae Radix	esculentoside N	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C(=O)OC)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1O)C)(CO)C)C1OC(C(O)C(OC2OC(C(O)C(O)C2O)CO)C1OC1OCC(O)C(O)C1O)CO
MOL003793	0.6761	0.3239	0.7519	Phytolaccae Radix	esculentoside N_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C(=O)OC)C(=O)O)C)(CC2)C)(CC1O)C)(CO)C
MOL003794	0.7230	0.2770	0.7229	Phytolaccae Radix	Jaligonic acid	99610	FALSE	C12(C3C(C4(C(=CC3)C3C(C(=O)O)(CC4)CCC(C3)(C(=O)O)C)C)(CCC1C(C(C(C2)O)O)(CO)C)C)C
MOL003795	0.9200	0.0800	0.9775	Bombyx Mori L.	CPI	6931663	FALSE	C1(CCCCN1)C(=O)O
MOL003795	0.9200	0.0800	0.9775	Lablab Semen Album	CPI	6931663	FALSE	C1(CCCCN1)C(=O)O
MOL003795	0.9200	0.0800	0.9775	Phytolaccae Radix	CPI	6931663	FALSE	C1(CCCCN1)C(=O)O
MOL003796	0.7794	0.2206	0.8922	Phytolaccae Radix	Xanthomicrol	73207	FALSE	c12c(c(c(c(c1OC)OC)OC)O)c(=O)cc(o2)c1ccc(cc1)O
MOL003797	0.2609	0.7391	0.6703	Phytolaccae Radix	2-[[(1R,4aS,8aR)-5,5,8a-trimethyl-2-methylene-decalin-1-yl]methyl]hydroquinone	10946969	FALSE	Oc1c(CC2C3(C(C(CCC3)(C)C)CCC2=C)C)cc(O)cc1
MOL003798	0.3559	0.6441	0.6269	Phytolaccae Radix	A-SPINASTEROL	Not Available	FALSE	C1C(CC2(C(C1)(C1(C(CC2)C2(C(CC1)(C(CC2)(C(/C=C/C(C(C)C)CC)C)C)C)C)C)C)O
MOL003799	0.8928	0.1072	0.9020	Phytolaccae Radix	Glutamyl histidine	Not Available	FALSE	c1c([nH]cn1)CC(NC(=O)CCC(N)C(=O)O)C(=O)O
MOL003800	0.8970	0.1030	0.9325	Phytolaccae Radix	CIR	6992098	FALSE	C(=O)(C(N)CCCNC(=O)N)O
MOL003800	0.8970	0.1030	0.9325	Lycii Fructus	CIR	6992098	FALSE	C(=O)(C(N)CCCNC(=O)N)O
MOL003800	0.8970	0.1030	0.9325	Trichosanthis Radix	CIR	6992098	FALSE	C(=O)(C(N)CCCNC(=O)N)O
MOL003802	0.9322	0.0678	0.9555	Campsis Flos	(2R)-2-ethylhexan-1-ol	6991979	FALSE	C(C(CCCC)CC)O
MOL003802	0.9322	0.0678	0.9555	Ephedra Herba	(2R)-2-ethylhexan-1-ol	6991979	FALSE	C(C(CCCC)CC)O
MOL003802	0.9322	0.0678	0.9555	Mori Fructus	(2R)-2-ethylhexan-1-ol	6991979	FALSE	C(C(CCCC)CC)O
MOL003802	0.9322	0.0678	0.9555	Phytolaccae Radix	(2R)-2-ethylhexan-1-ol	6991979	FALSE	C(C(CCCC)CC)O
MOL003803	0.6811	0.3189	0.7683	Phytolaccae Radix	phytolaccagenic acid	Not Available	FALSE	C1C(C(C2(C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C(=O)OC)C)C(=O)O)C)C)C)(C)CO)O

MOL003804	0.6380	0.3620	0.8358	Phytolaccae Radix	Phytolaccasaponin G	Not Available	FALSE	C1(C(CC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C)(C(=O)OC)CC4C3=CCC21)C)O)OC1C(O)C(O)C(O)CO1
MOL003805	0.6761	0.3239	0.7519	Phytolaccae Radix	Phytolaccasaponin G_qt	Not Available	FALSE	C1(C(CC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C)(C(=O)OC)CC4C3=CCC21)C)O)O
MOL003806	0.6761	0.3239	0.7519	Phytolaccae Radix	phytolaccagenin	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C(=O)OC)C(=O)O)C)(CC2)C)(CC1O)C)(CO)C
MOL003807	0.7134	0.2866	0.7483	Phytolaccae Radix	esculentic acid	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C(=O)O)C(=O)O)C)(CC2)C)(CC1)C)(CO)C
MOL003808	0.6380	0.3620	0.8358	Phytolaccae Radix	esculentoside B	Not Available	FALSE	C1OC(C(C(C1O)O)O)OC1C(CC2(C(C1(C)CO)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C(=O)OC)C(=O)O)C)C)C)O
MOL003809	0.6761	0.3239	0.7519	Phytolaccae Radix	esculentoside G_qt	Not Available	FALSE	OC1C(CC2(C(C1(C)CO)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C(=O)OC)C(=O)O)C)C)C)O
MOL003810	0.7173	0.2827	0.8479	Phytolaccae Radix	esculentoside C	Not Available	FALSE	C1OC(C(C(C1OC1C(C(C(C(O1)CO)O)O)O)O)O)OC1C(CC2(C(C1(C)CO)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C(=O)OC)C(=O)O)C)C)C)O
MOL003811	0.6761	0.3239	0.7519	Phytolaccae Radix	esculentoside C_qt	Not Available	FALSE	OC1C(CC2(C(C1(C)CO)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C(=O)OC)C(=O)O)C)C)C)O
MOL003812	0.6402	0.3598	0.8478	Phytolaccae Radix	esculentoside D2	Not Available	FALSE	C1(OC(C(C(C1O)O)O)O)OC1C(CC2(C(C1(C)CO)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C(=O)OC)C(=O)O)C)C)C)O)CO
MOL003813	0.7024	0.2976	0.8495	Phytolaccae Radix	esculentoside D2	Not Available	FALSE	C1OC(C(C(C1O)O)OC1C(C(C(CO1)O)O)O)OC1C(CC2(C(C1(C)CO)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C(=O)OC)C(=O)O)C)C)C)O
MOL003814	0.7034	0.2966	0.8336	Phytolaccae Radix	esculentoside E	Not Available	FALSE	C1(C(C(C(OC1)OC1C(C2C(CC1O)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C(=O)O)C(=O)O)C)C)(CO)C)O)O)O
MOL003815	0.7230	0.2770	0.7229	Phytolaccae Radix	esculentoside P_qt	Not Available	FALSE	OC1C(C2C(CC1O)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C(=O)O)C(=O)O)C)C)(CO)C
MOL003816	0.7436	0.2564	0.8438	Phytolaccae Radix	esculentoside F	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C(=O)O)C(=O)O)C)(CC2)C)(CC1O)C)(CO)C)C1OCC(OC2OC(C(O)C(O)C2O)CO)C(O)C1O
MOL003817	0.7230	0.2770	0.7229	Phytolaccae Radix	esculentoside F_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C(=O)O)C(=O)O)C)(CC2)C)(CC1O)C)(CO)C
MOL003818	0.7724	0.2276	0.8213	Phytolaccae Radix	esculentoside G	Not Available	FALSE	C1OC(C(C(C1OC1C(C(C(C(C1)CO)O)O)O)O)O)OC1C(CC2(C(C1(C)CO)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C(=O)OC)C(=O)OC1OC(C(C(C1O)O)O)CO)C)C)C)O
MOL003819	0.7554	0.2446	0.8238	Phytolaccae Radix	esculentoside H	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C(=O)OC)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1O)C)(CO)C)C1OCC(OC2OC(C(O)C(O)C2O)CO)C(O)C1O

MOL003820	0.7548	0.2452	0.8236	Phytolaccae Radix	esculentoside I	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C(=O)OC)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1O)C)(CO)C)C1OC(C(OC2OC(C(O)C(O)C2O)CO)C(O)C1O)CO
MOL003821	0.7834	0.2166	0.8309	Phytolaccae Radix	esculentoside J	Not Available	FALSE	C1OC(C(C(C1OC1C(C(C(C(C1)CO)O)O)O)O)OC1C(CC2(C(C1(C)CO)CCC1(C2CC=C2C1CCC1(C2CC(CC1)(C)CO)C(=O)OC1OC(C(C(C1O)O)O)CO)C)O
MOL003822	0.7219	0.2781	0.7250	Phytolaccae Radix	esculentoside J_qt	Not Available	FALSE	OC1C(CC2(C(C1(C)CO)CCC1(C2CC=C2C1CCC1(C2CC(CC1)(C)CO)C(=O)O)C)C)O
MOL003823	0.7336	0.2664	0.7967	Phytolaccae Radix	esculentoside K	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C(=O)OC)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(CO)C)C1OC(C(O)C(OC2OC(C(O)C(O)C2O)CO)C1OC1OCC(O)C(O)C1O)CO
MOL003824	0.6772	0.3228	0.7807	Phytolaccae Radix	esculentoside L_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C(=O)OC)C(=O)O)C)(CC2)C)(CC1)C)(CO)C
MOL003825	0.7369	0.2631	0.8197	Phytolaccae Radix	esculentoside L	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C(=O)OC)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(CO)C)C1OCC(OC2OC(C(O)C(O)C2O)CO)C(O)C1O
MOL003826	0.7503	0.2497	0.8212	Phytolaccae Radix	esculentoside M	Not Available	FALSE	C1OC(C(C(C1OC1C(C(C(C(O1)CO)O)O)O)O)O)OC1C(CC2(C(C1(C)CO)CCC1(C2C(=O)C=C2C1(CCC1(C2CC(CC1)(C)C(=O)OC)C(=O)OC1OC(C(C(C1O)O)O)CO)C)C)O
MOL003827	0.6547	0.3453	0.7309	Phytolaccae Radix	esculentoside M_qt	Not Available	FALSE	OC1C(CC2(C(C1(C)CO)CCC1(C2C(=O)C=C2C1(CCC1(C2CC(CC1)(C)C(=O)OC)C(=O)O)C)C)O
MOL003828	0.6907	0.3093	0.7842	Phytolaccae Radix	esculentoside O	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C(=O)O)C(=O)O)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1O
MOL003829	0.7157	0.2843	0.8439	Phytolaccae Radix	esculentoside P	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C(=O)O)C(=O)O)C)(CC2)C)(CC1O)C)(CO)C)C1OC(C(O)C(O)C1O)CO
MOL003830	0.7718	0.2282	0.8252	Phytolaccae Radix	esculentoside Q	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C(=O)O)C(=O)O)C)(CC2)C)(CC1O)C)(CO)C)C1OC(C(O)C(OC2OCC(OC3OC(C(O)C(O)C3O)CO)C(O)C2O)C1O)CO
MOL003831	0.7230	0.2770	0.7229	Phytolaccae Radix	esculentoside Q_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C(=O)O)C(=O)O)C)(CC2)C)(CC1O)C)(CO)C
MOL003832	0.7173	0.2827	0.8479	Phytolaccae Radix	esculentoside A	Not Available	FALSE	C1(CCC2(C(C1)C1=CCC3C(C1(CC2)C)(CCC1C3(CC(C(C1(C)CO)OC1OCC(C(C1O)O)OC1OC(C(C(C1O)O)O)CO)O)C)C)C(=O)O)(C(=O)OC)C
MOL003833	0.6761	0.3239	0.7519	Phytolaccae Radix	esculentoside A_qt	Not Available	FALSE	C1(CCC2(C(C1)C1=CCC3C(C1(CC2)C)(CCC1C3(CC(C(C1(C)CO)O)O)C)C)C(=O)O)(C(=O)OC)C
MOL003834	0.6547	0.3453	0.7309	Phytolaccae Radix	esculentagenin	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3=O)C3C(CC4)(CCC(C3)(C)C(=O)OC)C(=O)O)C)(CC2)C)(CC1O)C)(CO)C

MOL003835	0.7425	0.2575	0.8215	Phytolaccae Radix	Esculentoside L1	Not Available	FALSE	C1(CCC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C(=O)OC5C(O)C(O)C(O)C(O5)CO)CCC(C)(C(=O)OC)CC4C3=CCC21)C)OC1C(OC2C(O)C(O)C(O)C(O2)CO)C(O)C(O)CO1
MOL003836	0.6772	0.3228	0.7807	Phytolaccae Radix	Esculentoside L1_qt	Not Available	FALSE	C1(CCC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C)(C(=O)OC)CC4C3=CCC21)C)O
MOL003837	0.9567	0.0433	0.8665	Impatiens Balsamina	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Artemisia Annua L.	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Prunellae Spica	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Calendula Officinalis	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Semen Aesculi	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Perilla Frutescens	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Folium Artemisiae Argyi	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Rubi Fructus	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Lunulatae Herba	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Cichorii Radix	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Radix Bupleuri	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Mori Cortex	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Inulae Herba	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Cimicifugae Rhizoma	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Trollius Chinensis	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Phytolaccae Radix	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Ailanthi Altissimae Fructus	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Chaenomeles Sinensis (Thouin) Koehne	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Actinidia Chinensis Planch	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Fraxini Cortex	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Ajugae Decumbentis Herba	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Violsse Herba	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Morindae Officinalis Radix	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Semen Euphorbiae	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O
MOL003837	0.9567	0.0433	0.8665	Saxifraga Stolonifera	esculetin	5281416	TRUE	c1(c(cc2c(c1)ccc(=O)o2)O)O

MOL003838	0.6641	0.3359	0.7887	Phytolaccae Radix	(4aS,6aR,6bR,8aR,9R,10S,12aS,13R,14aS,14bS)-10-acetoxy-13-hydroxy-2,2,6b,9,12a,14a-hexamethyl-9-methylol-1,3,4,5,6a,7,8,8a,10,11,12,13,14,14b-tetradecahydropicene-4a-carboxylic acid	10052734	FALSE	OC1C2C3(C(C(C(OC(=O)C)CC3)(CO)C)CCC2(C2=CCC3(C(C2(C1)C)CC(CC3)(C)C)C(=O)O)C)C
MOL003839	0.8709	0.1291	0.8054	Radix Bupleuri	(-)-Guaia-1(10),11-dien-15-al	Not Available	FALSE	C12=C(CCC(CC1C(CC2)C)C(=C)C)C=O
MOL003839	0.8709	0.1291	0.8054	Mori Follum	(-)-Guaia-1(10),11-dien-15-al	Not Available	FALSE	C12=C(CCC(CC1C(CC2)C)C(=C)C)C=O
MOL003840	0.7324	0.2676	0.8160	Mori Cortex	1'-Methoxy-2'-hydroxydihydromollugin	Not Available	FALSE	c1cccc2c1c(c(c1c2OC(C(C1OC)O)(C)C)C(=O)OC)O
MOL003840	0.7324	0.2676	0.8160	Polygoni Avicularis Herba	1'-Methoxy-2'-hydroxydihydromollugin	Not Available	FALSE	c1cccc2c1c(c(c1c2OC(C(C1OC)O)(C)C)C(=O)OC)O
MOL003840	0.7324	0.2676	0.8160	Mori Follum	1'-Methoxy-2'-hydroxydihydromollugin	Not Available	FALSE	c1cccc2c1c(c(c1c2OC(C(C1OC)O)(C)C)C(=O)OC)O
MOL003842	0.5705	0.4295	0.6618	Mori Follum	Albanol	Not Available	FALSE	c1cc(c(cc1O)O)C12C3C(c4c(O1)cc(cc4)O)CC(=CC3c1c(O2)cc(cc1O)c1cc2c(o1)cc(cc2)O)C
MOL003843	0.7038	0.2962	0.8024	Mori Follum	Ecdysterone-3-O-beta-D-glucopyranoside	Not Available	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C(CC2)C(O)C(CCC(C)(O)C)O)C)O)C)OC1OC(C(C(C1O)O)O)CO)O

MOL003843	0.7038	0.2962	0.8024	Achyranthis Asperae Herba	Ecdysterone-3-O-beta-D-glucopyranoside	Not Available	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C(CC2)C(O)C(CCC(C)(O)C)O)C)O)C)OC1OC(C(C(C1O)O)O)CO)O
MOL003844	0.6426	0.3574	0.7202	Mori Follum	Ecdysterone-3-O-beta-D-glucopyranoside_qt	Not Available	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C(CC2)C(O)C(CCC(C)(O)C)O)C)O)C)O)O
MOL003844	0.6426	0.3574	0.7202	Achyranthis Asperae Herba	Ecdysterone-3-O-beta-D-glucopyranoside_qt	Not Available	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C(CC2)C(O)C(CCC(C)(O)C)O)C)O)C)O)O
MOL003845	0.8872	0.1128	0.6403	Panax Ginseng C. A. Mey.	Folinic acid	Not Available	FALSE	n1c(nc2c(c1O)N(CC(N2)CNc1ccc(C(=O)NC(C(=O)O)CCC(=O)O)cc1)C=O)N
MOL003845	0.8872	0.1128	0.6403	Mori Follum	Folinic acid	Not Available	FALSE	n1c(nc2c(c1O)N(CC(N2)CNc1ccc(C(=O)NC(C(=O)O)CCC(=O)O)cc1)C=O)N
MOL003846	0.9234	0.0766	0.8840	Sojae Semen Nigrum	8-[(2S)-2,3-dihydroxy-3-methyl-butoxy]-4-methoxy-1-methyl-carbostyril	673471	TRUE	c1cc(c2c(c1)c(cc(=O)n2C)OC)OCC(O)C(C)(O)C
MOL003846	0.9234	0.0766	0.8840	Mori Follum	8-[(2S)-2,3-dihydroxy-3-methyl-butoxy]-4-methoxy-1-methyl-carbostyril	673471	TRUE	c1cc(c2c(c1)c(cc(=O)n2C)OC)OCC(O)C(C)(O)C
MOL003846	0.9234	0.0766	0.8840	Sesami Nigrum Semen	8-[(2S)-2,3-dihydroxy-3-methyl-butoxy]-4-methoxy-1-methyl-carbostyril	673471	TRUE	c1cc(c2c(c1)c(cc(=O)n2C)OC)OCC(O)C(C)(O)C
MOL003847	0.1344	0.8656	0.6883	Mori Follum	Inophyllum E	Not Available	FALSE	c1cc(ccc1)c1c2c(oc(=O)c1)c1c(c3c2OC(C=C3)(C)C)OC(C(C1=O)C)C
MOL003847	0.1344	0.8656	0.6883	Achyranthis Bidentatae Radix	Inophyllum E	Not Available	FALSE	c1cc(ccc1)c1c2c(oc(=O)c1)c1c(c3c2OC(C=C3)(C)C)OC(C(C1=O)C)C
MOL003848	0.1941	0.8059	0.7153	Papaveris Pericarpium	Insularine	Not Available	FALSE	c12ccc(cc1)Oc1c3c(cc(c1OC)OC)CCN(C3Cc1cc3c(Oc4c5C(C2)N(CCc5cc(c4OC3)OC)C)cc1)C

MOL003848	0.1941	0.8059	0.7153	Mori Follum	Insularine	Not Available	FALSE	c12ccc(cc1)Oc1c3c(cc(c1OC)OC)CCN(C3Cc1cc3c(Oc4c5C(C2)N(CCc5cc(c4OC3)OC)C)cc1)C
MOL003850	0.2061	0.7939	0.7139	Mori Follum	26-Hydroxy-dammara-20,24-dien-3-one	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(=C)CC/C=C(\C)/CO)C)C)C)(C)C
MOL003851	0.6046	0.3954	0.7597	Mori Follum	Isoramanone	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CC(C1(C3(CCC1C(=O)C)O)C)O)O
MOL003851	0.6046	0.3954	0.7597	Inulae Flos	Isoramanone	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CC(C1(C3(CCC1C(=O)C)O)C)O)O
MOL003851	0.6046	0.3954	0.7597	Houttuyniae Herba	Isoramanone	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CC(C1(C3(CCC1C(=O)C)O)C)O)O
MOL003851	0.6046	0.3954	0.7597	Pyrrosiae Folium	Isoramanone	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CC(C1(C3(CCC1C(=O)C)O)C)O)O
MOL003853	0.5156	0.4844	0.6592	Mori Cortex	Kuwanon H	5281668	FALSE	c1(c(cc(c2c1oc(c(c2=O)CC=C(C)C)c1c(O)cc(cc1)O)O)O)C1C(C(CC(=C1)C)c1c(O)cc(cc1)O)C(=O)c1ccc(c(c1O)CC=C(C)C)O
MOL003853	0.5156	0.4844	0.6592	Mori Follum	Kuwanon H	5281668	FALSE	c1(c(cc(c2c1oc(c(c2=O)CC=C(C)C)c1c(O)cc(cc1)O)O)O)C1C(C(CC(=C1)C)c1c(O)cc(cc1)O)C(=O)c1ccc(c(c1O)CC=C(C)C)O
MOL003854	0.5209	0.4791	0.7951	Mori Follum	Kwangsine	5318907	FALSE	Oc1c(c2c(O)ccc3c2c2c([nH]3)c3c(c(c2)C)OC(C=C3)(C)C)c2c(cc1)[nH]c1c2cc(c2c1C=CC(O2)(C)C)C
MOL003855	0.7613	0.2387	0.8412	Mori Follum	Macranthoidin A_qt	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)CO)O)C)C)C)C(=O)O
MOL003856	0.8319	0.1681	0.8483	Mori Cortex	Moracin B	5319887	FALSE	c1(c(cc2c(c1)cc(o2)c1cc(cc(c1)O)OC)OC)O
MOL003856	0.8319	0.1681	0.8483	Mori Follum	Moracin B	5319887	FALSE	c1(c(cc2c(c1)cc(o2)c1cc(cc(c1)O)OC)OC)O
MOL003857	0.7141	0.2859	0.7059	Mori Cortex	Moracin C	155248	FALSE	c1c(cc2c(c1)cc(o2)c1cc(c(c(c1)O)CC=C(C)C)O)O
MOL003857	0.7141	0.2859	0.7059	Mori Follum	Moracin C	155248	FALSE	c1c(cc2c(c1)cc(o2)c1cc(c(c(c1)O)CC=C(C)C)O)O
MOL003858	0.6129	0.3871	0.8241	Mori Follum	Moracin D	641378	FALSE	c1c(cc2c(c1)cc(o2)c1cc2c(c(c1)O)C=CC(O2)(C)C)O
MOL003858	0.6129	0.3871	0.8241	Mori Cortex	Moracin D	641378	FALSE	c1c(cc2c(c1)cc(o2)c1cc2c(c(c1)O)C=CC(O2)(C)C)O
MOL003859	0.5471	0.4529	0.8220	Mori Follum	Moracin E	5319888	FALSE	c1c(cc2c(c1)cc(o2)c1c2c(cc(c1)O)OC(C=C2)(C)C)O
MOL003860	0.9265	0.0735	0.8801	Mori Cortex	Moracin F	5319889	FALSE	COc1c(OC)cc2c(c1)oc(c2)c1cc(cc(c1)O)O
MOL003860	0.9265	0.0735	0.8801	Mori Follum	Moracin F	5319889	FALSE	COc1c(OC)cc2c(c1)oc(c2)c1cc(cc(c1)O)O
MOL003861	0.6710	0.3290	0.8055	Mori Follum	Moracin G	5319890	FALSE	c12c(ccc3c1oc(c3)c1cc(cc(c1)O)O)OCC(=CC2)C
MOL003862	0.5480	0.4520	0.7348	Mori Follum	Moracin H	5319891	FALSE	c12c(cc(c3c1oc(c3)c1cc(cc(c1)O)O)O)OCC(=CC2)C
MOL003863	0.5684	0.4316	0.7885	Mori Follum	Morellic acid	Not Available	FALSE	C1(C=CC2C(O1)C(C1(C2O)C(=O)C2=CC3C(=O)C4(C2(O1)C(C(O4)(C)C)C3)C/C=C(\C(=O)O)/C)CC=C(C)C)C)C
MOL003864	0.8819	0.1181	0.8412	Mori Follum	Morindon	442756	FALSE	Oc1c(c2c(cc1)C(=O)c1c(C2=O)ccc(c1O)C)O
MOL003864	0.8819	0.1181	0.8412	Morindae Officinalis Radix	Morindon	442756	FALSE	Oc1c(c2c(cc1)C(=O)c1c(C2=O)ccc(c1O)C)O
MOL003865	0.7794	0.2206	0.8308	Mori Cortex	Moscatin	194774	FALSE	c1cc2c(c(c1)O)c1c(OC)cc(cc1cc2)O
MOL003865	0.7794	0.2206	0.8308	Mori Follum	Moscatin	194774	FALSE	c1cc2c(c(c1)O)c1c(OC)cc(cc1cc2)O
MOL003867	0.8899	0.1101	0.7407	Cortex Moutan	Paeonolide	442923	FALSE	c1c(ccc(c1OC1C(C(C(C(O1)COC1C(C(C(CO1)O)O)O)O)O)O)C(=O)C)OC

MOL003867	0.8899	0.1101	0.7407	Radix Paeoniae Rubra	Paeonolide	442923	FALSE	c1c(ccc(c1OC1C(C(C(C(O1)COC1C(C(C(CO1)O)O)O)O)O)O)C(=O)C)OC
MOL003867	0.8899	0.1101	0.7407	Mori Follum	Paeonolide	442923	FALSE	c1c(ccc(c1OC1C(C(C(C(O1)COC1C(C(C(CO1)O)O)O)O)O)O)C(=O)C)OC
MOL003869	0.8229	0.1771	0.6402	Mori Follum	3,4-Dihydroxydihydgaroaroiuran	Not Available	FALSE	C1(C(C23C(CC1)(CCC(C2)C(C3)(C)C)C)(O)C)O
MOL003870	0.9060	0.0940	0.9341	Mori Follum	gynesine	5571	FALSE	c1(c[n+](ccc1)C)C(=O)O
MOL003870	0.9060	0.0940	0.9341	Arisaematis Rhizoma	gynesine	5571	FALSE	c1(c[n+](ccc1)C)C(=O)O
MOL003870	0.9060	0.0940	0.9341	Arum Ternatum Thunb.	gynesine	5571	FALSE	c1(c[n+](ccc1)C)C(=O)O
MOL003870	0.9060	0.0940	0.9341	Dictamni Cortex	gynesine	5571	FALSE	c1(c[n+](ccc1)C)C(=O)O
MOL003870	0.9060	0.0940	0.9341	Cannabis Sativa L.	gynesine	5571	FALSE	c1(c[n+](ccc1)C)C(=O)O
MOL003870	0.9060	0.0940	0.9341	Lablab Semen Album	gynesine	5571	FALSE	c1(c[n+](ccc1)C)C(=O)O
MOL003871	0.9508	0.0492	0.9163	Mori Follum	Chlorogenic acid	Not Available	FALSE	C1C(O)(C(=O)O)C(C)(C(O)C1O)OC(=O)/C=C/c1ccc(c(c1)O)O
MOL003872	0.9367	0.0633	0.7871	Mori Follum	α－ionone	54682930	FALSE	c1ccc2c(c1)c(cc(=O)o2)O
MOL003872	0.9367	0.0633	0.7871	Bombyx Mori L.	α－ionone	54682930	FALSE	c1ccc2c(c1)c(cc(=O)o2)O
MOL003873	0.9247	0.0753	0.9448	Mori Follum	Inositol	892	FALSE	C1(C(C(C(C(C1O)O)O)O)O)O
MOL003875	0.9613	0.0387	0.8203	Mori Follum	7-Hydroxycoumarin	68348948	FALSE	C1(=C)C=Cc2c(O1)cc(cc2)O
MOL003876	0.8829	0.1171	0.8565	Mori Follum	(2R)-2-[[4-[[(6S)-2-amino-5-formyl-4-keto-1,6,7,8-tetrahydropteridin-6-yl]methylamino]benzoyl]amino]glutaric acid	3033683	FALSE	n1c2c(c(=O)[nH]c1N)N(C(CN2)CNc1ccc(cc1)C(=O)NC(C(=O)O)CCC(=O)O)C=O
MOL003877	0.9325	0.0675	0.9682	Mori Fructus	Fuseloel	31260	FALSE	CC(C)CCO
MOL003877	0.9325	0.0675	0.9682	Campsis Flos	Fuseloel	31260	FALSE	CC(C)CCO
MOL003877	0.9325	0.0675	0.9682	Cornus Officinalis Sieb. Et Zucc.	Fuseloel	31260	FALSE	CC(C)CCO
MOL003877	0.9325	0.0675	0.9682	Sesami Nigrum Semen	Fuseloel	31260	FALSE	CC(C)CCO
MOL003877	0.9325	0.0675	0.9682	Capsici Fructus	Fuseloel	31260	FALSE	CC(C)CCO
MOL003877	0.9325	0.0675	0.9682	Ginkgo Folium	Fuseloel	31260	FALSE	CC(C)CCO
MOL003877	0.9325	0.0675	0.9682	Rose Rugosae Flos	Fuseloel	31260	FALSE	CC(C)CCO
MOL003877	0.9325	0.0675	0.9682	Mori Follum	Fuseloel	31260	FALSE	CC(C)CCO

MOL003879	0.6785	0.3215	0.7820	Mori Follum	4-Prenylresveratrol	Not Available	FALSE	c1(cc(cc(c1CC=C(C)C)O)/C=C\c1ccc(cc1)O)O
MOL003880	0.9296	0.0704	0.8279	Mori Follum	5-Hydroxycoumarin	5318179	FALSE	c1ccc2c(c1O)ccc(=O)o2
MOL003881	0.9514	0.0486	0.8236	Mori Follum	6-Hydroxycoumarin	99477	FALSE	c1(ccc2c(c1)ccc(=O)o2)O
MOL003881	0.9514	0.0486	0.8236	Cortex Moutan	6-Hydroxycoumarin	99477	FALSE	c1(ccc2c(c1)ccc(=O)o2)O
MOL003882	0.1682	0.8318	0.7663	Mori Follum	7alpha,21S,25-Trihydroxy-3beta-acetoxy-21S,23R-epoxy-9(11)-en-dammarane	Not Available	FALSE	C1C(C(C2C(C1)(C1=CCC3C(C1(C(C2)O)C)(CCC3C1CC(OC1O)CC(C)(C)O)C)C)(C)C)OC(=O)C
MOL003882	0.1682	0.8318	0.7663	Trigonellae Semen	7alpha,21S,25-Trihydroxy-3beta-acetoxy-21S,23R-epoxy-9(11)-en-dammarane	Not Available	FALSE	C1C(C(C2C(C1)(C1=CCC3C(C1(C(C2)O)C)(CCC3C1CC(OC1O)CC(C)(C)O)C)C)(C)C)OC(=O)C
MOL003883	0.8447	0.1553	0.8028	Asparagi Radix	Nyasol	6438674	FALSE	Oc1ccc(C(/C=C/c2ccc(O)cc2)C=C)cc1
MOL003883	0.8447	0.1553	0.8028	Anemarrhenae Rhizoma	Nyasol	6438674	FALSE	Oc1ccc(C(/C=C/c2ccc(O)cc2)C=C)cc1
MOL003884	0.7787	0.2213	0.8704	Asparagi Radix	Nevadensin	160921	FALSE	c1(cc(=O)c2c(c(c(c(c2o1)OC)O)OC)O)c1ccc(cc1)OC
MOL003885	0.2872	0.7128	0.7586	Herba Solani Lyrati	Yamogenin	Not Available	FALSE	C12(C(C3C(C4(C(=CC3)CC(CC4)O)C)CC2)CC2C1C(C1(O2)OCC(CC1)C)C)C
MOL003885	0.2872	0.7128	0.7586	Dioscoreae Hypoglaucae Rhizoma	Yamogenin	Not Available	FALSE	C12(C(C3C(C4(C(=CC3)CC(CC4)O)C)CC2)CC2C1C(C1(O2)OCC(CC1)C)C)C
MOL003885	0.2872	0.7128	0.7586	Tribulifructus	Yamogenin	Not Available	FALSE	C12(C(C3C(C4(C(=CC3)CC(CC4)O)C)CC2)CC2C1C(C1(O2)OCC(CC1)C)C)C
MOL003885	0.2872	0.7128	0.7586	Polygonati Odorati Rhizoma	Yamogenin	Not Available	FALSE	C12(C(C3C(C4(C(=CC3)CC(CC4)O)C)CC2)CC2C1C(C1(O2)OCC(CC1)C)C)C
MOL003885	0.2872	0.7128	0.7586	Asparagi Radix	Yamogenin	Not Available	FALSE	C12(C(C3C(C4(C(=CC3)CC(CC4)O)C)CC2)CC2C1C(C1(O2)OCC(CC1)C)C)C
MOL003885	0.2872	0.7128	0.7586	Smilax China	Yamogenin	Not Available	FALSE	C12(C(C3C(C4(C(=CC3)CC(CC4)O)C)CC2)CC2C1C(C1(O2)OCC(CC1)C)C)C

MOL003885	0.2872	0.7128	0.7586	Dioscoreaebulbiferae	Yamogenin	Not Available	FALSE	C12(C(C3C(C4(C(=CC3)CC(CC4)O)C)CC2)CC2C1C(C1(O2)OCC(CC1)C)C)C
MOL003885	0.2872	0.7128	0.7586	Trigonellae Semen	Yamogenin	Not Available	FALSE	C12(C(C3C(C4(C(=CC3)CC(CC4)O)C)CC2)CC2C1C(C1(O2)OCC(CC1)C)C)C
MOL003885	0.2872	0.7128	0.7586	Dioscoreae Septemlo Bae Rhizoma	Yamogenin	Not Available	FALSE	C12(C(C3C(C4(C(=CC3)CC(CC4)O)C)CC2)CC2C1C(C1(O2)OCC(CC1)C)C)C
MOL003886	0.3326	0.6674	0.6585	Asparagi Radix	diosgenin glucoside	Not Available	FALSE	O1C2C(C3(C(C4C(CC3)C3(C(=CC4)CC(OC4OC(C(O)C(O)C4O)CO)CC3)C)C2)C)C(C21OCC(CC2)C)C
MOL003887	0.6900	0.3100	0.8595	Smilax China	Gracillin	Not Available	FALSE	O1C2C(C3(C(C4C(CC3)C3(C(=CC4)CC(OC4OC(C(O)C(OC5OC(C(O)C(O)C5O)CO)C4OC4OC(C(O)C(O)C4O)C)CO)CC3)C)C2)C)C(C21OCC(CC2)C)C
MOL003887	0.6900	0.3100	0.8595	Dioscoreae Septemlo Bae Rhizoma	Gracillin	Not Available	FALSE	O1C2C(C3(C(C4C(CC3)C3(C(=CC4)CC(OC4OC(C(O)C(OC5OC(C(O)C(O)C5O)CO)C4OC4OC(C(O)C(O)C4O)C)CO)CC3)C)C2)C)C(C21OCC(CC2)C)C
MOL003887	0.6900	0.3100	0.8595	Dioscoreae Hypoglaucae Rhizoma	Gracillin	Not Available	FALSE	O1C2C(C3(C(C4C(CC3)C3(C(=CC4)CC(OC4OC(C(O)C(OC5OC(C(O)C(O)C5O)CO)C4OC4OC(C(O)C(O)C4O)C)CO)CC3)C)C2)C)C(C21OCC(CC2)C)C
MOL003887	0.6900	0.3100	0.8595	Asparagi Radix	Gracillin	Not Available	FALSE	O1C2C(C3(C(C4C(CC3)C3(C(=CC4)CC(OC4OC(C(O)C(OC5OC(C(O)C(O)C5O)CO)C4OC4OC(C(O)C(O)C4O)C)CO)CC3)C)C2)C)C(C21OCC(CC2)C)C
MOL003888	0.7178	0.2822	0.8077	Polygonati Rhizoma	methylprotodioscin	Not Available	FALSE	C12(C(C3C(CC2)C2(C(=CC3)CC(CC2)OC2C(C(C(O2)CO)OC2C(C(C(C(O2)C)O)O)O)O)OC2C(C(C(O2)C)O)O)O)C)CC2C1C(C(O2)(CCC(COC1OC(C(C(C1O)O)O)CO)C)OC)C)C
MOL003888	0.7178	0.2822	0.8077	Smilax China	methylprotodioscin	Not Available	FALSE	C12(C(C3C(CC2)C2(C(=CC3)CC(CC2)OC2C(C(C(O2)CO)OC2C(C(C(C(O2)C)O)O)O)O)OC2C(C(C(O2)C)O)O)O)C)CC2C1C(C(O2)(CCC(COC1OC(C(C(C1O)O)O)CO)C)OC)C)C
MOL003888	0.7178	0.2822	0.8077	Asparagi Radix	methylprotodioscin	Not Available	FALSE	C12(C(C3C(CC2)C2(C(=CC3)CC(CC2)OC2C(C(C(O2)CO)OC2C(C(C(C(O2)C)O)O)O)O)OC2C(C(C(O2)C)O)O)O)C)CC2C1C(C(O2)(CCC(COC1OC(C(C(C1O)O)O)CO)C)OC)C)C
MOL003889	0.2233	0.7767	0.7590	Polygonati Rhizoma	methylprotodioscin_qt	Not Available	FALSE	C12(C(C3C(CC2)C2(C(=CC3)CC(CC2)O)C)CC2C1C(C(O2)(CCC(CO)C)OC)C)C
MOL003889	0.2233	0.7767	0.7590	Asparagi Radix	methylprotodioscin_qt	Not Available	FALSE	C12(C(C3C(CC2)C2(C(=CC3)CC(CC2)O)C)CC2C1C(C(O2)(CCC(CO)C)OC)C)C
MOL003889	0.2233	0.7767	0.7590	Smilax China	methylprotodioscin_qt	Not Available	FALSE	C12(C(C3C(CC2)C2(C(=CC3)CC(CC2)O)C)CC2C1C(C(O2)(CCC(CO)C)OC)C)C
MOL003890	0.7505	0.2495	0.8070	Asparagi Radix	pseudoprotodioscin	Not Available	FALSE	C12(C(C3C(CC2)C2(C(=CC3)CC(CC2)OC2C(C(C(O2)CO)OC2C(C(C(C(O2)C)O)O)O)O)OC2C(C(C(O2)C)O)O)O)C)CC2C1C(=C(O2)CCC(COC1OC(C(C(C1O)O)O)CO)C)C

MOL003891	0.2744	0.7256	0.7812	Asparagi Radix	pseudoprotodioscin_qt	Not Available	FALSE	C12(C(C3C(CC2)C2(C(=CC3)CC(CC2)O)C)CC2C1C(=C(O2)CCC(CO)C)C)C
MOL003891	0.2744	0.7256	0.7812	Smilax China	pseudoprotodioscin_qt	Not Available	FALSE	C12(C(C3C(CC2)C2(C(=CC3)CC(CC2)O)C)CC2C1C(=C(O2)CCC(CO)C)C)C
MOL003892	0.3012	0.6988	0.7449	Asparagi Radix	Sarsapogenine	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(O)CC5)C)CC3)C2)C)C(C21OCC(CC2)C)C
MOL003892	0.3012	0.6988	0.7449	Anemarrhenae Rhizoma	Sarsapogenine	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(O)CC5)C)CC3)C2)C)C(C21OCC(CC2)C)C
MOL003893	0.3012	0.6988	0.7449	Asparagi Radix	sarsasopogenin	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(O)CC5)C)CC3)C2)C)C(C21OCC(CC2)C)C
MOL003894	0.3012	0.6988	0.7449	Anemarrhenae Rhizoma	Smilagenin	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(O)CC5)C)CC3)C2)C)C(C21OCC(CC2)C)C
MOL003894	0.3012	0.6988	0.7449	Allium Azureum Ledeb.	Smilagenin	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(O)CC5)C)CC3)C2)C)C(C21OCC(CC2)C)C
MOL003894	0.3012	0.6988	0.7449	Smilacis Glabrae Rhixoma	Smilagenin	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(O)CC5)C)CC3)C2)C)C(C21OCC(CC2)C)C
MOL003894	0.3012	0.6988	0.7449	Trigonellae Semen	Smilagenin	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(O)CC5)C)CC3)C2)C)C(C21OCC(CC2)C)C
MOL003894	0.3012	0.6988	0.7449	Asparagi Radix	Smilagenin	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(O)CC5)C)CC3)C2)C)C(C21OCC(CC2)C)C
MOL003895	0.9008	0.0992	0.9436	Codonopsis Radix	5-Methoxymethyl furfural	74711	FALSE	c1(oc(cc1)C=O)COC
MOL003895	0.9008	0.0992	0.9436	Asparagi Radix	5-Methoxymethyl furfural	74711	FALSE	c1(oc(cc1)C=O)COC
MOL003895	0.9008	0.0992	0.9436	Bomboo Juice	5-Methoxymethyl furfural	74711	FALSE	c1(oc(cc1)C=O)COC
MOL003896	0.7635	0.2365	0.9208	Asparagi Radix	7-Methoxy-2-methyl isoflavone	354368	FALSE	c1c(ccc2c1oc(c(c2=O)c1ccccc1)C)OC
MOL003896	0.7635	0.2365	0.9208	Codonopsis Radix	7-Methoxy-2-methyl isoflavone	354368	FALSE	c1c(ccc2c1oc(c(c2=O)c1ccccc1)C)OC
MOL003896	0.7635	0.2365	0.9208	licorice	7-Methoxy-2-methyl isoflavone	354368	FALSE	c1c(ccc2c1oc(c(c2=O)c1ccccc1)C)OC
MOL003897	0.7915	0.2085	0.6415	Asparagi Radix	9,10-Dihydrophenanthrene	13058	FALSE	c1cccc2c3ccccc3CCc12

MOL003898	0.6040	0.3960	0.8203	Asparagi Radix	Aspafilioside A	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(OC4OC(C(OC6OCC(O)C(O)C6O)C(O)C4O)CO)CC5)C)CC3)C2)C)C(C21OCC(CC2)C)C
MOL003899	0.3012	0.6988	0.7449	Asparagi Radix	Aspafilioside A_qt	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(O)CC5)C)CC3)C2)C)C(C21OCC(CC2)C)C
MOL003900	0.7201	0.2799	0.8023	Asparagi Radix	Asparaside A	Not Available	FALSE	C1(C(C(OC(C1O)CO)OC1C(OC(C(C1O)O)C)OC1C(C(C(OC1CO)OC1CC2C(CC1)(C1C(CC2)C2C(CC1)(C1C(C2)OC(C1C)(OC)CCC(C)OC1OC(C(C(C1O)O)O)CO)C)C)O)O)O)O
MOL003901	0.2933	0.7067	0.7299	Asparagi Radix	Asparaside A_qt	Not Available	FALSE	OC1CC2C(CC1)(C1C(CC2)C2C(CC1)(C1C(C2)OC(C1C)(OC)CCC(C)O)C)C
MOL003905	0.5507	0.4493	0.8403	Lepidii Semen Descurainiae Semen	K-STROPHANTHOSIDE	Not Available	FALSE	OC12C3C(C4(C(O)(CC3)CC(OC3OC(C(OC5OC(C(O)C(O)C5O)CO)C(OC)C3)C)CC4)C=O)CCC1(C(CC2)C1=CC(=O)OC1)C
MOL003906	0.6450	0.3550	0.7872	Lepidii Semen Descurainiae Semen	K-STROPHANTHOSIDE_qt	Not Available	FALSE	OC12C3C(C4(C(O)(CC3)CC(O)CC4)C=O)CCC1(C(CC2)C1=CC(=O)OC1)C
MOL003907	0.6114	0.3886	0.8401	Lepidii Semen Descurainiae Semen	erysimoside	12308885	FALSE	C12(C3C(C4(C(CC3)(C(CC4)C3=CC(=O)OC3)C)O)CCC1(CC(CC2)OC1CC(C(C(O1)C)OC1OC(C(C(C1O)O)O)CO)O)O)C=O
MOL003908	0.6450	0.3550	0.7872	Lepidii Semen Descurainiae Semen	Cynotoxin	6185	FALSE	C12(C3C(C4(C(CC3)(C(CC4)C3=CC(=O)OC3)C)O)CCC1(CC(CC2)O)O)C=O
MOL003909	0.6175	0.3825	0.8374	Lepidii Semen Descurainiae Semen	evobioside	Not Available	FALSE	C1(CCC2(C(C1)CCC1C3(CCC(C4=CC(=O)OC4)C3(C)CCC21)O)C)OC1C(O)C(O)C(OC2C(O)C(O)C(O)C(O2)C)C(O1)CO
MOL003910	0.3527	0.6473	0.7936	Lepidii Semen Descurainiae Semen	evobioside_qt	12305991	FALSE	C1(CCC2(C(C1)CCC1C3(CCC(C4=CC(=O)OC4)C3(C)CCC21)O)C)O
MOL003911	0.3828	0.6172	0.6210	Lepidii Semen Descurainiae Semen	evomonoside	Not Available	FALSE	C12(C3C(C4(C(CC3)CC(CC4)OC3C(C(C(O3)C)O)O)O)C)CCC1(C(CC2)C1=CC(=O)OC1)C)O
MOL003912	0.3527	0.6473	0.7936	Cichorii Radix	DTX	4369270	FALSE	C12(C3C(C4(C(CC3)CC(CC4)O)C)CCC1(C(CC2)C1=CC(=O)OC1)C)O
MOL003912	0.3527	0.6473	0.7936	Lepidii Semen Descurainiae Semen	DTX	4369270	FALSE	C12(C3C(C4(C(CC3)CC(CC4)O)C)CCC1(C(CC2)C1=CC(=O)OC1)C)O
MOL003913	0.5157	0.4843	0.7078	Lepidii Semen Descurainiae Semen	Helveticoside	441860	FALSE	C12(C3C(C4(C(CC3)(C(CC4)C3=CC(=O)OC3)C)O)CCC1(CC(CC2)OC1CC(C(C(O1)C)O)O)O)C=O
MOL003914	0.6450	0.3550	0.7872	Lepidii Semen Descurainiae Semen	STOCK1N-70051	7059642	FALSE	C12(C3C(C4(C(CC3)(C(CC4)C3=CC(=O)OC3)C)O)CCC1(CC(CC2)O)O)C=O
MOL003915	0.9415	0.0585	0.9609	Lepidii Semen Descurainiae Semen	WLN: NC1R	8794	FALSE	C(c1ccccc1)C#N
MOL003917	0.9362	0.0638	0.9547	Lepidii Semen Descurainiae Semen	3-(4-Hydroxyphenyl)propionitrile	87079	FALSE	c1(ccc(cc1)O)CCC#N

MOL003918	0.9177	0.0823	0.9438	Lepidii Semen Descurainiae Semen	WLN: SCN2R	16741	FALSE	c1(ccccc1)CCN=C=S
MOL003918	0.9177	0.0823	0.9438	Sinapis Semen	WLN: SCN2R	16741	FALSE	c1(ccccc1)CCN=C=S
MOL003919	0.9082	0.0918	0.9071	Lepidii Semen Descurainiae Semen	Methyl sebacate	7829	FALSE	C(=O)(CCCCCCCCC(=O)OC)OC
MOL003921	0.9163	0.0837	0.9076	Lepidii Semen Descurainiae Semen	Sinapinic acid	1549091	FALSE	C(=O)(/C=C\c1cc(c(c(c1)OC)O)OC)O
MOL003922	0.8264	0.1736	0.9611	Lepidii Semen Descurainiae Semen	Crotonitrile	637921	FALSE	C(#N)/C=C/C
MOL003923	0.8985	0.1015	0.9337	Lepidii Semen Descurainiae Semen	Tropeolin	18170	FALSE	S(C#N)Cc1ccccc1
MOL003924	0.9148	0.0852	0.9314	Arisaematis Rhizoma	Methyl azelate	15612	FALSE	C(=O)(CCCCCCCC(=O)OC)OC
MOL003924	0.9148	0.0852	0.9314	Sterculiae Lychnophorae Semen	Methyl azelate	15612	FALSE	C(=O)(CCCCCCCC(=O)OC)OC
MOL003924	0.9148	0.0852	0.9314	Impatientis Semen	Methyl azelate	15612	FALSE	C(=O)(CCCCCCCC(=O)OC)OC
MOL003924	0.9148	0.0852	0.9314	Perillae Fructus	Methyl azelate	15612	FALSE	C(=O)(CCCCCCCC(=O)OC)OC
MOL003924	0.9148	0.0852	0.9314	Calyx Seu Fructus Physalis	Methyl azelate	15612	FALSE	C(=O)(CCCCCCCC(=O)OC)OC
MOL003924	0.9148	0.0852	0.9314	Lepidii Semen Descurainiae Semen	Methyl azelate	15612	FALSE	C(=O)(CCCCCCCC(=O)OC)OC
MOL003924	0.9148	0.0852	0.9314	Trollius Chinensis	Methyl azelate	15612	FALSE	C(=O)(CCCCCCCC(=O)OC)OC
MOL003925	0.8575	0.1425	0.6908	Lepidii Semen Descurainiae Semen	10-hexadecenoic acid	5312412	FALSE	C(=O)(CCCCCCCC/C=C/CCCCC)O
MOL003926	0.9110	0.0890	0.8732	Lepidii Semen Descurainiae Semen	Dimethyl undecanedioate	78321	FALSE	C(=O)(CCCCCCCCCC(=O)OC)OC
MOL003927	0.7026	0.2974	0.6091	Lepidii Semen Descurainiae Semen	Dihomolinolenic acid	5312529	FALSE	C(=O)(CCCCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL003927	0.7026	0.2974	0.6091	Platycladi Semen	Dihomolinolenic acid	5312529	FALSE	C(=O)(CCCCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL003928	0.9149	0.0851	0.9517	Lepidii Semen Descurainiae Semen	Butenylisothiocyanate	6439701	FALSE	C(=C\CC)/N=C=S
MOL003929	0.8902	0.1098	0.8812	Lepidii Semen Descurainiae Semen	mustard oil	5971	FALSE	C(C=C)N=C=S
MOL003929	0.8902	0.1098	0.8812	Sinapis Semen	mustard oil	5971	FALSE	C(C=C)N=C=S
MOL003930	0.9228	0.0772	0.9563	Lepidii Semen Descurainiae Semen	Urogran	2346	FALSE	c1(ccccc1)CN=C=S
MOL003930	0.9228	0.0772	0.9563	Sinapis Semen	Urogran	2346	FALSE	c1(ccccc1)CN=C=S

MOL003931	0.8316	0.1684	0.9610	Lepidii Semen Descurainiae Semen	Allylnitrile	8009	FALSE	C(#N)CC=C
MOL003932	0.9356	0.0644	0.9520	Lepidii Semen Descurainiae Semen	WLN: SH1R	7509	FALSE	C(c1ccccc1)S
MOL003933	0.9464	0.0536	0.9093	Lepidii Semen Descurainiae Semen	ST5407144	2822957	FALSE	C(=O)(c1cc(c(cc1)OC)OCC)O
MOL003934	0.9239	0.0761	0.9138	Lepidii Semen Descurainiae Semen	4-O-Methylgallic acid	78016	FALSE	C(=O)(c1cc(c(c(c1)O)OC)O)O
MOL003935	0.9184	0.0816	0.8987	Ephedra Herba	2,6-Dimethyl-1,3,5,7-octatetraene, E,E-	5368451	FALSE	C=C(/C=C/C=C(/C=C)\C)C
MOL003935	0.9184	0.0816	0.8987	Evodiae Fructus	2,6-Dimethyl-1,3,5,7-octatetraene, E,E-	5368451	FALSE	C=C(/C=C/C=C(/C=C)\C)C
MOL003936	0.9314	0.0686	0.9505	Evodiae Fructus	1,2,3-Trimethylcyclopentene	Not Available	FALSE	C1(=C(CCC1C)C)C
MOL003937	0.8550	0.1450	0.6445	Ligustici Rhizoma Et Radix	Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-7-methyl-4-methylene-1-(1-methylethyl)-, (1alpha,4abeta,8aalpha)-	92313	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C
MOL003937	0.8550	0.1450	0.6445	Anisi Stellati Fructus	Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-7-methyl-4-methylene-1-(1-methylethyl)-, (1alpha,4abeta,8aalpha)-	92313	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C

MOL003937	0.8550	0.1450	0.6445	Chrysanthemi Flos	Naphthalene, 1,2,3,4,4a,5,6, 8a-octahydro- 7-methyl-4- methylene-1- (1- methylethyl)-, (1alpha,4abet a,8aalpha)-	92313	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C
MOL003937	0.8550	0.1450	0.6445	Evodiae Fructus	Naphthalene, 1,2,3,4,4a,5,6, 8a-octahydro- 7-methyl-4- methylene-1- (1- methylethyl)-, (1alpha,4abet a,8aalpha)-	92313	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C
MOL003937	0.8550	0.1450	0.6445	Tamaricis Cacumen	Naphthalene, 1,2,3,4,4a,5,6, 8a-octahydro- 7-methyl-4- methylene-1- (1- methylethyl)-, (1alpha,4abet a,8aalpha)-	92313	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C

MOL003937	0.8550	0.1450	0.6445	Cyperi Rhizoma	Naphthalene, 1,2,3,4,4a,5,6, 8a-octahydro- 7-methyl-4- methylene-1- (1- methylethyl)-, (1alpha,4abet a,8aalpha)-	92313	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C
MOL003937	0.8550	0.1450	0.6445	Kaempferiae Rhizoma	Naphthalene, 1,2,3,4,4a,5,6, 8a-octahydro- 7-methyl-4- methylene-1- (1- methylethyl)-, (1alpha,4abet a,8aalpha)-	92313	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C
MOL003937	0.8550	0.1450	0.6445	Zanthoxyli Pericarpium	Naphthalene, 1,2,3,4,4a,5,6, 8a-octahydro- 7-methyl-4- methylene-1- (1- methylethyl)-, (1alpha,4abet a,8aalpha)-	92313	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C

MOL003937	0.8550	0.1450	0.6445	Ailanthi Cortex	Naphthalene, 1,2,3,4,4a,5,6, 8a-octahydro- 7-methyl-4- methylene-1- (1- methylethyl)-, (1alpha,4abet a,8aalpha)-	92313	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C
MOL003937	0.8550	0.1450	0.6445	Caryophylliflos	Naphthalene, 1,2,3,4,4a,5,6, 8a-octahydro- 7-methyl-4- methylene-1- (1- methylethyl)-, (1alpha,4abet a,8aalpha)-	92313	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C
MOL003937	0.8550	0.1450	0.6445	Schizonepetae Spica	Naphthalene, 1,2,3,4,4a,5,6, 8a-octahydro- 7-methyl-4- methylene-1- (1- methylethyl)-, (1alpha,4abet a,8aalpha)-	92313	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C

MOL003937	0.8550	0.1450	0.6445	Rubi Fructus	Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-7-methyl-4-methylene-1-(1-methylethyl)-, (1alpha,4abeta,8aalpha)-	92313	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C
MOL003937	0.8550	0.1450	0.6445	Pogostemon Cablin (Blanco) Benth.	Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-7-methyl-4-methylene-1-(1-methylethyl)-, (1alpha,4abeta,8aalpha)-	92313	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C
MOL003937	0.8550	0.1450	0.6445	Lysimachiae Herba	Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-7-methyl-4-methylene-1-(1-methylethyl)-, (1alpha,4abeta,8aalpha)-	92313	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C

MOL003937	0.8550	0.1450	0.6445	Citri Grandis Exocarpium	Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-7-methyl-4-methylene-1-(1-methylethyl)-, (1alpha,4abeta,8aalpha)-	92313	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C
MOL003937	0.8550	0.1450	0.6445	Folium Artemisiae Argyi	Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro-7-methyl-4-methylene-1-(1-methylethyl)-, (1alpha,4abeta,8aalpha)-	92313	FALSE	C1(CCC(=C)C2CCC(=CC12)C)C(C)C
MOL003938	0.7344	0.2656	0.7235	Evodiae Fructus	nerolidyl acetate	Not Available	FALSE	C(C(OC(=O)C)(C=C)C)C/C=C(/CCC=C(C)C)\C
MOL003938	0.7344	0.2656	0.7235	Citrus Aurantium	nerolidyl acetate	Not Available	FALSE	C(C(OC(=O)C)(C=C)C)C/C=C(/CCC=C(C)C)\C
MOL003939	0.6964	0.3036	0.8691	Evodiae Fructus	Nantenin	Not Available	FALSE	C1CC2C3C(N1C)CC1(C3C(C(C2)OC)OC)CC2(C1)OC
MOL003939	0.6964	0.3036	0.8691	Corydalis Rhizoma	Nantenin	Not Available	FALSE	C1CC2C3C(N1C)CC1(C3C(C(C2)OC)OC)CC2(C1)OC
MOL003941	0.6230	0.3770	0.7072	Evodiae Fructus	Rutaevine acetate	Not Available	FALSE	C1(=O)CC2C3(CO1)C(C(=O)C(C1(C3CCC3(C41C(C(=O)OC3c1ccoc1)O4)C)C)OC(=O)C)C(O2)(C)C
MOL003942	0.7882	0.2118	0.7008	Evodiae Fructus	Rutaevine	Not Available	FALSE	C1(=O)CC2C3(CO1)C(C(=O)C(C1(C3CCC3C41C(C(=O)OC3c1ccoc1)O4)C)O)C(O2)(C)C
MOL003943	0.8443	0.1557	0.7857	Evodiae Fructus	Rutalinidine	51380995	FALSE	c1(ccc2c(c1)c(=O)c1c(n2C)OC(C1)C(C)(C)O)O
MOL003945	0.6220	0.3780	0.7816	Evodiae Fructus	Tetrahydromagnolol	5321851	FALSE	c1c(CCC)cc(c(c1)O)c1c(ccc(CCC)c1)O
MOL003946	0.9653	0.0347	0.6884	Evodiae Fructus	1-bromo-2,2,3,3-tetramethyl-1-prop-1-ynylcyclopropane	570815	FALSE	C1(C(C1(C)C)(C)C)(C#CC)Br

MOL003947	0.0955	0.9045	0.6713	Evodiae Fructus	1-methyl-2-[(Z)-pentadec-10-enyl]-4-quinolone	5319752	FALSE	c1c2c(ccc1)c(=O)cc(n2C)CCCCCCCCC/C=C\CCCC
MOL003948	0.9594	0.0406	0.9487	Radix Clematidis	Cuminol	325	FALSE	c1(ccc(cc1)CO)C(C)C
MOL003948	0.9594	0.0406	0.9487	Zanthoxyli Pericarpium	Cuminol	325	FALSE	c1(ccc(cc1)CO)C(C)C
MOL003948	0.9594	0.0406	0.9487	Ephedra Herba	Cuminol	325	FALSE	c1(ccc(cc1)CO)C(C)C
MOL003948	0.9594	0.0406	0.9487	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Cuminol	325	FALSE	c1(ccc(cc1)CO)C(C)C
MOL003948	0.9594	0.0406	0.9487	Evodiae Fructus	Cuminol	325	FALSE	c1(ccc(cc1)CO)C(C)C
MOL003948	0.9594	0.0406	0.9487	Moslae Herba	Cuminol	325	FALSE	c1(ccc(cc1)CO)C(C)C
MOL003949	0.9485	0.0515	0.9541	Evodiae Fructus	Dimethyl anthranilate	6826	FALSE	c1(c(cccc1)NC)C(=O)OC
MOL003949	0.9485	0.0515	0.9541	Citrus Reticulata	Dimethyl anthranilate	6826	FALSE	c1(c(cccc1)NC)C(=O)OC
MOL003950	0.1196	0.8804	0.7930	Evodiae Fructus	1-methyl-2-[(Z)-undec-6-enyl]-4-quinolone	5319810	FALSE	c1ccc2c(c1)c(=O)cc(n2C)CCCCC/C=C\CCCC
MOL003951	0.9501	0.0499	0.9717	Evodiae Fructus	Benzyl isovalerate	7651	FALSE	c1(COC(=O)CC(C)C)ccccc1
MOL003951	0.9501	0.0499	0.9717	Artemisia Annua L.	Benzyl isovalerate	7651	FALSE	c1(COC(=O)CC(C)C)ccccc1
MOL003952	0.6081	0.3919	0.7154	Evodiae Fructus	[(E)-3-phenylprop-2-enyl] (Z)-3-phenylprop-2-enoate	1550888	FALSE	c1(/C=C\C(=O)OC/C=C/c2ccccc2)ccccc1
MOL003953	0.9613	0.0387	0.8133	Evodiae Fructus	AI3-23133	89664	FALSE	C1(C2C(=CC(C1C2)O)C)(C)C
MOL003954	0.9419	0.0581	0.9433	Evodiae Fructus	cyclohexene,3-butyl-	Not Available	FALSE	C1=CC(CCC1)CCCC
MOL003955	0.8679	0.1321	0.7686	Rhizoma Dioscoreae	D-Cystine	6992103	FALSE	S(SCC(N)C(=O)O)CC(N)C(=O)O
MOL003955	0.8679	0.1321	0.7686	Bamusaeconcretiosilicea	D-Cystine	6992103	FALSE	S(SCC(N)C(=O)O)CC(N)C(=O)O
MOL003955	0.8679	0.1321	0.7686	Evodiae Fructus	D-Cystine	6992103	FALSE	S(SCC(N)C(=O)O)CC(N)C(=O)O
MOL003955	0.8679	0.1321	0.7686	Cornus Officinalis Sieb. Et Zucc.	D-Cystine	6992103	FALSE	S(SCC(N)C(=O)O)CC(N)C(=O)O
MOL003955	0.8679	0.1321	0.7686	Capsellae Herba	D-Cystine	6992103	FALSE	S(SCC(N)C(=O)O)CC(N)C(=O)O
MOL003956	0.8155	0.1845	0.7164	Evodiae Fructus	dihydrorutaecarpine	Not Available	FALSE	N1C2N(C(=O)c3ccccc13)CCc1c2[nH]c2c1cccc2
MOL003957	0.0967	0.9033	0.6296	Evodiae Fructus	1-methyl-2-pentadecyl-4-quinolone	5319753	FALSE	c1cc2c(cc1)c(=O)cc(n2C)CCCCCCCCCCCCCCC

MOL003958	0.7690	0.2310	0.7782	Evodiae Fructus	Evodiamine	Not Available	FALSE	N12C(c3c(c4c([nH]3)ccc(c4)O)CC2)N(c2c(C1=O)cccc2)C
MOL003959	0.6358	0.3642	0.7390	Citri Reticulatae Semen	limonin	Not Available	FALSE	O1C23C4(C(C56C(CC4=O)C(OC5CC(=O)OC6)(C)C)CCC2(C(OC(=O)C13)c1ccoc1)C)C
MOL003959	0.6358	0.3642	0.7390	Dictamni Cortex	limonin	Not Available	FALSE	O1C23C4(C(C56C(CC4=O)C(OC5CC(=O)OC6)(C)C)CCC2(C(OC(=O)C13)c1ccoc1)C)C
MOL003959	0.6358	0.3642	0.7390	Citri Exocarpium Rubrum	limonin	Not Available	FALSE	O1C23C4(C(C56C(CC4=O)C(OC5CC(=O)OC6)(C)C)CCC2(C(OC(=O)C13)c1ccoc1)C)C
MOL003959	0.6358	0.3642	0.7390	Aurantii Fructus Immaturus	limonin	Not Available	FALSE	O1C23C4(C(C56C(CC4=O)C(OC5CC(=O)OC6)(C)C)CCC2(C(OC(=O)C13)c1ccoc1)C)C
MOL003959	0.6358	0.3642	0.7390	Cortex Periplocae Radicis	limonin	Not Available	FALSE	O1C23C4(C(C56C(CC4=O)C(OC5CC(=O)OC6)(C)C)CCC2(C(OC(=O)C13)c1ccoc1)C)C
MOL003959	0.6358	0.3642	0.7390	Coptidis Rhizoma	limonin	Not Available	FALSE	O1C23C4(C(C56C(CC4=O)C(OC5CC(=O)OC6)(C)C)CCC2(C(OC(=O)C13)c1ccoc1)C)C
MOL003959	0.6358	0.3642	0.7390	Citri Fructus	limonin	Not Available	FALSE	O1C23C4(C(C56C(CC4=O)C(OC5CC(=O)OC6)(C)C)CCC2(C(OC(=O)C13)c1ccoc1)C)C
MOL003959	0.6358	0.3642	0.7390	Citrus Aurantium	limonin	Not Available	FALSE	O1C23C4(C(C56C(CC4=O)C(OC5CC(=O)OC6)(C)C)CCC2(C(OC(=O)C13)c1ccoc1)C)C
MOL003959	0.6358	0.3642	0.7390	Phellodendri Amurensis Cortex	limonin	Not Available	FALSE	O1C23C4(C(C56C(CC4=O)C(OC5CC(=O)OC6)(C)C)CCC2(C(OC(=O)C13)c1ccoc1)C)C
MOL003959	0.6358	0.3642	0.7390	Evodiae Fructus	limonin	Not Available	FALSE	O1C23C4(C(C56C(CC4=O)C(OC5CC(=O)OC6)(C)C)CCC2(C(OC(=O)C13)c1ccoc1)C)C
MOL003960	0.8752	0.1248	0.8013	Evodiae Fructus	1-(5,7,8-trimethoxy-2,2-dimethylchromen-6-yl)ethanone	624052	FALSE	C1(C=Cc2c(O1)c(c(c(c2OC)C(=O)C)OC)OC)(C)C
MOL003961	0.8925	0.1075	0.8582	Evodiae Fructus	Geranyl isobutyrate	6086514	FALSE	C(=O)(OC/C=C(/CCC=C(C)C)\C)C(C)C
MOL003962	0.9117	0.0883	0.8972	Evodiae Fructus	Geranyl propionate	5355853	FALSE	C(=C\COC(=O)CC)(/CCC=C(C)C)\C
MOL003962	0.9117	0.0883	0.8972	Flos Genkwa	Geranyl propionate	5355853	FALSE	C(=C\COC(=O)CC)(/CCC=C(C)C)\C
MOL003962	0.9117	0.0883	0.8972	Zingiber Officinale Roscoe	Geranyl propionate	5355853	FALSE	C(=C\COC(=O)CC)(/CCC=C(C)C)\C
MOL003963	0.8070	0.1930	0.8041	Evodiae Fructus	hydroxyevodiamine	Not Available	FALSE	N12C(c3c(c4c([nH]3)ccc(c4)O)CC2)N(c2c(C1=O)cccc2)C
MOL003964	0.1285	0.8715	0.7445	Evodiae Fructus	1-methyl-2-undecyl-4-quinolone	5319811	FALSE	c1ccc2c(c1)c(=O)cc(n2C)CCCCCCCCCCC
MOL003966	0.9225	0.0775	0.9610	Bombyx Mori L.	1-Penten-3-one	15394	FALSE	C(=O)(CC)C=C

MOL003966	0.9225	0.0775	0.9610	Evodiae Fructus	1-Penten-3-one	15394	FALSE	C(=O)(CC)C=C
MOL003966	0.9225	0.0775	0.9610	Capsici Fructus	1-Penten-3-one	15394	FALSE	C(=O)(CC)C=C
MOL003967	0.8470	0.1530	0.8324	Evodiae Fructus	Neryl 3-methylbutyrate	6429039	FALSE	O(C(=O)CC(C)C)C/C=C(\CCC=C(C)C)/C
MOL003968	0.8402	0.1598	0.8191	Evodiae Fructus	(Z)-3,7-Dimethylocta-2,6-dienyl valerate	6436375	FALSE	C(=O)(CCCC)OC/C=C(\CCC=C(C)C)/C
MOL003968	0.8402	0.1598	0.8191	Flos Genkwa	(Z)-3,7-Dimethylocta-2,6-dienyl valerate	6436375	FALSE	C(=O)(CCCC)OC/C=C(\CCC=C(C)C)/C
MOL003969	0.8929	0.1071	0.9599	Bamusaeconcretiosilicea	L-Serin	6857581	FALSE	OCC(N)C(=O)O
MOL003969	0.8929	0.1071	0.9599	Rhizoma Dioscoreae	L-Serin	6857581	FALSE	OCC(N)C(=O)O
MOL003969	0.8929	0.1071	0.9599	Cornus Officinalis Sieb. Et Zucc.	L-Serin	6857581	FALSE	OCC(N)C(=O)O
MOL003969	0.8929	0.1071	0.9599	Trichosanthes Kirilowii Maxim	L-Serin	6857581	FALSE	OCC(N)C(=O)O
MOL003969	0.8929	0.1071	0.9599	Evodiae Fructus	L-Serin	6857581	FALSE	OCC(N)C(=O)O
MOL003969	0.8929	0.1071	0.9599	Arum Ternatum Thunb.	L-Serin	6857581	FALSE	OCC(N)C(=O)O
MOL003969	0.8929	0.1071	0.9599	Radix Salviae	L-Serin	6857581	FALSE	OCC(N)C(=O)O
MOL003969	0.8929	0.1071	0.9599	Santalum Album L.	L-Serin	6857581	FALSE	OCC(N)C(=O)O
MOL003970	0.9306	0.0694	0.9817	Evodiae Fructus	4-[(1S)-1-hydroxy-2-methylaminoethyl]phenol	667452	FALSE	c1(C(CNC)O)ccc(cc1)O
MOL003970	0.9306	0.0694	0.9817	Aurantii Fructus Immaturus	4-[(1S)-1-hydroxy-2-methylaminoethyl]phenol	667452	FALSE	c1(C(CNC)O)ccc(cc1)O
MOL003971	0.9046	0.0954	0.9687	Arum Ternatum Thunb.	Threonin	6971019	FALSE	OC(C(N)C(=O)O)C
MOL003971	0.9046	0.0954	0.9687	Cornus Officinalis Sieb. Et Zucc.	Threonin	6971019	FALSE	OC(C(N)C(=O)O)C
MOL003971	0.9046	0.0954	0.9687	Euryales Semen	Threonin	6971019	FALSE	OC(C(N)C(=O)O)C
MOL003971	0.9046	0.0954	0.9687	Rhizoma Dioscoreae	Threonin	6971019	FALSE	OC(C(N)C(=O)O)C
MOL003971	0.9046	0.0954	0.9687	Trichosanthes Kirilowii Maxim	Threonin	6971019	FALSE	OC(C(N)C(=O)O)C
MOL003971	0.9046	0.0954	0.9687	Santalum Album L.	Threonin	6971019	FALSE	OC(C(N)C(=O)O)C
MOL003971	0.9046	0.0954	0.9687	Radix Salviae	Threonin	6971019	FALSE	OC(C(N)C(=O)O)C
MOL003971	0.9046	0.0954	0.9687	Bamusaeconcretiosilicea	Threonin	6971019	FALSE	OC(C(N)C(=O)O)C

MOL003971	0.9046	0.0954	0.9687	Evodiae Fructus	Threonin	6971019	FALSE	OC(C(N)C(=O)O)C
MOL003971	0.9046	0.0954	0.9687	Vigna Radiata	Threonin	6971019	FALSE	OC(C(N)C(=O)O)C
MOL003972	0.3946	0.6054	0.8176	Evodiae Fructus	1-methyl-2-nonyl-4-quinolone	13967189	FALSE	n1(c(cc(=O)c2ccccc12)CCCCCCCCC)C
MOL003973	0.9440	0.0560	0.8545	Folium Ilicis Cornutae	caffeine	2519	TRUE	O=c1n(C)c2c(n(C)cn2)c(=O)n1C
MOL003973	0.9440	0.0560	0.8545	Corayceps	caffeine	2519	TRUE	O=c1n(C)c2c(n(C)cn2)c(=O)n1C
MOL003973	0.9440	0.0560	0.8545	Evodiae Fructus	caffeine	2519	TRUE	O=c1n(C)c2c(n(C)cn2)c(=O)n1C
MOL003973	0.9440	0.0560	0.8545	Semen Firmianae	caffeine	2519	TRUE	O=c1n(C)c2c(n(C)cn2)c(=O)n1C
MOL003973	0.9440	0.0560	0.8545	Curculiginis Rhizome	caffeine	2519	TRUE	O=c1n(C)c2c(n(C)cn2)c(=O)n1C
MOL003974	0.1580	0.8420	0.7212	Evodiae Fructus	Evocarpine	5317303	FALSE	n1(c(cc(=O)c2ccccc12)CCCCCCC/C=C\CCCC)C
MOL003976	0.8076	0.1924	0.7081	Evodiae Fructus	12alpha-Hydroxyevodol	Not Available	FALSE	C1(=O)CC2C3(CO1)C(=C(C(=O)C1(C3CC(C3(C41C(C(=O)OC3c1cocc1)O4)C)O)C)O)O)C(O2)(C)C
MOL003977	0.8760	0.1240	0.7294	Evodiae Fructus	13-Methylmyristate	151014	FALSE	C(CCC(=O)O)CCCCCCCCC(C)C
MOL003979	0.8918	0.1082	0.8917	Evodiae Fructus	1,9-Decadiyne	74400	FALSE	C(CCCC#C)CCC#C
MOL003980	0.8522	0.1478	0.8618	Evodiae Fructus	3-isopropylidene-5-methylhexa-1,4-diene	578220	FALSE	C=CC(=C(C)C)C=C(C)C
MOL003981	0.8870	0.1130	0.9296	Evodiae Fructus	2,4-DIMETHYLFURAN	19462	FALSE	o1c(cc(c1)C)C
MOL003982	0.9124	0.0876	0.9637	Evodiae Fructus	2,5-Dimethyl-1,5-hexadiene-3,4-diol	13682637	FALSE	C=C(C(C(C(=C)C)O)O)C
MOL003984	0.9190	0.0810	0.9275	Rose Rugosae Flos	2,6-dimethylocta-2,6-diene	5365898	FALSE	CC(=CCC/C(=C/C)/C)C
MOL003984	0.9190	0.0810	0.9275	Evodiae Fructus	2,6-dimethylocta-2,6-diene	5365898	FALSE	CC(=CCC/C(=C/C)/C)C
MOL003985	0.9606	0.0394	0.7978	licorice	2-Caren-10-al	12678291	FALSE	C12C=C(CCC1C2(C)C)C=O
MOL003985	0.9606	0.0394	0.7978	Ephedra Herba	2-Caren-10-al	12678291	FALSE	C12C=C(CCC1C2(C)C)C=O
MOL003985	0.9606	0.0394	0.7978	Evodiae Fructus	2-Caren-10-al	12678291	FALSE	C12C=C(CCC1C2(C)C)C=O
MOL003986	0.8996	0.1004	0.9682	Evodiae Fructus	3-ethylcyclopent-2-en-1-one	557256	FALSE	C1(=O)C=C(CC1)CC
MOL003987	0.9077	0.0923	0.9071	Evodiae Fructus	2-Decyne	75424	FALSE	C(CCC#CC)CCCC

MOL003988	0.9199	0.0801	0.7128	Evodiae Fructus	2-Hydroxy-3-formyl-7-methoxycarbazole	189687	FALSE	c1c(cc2c(c1)c1c([nH]2)cc(c(c1)C=O)O)OC
MOL003989	0.9228	0.0772	0.9539	Evodiae Fructus	2-Methylpent-2-enal	5319754	FALSE	CC/C=C(/C=O)\C
MOL003989	0.9228	0.0772	0.9539	Apocyniveneti Folium	2-Methylpent-2-enal	5319754	FALSE	CC/C=C(/C=O)\C
MOL003989	0.9228	0.0772	0.9539	Allium Azureum Ledeb.	2-Methylpent-2-enal	5319754	FALSE	CC/C=C(/C=O)\C
MOL003990	0.9256	0.0744	0.9514	Evodiae Fructus	2-Methyl-6-hepten-3-ol	Not Available	FALSE	CC(C(CCC=C)O)C
MOL003991	0.6924	0.3076	0.8209	Rubia Cordifolia	Tectochinon	6773	FALSE	c1cc2c(cc1)C(=O)c1c(C2=O)ccc(c1)C
MOL003991	0.6924	0.3076	0.8209	Evodiae Fructus	Tectochinon	6773	FALSE	c1cc2c(cc1)C(=O)c1c(C2=O)ccc(c1)C
MOL003991	0.6924	0.3076	0.8209	Morindae Officinalis Radix	Tectochinon	6773	FALSE	c1cc2c(cc1)C(=O)c1c(C2=O)ccc(c1)C
MOL003992	0.7783	0.2217	0.6963	Morindae Officinalis Radix	2-PENTADECANONE	61303	FALSE	C(CCCCCCCC)CCCCC(=O)C
MOL003992	0.7783	0.2217	0.6963	Ephedra Herba	2-PENTADECANONE	61303	FALSE	C(CCCCCCCC)CCCCC(=O)C
MOL003992	0.7783	0.2217	0.6963	Folium Ilicis Cornutae	2-PENTADECANONE	61303	FALSE	C(CCCCCCCC)CCCCC(=O)C
MOL003992	0.7783	0.2217	0.6963	Ginseng Folium	2-PENTADECANONE	61303	FALSE	C(CCCCCCCC)CCCCC(=O)C
MOL003992	0.7783	0.2217	0.6963	Rose Rugosae Flos	2-PENTADECANONE	61303	FALSE	C(CCCCCCCC)CCCCC(=O)C
MOL003992	0.7783	0.2217	0.6963	Evodiae Fructus	2-PENTADECANONE	61303	FALSE	C(CCCCCCCC)CCCCC(=O)C
MOL003993	0.8677	0.1323	0.8275	Evodiae Fructus	TRIDECANONE	11622	FALSE	C(CCCCCCCC)CCC(=O)C
MOL003993	0.8677	0.1323	0.8275	Rose Rugosae Flos	TRIDECANONE	11622	FALSE	C(CCCCCCCC)CCC(=O)C
MOL003993	0.8677	0.1323	0.8275	Junci Medulla	TRIDECANONE	11622	FALSE	C(CCCCCCCC)CCC(=O)C

MOL003993	0.8677	0.1323	0.8275	Momordicae Fructus	TRIDECANONE	11622	FALSE	C(CCCCCCCC)CCC(=O)C
MOL003993	0.8677	0.1323	0.8275	Zingiber Officinale Roscoe	TRIDECANONE	11622	FALSE	C(CCCCCCCC)CCC(=O)C
MOL003993	0.8677	0.1323	0.8275	Lysimachiae Foenigraeci Herba	TRIDECANONE	11622	FALSE	C(CCCCCCCC)CCC(=O)C
MOL003994	0.2694	0.7306	0.6107	Evodiae Fructus	24-methyl-31-norlanost-9(11)-enol	Not Available	FALSE	C1C=C2C(C3(C1(C(CC3)C(C)CCC(C(C)C)C)C)C)CCC1C2(CCC(C1C)O)C
MOL003995	0.9090	0.0910	0.9037	Evodiae Fructus	3,3-Dimethylallyl-p-propenyl phenyl ether	5316879	FALSE	c1c(ccc(c1)OCC=C(C)C)/C=C/C
MOL003996	0.9491	0.0509	0.9764	Evodiae Fructus	3-Cyclohexen-1-carboxaldehyde,3,4-dimethyl-	Not Available	FALSE	C1(CC(=C(CC1)C)C)C=O
MOL003997	0.8706	0.1294	0.9663	Chaenomeles Sinensis (Thouin) Koehne	3-Furaldehyde	10351	FALSE	c1(ccoc1)C=O
MOL003997	0.8706	0.1294	0.9663	Schisandrae Chinensis Fructus	3-Furaldehyde	10351	FALSE	c1(ccoc1)C=O
MOL003997	0.8706	0.1294	0.9663	Evodiae Fructus	3-Furaldehyde	10351	FALSE	c1(ccoc1)C=O
MOL003998	0.8937	0.1063	0.9706	Lilii Bulbus	(3S)-3-methyl-2,3-dihydrofuran	11423556	FALSE	O1CC(C=C1)C
MOL003998	0.8937	0.1063	0.9706	Evodiae Fructus	(3S)-3-methyl-2,3-dihydrofuran	11423556	FALSE	O1CC(C=C1)C
MOL003999	0.9273	0.0727	0.8717	Evodiae Fructus	3,3-diethyl-4,5-dimethylhex-4-en-2-one	549557	FALSE	CC(=O)C(C(=C(C)C)C)(CC)CC
MOL003999	0.9273	0.0727	0.8717	Morindae Officinalis Radix	3,3-diethyl-4,5-dimethylhex-4-en-2-one	549557	FALSE	CC(=O)C(C(=C(C)C)C)(CC)CC

MOL004000	0.9619	0.0381	0.9706	Evodiae Fructus	(3R,6S)-3-hydroperoxy-6-isopropenyl-3-methylcyclohexene	10419566	FALSE	C1(C=CC(CC1)C(=C)C)(C)OO
MOL004001	0.8960	0.1040	0.7959	Evodiae Fructus	5,8-tetradecadienoic acid	5312408	FALSE	C(=O)(CCC/C=C/C/C=C/CCCCC)O
MOL004002	0.1103	0.8897	0.7588	Evodiae Fructus	5alpha-O-(3'-Methylamino-3'-phenylpropionyl)nicotaxine	Not Available	FALSE	c1(cnccc1)C(=O)OC1C(C2=C(C(=O)CC(C2(C)C)C(C2C1(CCC(C12CO1)OC(=O)CC(c1ccccc1)NC)C)OC(=O)C)C)OC(=O)C
MOL004003	0.8953	0.1047	0.8320	Evodiae Fructus	6,11-Dimethyl-2,6,10-dodecatrien-1-ol	5365863	FALSE	C(/C=C/CC/C(=C/CCC=C(C)C)/C)O
MOL004004	0.9370	0.0630	0.8626	Plantaginis Herba	6-OH-Luteolin	5281642	FALSE	c1(c(c(c2c(c1)oc(cc2=O)c1cc(c(cc1)O)O)O)O)O)O
MOL004004	0.9370	0.0630	0.8626	Oroxyli Semen	6-OH-Luteolin	5281642	FALSE	c1(c(c(c2c(c1)oc(cc2=O)c1cc(c(cc1)O)O)O)O)O)O
MOL004004	0.9370	0.0630	0.8626	Evodiae Fructus	6-OH-Luteolin	5281642	FALSE	c1(c(c(c2c(c1)oc(cc2=O)c1cc(c(cc1)O)O)O)O)O)O
MOL004005	0.3697	0.6303	0.7247	Evodiae Fructus	6alpha-Acetoxy-5-epilimonin	Not Available	FALSE	C1C2C(C3(C(C1)(C(OC(=O)C3C)c1cocc1)C)C)(C(=O)C(C1C32COC(=O)CC3OC1(C)C)OC(=O)C)C
MOL004006	0.6686	0.3314	0.6222	Lysimachiae Foenigraeci Herba	7-Hexadecyne	549042	FALSE	CCCCCCC#CCCCCCCCC
MOL004006	0.6686	0.3314	0.6222	Momordicae Fructus	7-Hexadecyne	549042	FALSE	CCCCCCC#CCCCCCCCC
MOL004006	0.6686	0.3314	0.6222	Evodiae Fructus	7-Hexadecyne	549042	FALSE	CCCCCCC#CCCCCCCCC
MOL004007	0.9103	0.0897	0.8300	Evodiae Fructus	1,1-Dimethyl-2-(3-methyl-1,3-butadiene)-cyclo-propane	Not Available	FALSE	C1(/C=C/C(=C)C)CC1(C)C

MOL004008	0.8775	0.1225	0.8120	Evodiae Fructus	7R,8R-8-hydroxy-4-isopropylidene-7-methylbicyclo[5.3.1]undec-1-ene	21160893	FALSE	C12=CCC(=C(C)C)CCC(C(CC1)O)(C2)C
MOL004009	0.8494	0.1506	0.7126	Evodiae Fructus	(9S,10S)-9,10-dihydroxyoctadecanoic acid	12235230	FALSE	CCCCCCCCC(C(CCCCCCCC(=O)O)O)O
MOL004010	0.8912	0.1088	0.8553	Evodiae Fructus	Arachidoside	Not Available	FALSE	c1(c2c(cc(c1)O)OC(C(C2)O)c1ccc(c(c1)OC)O)O
MOL004011	0.9486	0.0514	0.9681	Evodiae Fructus	Nevoli oil	8635	FALSE	c1(c(cccc1)N)C(=O)OC
MOL004011	0.9486	0.0514	0.9681	Citri Grandis Exocarpium	Nevoli oil	8635	FALSE	c1(c(cccc1)N)C(=O)OC
MOL004012	0.9631	0.0369	0.8871	Evodiae Fructus	Bicyclo[3.3.0]octan-3-one, 7-ethylidene-	Not Available	FALSE	C12CC(=O)CC1C/C(=C\C)/C2
MOL004013	0.2098	0.7902	0.6866	Evodiae Fructus	1,3,4-Tridehydrofangchinolium hydroxide	Not Available	FALSE	c1c2c3c(c(c1OC)O)Oc1c(OC)cc4c(c1)C(N(CC4)C)Cc1ccc(Oc4c(ccc(CC3=[N+](CC2)C)c4)OC)cc1
MOL004014	0.5202	0.4798	0.7733	Evodiae Fructus	Evodiamide	189454	FALSE	c1ccc2c(c1)c(c[nH]2)CCN(C)C(=O)c1ccccc1NC
MOL004015	0.7108	0.2892	0.7089	Dictamni Cortex	Rutaevin	Not Available	FALSE	C123C(C(=O)C(C4(C1CCC1(C54C(C(=O)OC1c1occc1)O5)C)C)O)C(OC2CC(=O)OC3)(C)C
MOL004015	0.7108	0.2892	0.7089	Evodiae Fructus	Rutaevin	Not Available	FALSE	C123C(C(=O)C(C4(C1CCC1(C54C(C(=O)OC1c1occc1)O5)C)C)O)C(OC2CC(=O)OC3)(C)C
MOL004016	0.6798	0.3202	0.7061	Evodiae Fructus	Exaltolide	Not Available	FALSE	C123C(=C(C(=O)C4(C1CCC1(C54C(C(=O)OC1c1cocc1)O5)C)C)O)C(OC2CC(=O)OC3)(C)C
MOL004017	0.7640	0.2360	0.6701	Evodiae Fructus	Fordimine	Not Available	FALSE	C1CNC23C(C(Cc4c2ccc(=O)[nH]4)C=C(C3)C)C1
MOL004018	0.4789	0.5211	0.7888	Evodiae Fructus	Goshuyuamide I	5317827	FALSE	c1ccc2c(c1)c1c([nH]2)CN(CC1)C(=O)c1ccccc1NC
MOL004019	0.4985	0.5015	0.7452	Evodiae Fructus	Goshuyuamide II	5317828	FALSE	c1ccc2c(c1)c(c[nH]2)CCn1c(=O)n(c2c(c1=O)cccc2)C
MOL004020	0.9423	0.0577	0.9104	Rhododendri Daurici Folium	gossypetin	5280647	FALSE	c1c(c(c2c(c1O)c(=O)c(c(o2)c1ccc(c(c1)O)O)O)O)O
MOL004020	0.9423	0.0577	0.9104	Equiseti Hiemalis Herba	gossypetin	5280647	FALSE	c1c(c(c2c(c1O)c(=O)c(c(o2)c1ccc(c(c1)O)O)O)O)O
MOL004020	0.9423	0.0577	0.9104	Evodiae Fructus	gossypetin	5280647	FALSE	c1c(c(c2c(c1O)c(=O)c(c(o2)c1ccc(c(c1)O)O)O)O)O
MOL004021	0.6900	0.3100	0.6610	Evodiae Fructus	Gravacridonechlirine	Not Available	FALSE	c1ccc2c(c1)n(c1c(c2=O)c(cc2c1CC(O2)C(CO)(Cl)C)O)C

MOL004022	0.8649	0.1351	0.6821	Evodiae Fructus	Methyl 3,3,6-tri-O-galloyl-beta-D-glucopyranoside	Not Available	FALSE	c1(c(cc(cc1O)C(=O)OCC1C(C(C(C(O1)OC)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O)O
MOL004023	0.9606	0.0394	0.9653	Evodiae Fructus	Veratral	8419	FALSE	c1(ccc(c(c1)OC)OC)C=O
MOL004024	0.9267	0.0733	0.7612	Evodiae Fructus	MeODMT	1832	FALSE	c12c([nH]cc1CCN(C)C)ccc(c2)OC
MOL004025	0.7363	0.2637	0.7074	Evodiae Fructus	N-(2-Methylamino benzoyl)tryptamine	5319506	FALSE	N(CCc1c[nH]c2ccccc12)C(=O)c1c(cccc1)NC
MOL004026	0.9509	0.0491	0.9695	Evodiae Fructus	o-Amino-N-methylbenzamide	308072	FALSE	C(=O)(c1c(N)cccc1)NC
MOL004027	0.3621	0.6379	0.6224	Cyperi Rhizoma	1,4-Epoxy-16-hydroxyheneicos-1,3,12,14,18-pentaene	Not Available	FALSE	c1coc(c1)CCCCCCC/C=C/C=C/C(C/C=C/CC)O
MOL004028	0.7231	0.2769	0.8260	Cyperi Rhizoma	3-O-(2-rhamnosylglucosyl) oleanolic acid	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(OC6C(O)(C(O)C(O)C(O6)CO)C6C(O)C(O)C(O)C(O6)C)CCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)C)C)C)O
MOL004029	0.8976	0.1024	0.8266	Cyperi Rhizoma	Visnagin	6716	FALSE	c12c(c3c(cc1oc(cc2=O)C)occ3)OC
MOL004029	0.8976	0.1024	0.8266	Cimicifugae Rhizoma	Visnagin	6716	FALSE	c12c(c3c(cc1oc(cc2=O)C)occ3)OC
MOL004030	0.8516	0.1484	0.8132	Cyperi Rhizoma	(4aR,7R)-7-isopropenyl-1,4a-dimethyl-3,4,5,6,7,8-hexahydronaphthalen-2-one	10632629	FALSE	C1C(CC2=C(C(=O)CCC2(C1)C)C)C(=C)C
MOL004031	0.8626	0.1374	0.6836	Cyperi Rhizoma	(6S)-1-isopropyl-3-isopropylidene-6-methyl-6-vinylcyclohexene	80048	FALSE	C1(CCC(=C(C)C)C=C1C(C)C)(C)C=C

MOL004031	0.8626	0.1374	0.6836	Ligustici Rhizoma Et Radix	(6S)-1-isopropyl-3-isopropylidene-6-methyl-6-vinylcyclohexene	80048	FALSE	C1(CCC(=C(C)C)C=C1C(C)C)(C)C=C
MOL004031	0.8626	0.1374	0.6836	Hippophae Fructus	(6S)-1-isopropyl-3-isopropylidene-6-methyl-6-vinylcyclohexene	80048	FALSE	C1(CCC(=C(C)C)C=C1C(C)C)(C)C=C
MOL004032	0.8707	0.1293	0.8244	Cyperi Rhizoma	(4aS,6R,8aS)-4a-hydroxy-6-isopropenyl-4,8a-dimethyl-5,6,7,8-tetrahydro-1H-naphthalen-2-one	11651583	FALSE	C1(=O)C=C(C2(C(C1)(CCC(C2)C(=C)C)C)O)C
MOL004033	0.8219	0.1781	0.6554	Cyperi Rhizoma	α-Selinene	12309811	FALSE	C12(C(CC(CC1)C(=C)C)C(=CCC2)C)C
MOL004033	0.8219	0.1781	0.6554	Lysimachiae Herba	α-Selinene	12309811	FALSE	C12(C(CC(CC1)C(=C)C)C(=CCC2)C)C
MOL004033	0.8219	0.1781	0.6554	Nardostachyos Radix Et Rhizoma	α-Selinene	12309811	FALSE	C12(C(CC(CC1)C(=C)C)C(=CCC2)C)C
MOL004034	0.8437	0.1563	0.7357	Cyperi Rhizoma	Ammiol	621572	FALSE	o1c2c(c(OC)c3c(occ3)c2OC)c(=O)cc1CO
MOL004035	0.8383	0.1617	0.6248	Cyperi Rhizoma	4,5-secoeudesmane	Not Available	FALSE	C(CCCC)C1(CCC(C(C)C)CC1)C
MOL004036	0.8604	0.1396	0.8291	Cyperi Rhizoma	Eudesma-4,6-dien-3-one	6428385	FALSE	C1C(=CC2=C(C(=O)CCC2(C1)C)C)C(C)C
MOL004037	0.8568	0.1432	0.6274	Cyperi Rhizoma	beta-muurolene	25203009	FALSE	C12C(CC=C(C1CC=C(C2)C)C)C(C)C
MOL004038	0.8707	0.1293	0.8244	Cyperi Rhizoma	beta-Rotunol	5321005	FALSE	C1(=O)C=C(C2(C(C1)(CCC(C2)C(=C)C)C)O)C
MOL004039	0.9433	0.0567	0.8330	Cyperi Rhizoma	4,7-dimethyl-1-tetralone	71608071	FALSE	C1(=O)CCC(c2ccc(cc12)C)C
MOL004040	0.9122	0.0878	0.7803	Cyperi Rhizoma	cyperenoic acid	Not Available	FALSE	OC(=O)C1=C2C3(C(C(C2)CCC3C)(C)C)CC1
MOL004041	0.8612	0.1388	0.8021	Cyperi Rhizoma	Cyperol	14076601	FALSE	C1C(C(=C2C(C1)(CCC(C2)C(=C)C)C)C)O
MOL004042	0.8946	0.1054	0.7840	Cyperi Rhizoma	Cyperolone	5316283	FALSE	C12(C(CCC(C1)C(=C)C)(C)CCC2O)C(=O)C

MOL004043	0.8615	0.1385	0.7207	Cyperi Rhizoma	cyperotundone	Not Available	FALSE	O=C1CC23C(C(CC3=C1C)CCC2C)(C)C
MOL004044	0.8705	0.1295	0.6203	Cyperi Rhizoma	cyprotene	Not Available	FALSE	C12(C(CCC(C/C/1=C/C)C2(C)C)C)C
MOL004046	0.8273	0.1727	0.7143	Cyperi Rhizoma	Dimethyl tetrasulfide	79828	FALSE	CSSSSC
MOL004046	0.8273	0.1727	0.7143	Allium Azureum Ledeb.	Dimethyl tetrasulfide	79828	FALSE	CSSSSC
MOL004046	0.8273	0.1727	0.7143	Allii Tuberosi Semen	Dimethyl tetrasulfide	79828	FALSE	CSSSSC
MOL004046	0.8273	0.1727	0.7143	Allii Sativi Bulbus	Dimethyl tetrasulfide	79828	FALSE	CSSSSC
MOL004047	0.8148	0.1852	0.6020	Cyperi Rhizoma	epi-alpha-selinene	25200351	FALSE	C12(C(CC(CC1)C(C)C)C(=CCC2)C)C
MOL004048	0.9462	0.0538	0.9703	Cornus Officinalis Sieb. Et Zucc.	keto-L-fructose	5460024	FALSE	OCC(C(C(C(=O)CO)O)O)O
MOL004048	0.9462	0.0538	0.9703	Cyperi Rhizoma	keto-L-fructose	5460024	FALSE	OCC(C(C(C(=O)CO)O)O)O
MOL004050	0.8579	0.1421	0.6955	Cyperi Rhizoma	gamma-Calacorene	14038842	FALSE	C1(c2c(C(=CC1)C(C)C)cc(cc2)C)C
MOL004051	0.8911	0.1089	0.7832	Cyperi Rhizoma	(1S,3aS,4S,7R,8aS)-7-isopropenyl-1,4-dimethyl-2,3,3a,5,6,7,8,8a-octahydroazulene-1,4-diol	10633702	FALSE	OC1(C2C(C(O)(CCC(C2)C(=C)C)C)CC1)C
MOL004052	0.8651	0.1349	0.7681	Cyperi Rhizoma	isocyperol	14076604	FALSE	OC1C(=C)C2C(CCC(C2)C(=C)C)(CC1)C
MOL004053	0.7627	0.2373	0.8946	Cyperi Rhizoma	Isodalbergin	5318543	FALSE	c1cc(ccc1)c1c2c(oc(=O)c1)cc(c(c2)OC)O
MOL004054	0.9122	0.0878	0.8565	Cyperi Rhizoma	isokobusone	1493936	FALSE	O=C1C2C(C(C2)(C)C)CCC(=C)C(O)CC1
MOL004055	0.9466	0.0534	0.7515	Cyperi Rhizoma	6-[(3S,5R)-1-methyl-5-methylol-3-piperidyl]-2-pyridone	11447394	FALSE	C1(CN(CC(C1)c1[nH]c(=O)ccc1)C)CO
MOL004056	0.8553	0.1447	0.6426	Campsis Flos	α-Cadinene	12306048	FALSE	C12C(CC=C(C1CCC(=C2)C)C)C(C)C
MOL004056	0.8553	0.1447	0.6426	Moslae Herba	α-Cadinene	12306048	FALSE	C12C(CC=C(C1CCC(=C2)C)C)C(C)C
MOL004056	0.8553	0.1447	0.6426	Ailanthi Cortex	α-Cadinene	12306048	FALSE	C12C(CC=C(C1CCC(=C2)C)C)C(C)C
MOL004056	0.8553	0.1447	0.6426	Cyperi Rhizoma	α-Cadinene	12306048	FALSE	C12C(CC=C(C1CCC(=C2)C)C)C(C)C
MOL004058	0.8659	0.1341	0.7864	Cyperi Rhizoma	Khell	3828	FALSE	c12c(c(c3c(c1OC)cco3)OC)oc(cc2=O)C
MOL004059	0.9141	0.0859	0.7842	Cyperi Rhizoma	khellol glucoside	70697662	FALSE	O1C(C(O)C(O)C(O)C1OCc1oc2c(c(=O)c1)c(OC)c1c(occ1)c2)CO
MOL004060	0.8634	0.1366	0.8008	Cyperi Rhizoma	Khellol	164613	FALSE	OCc1oc2c(c(=O)c1)c(OC)c1c(occ1)c2

MOL004061	0.8846	0.1154	0.7905	Cyperi Rhizoma	kobusone	Not Available	FALSE	O1C2(C1CCC(=O)C1C(C((C1)(C)C)CC2)C
MOL004062	0.6690	0.3310	0.7422	Cyperi Rhizoma	Koelreuteria saponin A	Not Available	FALSE	C1(C(C(C(OC1)OC1C(C2C(CC1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(CO)C)C)O)O
MOL004065	0.8841	0.1159	0.7226	Cyperi Rhizoma	mustakone	Not Available	FALSE	C12(C3C(=O)C=C(C1C3C(CC2)C(C)C)C)C
MOL004066	0.7759	0.2241	0.7055	Cyperi Rhizoma	nootkatene	25200342	FALSE	C12(C(CC=CC2=CCC(C1)C(=C)C)C)C
MOL004067	0.8057	0.1943	0.7686	Radix Bupleuri	()-Nootkatone	1268142	FALSE	O=C1CC(C2(CC(CCC2=C1)C(=C)C)C)C
MOL004067	0.8057	0.1943	0.7686	Cyperi Rhizoma	()-Nootkatone	1268142	FALSE	O=C1CC(C2(CC(CCC2=C1)C(=C)C)C)C
MOL004067	0.8057	0.1943	0.7686	Siphonostegiae Herba	()-Nootkatone	1268142	FALSE	O=C1CC(C2(CC(CCC2=C1)C(=C)C)C)C
MOL004068	0.2931	0.7069	0.8132	Cyperi Rhizoma	rosenonolactone	Not Available	FALSE	O1C23C4(C(CC(CC4)(C)C=C)C(=O)CC2C(CCC3)(C1=O)C)C
MOL004070	0.8278	0.1722	0.7148	Cyperi Rhizoma	rotundenol	Not Available	FALSE	C1(CCC2C3(C(C(=C)C(CC12)CC3)O)C)C
MOL004071	0.3741	0.6259	0.7535	Cyperi Rhizoma	Hyndarin	72301	FALSE	O(C1C2CN3C(CC2CC1OC)C1(CC3)CC(OC)C(OC)C1)C
MOL004071	0.3741	0.6259	0.7535	Corydalis Rhizoma	Hyndarin	72301	FALSE	O(C1C2CN3C(CC2CC1OC)C1(CC3)CC(OC)C(OC)C1)C
MOL004072	0.6562	0.3438	0.7570	Cyperi Rhizoma	Rouhuoside	Not Available	FALSE	c1(cc(c2c(c1CC=C(C)C)oc(c(c2=O)OC1OC(C(C(C1O)O)OC1OC(C(C(C1O)O)O)CO)C)c1ccc(cc1)O)O)OC1OC(C(C(C1O)O)O)CO
MOL004075	0.9050	0.0950	0.7773	Cyperi Rhizoma	sugebiol	Not Available	FALSE	C1(C(=C2C3(C1)C(CCC(C2O)C3(C)C)C)C)O
MOL004076	0.9011	0.0989	0.7821	Cyperi Rhizoma	sugeonol	Not Available	FALSE	OC1C2C(C3(C(CC2)C)C1=C(C(=O)C3)C)(C)C
MOL004077	0.7489	0.2511	0.7456	Cyperi Rhizoma	sugeonyl acetate	Not Available	FALSE	O(C1C2C(C3(C(CC2)C)C1=C(C(=O)C3)C)(C)C)C(=O)C
MOL004078	0.9208	0.0792	0.7929	Cyperi Rhizoma	sugetriol	Not Available	FALSE	OC1C2C(C3(C(C(O)C2)C)C1=C(C(O)C3)C)(C)C
MOL004079	0.8644	0.1356	0.6151	Tamaricis Cacumen	(E)-calamenene	6429022	FALSE	C1(CCC(c2c1cc(cc2)C)C)C(C)C
MOL004079	0.8644	0.1356	0.6151	Cyperi Rhizoma	(E)-calamenene	6429022	FALSE	C1(CCC(c2c1cc(cc2)C)C)C(C)C
MOL004079	0.8644	0.1356	0.6151	Rhododendri Daurici Folium	(E)-calamenene	6429022	FALSE	C1(CCC(c2c1cc(cc2)C)C)C(C)C
MOL004080	0.9100	0.0900	0.8962	Cyperi Rhizoma	Vanay	5541	FALSE	O(C(COC(=O)C)COC(=O)C)C(=O)C
MOL004081	0.8521	0.1479	0.8802	Inulae Flos	4',5-dimethoxyquercetin	15227607	FALSE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)OC)OC)O
MOL004083	0.9056	0.0944	0.8845	Inulae Flos	Tamarixetin	5281699	FALSE	o1c(c2cc(O)c(OC)cc2)c(O)c(=O)c2c1cc(O)cc2O
MOL004083	0.9056	0.0944	0.8845	Artemisia Annua L.	Tamarixetin	5281699	FALSE	o1c(c2cc(O)c(OC)cc2)c(O)c(=O)c2c1cc(O)cc2O
MOL004084	0.9110	0.0890	0.8807	Inulae Flos	Spinacetin	5321435	FALSE	O1C2(C(=O)C(O)C1C1C(OC)C(O)CC1)C(O)C(OC)C(O)C2
MOL004085	0.3451	0.6549	0.7434	Inulae Flos	taraxasterol	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(C5C(CC4)(CCC(=C)C5C)C)CC3)C)(CC2)C)(CC1)C)(C)C)C(=O)C
MOL004086	0.8307	0.1693	0.8110	Inulae Flos	ivangustin	13895670	FALSE	O1C2C(C(=C)C1=O)CC1=C(CCC(C1(C2)C)O)C
MOL004087	0.8498	0.1502	0.7183	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	1,5-di-O-Caffeoylquinic acid	6474640	FALSE	O(C1(CC(OC(=O)/C=C/c2cc(O)c(O)cc2)C(O)C(O)C1)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1

MOL004087	0.8498	0.1502	0.7183	Xanthii Fructus	1,5-di-O-Caffeoylquinic acid	6474640	FALSE	O(C1(CC(OC(=O)/C=C/c2cc(O)c(O)cc2)C(O)C(O)C1)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL004087	0.8498	0.1502	0.7183	Inulae Flos	1,5-di-O-Caffeoylquinic acid	6474640	FALSE	O(C1(CC(OC(=O)/C=C/c2cc(O)c(O)cc2)C(O)C(O)C1)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL004088	0.9193	0.0807	0.8292	Inulae Flos	britannilactone	44575246	FALSE	O1C2C(C(O)C(=C(C2)C)C(CCCO)C)C(=C)C1=O
MOL004089	0.7601	0.2399	0.7892	Inulae Herba	inulicin	Not Available	FALSE	C12C(C(C(C(=C(C1)C)CCCOC(=O)C)C)O)C(=C)C(=O)O2
MOL004089	0.7601	0.2399	0.7892	Inulae Flos	inulicin	Not Available	FALSE	C12C(C(C(C(=C(C1)C)CCCOC(=O)C)C)O)C(=C)C(=O)O2
MOL004090	0.7601	0.2399	0.7892	Inulae Flos	3-[(3aS,4R,5R,8aR)-4-hydroxy-5,7-dimethyl-3-methylene-2-oxo-4,5,8,8a-tetrahydro-3aH-cyclohepta[b]furan-6-yl]propyl acetate	442263	FALSE	O1C2C(C(O)C(C(=C(C2)C)CCCOC(=O)C)C)C(=C)C1=O
MOL004091	0.6867	0.3133	0.6659	Inulae Flos	inuchinenolide C	46906384	FALSE	O1C2C(C(OC(=O)C)C=C(C(C2)C)CCC(=O)C)C(=C)C1=O
MOL004092	0.5716	0.4284	0.6610	Inulae Flos	[(3aR,4R,7aR)-5-[(1S)-4-acetoxy-1-methyl-butyl]-6-methyl-3-methylene-2-oxo-3a,4,7,7a-tetrahydrobenzofuran-4-yl] acetate	10360513	FALSE	O1C(=O)C(=C)C2C1CC(=C(C2OC(=O)C)C(CCCOC(=O)C)C)C
MOL004093	0.8934	0.1066	0.8957	Rhododendri Daurici Folium	Azaleatin	5281604	FALSE	c1c(cc2c(c1OC)c(=O)c(c(o2)c1cc(c(cc1)O)O)O)O
MOL004093	0.8934	0.1066	0.8957	Inulae Flos	Azaleatin	5281604	FALSE	c1c(cc2c(c1OC)c(=O)c(c(o2)c1cc(c(cc1)O)O)O)O

MOL004094	0.5670	0.4330	0.6041	Inulae Herba	Britanin	5315501	FALSE	C1(CC(C2(C1C(CC1C(C(=C)C(=O)O1)C2OC(=O)C)C)C)O)OC(=O)C
MOL004094	0.5670	0.4330	0.6041	Inulae Flos	Britanin	5315501	FALSE	C1(CC(C2(C1C(CC1C(C(=C)C(=O)O1)C2OC(=O)C)C)C)O)OC(=O)C
MOL004095	0.9550	0.0450	0.8963	Polygoni Avicularis Herba	Cinnamic acid, 3,4-dimethoxy-(8CI)	1585026	FALSE	C(=C\c1cc(c(cc1)OC)OC)\C(=O)O
MOL004095	0.9550	0.0450	0.8963	Inulae Flos	Cinnamic acid, 3,4-dimethoxy-(8CI)	1585026	FALSE	C(=C\c1cc(c(cc1)OC)OC)\C(=O)O
MOL004095	0.9550	0.0450	0.8963	Solidaginis Herba	Cinnamic acid, 3,4-dimethoxy-(8CI)	1585026	FALSE	C(=C\c1cc(c(cc1)OC)OC)\C(=O)O
MOL004095	0.9550	0.0450	0.8963	Eucommiae Cortex	Cinnamic acid, 3,4-dimethoxy-(8CI)	1585026	FALSE	C(=C\c1cc(c(cc1)OC)OC)\C(=O)O
MOL004096	0.3733	0.6267	0.7414	Inulae Flos	epifriedelanol acetate	13688752	FALSE	C1C(C(C2(C(C1)C1(C(CC2)C2(C(CC1)(C1C(CC2)(CCC(C1)(C)C)C)C)C)C)C)OC(=O)C
MOL004096	0.3733	0.6267	0.7414	Asteris Radix Et Rhizoma	epifriedelanol acetate	13688752	FALSE	C1C(C(C2(C(C1)C1(C(CC2)C2(C(CC1)(C1C(CC2)(CCC(C1)(C)C)C)C)C)C)C)OC(=O)C
MOL004097	0.8363	0.1637	0.7809	Inulae Flos	Inumakilactone E	Not Available	FALSE	C1CC2(C3C(C1O)(c1c(C(C3OC2=O)O)c(oc(=O)c1)C(C)CO)C)C
MOL004097	0.8363	0.1637	0.7809	Inulae Herba	Inumakilactone E	Not Available	FALSE	C1CC2(C3C(C1O)(c1c(C(C3OC2=O)O)c(oc(=O)c1)C(C)CO)C)C
MOL004098	0.8202	0.1798	0.7460	Inulae Flos	6-O-p-Hydroxybenzoyl ajugol	Not Available	FALSE	C12C(C(OC=C1)OC1OC(C(C(C1O)O)O)CO)C(CC2OC(=O)c1ccc(cc1)O)(O)C
MOL004099	0.9085	0.0915	0.8281	Schizonepetae Herba	Luteolin 8-O-beta-D-galatoside	5319115	FALSE	C1(C(C(C(C(O1)Oc1cc2c(c(c1)O)c(=O)cc(o2)c1cc(c(cc1)O)O)O)O)O)CO
MOL004099	0.9085	0.0915	0.8281	Inulae Flos	Luteolin 8-O-beta-D-galatoside	5319115	FALSE	C1(C(C(C(C(O1)Oc1cc2c(c(c1)O)c(=O)cc(o2)c1cc(c(cc1)O)O)O)O)O)CO
MOL004100	0.9197	0.0803	0.8086	Panax Ginseng C. A. Mey.	N-Salicylidene-salicylamine	Not Available	FALSE	c1ccc(c(c1)/C=N\Cc1c(cccc1)O)O
MOL004100	0.9197	0.0803	0.8086	Inulae Flos	N-Salicylidene-salicylamine	Not Available	FALSE	c1ccc(c(c1)/C=N\Cc1c(cccc1)O)O

MOL004101	0.9522	0.0478	0.8512	Inulae Flos	Melilotoside	5280759	FALSE	C1(C(C(C(OC1CO)Oc1ccccc1/C=C/C(=O)O)O)O)O
MOL004102	0.9471	0.0529	0.9324	Inulae Flos	2-Coumarate	Not Available	FALSE	Oc1ccccc1/C=C/C(=O)O
MOL004102	0.9471	0.0529	0.9324	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	2-Coumarate	Not Available	FALSE	Oc1ccccc1/C=C/C(=O)O
MOL004103	0.6786	0.3214	0.7191	Inulae Flos	Paucin	161538	FALSE	C12C(CC3C(CC1C)OC(=O)C3=C)(C(=O)CC2OC1C(C(C(C(O1)COC(=O)C)O)O)O)C
MOL004104	0.8863	0.1137	0.9380	Inulae Flos	Pratol	5320693	FALSE	c1(ccc2c(c1)oc(cc2=O)c1ccc(cc1)OC)O
MOL004105	0.8973	0.1027	0.7252	Inulae Flos	Quercetin-3-L-arabinon-7-D-glucoside	Not Available	FALSE	c1(c(ccc(c1)C1=C(OC(=O)CC(=O)OC2OC(C(C(C2O)O)O)CO)C(=O)C2C(O1)C=C(C=C2O)O)O)O
MOL004106	0.8980	0.1020	0.7502	Inulae Flos	Quercetin-3-L-arabinon-7-D-glucoside_qt	Not Available	FALSE	c1(c(ccc(c1)C1=C(OC(=O)CC(=O)O)C(=O)C2C(O1)C=C(C=C2O)O)O)O
MOL004107	0.5333	0.4667	0.7310	Smilacis Glabrae Rhixoma	Syrionylglycerol-beta-syringaresinol	Not Available	FALSE	C1(C(C(OC(C1O)CO)Oc1c(cc(cc1OC)C1OCC2C1COC2c1cc(c(c(c1)OC)OC(CO)C(c1cc(c(c(c1)OC)OC1C(C(C(C(O1)CO)O)O)O)OC)O)OC)OC)O)O
MOL004107	0.5333	0.4667	0.7310	Inulae Flos	Syrionylglycerol-beta-syringaresinol	Not Available	FALSE	C1(C(C(OC(C1O)CO)Oc1c(cc(cc1OC)C1OCC2C1COC2c1cc(c(c(c1)OC)OC(CO)C(c1cc(c(c(c1)OC)OC1C(C(C(C(O1)CO)O)O)O)OC)O)OC)OC)O)O
MOL004107	0.5333	0.4667	0.7310	Sojae Semen Nigrum	Syrionylglycerol-beta-syringaresinol	Not Available	FALSE	C1(C(C(OC(C1O)CO)Oc1c(cc(cc1OC)C1OCC2C1COC2c1cc(c(c(c1)OC)OC(CO)C(c1cc(c(c(c1)OC)OC1C(C(C(C(O1)CO)O)O)O)OC)O)OC)OC)O)O
MOL004107	0.5333	0.4667	0.7310	Rhododendri Daurici Folium	Syrionylglycerol-beta-syringaresinol	Not Available	FALSE	C1(C(C(OC(C1O)CO)Oc1c(cc(cc1OC)C1OCC2C1COC2c1cc(c(c(c1)OC)OC(CO)C(c1cc(c(c(c1)OC)OC1C(C(C(C(O1)CO)O)O)O)OC)O)OC)OC)O)O
MOL004109	0.5670	0.4330	0.6041	Inulae Flos	[(3aS,5R,5aS,6S,8S,8aR,9S,9aR)-6-acetoxy-8-hydroxy-5,8a-dimethyl-1-methylene-2-oxo-4,5,5a,6,7,8,9,9a-octahydro-3aH-azuleno[6,5-b]furan-9-yl] acetate	24721441	FALSE	C12(C(C(CC2O)OC(=O)C)C(CC2C(C1OC(=O)C)C(=C)C(=O)O2)C)C

MOL004110	0.9208	0.0792	0.8007	Inulae Flos	Isotrifolin	5484006	FALSE	O1C(C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1)C(O)CO
MOL004111	0.4108	0.5892	0.7050	Inulae Herba	ZINC04027388	7077273	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC(=C)C5C)C)CC3)C)(CC2)C)(CC1)C)(C)C
MOL004111	0.4108	0.5892	0.7050	Inulae Flos	ZINC04027388	7077273	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC(=C)C5C)C)CC3)C)(CC2)C)(CC1)C)(C)C
MOL004112	0.9399	0.0601	0.9172	Inulae Herba	Patuletin	5281678	FALSE	o1c2c(c(=O)c(O)c1c1cc(O)c(O)cc1)c(O)c(OC)c(O)c2
MOL004112	0.9399	0.0601	0.9172	Eriocauli Flos	Patuletin	5281678	FALSE	o1c2c(c(=O)c(O)c1c1cc(O)c(O)cc1)c(O)c(OC)c(O)c2
MOL004112	0.9399	0.0601	0.9172	Inulae Flos	Patuletin	5281678	FALSE	o1c2c(c(=O)c(O)c1c1cc(O)c(O)cc1)c(O)c(OC)c(O)c2
MOL004112	0.9399	0.0601	0.9172	Artemisia Annua L.	Patuletin	5281678	FALSE	o1c2c(c(=O)c(O)c1c1cc(O)c(O)cc1)c(O)c(OC)c(O)c2
MOL004113	0.9205	0.0795	0.9242	Curculiginis Rhizome	(E)-6-Methyl-3,5-heptadien-2-one	5319674	FALSE	CC(=CC/C=C/C(=O)CC)C
MOL004114	0.9055	0.0945	0.8299	Curculiginis Rhizome	3,2',4',6'-Tetrahydroxy-4,3'-dimethoxy chalcone	5321858	FALSE	C(=C\c1cc(c(cc1)OC)O)/C(=O)c1c(c(c(cc1O)O)OC)O
MOL004115	0.5932	0.4068	0.6751	Curculiginis Rhizome	3,3',5,5'-tetramethoxy-7,9'7',9-diepoxy-lignan-4,4'-di-O-β-D-glucopyranoside	Not Available	FALSE	c1(cc(c(c(c1)OC)OC1OC(C(C(C1O)O)O)CO)OC)C1C2C(CO1)C(OC2)c1cc(c(c(c1)OC)OC1OC(C(C(C1O)O)O)CO)OC
MOL004116	0.9006	0.0994	0.9292	Curculiginis Rhizome	methyl 5-acetyl-1,2,3,5,6-oxatetrazinane-3-carboxylate	14308995	FALSE	O1NN(CN(N1)C(=O)OC)C(=O)C
MOL004119	0.8851	0.1149	0.9621	Momordicae Fructus	5-METHYLFURFURAL	12097	FALSE	c1cc(oc1C)C=O
MOL004119	0.8851	0.1149	0.9621	Curculiginis Rhizome	5-METHYLFURFURAL	12097	FALSE	c1cc(oc1C)C=O
MOL004119	0.8851	0.1149	0.9621	Ginkgo Folium	5-METHYLFURFURAL	12097	FALSE	c1cc(oc1C)C=O

MOL004119	0.8851	0.1149	0.9621	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	5-METHYLFURFURAL	12097	FALSE	c1cc(oc1C)C=O
MOL004119	0.8851	0.1149	0.9621	Mume Fructus	5-METHYLFURFURAL	12097	FALSE	c1cc(oc1C)C=O
MOL004119	0.8851	0.1149	0.9621	Campsis Flos	5-METHYLFURFURAL	12097	FALSE	c1cc(oc1C)C=O
MOL004120	0.8660	0.1340	0.6416	Curculiginis Rhizome	Curculigin C	132568	FALSE	C1C(C(C(C(O1)OCC1C(C(C(C(O1)Oc1c(Cl)c(c(c(c1Cl)C)Cl)OC)O)O)O)O)O)O
MOL004121	0.9404	0.0596	0.9062	Curculiginis Rhizome	2,4,6-Trichloro-3-methoxy-5-methylphenol	617690	FALSE	Oc1c(Cl)c(c(c(c1Cl)C)Cl)OC
MOL004122	0.6796	0.3204	0.8200	Curculiginis Rhizome	Curculigosaponin G	Not Available	FALSE	C1(C(C(C(C(O1)OC1C(OC(C(C1O)O)CO)OC1C(C2C3(CC1)C1(C(CC2)C2(C(CC1O)(C(C(C2)O)C(CCC(=O)C(C)C)C)C)C)C3)(C)C)O)O)O)C
MOL004123	0.3777	0.6223	0.7052	Curculiginis Rhizome	Curculigosaponin G_qt	Not Available	FALSE	OC1C(C2C3(CC1)C1(C(CC2)C2(C(CC1O)(C(C(C2)O)C(CCC(=O)C(C)C)C)C)C)C3)(C)C
MOL004124	0.8332	0.1668	0.7458	Curculiginis Rhizome	Curculigoside B	132567	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(COC(=O)c2c(OC)cccc2O)cc(O)cc1)CO
MOL004125	0.9164	0.0836	0.7620	Curculiginis Rhizome	Curculigoside B_qt	Not Available	FALSE	Oc1c(COC(=O)c2c(OC)cccc2O)cc(O)cc1
MOL004126	0.7368	0.2632	0.6803	Curculiginis Rhizome	Curculigoside	158845	FALSE	c1(ccc(c(c1)COC(=O)c1c(OC)cccc1OC)OC1OC(C(C(C1O)O)O)CO)O
MOL004127	0.8667	0.1333	0.7820	Curculiginis Rhizome	Curcumadiol	Not Available	FALSE	C12C(C(CC2)(O)C)CC(=CCC1(C)O)C(C)C

MOL004128	0.2036	0.7964	0.8533	Curculiginis Rhizome	4H-Dibenzo(de,g)quinoline, 9-(4,5-dimethoxy-2-((1,2,3,4-tetrahydro-5,6,7-trimethoxy-2-methyl-1-isoquinolinyl)methyl)phenoxy)-5,6,6a,7-tetrahydro-1,2,3,10-tetramethoxy-6-methyl-, (S-(R*,R*))-	3082725	FALSE	COc1c(OC)c2c3c(c1OC)CCN(C3Cc1c2cc(c(c1)Oc1c(cc(c(c1)OC)OC)CC1c2c(c(c(c(c2)OC)OC)OC)CCN1C)OC)C
MOL004129	0.9098	0.0902	0.7826	Curculiginis Rhizome	Curculigoside_qt	Not Available	FALSE	c1(ccc(c(c1)COC(=O)c1c(OC)cccc1OC)O)O
MOL004130	0.9391	0.0609	0.9432	Curculiginis Rhizome	TETRAMETHYLSUCCINAMIDE	23752	FALSE	C(=O)(N(C)C)CCC(=O)N(C)C
MOL004131	0.9132	0.0868	0.9403	Curculiginis Rhizome	N-acetyl-N-hydroxy-2-carbamic acid methylester	14308994	FALSE	CC(=O)N(O)C(=O)OC
MOL004132	0.9472	0.0528	0.8218	Curculiginis Rhizome	1-Bromo-2-methoxynaphthalene	72860	FALSE	c12c(ccc(c1Br)OC)cccc2
MOL004133	0.9273	0.0727	0.9234	Curculiginis Rhizome	orcinol glucoside	12315192	FALSE	c1(cc(O)cc(C)c1)OC1C(O)C(O)C(O)C(O1)CO
MOL004134	0.8753	0.1247	0.9530	Curculiginis Rhizome	Orcin	10436	FALSE	c1(cc(O)cc(C)c1)O
MOL004134	0.8753	0.1247	0.9530	Rhododendri Daurici Folium	Orcin	10436	FALSE	c1(cc(O)cc(C)c1)O
MOL004135	0.7705	0.2295	0.8051	Curculiginis Rhizome	2,3,4,7-tetramethoxyxanthone	370636	FALSE	c1c(ccc2c1c(=O)c1c(o2)c(c(c(c1)OC)OC)OC)OC
MOL004136	0.8719	0.1281	0.6902	Curculiginis Rhizome	lycorine	Not Available	FALSE	c1c2c(cc3c1C1C4N(C3)CCC4=CC(C1O)O)OCO2
MOL004137	0.3077	0.6923	0.7078	Curculiginis Rhizome	yuccagenin	Not Available	FALSE	C1C2(C(=CCC3C2CCC2(C3CC3C2C(C2(O3)OCC(CC2)C)C)C)CC(C1O)O)C
MOL004138	0.9301	0.0699	0.8380	Curculiginis Rhizome	corchioside A	Not Available	FALSE	c1(cc(cc(c1)O)C)OC1C(C(C(C(O1)COC1C(C(C(CO1)O)O)O)O)O)O)O

MOL004139	0.8861	0.1139	0.6735	Curculiginis Rhizome	curculigine A	Not Available	FALSE	c1(c(c(c(c(c1)OC)Cl)C)Cl)OC1C(C(C(C(O1)COC1C(C(C(C(O1)CO)O)O)O)O)O)O
MOL004140	0.9533	0.0467	0.9482	Curculiginis Rhizome	2,4-dichloro-5-methoxy-3-methylphenol	21475016	FALSE	c1(c(c(c(c(c1)OC)Cl)C)Cl)O
MOL004141	0.8828	0.1172	0.6476	Curculiginis Rhizome	curculigine B	Not Available	FALSE	c1(c(c(c(c(c1)OC)Cl)C)Cl)OC1C(C(C(C(O1)COC1OCC(C1O)(O)CO)O)O)O
MOL004143	0.4988	0.5012	0.7081	Curculiginis Rhizome	curculigosaponin A	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(C3)C(CC2(C1(CC(C2C(CCC(=O)C(C)C)C)O)C)C)O)OC1C(C(C(C(O1)CO)O)O)O
MOL004144	0.3777	0.6223	0.7052	Curculiginis Rhizome	curculigosaponin E_qt	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(C3)C(CC2(C1(CC(C2C(CCC(=O)C(C)C)C)O)C)C)O)O
MOL004145	0.4481	0.5519	0.7322	Curculiginis Rhizome	curculigosaponin B	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(C3)C(CC2(C1(CC(C2C(CCC(=O)C(C)C)C)OC1C(C(C(CO1)O)O)O)C)C)O)O
MOL004146	0.6699	0.3301	0.7293	Curculiginis Rhizome	curculigosaponin C	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(C3)C(CC2(C1(CC(C2C(CCC(=O)C(C)C)C)OC1C(C(C(CO1)O)O)O)C)C)O)OC1C(C(C(C(O1)CO)O)O)O
MOL004147	0.7040	0.2960	0.8230	Curculiginis Rhizome	curculigosaponin D	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(C3)C(CC2(C1(CC(C2C(CCC(=O)C(C)C)C)O)C)C)O)OC1C(C(C(C(O1)CO)O)O)O)OC1C(C(C(C(O1)CO)O)O)O
MOL004148	0.7154	0.2846	0.8139	Curculiginis Rhizome	curculigosaponin E	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(C3)C(CC2(C1(CC(C2C(CCC(=O)C(C)C)C)OC1C(C(C(CO1)O)O)O)C)C)O)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O)O
MOL004149	0.7313	0.2687	0.8054	Curculiginis Rhizome	curculigosaponin F	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(C3)C(CC2(C1(CC(C2C(CCC(=O)C(C)C)C)O)C)C)O)OC1C(C(C(C(O1)CO)O)O)O)OC1C(C(C(C(O1)CO)O)OC1C(C(C(C(O1)CO)O)O)O)O)O
MOL004150	0.3777	0.6223	0.7052	Curculiginis Rhizome	curculigosaponin J_qt	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(C3)C(CC2(C1(CC(C2C(CCC(=O)C(C)C)C)O)C)C)O)O
MOL004151	0.6796	0.3204	0.8200	Curculiginis Rhizome	curculigosaponin G	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(C3)C(CC2(C1(CC(C2C(CCC(=O)C(C)C)C)O)C)C)O)OC1C(C(C(C(O1)CO)O)O)O)OC1OC(C(C(C1O)O)O)C
MOL004152	0.7291	0.2709	0.8109	Curculiginis Rhizome	curculigosaponin H	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(C3)C(CC2(C1(CC(C2C(CCC(=O)C(C)C)C)OC1C(C(C(CO1)O)O)O)C)C)O)OC1C(C(C(C(O1)CO)O)O)OC1OC(C(C(C1O)O)O)C
MOL004154	0.2819	0.7181	0.6714	Asari Radix Et Rhizoma	Cynanuriculoside A_qt	Not Available	FALSE	C1(CC2=CCC3(C(C2(CC1)C)CC(C1(C3(O)CCC1O)C)C(=O)C)OC(=O)/C=C(/C(C)C)\C)O)OC1OC(C(C(C1)OC)OC1OC(C(C(C1)OC)OC1OC(C(C(C1)OC)O)O)O)O)O
MOL004154	0.2819	0.7181	0.6714	Schizonepetae Herba	Cynanuriculoside A_qt	Not Available	FALSE	C1(CC2=CCC3(C(C2(CC1)C)CC(C1(C3(O)CCC1O)C)C(=O)C)OC(=O)/C=C(/C(C)C)\C)O)OC1OC(C(C(C1)OC)OC1OC(C(C(C1)OC)OC1OC(C(C(C1)OC)O)O)O)O)O
MOL004154	0.2819	0.7181	0.6714	Curculiginis Rhizome	Cynanuriculoside A_qt	Not Available	FALSE	C1(CC2=CCC3(C(C2(CC1)C)CC(C1(C3(O)CCC1O)C)C(=O)C)OC(=O)/C=C(/C(C)C)\C)O)OC1OC(C(C(C1)OC)OC1OC(C(C(C1)OC)OC1OC(C(C(C1)OC)O)O)O)O)O

MOL004155	0.7283	0.2717	0.8132	Curculiginis Rhizome	curculigosaponin I	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(C3)C(CC2(C1(CC(C2C(CCC(=O)C(C)C)C)O)C)C)O)OC1C(C(C(C(O1)CO)O)O)O)OC1C(C(C(C(O1)C)O)OC1C(C(C(C(O1)CO)O)O)O)O
MOL004156	0.7460	0.2540	0.7971	Curculiginis Rhizome	curculigosaponin J	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(C3)C(CC2(C1(CC(C2C(CCC(=O)C(C)C)C)OC1C(C(C(CO1)O)O)O)C)C)O)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)C)O)OC1C(C(C(C(O1)CO)O)O)O)O
MOL004157	0.7443	0.2557	0.8062	Curculiginis Rhizome	curculigosaponin K	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(C3)C(CC2(C1(CC(C2C(CCC(C(C)C)O)C)O)C)C)O)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)OC1C(C(C(C(O1)CO)O)O)O)O
MOL004158	0.4221	0.5779	0.6960	Curculiginis Rhizome	curculigosaponin L_qt	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(C3)C(CC2(C1(CC(C2C(CCC(C(C)C)O)C)O)C)C)O)O
MOL004159	0.7070	0.2930	0.8122	Curculiginis Rhizome	curculigosaponin L	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(C3)C(CC2(C1(CC(C2C(CCC(C(C)C)O)C)O)C)C)O)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)C)O)O)O
MOL004160	0.7359	0.2641	0.7930	Curculiginis Rhizome	curculigosaponin M	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(C3)C(CC2(C1(CC(C2C(CCC=C(C)C)C)OC1C(C(C(CO1)O)O)O)C)C)O)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)OC1C(C(C(C(O1)CO)O)O)O)O
MOL004161	0.3953	0.6047	0.7219	Curculiginis Rhizome	curculigosaponin M_qt	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(C3)C(CC2(C1(CC(C2C(CCC=C(C)C)C)O)C)C)O)O
MOL004162	0.3777	0.6223	0.7052	Curculiginis Rhizome	Curculigenin A	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(C3)C(CC2(C1(CC(C2C(CCC(=O)C(C)C)C)O)C)C)O)O
MOL004163	0.4221	0.5779	0.6960	Curculiginis Rhizome	Curculigenin B	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(C3)C(CC2(C1(CC(C2C(CCC(C(C)C)O)C)O)C)C)O)O
MOL004164	0.3953	0.6047	0.7219	Curculiginis Rhizome	Curculigenin C	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(C3)C(CC2(C1(CC(C2C(CCC=C(C)C)C)O)C)C)O)O
MOL004165	0.7917	0.2083	0.6923	Curculiginis Rhizome	[5-hydroxy-2-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl] methyl 3-hydroxy-2,6-dimethoxybenzoate	11503965	FALSE	c1(c(ccc(c1OC)O)OC)C(=O)OCc1c(OC2OC(C(C(C2O)O)O)CO)ccc(c1)O
MOL004166	0.9025	0.0975	0.7994	Curculiginis Rhizome	Curculigoside C_qt	Not Available	FALSE	c1(c(ccc(c1OC)O)OC)C(=O)OCc1c(O)ccc(c1)O
MOL004167	0.9411	0.0589	0.8375	Curculiginis Rhizome	2,6-Dimethoxybenzoic acid	15109	FALSE	c1(c(cccc1OC)OC)C(=O)O

MOL004168	0.3558	0.6442	0.6990	Curculiginis Rhizome	curculigol	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C(CC2)C(O)(C)CCC(C(C)C)C)C)C)C3)(C)C)O
MOL004169	0.9241	0.0759	0.9236	Curculiginis Rhizome	2-PROPYL-1-HEPTANOL	38988758	FALSE	C(CCCCC)(CCC)CO
MOL004170	0.9104	0.0896	0.7564	Gossampiniflos	DBQ	12867	FALSE	C1(=CC(=O)C=C(C1=O)C(C)(C)C)C(C)(C)C
MOL004170	0.9104	0.0896	0.7564	Curculiginis Rhizome	DBQ	12867	FALSE	C1(=CC(=O)C=C(C1=O)C(C)(C)C)C(C)(C)C
MOL004170	0.9104	0.0896	0.7564	Mahoniae Caulis	DBQ	12867	FALSE	C1(=CC(=O)C=C(C1=O)C(C)(C)C)C(C)(C)C
MOL004171	0.6575	0.3425	0.7331	Siegesbeckiae Herba	3-(alpha,4-Dihydroxy-3-methoxybenzyl)-4-(hydroxy-3-methoxybenzyl) tetrahydrofuran	44559616	FALSE	c1cc(cc(c1O)OC)CC1COCC1C(c1cc(c(cc1)O)OC)O
MOL004172	0.3961	0.6039	0.6868	Siegesbeckiae Herba	(1R)-1-[(2S,4aR,4bS,7R,8aS)-7-hydroxy-2,4b,8,8-tetramethyl-4,4a,5,6,7,8a,9,10-octahydro-3H-phenanthren-2-yl]ethane-1,2-diol	3037565	FALSE	C1C(C(C2C(C1)(C1C(=CC(CC1)(C(CO)O)C)CC2)C)(C)C)O
MOL004173	0.3961	0.6039	0.6868	Siegesbeckiae Herba	darutoside_qt	Not Available	FALSE	C1(C=C2C(CC1)C1(C(CC2)C(C(CC1)O)(C)C)C)(C)C(O)CO
MOL004174	0.8530	0.1470	0.6183	Schisandrae Chinensis Fructus	epsilon-Cadinene	12302130	FALSE	C1CC(C2C(C1=C)CCC(=C)C2)C(C)C
MOL004174	0.8530	0.1470	0.6183	Siegesbeckiae Herba	epsilon-Cadinene	12302130	FALSE	C1CC(C2C(C1=C)CCC(=C)C2)C(C)C
MOL004174	0.8530	0.1470	0.6183	Panax Ginseng C. A. Mey.	epsilon-Cadinene	12302130	FALSE	C1CC(C2C(C1=C)CCC(=C)C2)C(C)C
MOL004175	0.7404	0.2596	0.7552	Mori Cortex	NSC733507	471426	FALSE	C12=CCC3C4(C(C(C(C(C4)O)O)(C)C)CCC3(C1(CCC1(C2C(C(CC1)C)(O)C)C(=O)O)C)C)C
MOL004175	0.7404	0.2596	0.7552	Siegesbeckiae Herba	NSC733507	471426	FALSE	C12=CCC3C4(C(C(C(C(C4)O)O)(C)C)CCC3(C1(CCC1(C2C(C(CC1)C)(O)C)C(=O)O)C)C)C

MOL004175	0.7404	0.2596	0.7552	Potentillae Discoloris Herba	NSC733507	471426	FALSE	C12=CCC3C4(C(C(C(C(C4)O)O)(C)C)CCC3(C1(CCC1(C2C(C(CC1)C)(O)C)C(=O)O)C)C)C
MOL004175	0.7404	0.2596	0.7552	Ardisiae Japonicae Herba	NSC733507	471426	FALSE	C12=CCC3C4(C(C(C(C(C4)O)O)(C)C)CCC3(C1(CCC1(C2C(C(CC1)C)(O)C)C(=O)O)C)C)C
MOL004175	0.7404	0.2596	0.7552	Potentillae Chinensis Herba	NSC733507	471426	FALSE	C12=CCC3C4(C(C(C(C(C4)O)O)(C)C)CCC3(C1(CCC1(C2C(C(CC1)C)(O)C)C(=O)O)C)C)C
MOL004175	0.7404	0.2596	0.7552	Radix Salviae	NSC733507	471426	FALSE	C12=CCC3C4(C(C(C(C(C4)O)O)(C)C)CCC3(C1(CCC1(C2C(C(CC1)C)(O)C)C(=O)O)C)C)C
MOL004176	0.7993	0.2007	0.6640	Siegesbeckiae Herba	germacrane D	Not Available	FALSE	C1(CCC(CCC(CCC1)C)C(C)C)C
MOL004177	0.6584	0.3416	0.7140	Siegesbeckiae Herba	15alpha-Hydroxy-ent-kaur-16-en-19-oic acid	Not Available	FALSE	C1CC(C2C(C1)(C1C3(CC2)CC(CC1)C(=C)C3O)C)(C)C(=O)O
MOL004178	0.9044	0.0956	0.8197	Polygoni Orientalis Fructus	orientin	5281675	FALSE	c1(cc(=O)c2c(o1)c(c(cc2O)O)C1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL004178	0.9044	0.0956	0.8197	Crataegi Folium	orientin	5281675	FALSE	c1(cc(=O)c2c(o1)c(c(cc2O)O)C1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL004178	0.9044	0.0956	0.8197	Trollius Chinensis	orientin	5281675	FALSE	c1(cc(=O)c2c(o1)c(c(cc2O)O)C1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL004178	0.9044	0.0956	0.8197	Siegesbeckiae Herba	orientin	5281675	FALSE	c1(cc(=O)c2c(o1)c(c(cc2O)O)C1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL004178	0.9044	0.0956	0.8197	Cannabis Sativa L.	orientin	5281675	FALSE	c1(cc(=O)c2c(o1)c(c(cc2O)O)C1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL004178	0.9044	0.0956	0.8197	Abrus Precatorius L.	orientin	5281675	FALSE	c1(cc(=O)c2c(o1)c(c(cc2O)O)C1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL004178	0.9044	0.0956	0.8197	Drynariae Rhizoma	orientin	5281675	FALSE	c1(cc(=O)c2c(o1)c(c(cc2O)O)C1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL004178	0.9044	0.0956	0.8197	Santalum Album L.	orientin	5281675	FALSE	c1(cc(=O)c2c(o1)c(c(cc2O)O)C1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL004178	0.9044	0.0956	0.8197	Commelinae Herba	orientin	5281675	FALSE	c1(cc(=O)c2c(o1)c(c(cc2O)O)C1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL004178	0.9044	0.0956	0.8197	Spirodelae Herba	orientin	5281675	FALSE	c1(cc(=O)c2c(o1)c(c(cc2O)O)C1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)O
MOL004179	0.8274	0.1726	0.7024	Siegesbeckiae Herba	Vernolic acid	5281128	FALSE	C1(C(O1)CCCCC)C/C=C\CCCCCCCC(=O)O
MOL004180	0.4025	0.5975	0.8482	Siegesbeckiae Herba	Coronaridine	Not Available	FALSE	c1ccc2c(c1)c1c([nH]2)C2(C(=O)OC)C3C(CC(CN3CC1)C2)CC

MOL004182	0.5397	0.4603	0.7385	Siegesbeckiae Herba	(1R)-1-[(2S,4aR,4bS,6S,8R,8aS)-6-hydroxy-2,4b,8-trimethyl-8-methylol-4,4a,5,6,7,8a,9,10-octahydro-3H-phenanthren-2-yl]ethane-1,2-diol	15736732	FALSE	OC1CC2(C(C(C1)(CO)C)CCC1=CC(CCC21)(C(O)CO)C)C
MOL004183	0.8030	0.1970	0.6332	Siegesbeckiae Herba	Orixine	Not Available	FALSE	O1COc2c1ccc1c2nc(c(c1OC)CC(O)C(C)(C)O)OC
MOL004184	0.5576	0.4424	0.7334	Siegesbeckiae Herba	Siegesesteric acid II	Not Available	FALSE	C1CC(C2C(C1)(C1C3(CC2)CC(CC1)C(C3)COCC)C)(C(=O)O)C
MOL004185	0.6007	0.3993	0.7626	Siegesbeckiae Herba	Siegesmethyletheric acid	Not Available	FALSE	C1CC(C2C(C1)(C1C3(CC2)CC(CC1)C(C3)COC)C)(C(=O)O)C
MOL004188	0.9125	0.0875	0.7646	Siegesbeckiae Herba	chromolaevanedione	25084009	FALSE	O=C1C2C(C2CC1)C(C(C)C)CCC(=O)C
MOL004189	0.3736	0.6264	0.7967	Siegesbeckiae Herba	darutigenol B	Not Available	FALSE	O1C23C(C4(C(C(C(O)CC4)(C)C)CC3)C)CCC(C2)(C1CO)C
MOL004190	0.5145	0.4855	0.7448	Corydalis Rhizoma	(-)-alpha-N-methylcanadine	Not Available	FALSE	c1c(c(c2c(c1)CC1[N+](C2)(CCc2c1cc1c(c2)OCO1)C)OC)OC
MOL004191	0.5555	0.4445	0.6812	Corydalis Rhizoma	Capaurine	94149	FALSE	c12c3N(CC4c(c3)ccc(c4OC)OC)CCC1cc(c(c2O)OC)OC
MOL004192	0.5466	0.4534	0.7033	Corydalis Rhizoma	caseanidine	Not Available	FALSE	c12c(CCN3Cc4c(CC13)ccc(c4OC)OC)ccc(c2O)OC
MOL004193	0.5784	0.4216	0.7663	Corydalis Rhizoma	Clarkeanidine	127376	FALSE	c12c(CCN3Cc4c(CC13)ccc(c4O)OC)ccc(c2O)OC
MOL004194	0.1836	0.8164	0.6830	Corydalis Rhizoma	corybulbine	Not Available	FALSE	c1(c2c(ccc1OC)CC1N(C2)CCc2c1cc(c(c2)OC)OC)OC
MOL004195	0.2168	0.7832	0.6854	Corydalis Rhizoma	CORYDALINE	101301	FALSE	C12c3c(cc(c(c3)OC)OC)CCN1Cc1c(C2C)ccc(c1OC)OC
MOL004196	0.3371	0.6629	0.7430	Corydalis Rhizoma	Corydalmine	Not Available	FALSE	c1c(c(c2c(c1)CC1C(C2)CCc2c1cc(c(c2)OC)OC)OC)O
MOL004197	0.6195	0.3805	0.8165	Corydalis Rhizoma	Corydine	10153	FALSE	c12c3c4c(CC1N(CCc2cc(c3O)OC)C)ccc(c4OC)OC
MOL004198	0.7737	0.2263	0.7864	Corydalis Rhizoma	18797-79-0	Not Available	FALSE	c1cc2c(c3c1C1(C(N(C3)C)c3c(CC1O)cc1c(c3)OCO1)C)OCO2
MOL004199	0.8202	0.1798	0.7810	Corydalis Rhizoma	Corynoloxine	Not Available	FALSE	c12c(cc3c(c1)C1C4(C(C3)OC(c3c4ccc4c3OCO4)N1C)C)OCO2

MOL004200	0.3857	0.6143	0.7192	Corydalis Rhizoma	methyl-[2-(3,4,6,7-tetramethoxy-1-phenanthryl)ethyl]amine	11462401	FALSE	c1(cc(c(c2c3cc(c(cc3ccc12)OC)OC)OC)OC)CCNC
MOL004201	0.7159	0.2841	0.8595	Corydalis Rhizoma	4H-Dibenzo(de,g)quinoline-1,11-diol, 5,6,6a,7-tetrahydro-2,10-dimethoxy-6-methyl-, (S)-	160500	FALSE	N1(CCc2c3c(c4c(CC13)ccc(c4O)OC)c(c(c2)OC)O)C
MOL004202	0.4897	0.5103	0.8234	Corydalis Rhizoma	dehydrocavidine	Not Available	FALSE	C12c3c(cc(c(c3)OC)OC)C=CN1Cc1c(C2C)ccc2c1OCO2
MOL004203	0.5071	0.4929	0.7217	Corydalis Rhizoma	Dehydrocorybulbine	5316439	FALSE	c1(c2c(ccc1OC)c(c1[n+](c2)CCc2c1cc(c(c2)O)OC)C)OC
MOL004204	0.3852	0.6148	0.6942	Corydalis Rhizoma	dehydrocorydaline	34781	FALSE	c12c3c(cc(c(c3)OC)OC)CC[n+]1cc1c(c2C)ccc(c1OC)OC
MOL004205	0.5808	0.4192	0.7417	Corydalis Rhizoma	Dehydrocorydalmine	3083983	FALSE	c1c(c(c2c(c1)cc1[n+](c2)CCc2c1cc(c(c2)OC)OC)OC)O
MOL004206	0.4704	0.5296	0.7446	Corydalis Rhizoma	Dehydroglaucine	Not Available	FALSE	c12c3c(N(CC1)C)cc1c(c3c(c(c2)OC)OC)cc(c(c1)OC)OC
MOL004207	0.7078	0.2922	0.8334	Corydalis Rhizoma	Dehydronantenine	Not Available	FALSE	c12c3c(cc4c1cc1c(c4)OCO1)N(CCc3cc(c2OC)OC)C
MOL004208	0.6164	0.3836	0.7154	Corydalis Rhizoma	demethylcorydalmatine	Not Available	FALSE	c1c(c(c2c(c1)CC1N(C2)CCc2c1cc(c(c2)OC)OC)O)O
MOL004209	0.5072	0.4928	0.7188	Corydalis Rhizoma	13-methyldehydrocorydalmine	25254728	FALSE	c12c3c(cc(c(c3)OC)OC)CC[n+]1cc1c(c2C)ccc(c1OC)O
MOL004210	0.4913	0.5087	0.7927	Corydalis Rhizoma	(1S,8'R)-6,7-dimethoxy-2-methylspiro[3,4-dihydroisoquinoline-1,7'-6,8-dihydrocyclopenta[g][1,3]benzodioxole]-8'-ol	21770852	FALSE	O1COc2c1ccc1CC3(C(c21)O)N(CCc1cc(c(cc31)OC)OC)C

MOL004211	0.4336	0.5664	0.7651	Thalictri Glandulosissimi Et	Glauvent	16754	TRUE	c12c3C(Cc4c1cc(c(c4)OC)OC)N(CCc3cc(c2OC)OC)C
MOL004211	0.4336	0.5664	0.7651	Corydalis Rhizoma	Glauvent	16754	TRUE	c12c3C(Cc4c1cc(c(c4)OC)OC)N(CCc3cc(c2OC)OC)C
MOL004212	0.8199	0.1801	0.7643	Corydalis Rhizoma	Streptomycin C	23267	FALSE	C1(C(OC2C(C(C(C(C2O)O)NC(=N)N)O)NC(=N)N)OC(C1(C=O)O)CO)OC1C(C(C(C(O1)CO)O)O)NC
MOL004214	0.2176	0.7824	0.7514	Corydalis Rhizoma	isocorybulbine	Not Available	FALSE	c1c(c(c2c(c1)C(C1(C(C2)CCc2c1cc(c(c2)OC)O)C)C)OC)OC
MOL004215	0.4425	0.5575	0.7586	Corydalis Rhizoma	leonticine	Not Available	FALSE	c1(c(c(ccc1OC)CCN(C)C)/C=C\c1ccc(cc1)OC)O
MOL004216	0.4968	0.5032	0.7394	Corydalis Rhizoma	13-methylpalmatrubine	12275616	FALSE	c12c3c(cc(c(c3)OC)OC)CC[n+]1cc1c(c2C)ccc(c1O)OC
MOL004217	0.8138	0.1862	0.7299	Folium Nelumbinis	Micheline B	Not Available	FALSE	n1ccc2c3c(c4c(C(=O)c13)cccc4)c1OCOc1c2
MOL004217	0.8138	0.1862	0.7299	Linderae Radix	Micheline B	Not Available	FALSE	n1ccc2c3c(c4c(C(=O)c13)cccc4)c1OCOc1c2
MOL004217	0.8138	0.1862	0.7299	Nelumbinis Plumula	Micheline B	Not Available	FALSE	n1ccc2c3c(c4c(C(=O)c13)cccc4)c1OCOc1c2
MOL004217	0.8138	0.1862	0.7299	Zanthoxylum Nitidum	Micheline B	Not Available	FALSE	n1ccc2c3c(c4c(C(=O)c13)cccc4)c1OCOc1c2
MOL004217	0.8138	0.1862	0.7299	Stemonae Radix	Micheline B	Not Available	FALSE	n1ccc2c3c(c4c(C(=O)c13)cccc4)c1OCOc1c2
MOL004217	0.8138	0.1862	0.7299	Broussonetiae Fructus	Micheline B	Not Available	FALSE	n1ccc2c3c(c4c(C(=O)c13)cccc4)c1OCOc1c2
MOL004217	0.8138	0.1862	0.7299	Corydalis Rhizoma	Micheline B	Not Available	FALSE	n1ccc2c3c(c4c(C(=O)c13)cccc4)c1OCOc1c2
MOL004218	0.6474	0.3526	0.6611	Corydalis Rhizoma	31098-60-9	Not Available	FALSE	c12c(CCN3Cc4c(CC13)c(c(c(c4)OC)OC)CO)cc1OCOc1c2OC
MOL004220	0.6157	0.3843	0.7193	Corydalis Rhizoma	N-methyllaurotetanine	6543699	FALSE	c1(c(cc2c(c1)c1c3C(C2)N(CCc3cc(c1OC)OC)C)O)OC
MOL004221	0.5998	0.4002	0.8710	Corydalis Rhizoma	norglaucing	Not Available	FALSE	c1(c(cc2c(c1)c1c3C(C2)NCCc3cc(c1OC)OC)OC)OC
MOL004222	0.6586	0.3414	0.8272	Corydalis Rhizoma	Oxoglaucine	Not Available	FALSE	c1(c(cc2c(c1)c1c3c(c2=O)ncc3cc(c1OC)OC)OC)OC
MOL004223	0.5909	0.4091	0.6848	Corydalis Bungeanae Herba	18797-80-3	Not Available	FALSE	c12c(cc3c(c1)C1C(C(C3)OC(=O)C)(c3c(CN1C)c1c(cc3)OCO1)C)OCO2
MOL004223	0.5909	0.4091	0.6848	Corydalis Rhizoma	18797-80-3	Not Available	FALSE	c12c(cc3c(c1)C1C(C(C3)OC(=O)C)(c3c(CN1C)c1c(cc3)OCO1)C)OCO2
MOL004224	0.6377	0.3623	0.7819	Corydalis Rhizoma	pontevedrine	Not Available	FALSE	c1(c(cc2c(c1)c1c3c(c2)n(c(=O)c(=O)c3cc(c1OC)OC)C)OC)OC
MOL004225	0.8843	0.1157	0.7144	Corydalis Rhizoma	pseudocoptisine	Not Available	FALSE	c12c(cc3c(c1)cc1[n+](c3)CCc3c1cc1c(c3)OCO1)OCO2
MOL004227	0.2633	0.7367	0.7180	Corydalis Rhizoma	Sanguidimerine	Not Available	FALSE	C(C(=O)CC1N(c2c3c(ccc2c2c1c1c(cc2)OCO1)cc1OCOc1c3)C)C1N(c2c3c(ccc2c2c1c1c(cc2)OCO1)cc1OCOc1c3)C
MOL004228	0.2852	0.7148	0.7631	Corydalis Rhizoma	saulatine	Not Available	FALSE	c1c2c(cc(c1OC)OC)C(=O)C1C(C(=O)Cc3c1cc(c(c3)OC)OC)CC2
MOL004229	0.7980	0.2020	0.6731	Corydalis Rhizoma	Spallidamine	Not Available	FALSE	c1cc2c(c3N(C(c4c5c(ccc4c13)OCO5)CC(=O)O)C)cc1OCOc1c2
MOL004230	0.8577	0.1423	0.7648	Corydalis Rhizoma	stylopine	Not Available	FALSE	c12c(CCN3Cc4c(CC13)ccc1OCOc41)cc1OCOc1c2
MOL004230	0.8577	0.1423	0.7648	Corydalis Bungeanae Herba	stylopine	Not Available	FALSE	c12c(CCN3Cc4c(CC13)ccc1OCOc41)cc1OCOc1c2

MOL004231	0.7911	0.2089	0.7867	Corydalis Rhizoma	Tetrahydrocorysamine	Not Available	FALSE	c12c(cc3c(c1)C1N(CC3)Cc3c(C1C)ccc1c3OCO1)OCO2
MOL004232	0.6460	0.3540	0.6832	Corydalis Rhizoma	tetrahydroprotopapaverine	40512630	FALSE	C1(N(CCc2cc(c(cc12)O)O)C)Cc1cc(c(cc1)OC)OC
MOL004233	0.6250	0.3750	0.8061	Corydalis Rhizoma	ST057701	6992288	FALSE	c12c3c(c(cc1CCN(C2Cc1c3cc(c(c1)OC)OC)C)OC)O
MOL004234	0.4244	0.5756	0.7712	Corydalis Rhizoma	2,3,9,10-tetramethoxy-13-methyl-5,6-dihydroisoquinolino[2,1-b]isoquinolin-8-one	10362429	FALSE	c1c(c(c2c(c1)c(c1n(c2=O)CCc2c1cc(c(c2)OC)OC)C)OC)OC
MOL004235	0.3959	0.6041	0.7184	Corydalis Rhizoma	104387-15-7	128558	FALSE	c12c(CCN3Cc4c(C(C13)C)ccc(c4OC)O)cc(c(c2)OC)OC
MOL004236	0.6584	0.3416	0.7064	Curcumae Radix	(1E,6E)-1-(4-Hydroxy-3-methoxyphenyl)-7-(3,4-dihydroxyphenyl)-1,6-heptadiene-3,5-dione	Not Available	FALSE	C(=C\C(=O)CC(=O)/C=C\c1cc(c(cc1)O)O)\c1cc(c(cc1)O)OC
MOL004237	0.8553	0.1447	0.6660	Ligustici Rhizoma Et Radix	δ-elemene	12309451	FALSE	C1(C(C=C(CC1)C(C)C)C(=C)C)(C=C)C
MOL004237	0.8553	0.1447	0.6660	Curcumae Radix	δ-elemene	12309451	FALSE	C1(C(C=C(CC1)C(C)C)C(=C)C)(C=C)C
MOL004237	0.8553	0.1447	0.6660	Panax Ginseng C. A. Mey.	δ-elemene	12309451	FALSE	C1(C(C=C(CC1)C(C)C)C(=C)C)(C=C)C
MOL004238	0.8264	0.1736	0.6799	Curcumae Radix	(4aR,8aS)-7-isopropylidene-4a-methyl-1-methylenedecalin	10655819	FALSE	C12(C(CC(=C(C)C)CC1)C(=C)CCC2)C
MOL004239	0.8895	0.1105	0.8020	Curcumae Radix	(1S,4S,6R,7R)-4-(1-hydroxy-1-methylethyl)-1-methyl-7-(3-oxobutyl)-3-norcaranone	154167	FALSE	C12(C(CC(C(=O)C1)C(C)(C)O)C2CCC(=O)C)C

MOL004240	0.8895	0.1105	0.8020	Curcumae Radix	(1S,4R,6R,7R)-4-(1-hydroxy-1-methylethyl)-1-methyl-7-(3-oxobutyl)-3-norcaranone	154168	FALSE	C12(C(CC(C(=O)C1)C(C)(C)O)C2CCC(=O)C)C
MOL004241	0.8952	0.1048	0.7911	Curcumae Radix	curcolactone	Not Available	FALSE	C12(C(CC3=C(C(=O)OC3C1)C)C(CCC2O)(C)O)C
MOL004242	0.5470	0.4530	0.7508	Curcumae Radix	(E)-1,7-bis-(4-hydroxy-3-methoxyphenyl)-1-heptene-3,5-dione	Not Available	FALSE	C(=C\C(=O)CC(=O)CCc1cc(c(cc1)O)OC)\c1cc(c(cc1)O)OC
MOL004243	0.8443	0.1557	0.8355	Curcumae Radix	Curcolone	12304272	FALSE	OC1C2(C(=C(CC1)C)C(=O)c1c(occ1C)C2)C
MOL004244	0.8811	0.1189	0.8282	Curcumae Radix	(4aR,5R,8R,8aR)-5,8-dihydroxy-3,5,8a-trimethyl-6,7,8,9-tetrahydro-4aH-benzo[f]benzofuran-4-one	10683031	FALSE	OC1(C2C(C(O)CC1)(Cc1occ(c1C2=O)C)C)C
MOL004245	0.8667	0.1333	0.7820	Curcumae Radix	curcumadiol	Not Available	FALSE	OC1(C2C(CC1)C(O)(CC=C(C2)C(C)C)C)C
MOL004246	0.8852	0.1148	0.8760	Curcumae Radix	(6S)-2-isopropyliden e-6-methyl-5-(3-oxobutyl)cyclohept-4-en-1-one	21769417	FALSE	C1(=O)C(=C(C)C)CC=C(C(C1)C)CCC(=O)C
MOL004247	0.8848	0.1152	0.6967	Curcumae Radix	Curcumalactone	15071433	FALSE	C1CC(C2(C1C(=C)C)CC(C(=O)O2)C(C)C)C
MOL004248	0.8931	0.1069	0.7350	Curcumae Radix	(5R,6S,9S)-9-isopropenyl-3-isopropyliden e-6-methyl-1-oxaspiro[4.4]nonan-2-one	10014272	FALSE	C1CC(C2(C1C(=C)C)CC(=C(C)C)C(=O)O2)C

MOL004249	0.8935	0.1065	0.7768	Curcumae Radix	Curcumenol	Not Available	FALSE	O1C23C(CCC2C)C(=CC1(O)C(=C(C)C)C3)C
MOL004250	0.9149	0.0851	0.7692	Curcumae Radix	Curcumenolactone A	10083354	FALSE	C12(C(CC3=C(C(=O)OC3C1)C)C2CCC(=O)C)C
MOL004251	0.9149	0.0851	0.7692	Curcumae Radix	Curcumenolactone B	10264037	FALSE	C12(C(CC3=C(C(=O)OC3C1)C)C2CCC(=O)C)C
MOL004253	0.9234	0.0766	0.7671	Curcumae Radix	Curcumenolactone C	Not Available	FALSE	C12(C(CC3=C(C(=O)OC3(C1)O)C)C2CCC(=O)C)C
MOL004254	0.8695	0.1305	0.7531	Curcumae Radix	curcumol	Not Available	FALSE	O1C23C(CCC3C)C(=C)CC1(O)C(C2)C(C)C
MOL004255	0.8619	0.1381	0.8526	Curcumae Radix	curdione	Not Available	FALSE	C1C(C(=O)C/C(=C/CCC(C1=O)C)/C)C(C)C
MOL004256	0.8951	0.1049	0.8904	Curcumae Radix	Curmadione	Not Available	FALSE	O=C1CC(C(=CCC1=C(C)C)CC(=O)CC)C
MOL004257	0.7736	0.2264	0.7667	Curcumae Radix	Curzeone	Not Available	FALSE	o1c2c(c(c1)C)c1c(c(c2)C)CCC(C1=O)C
MOL004258	0.8729	0.1271	0.6809	Curcumae Radix	curzerene	Not Available	FALSE	o1c2CC(C(Cc2c(c1)C)C(=C)C)(C)C=C
MOL004259	0.4855	0.5145	0.7066	Curcumae Radix	cyclocurcumin	Not Available	FALSE	C1C(=O)C=C(OC1c1cc(c(cc1)O)OC)/C=C\c1cc(c(cc1)O)OC
MOL004260	0.5123	0.4877	0.7386	Curcumae Radix	(E)-1,7-Diphenyl-3-hydroxy-1-hepten-5-one	44559751	FALSE	C(=C\C(CC(=O)CCc1ccccc1)O)/c1ccccc1
MOL004261	0.8834	0.1166	0.8625	Curcumae Radix	(6E,10S)-3-isopropylidene-6,10-dimethyl-cyclodec-6-ene-1,4-quinone	10421549	FALSE	O=C1C(CC/C=C(/CC(=O)C(=C(C)C)C1)\C)C
MOL004262	0.8647	0.1353	0.6853	Curcumae Radix	deta-elemene	Not Available	FALSE	C1(C(CC(=C(C)C)CC1)C(=C)C)(C=C)C
MOL004264	0.8890	0.1110	0.8341	Curcumae Radix	Epicurzerenone	5317062	FALSE	o1c2CC(C(C(=O)c2c(c1)C)C(=C)C)(C)C=C
MOL004265	0.9433	0.0567	0.9090	Cimicifugae Rhizoma	Ethyl ferulate	736681	FALSE	c1(cc(c(cc1)O)OC)/C=C/C(=O)OCC
MOL004265	0.9433	0.0567	0.9090	Curcumae Radix	Ethyl ferulate	736681	FALSE	c1(cc(c(cc1)O)OC)/C=C/C(=O)OCC
MOL004266	0.9479	0.0521	0.9311	Curcumae Radix	ethyl (Z)-3-(4-methoxyphenyl)prop-2-enoate	13010829	FALSE	C(=O)(/C=C\c1ccc(cc1)OC)OCC
MOL004267	0.8129	0.1871	0.6579	Curcumae Radix	Eudesma-4(14),11-diene	12309816	FALSE	C12(C(CC(CC1)C(=C)C)C(=C)CCC2)C

MOL004268	0.6158	0.3842	0.7137	Curcumae Radix	(E)-7-(3,4-dihydroxyphenyl)-5-hydroxy-1-phenyl-1-heptene	44560893	FALSE	C(=C\CCC(CCc1cc(c(cc1)O)O)O)/c1ccccc1
MOL004269	0.8073	0.1927	0.6924	Curcumae Radix	Furanodiene	Not Available	FALSE	o1c2c(c(c1)C)C/C=C(\CC/C=C(/C2)\C)/C
MOL004270	0.8200	0.1800	0.7889	Curcumae Radix	Furanogermenone	6439596	FALSE	c12c(occ1C)C/C(=C\CCC(C(=O)C2)C)/C
MOL004271	0.8997	0.1003	0.8731	Curcumae Radix	germacrone-13-al	46173921	FALSE	O=C1/C(=C(\CO)/C)/C/C=C(/CC/C=C(/C1)\C)\C
MOL004272	0.8406	0.1594	0.8143	Curcumae Radix	Germacrone-4,5-epoxide	Not Available	FALSE	C1(=O)CCC2(C)C(CC(C(C)C)CCC1C)O2
MOL004273	0.7991	0.2009	0.7536	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	glechomanolide	Not Available	FALSE	O1C2C(=C(C1=O)C)C/C=C(\CC/C=C(\C2)/C)/C
MOL004273	0.7991	0.2009	0.7536	Curcumae Radix	glechomanolide	Not Available	FALSE	O1C2C(=C(C1=O)C)C/C=C(\CC/C=C(\C2)/C)/C
MOL004274	0.6371	0.3629	0.7426	Curcumae Radix	(E)-7-Hydroxy-1,7-bis-(4-hydroxy-3-methoxyphenyl)-1-heptene-3,5-dione	Not Available	FALSE	C(=C\C(=O)CC(=O)CC(c1cc(c(cc1)O)OC)O)\c1cc(c(cc1)O)OC
MOL004275	0.8564	0.1436	0.7051	Panax Ginseng C. A. Mey.	(1R,4E,7E,11R)-1,5,9,9-tetramethyl-12-oxabicyclo[9.1.0]dodeca-4,7-diene	14038843	FALSE	C1C(/C=C/C/C(=C/CCC2(C1O2)C)/C)(C)C
MOL004275	0.8564	0.1436	0.7051	Curcumae Radix	(1R,4E,7E,11R)-1,5,9,9-tetramethyl-12-oxabicyclo[9.1.0]dodeca-4,7-diene	14038843	FALSE	C1C(/C=C/C/C(=C/CCC2(C1O2)C)/C)(C)C

MOL004275	0.8564	0.1436	0.7051	Schizonepetae Herba	(1R,4E,7E,11R)-1,5,9,9-tetramethyl-12-oxabicyclo[9.1.0]dodeca-4,7-diene	14038843	FALSE	C1C(/C=C/C/C(=C/CCC2(C1O2)C)/C)(C)C
MOL004277	0.8922	0.1078	0.8832	Curcumae Radix	Isocurcumadione	Not Available	FALSE	C1(=O)C=C(C(CCC1=C(C)C)CCC(=O)C)C
MOL004278	0.8250	0.1750	0.8098	Curcumae Radix	Furanodienone	5317425	FALSE	C1/C(=C\C(=O)c2c(C/C(=C/C1)/C)occ2C)/C
MOL004279	0.8880	0.1120	0.6687	Curcumae Radix	Isospathulenol	Not Available	FALSE	C1CC(C2C3C(CCC(=C12)C)C3(C)C)(O)C
MOL004280	0.8970	0.1030	0.8021	Curcumae Radix	(3S,3aS,8R,8aR)-3,8-dihydroxy-5-isopropylidene-3,8-dimethyl-1,2,3a,4,7,8a-hexahydroazulen-6-one	14632998	FALSE	C1(CCC2C(CC(=O)C(=C(C)C)CC12)(C)O)(C)O
MOL004281	0.8350	0.1650	0.7979	A. Dahurica (Fisch.) Benth. Et Hook	Lauryl acetate	8205	FALSE	C(CCCCCCCC)CCCOC(=O)C
MOL004281	0.8350	0.1650	0.7979	Curcumae Radix	Lauryl acetate	8205	FALSE	C(CCCCCCCC)CCCOC(=O)C
MOL004282	0.8487	0.1513	0.7300	Curcumae Radix	(1S,4aR,8aR)-7-isopropylidene-1,4a-dimethyl-1-decalinol	22211695	FALSE	C1CCC(C2C1(CCC(=C(C)C)C2)C)(O)C
MOL004285	0.9597	0.0403	0.9191	Curcumae Radix	MBP	8575	FALSE	c1(c(cccc1)C(=O)O)C(=O)OCCCC
MOL004285	0.9597	0.0403	0.9191	Momordicae Fructus	MBP	8575	FALSE	c1(c(cccc1)C(=O)O)C(=O)OCCCC
MOL004285	0.9597	0.0403	0.9191	Saussureae Involucratae Herba	MBP	8575	FALSE	c1(c(cccc1)C(=O)O)C(=O)OCCCC
MOL004286	0.8885	0.1115	0.7898	Curcumae Radix	Neocurcumenol	Not Available	FALSE	C1(=C2C3(CC(=C(C)C)C(C1)(O)O3)C(CC2)C)C
MOL004287	0.8619	0.1381	0.8526	Curcumae Radix	neocurdione	Not Available	FALSE	O=C1CC(C(C)C)C(=O)C/C(=C/CCC1C)/C

MOL004288	0.9016	0.0984	0.8257	Curcumae Radix	(3S,3aS)-3-hydroxy-5-isopropylidene-3,8-dimethyl-2,3a,4,7-tetrahydro-1H-azulen-6-one	14543200	FALSE	C1(CCC2=C(CC(=O)C(=C(C)C)CC12)C)(C)O
MOL004289	0.8970	0.1030	0.8021	Curcumae Radix	neozedoarondiol	Not Available	FALSE	C12C(CC(=C(C)C)C(=O)CC1(C)O)C(CC2)(C)O
MOL004290	0.4900	0.5100	0.7197	Curcumae Radix	1-(4-hydroxy-3,5-dimethoxyphenyl)-7-(4-hydroxy-3-methoxy-phenyl)-(1e,6e)-1,6-heptadiene-3,5-dione	Not Available	FALSE	C(=C\C(=O)CC(=O)/C=C\c1cc(c(cc1)O)OC)\c1cc(c(c(c1)OC)O)OC
MOL004291	0.8868	0.1132	0.7704	Curcumae Radix	Oxycurcumenol	Not Available	FALSE	C1CC(C23CC4(C(C=C(C12)C)(O3)O)OC4(C)C)C
MOL004292	0.4655	0.5345	0.7313	Curcumae Radix	Parviflorene F	12191212	FALSE	OC1C(C(C)C)c2c(c3c1cc1c(CC(c4c1c(O)cc(c4)C)C(C)C)c3)c(O)cc(c2)C
MOL004294	0.9002	0.0998	0.9391	Curcumae Radix	Perillen	68316	FALSE	c1cocc1CCC=C(C)C
MOL004294	0.9002	0.0998	0.9391	Zanthoxyli Pericarpium	Perillen	68316	FALSE	c1cocc1CCC=C(C)C
MOL004294	0.9002	0.0998	0.9391	Caryophylliflos	Perillen	68316	FALSE	c1cocc1CCC=C(C)C
MOL004295	0.6601	0.3399	0.7114	Curcumae Radix	1-(4-Hydroxy-3-methoxyphenyl)-7-(3,4-dihydroxyphe ny)-1,6-heptadiene-3,5-dione	Not Available	FALSE	c1(ccc(cc1)/C=C\C(=O)CC(=O)/C=C\c1cc(c(c(c1)O)O)OC)O
MOL004296	0.7158	0.2842	0.6382	Curcumae Radix	1-Phenylnaphthalene	11795	FALSE	c1(c2c(ccc1)cccc2)c1ccccc1
MOL004297	0.9266	0.0734	0.8832	Curcumae Radix	THAP	68073	FALSE	c1(c(cc(cc1O)O)O)C(=O)C
MOL004298	0.9444	0.0556	0.9017	Curcumae Radix	(Z)-p-Methoxycinnamic acid	1550936	FALSE	C(=O)(/C=C\c1ccc(cc1)OC)O

MOL004299	0.7625	0.2375	0.6683	Curcumae Radix	Pyrocurzerenone	12314812	FALSE	o1c2c(c(c1)C)c1c(c(c2)C)CCC(=C1)C
MOL004300	0.8872	0.1128	0.7983	Curcumae Radix	(6S)-6-[(1S,2R,4S,5R,6S)-4,5-dihydroxy-5-methyl-7-oxabicyclo[4.1.0]heptan-2-yl]-2-methylhept-2-en-4-one	14543236	FALSE	CC(=CC(=O)CC(C)C1C2C(C(C(C1)O)(C)O)O2)C
MOL004301	0.6253	0.3747	0.7121	Curcumae Radix	1-(4-hydroxy-3-methoxyphenyl)-7-(4-hydroxyphenyl)heptane-3,5-dione	9906039	FALSE	O=C(CCc1cc(OC)c(O)cc1)CC(=O)CCc1ccc(O)cc1
MOL004302	0.4928	0.5072	0.6866	Curcumae Radix	Trans,trans-1,7-diphenyl-1,3-heptadien-5-ol	44560847	FALSE	C(=C\C=C\C(CCc1ccccc1)O)/c1ccccc1
MOL004303	0.6854	0.3146	0.7506	Curcumae Radix	1,5-Bis(4-hydroxy-3-methoxyphenyl)-1,4-pentadien-3-one	Not Available	FALSE	C(=C\C(=O)/C=C\c1cc(c(cc1)O)OC)\c1cc(c(cc1)O)OC
MOL004304	0.7779	0.2221	0.8106	Curcumae Radix	zederone	Not Available	FALSE	O1C2(C1C(=O)c1c(occ1C)C/C(=C/CC2)/C)C
MOL004305	0.9062	0.0938	0.7341	Curcumae Radix	Zedoalactone A	15226639	FALSE	O1C2C(=C(C1=O)C)CC1C(CCC1C(C2)(C)O)(C)O
MOL004306	0.9179	0.0821	0.7658	Curcumae Radix	Zedoalactone B	15226640	FALSE	O1C2=CC(C3(CCC(C3CC2=C(C1=O)C)(C)O)O)(C)O
MOL004307	0.9069	0.0931	0.7522	Curcumae Radix	zedoalactone C	Not Available	FALSE	C12C(CC3=C(C(=O)OC3CC1(O)C)C)C(CC2)O
MOL004308	0.9179	0.0821	0.7658	Curcumae Radix	zedoalactone D	71725779	FALSE	C12(C(CC3=C(C(=O)OC3=CC1(C)O)C)C(CC2)(C)O)O
MOL004309	0.8994	0.1006	0.7622	Curcumae Radix	zedoalactone E	Not Available	FALSE	C12(C(CC3=C(C(=O)OC3=CC1C)C)C(CC2)(C)O)O
MOL004310	0.7999	0.2001	0.8439	Curcumae Radix	Zedoarol	46173920	FALSE	OC12C(CCC1C)C(=C)Cc1occ(c1C2=O)C

MOL004311	0.9227	0.0773	0.8181	Curcumae Radix	Zedoarolide A	Not Available	FALSE	C1(C2(C(=C(C(=O)O2)C)CC2C3(C1(O3)C)CCC2(C)O)O)O
MOL004312	0.3873	0.6127	0.7862	Curcumae Radix	1,7-Bis(4-hydroxy-3-methoxyphenyl)-1,4,6-heptatrien-3-one	Not Available	FALSE	C(=C\C(=O)/C=C/C=C\c1cc(c(cc1)O)OC)\c1cc(c(cc1)O)OC
MOL004313	0.9242	0.0758	0.7454	Curcumae Radix	Zedoarolide B	Not Available	FALSE	C1(C2C(CC3=C(C(=O)OC3(C1)O)C)C(CC2)(C)O)(C)O
MOL004314	0.8523	0.1477	0.7545	Curcumae Radix	Zerumbone	5470187	FALSE	C1(/C=C/C(=O)/C(=C/CC/C(=C/C1)/C)/C)(C)C
MOL004316	0.3297	0.6703	0.7529	Curcumae Radix	1,7-Diphenyl-3-acetoxy-6(E)-hepten	Not Available	FALSE	C(CC(CC/C=C\c1ccccc1)OC(=O)C)c1ccccc1
MOL004317	0.4548	0.5452	0.7392	Curcumae Radix	1,7-Diphenyl-6(E)-hepten-3one	Not Available	FALSE	C(CC(=O)CC/C=C\c1ccccc1)c1ccccc1
MOL004318	0.8590	0.1410	0.8473	Curcumae Radix	(1a,4b,5a,10b)1,10,4,5-Diepoxy-7(11)-germacren-8-one	Not Available	FALSE	C12CCC3(C)C(CC(=C(C)C)C(=O)CC1(C)O2)O3
MOL004319	0.6371	0.3629	0.7426	Curcumae Radix	1-Hydroxy-1,7-bis(4-hydroxy-3-methoxyphernyl)-6-heptene-3,5-dione	Not Available	FALSE	C(CC(=O)CC(=O)/C=C\c1cc(c(cc1)O)OC)(c1cc(c(cc1)O)OC)O
MOL004320	0.9138	0.0862	0.9654	Curcumae Radix	MEK	6569	FALSE	C(=O)(CC)C
MOL004320	0.9138	0.0862	0.9654	Rubi Fructus	MEK	6569	FALSE	C(=O)(CC)C
MOL004320	0.9138	0.0862	0.9654	Sesami Nigrum Semen	MEK	6569	FALSE	C(=O)(CC)C
MOL004320	0.9138	0.0862	0.9654	Capsici Fructus	MEK	6569	FALSE	C(=O)(CC)C
MOL004321	0.9366	0.0634	0.8288	Curcumae Radix	3,7-Dimethyl-5-indanecarboxylic acid	Not Available	FALSE	C1CC(c2cc(cc(c12)C)C(=O)O)C
MOL004322	0.8563	0.1437	0.6754	Curcumae Radix	hexadec-3-enoic acid	5312418	FALSE	OC(=O)C/C=C/CCCCCCCCCCCC

MOL004324	0.5657	0.4343	0.7378	Curcumae Radix	4,5-Epoxy-12-acetoxy-7a,11a-dihydrogermacradien-8-one	Not Available	FALSE	C\1=C/CC2(C)/C(=C/C(C(COC(=O)C)C)C(=O)CC1C)/O2
MOL004325	0.8878	0.1122	0.8510	Curcumae Radix	4,5-Epoxy-12-hydroxy-1(10),7(11)-germacradien-8-one	Not Available	FALSE	C\1=C(/CC(=O)/C(=C(/CO)\C)/CC2C(CC1)(C)O2)\C
MOL004326	0.8935	0.1065	0.7768	Curcumae Radix	4-Epi-curcumenol	Not Available	FALSE	C1=C(C2C3(CC(=C(C)C)C1(O)O3)C(CC2)C)C
MOL004327	0.8731	0.1269	0.7044	Curcumae Radix	(1S,6R,7R)-7-[(3S)-3-hydroxybutyl]-4-isopropylidene-1-methyl-3-norcaranone	153942	FALSE	C12(C(CC(=C(C)C)C(=O)C1)C2CCC(C)O)C
MOL004328	0.9396	0.0604	0.8008	Curcumae Radix	naringenin	439246	FALSE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL004328	0.9396	0.0604	0.8008	Smilacis Glabrae Rhixoma	naringenin	439246	FALSE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL004328	0.9396	0.0604	0.8008	Allium Azureum Ledeb.	naringenin	439246	FALSE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL004328	0.9396	0.0604	0.8008	Aurantii Fructus Immaturus	naringenin	439246	FALSE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL004328	0.9396	0.0604	0.8008	Euphorbiae Helioscopiae Herba	naringenin	439246	FALSE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL004328	0.9396	0.0604	0.8008	Aurantii Fructus	naringenin	439246	FALSE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL004328	0.9396	0.0604	0.8008	licorice	naringenin	439246	FALSE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL004328	0.9396	0.0604	0.8008	Citri Exocarpium Rubrum	naringenin	439246	FALSE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL004328	0.9396	0.0604	0.8008	Lunulatae Herba	naringenin	439246	FALSE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL004328	0.9396	0.0604	0.8008	Hedysari Radix	naringenin	439246	FALSE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL004328	0.9396	0.0604	0.8008	Citrus Reticulata	naringenin	439246	FALSE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL004328	0.9396	0.0604	0.8008	Canarii Fructus	naringenin	439246	FALSE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL004328	0.9396	0.0604	0.8008	Citri Reticulatae Pericarpium Viride	naringenin	439246	FALSE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL004328	0.9396	0.0604	0.8008	Hoveniae Dulcis Semen	naringenin	439246	FALSE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL004328	0.9396	0.0604	0.8008	Ephedrae Radix Et Rhizoma	naringenin	439246	FALSE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL004328	0.9396	0.0604	0.8008	Menthae Herba	naringenin	439246	FALSE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL004328	0.9396	0.0604	0.8008	Citrus Aurantium	naringenin	439246	FALSE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL004328	0.9396	0.0604	0.8008	Drynariae Rhizoma	naringenin	439246	FALSE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL004328	0.9396	0.0604	0.8008	Citri Grandis Exocarpium	naringenin	439246	FALSE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O
MOL004328	0.9396	0.0604	0.8008	Choerospondiatis Fructus	naringenin	439246	FALSE	C1(CC(=O)c2c(cc(cc2O1)O)O)c1ccc(cc1)O

MOL004329	0.9574	0.0426	0.8343	Curcumae Radix	6-methyl-7-(3-oxobutyl)-bicyclo[4,1,0]heptan-3-one	Not Available	FALSE	C12CC(=O)CCC1(C2CCC(=O)C)C
MOL004330	0.8596	0.1404	0.7530	Curcumae Radix	8-Hydroxycadalene	14107524	FALSE	c1(C)ccc(C(C)C)c2cc(C)cc(c12)O
MOL004331	0.8987	0.1013	0.8777	Curcumae Radix	a Atlantone	Not Available	FALSE	O=C(CC(C1=CC=C(CC1)C)C)C=C(C)C
MOL004332	0.7254	0.2746	0.7082	Curcumae Radix	(1E,4E)-1-(4-Hydroxy-3-methoxyphenyl)-5-(4-hydroxyphenyl)-1,4-pentadien-3-one	Not Available	FALSE	C(=C\C(=O)/C=C\c1ccc(cc1)O)\c1cc(c(cc1)O)OC
MOL004333	0.8876	0.1124	0.8394	Momordicae Fructus	ar-turmerone	160512	FALSE	O=C(CC(c1ccc(cc1)C)C)C=C(C)C
MOL004333	0.8876	0.1124	0.8394	Curcumae Radix	ar-turmerone	160512	FALSE	O=C(CC(c1ccc(cc1)C)C)C=C(C)C
MOL004334	0.8219	0.1781	0.6554	Curcumae Radix	a-Selinene	12309810	FALSE	C12(C(CC(CC1)C(=C)C)C(=CCC2)C)C
MOL004335	0.9025	0.0975	0.8750	Curcumae Radix	(6S)-2-methyl-6-[(1R)-4-methyl-1-cyclohexa-2,4-dienyl]hept-2-en-4-one	11820691	FALSE	C1(C=CC(=CC1)C)C(CC(=O)C=C(C)C)C
MOL004336	0.8989	0.1011	0.8670	Curcumae Radix	6-methyl-2-[(1R)-4-methyl-1-cyclohex-3-enyl]hepta-1,5-dien-4-one	181580	FALSE	C1=C(CCC(C1)C(=C)CC(=O)C=C(C)C)C
MOL004337	0.8705	0.1295	0.7191	Curcumae Radix	b-Elemenone	12314814	FALSE	C1(CC(=O)C(=C(C)C)CC1C(=C)C)(C=C)C

MOL004338	0.9183	0.0817	0.8570	Curcumae Radix	(6S)-6-[(1R,4R,5S)-4,5-dihydroxy-4-methyl-1-cyclohex-2-enyl]-2-methylhept-2-en-4-one	14287398	FALSE	CC(=CC(=O)CC(C)C1C=CC(C(C1)O)(C)O)C
MOL004339	0.9183	0.0817	0.8570	Curcumae Radix	(6S)-6-[(1R,4S,5R)-4,5-dihydroxy-4-methyl-1-cyclohex-2-enyl]-2-methylhept-2-en-4-one	14287400	FALSE	CC(=CC(=O)CC(C)C1C=CC(C(C1)O)(C)O)C
MOL004340	0.9183	0.0817	0.8570	Curcumae Radix	(6S)-6-[(1R,4R,5R)-4,5-dihydroxy-4-methyl-1-cyclohex-2-enyl]-2-methylhept-2-en-4-one	14287399	FALSE	CC(=CC(=O)CC(C)C1C=CC(C(C1)O)(C)O)C
MOL004341	0.8985	0.1015	0.8622	Curcumae Radix	Cadalenequinone	Not Available	FALSE	c1(C=O)ccc(C(C=O)C)c2cc(C)ccc12
MOL004342	0.8343	0.1657	0.6242	Curcumae Radix	calarenepoxide	Not Available	FALSE	C1CC23C(C(CCC2O3)C)(C2C1C2(C)C)C
MOL004343	0.5661	0.4339	0.6832	Curcumae Radix	Calebin-A	637429	FALSE	O(c1cc(ccc1O)/C=C/C(=O)COC(=O)/C=C/c1cc(OC)c(O)cc1)C
MOL004344	0.8035	0.1965	0.6474	Curcumae Radix	caryophyllene oxide	Not Available	FALSE	O1C2(C1CCC(=C)C1C(C(C1)(C)C)CC2)C
MOL004346	0.2582	0.7418	0.7662	Houttuyniae Herba	16'-Decarbomethoxy-19,20-dihydroconoduramine	Not Available	FALSE	c1ccc2c(c1)c1c([nH]2)C(CC2C(CN(C(C1)C2C(=O)OC)C)CC)c1cc(c2c(c1)C1C(N2)C2C3N(CC1)CC(CC3CC)C2)OC
MOL004347	0.6709	0.3291	0.7196	Houttuyniae Herba	Laurifoline	Not Available	FALSE	c1(cc2c(cc1OC)C1c3c(c2)[N+](CCc3cc(c1O)OC)(C)C)O
MOL004348	0.9270	0.0730	0.9487	Ranunculi Ternati Radix	Abiol	7456	FALSE	c1(ccc(cc1)O)C(=O)OC
MOL004348	0.9270	0.0730	0.9487	Daturae Flos	Abiol	7456	FALSE	c1(ccc(cc1)O)C(=O)OC

MOL004348	0.9270	0.0730	0.9487	Trollius Chinensis	Abiol	7456	FALSE	c1(ccc(cc1)O)C(=O)OC
MOL004348	0.9270	0.0730	0.9487	Houttuyniae Herba	Abiol	7456	FALSE	c1(ccc(cc1)O)C(=O)OC
MOL004348	0.9270	0.0730	0.9487	Pseudolaricis Cortex	Abiol	7456	FALSE	c1(ccc(cc1)O)C(=O)OC
MOL004349	0.3315	0.6685	0.6535	Houttuyniae Herba	Ruvoside	Not Available	FALSE	C1(C(C(OC(C1O)C)OC1CCC2(C(C1)CCC1C2CCC2(C1(CCC2C1=CC(=O)OC1)O)C)CO)O)OC
MOL004349	0.3315	0.6685	0.6535	Ginkgo Semen	Ruvoside	Not Available	FALSE	C1(C(C(OC(C1O)C)OC1CCC2(C(C1)CCC1C2CCC2(C1(CCC2C1=CC(=O)OC1)O)C)CO)O)OC
MOL004349	0.3315	0.6685	0.6535	Jujubae Fructus	Ruvoside	Not Available	FALSE	C1(C(C(OC(C1O)C)OC1CCC2(C(C1)CCC1C2CCC2(C1(CCC2C1=CC(=O)OC1)O)C)CO)O)OC
MOL004349	0.3315	0.6685	0.6535	Gynostemmae Pentaphylli Herba	Ruvoside	Not Available	FALSE	C1(C(C(OC(C1O)C)OC1CCC2(C(C1)CCC1C2CCC2(C1(CCC2C1=CC(=O)OC1)O)C)CO)O)OC
MOL004350	0.5248	0.4752	0.7612	Houttuyniae Herba	Ruvoside_qt	Not Available	FALSE	OC1CCC2(C(C1)CCC1C2CCC2(C1(CCC2C1=CC(=O)OC1)O)C)CO
MOL004350	0.5248	0.4752	0.7612	Ginkgo Semen	Ruvoside_qt	Not Available	FALSE	OC1CCC2(C(C1)CCC1C2CCC2(C1(CCC2C1=CC(=O)OC1)O)C)CO
MOL004350	0.5248	0.4752	0.7612	Jujubae Fructus	Ruvoside_qt	Not Available	FALSE	OC1CCC2(C(C1)CCC1C2CCC2(C1(CCC2C1=CC(=O)OC1)O)C)CO
MOL004350	0.5248	0.4752	0.7612	Gynostemmae Pentaphylli Herba	Ruvoside_qt	Not Available	FALSE	OC1CCC2(C(C1)CCC1C2CCC2(C1(CCC2C1=CC(=O)OC1)O)C)CO
MOL004351	0.9097	0.0903	0.7865	Houttuyniae Herba	C09747	Not Available	FALSE	O1C2(C3(C4(C(OC2C(O)C3)C=C(C(=O)C4O)C)CO)C)C1
MOL004353	0.8885	0.1115	0.8071	Houttuyniae Herba	quercetin-3-O-β-D-galactoside-7-O-β-D-glucoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(=O)c2c(oc1c1cc(O)c(O)cc1)cc(OC1OC(C(O)C(O)C1O)CO)cc2O)CO
MOL004354	0.9208	0.0792	0.7851	Anisi Stellati Fructus	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-[(2R,3R,4S,5R)-3,4,5-trihydroxytetrahydropyran-2-yl]oxy-chromone	10274530	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(CO1)O)O)O)c1cc(c(cc1)O)O

MOL004354	0.9208	0.0792	0.7851	Houttuyniae Herba	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-[(2R,3R,4S,5R)-3,4,5-trihydroxytetrahydropyran-2-yl]oxy-chromone	10274530	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(C(C(CO1)O)O)O)c1cc(c(cc1)O)O
MOL004355	0.2168	0.7832	0.6260	Gossampiniflos	Spinasterol	5281331	FALSE	C12=CCC3C(C2CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C)(CCC(C3)O)C
MOL004355	0.2168	0.7832	0.6260	Gynostemmae Pentaphylli Herba	Spinasterol	5281331	FALSE	C12=CCC3C(C2CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C)(CCC(C3)O)C
MOL004355	0.2168	0.7832	0.6260	Lysimachiae Foenigraeci Herba	Spinasterol	5281331	FALSE	C12=CCC3C(C2CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C)(CCC(C3)O)C
MOL004355	0.2168	0.7832	0.6260	Achyranthis Bidentatae Radix	Spinasterol	5281331	FALSE	C12=CCC3C(C2CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C)(CCC(C3)O)C
MOL004355	0.2168	0.7832	0.6260	Gypsophila Licentiana Hand.-Mazz.	Spinasterol	5281331	FALSE	C12=CCC3C(C2CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C)(CCC(C3)O)C
MOL004355	0.2168	0.7832	0.6260	Prunellae Spica	Spinasterol	5281331	FALSE	C12=CCC3C(C2CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C)(CCC(C3)O)C
MOL004355	0.2168	0.7832	0.6260	Trichosanthis Radix	Spinasterol	5281331	FALSE	C12=CCC3C(C2CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C)(CCC(C3)O)C
MOL004355	0.2168	0.7832	0.6260	Solidaginis Herba	Spinasterol	5281331	FALSE	C12=CCC3C(C2CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C)(CCC(C3)O)C
MOL004355	0.2168	0.7832	0.6260	Platycodon Grandiforus	Spinasterol	5281331	FALSE	C12=CCC3C(C2CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C)(CCC(C3)O)C
MOL004355	0.2168	0.7832	0.6260	Houttuyniae Herba	Spinasterol	5281331	FALSE	C12=CCC3C(C2CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C)(CCC(C3)O)C
MOL004355	0.2168	0.7832	0.6260	Calyx Cucumis	Spinasterol	5281331	FALSE	C12=CCC3C(C2CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C)(CCC(C3)O)C
MOL004355	0.2168	0.7832	0.6260	Codonopsis Radix	Spinasterol	5281331	FALSE	C12=CCC3C(C2CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C)(CCC(C3)O)C
MOL004355	0.2168	0.7832	0.6260	Ampelopsis Japonica	Spinasterol	5281331	FALSE	C12=CCC3C(C2CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C)(CCC(C3)O)C
MOL004355	0.2168	0.7832	0.6260	Trichosanthes Kirilowii Maxim	Spinasterol	5281331	FALSE	C12=CCC3C(C2CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C)(CCC(C3)O)C
MOL004355	0.2168	0.7832	0.6260	Asteris Radix Et Rhizoma	Spinasterol	5281331	FALSE	C12=CCC3C(C2CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C)(CCC(C3)O)C
MOL004355	0.2168	0.7832	0.6260	Radix Paeoniae Rubra	Spinasterol	5281331	FALSE	C12=CCC3C(C2CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C)(CCC(C3)O)C

MOL004355	0.2168	0.7832	0.6260	Perillae Fructus	Spinasterol	5281331	FALSE	C12=CCC3C(C2CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C)(CCC(C3)O)C
MOL004356	0.8822	0.1178	0.8398	Houttuyniae Herba	KAEMPFEROL 3-O-GLUCORHAMNOSIDE	Not Available	FALSE	c12c(c(cc(c1)O)O)c(=O)c(c(o2)c1ccc(cc1)O)OC1C(C(C(C(O1)C)O)O)O
MOL004358	0.9206	0.0794	0.9427	Houttuyniae Herba	linalool	Not Available	FALSE	C=CC(C)(O)CC=C(C)C
MOL004359	0.8915	0.1085	0.8920	Houttuyniae Herba	Houttuynin	122640	FALSE	CCCCCCCCCC(=O)CC=O
MOL004362	0.8822	0.1178	0.8398	Anemarrhenae Rhizoma	Afzelin	5316673	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)C)c1ccc(cc1)O
MOL004362	0.8822	0.1178	0.8398	Mume Fructus	Afzelin	5316673	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)C)c1ccc(cc1)O
MOL004362	0.8822	0.1178	0.8398	Lysimachiae Foenigraeci Herba	Afzelin	5316673	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)C)c1ccc(cc1)O
MOL004362	0.8822	0.1178	0.8398	Drynariae Rhizoma	Afzelin	5316673	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)C)c1ccc(cc1)O
MOL004362	0.8822	0.1178	0.8398	Semen Pruni	Afzelin	5316673	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)C)c1ccc(cc1)O
MOL004362	0.8822	0.1178	0.8398	Houttuyniae Herba	Afzelin	5316673	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)C)c1ccc(cc1)O
MOL004362	0.8822	0.1178	0.8398	Impatientis Semen	Afzelin	5316673	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)C)c1ccc(cc1)O
MOL004364	0.9581	0.0419	0.9734	Radix Angelicae Biseratae	3,5-Dimethoxytoluene	77844	FALSE	c1(cc(cc(c1)C)OC)OC
MOL004364	0.9581	0.0419	0.9734	Magnoliae Flos	3,5-Dimethoxytoluene	77844	FALSE	c1(cc(cc(c1)C)OC)OC
MOL004364	0.9581	0.0419	0.9734	Epimrdii Herba	3,5-Dimethoxytoluene	77844	FALSE	c1(cc(cc(c1)C)OC)OC
MOL004364	0.9581	0.0419	0.9734	Asari Radix Et Rhizoma	3,5-Dimethoxytoluene	77844	FALSE	c1(cc(cc(c1)C)OC)OC
MOL004365	0.9543	0.0457	0.9542	Epimrdii Herba	Isomenthol	19244	FALSE	C1(C(CCC(C1)C)C(C)C)O
MOL004365	0.9543	0.0457	0.9542	Arecae Semen	Isomenthol	19244	FALSE	C1(C(CCC(C1)C)C(C)C)O
MOL004366	0.9357	0.0643	0.9446	Epimrdii Herba	Octyl formate	8176	FALSE	C(CCCCC)CCOC=O
MOL004367	0.8013	0.1987	0.7010	Eucommiae Cortex	olivil	Not Available	FALSE	O1C(C(C(O)(C1)Cc1cc(OC)c(O)cc1)CO)c1cc(OC)c(O)cc1
MOL004367	0.8013	0.1987	0.7010	Epimrdii Herba	olivil	Not Available	FALSE	O1C(C(C(O)(C1)Cc1cc(OC)c(O)cc1)CO)c1cc(OC)c(O)cc1
MOL004368	0.9265	0.0735	0.8040	Choerospondiatis Fructus	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O

MOL004368	0.9265	0.0735	0.8040	Houttuyniae Herba	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Uncariae Ramulus Cumuncis	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Achyranthis Bidentatae Radix	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Radix Bupleuri	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Crataegi Folium	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Forsythiae Fructus	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Lysimachiae Herba	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Eriobotryae Folium	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Lunulatae Herba	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Polygoni Cuspidati Rhizoma Et Radix	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Nelumbinis Plumula	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Prunellae Spica	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Eucommiae Folium	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Geranium Wilfordii Maxim.	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Lonicerae Japonicae Flos	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Apocyniveneti Folium	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Bidentis Bipinnatae Herba	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Farfarae Flos	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Astragali Cpmplanatisemen	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Rubi Fructus	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Dioscoreaebulbiferae	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O

MOL004368	0.9265	0.0735	0.8040	Herba Pyrolae	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Bistortae Rhizoma	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Euonymi Alati Ramulus	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Cuscutae Semen	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Agrimonia Eupatoria	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Canarii Fructus	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Microctis Folium	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Gnaphalii Affinis Herba	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Kaki Calyx	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Bruceae Fructus	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Artemisia Annua L.	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Epimrdii Herba	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Ailanthi Altissimae Fructus	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Receptaculum Nelumbinis	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Folium Ilicis Cornutae	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Phellodendri Amurensis Cortex	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Rhododendri Daurici Folium	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Saururi Herba	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Pogostemon Cablin (Blanco) Benth.	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Solanum Nigrum Linn.	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Leonuri Herba	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O

MOL004368	0.9265	0.0735	0.8040	Ilicis Cornutae Folium Immayuri	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Zanthoxyli Pericarpium	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Gossampiniflos	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Polygoni Avicularis Herba	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Euphorbiae Helioscopiae Herba	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Phyllanthi Fructus	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Amomum Tsao-Ko Crevostet	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004368	0.9265	0.0735	0.8040	Folium Nelumbinis	Hyperin	5281643	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O
MOL004369	0.9133	0.0867	0.8176	Choerospondiatis Fructus	quercetin-3-rhamnooside	40486293	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O)C(O1)C)c1cc(O)c(O)cc1
MOL004369	0.9133	0.0867	0.8176	Epimrdii Herba	quercetin-3-rhamnooside	40486293	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O)C(O1)C)c1cc(O)c(O)cc1
MOL004370	0.9267	0.0733	0.8867	Epimrdii Herba	Robinetin	5281692	FALSE	o1c(c2cc(O)c(O)c(O)c2)c(O)c(=O)c2c1cc(O)cc2
MOL004370	0.9267	0.0733	0.8867	Capsellae Herba	Robinetin	5281692	FALSE	o1c(c2cc(O)c(O)c(O)c2)c(O)c(=O)c2c1cc(O)cc2
MOL004371	0.6489	0.3511	0.7565	Epimrdii Herba	rouhuoside	Not Available	FALSE	c1(c(c(=O)c2c(o1)c(c(cc2O)OC1C(O)C(O)C(O)C(O1)CO)CC=C(C)C)OC1C(O)C(O)C(OC2C(O)C(O)C(O)C(O2)C)C(O1)CO)c1ccc(cc1)O
MOL004372	0.5916	0.4084	0.7522	Epimrdii Herba	Sagittatoside A	Not Available	FALSE	O(C1C(O)C(O)C(OC1Oc1c(oc2c(c1=O)c(O)cc(O)c2CC=C(C)C)c1ccc(OC)cc1)C)C1OC(C(O)C(O)C1O)CO
MOL004373	0.3879	0.6121	0.7334	Anemarrhenae Rhizoma	Anhydroicaritin	5318980	FALSE	Oc1c(oc2c(c1=O)c(O)cc(O)c2CC=C(C)C)c1ccc(OC)cc1
MOL004373	0.3879	0.6121	0.7334	Epimrdii Herba	Anhydroicaritin	5318980	FALSE	Oc1c(oc2c(c1=O)c(O)cc(O)c2CC=C(C)C)c1ccc(OC)cc1
MOL004373	0.3879	0.6121	0.7334	Semen Pharbitidis	Anhydroicaritin	5318980	FALSE	Oc1c(oc2c(c1=O)c(O)cc(O)c2CC=C(C)C)c1ccc(OC)cc1
MOL004373	0.3879	0.6121	0.7334	Herba Sarcandrae	Anhydroicaritin	5318980	FALSE	Oc1c(oc2c(c1=O)c(O)cc(O)c2CC=C(C)C)c1ccc(OC)cc1
MOL004374	0.5659	0.4341	0.7268	Epimrdii Herba	sagittatoside B	Not Available	FALSE	O(C1C(O)C(O)C(OC1Oc1c(oc2c(c1=O)c(O)cc(O)c2CC=C(C)C)c1ccc(OC)cc1)C)C1OCC(O)C(O)C1O
MOL004375	0.9140	0.0860	0.8280	Ilicis Purpureae Folium	Trifolin	5282149	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)CO
MOL004375	0.9140	0.0860	0.8280	Kaki Calyx	Trifolin	5282149	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)CO
MOL004375	0.9140	0.0860	0.8280	Epimrdii Herba	Trifolin	5282149	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)CO

MOL004375	0.9140	0.0860	0.8280	Lysimachiae Herba	Trifolin	5282149	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)CO
MOL004375	0.9140	0.0860	0.8280	Eriobotryae Folium	Trifolin	5282149	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)CO
MOL004375	0.9140	0.0860	0.8280	Hemerocallis Radix	Trifolin	5282149	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)CO
MOL004375	0.9140	0.0860	0.8280	Gentianae Radix Et Rhozima	Trifolin	5282149	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)CO
MOL004375	0.9140	0.0860	0.8280	Astragali Cpmplanatisemen	Trifolin	5282149	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)CO
MOL004376	0.5740	0.4260	0.7474	Epimrdii Herba	wanepimedoside A	Not Available	FALSE	O(C1C(O)C(O)C(OC1Oc1c(oc2c(c1=O)c(O)cc(O)c2CCC(O)(C)C)c1ccc(OC)cc1)C)C1OC(C(O)C(O)C1O)C
MOL004379	0.4176	0.5824	0.7534	Epimrdii Herba	wushanicariin_qt	Not Available	FALSE	Oc1c(CC=C(C)C)cc2c(oc(cc2=O)c2cc(O)c(OC)c(O)c2)c1
MOL004380	0.3778	0.6222	0.7975	Epimrdii Herba	C-Homoerythrinan, 1,6-didehydro-3,15,16-trimethoxy-, (3.beta.)-	Not Available	FALSE	c12c(cc(c(c1)OC)OC)CCCN1C32C(=CCC(C3)OC)CC1
MOL004381	0.4523	0.5477	0.7301	Epimrdii Herba	Besigomsin	Not Available	FALSE	c1(c(c2c(cc1OC)CC(C(Cc1c2c(OC)c2c(c1)OCO2)C)(C)O)OC)OC
MOL004382	0.1509	0.8491	0.7044	Epimrdii Herba	Yinyanghuo A	Not Available	FALSE	O1C(C=Cc2c1c(CC(O)C(=C)C)cc(c2)c1oc2c(c(=O)c1)c(O)cc(O)c2)(C)C
MOL004384	0.3325	0.6675	0.8340	Epimrdii Herba	Yinyanghuo C	5315395	FALSE	C1(cc(c2c(c1)oc(cc2=O)c1cc(c(c1)CC=C(C)C)O)O)O
MOL004385	0.5090	0.4910	0.6439	Epimrdii Herba	Yinyanghuo D	5315396	FALSE	C1(cc(c2c(c1)oc(cc2=O)c1cc(c(c1)CC=C(C)C)O)O)O
MOL004385	0.5090	0.4910	0.6439	licorice	Yinyanghuo D	5315396	FALSE	C1(cc(c2c(c1)oc(cc2=O)c1cc(c(c1)CC=C(C)C)O)O)O
MOL004386	0.3746	0.6254	0.8120	Epimrdii Herba	Yinyanghuo E	5315397	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1cc(c2c(c1)C=CC(O2)(C)C)O)O)O
MOL004387	0.7290	0.2710	0.8055	Epimrdii Herba	Yixinoside A	Not Available	FALSE	C1(OC(C(C(C1O)O)O)OC1C(C(C(OC1OC1C(C2CCC3(C(C2(C(C1)O)C)CC(C1C3(CCC1C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1OC(C(C(C1O)O)O)C)O)O)O)C)C)(C)C)CO)O)O)CO

MOL004388	0.6742	0.3258	0.7137	Epimrdii Herba	6-hydroxy-11,12-dimethoxy-2,2-dimethyl-1,8-dioxo-2,3,4,8-tetrahydro-1H-isochromeno[3,4-h]isoquinolin-2-ium	12115137	FALSE	o1c(=O)c2c(c3c4C(=O)[N+](CCc4cc(c13)O)(C)C)c(c(cc2)OC)OC
MOL004389	0.9338	0.0662	0.8991	Epimrdii Herba	3-Hexenyl-beta-glucopyranoside	5318046	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)CC/C=C/CC
MOL004391	0.2145	0.7855	0.7961	Epimrdii Herba	8-(3-methylbut-2-enyl)-2-phenyl-chromone	17861868	FALSE	c1(cc(=O)c2cccc(c2o1)CC=C(C)C)c1ccccc1
MOL004392	0.5760	0.4240	0.7787	Epimrdii Herba	acuminatoside	Not Available	FALSE	O(C1C(O)C(O)C(OC1Oc1c(c2oc(c(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)C)C)c(=O)c2c(O)c1)c1ccc(OC)cc1)CC=C(C)C)CO)C1OC(C(O)C(O)C1O)CO
MOL004393	0.3359	0.6641	0.8190	Epimrdii Herba	anhydroicaritin	14583584	FALSE	c12c(CCC(O1)(C)C)c1c(c(=O)c(c(o1)c1ccc(cc1)OC)O)c(c2)O
MOL004394	0.5616	0.4384	0.7311	Epimrdii Herba	Anhydroicaritin-3-O-alpha-L-rhamnoside	Not Available	FALSE	C1(C(C(C(C(O1)Oc1cc(c2c(c1CC=C(C)C)oc(c(c2=O)OC1OC(C(C(C1O)O)O)C)c1ccc(cc1)OC)O)O)O)O)CO
MOL004395	0.3020	0.6980	0.6522	Epimrdii Herba	artonin U	44258358	FALSE	O1c2c(CC=C(C)C)c(OC)cc(O)c2c(=O)cc1c1ccc(O)cc1
MOL004396	0.8613	0.1387	0.8259	Epimrdii Herba	1,2-bis(4-hydroxy-3-methoxyphenyl)propan-1,3-diol	12468616	FALSE	C(C(CO)c1cc(c(cc1)O)OC)(O)c1cc(c(cc1)O)OC
MOL004397	0.5737	0.4263	0.7560	Epimrdii Herba	baohuoside Ⅵ	Not Available	FALSE	O(C1C(O)C(O)C(OC1Oc1c(oc2c(c1=O)c(O)cc(OC1OC(C(O)C(O)C1O)CO)c2CC=C(C)C)c1ccc(OC)cc1)C)C1OC(C(O)C(O)C1O)C

MOL004398	0.4007	0.5993	0.7065	Anemarrhenae Rhizoma	3,5,7-Trihydroxy-4'-methoxyl-8-prenylflavone-3-O-rhamnopyranoside	5488822	TRUE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2CC=C(C)C)c1ccc(OC)cc1)C
MOL004398	0.4007	0.5993	0.7065	Epimrdii Herba	3,5,7-Trihydroxy-4'-methoxyl-8-prenylflavone-3-O-rhamnopyranoside	5488822	TRUE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2CC=C(C)C)c1ccc(OC)cc1)C
MOL004399	0.5632	0.4368	0.7503	Epimrdii Herba	Baohuoside VI	11972471	FALSE	C1(C(C(OC(C1O)CO)Oc1cc(c2c(c1CC=C(C)C)oc(c(c2=O)OC1OC(C(C(C1O)O)OC1OC(C(C(C1O)O)O)C)C)c1ccc(cc1)OC)O)O)O
MOL004400	0.9223	0.0777	0.8896	Epimrdii Herba	Bilobanol	Not Available	FALSE	C1C(CC=C(C1O)C)c1cc(oc1)CC(C)C
MOL004401	0.4177	0.5823	0.6186	Epimrdii Herba	bilobetin	5315459	FALSE	c12c(c3c(ccc(c3)c3oc4c(c(=O)c3)c(cc(c4)O)O)OC)c(cc(c1c(=O)cc(o2)c1ccc(cc1)O)O)O
MOL004401	0.4177	0.5823	0.6186	Ginkgo Semen	bilobetin	5315459	FALSE	c12c(c3c(ccc(c3)c3oc4c(c(=O)c3)c(cc(c4)O)O)OC)c(cc(c1c(=O)cc(o2)c1ccc(cc1)O)O)O
MOL004401	0.4177	0.5823	0.6186	Ranunculi Ternati Radix	bilobetin	5315459	FALSE	c12c(c3c(ccc(c3)c3oc4c(c(=O)c3)c(cc(c4)O)O)OC)c(cc(c1c(=O)cc(o2)c1ccc(cc1)O)O)O
MOL004401	0.4177	0.5823	0.6186	Ginkgo Folium	bilobetin	5315459	FALSE	c12c(c3c(ccc(c3)c3oc4c(c(=O)c3)c(cc(c4)O)O)OC)c(cc(c1c(=O)cc(o2)c1ccc(cc1)O)O)O
MOL004403	0.5235	0.4765	0.7250	Epimrdii Herba	caohuoside B	Not Available	FALSE	O(C1C(OC(=O)C)C(OC(Oc2c(oc3c(c2=O)c(O)cc(OC2OC(C(O)C(O)C2O)CO)c3CC=C(C)C)c2ccc(OC)cc2)C1O)C)C1OC(C(OC(=O)C)C(O)C1O)COC(=O)C
MOL004404	0.4383	0.5617	0.6350	Epimrdii Herba	caohuoside D	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(CCC(OC)(C)C)c2oc(c(O)c(=O)c2c(O)c1)c1ccc(OC)cc1)CO

MOL004405	0.5737	0.4263	0.7560	Epimrdii Herba	3-[(2S,3R,4R,5R,6S)-4,5-dihydroxy-6-methyl-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-tetrahydropyran-2-yl]oxy-5-hydroxy-2-(4-methoxyphenyl)-8-(3-methylbut-2-enyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran	24721194	FALSE	c12c(c(=O)c(c(o2)c2ccc(cc2)OC)OC2C(OC3C(C(C(C(O3)C)O)O)O)C(C(C(O2)C)O)O)c(cc(c1CC=C(C)C)OC1OC(C(C(C1O)O)O)CO)O
MOL004406	0.7542	0.2458	0.7285	Epimrdii Herba	2,15-Hexadecanedione	458096	FALSE	C(=O)(CCCCCCCCCCCCC(=O)C)C
MOL004407	0.5614	0.4386	0.7376	Epimrdii Herba	Epimedin B	25087708	FALSE	c1(ccc2c(c1CC=C(C)C)oc(c(c2=O)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)C)O)O)c1ccc(cc1)OC)OC1OC(C(C(C1O)O)O)CO
MOL004408	0.2408	0.7592	0.7544	Epimrdii Herba	Epimedin C_qt	Not Available	FALSE	c1(ccc2c(c1CC=C(C)C)oc(c(c2=O)O)c1ccc(cc1)OC)O
MOL004409	0.5175	0.4825	0.7356	Epimrdii Herba	Epimedin C	5317090	FALSE	c1(ccc2c(c1CC=C(C)C)oc(c(c2=O)OC1OC(C(CC1OC1OC(C(C(C1O)O)O)C)O)C)c1ccc(cc1)OC)OC1OC(C(C(C1O)O)O)CO
MOL004410	0.9161	0.0839	0.9602	Epimrdii Herba	epimedokoreanone A	54728446	FALSE	c1(=O)cc(c(c(o1)C)O)O

MOL004411	0.7171	0.2829	0.7650	Epimrdii Herba	(2S,3S)-3,5-dihydroxy-2-(4-hydroxyphenyl)-8-(3-methylbut-2-enyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]oxy-chroman-4-one	7163182	FALSE	c1(cc(c2c(c1CC=C(C)C)OC(C(C2=O)O)c1ccc(cc1)O)O)OC1OC(C(C(C1O)O)O)CO
MOL004413	0.7150	0.2850	0.7646	Epimrdii Herba	epimedoside C	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(c2oc(c(O)c(=O)c2c(O)c1)c1ccc(O)cc1)CC=C(C)C)CO
MOL004414	0.6483	0.3517	0.7563	Epimrdii Herba	epimedoside D	Not Available	FALSE	O(C1C(O)C(O)COC1Oc1c(=O)c2c(oc1c1ccc(O)cc1)c(c(OC1OC(C(O)C(O)C1O)CO)cc2O)CC=C(C)C)C1OC(C(O)C(O)C1O)C
MOL004415	0.6447	0.3553	0.7553	Epimrdii Herba	Epimedoside E	Not Available	FALSE	O(C1C(O)C(O)C(OC1Oc1c(=O)c2c(oc1c1ccc(O)cc1)c(c(OC1OC(C(O)C(O)C1O)CO)cc2O)CC=C(C)C)C)C1OCC(O)C(O)C1O
MOL004417	0.4145	0.5855	0.7014	Epimrdii Herba	epimedoside	Not Available	FALSE	O(C1C(OC(=O)C)C(OC(Oc2c(oc3c(c2=O)c(O)cc(O)c3CC=C(C)C)c2ccc(OC)cc2)C1O)C)C1OC(C(O)C(O)C1O)COC(=O)C
MOL004418	0.9305	0.0695	0.9452	Semiaquilegiae Radix	DOB	1491	FALSE	c1(c(cc(cc1)O)O)C(=O)O
MOL004418	0.9305	0.0695	0.9452	Sterculiae Lychnophorae Semen	DOB	1491	FALSE	c1(c(cc(cc1)O)O)C(=O)O
MOL004418	0.9305	0.0695	0.9452	Radix Euphorbiae Pekinensis	DOB	1491	FALSE	c1(c(cc(cc1)O)O)C(=O)O
MOL004418	0.9305	0.0695	0.9452	Epimrdii Herba	DOB	1491	FALSE	c1(c(cc(cc1)O)O)C(=O)O
MOL004419	0.8608	0.1392	0.6197	Epimrdii Herba	globulol	11996452	FALSE	OC1(C2C(C3C(C3CC1)(C)C)C(CC2)C)C
MOL004419	0.8608	0.1392	0.6197	Linderae Radix	globulol	11996452	FALSE	OC1(C2C(C3C(C3CC1)(C)C)C(CC2)C)C
MOL004419	0.8608	0.1392	0.6197	Ardisiae Japonicae Herba	globulol	11996452	FALSE	OC1(C2C(C3C(C3CC1)(C)C)C(CC2)C)C
MOL004419	0.8608	0.1392	0.6197	Citrus Aurantium	globulol	11996452	FALSE	OC1(C2C(C3C(C3CC1)(C)C)C(CC2)C)C
MOL004419	0.8608	0.1392	0.6197	Litchi Semen	globulol	11996452	FALSE	OC1(C2C(C3C(C3CC1)(C)C)C(CC2)C)C
MOL004419	0.8608	0.1392	0.6197	Nardostachyos Radix Et Rhizoma	globulol	11996452	FALSE	OC1(C2C(C3C(C3CC1)(C)C)C(CC2)C)C
MOL004419	0.8608	0.1392	0.6197	Ailanthi Cortex	globulol	11996452	FALSE	OC1(C2C(C3C(C3CC1)(C)C)C(CC2)C)C
MOL004421	0.5656	0.4344	0.7549	Epimrdii Herba	hexandraside D	Not Available	FALSE	O(C1C(O)C(OC(Oc2c(=O)c3c(oc2c2ccc(OC)cc2)c(c(OC2OC(C(O)C(O)C2O)CO)cc3O)CC=C(C)C)C1O)C)C1OC(C(O)C(O)C1O)C

MOL004422	0.7128	0.2872	0.7667	Epimrdii Herba	Hexandraside E	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(c2oc(c(OC3OC(C(O)C(O)C3O)CO)c(=O)c2c(O)c1)c1ccc(O)cc1)CC=C(C)C)CO
MOL004423	0.5876	0.4124	0.7545	Epimrdii Herba	hexandraside F	Not Available	FALSE	O(C1C(O)C(OC(Oc2c(=O)c3c(oc2c2ccc(OC)cc2)c(c(OC2OC(C(O)C(O)C2O)CO)cc3O)CC=C(C)C)C1O)C)C1OC(C(O)C(O)C1O)CO
MOL004424	0.7832	0.2168	0.6095	Epimrdii Herba	Icaride A2	15690604	FALSE	c1(c(c(cc(c1)C1OC(C(C1CO)CO)c1cc(c(c(c1)OC)O)OC)OC)O)OC
MOL004425	0.5614	0.4386	0.7313	Epimrdii Herba	Icariin	5318997	FALSE	c12c(c(=O)c(c(o2)c2ccc(cc2)OC)OC2C(C(C(C(O2)C)O)O)O)c(cc(c1CC=C(C)C)OC1OC(C(C(C1O)O)O)CO)O
MOL004426	0.8326	0.1674	0.7743	Epimrdii Herba	Icariresinol	Not Available	FALSE	O1C(C(C(C1)(Cc1cc(c(cc1)O)OC)O)(CO)CC(=O)O)c1cc(c(cc1)O)OC
MOL004427	0.8166	0.1834	0.7157	Epimrdii Herba	Icariside A7	5318401	FALSE	c1c(c(c(c2c1ccc1c2cc(c(c1)O)OC)OC)OC)OC1OC(C(C(C1O)O)O)CO
MOL004428	0.6462	0.3538	0.7594	Epimrdii Herba	3,4,6-trimethoxyphenanthrene-2,7-diol	356766	FALSE	Oc1cc2c(c(c1OC)OC)c1c(cc2)cc(c(c1)OC)O
MOL004429	0.7916	0.2084	0.7018	Epimrdii Herba	icariside C1	Not Available	FALSE	O1C(OC(C(O)(C)C)CC/C(=C/CCC(O)(C)C=C)/C)C(O)C(O)C(O)C1CO
MOL004430	0.4877	0.5123	0.7176	Epimrdii Herba	icariside I	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(c2oc(c(O)c(=O)c2c(O)c1)c1ccc(OC)cc1)CC=C(C)C)CO
MOL004431	0.4007	0.5993	0.7065	Epimrdii Herba	icariside II	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2CC=C(C)C)c1ccc(OC)cc1)C
MOL004432	0.5969	0.4031	0.7417	Epimrdii Herba	4H-1-Benzopyran-4-one, 3-((6-deoxy-alpha-L-mennopyranosyl)oxy)-5,7-dihydroxy-2-(4-hydroxyphenyl)-8-(3-methyl-2-butenyl)-	5481982	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2CC=C(C)C)c1ccc(O)cc1)C

MOL004433	0.6759	0.3241	0.7666	Epimrdii Herba	3-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-6-methylol-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-tetrahydropyran-2-yl]oxy-5,7-dihydroxy-2-(4-hydroxyphenyl)-8-(3-methylbut-2-enyl)chromone	5318411	FALSE	c1(c(c(=O)c2c(o1)c(c(cc2O)O)CC=C(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO)c1ccc(cc1)O
MOL004434	0.6363	0.3637	0.7650	Epimrdii Herba	Ikarisoside C	Not Available	FALSE	O(C1CC(C(O)C(O)C1O)CO)c1c(c2oc(c(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)C)c(=O)c2c(O)c1)c1ccc(O)cc1)CC=C(C)C
MOL004435	0.6642	0.3358	0.7618	Epimrdii Herba	Ikarisoside F	5318413	FALSE	c1(c(c(=O)c2c(o1)c(c(cc2O)O)CC=C(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)C)O)O)c1ccc(cc1)O
MOL004436	0.2366	0.7634	0.6622	Epimrdii Herba	Ikshusterol	Not Available	FALSE	C1C(CC2=CC(C3C(C2(C1)C)CCC1(C3CCC1C(C)CCC(C(C)C)CC)C)O)O
MOL004437	0.8468	0.1532	0.8032	Epimrdii Herba	Lespedin	5486199	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(=O)c2c(oc1c1ccc(O)cc1)cc(OC1OC(C(O)C(O)C1O)C)cc2O)C
MOL004438	0.4449	0.5551	0.6907	Epimrdii Herba	korepimedoside A	Not Available	FALSE	c1(ccc(cc1)C1C(C(=O)c2c(O1)c(c(cc2O)O)CC=C(C)C)OC1C(C(C(C(O1)C)OC(=O)C)OC1C(C(C(C(O1)OC(=O)C)O)O)O)O)OC
MOL004439	0.5220	0.4780	0.7288	Epimrdii Herba	korepimedoside B	Not Available	FALSE	O(C1C(OC(=O)C)C(OC(Oc2c(oc3c(c2=O)c(O)cc(OC2OC(C(O)C(O)C2O)CO)c3CC=C(C)C)c2ccc(OC)cc2)C1O)C)C1OC(C(O)C(O)C1OC(=O)C)COC(=O)C
MOL004440	0.2986	0.7014	0.7744	Fritillariae Thunbrgii Bulbus	Peimisine	161294	FALSE	O1C2(C(=C3C(C4C(C5(C(C(=O)C4)CC(O)CC5)C)C3)CC2)C)C(C2NCC(CC12)C)C
MOL004440	0.2986	0.7014	0.7744	Fritillariaeussuriensis Bulbus	Peimisine	161294	FALSE	O1C2(C(=C3C(C4C(C5(C(C(=O)C4)CC(O)CC5)C)C3)CC2)C)C(C2NCC(CC12)C)C
MOL004440	0.2986	0.7014	0.7744	Fritillariae Pallidiflorae Bulbus	Peimisine	161294	FALSE	O1C2(C(=C3C(C4C(C5(C(C(=O)C4)CC(O)CC5)C)C3)CC2)C)C(C2NCC(CC12)C)C

MOL004440	0.2986	0.7014	0.7744	Fritiliariae Irrhosae Bulbus	Peimisine	161294	FALSE	O1C2(C(=C3C(C4C(C5(C(C(=O)C4)CC(O)CC5)C)C3)CC2)C)C(C2NCC(CC12)C)C
MOL004443	0.9080	0.0920	0.7621	Fritillariae Thunbrgii Bulbus	Zhebeiresinol	Not Available	FALSE	c1(c(cc(cc1OC)C1C2C(CO1)C(=O)OC2)OC)O
MOL004444	0.4653	0.5347	0.7403	Fritillariae Thunbrgii Bulbus	Ziebeimine	Not Available	FALSE	OC1C2C(C3C(C4C(C3)C3=C(CC4)C(C4N(C3)CC(CC4)C)C)C1)(CCC(O)C2)C
MOL004445	0.5559	0.4441	0.7268	Fritillariae Thunbrgii Bulbus	Verticine	Not Available	FALSE	OC1C2C(C3C(C4C(C3)C3C(CC4)C(O)(C4N(C3)CC(CC4)C)C)C1)(CCC(O)C2)C
MOL004445	0.5559	0.4441	0.7268	Fritillariaeussuriensis Bulbus	Verticine	Not Available	FALSE	OC1C2C(C3C(C4C(C3)C3C(CC4)C(O)(C4N(C3)CC(CC4)C)C)C1)(CCC(O)C2)C
MOL004445	0.5559	0.4441	0.7268	Fritiliariae Irrhosae Bulbus	Verticine	Not Available	FALSE	OC1C2C(C3C(C4C(C3)C3C(CC4)C(O)(C4N(C3)CC(CC4)C)C)C1)(CCC(O)C2)C
MOL004446	0.8916	0.1084	0.8282	Fritillariae Thunbrgii Bulbus	6-Methoxyl-2-acetyl-3-methyl-1,4-naphthoquinone-8-O-beta-D-glucopyranoside	5319462	FALSE	C1(C(OC(C(C1O)O)CO)Oc1cc(cc2c1C(=O)C(=C(C2=O)C)C(=O)C)OC)O
MOL004447	0.9263	0.0737	0.8256	Fritillariae Thunbrgii Bulbus	6-Methoxyl-2-acetyl-3-methyl-1,4-naphthoquinone-8-O-beta-D-glucopyranoside_qt	67877406	FALSE	c1(cc(cc2c1C(=O)C(=C(C2=O)C)C(=O)C)OC)O
MOL004448	0.3950	0.6050	0.6667	Fritillariaeussuriensis Bulbus	Solatubin	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC2C1C(C1N2CC(CC1)C)C)C)O
MOL004448	0.3950	0.6050	0.6667	Fritillariae Thunbrgii Bulbus	Solatubin	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC2C1C(C1N2CC(CC1)C)C)C)O
MOL004448	0.3950	0.6050	0.6667	Fritiliariae Irrhosae Bulbus	Solatubin	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC2C1C(C1N2CC(CC1)C)C)C)O
MOL004448	0.3950	0.6050	0.6667	Solanum Nigrum Linn.	Solatubin	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC2C1C(C1N2CC(CC1)C)C)C)O
MOL004451	0.5462	0.4538	0.7618	Fritillariae Thunbrgii Bulbus	Peiminine	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2=O)C2C(C1)C1C(CC2)C(C2N(C1)CC(CC2)C)(O)C)C)O
MOL004452	0.6131	0.3869	0.7051	Fritillariae Thunbrgii Bulbus	Peiminoside	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2O)C2C(C1)C1C(CC2)C(C2N(C1)CC(CC2)C)(O)C)C)OC1C(C(C(C(O1)CO)O)O)O
MOL004453	0.5559	0.4441	0.7268	Fritillariae Thunbrgii Bulbus	Peiminoside_qt	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2O)C2C(C1)C1C(CC2)C(C2N(C1)CC(CC2)C)(O)C)C)O
MOL004454	0.7713	0.2287	0.6307	Arecae Semen	ODD	5282800	FALSE	C(CC/C=C/C=C\CCCCC)CCCCCC(=O)O

MOL004454	0.7713	0.2287	0.6307	Violsse Herba	ODD	5282800	FALSE	C(CC/C=C/C=C\CCCCC)CCCCCC(=O)O
MOL004454	0.7713	0.2287	0.6307	Fructussophorae	ODD	5282800	FALSE	C(CC/C=C/C=C\CCCCC)CCCCCC(=O)O
MOL004454	0.7713	0.2287	0.6307	Abutili Semen	ODD	5282800	FALSE	C(CC/C=C/C=C\CCCCC)CCCCCC(=O)O
MOL004454	0.7713	0.2287	0.6307	Ricini Semen	ODD	5282800	FALSE	C(CC/C=C/C=C\CCCCC)CCCCCC(=O)O
MOL004455	0.9477	0.0523	0.9246	Violsse Herba	p-Allyltoluene	76851	FALSE	c1(ccc(cc1)C)CC=C
MOL004456	0.9323	0.0677	0.8757	Semen Aesculi	Esculin	5281417	FALSE	[illegible]
MOL004456	0.9323	0.0677	0.8757	Cichorii Radix	Esculin	5281417	FALSE	[illegible]
MOL004456	0.9323	0.0677	0.8757	Fraxini Cortex	Esculin	5281417	FALSE	[illegible]
MOL004456	0.9323	0.0677	0.8757	Violsse Herba	Esculin	5281417	FALSE	[illegible]
MOL004456	0.9323	0.0677	0.8757	Semen Euphorbiae	Esculin	5281417	FALSE	[illegible]
MOL004456	0.9323	0.0677	0.8757	Rubi Fructus	Esculin	5281417	FALSE	[illegible]
MOL004457	0.4747	0.5253	0.6438	Violsse Herba	trans-10, cis-12 octadecadienoic acid, methyl ester	5471014	FALSE	C(C/C=C/C=C\CCCCC)CCCCCCC(=O)OC
MOL004459	0.8675	0.1325	0.8116	Hyperici Japonici Herber	Tridecanol	8207	FALSE	OCCCCCCCCCCCCCC
MOL004459	0.8675	0.1325	0.8116	Violsse Herba	Tridecanol	8207	FALSE	OCCCCCCCCCCCCC
MOL004461	0.9080	0.0920	0.9727	Violsse Herba	(2R,6R)-2,6-dimethylcyclohexan-1-ol	6992793	FALSE	C1(CCCC(C1O)C)C
MOL004462	0.9297	0.0703	0.9616	Bomboo Juice	Otan	670	FALSE	C(C(=O)CO)O
MOL004462	0.9297	0.0703	0.9616	Zanthoxyli Pericarpium	Otan	670	FALSE	C(C(=O)CO)O
MOL004463	0.9252	0.0748	0.9659	Bomboo Juice	1-[(2S)-oxolan-2-yl]ethanone	11170944	FALSE	C(=O)(C)C1OCCC1
MOL004464	0.9247	0.0753	0.9738	Bomboo Juice	MEHQ	9015	FALSE	c1cc(ccc1OC)O
MOL004464	0.9247	0.0753	0.9738	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	MEHQ	9015	FALSE	c1cc(ccc1OC)O
MOL004464	0.9247	0.0753	0.9738	Cannabis Sativa L.	MEHQ	9015	FALSE	c1cc(ccc1OC)O
MOL004465	0.9587	0.0413	0.9692	Bomboo Juice	N-Methylphenethylamine	11503	FALSE	c1(ccccc1)CCNC
MOL004466	0.9525	0.0475	0.9417	Bomboo Juice	Sympamin	5826	FALSE	NC(Cc1ccccc1)C
MOL004467	0.9525	0.0475	0.9417	Bomboo Juice	Levamfetamine	32893	FALSE	c1(ccccc1)CC(C)N
MOL004468	0.9155	0.0845	0.9672	Bomboo Juice	(2R)-butan-2-amine	2724537	FALSE	C(CC)(C)N
MOL004469	0.9243	0.0757	0.9779	Bomboo Juice	N-Methylvalerolactam	13603	FALSE	N1(C(=O)CCCC1)C
MOL004470	0.8873	0.1127	0.9598	Sojae Semen Nigrum	PPI	1032	FALSE	C(=O)(CC)O

MOL004470	0.8873	0.1127	0.9598	Paederiae Scandentis Herba	PPI	1032	FALSE	C(=O)(CC)O
MOL004470	0.8873	0.1127	0.9598	Apocyniveneti Folium	PPI	1032	FALSE	C(=O)(CC)O
MOL004470	0.8873	0.1127	0.9598	Ginkgo Semen	PPI	1032	FALSE	C(=O)(CC)O
MOL004470	0.8873	0.1127	0.9598	Bomboo Juice	PPI	1032	FALSE	C(=O)(CC)O
MOL004471	0.9267	0.0733	0.9601	Bomboo Juice	Methyl propylate	11124	FALSE	C(=O)(CC)OC
MOL004471	0.9267	0.0733	0.9601	Puerariae Flos	Methyl propylate	11124	FALSE	C(=O)(CC)OC
MOL004472	0.8602	0.1398	0.6668	Zanthoxyli Pericarpium	Azeton	180	TRUE	CC(=O)C
MOL004472	0.8602	0.1398	0.6668	Oroxyli Semen	Azeton	180	TRUE	CC(=O)C
MOL004472	0.8602	0.1398	0.6668	Bomboo Juice	Azeton	180	TRUE	CC(=O)C
MOL004473	0.9607	0.0393	0.9534	Bomboo Juice	2-(p-Tolyl)ethylamine	76751	FALSE	c1(ccc(cc1)C)CCN
MOL004474	0.9426	0.0574	0.9556	Apocyniveneti Folium	Maruzen M	31242	FALSE	c1(ccc(cc1)CC)O
MOL004474	0.9426	0.0574	0.9556	Bomboo Juice	Maruzen M	31242	FALSE	c1(ccc(cc1)CC)O
MOL004474	0.9426	0.0574	0.9556	Angelicae Sinensis Radix	Maruzen M	31242	FALSE	c1(ccc(cc1)CC)O
MOL004475	0.9334	0.0666	0.9517	Bomboo Juice	DIBUTYLAMINE	8148	FALSE	C(CCC)NCCCC
MOL004476	0.9221	0.0779	0.9679	Bomboo Juice	Methyl formyl	10795	FALSE	C(C)(OC)OC
MOL004477	0.8521	0.1479	0.6657	Bomboo Juice	OME	887	FALSE	CO
MOL004477	0.8521	0.1479	0.6657	Morindae Officinalis Radix	OME	887	FALSE	CO
MOL004478	0.9300	0.0700	0.9694	Bomboo Juice	2-Oxobutanol	521300	FALSE	C(C(=O)CC)O
MOL004479	0.8896	0.1104	0.9551	Angelicae Sinensis Radix	o-cresol	335	FALSE	c1(c(cccc1)C)O
MOL004479	0.8896	0.1104	0.9551	Bomboo Juice	o-cresol	335	FALSE	c1(c(cccc1)C)O
MOL004479	0.8896	0.1104	0.9551	Campsis Flos	o-cresol	335	FALSE	c1(c(cccc1)C)O
MOL004480	0.8662	0.1338	0.6765	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	acetic acid	21980959	FALSE	C(=O)(C)O
MOL004480	0.8662	0.1338	0.6765	Citri Sarcodactylis Fructus	acetic acid	21980959	FALSE	C(=O)(C)O
MOL004480	0.8662	0.1338	0.6765	Caryophylliflos	acetic acid	21980959	FALSE	C(=O)(C)O
MOL004480	0.8662	0.1338	0.6765	Hippophae Fructus	acetic acid	21980959	FALSE	C(=O)(C)O
MOL004480	0.8662	0.1338	0.6765	Ephedra Herba	acetic acid	21980959	FALSE	C(=O)(C)O
MOL004480	0.8662	0.1338	0.6765	Linderae Radix	acetic acid	21980959	FALSE	C(=O)(C)O
MOL004480	0.8662	0.1338	0.6765	Campsis Flos	acetic acid	21980959	FALSE	C(=O)(C)O
MOL004480	0.8662	0.1338	0.6765	Panacis Japonici Rhizoma	acetic acid	21980959	FALSE	C(=O)(C)O
MOL004480	0.8662	0.1338	0.6765	Maydis Seigma	acetic acid	21980959	FALSE	C(=O)(C)O
MOL004480	0.8662	0.1338	0.6765	Stemonae Radix	acetic acid	21980959	FALSE	C(=O)(C)O
MOL004480	0.8662	0.1338	0.6765	Mume Flos	acetic acid	21980959	FALSE	C(=O)(C)O
MOL004480	0.8662	0.1338	0.6765	Paederiae Scandentis Herba	acetic acid	21980959	FALSE	C(=O)(C)O
MOL004480	0.8662	0.1338	0.6765	Mori Fructus	acetic acid	21980959	FALSE	C(=O)(C)O
MOL004480	0.8662	0.1338	0.6765	Bomboo Juice	acetic acid	21980959	FALSE	C(=O)(C)O
MOL004480	0.8662	0.1338	0.6765	Folium Artemisiae Argyi	acetic acid	21980959	FALSE	C(=O)(C)O

MOL004480	0.8662	0.1338	0.6765	Portulacae Herba	acetic acid	21980959	FALSE	C(=O)(C)O
MOL004481	0.8679	0.1321	0.7686	Bomboo Juice	(2S)-2-amino-3-[(2R)-2-amino-3-hydroxy-3-oxopropyl]disulfanylpropanoic acid	6991966	FALSE	C(=O)(C(N)CSSCC(N)C(=O)O)O
MOL004481	0.8679	0.1321	0.7686	Arum Ternatum Thunb.	(2S)-2-amino-3-[(2R)-2-amino-3-hydroxy-3-oxopropyl]disulfanylpropanoic acid	6991966	FALSE	C(=O)(C(N)CSSCC(N)C(=O)O)O
MOL004481	0.8679	0.1321	0.7686	Santalum Album L.	(2S)-2-amino-3-[(2R)-2-amino-3-hydroxy-3-oxopropyl]disulfanylpropanoic acid	6991966	FALSE	C(=O)(C(N)CSSCC(N)C(=O)O)O
MOL004481	0.8679	0.1321	0.7686	Euryales Semen	(2S)-2-amino-3-[(2R)-2-amino-3-hydroxy-3-oxopropyl]disulfanylpropanoic acid	6991966	FALSE	C(=O)(C(N)CSSCC(N)C(=O)O)O
MOL004481	0.8679	0.1321	0.7686	Vigna Radiata	(2S)-2-amino-3-[(2R)-2-amino-3-hydroxy-3-oxopropyl]disulfanylpropanoic acid	6991966	FALSE	C(=O)(C(N)CSSCC(N)C(=O)O)O
MOL004481	0.8679	0.1321	0.7686	Radix Salviae	(2S)-2-amino-3-[(2R)-2-amino-3-hydroxy-3-oxopropyl]disulfanylpropanoic acid	6991966	FALSE	C(=O)(C(N)CSSCC(N)C(=O)O)O

MOL004482	0.9299	0.0701	0.9642	Bomboo Juice	Acetol	8299	FALSE	C(C(=O)C)O
MOL004482	0.9299	0.0701	0.9642	Santalum Album L.	Acetol	8299	FALSE	C(C(=O)C)O
MOL004482	0.9299	0.0701	0.9642	Citri Sarcodactylis Fructus	Acetol	8299	FALSE	C(C(=O)C)O
MOL004483	0.9283	0.0717	0.9591	Radix Cynanchi Paniculati	CREOSOL	7144	FALSE	c1(c(ccc(c1)C)O)OC
MOL004483	0.9283	0.0717	0.9591	Bomboo Juice	CREOSOL	7144	FALSE	c1(c(ccc(c1)C)O)OC
MOL004484	0.9244	0.0756	0.9536	Bomboo Juice	(2S)-heptan-2-amine	2734517	FALSE	CC(CCCCC)N
MOL004485	0.9251	0.0749	0.9620	Bomboo Juice	3,3-Dimethylbutylamine	19709	FALSE	C(CC(C)(C)C)N
MOL004486	0.7356	0.2644	0.8432	Anemarrhenae Rhizoma	(25R,S)-5alpha-Spirostane-2alpha,3beta-diol 3-O-[O-beta-D-glucopyranosyl-(1-2)-O-beta-D-glucopyranosyl-(1-4)-beta-D-galactopyranoside]	Not Available	FALSE	C1(C(CC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)OC1OC(C(C(C1O)O)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO)CO)O
MOL004487	0.3332	0.6668	0.6949	Allium Azureum Ledeb.	gitogenin	Not Available	FALSE	C1(C(CC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)O)O
MOL004487	0.3332	0.6668	0.6949	Anemarrhenae Rhizoma	gitogenin	Not Available	FALSE	C1(C(CC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)O)O
MOL004488	0.7305	0.2695	0.8301	Anemarrhenae Rhizoma	Anemarsaponin F	Not Available	FALSE	C1CC2(OCC1C)OC1C(C2C)C2(C(C1)C1C(CC2)C2(C(CC1)CC(C(C2)O)OC1OC(C(C(C1O)O)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)OC1OCC(C(C1O)O)O)O)CO)CO)C)C
MOL004489	0.3332	0.6668	0.6949	Anemarrhenae Rhizoma	Anemarsaponin F_qt	Not Available	FALSE	C1CC2(OCC1C)OC1C(C2C)C2(C(C1)C1C(CC2)C2(C(CC1)CC(C(C2)O)O)C)C
MOL004490	0.7247	0.2753	0.8298	Anemarrhenae Rhizoma	Anemarsaponin G	Not Available	FALSE	C1CC2(OCC1C)OC1C(C2C)C2(C(C1)C1C(CC2)C2(C(=CC1)CC(C(C2)O)OC1OC(C(C(C1O)O)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)OC1OCC(C(C1O)O)O)O)CO)CO)C)C
MOL004491	0.3077	0.6923	0.7078	Anemarrhenae Rhizoma	Anemarsaponin G_qt	Not Available	FALSE	C1CC2(OCC1C)OC1C(C2C)C2(C(C1)C1C(CC2)C2(C(=CC1)CC(C(C2)O)O)C)C
MOL004493	0.9236	0.0764	0.9697	Anemarrhenae Rhizoma	PAU	6613	FALSE	C(C(CO)(C)C)(C(=O)NCCC(=O)O)O
MOL004493	0.9236	0.0764	0.9697	Maydis Seigma	PAU	6613	FALSE	C(C(CO)(C)C)(C(=O)NCCC(=O)O)O
MOL004493	0.9236	0.0764	0.9697	Ginkgo Semen	PAU	6613	FALSE	C(C(CO)(C)C)(C(=O)NCCC(=O)O)O

MOL004494	0.7063	0.2937	0.8303	Anemarrhenae Rhizoma	Desglucolanatigonin II	Not Available	FALSE	C1(C(C(OC(C1O)CO)OC1C(C(C(OC1OC1C(C(C(OC1CO)OC1CC2CCC3C(C2(CC1)C)CCC1(C3CC2C1C(C1(O2)OCC(CC1)C)C)C)O)O)CO)O)OC1OCC(C(C1O)O)O)O)O
MOL004495	0.3012	0.6988	0.7449	Anemarrhenae Rhizoma	tigogenin	Not Available	FALSE	OC1CC2CCC3C(C2(CC1)C)CCC1(C3CC2C1C(C1(O2)OCC(CC1)C)C)C
MOL004495	0.3012	0.6988	0.7449	Solanum Nigrum Linn.	tigogenin	Not Available	FALSE	OC1CC2CCC3C(C2(CC1)C)CCC1(C3CC2C1C(C1(O2)OCC(CC1)C)C)C
MOL004495	0.3012	0.6988	0.7449	Allium Azureum Ledeb.	tigogenin	Not Available	FALSE	OC1CC2CCC3C(C2(CC1)C)CCC1(C3CC2C1C(C1(O2)OCC(CC1)C)C)C
MOL004495	0.3012	0.6988	0.7449	Radix Salviae	tigogenin	Not Available	FALSE	OC1CC2CCC3C(C2(CC1)C)CCC1(C3CC2C1C(C1(O2)OCC(CC1)C)C)C
MOL004495	0.3012	0.6988	0.7449	Herba Solani Lyrati	tigogenin	Not Available	FALSE	OC1CC2CCC3C(C2(CC1)C)CCC1(C3CC2C1C(C1(O2)OCC(CC1)C)C)C
MOL004497	0.8743	0.1257	0.6313	Anemarrhenae Rhizoma	Hippeastrine	Not Available	FALSE	C12C(CC3C(C1)C1C(OC3=O)C(C=C3C1N(CC3)C)O)OCO2
MOL004499	0.6612	0.3388	0.7615	Pyrrosiae Folium	Isomangiferolic acid	Not Available	FALSE	C1C(C(C2C3(C1)C1C(C(CC2)C2C(CC1)(C(CC2)C(CC/C=C(\C(=O)O)/C)C)C)C3)(C)C)O
MOL004499	0.6612	0.3388	0.7615	Anemarrhenae Rhizoma	Isomangiferolic acid	Not Available	FALSE	C1C(C(C2C3(C1)C1C(C(CC2)C2C(CC1)(C(CC2)C(CC/C=C(\C(=O)O)/C)C)C)C3)(C)C)O
MOL004500	0.6943	0.3057	0.8620	Anemarrhenae Rhizoma	Markogenin-3-O-beta-D-glucopyranosyl-(1-2)-beta-D-galactopyranoside	Not Available	FALSE	O1C(C(C(C(C1OC1C(O)CC2(C(C1)CCC1C2CCC2(C1CC1C2C(C2(O1)OCC(CC2)C)C)C)C)OC1OC(C(C(C1O)O)O)CO)O)O)O
MOL004501	0.3332	0.6668	0.6949	Anemarrhenae Rhizoma	Markogenin-3-O-beta-D-glucopyranosyl-(1-2)-beta-D-galactopyranoside_qt	Not Available	FALSE	OC1C(O)CC2(C(C1)CCC1C2CCC2(C1CC1C2C(C2(O1)OCC(CC2)C)C)C)C
MOL004502	0.7029	0.2971	0.6661	Radix Salviae	Monomethyllithospermate	Not Available	FALSE	c12c(c(ccc1/C=C/C(=O)OC(C(=O)O)Cc1ccc(c(c1)O)O)O)OC(C2C(=O)OC)c1ccc(c(c1)O)O
MOL004502	0.7029	0.2971	0.6661	Anemarrhenae Rhizoma	Monomethyllithospermate	Not Available	FALSE	c12c(c(ccc1/C=C/C(=O)OC(C(=O)O)Cc1ccc(c(c1)O)O)O)OC(C2C(=O)OC)c1ccc(c(c1)O)O
MOL004503	0.9673	0.0327	0.8769	Anemarrhenae Rhizoma	D-Nicotine	157672	FALSE	c1(cccnc1)C1CCCN1C
MOL004504	0.6898	0.3102	0.8566	Anemarrhenae Rhizoma	Sarsasapogenin 3-O-4G-rhamnosylsophoroside	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)CCC(CO2)C)C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)OC1OC(C(C(C1O)O)O)C)CO

MOL004505	0.6673	0.3327	0.8540	Anemarrhenae Rhizoma	Smilagenin-3-O[beta-D-glucopyranosyl-(1-2)]-beta-D-mannopyranoside	Not Available	FALSE	C1(CCC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL004506	0.2892	0.7108	0.7392	Anemarrhenae Rhizoma	Smilagenin-3-O[beta-D-glucopyranosyl-(1-2)]-beta-D-mannopyranoside_qt	Not Available	FALSE	C1(CCC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)O
MOL004507	0.2799	0.7201	0.7501	Anemarrhenae Rhizoma	Smilagenone	Not Available	FALSE	C1C(=O)CC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C
MOL004509	0.6774	0.3226	0.8508	Anemarrhenae Rhizoma	Timosaponin A III	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL004510	0.3012	0.6988	0.7449	Anemarrhenae Rhizoma	Timosaponin A III_qt	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)O
MOL004511	0.3367	0.6633	0.6320	Anemarrhenae Rhizoma	Timosaponin A-1	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)OC1OC(C(C(C1O)O)O)CO
MOL004512	0.3012	0.6988	0.7449	Anemarrhenae Rhizoma	Timosaponin A-1_qt	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)O
MOL004513	0.7688	0.2312	0.8184	Anemarrhenae Rhizoma	Timosaponin B III	Not Available	FALSE	O(C1C(OC2C(O)C(O)C(O)C(O2)CO)C(O)C(O)C(O1)CO)C1CCC2(C(C1)CCC1C3CC4OC(=C(C4C3(C)CCC21)C)CCC(COC1C(O)C(O)C(O)C(O1)CO)C)C
MOL004514	0.2792	0.7208	0.7661	Anemarrhenae Rhizoma	Timosaponin B III_qt	Not Available	FALSE	OC1CCC2(C(C1)CCC1C3CC4OC(=C(C4C3(C)CCC21)C)CCC(CO)C)C
MOL004515	0.7696	0.2304	0.8028	Anemarrhenae Rhizoma	Timosaponin BII	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C2C(CC1)(C)C1C(C2)OC(C1C)(CCC(COC1OC(C(C(C1O)O)O)CO)C)O)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL004516	0.3339	0.6661	0.7367	Anemarrhenae Rhizoma	Timosaponin BII_qt	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C2C(CC1)(C)C1C(C2)OC(C1C)(CCC(CO)C)O)C)O
MOL004517	0.8645	0.1355	0.7802	Anemarrhenae Rhizoma	Xuelianlactone	Not Available	FALSE	C1(=C)C2C(C3C(C(C1)O)C(C(=O)O3)C)C(=C)CC2
MOL004518	0.9223	0.0777	0.8605	Anemarrhenae Rhizoma	4-O-beta-D-Glucopyranosyl methyl gallate	5317705	FALSE	c1(c(c(cc(c1)C(=O)OC)O)OC1OC(C(C(C1O)O)O)CO)O
MOL004519	0.3332	0.6668	0.6949	Anemarrhenae Rhizoma	markogenin	Not Available	FALSE	C1(C(CC2(C(C1)CCC1C3CC4OC5(C(C4C3(C)CCC21)C)OCC(CC5)C)C)O)O

MOL004520	0.3332	0.6668	0.6949	Trigonellae Semen	neogitogenin	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(O)C(O)C5)C)CC3)C2)C)C(C21OCC(CC2)C)C
MOL004520	0.3332	0.6668	0.6949	Anemarrhenae Rhizoma	neogitogenin	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(O)C(O)C5)C)CC3)C2)C)C(C21OCC(CC2)C)C
MOL004521	0.6774	0.3226	0.8508	Anemarrhenae Rhizoma	xilingsaponin A	Not Available	FALSE	C12(C3C(CC1C1C(CC2)C2(C(CC1)CC(CC2)OC1C(OC2OC(C(C(C2O)O)O)CO)C(C(C(O1)CO)O)O)C)OC1(C3C)CCC(CO1)C)C
MOL004523	0.7253	0.2747	0.8562	Anemarrhenae Rhizoma	Anemarrhenasaponin-I	Not Available	FALSE	O(C1C(OC(C(C1O)O)CO)OC1CC2C(CC1)(C1C(CC2)C2C(CC1)(C1C(C2O)OC(C1C)(CCC(C)C)O)C)C)C1OC(C(C(C1O)O)O)CO
MOL004524	0.3869	0.6131	0.7556	Anemarrhenae Rhizoma	Anemarrhenasaponin-I_qt	Not Available	FALSE	OC1CC2C(CC1)(C1C(CC2)C2C(CC1)(C1C(C2O)OC(C1C)(CCC(C)C)O)C)C
MOL004525	0.9113	0.0887	0.8402	Anemarrhenae Rhizoma	Chinoinin	5281647	FALSE	c1(cc2c(cc1O)c(=O)c1c(o2)cc(c(c1O)C1OC(C(C(C1O)O)O)CO)O)O
MOL004525	0.9113	0.0887	0.8402	Drynariae Rhizoma	Chinoinin	5281647	FALSE	c1(cc2c(cc1O)c(=O)c1c(o2)cc(c(c1O)C1OC(C(C(C1O)O)O)CO)O)O
MOL004525	0.9113	0.0887	0.8402	Gossampiniflos	Chinoinin	5281647	FALSE	c1(cc2c(cc1O)c(=O)c1c(o2)cc(c(c1O)C1OC(C(C(C1O)O)O)CO)O)O
MOL004525	0.9113	0.0887	0.8402	Belamcandae Rhizome	Chinoinin	5281647	FALSE	c1(cc2c(cc1O)c(=O)c1c(o2)cc(c(c1O)C1OC(C(C(C1O)O)O)CO)O)O
MOL004525	0.9113	0.0887	0.8402	Pyrrosiae Folium	Chinoinin	5281647	FALSE	c1(cc2c(cc1O)c(=O)c1c(o2)cc(c(c1O)C1OC(C(C(C1O)O)O)CO)O)O
MOL004525	0.9113	0.0887	0.8402	Gentianae Radix Et Rhozima	Chinoinin	5281647	FALSE	c1(cc2c(cc1O)c(=O)c1c(o2)cc(c(c1O)C1OC(C(C(C1O)O)O)CO)O)O
MOL004526	0.8900	0.1100	0.7566	Anemarrhenae Rhizoma	Neomangiferin	Not Available	FALSE	C1(C(OC(C(C1O)O)Oc1c(cc2c(c1)c(=O)c1c(o2)cc(c(c1O)C1C(C(C(C(O1)CO)O)O)O)O)O)CO)O
MOL004527	0.8992	0.1008	0.8298	Ilicis Cornutae Folium Immayuri	Isomangiferin	5318597	FALSE	c12c(cc(c(c1)O)O)c(=O)c1c(o2)c(c(cc1O)O)C1OC(C(C(C1O)O)O)CO
MOL004527	0.8992	0.1008	0.8298	Pyrrosiae Folium	Isomangiferin	5318597	FALSE	c12c(cc(c(c1)O)O)c(=O)c1c(o2)c(c(cc1O)O)C1OC(C(C(C1O)O)O)CO
MOL004527	0.8992	0.1008	0.8298	Drynariae Rhizoma	Isomangiferin	5318597	FALSE	c12c(cc(c(c1)O)O)c(=O)c1c(o2)c(c(cc1O)O)C1OC(C(C(C1O)O)O)CO
MOL004527	0.8992	0.1008	0.8298	Anemarrhenae Rhizoma	Isomangiferin	5318597	FALSE	c12c(cc(c(c1)O)O)c(=O)c1c(o2)c(c(cc1O)O)C1OC(C(C(C1O)O)O)CO
MOL004527	0.8992	0.1008	0.8298	Eucommiae Cortex	Isomangiferin	5318597	FALSE	c12c(cc(c(c1)O)O)c(=O)c1c(o2)c(c(cc1O)O)C1OC(C(C(C1O)O)O)CO
MOL004528	0.5614	0.4386	0.7313	Anemarrhenae Rhizoma	Icariin I	Not Available	FALSE	C1(C(C(OC(C1O)CO)OC1c(c2c(c(c1O)c(=O)c(c(o2)c1ccc(cc1)OC)OC1C(C(C(C(O1)C)O)O)O)CC=C(C)C)O)O
MOL004529	0.6774	0.3226	0.8508	Anemarrhenae Rhizoma	Timosaponin A-III	Not Available	FALSE	O(C1C(OC2C(O)C(O)C(O)C(O2)CO)C(O)C(O)C(O1)CO)C1CCC2(C(C1)CCC1C3CC4OC5(C(C4C3(C)CCC21)C)OCC(CC5)C)C
MOL004530	0.3012	0.6988	0.7449	Anemarrhenae Rhizoma	Timosaponin A-III_qt	Not Available	FALSE	OC1CCC2(C(C1)CCC1C3CC4OC5(C(C4C3(C)CCC21)C)OCC(CC5)C)C

MOL004531	0.7688	0.2312	0.8184	Anemarrhenae Rhizoma	Anemarsaponin B	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(OC4OC(C(O)C(O)C4OC4OC(C(O)C(O)C4O)CO)CO)CC5)C)CC3)C2)C)C(=C1CCC(COC1OC(C(O)C(O)C1O)CO)C)C
MOL004532	0.2792	0.7208	0.7661	Anemarrhenae Rhizoma	Anemarsaponin B_qt	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(O)CC5)C)CC3)C2)C)C(=C1CCC(CO)C)C
MOL004534	0.6848	0.3152	0.8694	Anemarrhenae Rhizoma	Anemarrhenasaponin-Ia	Not Available	FALSE	O(C1C(OC(C(C1O)O)CO)OC1CC2C(CC1)(C1C(CC2)C2C(CC1)(C1C(C2O)OC(C1C)(CCC(C)C)OC)C)C1OC(C(C(C1O)O)O)CO
MOL004535	0.2525	0.7475	0.7387	Anemarrhenae Rhizoma	Anemarrhenasaponin-Ia_qt	Not Available	FALSE	OC1CC2C(CC1)(C1C(CC2)C2C(CC1)(C1C(C2O)OC(C1C)(CCC(C)C)OC)C)C
MOL004536	0.7585	0.2415	0.7345	Anemarrhenae Rhizoma	Glycerite	Not Available	FALSE	c1(cc(cc(c1O)O)C(=O)Oc1cc(cc(c1O)O)C(=O)OCC1C(C(C(C(O1)OC(=O)c1cc(c(c(c1)OC(=O)c1cc(c(c(c1)O)O)O)O)O)OC(=O)c1cc(c(c(c1)OC(=O)c1cc(c(c(c1)O)O)O)O)O)OC(=O)c1cc(c(c(c1)OC(=O)c1cc(c(c(c1)O)O)O)O)O)OC(=O)c1c(c(c(cc1)CC(=O)c1cc(c(c(c1)O)O)O)O)O)O
MOL004537	0.7688	0.2312	0.8184	Anemarrhenae Rhizoma	Anemarsaponin B	Not Available	FALSE	O(C1C(OC(C(C1O)O)CO)OC1CC2C(CC1)(C1C(CC2)C2C(CC1)(C1C(C2)OC(=C1C)CCC(COC1OC(C(C(C1O)O)O)CO)C)C)C)C1OC(C(C(C1O)O)O)CO
MOL004538	0.2792	0.7208	0.7661	Anemarrhenae Rhizoma	Anemarsaponin B_qt	Not Available	FALSE	OC1CC2C(CC1)(C1C(CC2)C2C(CC1)(C1C(C2)OC(=C1C)CCC(CO)C)C)C
MOL004539	0.7470	0.2530	0.8218	Anemarrhenae Rhizoma	Anemarsaponin C	Not Available	FALSE	O(C1C(OC(C(C1O)O)CO)OC1CC2C(CC1)(C1C(CC2)C2C(CC1)(C1C(O2)CC(=C1C)CCC(COC1OC(C(C(C1O)C)O)CO)C)C)C)C1OC(C(C(C1O)O)O)CO
MOL004540	0.2780	0.7220	0.6588	Anemarrhenae Rhizoma	Anemarsaponin C_qt	Not Available	FALSE	OC1CC2C(CC1)(C1C(CC2)C2C(CC1)(C1C(O2)CC(=C1C)CCC(CO)C)C)C
MOL004541	0.7358	0.2642	0.8196	Anemarrhenae Rhizoma	Anemarsaponin E	Not Available	FALSE	O(C1C(OC(C(C1O)O)CO)OC1CC2C(CC1)(C1C(CC2)C2C(CC1)(C1C(C2)OC(C1C)(CCC(COC1OC(C(C(C1O)O)O)CO)C)OC)C)C)C1OC(C(C(C1O)O)O)CO
MOL004542	0.2453	0.7547	0.7378	Anemarrhenae Rhizoma	Anemarsaponin E_qt	Not Available	FALSE	OC1CC2C(CC1)(C1C(CC2)C2C(CC1)(C1C(C2)OC(C1C)(CCC(CO)C)OC)C)C
MOL004543	0.7411	0.2589	0.8486	Boehmeriae Rhizoma Et Radix	Anemosapogenin	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=C)C)C(=O)O)C)C)(C)CO)O
MOL004544	0.9313	0.0687	0.9526	Boehmeriae Rhizoma Et Radix	Quinic acid	37439	FALSE	C1(C(C(CC(C1)(O)C(=O)O)O)O)O
MOL004549	0.9517	0.0483	0.9219	Boehmeriae Rhizoma Et Radix	M-COUMARIC ACID	637541	FALSE	C(=O)(/C=C/c1cc(ccc1)O)O
MOL004549	0.9517	0.0483	0.9219	Hordei Fructus Germinatus	M-COUMARIC ACID	637541	FALSE	C(=O)(/C=C/c1cc(ccc1)O)O
MOL004550	0.7612	0.2388	0.8406	Potentillae Chinensis Herba	Pomolic acid	382831	FALSE	OC1(C2C3=CCC4C(C3(CCC2(CCC1C)C(=O)O)C)(CCC1C4(CCC(O)C1(C)C)C)C)C

MOL004550	0.7612	0.2388	0.8406	Eriobotryae Folium	Pomolic acid	382831	FALSE	OC1(C2C3=CCC4C(C3(CCC2(CCC1C)C(=O)O)C)(CCC1C4(CCC(O)C1(C)C)C)C)C
MOL004550	0.7612	0.2388	0.8406	Potentillae Discoloris Herba	Pomolic acid	382831	FALSE	OC1(C2C3=CCC4C(C3(CCC2(CCC1C)C(=O)O)C)(CCC1C4(CCC(O)C1(C)C)C)C)C
MOL004550	0.7612	0.2388	0.8406	Radix Sanguisorbae	Pomolic acid	382831	FALSE	OC1(C2C3=CCC4C(C3(CCC2(CCC1C)C(=O)O)C)(CCC1C4(CCC(O)C1(C)C)C)C)C
MOL004550	0.7612	0.2388	0.8406	Uncariae Ramulus Cumuncis	Pomolic acid	382831	FALSE	OC1(C2C3=CCC4C(C3(CCC2(CCC1C)C(=O)O)C)(CCC1C4(CCC(O)C1(C)C)C)C)C
MOL004550	0.7612	0.2388	0.8406	Rosae Laevigatae Fructus	Pomolic acid	382831	FALSE	OC1(C2C3=CCC4C(C3(CCC2(CCC1C)C(=O)O)C)(CCC1C4(CCC(O)C1(C)C)C)C)C
MOL004550	0.7612	0.2388	0.8406	Ilicis Purpureae Folium	Pomolic acid	382831	FALSE	OC1(C2C3=CCC4C(C3(CCC2(CCC1C)C(=O)O)C)(CCC1C4(CCC(O)C1(C)C)C)C)C
MOL004550	0.7612	0.2388	0.8406	Boehmeriae Rhizoma Et Radix	Pomolic acid	382831	FALSE	OC1(C2C3=CCC4C(C3(CCC2(CCC1C)C(=O)O)C)(CCC1C4(CCC(O)C1(C)C)C)C)C
MOL004551	0.8521	0.1479	0.7960	Boehmeriae Rhizoma Et Radix	BB_NC-1760	10178463	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)c1cc(cc(c1)/C=C\c1ccc(cc1)O)O
MOL004552	0.4571	0.5429	0.8046	Gardeniae Fructus	Isoimperatorin	Not Available	FALSE	C1(=C)C=Cc2c(O1)cc1c(c2OCC=C(C)C)C=CC1
MOL004553	0.9380	0.0620	0.8491	Gardeniae Fructus	Gardenone	Not Available	FALSE	C1C(=O)CC2C(C1(C)C)COC(C2)OCC
MOL004554	0.8993	0.1007	0.7916	Gardeniae Fructus	GARDENOSIDE	Not Available	FALSE	C1(C(OC(C(C1O)O)OC1OCC(C2C1C(=CCC2)CO)C(=O)OC)CO)O
MOL004555	0.9318	0.0682	0.8451	Gardeniae Fructus	GARDENOSIDE_qt	Not Available	FALSE	OC1OCC(C2C1C(=CCC2)CO)C(=O)OC
MOL004556	0.6188	0.3812	0.7566	Gardeniae Fructus	crocin	5281233	FALSE	O1C(OCC2OC(OC(=O)/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C(=O)OC3OC(C(O)C(O)C3O)COC3OC(C(O)C(O)C3O)CO)\C)\C)/C)/C)C(O)C(O)C2O)C(O)C(O)C(O)C1CO
MOL004557	0.9113	0.0887	0.8440	Figwort Root	geniposide	107848	FALSE	C1(C(OC(C(C1O)O)OC1OC=C(C2C1C(=CC2)CO)C(=O)OC)CO)O
MOL004557	0.9113	0.0887	0.8440	Gardeniae Fructus	geniposide	107848	FALSE	C1(C(OC(C(C1O)O)OC1OC=C(C2C1C(=CC2)CO)C(=O)OC)CO)O
MOL004557	0.9113	0.0887	0.8440	Paederiae Scandentis Herba	geniposide	107848	FALSE	C1(C(OC(C(C1O)O)OC1OC=C(C2C1C(=CC2)CO)C(=O)OC)CO)O
MOL004557	0.9113	0.0887	0.8440	Plantaginis Semen	geniposide	107848	FALSE	C1(C(OC(C(C1O)O)OC1OC=C(C2C1C(=CC2)CO)C(=O)OC)CO)O
MOL004557	0.9113	0.0887	0.8440	Eucommiae Cortex	geniposide	107848	FALSE	C1(C(OC(C(C1O)O)OC1OC=C(C2C1C(=CC2)CO)C(=O)OC)CO)O
MOL004557	0.9113	0.0887	0.8440	Hedyotis Diffusae Herba	geniposide	107848	FALSE	C1(C(OC(C(C1O)O)OC1OC=C(C2C1C(=CC2)CO)C(=O)OC)CO)O

MOL004559	0.9160	0.0840	0.8659	Gardeniae Fructus	(1S,4aS,5R,7S,7aS)-5,7-dihydroxy-7-methyl-1-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4a,5,6,7a-tetrahydro-1H-cyclopenta[d]pyran-4-carboxylic acid	11948668	FALSE	OC1(C2C(C(O)C1)C(=COC2OC1OC(C(O)C(O)C1O)CO)C(=O)O)C
MOL004560	0.9469	0.0531	0.8307	Gardeniae Fructus	SHANZHISIDE_qt	Not Available	FALSE	OC1(C2C(C(O)C1)C(=COC2O)C(=O)O)C
MOL004562	0.7218	0.2782	0.8071	Smilax China	methylprotogracillin	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(=CC4)CC(OC4OC(C(O)C(OC6OC(C(O)C(O)C6O)CO)C4OC4OC(C(O)C(O)C4O)C)CO)CC5)C)CC3)C2)C)C(C1(OC)CCC(COC1OC(C(O)C(O)C1O)CO)C)C
MOL004563	0.2233	0.7767	0.7590	Smilax China	methylprotogracillin_qt	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(=CC4)CC(O)CC5)C)CC3)C2)C)C(C1(OC)CCC(CO)C)C
MOL004564	0.9206	0.0794	0.8973	Smilax China	Kaempferid	5281666	TRUE	o1c2c(c(=O)c(O)c1c1ccc(OC)cc1)c(O)cc(O)c2
MOL004564	0.9206	0.0794	0.8973	Tamaricis Cacumen	Kaempferid	5281666	TRUE	o1c2c(c(=O)c(O)c1c1ccc(OC)cc1)c(O)cc(O)c2
MOL004564	0.9206	0.0794	0.8973	Astragali Cpmplanatisemen	Kaempferid	5281666	TRUE	o1c2c(c(=O)c(O)c1c1ccc(OC)cc1)c(O)cc(O)c2
MOL004564	0.9206	0.0794	0.8973	Kaempferiae Rhizoma	Kaempferid	5281666	TRUE	o1c2c(c(=O)c(O)c1c1ccc(OC)cc1)c(O)cc(O)c2
MOL004564	0.9206	0.0794	0.8973	Capsellae Herba	Kaempferid	5281666	TRUE	o1c2c(c(=O)c(O)c1c1ccc(OC)cc1)c(O)cc(O)c2
MOL004566	0.7505	0.2495	0.8070	Smilax China	pseudoprotodioscin	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(=CC4)CC(OC4OC(C(OC6OC(C(O)C(O)C6O)C)C(O)C4OC4OC(C(O)C(O)C4O)C)CO)CC5)C)CC3)C2)C)C(=C1CCC(COC1OC(C(O)C(O)C1O)CO)C)C
MOL004567	0.8829	0.1171	0.8398	Smilacis Glabrae Rhixoma	isoengelitin	Not Available	FALSE	O1C(OC2C(Oc3c(C2=O)c(O)cc(O)c3)c2ccc(O)cc2)C(O)C(O)C(O)C1C
MOL004567	0.8829	0.1171	0.8398	Smilax China	isoengelitin	Not Available	FALSE	O1C(OC2C(Oc3c(C2=O)c(O)cc(O)c3)c2ccc(O)cc2)C(O)C(O)C(O)C1C
MOL004568	0.8829	0.1171	0.8398	Herba Sarcandrae	Engelitin	6453452	FALSE	c1(cc(c2c(c1)OC(C(C2=O)OC1C(C(C(C(O1)C)O)O)O)c1ccc(cc1)O)O)O
MOL004568	0.8829	0.1171	0.8398	Smilax China	Engelitin	6453452	FALSE	c1(cc(c2c(c1)OC(C(C2=O)OC1C(C(C(C(O1)C)O)O)O)c1ccc(cc1)O)O)O

MOL004569	0.9230	0.0770	0.8944	Hoveniae Dulcis Semen	Aromadedrin	122850	FALSE	c1(cc(c2c(c1)OC(C(C2=O)O)c1ccc(cc1)O)O)O
MOL004569	0.9230	0.0770	0.8944	Polygoni Orientalis Fructus	Aromadedrin	122850	FALSE	c1(cc(c2c(c1)OC(C(C2=O)O)c1ccc(cc1)O)O)O
MOL004569	0.9230	0.0770	0.8944	Gossampiniflos	Aromadedrin	122850	FALSE	c1(cc(c2c(c1)OC(C(C2=O)O)c1ccc(cc1)O)O)O
MOL004569	0.9230	0.0770	0.8944	Smilacis Glabrae Rhixoma	Aromadedrin	122850	FALSE	c1(cc(c2c(c1)OC(C(C2=O)O)c1ccc(cc1)O)O)O
MOL004569	0.9230	0.0770	0.8944	Ephedrae Radix Et Rhizoma	Aromadedrin	122850	FALSE	c1(cc(c2c(c1)OC(C(C2=O)O)c1ccc(cc1)O)O)O
MOL004569	0.9230	0.0770	0.8944	Smilax China	Aromadedrin	122850	FALSE	c1(cc(c2c(c1)OC(C(C2=O)O)c1ccc(cc1)O)O)O
MOL004570	0.9180	0.0820	0.8493	Polygoni Cuspidati Rhizoma Et Radix	5-[(Z)-2-(3,4-dihydroxyphenyl)vinyl]resorcinol	6603962	FALSE	c1(c(ccc(c1)/C=C\c1cc(cc(c1)O)O)O)O
MOL004570	0.9180	0.0820	0.8493	Smilax China	5-[(Z)-2-(3,4-dihydroxyphenyl)vinyl]resorcinol	6603962	FALSE	c1(c(ccc(c1)/C=C\c1cc(cc(c1)O)O)O)O
MOL004571	0.9137	0.0863	0.8009	Smilax China	(2R,3S)-2-(3,5-dihydroxyphenyl)chroman-3,5,7-triol	Not Available	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1cc(cc(c1)O)O)O)O
MOL004572	0.8829	0.1171	0.8398	Smilacis Glabrae Rhixoma	engeletin	Not Available	FALSE	O1C(OC2C(Oc3c(C2=O)c(O)cc(O)c3)c2ccc(O)cc2)C(O)C(O)C(O)C1C
MOL004572	0.8829	0.1171	0.8398	Smilax China	engeletin	Not Available	FALSE	O1C(OC2C(Oc3c(C2=O)c(O)cc(O)c3)c2ccc(O)cc2)C(O)C(O)C(O)C1C
MOL004573	0.9470	0.0530	0.7029	Smilax China	Gramin	6890	TRUE	c1ccc2c(c1)[nH]cc2CN(C)C
MOL004573	0.9470	0.0530	0.7029	Dioscoreae Septemlo Bae Rhizoma	Gramin	6890	TRUE	c1ccc2c(c1)[nH]cc2CN(C)C
MOL004574	0.9569	0.0431	0.8267	Smilax China	Moracin M	185848	FALSE	c1c(cc2c(c1)cc(o2)c1cc(cc(c1)O)O)O
MOL004574	0.9569	0.0431	0.8267	Mori Cortex	Moracin M	185848	FALSE	c1c(cc2c(c1)cc(o2)c1cc(cc(c1)O)O)O
MOL004575	0.9114	0.0886	0.8248	Smilax China	astilbin	119258	FALSE	O1C(OC2C(Oc3c(C2=O)c(O)cc(O)c3)c2cc(O)c(O)cc2)C(O)C(O)C(O)C1C
MOL004575	0.9114	0.0886	0.8248	Smilacis Glabrae Rhixoma	astilbin	119258	FALSE	O1C(OC2C(Oc3c(C2=O)c(O)cc(O)c3)c2cc(O)c(O)cc2)C(O)C(O)C(O)C1C
MOL004576	0.9461	0.0539	0.9148	Smilax China	taxifolin	439533	FALSE	OC1C(Oc2c(C1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1
MOL004576	0.9461	0.0539	0.9148	Fructus Ligustri Lucidi	taxifolin	439533	FALSE	OC1C(Oc2c(C1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1
MOL004576	0.9461	0.0539	0.9148	Polygoni Orientalis Fructus	taxifolin	439533	FALSE	OC1C(Oc2c(C1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1
MOL004576	0.9461	0.0539	0.9148	Ephedrae Radix Et Rhizoma	taxifolin	439533	FALSE	OC1C(Oc2c(C1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1
MOL004576	0.9461	0.0539	0.9148	Smilacis Glabrae Rhixoma	taxifolin	439533	FALSE	OC1C(Oc2c(C1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1
MOL004577	0.5466	0.4534	0.7939	Smilax China	maackoline	Not Available	FALSE	c1c(c(cc(c1)C1OCC2C1c1c(C2c2cc(c(c(c2)OC)O)OC)c(cc(c1)O)O)O)O

MOL004579	0.8976	0.1024	0.8970	Smilax China	dihydrokaempferide	Not Available	FALSE	O1C(C(O)C(=O)c2c1cc(O)cc2O)c1ccc(OC)cc1
MOL004579	0.8976	0.1024	0.8970	Iridis Tectori Rhizoma	dihydrokaempferide	Not Available	FALSE	O1C(C(O)C(=O)c2c1cc(O)cc2O)c1ccc(OC)cc1
MOL004580	0.9461	0.0539	0.9148	Sophorae Flavescentis Radix	cis-Dihydroquercetin	443758	FALSE	c12c(OC(C(C1=O)O)c1cc(c(cc1)O)O)cc(cc2O)O
MOL004580	0.9461	0.0539	0.9148	Smilacis Glabrae Rhixoma	cis-Dihydroquercetin	443758	FALSE	c12c(OC(C(C1=O)O)c1cc(c(cc1)O)O)cc(cc2O)O
MOL004580	0.9461	0.0539	0.9148	Smilax China	cis-Dihydroquercetin	443758	FALSE	c12c(OC(C(C1=O)O)c1cc(c(cc1)O)O)cc(cc2O)O
MOL004580	0.9461	0.0539	0.9148	Platycodon Grandiforus	cis-Dihydroquercetin	443758	FALSE	c12c(OC(C(C1=O)O)c1cc(c(cc1)O)O)cc(cc2O)O
MOL004581	0.9556	0.0444	0.8111	Nardostachyos Radix Et Rhizoma	[(1R,5S)-7,7-dimethyl-4-bicyclo[3.1.1]hept-3-enyl]methyl acetate	11435490	FALSE	C12CC(CC=C1COC(=O)C)C2(C)C
MOL004581	0.9556	0.0444	0.8111	Radix Bupleuri	[(1R,5S)-7,7-dimethyl-4-bicyclo[3.1.1]hept-3-enyl]methyl acetate	11435490	FALSE	C12CC(CC=C1COC(=O)C)C2(C)C
MOL004581	0.9556	0.0444	0.8111	Coriandri Sativi Herba	[(1R,5S)-7,7-dimethyl-4-bicyclo[3.1.1]hept-3-enyl]methyl acetate	11435490	FALSE	C12CC(CC=C1COC(=O)C)C2(C)C
MOL004581	0.9556	0.0444	0.8111	A. Dahurica (Fisch.) Benth. Et Hook	[(1R,5S)-7,7-dimethyl-4-bicyclo[3.1.1]hept-3-enyl]methyl acetate	11435490	FALSE	C12CC(CC=C1COC(=O)C)C2(C)C
MOL004582	0.9193	0.0807	0.6927	Radix Bupleuri	Methyl naphthalene	7002	FALSE	c12c(cccc1C)cccc2

MOL004582	0.9193	0.0807	0.6927	Ginkgo Folium	Methyl naphthalene	7002	FALSE	c12c(cccc1C)cccc2
MOL004582	0.9193	0.0807	0.6927	Codonopsis Radix	Methyl naphthalene	7002	FALSE	c12c(cccc1C)cccc2
MOL004582	0.9193	0.0807	0.6927	Gossampiniflos	Methyl naphthalene	7002	FALSE	c12c(cccc1C)cccc2
MOL004582	0.9193	0.0807	0.6927	Radix Cynanchi Paniculati	Methyl naphthalene	7002	FALSE	c12c(cccc1C)cccc2
MOL004582	0.9193	0.0807	0.6927	Pollen Typhae	Methyl naphthalene	7002	FALSE	c12c(cccc1C)cccc2
MOL004582	0.9193	0.0807	0.6927	Ranunculi Ternati Radix	Methyl naphthalene	7002	FALSE	c12c(cccc1C)cccc2
MOL004582	0.9193	0.0807	0.6927	Gnaphalii Affinis Herba	Methyl naphthalene	7002	FALSE	c12c(cccc1C)cccc2
MOL004582	0.9193	0.0807	0.6927	Achyranthis Asperae Herba	Methyl naphthalene	7002	FALSE	c12c(cccc1C)cccc2
MOL004582	0.9193	0.0807	0.6927	Cornus Officinalis Sieb. Et Zucc.	Methyl naphthalene	7002	FALSE	c12c(cccc1C)cccc2
MOL004583	0.7414	0.2586	0.8453	Radix Bupleuri	11α-methoxysaikosaponin f	Not Available	FALSE	O(C1C2C(C3(C(=C1)C1C(C(O)C3)(CCCC1)CO)C)(CCC1C2(CCC(OC2OC(C(OC3OC(C(O)C(O)C3O)C)C(O)C2O)COC2OC(C(O)C(O)C2O)CO)C1(C)C)C)C)C
MOL004584	0.3920	0.6080	0.7136	Radix Bupleuri	11α-methoxysaikosaponin f_qt	Not Available	FALSE	O(C1C=C2C(C3(C1C1(C(CC3)C(C(O)CC1)(C)C)C)C)(CC(O)C1(C2CCCC1)CO)C)C
MOL004585	0.8907	0.1093	0.8630	Radix Bupleuri	2,4-Dodecadienal	5367530	FALSE	C(CCCCCC)/C=C/C=C/C=O
MOL004585	0.8907	0.1093	0.8630	Mahoniae Folum	2,4-Dodecadienal	5367530	FALSE	C(CCCCCC)/C=C/C=C/C=O
MOL004586	0.9208	0.0792	0.9224	Radix Bupleuri	trans,trans-nona-2,4-dienol	5364586	FALSE	OC/C=C/C=C/CCCC
MOL004587	0.9184	0.0816	0.9509	Radix Bupleuri	Heptenoic acid	5282709	FALSE	OC(=O)/C=C/CCCC
MOL004587	0.9184	0.0816	0.9509	Astragali Cpmplanatisemen	Heptenoic acid	5282709	FALSE	OC(=O)/C=C/CCCC
MOL004588	0.8767	0.1233	0.9691	Radix Bupleuri	(2R)-2-methylcyclopentan-1-one	642552	FALSE	O=C1C(CCC1)C
MOL004589	0.9243	0.0757	0.9242	Herbahypericiperforati	Methylheptane	11594	FALSE	C(C(C)C)CCCC
MOL004589	0.9243	0.0757	0.9242	Rose Rugosae Flos	Methylheptane	11594	FALSE	C(C(C)C)CCCC

MOL004589	0.9243	0.0757	0.9242	Radix Bupleuri	Methylheptane	11594	FALSE	C(C(C)C)CCCC
MOL004589	0.9243	0.0757	0.9242	Sesami Nigrum Semen	Methylheptane	11594	FALSE	C(C(C)C)CCCC
MOL004589	0.9243	0.0757	0.9242	Eucommiae Folium	Methylheptane	11594	FALSE	C(C(C)C)CCCC
MOL004589	0.9243	0.0757	0.9242	licorice	Methylheptane	11594	FALSE	C(C(C)C)CCCC
MOL004591	0.9250	0.0750	0.9400	Radix Bupleuri	Nonenoic acid	5312586	FALSE	OC(=O)/C=C/CCCCCC
MOL004591	0.9250	0.0750	0.9400	Capsici Fructus	Nonenoic acid	5312586	FALSE	OC(=O)/C=C/CCCCCC
MOL004592	0.9200	0.0800	0.9494	Radix Bupleuri	2-Octenoic acid	5282714	FALSE	OC(=O)/C=C/CCCCC
MOL004592	0.9200	0.0800	0.9494	Schizonepetae Herba	2-Octenoic acid	5282714	FALSE	OC(=O)/C=C/CCCCC
MOL004593	0.6300	0.3700	0.8381	Radix Bupleuri	3'-O-Acetylsaikosaponin D	Not Available	FALSE	O1C23C(C4(C(C5(C(CC4)C(C(OC4OC(C(O)C(OC6OC(C(O)C(OC(=O)C)C6O)CO)C4O)C)CC5)(CO)C)C)C=C3)C)(CC(O)C3(C2CC(CC3)(C)C)C1)C
MOL004594	0.4807	0.5193	0.7893	Radix Bupleuri	3'-O-Acetylsaikosaponin D_qt	Not Available	FALSE	O1C23C(C4(C(C=C3)C3(C(CC4)C(C(O)CC3)(CO)C)C)C)(CC(O)C3(C2CC(C)(CC3)C)C1)C
MOL004595	0.6250	0.3750	0.8474	Radix Bupleuri	3',6'-O,O-diacetylsaikosaponin b2	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=C5C(C(O)C4)(CCC(C5)(C)C)CO)C=C3)C)(CC2)C)(CC1)C)(CO)C)C1OC(C(O)C(OC2OC(C(O)C(OC(=O)C)C2O)COC(=O)C)C1O)C
MOL004596	0.4733	0.5267	0.7713	Radix Bupleuri	3',6'-O,O-diacetylsaikosaponin b2_qt	Not Available	FALSE	OC1C(C2C(C3C=CC4=C5C(C(O)CC4(C3(CC2)C)C)(CCC(C)(C5)C)CO)(CC1)C)(CO)C
MOL004597	0.6463	0.3537	0.8537	Radix Bupleuri	3'-O-acetylsaikosaponin b2	Not Available	FALSE	C(=O)(C)OC1C(C(OC(C1O)CO)OC1C(C(OC(C1O)C)OC1CCC2(C(C1(C)CO)CCC1(C3(CC(C4(CCC(CC4C3=CCC21)(C)C)CO)O)C)C)C)O)O
MOL004598	0.6490	0.3510	0.6178	Radix Bupleuri	3,5,6,7-tetramethoxy-2-(3,4,5-trimethoxyphenyl)chromone	389001	FALSE	COc1c(OC)c(c2c(c1)oc(c(c2=O)OC)c1cc(c(c(c1)OC)OC)OC)OC
MOL004599	0.9313	0.0687	0.8949	Radix Bupleuri	3,3,5-trimethylheptane	Not Available	FALSE	C(CC(CC)C)(CC)(C)C
MOL004600	0.8693	0.1307	0.9086	Radix Bupleuri	FLAVONE,3,5,7-TRIHYDROXY-3,4-DIMETHOXY	5380905	FALSE	c1(c2cc(c(cc2)OC)O)c(c(=O)c2c(o1)cc(cc2O)O)OC

MOL004601	0.9232	0.0768	0.9342	Radix Bupleuri	ZINC01716732	6994762	FALSE	C(CCCC(C)C)(CC)(C)O
MOL004602	0.7907	0.2093	0.6856	Radix Bupleuri	(3R)-3-methylcyclotridecan-1-one	12002600	FALSE	C1CCCC(=O)CC(CCCCCC1)C
MOL004603	0.9071	0.0929	0.9065	Radix Bupleuri	3-ETHYL-2-METHYL-1,3-HEXADIENE	5365710	FALSE	C(=C\CC)(\CC)/C(=C)C
MOL004604	0.9380	0.0620	0.9525	Radix Bupleuri	Heptan-3-on	7802	FALSE	CCCCC(=O)CC
MOL004605	0.8740	0.1260	0.7099	Radix Bupleuri	3-methyldodecane	Not Available	FALSE	C(CCCCCCCCC)(CC)C
MOL004606	0.7665	0.2335	0.6003	Radix Bupleuri	4,8-dimethyltridecane	Not Available	FALSE	C(CCCC(CCC)C)(CCCCC)C
MOL004606	0.7665	0.2335	0.6003	Hippophae Fructus	4,8-dimethyltridecane	Not Available	FALSE	C(CCCC(CCC)C)(CCCCC)C
MOL004607	0.9283	0.0717	0.9522	Radix Bupleuri	ZINC03860615	7057966	FALSE	C(C(CC)O)(CCC)C
MOL004608	0.9322	0.0678	0.9670	Schisandrae Chinensis Fructus	(5S)-5-butyloxolan-2-one	7057972	FALSE	O1C(CCCC)CCC1=O
MOL004608	0.9322	0.0678	0.9670	Radix Bupleuri	(5S)-5-butyloxolan-2-one	7057972	FALSE	O1C(CCCC)CCC1=O
MOL004609	0.8353	0.1647	0.8147	Artemisia Annua L.	Areapillin	158311	FALSE	o1c2c(c(O)c(OC)c(OC)c2)c(=O)cc1c1c(O)cc(O)c(OC)c1
MOL004609	0.8353	0.1647	0.8147	Artemisiae Scopariae Herba	Areapillin	158311	FALSE	o1c2c(c(O)c(OC)c(OC)c2)c(=O)cc1c1c(O)cc(O)c(OC)c1
MOL004609	0.8353	0.1647	0.8147	Radix Bupleuri	Areapillin	158311	FALSE	o1c2c(c(O)c(OC)c(OC)c2)c(=O)cc1c1c(O)cc(O)c(OC)c1
MOL004610	0.9285	0.0715	0.9483	Morindae Officinalis Radix	gamma-Undecalactone	441644	FALSE	O1C(CCCCCCC)CCC1=O
MOL004610	0.9285	0.0715	0.9483	Radix Bupleuri	gamma-Undecalactone	441644	FALSE	O1C(CCCCCCC)CCC1=O
MOL004611	0.9033	0.0967	0.7199	Radix Bupleuri	5-methyl-5-ethyldecane	Not Available	FALSE	C(CCCCC)(CCCC)(CC)C
MOL004612	0.8991	0.1009	0.8512	Radix Bupleuri	5-methyldecane	Not Available	FALSE	C(CCCCC)(CCCC)C
MOL004613	0.2371	0.7629	0.7492	Radix Bupleuri	6,7,3',8'-diligustilide	Not Available	FALSE	C1(=O)OC2(C3=C1C=CCC3)C1C(CCC3=C1C(=O)O/C/3=C/CCC)C2CCC

MOL004613	0.2371	0.7629	0.7492	Angelicae Sinensis Radix	6,7,3',8'-diligustilide	Not Available	FALSE	C1(=O)OC2(C3=C1C=CCC3)C1C(CCC3=C1C(=O)O/C/3=C/CCC)C2CCC
MOL004614	0.9699	0.0301	0.8114	Radix Bupleuri	Fraxidin Methyl Ether	3083928	FALSE	o1c2c(cc(OC)c(OC)c2OC)ccc1=O
MOL004615	0.8092	0.1908	0.6916	Radix Bupleuri	6-O-Vanilloylajugol	Not Available	FALSE	c1(ccc(cc1OC)C(=O)OC1CC(C2C1C=COC2OC1OC(C(C(C1O)O)O)CO)(O)C)O
MOL004616	0.9316	0.0684	0.9497	Radix Bupleuri	7-Octen-4-ol	Not Available	FALSE	C(CC(CCC=C)O)C
MOL004617	0.9607	0.0393	0.8491	Citri Sarcodactylis Fructus	Ayapanin	10748	FALSE	o1c2c(ccc(OC)c2)ccc1=O
MOL004617	0.9607	0.0393	0.8491	Artemisiae Scopariae Herba	Ayapanin	10748	FALSE	o1c2c(ccc(OC)c2)ccc1=O
MOL004617	0.9607	0.0393	0.8491	Siphonostegiae Herba	Ayapanin	10748	FALSE	o1c2c(ccc(OC)c2)ccc1=O
MOL004617	0.9607	0.0393	0.8491	Radix Bupleuri	Ayapanin	10748	FALSE	o1c2c(ccc(OC)c2)ccc1=O
MOL004617	0.9607	0.0393	0.8491	Folium Artemisiae Argyi	Ayapanin	10748	FALSE	o1c2c(ccc(OC)c2)ccc1=O
MOL004617	0.9607	0.0393	0.8491	Puerariae Flos	Ayapanin	10748	FALSE	o1c2c(ccc(OC)c2)ccc1=O
MOL004617	0.9607	0.0393	0.8491	Zanthoxyli Pericarpium	Ayapanin	10748	FALSE	o1c2c(ccc(OC)c2)ccc1=O
MOL004618	0.8242	0.1758	0.6432	Radix Bupleuri	7-Methyltridecane	33588	FALSE	C(CCCCCC)(CCCCCC)C
MOL004619	0.9213	0.0787	0.9445	Radix Bupleuri	8-NONENOIC ACID	35860	FALSE	C(=C)CCCCCCC(=O)O
MOL004620	0.9273	0.0727	0.9000	Radix Bupleuri	Ara-Furan-A	453548	FALSE	O1C(n2c3ncnc(N)c3nc2)C(O)C(O)C1CO
MOL004621	0.9412	0.0588	0.9665	Radix Bupleuri	Adonitol	6912	FALSE	OCC(O)C(O)C(O)CO
MOL004621	0.9412	0.0588	0.9665	Capsellae Herba	Adonitol	6912	FALSE	OCC(O)C(O)C(O)CO
MOL004623	0.9315	0.0685	0.9526	Panacis Quinquefolii Radix	Encecalin	114703	FALSE	c1(c(cc2c(c1)C=CC(O2)(C)C)OC)C(=O)C
MOL004623	0.9315	0.0685	0.9526	Radix Bupleuri	Encecalin	114703	FALSE	c1(c(cc2c(c1)C=CC(O2)(C)C)OC)C(=O)C
MOL004623	0.9315	0.0685	0.9526	Codonopsis Radix	Encecalin	114703	FALSE	c1(c(cc2c(c1)C=CC(O2)(C)C)OC)C(=O)C
MOL004624	0.7902	0.2098	0.8818	Schisandrae Chinensis Fructus	Longikaurin A	Not Available	FALSE	C123C(C(C(C45C1CCC(C4O)C(=C)C5=O)(OC3)O)O)C(CCC2)(C)C
MOL004624	0.7902	0.2098	0.8818	Radix Bupleuri	Longikaurin A	Not Available	FALSE	C123C(C(C(C45C1CCC(C4O)C(=C)C5=O)(OC3)O)O)C(CCC2)(C)C
MOL004625	0.7315	0.2685	0.7230	Radix Bupleuri	Longispinogenin 3-O-beta-D-glucuronopyranoside	Not Available	FALSE	O1C(C(C(C(C1OC1C(C2C(CC1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)CO)C)C)C)(C)C)O)O)O)C(=O)O
MOL004626	0.4206	0.5794	0.8041	Radix Bupleuri	Longispinogenin	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)CO)C)C)C)(C)C)O
MOL004626	0.4206	0.5794	0.8041	Schisandrae Chinensis Fructus	Longispinogenin	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)CO)C)C)C)(C)C)O
MOL004627	0.9406	0.0594	0.9621	Radix Bupleuri	Methyl hexoate	7824	FALSE	CCCCCC(=O)OC

MOL004627	0.9406	0.0594	0.9621	Hoveniae Dulcis Semen	Methyl hexoate	7824	FALSE	CCCCCC(=O)OC
MOL004627	0.9406	0.0594	0.9621	Meliae Azedarach Fructus	Methyl hexoate	7824	FALSE	CCCCCC(=O)OC
MOL004627	0.9406	0.0594	0.9621	Puerariae Flos	Methyl hexoate	7824	FALSE	CCCCCC(=O)OC
MOL004627	0.9406	0.0594	0.9621	Perillae Fructus	Methyl hexoate	7824	FALSE	CCCCCC(=O)OC
MOL004629	0.9480	0.0520	0.9630	Paederiae Scandentis Herba	PAC	999	FALSE	c1cccc(c1)CC(=O)O
MOL004629	0.9480	0.0520	0.9630	Gossampiniflos	PAC	999	FALSE	c1cccc(c1)CC(=O)O
MOL004629	0.9480	0.0520	0.9630	Citrus Aurantium	PAC	999	FALSE	c1cccc(c1)CC(=O)O
MOL004629	0.9480	0.0520	0.9630	Radix Bupleuri	PAC	999	FALSE	c1cccc(c1)CC(=O)O
MOL004631	0.9159	0.0841	0.8310	Radix Puerariae	7,8,4'-Trihydroxyisoflavone	5466139	FALSE	c12c(c(=O)c(co2)c2ccc(cc2)O)ccc(c1O)O
MOL004631	0.9159	0.0841	0.8310	Radix Bupleuri	7,8,4'-Trihydroxyisoflavone	5466139	FALSE	c12c(c(=O)c(co2)c2ccc(cc2)O)ccc(c1O)O
MOL004632	0.7171	0.2829	0.8626	Radix Bupleuri	Pulsatillic acid	10672073	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=C)C)C(=O)O)C)C)(CO)C
MOL004632	0.7171	0.2829	0.8626	Panacis Quinquefolii Radix	Pulsatillic acid	10672073	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=C)C)C(=O)O)C)C)(CO)C
MOL004632	0.7171	0.2829	0.8626	Schizonepetae Herba	Pulsatillic acid	10672073	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=C)C)C(=O)O)C)C)(CO)C
MOL004633	0.4807	0.5193	0.7893	Radix Bupleuri	Saikogenin F	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C3(C=C1)C1C(C(C2)O)(CCC(C1)(C)C)CO3)C)C)C)(C)CO)O
MOL004634	0.4807	0.5193	0.7893	Radix Bupleuri	Saikogenin G	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C3(C=C1)C1C(C(C2)O)(CCC(C1)(C)C)CO3)C)C)C)(C)CO)O
MOL004635	0.6551	0.3449	0.8394	Radix Bupleuri	saikosaponin a	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C3(C=C1)C1C(C(C2)O)(CCC(C1)(C)C)CO3)C)C)C)(C)CO)OC1OC(C(C(C1O)OC1OC(C(C(C1O)O)O)CO)O)C
MOL004636	0.6775	0.3225	0.8444	Radix Bupleuri	Saikosaponin B	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=C3C(C(C2)O)(CCC(C3)(C)C)CO)C=C1)C)C)C)(CO)C)OC1OC(C(C(C1O)OC1OC(C(C(C1O)O)O)CO)O)C
MOL004637	0.6551	0.3449	0.8394	Radix Bupleuri	Saikosaponin D	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C3(C=C1)C1C(C(C2)O)(CCC(C1)(C)C)CO3)C)C)C)(C)CO)OC1OC(C(C(C1O)OC1OC(C(C(C1O)O)O)CO)O)C
MOL004638	0.7527	0.2473	0.8381	Radix Bupleuri	Saikosaponin K	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=C3C(C(C2)O)(CCC(C3)(C)C)CO)C=C1)C)C)C)(C)CO)OC1OC(C(C(C1O)OC1OC(C(C(C1OC1OCC(C(C1O)O)O)O)O)O)C

MOL004639	0.7697	0.2303	0.7814	Radix Bupleuri	Saikosaponin V	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=C3C(C(C2)O)(CCC(C3)(C(=O)OCC2C(C(C(C(O2)OCC(C(O)C(CO)O)O)O)O)O)C)CO)C=C1)C)C)(C)CO)OC1OC(C(C(C1O)OC1OC(C(C(C1O)O)O)O)CO)O)C
MOL004640	0.7799	0.2201	0.8433	Radix Bupleuri	Saikosaponin f	Not Available	FALSE	O1C(C(C(C(C1C)O)O)O)OC1C(C(C(OC1COC1OC(C(C(C1O)O)O)CO)OC1C(C2C(C3C(CC2)(C2(C(=CC3)C3C(C(C2)O)(CCC(C3)(C)C)CO)C)C)(CC1)C)(C)C)O)O
MOL004641	0.4206	0.5794	0.8041	Radix Bupleuri	(3S,4aS,6aR,6bS,8S,8aS,12aS,14aR,14bR)-4,4,6a,6b,11,11,14b-heptamethyl-8a-methylol-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydropicene-3,8-diol	9868802	FALSE	OC1C(C)(C2C(C)(C3CC=C4C(C3(CC2)C)(CC(O)C2(CO)CCC(C)(C)CC42)C)CC1)C
MOL004642	0.6496	0.3504	0.8535	Radix Bupleuri	Saikosaponin t	Not Available	FALSE	O(C1C2C(C3(C(=C1)C1C(C(O)C3)(CCC(C1)(C)C)CO)C)(CCC1C2(CCC(OC2(OC(C(OC3OC(C(O)C(O)C3O)CO)C2O)CO)CO)C1(C)C)C)C)C
MOL004643	0.3620	0.6380	0.8140	Radix Bupleuri	Saikosaponin t_qt	Not Available	FALSE	O(C1C=C2C(C3(CCC4C(C13)(CCC(O)C4(C)C)C)C)(CC(O)C1(C2CC(CC1)(C)C)CO)C)C
MOL004644	0.8447	0.1553	0.7107	Radix Bupleuri	Sainfuran	185034	FALSE	c1(c(cc2c(c1)cc(o2)c1c(cc(cc1)OC)O)OC)O
MOL004644	0.8447	0.1553	0.7107	Hedysari Radix	Sainfuran	185034	FALSE	c1(c(cc2c(c1)cc(o2)c1c(cc(cc1)OC)O)OC)O
MOL004646	0.8668	0.1332	0.8240	Radix Bupleuri	Thymonin	442662	FALSE	c1(c(c(c2c(c1OC)oc(cc2=O)c1cc(c(cc1)O)OC)O)O)O
MOL004647	0.9052	0.0948	0.8291	Tamaricis Cacumen	TDA	12530	FALSE	CCCCCCCCCCCCCC(=O)O
MOL004647	0.9052	0.0948	0.8291	Aloe	TDA	12530	FALSE	CCCCCCCCCCCCCC(=O)O
MOL004647	0.9052	0.0948	0.8291	Ginkgo Folium	TDA	12530	FALSE	CCCCCCCCCCCCCC(=O)O
MOL004647	0.9052	0.0948	0.8291	Ginseng Folium	TDA	12530	FALSE	CCCCCCCCCCCCCC(=O)O
MOL004647	0.9052	0.0948	0.8291	Arecae Semen	TDA	12530	FALSE	CCCCCCCCCCCCCC(=O)O
MOL004647	0.9052	0.0948	0.8291	Foeniculi Fructus	TDA	12530	FALSE	CCCCCCCCCCCCCC(=O)O
MOL004647	0.9052	0.0948	0.8291	Panax Ginseng C. A. Mey.	TDA	12530	FALSE	CCCCCCCCCCCCCC(=O)O
MOL004647	0.9052	0.0948	0.8291	Physochlainae Radix	TDA	12530	FALSE	CCCCCCCCCCCCCC(=O)O
MOL004647	0.9052	0.0948	0.8291	Ardisiae Japonicae Herba	TDA	12530	FALSE	CCCCCCCCCCCCCC(=O)O
MOL004647	0.9052	0.0948	0.8291	Radix Bupleuri	TDA	12530	FALSE	CCCCCCCCCCCCCC(=O)O
MOL004648	0.3140	0.6860	0.6830	Radix Bupleuri	Troxerutin	Not Available	FALSE	C(/C=C(/C)\C=C\C=C(\C)/C=C/C1=C(C)CCCC1(C)C)CC(O)(O)O

MOL004649	0.9341	0.0659	0.8962	Typhonii Rhizoma	1-[(2R,3R,4S,5S)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]pyrimidine-2,4-dione	7059437	FALSE	C1(n2c(=O)[nH]c(=O)cc2)OC(C(C1O)O)CO
MOL004649	0.9341	0.0659	0.8962	Tribulifructus	1-[(2R,3R,4S,5S)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]pyrimidine-2,4-dione	7059437	FALSE	C1(n2c(=O)[nH]c(=O)cc2)OC(C(C1O)O)CO
MOL004649	0.9341	0.0659	0.8962	Arum Ternatum Thunb.	1-[(2R,3R,4S,5S)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]pyrimidine-2,4-dione	7059437	FALSE	C1(n2c(=O)[nH]c(=O)cc2)OC(C(C1O)O)CO
MOL004649	0.9341	0.0659	0.8962	Ampelopsis Japonica	1-[(2R,3R,4S,5S)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]pyrimidine-2,4-dione	7059437	FALSE	C1(n2c(=O)[nH]c(=O)cc2)OC(C(C1O)O)CO
MOL004649	0.9341	0.0659	0.8962	Fritiliariae Irrhosae Bulbus	1-[(2R,3R,4S,5S)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]pyrimidine-2,4-dione	7059437	FALSE	C1(n2c(=O)[nH]c(=O)cc2)OC(C(C1O)O)CO

MOL004649	0.9341	0.0659	0.8962	Farfarae Flos	1-[(2R,3R,4S,5S)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]pyrimidine-2,4-dione	7059437	FALSE	C1(n2c(=O)[nH]c(=O)cc2)OC(C(C1O)O)CO
MOL004649	0.9341	0.0659	0.8962	Radix Bupleuri	1-[(2R,3R,4S,5S)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]pyrimidine-2,4-dione	7059437	FALSE	C1(n2c(=O)[nH]c(=O)cc2)OC(C(C1O)O)CO
MOL004650	0.9595	0.0405	0.8932	Caryophylliflos	Acetovanillin	61229	FALSE	c1(c(cc(cc1)C=O)OC)OC(=O)C
MOL004650	0.9595	0.0405	0.8932	Radix Bupleuri	Acetovanillin	61229	FALSE	c1(c(cc(cc1)C=O)OC)OC(=O)C
MOL004650	0.9595	0.0405	0.8932	Benzoinum	Acetovanillin	61229	FALSE	c1(c(cc(cc1)C=O)OC)OC(=O)C
MOL004651	0.9026	0.0974	0.8939	Radix Bupleuri	cis-2-Undecenal	6431019	FALSE	O=C/C=C\CCCCCCCC
MOL004654	0.9327	0.0673	0.9488	Radix Bupleuri	2-HEPTENOL	5318017	FALSE	CCCC/C=C/CO
MOL004655	0.9049	0.0951	0.7119	Radix Bupleuri	PHPH	7095	FALSE	c1(c2ccccc2)ccccc1
MOL004656	0.9597	0.0403	0.9791	Radix Bupleuri	(5R)-5-isopropyl-2-methyl-1-cyclohex-2-enone	10888107	FALSE	O=C1CC(C(C)C)CC=C1C
MOL004657	0.8035	0.1965	0.6474	Achyranthis Asperae Herba	caryophyllene oxide	Not Available	FALSE	O1C2(C1CCC(=C)C1C(C(C1)(C)C)CC2)C
MOL004657	0.8035	0.1965	0.6474	Verbenae Herb	caryophyllene oxide	Not Available	FALSE	O1C2(C1CCC(=C)C1C(C(C1)(C)C)CC2)C
MOL004657	0.8035	0.1965	0.6474	Radix Bupleuri	caryophyllene oxide	Not Available	FALSE	O1C2(C1CCC(=C)C1C(C(C1)(C)C)CC2)C
MOL004658	0.8871	0.1129	0.6169	Radix Bupleuri	cedrenol	Not Available	FALSE	C123C(C(C(C1)C(CC2)C)(C)C)C=CC3(C)O
MOL004659	0.7431	0.2569	0.8394	Radix Bupleuri	chikusaikoside II	Not Available	FALSE	O1C(C(C(C1C)O)O)OC1C(C(C(OC1COC1OC(C(C(C1O)O)O)CO)OC1C(C2C(C3C(C4(C5(OCC6(C5CC(CC6)(C)C)C(C4)O)C=C3)C)(CC2)C)(CC1)C)(CO)C)O)O
MOL004660	0.4807	0.5193	0.7893	Radix Bupleuri	chikusaikoside II_qt	Not Available	FALSE	OC1C(C2C(C)(C3C=CC45OCC6(C5CC(CC6)(C)C)C(CC4(C)C3(CC2)C)O)CC1)(CO)C

MOL004661	0.9198	0.0802	0.9211	Citri Sarcodactylis Fructus	[(3R)-3,7-dimethyloct-6-enyl] acetate	6708682	FALSE	O(CCC(CCC=C(C)C)C)C(=O)C
MOL004661	0.9198	0.0802	0.9211	Radix Bupleuri	[(3R)-3,7-dimethyloct-6-enyl] acetate	6708682	FALSE	O(CCC(CCC=C(C)C)C)C(=O)C
MOL004662	0.9364	0.0636	0.9811	Radix Bupleuri	Cyclohexyliso cyanate	18502	FALSE	C1(CCCCC1)N=C=O
MOL004663	0.9684	0.0316	0.8940	Radix Bupleuri	Vinylxylene	33936	FALSE	c1(c(cccc1C=C)C)C
MOL004664	0.9168	0.0832	0.9577	Radix Clematidis	heptanoic acid	8094	FALSE	CCCCCCC(=O)O
MOL004664	0.9168	0.0832	0.9577	Ephedra Herba	heptanoic acid	8094	FALSE	CCCCCCC(=O)O
MOL004664	0.9168	0.0832	0.9577	Codonopsis Radix	heptanoic acid	8094	FALSE	CCCCCCC(=O)O
MOL004664	0.9168	0.0832	0.9577	Radix Cynanchi Paniculati	heptanoic acid	8094	FALSE	CCCCCCC(=O)O
MOL004664	0.9168	0.0832	0.9577	Radix Bupleuri	heptanoic acid	8094	FALSE	CCCCCCC(=O)O
MOL004664	0.9168	0.0832	0.9577	Zanthoxyli Pericarpium	heptanoic acid	8094	FALSE	CCCCCCC(=O)O
MOL004664	0.9168	0.0832	0.9577	Radix Cynanchi	heptanoic acid	8094	FALSE	CCCCCCC(=O)O
MOL004664	0.9168	0.0832	0.9577	Panacis Quinquefolii Radix	heptanoic acid	8094	FALSE	CCCCCCC(=O)O
MOL004664	0.9168	0.0832	0.9577	Achyranthis Bidentatae Radix	heptanoic acid	8094	FALSE	CCCCCCC(=O)O
MOL004665	0.9207	0.0793	0.9199	Chebulae Fructus	Ethyl geranate	5317247	FALSE	O(C(=O)/C=C(/CCC=C(C)C)\C)CC
MOL004665	0.9207	0.0793	0.9199	Gossampiniflos	Ethyl geranate	5317247	FALSE	O(C(=O)/C=C(/CCC=C(C)C)\C)CC
MOL004665	0.9207	0.0793	0.9199	Radix Bupleuri	Ethyl geranate	5317247	FALSE	O(C(=O)/C=C(/CCC=C(C)C)\C)CC
MOL004665	0.9207	0.0793	0.9199	Rose Rugosae Flos	Ethyl geranate	5317247	FALSE	O(C(=O)/C=C(/CCC=C(C)C)\C)CC
MOL004665	0.9207	0.0793	0.9199	Fructus Carotae	Ethyl geranate	5317247	FALSE	O(C(=O)/C=C(/CCC=C(C)C)\C)CC
MOL004665	0.9207	0.0793	0.9199	Zanthoxyli Pericarpium	Ethyl geranate	5317247	FALSE	O(C(=O)/C=C(/CCC=C(C)C)\C)CC
MOL004665	0.9207	0.0793	0.9199	Citri Fructus	Ethyl geranate	5317247	FALSE	O(C(=O)/C=C(/CCC=C(C)C)\C)CC
MOL004666	0.9432	0.0568	0.9570	Chaenomeles Sinensis (Thouin) Koehne	Ethyl protocatechua te	77547	FALSE	c1(cc(c(cc1)O)O)C(=O)OCC
MOL004666	0.9432	0.0568	0.9570	Radix Bupleuri	Ethyl protocatechua te	77547	FALSE	c1(cc(c(cc1)O)O)C(=O)OCC

MOL004666	0.9432	0.0568	0.9570	Abri Herba	Ethyl protocatechuate	77547	FALSE	c1(cc(c(cc1)O)O)C(=O)OCC
MOL004667	0.9547	0.0453	0.8201	Semen Aesculi	fraxetin	5273569	FALSE	o1c2c(cc(OC)c(O)c2O)ccc1=O
MOL004667	0.9547	0.0453	0.8201	Actinidia Chinensis Planch	fraxetin	5273569	FALSE	o1c2c(cc(OC)c(O)c2O)ccc1=O
MOL004667	0.9547	0.0453	0.8201	Fraxini Cortex	fraxetin	5273569	FALSE	o1c2c(cc(OC)c(O)c2O)ccc1=O
MOL004667	0.9547	0.0453	0.8201	Radix Bupleuri	fraxetin	5273569	FALSE	o1c2c(cc(OC)c(O)c2O)ccc1=O
MOL004668	0.9388	0.0612	0.9616	Rhizoma Dioscoreae	GLB	439353	FALSE	O1C(C(O)C(O)C(O)C1O)CO
MOL004668	0.9388	0.0612	0.9616	Corayceps	GLB	439353	FALSE	O1C(C(O)C(O)C(O)C1O)CO
MOL004668	0.9388	0.0612	0.9616	Rosae Laevigatae Fructus	GLB	439353	FALSE	O1C(C(O)C(O)C(O)C1O)CO
MOL004668	0.9388	0.0612	0.9616	Radix Bupleuri	GLB	439353	FALSE	O1C(C(O)C(O)C(O)C1O)CO
MOL004670	0.9584	0.0416	0.8279	Radix Bupleuri	cis-pinocampheol	90350	FALSE	C12CC(C(C(C1(C)C)C2)C)O
MOL004671	0.9482	0.0518	0.9563	Radix Bupleuri	ISOPULEGOL	170833	FALSE	OC1C(CCC(C1)C)C(=C)C
MOL004673	0.8468	0.1532	0.8032	Radix Bupleuri	kaempferitrin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(=O)c2c(oc1c1ccc(O)cc1)cc(OC1OC(C(O)C(O)C1O)C)cc2O)C
MOL004673	0.8468	0.1532	0.8032	Momordicae Fructus	kaempferitrin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(=O)c2c(oc1c1ccc(O)cc1)cc(OC1OC(C(O)C(O)C1O)C)cc2O)C
MOL004673	0.8468	0.1532	0.8032	Ardisiae Japonicae Herba	kaempferitrin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(=O)c2c(oc1c1ccc(O)cc1)cc(OC1OC(C(O)C(O)C1O)C)cc2O)C
MOL004674	0.8468	0.1532	0.8032	Radix Bupleuri	kaempferol-3,7-α-L-dirhamnoside	Not Available	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC1C(O)C(O)C(O)C(O1)C)OC1C(O)C(O)C(O)C(O1)C)c1ccc(cc1)O
MOL004675	0.8574	0.1426	0.8126	Radix Bupleuri	kaempferol-7-O-rhamnoside	Not Available	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC1OC(C(C(C1O)O)O)C)O)c1ccc(cc1)O
MOL004675	0.8574	0.1426	0.8126	Cotyledon Fimbriata Turcz.	kaempferol-7-O-rhamnoside	Not Available	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC1OC(C(C(C1O)O)O)C)O)c1ccc(cc1)O
MOL004676	0.8574	0.1426	0.8126	Radix Bupleuri	kaempferol-7-O-α-L-rhamnoside	Not Available	FALSE	O1C(C(C(C(C1Oc1cc(c2c(c1)oc(c(c2=O)O)c1ccc(cc1)O)O)O)O)O)C
MOL004677	0.8608	0.1392	0.6197	Ardisiae Japonicae Herba	ledol	Not Available	FALSE	OC1(C2C(C3C(C3CC1)(C)C)C(CC2)C)C
MOL004677	0.8608	0.1392	0.6197	Radix Bupleuri	ledol	Not Available	FALSE	OC1(C2C(C3C(C3CC1)(C)C)C(CC2)C)C
MOL004678	0.9526	0.0474	0.8049	Citri Fructus	Limetin	2775	FALSE	c12c(cc(cc1OC)OC)oc(=O)cc2
MOL004678	0.9526	0.0474	0.8049	Lobeliae Chinensis Herba	Limetin	2775	FALSE	c12c(cc(cc1OC)OC)oc(=O)cc2
MOL004678	0.9526	0.0474	0.8049	Schisandrae Chinensis Fructus	Limetin	2775	FALSE	c12c(cc(cc1OC)OC)oc(=O)cc2
MOL004678	0.9526	0.0474	0.8049	Citri Sarcodactylis Fructus	Limetin	2775	FALSE	c12c(cc(cc1OC)OC)oc(=O)cc2
MOL004678	0.9526	0.0474	0.8049	Radix Bupleuri	Limetin	2775	FALSE	c12c(cc(cc1OC)OC)oc(=O)cc2
MOL004680	0.9598	0.0402	0.9671	Radix Bupleuri	cis-p-2-Menthen-1-ol	122485	FALSE	C1=CC(CCC1C(C)C)(C)O

MOL004681	0.9485	0.0515	0.9615	Radix Bupleuri	(6S)-6-pentyl-5,6-dihydropyran-2-one	404821	FALSE	O1C(CCCCC)CC=CC1=O
MOL004682	0.9365	0.0635	0.9498	Ephedra Herba	Methyl octylate	8091	FALSE	CCCCCCCC(=O)OC
MOL004682	0.9365	0.0635	0.9498	Panacis Quinquefolii Radix	Methyl octylate	8091	FALSE	CCCCCCCC(=O)OC
MOL004682	0.9365	0.0635	0.9498	Platycladi Semen	Methyl octylate	8091	FALSE	CCCCCCCC(=O)OC
MOL004682	0.9365	0.0635	0.9498	Impatientis Semen	Methyl octylate	8091	FALSE	CCCCCCCC(=O)OC
MOL004682	0.9365	0.0635	0.9498	Hoveniae Dulcis Semen	Methyl octylate	8091	FALSE	CCCCCCCC(=O)OC
MOL004682	0.9365	0.0635	0.9498	Radix Bupleuri	Methyl octylate	8091	FALSE	CCCCCCCC(=O)OC
MOL004682	0.9365	0.0635	0.9498	Calyx Seu Fructus Physalis	Methyl octylate	8091	FALSE	CCCCCCCC(=O)OC
MOL004682	0.9365	0.0635	0.9498	Broussonetiae Fructus	Methyl octylate	8091	FALSE	CCCCCCCC(=O)OC
MOL004682	0.9365	0.0635	0.9498	Trollius Chinensis	Methyl octylate	8091	FALSE	CCCCCCCC(=O)OC
MOL004682	0.9365	0.0635	0.9498	Perillae Fructus	Methyl octylate	8091	FALSE	CCCCCCCC(=O)OC
MOL004683	0.4813	0.5187	0.6197	Broussonetiae Fructus	methyl (2E,4E)-octadeca-2,4-dienoate	6442145	FALSE	O(C(=O)/C=C/C=C/CCCCCCCCCCCCC)C
MOL004683	0.4813	0.5187	0.6197	Radix Bupleuri	methyl (2E,4E)-octadeca-2,4-dienoate	6442145	FALSE	O(C(=O)/C=C/C=C/CCCCCCCCCCCCC)C
MOL004685	0.9267	0.0733	0.9292	Radix Bupleuri	(E)-non-2-en-4-one	448996	FALSE	C/C=C/C(=O)CCCCC
MOL004686	0.9240	0.0760	0.9271	Campsis Flos	Nonenone	5317045	FALSE	CC(=O)/C=C/CCCCC
MOL004686	0.9240	0.0760	0.9271	Radix Bupleuri	Nonenone	5317045	FALSE	CC(=O)/C=C/CCCCC
MOL004686	0.9240	0.0760	0.9271	Achyranthis Bidentatae Radix	Nonenone	5317045	FALSE	CC(=O)/C=C/CCCCC
MOL004687	0.9324	0.0676	0.9460	Rose Rugosae Flos	2-octanone	8093	FALSE	CCCCCCC(=O)C
MOL004687	0.9324	0.0676	0.9460	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	2-octanone	8093	FALSE	CCCCCCC(=O)C
MOL004687	0.9324	0.0676	0.9460	Radix Bupleuri	2-octanone	8093	FALSE	CCCCCCC(=O)C

MOL004688	0.9488	0.0512	0.9516	Perilla Frutescens	Cumic acid	10820	FALSE	C(=O)(c1ccc(cc1)C(C)C)O
MOL004688	0.9488	0.0512	0.9516	Radix Bupleuri	Cumic acid	10820	FALSE	C(=O)(c1ccc(cc1)C(C)C)O
MOL004688	0.9488	0.0512	0.9516	Ligustici Rhizoma Et Radix	Cumic acid	10820	FALSE	C(=O)(c1ccc(cc1)C(C)C)O
MOL004690	0.9464	0.0536	0.9717	Trichosanthes Kirilowii Maxim	RNS	19233	FALSE	OC(C(O)C(O)C=O)C(O)C
MOL004690	0.9464	0.0536	0.9717	Sapindi Mukorossi Semen	RNS	19233	FALSE	OC(C(O)C(O)C=O)C(O)C
MOL004690	0.9464	0.0536	0.9717	Radix Bupleuri	RNS	19233	FALSE	OC(C(O)C(O)C=O)C(O)C
MOL004691	0.9429	0.0571	0.9672	Trichosanthes Kirilowii Maxim	aldehydo-D-ribose	5311110	FALSE	OCC(O)C(O)C(O)C=O
MOL004691	0.9429	0.0571	0.9672	Radix Bupleuri	aldehydo-D-ribose	5311110	FALSE	OCC(O)C(O)C(O)C=O
MOL004693	0.6775	0.3225	0.8444	Radix Bupleuri	saikosaponin b1	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=C5C(C(O)C4)(CCC(C5)(C)C)CO)C=C3)C)(CC2)C)(CC1)C)(CO)C)C1OC(C(O)C(OC2OC(C(O)C(O)C2O)CO)C1O)C
MOL004694	0.4733	0.5267	0.7713	Radix Bupleuri	saikosaponin b1_qt	57358160	FALSE	OC1C(C2C(CC1)(C1C=CC3=C4C(C(O)CC3(C1(CC2)C)C)(CCC(C4)(C)C)CO)C)(CO)C
MOL004695	0.6775	0.3225	0.8444	Radix Bupleuri	saikosaponin b2	Not Available	FALSE	C12(C(=C3C(C(C2)O)(CCC(C3)(C)C)CO)C=CC2C1(CCC1C2(CCC(C1(CO)C)OC1C(C(OC2C(C(C(C(O2)CO)O)O)O)O)C(C(O1)C)O)O)C)C)C
MOL004696	0.4733	0.5267	0.7713	Radix Bupleuri	saikosaponin b2_qt	Not Available	FALSE	C12(C(=C3C(C(O)C2)(CCC(C3)(C)C)CO)C=CC2C1(CCC1C2(CCC(C1(C)CO)O)C)C)C
MOL004697	0.6455	0.3545	0.8556	Radix Bupleuri	saikosaponin b3	Not Available	FALSE	O1C(C(C(C(C1CO)O)O)O)OC1C(C(OC(C1O)C)OC1C(C2C(C3C(CC2)(C2(C(=CC3OC)C3C(C(C2)O)(CC(C3)(C)C)CO)C)C)(CC1)C)(CO)C)O
MOL004698	0.4089	0.5911	0.7785	Radix Bupleuri	saikosaponin b3_qt	Not Available	FALSE	OC1C(C2C(CC1)(C1C(C=C3C4C(C(CC3(C1(CC2)C)C)O)(CCC(C4)(C)C)CO)OC)C)(CO)C
MOL004699	0.6455	0.3545	0.8556	Radix Bupleuri	saikosaponin b4	Not Available	FALSE	O1C(C(C(C(C1CO)O)O)O)OC1C(C(OC(C1O)C)OC1C(C2C(C3C(CC2)(C2(C(=CC3OC)C3C(C(C2)O)(CC(C3)(C)C)CO)C)C)(CC1)C)(CO)C)O
MOL004700	0.4089	0.5911	0.7785	Radix Bupleuri	saikosaponin b4_qt	Not Available	FALSE	OC1C(C2C(CC1)(C1C(C=C3C4C(C(CC3(C1(CC2)C)C)O)(CCC(C4)(C)C)CO)OC)C)(CO)C
MOL004701	0.7431	0.2569	0.8394	Radix Bupleuri	saikosaponin c	Not Available	FALSE	C12(C3(C4C(C(C2)O)(CO3)CCC(C4)(C)C)C=CC2C1(CCC1C2(CCC(C1(CO)C)OC1C(C(C(OC2C(C(C(C(O2)C)O)O)O)O)C(O1)COC1C(C(C(C(O1)CO)O)O)O)O)O)O)C)C
MOL004702	0.4807	0.5193	0.7893	Radix Bupleuri	saikosaponin c_qt	Not Available	FALSE	C12(C3(C=CC4C1(CCC1C4(CCC(C1(C)CO)O)C)C)C1C(C(O)C2)(CO3)CCC(C1)(C)C)C
MOL004703	0.6330	0.3670	0.8039	Radix Bupleuri	saikosaponin e	Not Available	FALSE	O1C(C(C(C(C1CO)O)O)O)OC1C(C(OC(C1O)C)OC1C(C2C(C3C(C4(C5(OCC6(C5CC(CC6)(C)C)C(C4)O)C=C3)C)(CC2)C)(CC1)C)(C)C)O
MOL004704	0.4567	0.5433	0.8175	Radix Bupleuri	saikosaponin e_qt	Not Available	FALSE	OC1C(C2CCC3(C4(C5(OCC6(C(C4)O)C5CC(CC6)(C)C)C=CC3C2(CC1)C)C)C)(C)C

MOL004705	0.9563	0.0437	0.8701	Ligustici Rhizoma Et Radix	(3E,6S,7R)-3-butylidene-6,7-dihydroxy-4,5,6,7-tetrahydroisobenzofuran-1-one	10036567	FALSE	O1/C(=C/CCC)/C2=C(C(O)C(O)CC2)C1=O
MOL004705	0.9563	0.0437	0.8701	Radix Bupleuri	(3E,6S,7R)-3-butylidene-6,7-dihydroxy-4,5,6,7-tetrahydroisobenzofuran-1-one	10036567	FALSE	O1/C(=C/CCC)/C2=C(C(O)C(O)CC2)C1=O
MOL004706	0.8895	0.1105	0.6520	Radix Bupleuri	spathulenol	9794468	FALSE	OC1(C2C3C(C3CCC(=C)C2CC1)(C)C)C
MOL004707	0.8265	0.1735	0.6775	Radix Bupleuri	tau-cadinol	12302227	FALSE	OC1(C2C(C(CC1)C(C)C)C=C(CC2)C)C
MOL004708	0.8265	0.1735	0.6775	Radix Bupleuri	δ-cadinol	51394521	FALSE	OC1(C2C(C(CC1)C(C)C)C=C(CC2)C)C
MOL004708	0.8265	0.1735	0.6775	Lycii Fructus	δ-cadinol	51394521	FALSE	OC1(C2C(C(CC1)C(C)C)C=C(CC2)C)C
MOL004708	0.8265	0.1735	0.6775	Farfarae Flos	δ-cadinol	51394521	FALSE	OC1(C2C(C(CC1)C(C)C)C=C(CC2)C)C
MOL004709	0.9566	0.0434	0.9769	Radix Bupleuri	(+)-trans-Carveol	443178	FALSE	OC1CC(CC=C1C)C(=C)C
MOL004709	0.9566	0.0434	0.9769	Citri Sarcodactylis Fructus	(+)-trans-Carveol	443178	FALSE	OC1CC(CC=C1C)C(=C)C
MOL004710	0.9508	0.0492	0.9234	Radix Bupleuri	DTR	6923517	FALSE	c1(c[nH]c2c1cccc2)CC(C(=O)O)N
MOL004711	0.9559	0.0441	0.9718	Radix Bupleuri	Veratryl alcohol	7118	FALSE	COc1ccc(CO)cc1OC
MOL004711	0.9559	0.0441	0.9718	Coriolus	Veratryl alcohol	7118	FALSE	COc1ccc(CO)cc1OC
MOL004712	0.9412	0.0588	0.9665	Radix Bupleuri	xylitol	6912	FALSE	OCC(O)C(O)C(O)CO
MOL004713	0.8475	0.1525	0.7107	Tamaricis Cacumen	alpha-Eudesmol	92762	FALSE	OC(C1CC2C(CC1)(CCC=C2C)C)(C)C
MOL004713	0.8475	0.1525	0.7107	Rhododendri Daurici Folium	alpha-Eudesmol	92762	FALSE	OC(C1CC2C(CC1)(CCC=C2C)C)(C)C
MOL004713	0.8475	0.1525	0.7107	Smilacis Glabrae Rhixoma	alpha-Eudesmol	92762	FALSE	OC(C1CC2C(CC1)(CCC=C2C)C)(C)C
MOL004713	0.8475	0.1525	0.7107	Magnolia Officinalis Rehd Et Wils.	alpha-Eudesmol	92762	FALSE	OC(C1CC2C(CC1)(CCC=C2C)C)(C)C
MOL004713	0.8475	0.1525	0.7107	Radix Bupleuri	alpha-Eudesmol	92762	FALSE	OC(C1CC2C(CC1)(CCC=C2C)C)(C)C

MOL004714	0.9599	0.0401	0.7620	Radix Bupleuri	(1R,4S)-7,7-dimethyl-2-methylenenorbornane	10887972	FALSE	C1(C2CCC1C(=C)C2)(C)C
MOL004715	0.8331	0.1669	0.6734	Radix Bupleuri	(4aS,9aS)-2,9,9-trimethyl-5-methylene-4,4a,6,7,8,9a-hexahydro-3H-benzo[7]annulene	24798713	FALSE	C12C(CCCC(=C)C1CCC(=C2)C)(C)C
MOL004716	0.9348	0.0652	0.8176	Santalum Album L.	(1S,4R)-2,3-dimethylbicyclo[2.2.1]hept-2-ene	11457687	FALSE	C12CC(CC1)C(=C2C)C
MOL004716	0.9348	0.0652	0.8176	Radix Bupleuri	(1S,4R)-2,3-dimethylbicyclo[2.2.1]hept-2-ene	11457687	FALSE	C12CC(CC1)C(=C2C)C
MOL004717	0.8219	0.1781	0.6554	Rubi Fructus	(3R,4aR,8aR)-3-isopropenyl-5,8a-dimethyl-2,3,4,4a,7,8-hexahydro-1H-naphthalene	10856614	FALSE	C12(C(CC(CC1)C(=C)C)C(=CCC2)C)C
MOL004717	0.8219	0.1781	0.6554	Radix Bupleuri	(3R,4aR,8aR)-3-isopropenyl-5,8a-dimethyl-2,3,4,4a,7,8-hexahydro-1H-naphthalene	10856614	FALSE	C12(C(CC(CC1)C(=C)C)C(=CCC2)C)C

MOL004717	0.8219	0.1781	0.6554	Ardisiae Japonicae Herba	(3R,4aR,8aR)-3-isopropenyl-5,8a-dimethyl-2,3,4,4a,7,8-hexahydro-1H-naphthalene	10856614	FALSE	C12(C(CC(CC1)C(=C)C)C(=CCC2)C)C
MOL004718	0.2168	0.7832	0.6260	Radix Bupleuri	α-spinasterol	Not Available	FALSE	OC1CC2C(C3C(=CC2)C2C(C(CC2)C(C)/C=C/C(C(C)C)CC)(CC3)C)(CC1)C
MOL004721	0.9391	0.0609	0.7437	Radix Bupleuri	β-fenchene	12309844	FALSE	C1(C2CC(C1)(C=C2)C)(C)C
MOL004722	0.8221	0.1779	0.7523	Radix Bupleuri	β-oplopenone	14038846	FALSE	C(=O)(C)C1CCC2C1C(CCC2=C)C(C)C
MOL004723	0.9571	0.0429	0.9579	Angelicae Sinensis Radix	beta-Terpinene	66841	FALSE	C1(=CCC(=C)CC1)C(C)C
MOL004723	0.9571	0.0429	0.9579	Artemisia Annua L.	beta-Terpinene	66841	FALSE	C1(=CCC(=C)CC1)C(C)C
MOL004723	0.9571	0.0429	0.9579	licorice	beta-Terpinene	66841	FALSE	C1(=CCC(=C)CC1)C(C)C
MOL004723	0.9571	0.0429	0.9579	Schisandrae Chinensis Fructus	beta-Terpinene	66841	FALSE	C1(=CCC(=C)CC1)C(C)C
MOL004723	0.9571	0.0429	0.9579	Radix Bupleuri	beta-Terpinene	66841	FALSE	C1(=CCC(=C)CC1)C(C)C
MOL004724	0.8550	0.1450	0.6445	Radix Bupleuri	γ-cadinene	12313023	FALSE	C12C(CCC(=C)C1CCC(=C2)C)C(C)C
MOL004725	0.9405	0.0595	0.9645	Amygdalus Communis Vas	(5S)-5-hexyloxolan-2-one	7057904	FALSE	O1C(CCCCCC)CCC1=O
MOL004725	0.9405	0.0595	0.9645	Malvae Fructus	(5S)-5-hexyloxolan-2-one	7057904	FALSE	O1C(CCCCCC)CCC1=O
MOL004725	0.9405	0.0595	0.9645	Radix Bupleuri	(5S)-5-hexyloxolan-2-one	7057904	FALSE	O1C(CCCCCC)CCC1=O
MOL004726	0.9285	0.0715	0.9668	Radix Bupleuri	(5S)-5-propyloxolan-2-one	5325912	FALSE	O1C(CCC1=O)CCC

MOL004727	0.8550	0.1450	0.6445	Perillae Fructus	(1R,4aR,8aS)-1-isopropyl-7-methyl-4-methylene-2,3,4a,5,6,8a-hexahydro-1H-naphthalene	6432308	FALSE	C(C)(C)C1C2C(C(=C)CC1)CCC(=C2)C
MOL004727	0.8550	0.1450	0.6445	Viticis Negundo Folium	(1R,4aR,8aS)-1-isopropyl-7-methyl-4-methylene-2,3,4a,5,6,8a-hexahydro-1H-naphthalene	6432308	FALSE	C(C)(C)C1C2C(C(=C)CC1)CCC(=C2)C
MOL004727	0.8550	0.1450	0.6445	Notoginseng Flos	(1R,4aR,8aS)-1-isopropyl-7-methyl-4-methylene-2,3,4a,5,6,8a-hexahydro-1H-naphthalene	6432308	FALSE	C(C)(C)C1C2C(C(=C)CC1)CCC(=C2)C
MOL004727	0.8550	0.1450	0.6445	Radix Bupleuri	(1R,4aR,8aS)-1-isopropyl-7-methyl-4-methylene-2,3,4a,5,6,8a-hexahydro-1H-naphthalene	6432308	FALSE	C(C)(C)C1C2C(C(=C)CC1)CCC(=C2)C
MOL004727	0.8550	0.1450	0.6445	Campsis Flos	(1R,4aR,8aS)-1-isopropyl-7-methyl-4-methylene-2,3,4a,5,6,8a-hexahydro-1H-naphthalene	6432308	FALSE	C(C)(C)C1C2C(C(=C)CC1)CCC(=C2)C
MOL004729	0.9401	0.0599	0.9676	Mori Fructus	NOJ	29435	FALSE	C1(C(C(C(CN1)O)O)O)CO
MOL004729	0.9401	0.0599	0.9676	Bombyx Mori L.	NOJ	29435	FALSE	C1(C(C(C(CN1)O)O)O)CO
MOL004729	0.9401	0.0599	0.9676	Mori Cortex	NOJ	29435	FALSE	C1(C(C(C(CN1)O)O)O)CO

MOL004730	0.4819	0.5181	0.6013	Bombyx Mori L.	13,2-hydroxy(13,2-R,S)pheophytin a	Not Available	FALSE	C12=C3C(=C(C(/C=c\4/c(c(/c(=C/c5c(c(c(/C=C\6/C(C(C1=N6)CCC(=O)OC/C=C(/CCCC(CCCC(CCCC(C)C)C)C)\C)C)[nH]5)C)C=C)/[nH]4)C)CC)N3)C)C(=O)C2(C(=O)OC)O
MOL004731	0.9280	0.0720	0.7273	Bombyx Mori L.	3S,5R-dihydroxy-6R,7-megstigmadien-9-one	13922639	FALSE	C1C(CC(C(=C=CC(=O)C)C1(C)C)(C)O)O
MOL004732	0.8323	0.1677	0.6950	Bombyx Mori L.	(E)-4-[(1R,4S,6R)-2,2,6-trimethyl-4-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxycyclohexyl]but-3-en-2-one	10339245	FALSE	O(C1CC(C(C(C1)C)/C=C/C(=O)C)(C)C)C1OC(C(O)C(O)C1O)CO
MOL004733	0.9112	0.0888	0.7888	Bombyx Mori L.	(E)-4-[(1R,4S,6R)-4-hydroxy-2,2,6-trimethylcyclohexyl]but-3-en-2-one	21630918	FALSE	OC1CC(C(C(C1)C)/C=C/C(=O)C)(C)C
MOL004734	0.9141	0.0859	0.9643	Angelicae Sinensis Radix	Butal	261	FALSE	C(CC)C=O
MOL004734	0.9141	0.0859	0.9643	Artemisiae Scopariae Herba	Butal	261	FALSE	C(CC)C=O
MOL004734	0.9141	0.0859	0.9643	Capsici Fructus	Butal	261	FALSE	C(CC)C=O
MOL004734	0.9141	0.0859	0.9643	Tamaricis Cacumen	Butal	261	FALSE	C(CC)C=O
MOL004734	0.9141	0.0859	0.9643	Bombyx Mori L.	Butal	261	FALSE	C(CC)C=O
MOL004735	0.8993	0.1007	0.9572	Ginkgo Folium	CHX	8078	FALSE	C1CCCCC1
MOL004735	0.8993	0.1007	0.9572	Panacis Japonici Rhizoma	CHX	8078	FALSE	C1CCCCC1
MOL004735	0.8993	0.1007	0.9572	Bombyx Mori L.	CHX	8078	FALSE	C1CCCCC1
MOL004736	0.9344	0.0656	0.9734	Bombyx Mori L.	FAG	72259	FALSE	C1C(C(C(NC1)CO)O)O
MOL004737	0.9035	0.0965	0.8952	Bombyx Mori L.	4-Undecanone	84467	FALSE	C(=O)(CCCCCCC)CCC
MOL004738	0.9479	0.0521	0.9617	Vigna Radiata	Spantol	4770	FALSE	c1(CCCOC(=O)N)ccccc1
MOL004738	0.9479	0.0521	0.9617	Euryales Semen	Spantol	4770	FALSE	c1(CCCOC(=O)N)ccccc1
MOL004738	0.9479	0.0521	0.9617	Bombyx Mori L.	Spantol	4770	FALSE	c1(CCCOC(=O)N)ccccc1

MOL004738	0.9479	0.0521	0.9617	Arum Ternatum Thunb.	Spantol	4770	FALSE	c1(CCCOC(=O)N)ccccc1
MOL004739	0.8955	0.1045	0.9646	Bombyx Mori L.	DAL	7311725	FALSE	C(C(=O)O)(C)N
MOL004739	0.8955	0.1045	0.9646	Trichosanthes Kirilowii Maxim	DAL	7311725	FALSE	C(C(=O)O)(C)N
MOL004739	0.8955	0.1045	0.9646	Euryales Semen	DAL	7311725	FALSE	C(C(=O)O)(C)N
MOL004739	0.8955	0.1045	0.9646	Santalum Album L.	DAL	7311725	FALSE	C(C(=O)O)(C)N
MOL004739	0.8955	0.1045	0.9646	Arum Ternatum Thunb.	DAL	7311725	FALSE	C(C(=O)O)(C)N
MOL004740	0.8713	0.1287	0.9580	Bombyx Mori L.	DUC	649	FALSE	N1C(=O)CCNC1=O
MOL004741	0.9666	0.0334	0.8450	Gossampiniflos	(7aR)-4,4,7a-trimethyl-6,7-dihydro-5H-benzofuran-2-one	6432173	FALSE	C12=CC(=O)OC1(CCCC2(C)C)C
MOL004741	0.9666	0.0334	0.8450	Junci Medulla	(7aR)-4,4,7a-trimethyl-6,7-dihydro-5H-benzofuran-2-one	6432173	FALSE	C12=CC(=O)OC1(CCCC2(C)C)C
MOL004741	0.9666	0.0334	0.8450	Saussureae Involucratae Herba	(7aR)-4,4,7a-trimethyl-6,7-dihydro-5H-benzofuran-2-one	6432173	FALSE	C12=CC(=O)OC1(CCCC2(C)C)C
MOL004741	0.9666	0.0334	0.8450	Folium Artemisiae Argyi	(7aR)-4,4,7a-trimethyl-6,7-dihydro-5H-benzofuran-2-one	6432173	FALSE	C12=CC(=O)OC1(CCCC2(C)C)C
MOL004741	0.9666	0.0334	0.8450	Cornus Officinalis Sieb. Et Zucc.	(7aR)-4,4,7a-trimethyl-6,7-dihydro-5H-benzofuran-2-one	6432173	FALSE	C12=CC(=O)OC1(CCCC2(C)C)C
MOL004741	0.9666	0.0334	0.8450	Bombyx Mori L.	(7aR)-4,4,7a-trimethyl-6,7-dihydro-5H-benzofuran-2-one	6432173	FALSE	C12=CC(=O)OC1(CCCC2(C)C)C
MOL004741	0.9666	0.0334	0.8450	Ilicis Purpureae Folium	(7aR)-4,4,7a-trimethyl-6,7-dihydro-5H-benzofuran-2-one	6432173	FALSE	C12=CC(=O)OC1(CCCC2(C)C)C

MOL004742	0.9263	0.0737	0.8059	Lysimachiae Foenigraeci Herba	(4E)-4-[(E)-but-2-enylidene]-3,5,5-trimethylcyclohex-2-en-1-one	18645216	FALSE	C\1(=C\C=C\C)/C(=CC(=O)CC1(C)C)C
MOL004742	0.9263	0.0737	0.8059	Bombyx Mori L.	(4E)-4-[(E)-but-2-enylidene]-3,5,5-trimethylcyclohex-2-en-1-one	18645216	FALSE	C\1(=C\C=C\C)/C(=CC(=O)CC1(C)C)C
MOL004742	0.9263	0.0737	0.8059	Chaenomeles Sinensis (Thouin) Koehne	(4E)-4-[(E)-but-2-enylidene]-3,5,5-trimethylcyclohex-2-en-1-one	18645216	FALSE	C\1(=C\C=C\C)/C(=CC(=O)CC1(C)C)C
MOL004743	0.9513	0.0487	0.9125	Bamusaeconcretiosilicea	Z-Leu-OH	74840	FALSE	c1(COC(=O)NC(CC(C)C)C(=O)O)ccccc1
MOL004743	0.9513	0.0487	0.9125	Bombyx Mori L.	Z-Leu-OH	74840	FALSE	c1(COC(=O)NC(CC(C)C)C(=O)O)ccccc1
MOL004743	0.9513	0.0487	0.9125	Vigna Radiata	Z-Leu-OH	74840	FALSE	c1(COC(=O)NC(CC(C)C)C(=O)O)ccccc1
MOL004743	0.9513	0.0487	0.9125	Humulus Scandens (Lour.) Merr.	Z-Leu-OH	74840	FALSE	c1(COC(=O)NC(CC(C)C)C(=O)O)ccccc1
MOL004743	0.9513	0.0487	0.9125	Silybum Marianum	Z-Leu-OH	74840	FALSE	c1(COC(=O)NC(CC(C)C)C(=O)O)ccccc1
MOL004743	0.9513	0.0487	0.9125	Euryales Semen	Z-Leu-OH	74840	FALSE	c1(COC(=O)NC(CC(C)C)C(=O)O)ccccc1
MOL004744	0.4825	0.5175	0.6586	Bombyx Mori L.	pheophytin a	Not Available	FALSE	C12=C3C(C(=O)C2C(=O)OC)C(/C(=C/C2=N/C(=C\c4[nH]c(/C=C/5\N=C1C(C5C)CCC(=O)OC/C=C(/CCCC(CCCC(CCCC(C)C)C)C)\C)c(c4C=C)C)/C(=C2CC)C)/[nH]3)C
MOL004745	0.4587	0.5413	0.6604	Bombyx Mori L.	pheophytin b	Not Available	FALSE	C12=C3C(C(=O)C2C(=O)OC)C(/C(=C/C2=N/C(=C\c4[nH]c(/C=C/5\N=C1C(C5C)CCC(=O)OC/C=C(/CCCC(CCCC(CCCC(C)C)C)C)\C)c(c4C=C)C)/C(=C2CC)C=O)/[nH]3)C
MOL004747	0.9216	0.0784	0.9444	Aconitum Kusnezoffii Reichb	(2R)-6-methylheptan-2-amine	6989209	FALSE	C(CCCC(C)N)(C)C
MOL004748	0.2774	0.7226	0.7376	Aconitum Kusnezoffii Reichb	3-deoxyaconitine	Not Available	FALSE	C123C4C(C(C2C(CN4CC)(CCC3OC)COC)OC)C2(C3C1CC(C3OC(=O)c1ccccc1)(C(C2O)OC)O)OC(=O)C
MOL004749	0.3064	0.6936	0.7733	Aconitum Kusnezoffii Reichb	3-acetylaconitine	Not Available	FALSE	C123C4C(C(CC3OC)OC(=O)C)(CN(C2C(C4OC)C2(C3C1CC(C3OC(=O)c1ccccc1)(C(C2O)OC)O)OC(=O)C)CC)COC

MOL004750	0.9073	0.0927	0.7496	Aconitum Kusnezoffii Reichb	Xenylamin	7102	FALSE	c1(c2ccccc2)ccc(cc1)N
MOL004751	0.8856	0.1144	0.9608	Aconitum Kusnezoffii Reichb	CPMO	75644	FALSE	C1(CC1)CO
MOL004752	0.7998	0.2002	0.7596	Saussureae Involucratae Herba	Ethyl tridecanoate	119908	FALSE	C(CCCCCCCCCC)CC(=O)OCC
MOL004752	0.7998	0.2002	0.7596	Aconitum Kusnezoffii Reichb	Ethyl tridecanoate	119908	FALSE	C(CCCCCCCCCC)CC(=O)OCC
MOL004753	0.9527	0.0473	0.9606	Aconitum Kusnezoffii Reichb	BDMA	7681	TRUE	c1(ccccc1)CN(C)C
MOL004754	0.9721	0.0279	0.9646	Aconitum Kusnezoffii Reichb	N-Methylhomoveratrylamine	77039	FALSE	c1(c(ccc(c1)CCNC)OC)OC
MOL004755	0.9138	0.0862	0.9001	Aconitum Kusnezoffii Reichb	Cruex	5634	FALSE	C(CCCCC=C)CCCC(=O)O
MOL004756	0.2059	0.7941	0.6754	Aconitum Kusnezoffii Reichb	crassicauline A	Not Available	FALSE	C123C4C5C(C6C1N(CC(C2C6OC)(CCC3OC)COC)CC)(CC(C(C4)(C5OC(=O)c1ccc(cc1)OC)O)OC)OC(=O)C
MOL004757	0.2904	0.7096	0.7131	Aconitum Kusnezoffii Reichb	yunaconitine	Not Available	FALSE	C123C4C(CN(C2C(C4OC)C2(C4C1CC(C4OC(=O)c1ccc(cc1)OC)(C(C2)OC)O)OC(=O)C)CC)(C(CC3OC)O)COC
MOL004758	0.6819	0.3181	0.9006	Aconitum Kusnezoffii Reichb	lepenine	Not Available	FALSE	OC1C23C4C5(C6C2N(CC(C3C6)(CC1)C)CC)CCC(C4O)C(=C)C5O
MOL004759	0.6982	0.3018	0.9249	Aconitum Kusnezoffii Reichb	napelline	Not Available	FALSE	C123C4C5(C6C1N(CC(C2C6)(CCC3O)C)CC)CC(C(C4)O)C(=C)C5O
MOL004760	0.9165	0.0835	0.9605	Aconitum Kusnezoffii Reichb	ACONITATE, CIS	643757	FALSE	C(=C(\CC(=O)O)/C(=O)O)/C(=O)O
MOL004760	0.9165	0.0835	0.9605	Sojae Semen Nigrum	ACONITATE, CIS	643757	FALSE	C(=C(\CC(=O)O)/C(=O)O)/C(=O)O
MOL004761	0.5045	0.4955	0.8424	Aconitum Kusnezoffii Reichb	denudatine	Not Available	FALSE	C123C4C5(C6C1N(CC(C2C6)(CCC3)C)CC)C(C(=C)C(C4O)CC5)O
MOL004762	0.6086	0.3914	0.7641	Aconitum Kusnezoffii Reichb	neoline	Not Available	FALSE	C123C4C(CN(C1C(C4OC)C1(C4C2CC(C4O)C(C1)OC)O)CC)(CCC3O)COC
MOL004763	0.7217	0.2783	0.8299	Aconitum Kusnezoffii Reichb	Izoteolin	133323	FALSE	Oc1c2c3C(N(CCc3cc1OC)C)Cc1c2cc(OC)c(O)c1
MOL004763	0.7217	0.2783	0.8299	Corydalis Rhizoma	Izoteolin	133323	FALSE	Oc1c2c3C(N(CCc3cc1OC)C)Cc1c2cc(OC)c(O)c1
MOL004763	0.7217	0.2783	0.8299	Corydalis Bungeanae Herba	Izoteolin	133323	FALSE	Oc1c2c3C(N(CCc3cc1OC)C)Cc1c2cc(OC)c(O)c1
MOL004764	0.9105	0.0895	0.8954	Farfarae Flos	Decylene	13381	FALSE	C(=C)CCCCCCCC
MOL004764	0.9105	0.0895	0.8954	Radix Angelicae Biseratae	Decylene	13381	FALSE	C(=C)CCCCCCCC
MOL004765	0.8907	0.1093	0.9587	Radix Angelicae Biseratae	2,5-Dihydrotoluene	78006	FALSE	C1C=CCC=C1C
MOL004767	0.9627	0.0373	0.9084	Radix Angelicae Biseratae	Durenol	10694	FALSE	c1(c(c(cc1C)C)C)O)C
MOL004768	0.9273	0.0727	0.9447	Radix Angelicae Biseratae	2-HEXENE	639661	FALSE	C/C=C/CCC

MOL004769	0.9141	0.0859	0.7649	Radix Angelicae Biseratae	TERT-BUTYLTOLUENE	33712	FALSE	c1(ccccc1C(C)(C)C)C
MOL004770	0.7122	0.2878	0.6149	Radix Angelicae Biseratae	2-cyclohexyldecane	Not Available	FALSE	C1(C(CCCCCCCC)C)CCCCC1
MOL004771	0.9173	0.0827	0.9095	Radix Angelicae Biseratae	Isononane	18591	FALSE	CC(CCCCCC)C
MOL004772	0.9569	0.0431	0.9542	Radix Angelicae Biseratae	o-Cresol, 6-ethyl-	519333	FALSE	c1(cccc(c1O)CC)C
MOL004773	0.9182	0.0818	0.8976	Radix Angelicae Biseratae	Nonane, 3-methyl-	12859936	FALSE	CCC(CCCCCC)C
MOL004774	0.8482	0.1518	0.7025	Radix Angelicae Biseratae	Diphencyprone	65057	FALSE	C1(=C(C1=O)c1ccccc1)c1ccccc1
MOL004774	0.8482	0.1518	0.7025	Eriobotryae Folium	Diphencyprone	65057	FALSE	C1(=C(C1=O)c1ccccc1)c1ccccc1
MOL004775	0.9228	0.0772	0.7358	Radix Angelicae Biseratae	Isobergapten	68082	FALSE	c12c3c(cc(c1ccc(=O)o2)OC)occ3
MOL004777	0.5976	0.4024	0.6280	Radix Angelicae Biseratae	Angelol D	44144314	FALSE	O(C(C(O)C(O)(C)C)c1c(OC)cc2oc(=O)ccc2c1)C(=O)/C(=C/C)/C
MOL004778	0.5976	0.4024	0.6280	Radix Angelicae Biseratae	[(1R,2R)-2,3-dihydroxy-1-(7-methoxy-2-oxochromen-6-yl)-3-methylbutyl] (Z)-2-methylbut-2-enoate	10362168	FALSE	O(C(C(O)C(O)(C)C)c1c(OC)cc2oc(=O)ccc2c1)C(=O)/C(=C\C)/C
MOL004779	0.9009	0.0991	0.9657	Radix Angelicae Biseratae	Angelic acid	643915	FALSE	C(=C\C)(\C(=O)O)/C
MOL004779	0.9009	0.0991	0.9657	Farfarae Flos	Angelic acid	643915	FALSE	C(=C\C)(\C(=O)O)/C
MOL004779	0.9009	0.0991	0.9657	Peucedani Radix	Angelic acid	643915	FALSE	C(=C\C)(\C(=O)O)/C
MOL004780	0.8179	0.1821	0.9381	Radix Angelicae Biseratae	Angelicone	616303	FALSE	o1c2c(c(OC)cc(OC)c2ccc1=O)C(=O)C=C(C)C
MOL004781	0.9253	0.0747	0.8964	Radix Angelicae Biseratae	Pimpinellin	Not Available	FALSE	C1(C(C(C2C(C1)c1c(C(=O)O2)cc(c(c1O)OC)O)O)O)CO
MOL004782	0.5940	0.4060	0.6384	Radix Angelicae Biseratae	[(1R,2R)-2,3-dihydroxy-1-(7-methoxy-2-oxochromen-6-yl)-3-methylbutyl] 3-methylbutanoate	21669996	FALSE	O(C(C(O)C(O)(C)C)c1c(OC)cc2oc(=O)ccc2c1)C(=O)CC(C)C

MOL004783	0.9234	0.0766	0.9148	Radix Clematidis	nonane	8141	FALSE	CCCCCCCCC
MOL004783	0.9234	0.0766	0.9148	Radix Angelicae Biseratae	nonane	8141	FALSE	CCCCCCCCC
MOL004783	0.9234	0.0766	0.9148	Peucedanidecursivi Radix	nonane	8141	FALSE	CCCCCCCCC
MOL004783	0.9234	0.0766	0.9148	Semen Pharbitidis	nonane	8141	FALSE	CCCCCCCCC
MOL004783	0.9234	0.0766	0.9148	Sesami Nigrum Semen	nonane	8141	FALSE	CCCCCCCCC
MOL004783	0.9234	0.0766	0.9148	Arisaematis Rhizoma	nonane	8141	FALSE	CCCCCCCCC
MOL004783	0.9234	0.0766	0.9148	Ganoderma	nonane	8141	FALSE	CCCCCCCCC
MOL004783	0.9234	0.0766	0.9148	Flos Genkwa	nonane	8141	FALSE	CCCCCCCCC
MOL004783	0.9234	0.0766	0.9148	Rose Rugosae Flos	nonane	8141	FALSE	CCCCCCCCC
MOL004783	0.9234	0.0766	0.9148	Hyperici Japonici Herber	nonane	8141	FALSE	CCCCCCCCC
MOL004783	0.9234	0.0766	0.9148	Smilacis Glabrae Rhixoma	nonane	8141	FALSE	CCCCCCCCC
MOL004783	0.9234	0.0766	0.9148	Peucedani Radix	nonane	8141	FALSE	CCCCCCCCC
MOL004786	0.9407	0.0593	0.9214	Radix Angelicae Biseratae	4-terpineol	Not Available	FALSE	C1CC(CC=C1C)(C(C)C)C
MOL004787	0.9169	0.0831	0.9128	Farfarae Flos	NONYLENE	31285	FALSE	C(=C)CCCCCCC
MOL004787	0.9169	0.0831	0.9128	Radix Angelicae Biseratae	NONYLENE	31285	FALSE	C(=C)CCCCCCC
MOL004788	0.9326	0.0674	0.9095	Kaempferiae Rhizoma	1-alpha-Terpinyl acetate	93317	FALSE	C1=C(CCC(C1)C(OC(=O)C)(C)C)C
MOL004788	0.9326	0.0674	0.9095	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	1-alpha-Terpinyl acetate	93317	FALSE	C1=C(CCC(C1)C(OC(=O)C)(C)C)C
MOL004788	0.9326	0.0674	0.9095	Zanthoxyli Pericarpium	1-alpha-Terpinyl acetate	93317	FALSE	C1=C(CCC(C1)C(OC(=O)C)(C)C)C
MOL004788	0.9326	0.0674	0.9095	Viticis Negundo Folium	1-alpha-Terpinyl acetate	93317	FALSE	C1=C(CCC(C1)C(OC(=O)C)(C)C)C
MOL004788	0.9326	0.0674	0.9095	Rubi Fructus	1-alpha-Terpinyl acetate	93317	FALSE	C1=C(CCC(C1)C(OC(=O)C)(C)C)C
MOL004788	0.9326	0.0674	0.9095	Radix Angelicae Biseratae	1-alpha-Terpinyl acetate	93317	FALSE	C1=C(CCC(C1)C(OC(=O)C)(C)C)C
MOL004788	0.9326	0.0674	0.9095	Artemisia Annua L.	1-alpha-Terpinyl acetate	93317	FALSE	C1=C(CCC(C1)C(OC(=O)C)(C)C)C
MOL004788	0.9326	0.0674	0.9095	Lilii Bulbus	1-alpha-Terpinyl acetate	93317	FALSE	C1=C(CCC(C1)C(OC(=O)C)(C)C)C
MOL004788	0.9326	0.0674	0.9095	Menthae Herba	1-alpha-Terpinyl acetate	93317	FALSE	C1=C(CCC(C1)C(OC(=O)C)(C)C)C

MOL004789	0.8750	0.1250	0.6912	Radix Angelicae Biseratae	Isobornyl isovalerate	Not Available	FALSE	C1C2CCC(C1OC(=O)CC(C)C)(C2(C)C)C
MOL004790	0.8919	0.1081	0.8478	Calyx Seu Fructus Physalis	1-Undecene	13190	FALSE	C(=C)CCCCCCCCC
MOL004790	0.8919	0.1081	0.8478	Farfarae Flos	1-Undecene	13190	FALSE	C(=C)CCCCCCCCC
MOL004790	0.8919	0.1081	0.8478	Radix Angelicae Biseratae	1-Undecene	13190	FALSE	C(=C)CCCCCCCCC
MOL004790	0.8919	0.1081	0.8478	Rose Rugosae Flos	1-Undecene	13190	FALSE	C(=C)CCCCCCCCC
MOL004791	0.7198	0.2802	0.6084	Radix Angelicae Biseratae	Ethol	2682	FALSE	OCCCCCCCCCCCCCCCC
MOL004791	0.7198	0.2802	0.6084	Angelicae Sinensis Radix	Ethol	2682	FALSE	OCCCCCCCCCCCCCCCC
MOL004791	0.7198	0.2802	0.6084	Fritiliariae Irrhosae Bulbus	Ethol	2682	FALSE	OCCCCCCCCCCCCCCCC
MOL004791	0.7198	0.2802	0.6084	Bidentis Bipinnatae Herba	Ethol	2682	FALSE	OCCCCCCCCCCCCCCCC
MOL004791	0.7198	0.2802	0.6084	Meliae Azedarach Fructus	Ethol	2682	FALSE	OCCCCCCCCCCCCCCCC
MOL004792	0.7905	0.2095	0.7355	Peucedani Radix	nodakenin	73191	FALSE	C1(C(C(C(C(O1)OC(C1Cc2c(O1)cc1c(c2)ccc(=O)o1)(C)C)O)O)O)CO
MOL004792	0.7905	0.2095	0.7355	Peucedanidecursivi Radix	nodakenin	73191	FALSE	C1(C(C(C(C(O1)OC(C1Cc2c(O1)cc1c(c2)ccc(=O)o1)(C)C)O)O)O)CO
MOL004792	0.7905	0.2095	0.7355	Radix Angelicae Biseratae	nodakenin	73191	FALSE	C1(C(C(C(C(O1)OC(C1Cc2c(O1)cc1c(c2)ccc(=O)o1)(C)C)O)O)O)CO
MOL004792	0.7905	0.2095	0.7355	Notopterygii Rhizoma Et Radix	nodakenin	73191	FALSE	C1(C(C(C(C(O1)OC(C1Cc2c(O1)cc1c(c2)ccc(=O)o1)(C)C)O)O)O)CO
MOL004793	0.8901	0.1099	0.8313	Peucedanidecursivi Radix	Marmesine	26305	FALSE	OC(C1Cc2c(O1)cc1c(c2)ccc(=O)o1)(C)C
MOL004793	0.8901	0.1099	0.8313	Peucedani Radix	Marmesine	26305	FALSE	OC(C1Cc2c(O1)cc1c(c2)ccc(=O)o1)(C)C
MOL004793	0.8901	0.1099	0.8313	Radix Angelicae Biseratae	Marmesine	26305	FALSE	OC(C1Cc2c(O1)cc1c(c2)ccc(=O)o1)(C)C
MOL004793	0.8901	0.1099	0.8313	A. Dahurica (Fisch.) Benth. Et Hook	Marmesine	26305	FALSE	OC(C1Cc2c(O1)cc1c(c2)ccc(=O)o1)(C)C
MOL004794	0.8820	0.1180	0.6133	Radix Angelicae Biseratae	Acenaphthene	6734	FALSE	c1cc2c3c(c1)cccc3CC2
MOL004795	0.9618	0.0382	0.8135	Impatientis Semen	2-Methoxynaphthoquinone	16871	FALSE	c12c(C(=O)C=C(C1=O)OC)cccc2
MOL004795	0.9618	0.0382	0.8135	Impatiens Balsamina	2-Methoxynaphthoquinone	16871	FALSE	c12c(C(=O)C=C(C1=O)OC)cccc2
MOL004796	0.4439	0.5561	0.6039	Arum Ternatum Thunb.	soya-cerebroside i	Not Available	FALSE	O1C(OCC(NC(=O)C(O)CCCCCCCCCCCCCCC)C(O)/C=C/CC/C=C/CCCCCCCCC)C(O)C(O)C(O)C1CO
MOL004796	0.4439	0.5561	0.6039	Impatiens Balsamina	soya-cerebroside i	Not Available	FALSE	O1C(OCC(NC(=O)C(O)CCCCCCCCCCCCCCC)C(O)/C=C/CC/C=C/CCCCCCCCC)C(O)C(O)C(O)C1CO
MOL004801	0.6612	0.3388	0.7258	licorice	2',7-Dihydroxy-4'-methoxyisoflavan-7-O-β-d-glucopyranoside	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)c1ccc2c(c1)OC(C(C2OC)c1ccccc1)O

MOL004802	0.9179	0.0821	0.9226	licorice	(E)-1-butoxyhex-2-ene	5364961	FALSE	C(/C=C/CCC)OCCCC
MOL004803	0.1036	0.8964	0.6604	licorice	3-Hydroxyglabrol	480854	FALSE	c12OC(C(C(=O)c1ccc(c2CC=C(C)C)O)O)c1cc(c(cc1)O)CC=C(C)C
MOL004804	0.7209	0.2791	0.7420	Abri Herba	18beta-glycyrrhetinic acid	10114	TRUE	OC1C(C2C(C3C(C4(C(=CC3=O)C3C(CC4)(CCC(C3)(C)C(=O)O)C)C)(CC2)C)(CC1)C)(C)C
MOL004804	0.7209	0.2791	0.7420	licorice	18beta-glycyrrhetinic acid	10114	TRUE	OC1C(C2C(C3C(C4(C(=CC3=O)C3C(CC4)(CCC(C3)(C)C(=O)O)C)C)(CC2)C)(CC1)C)(C)C
MOL004805	0.1280	0.8720	0.6461	licorice	(2S)-2-[4-hydroxy-3-(3-methylbut-2-enyl)phenyl]-8,8-dimethyl-2,3-dihydropyrano[2,3-f]chromen-4-one	197678	FALSE	O1C(CC(=O)c2c1c1c(OC(C=C1)(C)C)cc2)c1cc(c(O)cc1)CC=C(C)C
MOL004806	0.1143	0.8857	0.6313	licorice	euchrenone	Not Available	FALSE	c1(ccc2c(c1CC=C(C)C)OC(CC2=O)c1ccc(c(c1)/C=C\C)OC(C)C)O
MOL004807	0.9130	0.0870	0.9453	licorice	glucuronic acid	441478	FALSE	O1C(C(O)C(O)C(O)C1O)C(=O)O
MOL004807	0.9130	0.0870	0.9453	Polygonati Rhizoma	glucuronic acid	441478	FALSE	O1C(C(O)C(O)C(O)C1O)C(=O)O
MOL004807	0.9130	0.0870	0.9453	Polygonati Odorati Rhizoma	glucuronic acid	441478	FALSE	O1C(C(O)C(O)C(O)C1O)C(=O)O
MOL004807	0.9130	0.0870	0.9453	Sojae Semen Nigrum	glucuronic acid	441478	FALSE	O1C(C(O)C(O)C(O)C1O)C(=O)O
MOL004808	0.4308	0.5692	0.7212	licorice	glyasperin B	Not Available	FALSE	Oc1c(C2COc3c(C2=O)c(O)c(c(c3)OC)CC=C(C)C)ccc(O)c1
MOL004809	0.0878	0.9122	0.6959	licorice	glyasperin E	Not Available	FALSE	c1(c(cc2c(c1)oc(c(c2=O)c1ccccc1)Oc1ccc(cc1O)O)CC=C(C)C)OC
MOL004810	0.4481	0.5519	0.7978	licorice	glyasperin F	Not Available	FALSE	O1C(C=Cc2c1c(C1COc3c(C1=O)c(O)cc(O)c3)ccc2O)(C)C
MOL004811	0.2951	0.7049	0.7995	licorice	Glyasperin C	480859	FALSE	O1CC(Cc2c1cc(O)c(c2OC)CC=C(C)C)c1c(O)cc(O)c
MOL004812	0.1640	0.8360	0.8593	licorice	glyasperins D	Not Available	FALSE	O1CC(Cc2c1cc(OC)c(c2O)CC=C(C)C)c1c(O)cc(O)cc1
MOL004813	0.2038	0.7962	0.8259	licorice	glyasperins Z	Not Available	FALSE	O1CC(Cc2c1cc(cc2)O)c1c(O)c(c(OC)cc1)CC=C(C)C
MOL004814	0.9174	0.0826	0.7163	licorice	Isotrifoliol	5318679	FALSE	o1c2c(c3c1cc(O)cc3)c(=O)oc1c2c(OC)cc(O)c1

MOL004815	0.4200	0.5800	0.7818	licorice	(E)-1-(2,4-dihydroxyphenyl)-3-(2,2-dimethylchromen-6-yl)prop-2-en-1-one	10881804	FALSE	O1C(C=Cc2c1ccc(c2)/C=C/C(=O)c1c(O)cc(O)cc1)(C)C
MOL004817	0.1158	0.8842	0.6117	licorice	kanzonols K	Not Available	FALSE	c1(c(c(c2c(c1)occ(c2=O)c1ccc(c(c1O)CC=C(C)C)O)O)CC=C(C)C)OC
MOL004820	0.3776	0.6224	0.8477	licorice	kanzonols W	15380912	FALSE	O1C2C(CCC3C2C=CC(O3)(C)C)CC(C1=O)C1C(O)CC(O)C=C1
MOL004822	0.5625	0.4375	0.6010	licorice	(E)-1-(2,4-dihydroxyphenyl)-3-[4-hydroxy-3-(3-methylbut-2-enyl)phenyl]prop-2-en-1-one	11099375	FALSE	Oc1c(CC=C(C)C)cc(cc1)/C=C/C(=O)c1c(O)cc(O)cc1
MOL004823	0.1682	0.8318	0.7640	licorice	licoagropin	Not Available	FALSE	c1(ccc2c(c1CC=C(C)C)OCC1C2Oc2c1ccc(c2)C)C
MOL004824	0.4478	0.5522	0.7824	licorice	(2S)-6-(2,4-dihydroxyphenyl)-2-(2-hydroxypropan-2-yl)-4-methoxy-2,3-dihydrofuro[3,2-g]chromen-7-one	637112	FALSE	O1C(C(O)(C)C)Cc2c1cc1oc(=O)c(cc1c2OC)c1c(O)cc(O)cc1
MOL004827	0.4774	0.5226	0.7623	licorice	Semilicoisoflavone B	5481948	FALSE	c12c(cc(cc1O)O)occ(c2=O)c1cc(c2c(c1)C=CC(O2)(C)C)O
MOL004828	0.4649	0.5351	0.7709	licorice	Glepidotin A	5281619	TRUE	c1(cc(c2c(c1CC=C(C)C)oc(c(c2=O)O)c1ccccc1)O)O
MOL004829	0.4732	0.5268	0.7456	licorice	Glepidotin B	442411	FALSE	O1C(C(O)C(=O)c2c1c(CC=C(C)C)c(O)cc2O)c1ccccc1
MOL004830	0.9147	0.0853	0.9100	Polygonati Odorati Rhizoma	Octadiene	517653	FALSE	C(/C=C/C=C)CCC
MOL004830	0.9147	0.0853	0.9100	licorice	Octadiene	517653	FALSE	C(/C=C/C=C)CCC
MOL004832	0.9535	0.0465	0.9683	Eriobotryae Folium	WLN: 4OVR	8698	FALSE	c1c(cccc1)C(=O)OCCCC
MOL004832	0.9535	0.0465	0.9683	licorice	WLN: 4OVR	8698	FALSE	c1c(cccc1)C(=O)OCCCC
MOL004832	0.9535	0.0465	0.9683	Benzoinum	WLN: 4OVR	8698	FALSE	c1c(cccc1)C(=O)OCCCC
MOL004833	0.3227	0.6773	0.8248	licorice	Phaseolinisoflavan	162412	FALSE	O1CC(Cc2c1cc(O)cc2)c1c(O)c2c(OC(C=C2)(C)C)cc1

MOL004834	0.9006	0.0994	0.9076	licorice	3-(2-hydroxy-4-methoxyphenyl)-2H-chromen-7-ol	10378419	FALSE	c1(ccc2c(c1)OCC(=C2)c1ccc(cc1O)OC)O
MOL004835	0.8752	0.1248	0.7534	licorice	Glypallichalcone	5317768	FALSE	O(c1c(/C=C/C(=O)c2ccc(OC)cc2)ccc(O)c1)C
MOL004836	0.8928	0.1072	0.7720	licorice	echinatin	Not Available	FALSE	c1(c(cc(cc1)O)OC)/C=C\C(=O)c1ccc(cc1)O
MOL004837	0.8599	0.1401	0.9183	licorice	Karenzu DK2	8433	FALSE	c1cccc(c1)C(=O)CC(=O)c1ccccc1
MOL004838	0.5328	0.4672	0.7252	licorice	8-(6-hydroxy-2-benzofuranyl)-2,2-dimethyl-5-chromenol	10542808	FALSE	c1(ccc2c(c1)oc(c2)c1c2c(c(cc1)O)C=CC(O2)(C)C)O
MOL004839	0.8795	0.1205	0.9481	licorice	(1S,2S)-1,2-dimethylcyclopentane	641612	FALSE	C1(C(CCC1)C)C
MOL004840	0.2908	0.7092	0.7461	licorice	Liconeolignan	133867	FALSE	C12c(cc(c(c1)OC)OC)c(c(o2)c1cc(c(cc1)O)CC=C(C)C)O
MOL004841	0.8496	0.1504	0.8132	licorice	Licochalcone B	5318999	FALSE	C(=C\c1c(c(c(cc1)O)O)OC)/C(=O)c1ccc(cc1)O
MOL004842	0.4290	0.5710	0.6485	licorice	licochalcone C	Not Available	FALSE	C(=O)(/C=C\c1c(c(c(cc1)O)CC=C(C)C)OC)c1ccc(cc1)O
MOL004843	0.4394	0.5606	0.6326	licorice	licochalconeD	Not Available	FALSE	C(=O)(/C=C\c1c(c(c(cc1)O)O)OC)c1cc(c(cc1)O)CC=C(C)C
MOL004845	0.7129	0.2871	0.8580	licorice	apioglycyrrhizin	Not Available	FALSE	C1CC2(C(CC1(C)C(=O)O)C1=CC(=O)C3C(C1(CC2)C)(CCC1C3(CCC(C1(C)C)OC1OC(C(C(C1OC1OCC(C1O)(O)CO)O)O)C(=O)O)C)C)C
MOL004846	0.7209	0.2791	0.7420	licorice	apioglycyrrhizin_qt	Not Available	FALSE	C1CC2(C(CC1(C)C(=O)O)C1=CC(=O)C3C(C1(CC2)C)(CCC1C3(CCC(C1(C)C)O)C)C)C
MOL004847	0.9208	0.0792	0.9394	licorice	2,2-DIMETHYLPENTANE	11542	FALSE	C(C(C)(C)C)CC
MOL004848	0.4654	0.5346	0.6096	licorice	licochalcone G	49856081	FALSE	Oc1c(C(C)(C)C=C)cc(c(OC)c1)/C=C/C(=O)c1c(O)cc(O)cc1
MOL004849	0.4585	0.5415	0.7871	licorice	3-(2,4-dihydroxyphenyl)-8-(1,1-dimethylprop-2-enyl)-7-hydroxy-5-methoxy-coumarin	10090416	FALSE	c1(=O)c(cc2c(o1)c(c(cc2OC)O)C(C=C)(C)C)c1c(cc(cc1)O)O

MOL004850	0.7108	0.2892	0.7151	licorice	liquoric acid	Not Available	FALSE	C1(C(CCC2(C1CCC1(C2C(=O)C=C2C1(CC1C3(C2CC(C(C3)O1)(C)C(=O)O)C)C)C)O)(C)C
MOL004851	0.4331	0.5669	0.6042	licorice	Licoflavone	5319000	FALSE	c1(cc2c(cc1CC=C(C)C)c(=O)cc(o2)c1ccc(cc1)O)O
MOL004853	0.5698	0.4302	0.6175	licorice	Licoflavonol	5481964	FALSE	c1(c(c(c2c(c1)oc(c(c2=O)O)c1ccc(cc1)O)O)CC=C(C)C)O
MOL004855	0.2368	0.7632	0.8353	licorice	Licoricone	5319013	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1c(c(c(cc1O)OC)CC=C(C)C)OC
MOL004856	0.2828	0.7172	0.7306	licorice	Gancaonin A	5317478	FALSE	O1c2c(c(=O)c(c3ccc(OC)cc3)c1)c(O)c(c(O)c2)CC=C(C)C
MOL004857	0.4461	0.5539	0.6894	licorice	Gancaonin B	5317479	FALSE	c12c(cc(c(c1O)CC=C(C)C)O)occ(c2=O)c1cc(c(cc1)OC)O
MOL004858	0.5713	0.4287	0.6348	licorice	Gancaonin C	6450959	FALSE	c12c(c(c(cc1O)O)C/C=C(/CO)\C)occ(c2=O)c1ccc(cc1)O
MOL004859	0.9126	0.0874	0.9369	Ginkgo Folium	2,3-dimethylhexane	24884354	FALSE	C(CCC)(C(C)C)C
MOL004859	0.9126	0.0874	0.9369	licorice	2,3-dimethylhexane	24884354	FALSE	C(CCC)(C(C)C)C
MOL004860	0.5059	0.4941	0.6627	licorice	licorice glycoside E	Not Available	FALSE	O(C1C(O)C(O)C(OC1OC1ccc(C2Oc3c(C(=O)C2)ccc(O)c3)cc1)CO)C1OCC(O)(C1O)COC(=O)c1c2c([nH]c1)cccc2
MOL004861	0.5302	0.4698	0.6662	licorice	Gancaonin D	5317481	FALSE	c12c(c(c(cc1O)O)C/C=C(/CO)\C)occ(c2=O)c1cc(c(cc1)OC)O
MOL004862	0.1904	0.8096	0.6634	licorice	(2R)-2-[3,4-dihydroxy-5-(3-methylbut-2-enyl)phenyl]-5,7-dihydroxy-8-(3-methylbut-2-enyl)chroman-4-one	14539875	FALSE	c12c(c(c(cc1O)O)CC=C(C)C)OC(CC2=O)c1cc(c(c(c1)O)O)CC=C(C)C
MOL004863	0.6183	0.3817	0.7711	licorice	3-(3,4-dihydroxyphenyl)-5,7-dihydroxy-8-(3-methylbut-2-enyl)chromone	14604077	FALSE	c1(cc(ccc1O)c1coc2c(c(cc(c2c1=O)O)O)CC=C(C)C)O

MOL004864	0.2532	0.7468	0.7597	licorice	5,7-dihydroxy-3-(4-methoxyphenyl)-8-(3-methylbut-2-enyl)chromone	14604078	FALSE	c1cc(ccc1OC)c1coc2c(c(cc(c2c1=O)O)O)CC=C(C)C
MOL004865	0.4755	0.5245	0.7162	licorice	5,7-dihydroxy-3-(2-hydroxy-4-methoxy-phenyl)-6-(3-methylbut-2-enyl)chromone	14604080	FALSE	c1(c2c(cc(c1CC=C(C)C)O)occ(c2=O)c1c(cc(cc1)OC)O)O
MOL004866	0.6043	0.3957	0.7625	licorice	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6-(3-methylbut-2-enyl)chromone	14604081	FALSE	c1(c2c(cc(c1CC=C(C)C)O)oc(cc2=O)c1cc(c(O)cc1)O)O
MOL004867	0.6637	0.3363	0.7864	licorice	Gancaonin P	5481966	FALSE	c1(c2c(cc(c1CC=C(C)C)O)oc(c(c2=O)O)c1cc(c(O)cc1)O)O
MOL004871	0.9235	0.0765	0.9471	licorice	(3S)-2,3-dimethylpentane	22810194	FALSE	C(C(C)C)(CC)C
MOL004873	0.3833	0.6167	0.6699	licorice	Gancaonin U	480818	FALSE	C1c2c(c3c(c(c(c(CC=C(C)C)c3O)O)CC=C(C)C)C1)cc(c(c2)O)O
MOL004874	0.7166	0.2834	0.7761	licorice	Gancaonin V	480817	FALSE	c1c(c(cc2c3c(cc(c(c3CCc12)CC=C(C)C)O)O)O)O
MOL004875	0.4202	0.5798	0.7990	licorice	3-[4,6-dihydroxy-2-methoxy-3-(3-methylbut-2-enyl)phenyl]-7-hydroxy-chromone	10361658	FALSE	c1c(c(=O)c2c(o1)cc(cc2)O)c1c(c(c(cc1O)O)CC=C(C)C)OC
MOL004876	0.7373	0.2627	0.8470	Puerariae Flos	Glycyram	14982	FALSE	C12C(C3(C(=CC2=O)C2C(CC3)(CCC(C2)(C(=O)O)C)C)C)(CCC2C1(CCC(C2(C)C)OC1C(OC2OC(C(C(C2O)O)O)C(=O)O)C(C(C(O1)C(=O)O)O)O)C)C

MOL004876	0.7373	0.2627	0.8470	licorice	Glycyram	14982	FALSE	C12C(C3(C(=CC2=O)C2C(CC3)(CCC(C2)(C(=O)O)C)C)C)(CCC2C1(CCC(C2(C)C)OC1C(OC2OC(C(C(C2O)O)O)O)C(=O)O)C(C(C(O1)C(=O)O)O)O)C)C
MOL004877	0.0920	0.9080	0.6018	licorice	Licoricidin	480865	FALSE	c1(c2c(cc(c1CC=C(C)C)O)OCC(C2)c1ccc(c(c1O)CC=C(C)C)O)OC
MOL004878	0.3895	0.6105	0.7964	licorice	Glycycoumarin	5317756	FALSE	c1(=O)c(cc2c(o1)cc(c(c2OC)CC=C(C)C)O)c1c(cc(cc1)O)O
MOL004879	0.2261	0.7739	0.8453	licorice	Glycyrin	480787	FALSE	c1(=O)c(cc2c(o1)cc(c(c2OC)CC=C(C)C)OC)c1c(cc(cc1)O)O
MOL004880	0.9371	0.0629	0.8230	licorice	5,6,7,8-Tetrahydro-2,4-dimethylquinoline	5321849	FALSE	n1c(cc(c2CCCCc12)C)C
MOL004882	0.6031	0.3969	0.6361	licorice	Licocoumarone	503731	FALSE	c1(c2c(cc(c1CC=C(C)C)O)oc(c1ccc(cc1O)O)c2)OC
MOL004883	0.5734	0.4266	0.7064	licorice	Licoisoflavone	5281789	FALSE	c1(cc(c2c(c1)occ(c2=O)c1ccc(c(c1O)CC=C(C)C)O)O)O
MOL004884	0.4878	0.5122	0.8224	licorice	Licoisoflavone B	5481234	FALSE	c1c(c(=O)c2c(o1)cc(cc2O)O)c1ccc2c(C=CC(O2)(C)C)c1O
MOL004885	0.5107	0.4893	0.7924	licorice	licoisoflavanone	Not Available	FALSE	c12c(c(cc(c1)O)O)C(=O)C(CO2)c1c(c2c(cc1)OC(C=C2)(C)C)O
MOL004886	0.7427	0.2573	0.8427	licorice	licorice-saponin C2	Not Available	FALSE	C1CC2(C(=C3C(CC2)(C2(C(C=C3)C3(C(CC2)C(C(CC3)OC2OC(C(C(C2OC2OC(C(C(C2O)O)O)O)C(=O)O)O)O)O)C(=O)O)(C)C)C)C)CC1(C)C(=O)O)C
MOL004887	0.6885	0.3115	0.8557	licorice	licorice-saponin C2_qt	Not Available	FALSE	C1CC2(C(=C3C(CC2)(C2(C(C=C3)C3(C(CC2)C(C(CC3)O)(C)C)C)C)CC1(C)C(=O)O)C
MOL004888	0.7588	0.2412	0.8228	licorice	licorice-saponin F3	Not Available	FALSE	C12(CC(C3(C(C1)C1=CCC4C(C1(CC3)C)(CCC1C4(CCC(C1(C)C)OC1OC(C(C(C1OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C(=O)O)O)O)C(=O)O)O)O)C(=O)O)C)C)OC2=O)C
MOL004889	0.4044	0.5956	0.8078	licorice	licorice-saponin F3_qt	Not Available	FALSE	C12(CC(C3(C(C1)C1=CCC4C(C1(CC3)C)(CCC1C4(CCC(C1(C)C)O)O)C)C)C)OC2=O)C
MOL004890	0.9190	0.0810	0.9219	licorice	(4S)-2,4-dimethylhexane	22810193	FALSE	C(CC(C)C)(CC)C
MOL004890	0.9190	0.0810	0.9219	Equiseti Hiemalis Herba	(4S)-2,4-dimethylhexane	22810193	FALSE	C(CC(C)C)(CC)C
MOL004891	0.6481	0.3519	0.8465	licorice	shinpterocarpin	Not Available	FALSE	O1C2C(COc3c2ccc2OC(C=Cc32)(C)C)c2c1cc(O)cc2

MOL004892	0.7390	0.2610	0.8368	licorice	licorice-saponin G2	Not Available	FALSE	C1(CCC2(C(C1)C1=CC(=O)C3C(C1(CC2)C)(CCC1C3(CCC(C1(CO)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C(=O)O)O)O)C(=O)O)C)C)(C)C(=O)O
MOL004893	0.7164	0.2836	0.7081	licorice	licorice-saponin G2_qt	Not Available	FALSE	C1(CCC2(C(C1)C1=CC(=O)C3C(C1(CC2)C)(CCC1C3(CCC(C1(CO)C)O)C)C)(C)C(=O)O
MOL004894	0.7373	0.2627	0.8470	licorice	licorice-saponin H2	Not Available	FALSE	C1(CCC2(C(C1)C1=CC(=O)C3C(C1(CC2)C)(CCC1C3(CCC(C1(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C(=O)O)O)O)C(=O)O)C)C)(C)C(=O)O
MOL004895	0.7209	0.2791	0.7420	licorice	licorice-saponin H2_qt	Not Available	FALSE	C1(CCC2(C(C1)C1=CC(=O)C3C(C1(CC2)C)(CCC1C3(CCC(C1(C)C)O)C)C)(C)C(=O)O
MOL004896	0.7552	0.2448	0.8484	licorice	licorice-saponin J2	Not Available	FALSE	C1(CCC2(C(C1)C1=CCC3C(C1(CC2)C)(CCC1C3(CCC(C1(CO)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C(=O)O)O)O)C(=O)O)C)C)(C)C(=O)O
MOL004897	0.6962	0.3038	0.8140	licorice	licorice-saponin J2_qt	Not Available	FALSE	C1(CCC2(C(C1)C1=CCC3C(C1(CC2)C)(CCC1C3(CCC(C1(CO)C)O)C)C)(C)C(=O)O
MOL004898	0.6066	0.3934	0.6562	licorice	(E)-3-[3,4-dihydroxy-5-(3-methylbut-2-enyl)phenyl]-1-(2,4-dihydroxyphenyl)prop-2-en-1-one	11267805	FALSE	Oc1c(CC=C(C)C)cc(cc1O)/C=C/C(=O)c1c(O)cc(O)cc1
MOL004899	0.7426	0.2574	0.8517	licorice	licorice-saponin B2	Not Available	FALSE	C1CC2(C(CC1(C)C(=O)O)C1=CCC3C(C1(CC2)C)(CCC1C3(CCC(C1(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C(=O)O)O)O)C(=O)O)C)C)C
MOL004900	0.7557	0.2443	0.8397	licorice	licorice-saponin K2	Not Available	FALSE	C1(CCC2(C(=C3C(CC2)(C2(C(C=C3)C3(C(CC2)C(C(CC3)OC2OC(C(C(C2OC2OC(C(C(C2O)O)O)O)C(=O)O)O)O)C(=O)O)(CO)C)C)C)C)C1)C)(C)C(=O)O
MOL004901	0.7198	0.2802	0.8028	licorice	licorice-saponin K2_qt	Not Available	FALSE	C1(CCC2(C(=C3C(CC2)(C2(C(C=C3)C3(C(CC2)C(C(CC3)O)(CO)C)C)C)C)C1)C)(C)C(=O)O
MOL004902	0.3914	0.6086	0.7432	licorice	glycyrrhetol	Not Available	FALSE	C(C1(CCC2(CCC3(C4(CCC5C(C(O)CCC5(C4C(=O)C=C3C2C1)C)(C)C)C)C)C)C)O
MOL004903	0.7638	0.2362	0.6363	licorice	liquiritin	503737	FALSE	c12c(OC(CC1=O)c1ccc(cc1)OC1OC(C(C(C1O)O)O)CO)cc(cc2)O
MOL004903	0.7638	0.2362	0.6363	Rhapontici Radix	liquiritin	503737	FALSE	c12c(OC(CC1=O)c1ccc(cc1)OC1OC(C(C(C1O)O)O)CO)cc(cc2)O
MOL004904	0.4214	0.5786	0.8009	licorice	licopyranocoumarin	Not Available	FALSE	c12c(OC(CC1)(C)CO)cc1c(c2OC)cc(c(=O)o1)c1ccc(cc1O)O

MOL004905	0.4074	0.5926	0.7535	licorice	3,22-Dihydroxy-11-oxo-delta(12)-oleanene-27-alpha-methoxycarbonyl-29-oic acid	Not Available	FALSE	O1C2C3(C(C4=CC(=O)C5C(C4(CC3)C(=O)OC)(CCC3C5(CCC(O)C3(C)C)C)C)CC(C2)(C1=O)C)C
MOL004906	0.1197	0.8803	0.7823	licorice	Hispaglabridin B	15228661	FALSE	O1CC(Cc2c1c1c(OC(C=C1)(C)C)cc2)c1c(O)c2c(OC(C=C2)(C)C)cc1
MOL004907	0.8353	0.1647	0.8527	licorice	Glyzaglabrin	5317777	FALSE	O1c2c(O)c(c3c(=O)c4c(oc3)cc(O)cc4)ccc2OC1
MOL004908	0.3655	0.6345	0.8521	licorice	Glabridin	124052	FALSE	C12c3c(CC(CO3)c3c(cc(cc3)O)O)ccc1OC(C=C2)(C)C
MOL004909	0.3949	0.6051	0.7687	licorice	glabrolide	Not Available	FALSE	C12=CC(=O)C3C(C1(CCC1(C2CC2(CC1OC2=O)C)C)C)(C)CCC1C3(C)CCC(C1(C)C)O
MOL004910	0.3831	0.6169	0.8023	licorice	Glabranin	124049	FALSE	c1(c2c(c(cc1O)O)C(=O)CC(O2)c1ccccc1)CC=C(C)C
MOL004911	0.3241	0.6759	0.8393	licorice	Glabrene	480774	FALSE	C1CC(c2c(c1O)C=CC(O2)(C)C)C1=CC2(OC1)CC(CC2)(C)C
MOL004912	0.4324	0.5676	0.8263	licorice	Glabrone	5317652	FALSE	C1C(C(=O)c2c(o1)cc(cc2)O)c1ccc2c(C=CC(O2)(C)C)c1O
MOL004912	0.4324	0.5676	0.8263	Mori Cortex	Glabrone	5317652	FALSE	C1C(C(=O)c2c(o1)cc(cc2)O)c1ccc2c(C=CC(O2)(C)C)c1O
MOL004913	0.9359	0.0641	0.7137	licorice	1,3-dihydroxy-9-methoxy-6-benzofurano[3,2-c]chromenone	11558452	FALSE	c1(cc(c2c(c1)oc(=O)c1c2oc2c1ccc(c2)OC)O)O
MOL004914	0.9141	0.0859	0.6852	licorice	1,3-dihydroxy-8,9-dimethoxy-6-benzofurano[3,2-c]chromenone	11602329	FALSE	c1(cc(c2c(c1)oc(=O)c1c2oc2c1cc(c(c2)OC)OC)O)O
MOL004915	0.5009	0.4991	0.7021	licorice	Eurycarpin A	5317300	FALSE	O1c2c(c(=O)c(c3c(O)c(CC=C(C)C)c(O)cc3)c1)ccc(O)c2
MOL004916	0.8796	0.1204	0.7085	licorice	2-methyl-5-propyl -nonane	Not Available	FALSE	CC(CCC(CCCC)CCC)C
MOL004917	0.7526	0.2474	0.7706	licorice	glycyroside	Not Available	FALSE	C1OC(C(C1(CO)O)O)OC1C(C(C(OC1Oc1ccc2c(c1)occ(c2=O)c1ccc(cc1)OC)CO)O)O
MOL004918	0.9248	0.0752	0.9496	Zanthoxyli Pericarpium	HEX	8058	FALSE	CCCCCC
MOL004918	0.9248	0.0752	0.9496	Oroxyli Semen	HEX	8058	FALSE	CCCCCC
MOL004918	0.9248	0.0752	0.9496	Viticis Negundo Folium	HEX	8058	FALSE	CCCCCC
MOL004918	0.9248	0.0752	0.9496	Ginkgo Folium	HEX	8058	FALSE	CCCCCC
MOL004918	0.9248	0.0752	0.9496	Rose Rugosae Flos	HEX	8058	FALSE	CCCCCC

MOL004918	0.9248	0.0752	0.9496	licorice	HEX	8058	FALSE	CCCCCC
MOL004919	0.8982	0.1018	0.9549	Apocyniveneti Folium	Sextone B	7962	FALSE	C1(CCCCC1)C
MOL004919	0.8982	0.1018	0.9549	Allium Azureum Ledeb.	Sextone B	7962	FALSE	C1(CCCCC1)C
MOL004919	0.8982	0.1018	0.9549	licorice	Sextone B	7962	FALSE	C1(CCCCC1)C
MOL004920	0.8829	0.1171	0.9580	Ginkgo Folium	Methylcyclopentane	7296	FALSE	C1(CCCC1)C
MOL004920	0.8829	0.1171	0.9580	licorice	Methylcyclopentane	7296	FALSE	C1(CCCC1)C
MOL004922	0.8812	0.1188	0.7109	licorice	2-methyl-6-ethyl decane	Not Available	FALSE	CC(CCCC(CCCC)CC)C
MOL004924	0.7993	0.2007	0.6102	licorice	(-)-Medicocarpin	23724664	FALSE	C12C(c3c(O2)cc(cc3)OC)COc2c1ccc(c2)OC1OC(C(C(C1O)O)O)CO
MOL004925	0.8571	0.1429	0.8397	Crataegi Folium	vitexin	5280441	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2oc(cc(=O)c2c(O)cc1O)c1ccc(O)cc1
MOL004925	0.8571	0.1429	0.8397	Humulus Scandens (Lour.) Merr.	vitexin	5280441	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2oc(cc(=O)c2c(O)cc1O)c1ccc(O)cc1
MOL004925	0.8571	0.1429	0.8397	Sophorae Tonkinensis Radix Et Rhizome	vitexin	5280441	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2oc(cc(=O)c2c(O)cc1O)c1ccc(O)cc1
MOL004925	0.8571	0.1429	0.8397	Hordei Fructus Germinatus	vitexin	5280441	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2oc(cc(=O)c2c(O)cc1O)c1ccc(O)cc1
MOL004925	0.8571	0.1429	0.8397	Microctis Folium	vitexin	5280441	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2oc(cc(=O)c2c(O)cc1O)c1ccc(O)cc1
MOL004925	0.8571	0.1429	0.8397	Cannabis Sativa L.	vitexin	5280441	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2oc(cc(=O)c2c(O)cc1O)c1ccc(O)cc1
MOL004925	0.8571	0.1429	0.8397	Commelinae Herba	vitexin	5280441	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2oc(cc(=O)c2c(O)cc1O)c1ccc(O)cc1
MOL004925	0.8571	0.1429	0.8397	Viticis Fructus	vitexin	5280441	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2oc(cc(=O)c2c(O)cc1O)c1ccc(O)cc1
MOL004925	0.8571	0.1429	0.8397	Trigonellae Semen	vitexin	5280441	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2oc(cc(=O)c2c(O)cc1O)c1ccc(O)cc1
MOL004925	0.8571	0.1429	0.8397	Spirodelae Herba	vitexin	5280441	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2oc(cc(=O)c2c(O)cc1O)c1ccc(O)cc1
MOL004925	0.8571	0.1429	0.8397	licorice	vitexin	5280441	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2oc(cc(=O)c2c(O)cc1O)c1ccc(O)cc1
MOL004925	0.8571	0.1429	0.8397	Vigna Radiata	vitexin	5280441	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2oc(cc(=O)c2c(O)cc1O)c1ccc(O)cc1
MOL004925	0.8571	0.1429	0.8397	Artemisia Annua L.	vitexin	5280441	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2oc(cc(=O)c2c(O)cc1O)c1ccc(O)cc1
MOL004925	0.8571	0.1429	0.8397	Gossampiniflos	vitexin	5280441	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2oc(cc(=O)c2c(O)cc1O)c1ccc(O)cc1
MOL004925	0.8571	0.1429	0.8397	Santalum Album L.	vitexin	5280441	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2oc(cc(=O)c2c(O)cc1O)c1ccc(O)cc1

MOL004925	0.8571	0.1429	0.8397	Zanthoxylum Nitidum	vitexin	5280441	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2oc(cc(=O)c2c(O)cc1O)c1ccc(O)cc1
MOL004926	0.8307	0.1693	0.6649	licorice	4H-1-Benzopyran-4-one, 2-(4-(beta-D-glucopyranosyloxy)phenyl)-2,3-dihydro-5,7-dihydroxy-, (2S)-	157745	FALSE	c1c(cc2c(c1O)C(=O)CC(O2)c1ccc(cc1)OC1OC(C(C(C1O)O)O)CO)O
MOL004926	0.8307	0.1693	0.6649	Choerospondiatis Fructus	4H-1-Benzopyran-4-one, 2-(4-(beta-D-glucopyranosyloxy)phenyl)-2,3-dihydro-5,7-dihydroxy-, (2S)-	157745	FALSE	c1c(cc2c(c1O)C(=O)CC(O2)c1ccc(cc1)OC1OC(C(C(C1O)O)O)CO)O
MOL004927	0.0913	0.9087	0.7003	licorice	Hispaglabridin A	442774	FALSE	O1CC(Cc2c1c1c(OC(C=C1)(C)C)cc2)c1c(O)c(c(O)cc1)CC=C(C)C
MOL004928	0.8729	0.1271	0.7979	licorice	violanthin	Not Available	FALSE	C1(C(OC(C(C1O)O)CO)c1c(c2c(c(c1O)C1C(C(C(C(O1)C)O)O)O)oc(cc2=O)c1ccc(cc1)O)O)O
MOL004929	0.7837	0.2163	0.6681	licorice	Pentadecanol	12397	FALSE	C(CCCCCCCO)CCCCCCC
MOL004930	0.6193	0.3807	0.7535	licorice	Uralenol	5315126	FALSE	c1(c2cc(c(c(c2)O)O)CC=C(C)C)oc2c(c(=O)c1O)c(cc(c2)O)O
MOL004931	0.4984	0.5016	0.7553	licorice	Uralenol-3-methylether	5315127	FALSE	c12c(c(cc(c1)O)O)c(=O)c(c(o2)c1cc(c(c(c1)CC=C(C)C)O)O)OC
MOL004932	0.7373	0.2627	0.8470	licorice	glycyrrhizin	128229	FALSE	C1(CCC2(C(C1)C1=CC(=O)C3C(C1(CC2)C)(CCC1C3(CCC(C1(C)C)OC1OC(C(C(C1OC1OC(C(O)C(C1O)O)C(=O)O)O)O)C(=O)O)C)C)(C)C(=O)O
MOL004933	0.7295	0.2705	0.8445	licorice	uralsaponin B	Not Available	FALSE	C1C(CCC2(C1C1=CC(=O)C3C(C1(CC2)C)(CCC1C3(CCC(C1(C)C)OC1OC(C(C(C1O)OC1OC(C(C(C1O)O)O)C(=O)O)O)C(=O)O)C)C)(C)C(=O)O
MOL004934	0.9295	0.0705	0.9478	Rubi Fructus	Isohexane	7892	FALSE	C(CC(C)C)C
MOL004934	0.9295	0.0705	0.9478	licorice	Isohexane	7892	FALSE	C(CC(C)C)C
MOL004934	0.9295	0.0705	0.9478	Sesami Nigrum Semen	Isohexane	7892	FALSE	C(CC(C)C)C
MOL004934	0.9295	0.0705	0.9478	Hippophae Fructus	Isohexane	7892	FALSE	C(CC(C)C)C
MOL004935	0.5971	0.4029	0.7670	licorice	Sigmoidin-B	73205	FALSE	C1(CC(=O)c2c(O1)cc(cc2O)O)c1cc(c(c(c1)CC=C(C)C)O)O

MOL004936	0.5092	0.4908	0.6888	licorice	Uralene	192490	FALSE	c1cc2c(c(c1O)O)c(=O)c(c(o2)c1c(cc(c(c1)O)O)CC=C(C)C)OC
MOL004936	0.5092	0.4908	0.6888	Corayceps	Uralene	192490	FALSE	c1cc2c(c(c1O)O)c(=O)c(c(o2)c1c(cc(c(c1)O)O)CC=C(C)C)OC
MOL004937	0.9211	0.0789	0.9345	licorice	uralenneoside	Not Available	FALSE	O1C(C(C(C(C1)O)O)O)OC(=O)c1ccc(c(c1)O)O
MOL004938	0.8721	0.1279	0.7695	licorice	schaftoside	46928317	FALSE	c1(cc(=O)c2c(O)c(c(O)c(c2o1)OC1C(O)C(O)C(O)CO1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL004939	0.9380	0.0620	0.8698	Trigonellae Semen	Nortangeretin	96506	FALSE	c1(cc(=O)c2c(O)c(c(O)c(c2o1)O)O)c1ccc(O)cc1
MOL004939	0.9380	0.0620	0.8698	licorice	Nortangeretin	96506	FALSE	c1(cc(=O)c2c(O)c(c(O)c(c2o1)O)O)c1ccc(O)cc1
MOL004940	0.7883	0.2117	0.8197	licorice	neoliquiritin	51666249	FALSE	c1cc(cc2c1C(=O)CC(O2)c1ccc(cc1)O)OC1C(C(C(C(O1)CO)O)O)O
MOL004940	0.7883	0.2117	0.8197	Polygonati Rhizoma	neoliquiritin	51666249	FALSE	c1cc(cc2c1C(=O)CC(O2)c1ccc(cc1)O)OC1C(C(C(C(O1)CO)O)O)O
MOL004941	0.9203	0.0797	0.7746	licorice	(2R)-7-hydroxy-2-(4-hydroxyphenyl)chroman-4-one	928837	FALSE	c1cc(cc2c1C(=O)CC(O2)c1ccc(cc1)O)O
MOL004941	0.9203	0.0797	0.7746	Polygonati Rhizoma	(2R)-7-hydroxy-2-(4-hydroxyphenyl)chroman-4-one	928837	FALSE	c1cc(cc2c1C(=O)CC(O2)c1ccc(cc1)O)O
MOL004941	0.9203	0.0797	0.7746	Hedysari Radix	(2R)-7-hydroxy-2-(4-hydroxyphenyl)chroman-4-one	928837	FALSE	c1cc(cc2c1C(=O)CC(O2)c1ccc(cc1)O)O
MOL004941	0.9203	0.0797	0.7746	Sophorae Flavescentis Radix	(2R)-7-hydroxy-2-(4-hydroxyphenyl)chroman-4-one	928837	FALSE	c1cc(cc2c1C(=O)CC(O2)c1ccc(cc1)O)O
MOL004942	0.8795	0.1205	0.8097	licorice	(E)-dodec-2-ene	5352911	FALSE	C(CCCCCC)CC/C=C/C
MOL004942	0.8795	0.1205	0.8097	Arisaematis Rhizoma	(E)-dodec-2-ene	5352911	FALSE	C(CCCCCC)CC/C=C/C
MOL004943	0.8491	0.1509	0.7745	licorice	neoisoliquiritin	Not Available	FALSE	C1(Oc2cc(c(cc2)C(=O)/C=C\c2ccc(cc2)O)O)OC(C(C(C1O)O)O)CO
MOL004944	0.8941	0.1059	0.9624	licorice	Cyclobutanol, 1-ethyl-	145025	FALSE	C1(CCC1)(O)CC

MOL004945	0.3814	0.6186	0.6314	licorice	(2S)-7-hydroxy-2-(4-hydroxyphenyl)-8-(3-methylbut-2-enyl)chroman-4-one	193679	FALSE	C1(CC(=O)c2c(O1)c(c(cc2)O)CC=C(C)C)c1ccc(cc1)O
MOL004946	0.8358	0.1642	0.7709	licorice	2-Tetradecanone	75364	FALSE	C(CCCCCCCCC)CCC(=O)C
MOL004947	0.8729	0.1271	0.7980	licorice	Isoviolanthin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c(C2OC(C(O)C(O)C2O)C)c(O)c2c1oc(cc2=O)c1ccc(O)cc1
MOL004948	0.7090	0.2910	0.7637	licorice	Isoglycyrol	Not Available	FALSE	c1c2c(ccc1O)c1c(c3c(oc1=O)cc1c(CCC(O1)(C)C)c3OC)o2
MOL004949	0.5349	0.4651	0.6066	licorice	Isolicoflavonol	5318585	FALSE	c1c(cc2c(c1O)c(=O)c(c(o2)c1cc(c(cc1)O)CC=C(C)C)O)O
MOL004950	0.3675	0.6325	0.8559	licorice	isoglycycoumarin	14187587	FALSE	C1(CCc2c(O1)cc1c(c2OC)cc(c(=O)o1)c1c(cc(cc1)O)O)(C)C
MOL004951	0.7708	0.2292	0.6351	licorice	Isoliquiritin	Not Available	FALSE	C1(Oc2ccc(cc2)/C=C\C(=O)c2c(cc(cc2)O)O)OC(C(C(C1O)O)O)CO
MOL004952	0.8332	0.1668	0.7567	licorice	licuraside	14282455	FALSE	c1cc(ccc1O)/C=C/C(=O)c1c(cc(cc1)OC1C(C(C(C(O1)CO)O)O)OC1C(C(CO1)(CO)O)O)O
MOL004953	0.8299	0.1701	0.8108	licorice	Liquiritin apioside	Not Available	FALSE	C1(c2ccc(cc2)OC2C(C(C(C(O2)CO)O)O)OC2C(C(CO2)(CO)O)O)CC(=O)c2c(O1)cc(cc2)O
MOL004955	0.4151	0.5849	0.7579	licorice	isoglabrolide	Not Available	FALSE	C1(C2C(CCC1O)(C1C(CC2)(C2(C(=CC1=O)C13C(CC2)(CCC(C1)(C(=O)O3)C)C)C)C)(C)C
MOL004957	0.9033	0.0967	0.9275	licorice	HMO	3764	FALSE	Oc1ccc(cc1)c1c(=O)c2c(oc1)cc(OC)cc2
MOL004958	0.8801	0.1199	0.7779	licorice	Isoschaftoside	3084995	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c(C2OCC(O)C(O)C2O)c(O)c2c1oc(cc2=O)c1ccc(O)cc1
MOL004958	0.8801	0.1199	0.7779	Arisaematis Rhizoma	Isoschaftoside	3084995	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c(C2OCC(O)C(O)C2O)c(O)c2c1oc(cc2=O)c1ccc(O)cc1
MOL004958	0.8801	0.1199	0.7779	Acoritataninowii Rhizoma	Isoschaftoside	3084995	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c(C2OCC(O)C(O)C2O)c(O)c2c1oc(cc2=O)c1ccc(O)cc1
MOL004959	0.3778	0.6222	0.7752	licorice	1-Methoxyphaseollidin	480873	FALSE	O1C2C(c3c1c(c(O)cc3)CC=C(C)C)COc1c2c(OC)cc(O)c1
MOL004960	0.6559	0.3441	0.7196	licorice	22β-acetylglabric acid	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1=O)C1C(CC2)(C)C(CC(C1)(C)C(=O)O)OC(=O)C)C)C)(C)C)O
MOL004961	0.8589	0.1411	0.8813	Centipedae Herba	Quercetin der.	5316900	FALSE	c1(c(OC)c(=O)c2c(O)cc(O)cc2o1)c1ccc(c(c1)OC)O
MOL004961	0.8589	0.1411	0.8813	licorice	Quercetin der.	5316900	FALSE	c1(c(OC)c(=O)c2c(O)cc(O)cc2o1)c1ccc(c(c1)OC)O

MOL004962	0.6721	0.3279	0.7508	licorice	24-Hydroxy-11-deoxyglycyrrhetic acid	Not Available	FALSE	C1C2C(CCC1(C)C(=O)O)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(O)C)O)C)C)C)C
MOL004963	0.7164	0.2836	0.7081	Hemerocallis Radix	24-Hydroxyglycyrrhetic acid	Not Available	FALSE	C1C2(C(C(C(C1)O)(CO)C)CCC1(C2C(=O)C=C2C1(CCC1(C2CC(CC1)(C)C(=O)O)C)C)C)C
MOL004963	0.7164	0.2836	0.7081	licorice	24-Hydroxyglycyrrhetic acid	Not Available	FALSE	C1C2(C(C(C(C1)O)(CO)C)CCC1(C2C(=O)C=C2C1(CCC1(C2CC(CC1)(C)C(=O)O)C)C)C)C
MOL004964	0.8902	0.1098	0.9254	licorice	(Z)-1-(2,4-dihydroxyphenyl)-3-phenylprop-2-en-1-one	10331849	FALSE	c1(ccc(c(c1)O)C(=O)/C=C\c1ccccc1)O
MOL004966	0.2765	0.7235	0.6601	licorice	3'-Hydroxy-4'-O-Methylglabridin	15228662	FALSE	O1CC(Cc2c1c1c(OC(C=C1)(C)C)cc2)c1c(O)c(c(OC)cc1)O
MOL004967	0.9199	0.0801	0.9452	Semen Pharbitidis	3,3-Dimethylpentane	11229	FALSE	C(CC)(CC)(C)C
MOL004967	0.9199	0.0801	0.9452	Allium Azureum Ledeb.	3,3-Dimethylpentane	11229	FALSE	C(CC)(CC)(C)C
MOL004967	0.9199	0.0801	0.9452	licorice	3,3-Dimethylpentane	11229	FALSE	C(CC)(CC)(C)C
MOL004968	0.8663	0.1337	0.7840	licorice	3,4,3',4'-Tetrahydroxy-2-methoxychalcone	Not Available	FALSE	Oc1c(c(c(C/C=C\c2cc(O)c(O)cc2)cc1)OC)O
MOL004969	0.9516	0.0484	0.8791	licorice	2-Ethyl-p-xylene	15653	FALSE	c1(c(cc(cc1)C)CC)C
MOL004969	0.9516	0.0484	0.8791	Ephedra Herba	2-Ethyl-p-xylene	15653	FALSE	c1(c(cc(cc1)C)CC)C
MOL004970	0.9250	0.0750	0.9344	licorice	3-methylheptane	12263096	FALSE	C(CCCC)(CC)C
MOL004971	0.9230	0.0770	0.9455	Rose Rugosae Flos	3-methylhexane	13800357	FALSE	C(CCC)(CC)C

MOL004971	0.9230	0.0770	0.9455	Semen Pharbitidis	3-methylhexane	13800357	FALSE	C(CCC)(CC)C
MOL004971	0.9230	0.0770	0.9455	licorice	3-methylhexane	13800357	FALSE	C(CCC)(CC)C
MOL004971	0.9230	0.0770	0.9455	Capsici Fructus	3-methylhexane	13800357	FALSE	C(CCC)(CC)C
MOL004971	0.9230	0.0770	0.9455	Zanthoxyli Pericarpium	3-methylhexane	13800357	FALSE	C(CCC)(CC)C
MOL004972	0.9260	0.0740	0.9526	licorice	3-Methylpentane	7282	FALSE	C(CC)(CC)C
MOL004973	0.9220	0.0780	0.9470	Semen Pharbitidis	3-Ethylpentane	12048	FALSE	C(CC)(CC)CC
MOL004973	0.9220	0.0780	0.9470	licorice	3-Ethylpentane	12048	FALSE	C(CC)(CC)CC
MOL004974	0.2734	0.7266	0.8372	licorice	3'-Methoxyglabridin	15228663	FALSE	O1CC(Cc2c1c1c(OC(C=C1)(C)C)cc2)c1c(O)c(OC)c(O)cc1
MOL004975	0.3063	0.6937	0.7675	licorice	3β-formylglabrolide	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1=O)C1C(CC2)(C2CC(C1)(C(=O)O2)C)C)C)C)(C)C)OC=O
MOL004976	0.8104	0.1896	0.9014	licorice	Daidzein dimethyl ether	136419	FALSE	c12c(cc(cc2)OC)occ(c1=O)c1ccc(cc1)OC
MOL004977	0.1056	0.8944	0.7253	licorice	1-Methoxyficifolinol	480872	FALSE	c1c2c(c(c(c1O)CC=C(C)C)OC)C1C(CO2)c2c(cc(c(c2)CC=C(C)C)O)O1
MOL004978	0.1615	0.8385	0.8740	licorice	2-[(3R)-8,8-dimethyl-3,4-dihydro-2H-pyrano[6,5-f]chromen-3-yl]-5-methoxyphenol	9927807	FALSE	O1CC(Cc2c1c1c(OC(C=C1)(C)C)cc2)c1c(O)cc(OC)cc1
MOL004979	0.8817	0.1183	0.8693	licorice	4,2',4',alpha-Tetrahydroxydihydrochalcone	14632193	FALSE	OC(Cc1ccc(O)cc1)C(=O)c1c(O)cc(O)cc1

MOL004981	0.4516	0.5484	0.6069	licorice	1-(5-hydroxy-2,2-dimethylchromen-6-yl)-3-(4-hydroxyphenyl)prop-2-en-1-one	5889042	FALSE	O1C(C=Cc2c1ccc(c2O)C(=O)/C=C/c1ccc(O)cc1)(C)C
MOL004982	0.9208	0.0792	0.9742	Ardisiae Japonicae Herba	2,6,10-trimethyl-dodecane	Not Available	FALSE	C1(=C(OCC(C1=O)O)C)O
MOL004982	0.9208	0.0792	0.9742	Caryophylliflos	2,6,10-trimethyl-dodecane	Not Available	FALSE	C1(=C(OCC(C1=O)O)C)O
MOL004982	0.9208	0.0792	0.9742	Citri Sarcodactylis Fructus	2,6,10-trimethyl-dodecane	Not Available	FALSE	C1(=C(OCC(C1=O)O)C)O
MOL004982	0.9208	0.0792	0.9742	Ephedra Herba	2,6,10-trimethyl-dodecane	Not Available	FALSE	C1(=C(OCC(C1=O)O)C)O
MOL004982	0.9208	0.0792	0.9742	Momordicae Fructus	2,6,10-trimethyl-dodecane	Not Available	FALSE	C1(=C(OCC(C1=O)O)C)O
MOL004982	0.9208	0.0792	0.9742	licorice	2,6,10-trimethyl-dodecane	Not Available	FALSE	C1(=C(OCC(C1=O)O)C)O
MOL004982	0.9208	0.0792	0.9742	Magnolia Officinalis Rehd Et Wils.	2,6,10-trimethyl-dodecane	Not Available	FALSE	C1(=C(OCC(C1=O)O)C)O
MOL004983	0.9413	0.0587	0.8675	licorice	5,6,7,8-Tetrahydro-4-methylquinoline	185667	FALSE	n1ccc(c2CCCCc12)C
MOL004987	0.7121	0.2879	0.8745	licorice	11-deoxyglycyrrhetic acid	12305517	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C(=O)O)C)C)C)C)(C)C)O
MOL004987	0.7121	0.2879	0.8745	Eucommiae Cortex	11-deoxyglycyrrhetic acid	12305517	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C(=O)O)C)C)C)C)(C)C)O
MOL004988	0.1560	0.8440	0.7525	licorice	Kanzonol F	Not Available	FALSE	C1C2C(c3c(O1)cc(c(c3OC)CC=C(C)C)O)Oc1cc3c(C=CC(O3)(C)C)cc21
MOL004989	0.6390	0.3610	0.7778	licorice	6-prenylated eriodictyol	Not Available	FALSE	c1(c(c(c2c(c1)OC(CC2=O)c1ccc(c(c1)O)O)O)CC=C(C)C)O

MOL004990	0.9210	0.0790	0.9155	licorice	7,2',4'-trihydroxy—5-methoxy-3—arylcoumarin	25015742	FALSE	c1(=O)c(cc2c(o1)cc(cc2OC)O)c1ccc(cc1O)O
MOL004991	0.5362	0.4638	0.9052	licorice	7-Acetoxy-2-methylisoflavone	268208	FALSE	c1(ccc2c(c1)oc(c(c2=O)c1ccccc1)C)OC(=O)C
MOL004992	0.8317	0.1683	0.9391	licorice	7-hydroxy-2-methyl-3-phenyl-chromone	5380976	FALSE	c12c(c(=O)c(c(o1)C)c1ccccc1)ccc(c2)O
MOL004993	0.6141	0.3859	0.7890	licorice	8-prenylated eriodictyol	Not Available	FALSE	c1(cc(c2c(c1CC=C(C)C)OC(CC2=O)c1ccc(c(c1)O)O)O)O
MOL004994	0.7569	0.2431	0.6675	Notopterygii Rhizoma Et Radix	12-methyltetradecanoate	Not Available	FALSE	O(C(=O)CCCCCCCCCCC(CC)C)C
MOL004994	0.7569	0.2431	0.6675	Arisaematis Rhizoma	12-methyltetradecanoate	Not Available	FALSE	O(C(=O)CCCCCCCCCCC(CC)C)C
MOL004994	0.7569	0.2431	0.6675	licorice	12-methyltetradecanoate	Not Available	FALSE	O(C(=O)CCCCCCCCCCC(CC)C)C
MOL004995	0.0662	0.9338	0.7282	licorice	Kanzonol H	480863	FALSE	O1C(CCc2c1cc1OCC(Cc1c2OC)c1c(O)c(c(O)cc1)CC=C(C)C)(C)C
MOL004997	0.7197	0.2803	0.8508	licorice	Araboglycyrrhizin	Not Available	FALSE	C1C2C(CCC1(C(=O)O)C)(CCC1(C2=CC(=O)C2C1(CCC1C2(CCC(C1(C)C)OC1C(C(C(C(O1)C(=O)O)O)O)OC1OCC(C(C1O)O)O)C)C)C)C
MOL004998	0.7209	0.2791	0.7420	licorice	Araboglycyrrhizin_qt	Not Available	FALSE	C1C2C(CCC1(C(=O)O)C)(CCC1(C2=CC(=O)C2C1(CCC1C2(CCC(C1(C)C)O)C)C)C)C
MOL004999	0.4261	0.5739	0.7843	licorice	Artonin E	5481962	FALSE	O1C(C=Cc2c3oc(c(c(=O)c3c(O)cc12)CC=C(C)C)c1c(O)cc(O)c(O)c1)(C)C
MOL005000	0.2767	0.7233	0.7846	licorice	Gancaonin G	480780	FALSE	O1C2C(C(O)C(CC=C(C)C)C(OC)C2)C(=O)C(C2CCC(O)CC2)C1
MOL005001	0.1446	0.8554	0.6898	licorice	Gancaonin H	5481949	FALSE	O1C(C=Cc2c1c(O)cc(c2)c1c(=O)c2c(oc1)cc(O)c(c2O)CC=C(C)C)(C)C
MOL005002	0.7209	0.2791	0.7420	licorice	beta-Glycyrrhetinic acid	73398	FALSE	OC1C(C2C(C3C(C4(C(=CC3=O)C3C(CC4)(CCC(C3)(C)C(=O)O)C)C)(CC2)C)(CC1)C)(C)C
MOL005003	0.2287	0.7713	0.8341	licorice	Licoagrocarpin	15840593	FALSE	c1(ccc2c(c1CC=C(C)C)OCC1C2Oc2c1ccc(c2)OC)O
MOL005004	0.3600	0.6400	0.7092	licorice	Gancaonin I	480777	FALSE	O1C2C(C(OC)C(C(OC)C2)CC=C(C)C)CC1C1C(O)CC(O)C=C1
MOL005006	0.1507	0.8493	0.8220	licorice	Glyasperins K	Not Available	FALSE	O1c2c(C(=O)C(C1)c1ccc(cc1O)OC)cc(c(c2)OC)CC=C(C)C

MOL005007	0.3662	0.6338	0.8302	licorice	Glyasperins M	Not Available	FALSE	O1c2c(C(=O)C(C1)c1ccc3c(c1O)C=CC(O3)(C)C)c(cc(c2)O)OC
MOL005008	0.5312	0.4688	0.7135	licorice	Glycyrrhiza flavonol A	Not Available	FALSE	O1C(C(O)Cc2c1ccc(c2)c1oc2c(c(=O)c1O)c(O)cc(O)c2)(C)C
MOL005010	0.1016	0.8984	0.7517	licorice	Kanzonol E	15516846	FALSE	O1C(C=Cc2c1ccc(c2)c1oc2c(cc(CC=C(C)C)c(O)c2)c(=O)c1)(C)C
MOL005011	0.1183	0.8817	0.7497	licorice	Kanzonol Z	Not Available	FALSE	O1C(C=Cc2c3c(ccc12)C(=O)C(C(O3)c1cc(c(cc1)O)CC=C(C)C)O)(C)C
MOL005012	0.4641	0.5359	0.7800	licorice	Licoagroisoflavone	636883	FALSE	O1C(Cc2c1cc1occ(c(=O)c1c2O)c1ccc(O)cc1)C(=C)C
MOL005013	0.7285	0.2715	0.7144	licorice	18α-hydroxyglycyrrhetic acid	Not Available	FALSE	C1C2(C(CCC1(C(=O)O)C)(CCC1(C2=CC(=O)C2C1(CCC1C2(CCC(C1(C)C)O)C)C)C)C)O
MOL005014	0.4330	0.5670	0.6752	licorice	Licorice glycoside A	Not Available	FALSE	O(C1C(O)C(O)C(OC1Oc1ccc(/C=C\C(=O)c2ccc(O)cc2O)cc1)CO)C1OCC(O)(C1O)COC(=O)/C=C/c1cc(c(cc1)O)OC
MOL005015	0.0686	0.9314	0.6289	licorice	Licoriisoflavan A	196831	FALSE	c1(c(c(c2c(c1)OCC(C2)c1c(c(c(cc1)O)CC=C(C)C)O)OC)CC=C(C)C)OC
MOL005016	0.7940	0.2060	0.8962	licorice	Odoratin	13965473	FALSE	o1c2c(c(=O)c(c3cc(O)c(OC)cc3)c1)cc(OC)c(O)c2
MOL005017	0.7594	0.2406	0.7771	licorice	Phaseol	44257530	FALSE	o1c2c3c(oc(=O)c2c2c1cc(O)cc2)c(CC=C(C)C)c(O)cc3
MOL005018	0.1007	0.8993	0.7760	licorice	Xambioona	Not Available	FALSE	O1C(CC(=O)c2c1c1c(OC(C=C1)(C)C)cc2)c1cc2c(OC(C=C2)(C)C)cc1
MOL005019	0.3543	0.6457	0.6273	licorice	(2R)-7-hydroxy-2-[4-hydroxy-3-(3-methylbut-2-enyl)phenyl]chroman-4-one	7330518	FALSE	c1(ccc2c(c1)OC(CC2=O)c1ccc(c(c1)CC=C(C)C)O)O
MOL005020	0.5632	0.4368	0.6885	licorice	dehydroglyasperins C	Not Available	FALSE	c1(c(c(c2c(c1)OCC(=C2)c1ccc(cc1O)O)O)CC=C(C)C)O
MOL005021	0.9448	0.0552	0.9170	Herba Sarcandrae	Mipax	8554	FALSE	c1(ccccc1C(=O)OC)C(=O)OC
MOL005021	0.9448	0.0552	0.9170	Folium Ilicis Cornutae	Mipax	8554	FALSE	c1(ccccc1C(=O)OC)C(=O)OC
MOL005021	0.9448	0.0552	0.9170	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Mipax	8554	FALSE	c1(ccccc1C(=O)OC)C(=O)OC
MOL005021	0.9448	0.0552	0.9170	licorice	Mipax	8554	FALSE	c1(ccccc1C(=O)OC)C(=O)OC
MOL005022	0.9359	0.0641	0.7179	Gossampiniflos	1,8-DIMETHYLNAPHTHALENE	11287	FALSE	c12c(cccc1C)cccc2C
MOL005022	0.9359	0.0641	0.7179	Cornus Officinalis Sieb. Et Zucc.	1,8-DIMETHYLNAPHTHALENE	11287	FALSE	c12c(cccc1C)cccc2C

MOL005022	0.9359	0.0641	0.7179	Cannabis Sativa L.	1,8-DIMETHYLNAPHTHALENE	11287	FALSE	c12c(cccc1C)cccc2C
MOL005023	0.9161	0.0839	0.9654	Cannabis Sativa L.	(R)-2-butanol	84682	FALSE	C(CC)(C)O
MOL005024	0.8798	0.1202	0.9672	Cannabis Sativa L.	WLN: QR CG	7933	FALSE	c1c(cccc1Cl)O
MOL005025	0.9482	0.0518	0.9289	Cannabis Sativa L.	4-Hydroxy-2-methylacetophenone	70133	FALSE	c1(c(cc(cc1)O)C)C(=O)C
MOL005026	0.1503	0.8497	0.7281	Cannabis Sativa L.	tetrahydrocannabinol	16078	FALSE	C12c3c(OC(C1CCC(=C2)C)(C)C)cc(cc3O)CCCCC
MOL005027	0.2592	0.7408	0.8866	Cannabis Sativa L.	cannabidiol	36688143	FALSE	C1(c2c(cc(cc2O)CCCCC)O)C(CCC(=C1)C)C(=C)C
MOL005028	0.2107	0.7893	0.7879	Cannabis Sativa L.	Cannabinol	2543	FALSE	c12c3c(OC(c1ccc(c2)C)(C)C)cc(cc3O)CCCCC
MOL005029	0.1645	0.8355	0.8751	Cannabis Sativa L.	(2S)-7-amyl-2-methyl-2-(4-methylpent-3-enyl)chromen-5-ol	21668219	FALSE	O1C(CCC=C(C)C)(C=Cc2c1cc(CCCCC)cc2O)C
MOL005031	0.9441	0.0559	0.8276	Cannabis Sativa L.	zeatin	449093	FALSE	C(/C(=C/CNc1ncnc2nc[nH]c12)/C)O
MOL005033	0.5331	0.4669	0.7547	Aloe	2'-O-p-Coumaroylaloesin	Not Available	FALSE	O1C(C(OC(=O)/C=C/c2ccc(O)c(c2)OC)C(O)C(O)C1CO)c1c2oc(cc(=O)c2c(cc1O)C)CC(=O)C
MOL005034	0.8395	0.1605	0.8444	Aloe	5-HydroxyaloinA	11972367	FALSE	O1C(C2c3c(C(=O)c4c2c(O)ccc4O)c(O)cc(c3)CO)C(O)C(O)C(O)C1CO
MOL005035	0.5144	0.4856	0.7381	Aloe	6'-O-p-Coumaroylaloesin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1COC(=O)/C=C/c1ccc(c(c1)OC)O)c1c2oc(cc(=O)c2c(cc1O)C)CC(=O)C
MOL005036	0.8403	0.1597	0.8480	Aloe	7-hydroxyaloin	Not Available	FALSE	O1C(C2c3c(C(=O)c4c2ccc(O)c4O)c(O)cc(c3)CO)C(O)C(O)C(O)C1CO
MOL005037	0.9245	0.0755	0.8353	Aloe	Isoaloesin	11972379	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(c2c(oc(cc2=O)CC(=O)C)cc1O)C)CO
MOL005038	0.9507	0.0493	0.8853	Aloe	Isoaloesin_qt	Not Available	FALSE	Oc1c(c2c(oc(cc2=O)CC(=O)C)cc1O)C
MOL005039	0.8629	0.1371	0.7773	Aloe	aloveroside	Not Available	FALSE	C1CCC2C(C1OC1OC(C(C(C1O)O)O)C)C(C(CC2COC1OCC(C(C1O)O)OC1OC(C(C(C1O)O)O)CO)C(=O)C)O
MOL005040	0.9512	0.0488	0.8547	Aloe	aloveroside_qt	Not Available	FALSE	c1ccc2c(c1O)c(c(cc2CO)C(=O)C)O
MOL005041	0.6181	0.3819	0.7498	Aloe	elgnica	Not Available	FALSE	C1(CCCC2C1C(=O)C1C(C2(C2OC(C(C(C2O)O)O)CO)C2c(c3c(cc2)C(=O)c2c(C3=O)c(cc(c2)CO)O)O)cc(cc1O)CO)O
MOL005042	0.5074	0.4926	0.6186	Aloe	p-coumaroyl	Not Available	FALSE	c1c(cc(c(c1C)c1cc(cc(=O)o1)OC)OC1OC(C(C(C1OC(=O)/C=C/c1ccc(cc1)O)O)O)CO)O

MOL005044	0.8239	0.1761	0.8818	Aloe	Homonataloin	Not Available	FALSE	c1(c(ccc2C(c3cc(cc(c3C(=O)c12)O)C)C1C(O)C(O)C(O)C(O1)CO)O)OC
MOL005045	0.9596	0.0404	0.8482	Aloe	feroxidin	Not Available	FALSE	OC1CC(c2c(C1)cc(O)cc2O)C
MOL005046	0.8396	0.1604	0.8683	Aloe	10-.BETA.-D-Glucopyranosyl-1,8-dihydroxy-3-(hydroxymethyl)-9(10H)-anthracenone-, 10(S)-	12305761	FALSE	O1C(C2c3c(C(=O)c4c2cccc4O)c(O)cc(c3)CO)C(O)C(O)C(O)C1CO
MOL005047	0.8865	0.1135	0.8510	Aloe	Aloesin	160190	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2oc(cc(=O)c2c(cc1O)C)CC(=O)C
MOL005048	0.9246	0.0754	0.8090	Aloe	2H-Pyran-2-one, 6-(2-(beta-D-glucopyranosyloxy)-4-hydroxy-6-methylphenyl)-4-methoxy-	162305	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(c(cc(O)c1)C)c1oc(=O)cc(OC)c1)CO
MOL005049	0.9538	0.0462	0.7581	Aloe	6-(2,4-dihydroxy-6-methylphenyl)-4-methoxypyran-2-one	5242842	FALSE	Oc1c(c(cc(O)c1)C)c1oc(=O)cc(OC)c1
MOL005050	0.5424	0.4576	0.7480	Aloe	aloeresinA	Not Available	FALSE	c12c(C3C(C(C(C(O3)CO)O)O)OC(=O)/C=C\c3ccc(cc3)O)c(cc(c1c(=O)cc(o2)CC(=O)C)C)O
MOL005051	0.6374	0.3626	0.7418	Aloe	Aloeresin C	11972360	FALSE	O1C(C(OC(=O)/C=C/c2ccc(O)cc2)C(O)C(O)C1CO)c1c(OC2OC(C(O)C(O)C2O)CO)cc(c2c1oc(cc2=O)CC(=O)C)C
MOL005052	0.5424	0.4576	0.7480	Aloe	aloeresin C_qt	Not Available	FALSE	O1C(C(OC(=O)/C=C/c2ccc(O)cc2)C(O)C(O)C1CO)c1c(O)cc(c2c1oc(cc2=O)CC(=O)C)C
MOL005053	0.3270	0.6730	0.6726	Aloe	Aloeresin G	5317680	FALSE	O1C(C(OC(=O)/C=C/c2ccc(O)cc2)C(O)C(O)C1CO)c1c2oc(cc(=O)c2c(cc1OC)C)/C=C/C
MOL005054	0.9519	0.0481	0.7933	Aloe	Aloesone	5317700	FALSE	c1(cc(=O)c2c(o1)cc(cc2C)O)CC(=O)C
MOL005055	0.9153	0.0847	0.7947	Aloe	Helminthosporin	97560	FALSE	c1c(cc2c(c1O)C(=O)c1c(C2=O)c(ccc1O)O)C
MOL005057	0.8551	0.1449	0.6793	Aloe	2E,4E-hexadecadienoic acid	5312421	FALSE	C(CCCCCCCCC)C/C=C/C=C/C(=O)O

MOL005058	0.8452	0.1548	0.7046	Aloe	Isoeleutherol glucoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(OC)c3C(OC(=O)c3cc2ccc1)C)CO
MOL005059	0.9021	0.0979	0.8699	Aloe	Isoeleutherol glucosiden_qt	Not Available	FALSE	Oc1c2c(OC)c3C(OC(=O)c3cc2ccc1)C
MOL005060	0.8396	0.1604	0.8683	Aloe	Aloinum	14989	FALSE	O1C(C2c3c(C(=O)c4c2cccc4O)c(O)cc(c3)CO)C(O)C(O)C(O)C1CO
MOL005061	0.8438	0.1562	0.6497	Aloe	Campherenol	Not Available	FALSE	OC1C2(C(C(C1)CC2)(CCC=C(C)C)C)C
MOL005062	0.8518	0.1482	0.7162	Aloe	ANF	10731	FALSE	c1cccc2cc3ccccc3c(c12)O
MOL005063	0.9290	0.0710	0.9378	Rose Rugosae Flos	citronellyl formate	24884267	FALSE	O(CCC(CCC=C(C)C)C)C=O
MOL005063	0.9290	0.0710	0.9378	Geranium Wilfordii Maxim.	citronellyl formate	24884267	FALSE	O(CCC(CCC=C(C)C)C)C=O
MOL005064	0.6316	0.3684	0.7425	Geranium Wilfordii Maxim.	Dehydrogeraniin	Not Available	FALSE	O1C2(O)C(O)(O)C3c4c1c(O)c(O)cc4C(=O)OC1C4OC(=O)c5c6C7C(O)(O)C(Oc6c(O)c(O)c5)(O)C(=O)C=C7C(=O)OCC(OC1OC(=O)c1cc(O)c(O)c(O)c1)C4OC(=O)C3=CC2=O
MOL005065	0.7024	0.2976	0.7332	Geranium Wilfordii Maxim.	chebulagic acid	Not Available	FALSE	C12C3C(OC(=O)C(C4c5c(OC(=O)C4O)c(c(cc5C(=O)O2)O)O)CC(=O)O)C(OC1OC(=O)c1cc(c(c(c1)O)O)O)COC(=O)c1c(c2c(C(=O)O3)cc(c(c2O)O)O)c(c(c(c1)O)O)O
MOL005066	0.8720	0.1280	0.7603	Geranium Wilfordii Maxim.	chebulinic acid	Not Available	FALSE	C12C(C(OC(=O)C(C3c4c(OC(=O)C3O)c(c(cc4C(=O)O2)O)O)CC(=O)O)C(OC1OC(=O)c1cc(c(c(c1)O)O)O)COC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O
MOL005067	0.8897	0.1103	0.7181	Geranium Wilfordii Maxim.	furosin	Not Available	FALSE	O1C2(O)C(O)(O)C3c4c1c(O)c(O)cc4C(=O)OC1C(O)C(OC(=O)C3=CC2=O)C(OC1OC(=O)c1cc(O)c(O)c(O)c1)CO
MOL005068	0.8726	0.1274	0.8647	Geranium Wilfordii Maxim.	Isogermacrone	6453848	FALSE	O=C1C(=C(C)C)C/C=C(\CCC/C(=C\1)/C)/C
MOL005069	0.8517	0.1483	0.7291	Geranium Wilfordii Maxim.	mallotinic acid	Not Available	FALSE	O1C(OC(=O)c2c(c3c(O)c(O)c(O)cc3C=O)cc(O)c(Oc3c(cc(O)c(O)c3O)C(=O)O)c2)(c2c(cc(O)c(O)c2O)C(=O)O)C(O)C(O)C(O)C1C=O
MOL005070	0.5867	0.4133	0.7444	Geranium Wilfordii Maxim.	mallotusinic acid	Not Available	FALSE	O1C2(O)C(O)(O)C3c4c1c(O)c(O)cc4C(=O)OC1C4OC(=O)c5c(c6c(C(=O)OCC(OC1OC(=O)c1cc(O)c(O)c(O)c1)C4OC(=O)C3=CC2=O)cc(O)c(O)c6O)c(O)c(O)c(Oc1c(cc(O)c(O)c1O)C(=O)O)c5
MOL005071	0.9196	0.0804	0.8020	Farfarae Flos	Spiraein	5320844	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(O)cc(cc1)c1oc2c(c(=O)c1O)c(O)cc(O)c2)CO
MOL005071	0.9196	0.0804	0.8020	Geranium Wilfordii Maxim.	Spiraein	5320844	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(O)cc(cc1)c1oc2c(c(=O)c1O)c(O)cc(O)c2)CO
MOL005072	0.9418	0.0582	0.8731	Trigonellae Semen	brevifolin	66654	FALSE	O(c1c(c(O)cc(OC)c1)C(=O)C)C
MOL005072	0.9418	0.0582	0.8731	Phyllanthi Fructus	brevifolin	66654	FALSE	O(c1c(c(O)cc(OC)c1)C(=O)C)C
MOL005072	0.9418	0.0582	0.8731	Canarii Fructus	brevifolin	66654	FALSE	O(c1c(c(O)cc(OC)c1)C(=O)C)C
MOL005072	0.9418	0.0582	0.8731	Geranium Wilfordii Maxim.	brevifolin	66654	FALSE	O(c1c(c(O)cc(OC)c1)C(=O)C)C

MOL005073	0.8912	0.1088	0.8471	Geranium Wilfordii Maxim.	ethyl brevifolincarboxylate	Not Available	FALSE	o1c2c(C(CC2=O)C(=O)OCC)c2c(c1=O)cc(O)c(O)c2O
MOL005074	0.9348	0.0652	0.9698	Geranium Wilfordii Maxim.	SKM	8742	FALSE	C1(=CC(C(C(C1)O)O)O)C(=O)O
MOL005074	0.9348	0.0652	0.9698	Chaenomeles Sinensis (Thouin) Koehne	SKM	8742	FALSE	C1(=CC(C(C(C1)O)O)O)C(=O)O
MOL005074	0.9348	0.0652	0.9698	Ginkgo Folium	SKM	8742	FALSE	C1(=CC(C(C(C1)O)O)O)C(=O)O
MOL005074	0.9348	0.0652	0.9698	Anisi Stellati Fructus	SKM	8742	FALSE	C1(=CC(C(C(C1)O)O)O)C(=O)O
MOL005074	0.9348	0.0652	0.9698	Selaginella Doederleinii Hieron	SKM	8742	FALSE	C1(=CC(C(C(C1)O)O)O)C(=O)O
MOL005074	0.9348	0.0652	0.9698	Smilacis Glabrae Rhixoma	SKM	8742	FALSE	C1(=CC(C(C(C1)O)O)O)C(=O)O
MOL005074	0.9348	0.0652	0.9698	Rubi Fructus	SKM	8742	FALSE	C1(=CC(C(C(C1)O)O)O)C(=O)O
MOL005074	0.9348	0.0652	0.9698	Euphorbiae Humifusae Herba	SKM	8742	FALSE	C1(=CC(C(C(C1)O)O)O)C(=O)O
MOL005074	0.9348	0.0652	0.9698	Dioscoreaebulbiferae	SKM	8742	FALSE	C1(=CC(C(C(C1)O)O)O)C(=O)O
MOL005074	0.9348	0.0652	0.9698	Pseudolaricis Cortex	SKM	8742	FALSE	C1(=CC(C(C(C1)O)O)O)C(=O)O
MOL005074	0.9348	0.0652	0.9698	Chebulae Fructus	SKM	8742	FALSE	C1(=CC(C(C(C1)O)O)O)C(=O)O
MOL005075	0.9316	0.0684	0.9383	Geranium Wilfordii Maxim.	Rhodinol (6CI)	81263	FALSE	C(CCCC(=C)C)(CCO)C
MOL005076	0.9247	0.0753	0.9448	Geranium Wilfordii Maxim.	inositol	892	FALSE	C1(C(C(C(C(C1O)O)O)O)O)O
MOL005076	0.9247	0.0753	0.9448	Coriolus	inositol	892	FALSE	C1(C(C(C(C(C1O)O)O)O)O)O
MOL005077	0.8468	0.1532	0.8032	Semen Pruni	kaempferitrin	21159160	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC1C(C(C(C(O1)C)O)O)O)OC1C(C(C(C(O1)C)O)O)O)c1ccc(cc1)O
MOL005077	0.8468	0.1532	0.8032	Lysimachiae Foenigraeci Herba	kaempferitrin	21159160	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC1C(C(C(C(O1)C)O)O)O)OC1C(C(C(C(O1)C)O)O)O)c1ccc(cc1)O
MOL005077	0.8468	0.1532	0.8032	Semen Aesculi	kaempferitrin	21159160	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC1C(C(C(C(O1)C)O)O)O)OC1C(C(C(C(O1)C)O)O)O)c1ccc(cc1)O
MOL005077	0.8468	0.1532	0.8032	Celosia Cristata L.	kaempferitrin	21159160	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC1C(C(C(C(O1)C)O)O)O)OC1C(C(C(C(O1)C)O)O)O)c1ccc(cc1)O
MOL005077	0.8468	0.1532	0.8032	Geranium Wilfordii Maxim.	kaempferitrin	21159160	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC1C(C(C(C(O1)C)O)O)O)OC1C(C(C(C(O1)C)O)O)O)c1ccc(cc1)O
MOL005078	0.9339	0.0661	0.9529	Geranium Wilfordii Maxim.	(3S)-3,7-dimethyloct-6-enoic acid	6999955	FALSE	C(CCC=C(C)C)(CC(=O)O)C
MOL005079	0.8710	0.1290	0.6776	Geranium Wilfordii Maxim.	corilagin	Not Available	FALSE	O1C2C(O)C(OC(=O)c3c(c4c(C(=O)OC2)cc(O)c(O)c4O)c(O)c(O)c(O)c3)C(O)C1OC(=O)c1cc(O)c(O)c(O)
MOL005079	0.8710	0.1290	0.6776	Euphorbiae Helioscopiae Herba	corilagin	Not Available	FALSE	O1C2C(O)C(OC(=O)c3c(c4c(C(=O)OC2)cc(O)c(O)c4O)c(O)c(O)c(O)c3)C(O)C1OC(=O)c1cc(O)c(O)c(O)
MOL005079	0.8710	0.1290	0.6776	Granati Pericarpium	corilagin	Not Available	FALSE	O1C2C(O)C(OC(=O)c3c(c4c(C(=O)OC2)cc(O)c(O)c4O)c(O)c(O)c(O)c3)C(O)C1OC(=O)c1cc(O)c(O)c(O)

MOL005079	0.8710	0.1290	0.6776	Chebulae Fructus	corilagin	Not Available	FALSE	O1C2C(O)C(OC(=O)c3c(c4c(C(=O)OC2)cc(O)c(O)c4O)c(O)c(O)c(O)c3)C(O)C1OC(=O)c1cc(O)c(O)c(O)c1
MOL005079	0.8710	0.1290	0.6776	Phyllanthi Fructus	corilagin	Not Available	FALSE	O1C2C(O)C(OC(=O)c3c(c4c(C(=O)OC2)cc(O)c(O)c4O)c(O)c(O)c(O)c3)C(O)C1OC(=O)c1cc(O)c(O)c(O)c1
MOL005080	0.9286	0.0714	0.9428	Fraxini Cortex	DMBQ	68262	FALSE	C1(=CC(=O)C=C(C1=O)OC)OC
MOL005080	0.9286	0.0714	0.9428	Schizonepetae Herba	DMBQ	68262	FALSE	C1(=CC(=O)C=C(C1=O)OC)OC
MOL005080	0.9286	0.0714	0.9428	Zanthoxylum Nitidum	DMBQ	68262	FALSE	C1(=CC(=O)C=C(C1=O)OC)OC
MOL005081	0.9062	0.0938	0.8361	Zanthoxylum Nitidum	5,7-dimethoxy-8-((3-methylbut-2-en-1-yl)oxy)-2H-chromen-2-one	14841901	FALSE	c12c(c(cc(c1ccc(=O)o2)OC)OC)OCC=C(C)C
MOL005082	0.9697	0.0303	0.8050	Zanthoxylum Nitidum	5,7,8-Trimethoxycoumarin	6482974	FALSE	c12c(c(cc(c1ccc(=O)o2)OC)OC)OC
MOL005083	0.5963	0.4037	0.7793	Zanthoxylum Nitidum	6-methoxy-5,6-dihydrochelerythrine	Not Available	FALSE	O1c2cc3c4N(C(c5c(c4ccc3cc2OC1)ccc(OC)c5OC)OC)C
MOL005084	0.6891	0.3109	0.8038	Zanthoxylum Nitidum	7-demethyl-6-methoxy-5,6-dihydrochelerythrine	Not Available	FALSE	c1c2c(cc3c1ccc1c3N(C(c3c1ccc(c3O)OC)OC)C)OCO2
MOL005085	0.2642	0.7358	0.6620	Zanthoxylum Nitidum	Chelidimerine	Not Available	FALSE	c12c(c3c(C[N+]1(C)CC(=O)C[N+]1(Cc4c(c5c1c1c(cc5)cc5c(c1)OCO5)ccc1c4OCO1)C)c1c(cc3)OCO1)ccc1c2cc2c(c1)OCO2
MOL005086	0.6443	0.3557	0.8323	Zanthoxylum Nitidum	Dihydronitidine	99641	FALSE	O1c2cc3c4N(Cc5c(c4ccc3cc2OC1)cc(OC)c(OC)c5)C
MOL005087	0.9569	0.0431	0.9765	Capsellae Herba	Diosphenol	12095091	FALSE	C1(=O)C(=C(CCC1C(C)C)C)O
MOL005087	0.9569	0.0431	0.9765	Zanthoxylum Nitidum	Diosphenol	12095091	FALSE	C1(=O)C(=C(CCC1C(C)C)C)O
MOL005087	0.9569	0.0431	0.9765	Citri Sarcodactylis Fructus	Diosphenol	12095091	FALSE	C1(=O)C(=C(CCC1C(C)C)C)O
MOL005088	0.9295	0.0705	0.7880	Hordei Fructus Germinatus	Nivalenol	Not Available	FALSE	O1C2C(C3(C4(C1C(C3O)O)OC4)C)(C(C(=O)C(=C2)C)O)CO
MOL005088	0.9295	0.0705	0.7880	Zanthoxylum Nitidum	Nivalenol	Not Available	FALSE	O1C2C(C3(C4(C1C(C3O)O)OC4)C)(C(C(=O)C(=C2)C)O)CO
MOL005089	0.8857	0.1143	0.8322	Zanthoxylum Nitidum	Oxypaeoniflorin	Not Available	FALSE	c1(ccc(cc1)C(=O)OCC12C3(CC1C1(CC3(C)OC2O1)O)OC1C(C(C(C(O1)CO)O)O)O)O
MOL005090	0.9090	0.0910	0.7962	Zanthoxylum Nitidum	oxypaeoniflorin_qt	Not Available	FALSE	c1(ccc(cc1)C(=O)OCC12C3(O)CC1C1(CC3(C)OC2O1)O)O
MOL005090	0.9090	0.0910	0.7962	Radix Paeoniae Rubra	oxypaeoniflorin_qt	Not Available	FALSE	c1(ccc(cc1)C(=O)OCC12C3(O)CC1C1(CC3(C)OC2O1)O)O

MOL005090	0.9090	0.0910	0.7962	Cortex Moutan	oxypaeoniflorin_qt	Not Available	FALSE	c1(ccc(cc1)C(=O)OCC12C3(O)CC1C1(CC3(C)OC2O1)O)O
MOL005091	0.4441	0.5559	0.6655	Zanthoxylum Nitidum	Arnottianamide	3085181	FALSE	O1c2cc3c(N(C)C=O)c(c4c(O)c(OC)c(OC)cc4)ccc3cc2OC1
MOL005092	0.7751	0.2249	0.7618	Zanthoxylum Nitidum	Decarine	179640	FALSE	O1c2cc3c4ncc5c(c4ccc3cc2OC1)ccc(O)c5OC
MOL005093	0.8626	0.1374	0.9005	Capsellae Herba	Diosmin	5281613	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2oc(cc(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL005093	0.8626	0.1374	0.9005	Zanthoxyli Pericarpium	Diosmin	5281613	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2oc(cc(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL005093	0.8626	0.1374	0.9005	Citri Sarcodactylis Fructus	Diosmin	5281613	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2oc(cc(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL005093	0.8626	0.1374	0.9005	Zanthoxylum Nitidum	Diosmin	5281613	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2oc(cc(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL005093	0.8626	0.1374	0.9005	Lobeliae Chinensis Herba	Diosmin	5281613	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2oc(cc(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL005093	0.8626	0.1374	0.9005	Lygodii Spora	Diosmin	5281613	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2oc(cc(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL005093	0.8626	0.1374	0.9005	Menthae Herba	Diosmin	5281613	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2oc(cc(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL005094	0.8417	0.1583	0.7521	Zanthoxylum Nitidum	3-[(2R)-2,3-dihydroxy-3-methyl-butyl]-4-methoxy-1-methyl-carbostyril	161570	FALSE	n1(c(=O)c(c(c2ccccc12)OC)CC(C(C)(C)O)O)C
MOL005094	0.8417	0.1583	0.7521	Dichroae Radix	3-[(2R)-2,3-dihydroxy-3-methyl-butyl]-4-methoxy-1-methyl-carbostyril	161570	FALSE	n1(c(=O)c(c(c2ccccc12)OC)CC(C(C)(C)O)O)C
MOL005095	0.7337	0.2663	0.7678	Zanthoxylum Nitidum	fagaridine	5318563	FALSE	c1cc2c(c3[n+](cc4c(c(ccc4c13)O)OC)C)cc1OCOc1c2
MOL005096	0.8481	0.1519	0.7759	Dictamni Cortex	haplopine	165368	FALSE	c12c(c(c3c(n2)occ3)OC)ccc(c1OC)O
MOL005096	0.8481	0.1519	0.7759	Zanthoxylum Nitidum	haplopine	165368	FALSE	c12c(c(c3c(n2)occ3)OC)ccc(c1OC)O

MOL005097	0.3478	0.6522	0.8014	Zanthoxylum Nitidum	5-[(1S,3aS,4R,6aS)-1-(1,3-benzodioxol-5-yl)-1,3,3a,4,6,6a-hexahydrofuro[4,3-c]furan-4-yl]-2-methoxyphenol	21722937	FALSE	O1COc2c1ccc(c2)C1OCC2C1COC2c1ccc(c(c1)O)OC
MOL005098	0.5599	0.4401	0.7818	Zanthoxylum Nitidum	chelerythrine methanolate	Not Available	FALSE	O1c2cc3c4N(C(C5C(c4ccc3cc2OC1)C=CC(=C5OC)OC)OC)C
MOL005100	0.9131	0.0869	0.9366	Herba Clinopodii Polycephali.	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	676152	TRUE	c12c(OC(CC1=O)c1cc(c(cc1)OC)O)cc(cc2O)O
MOL005100	0.9131	0.0869	0.9366	Citri Fructus Retinervus	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	676152	TRUE	c12c(OC(CC1=O)c1cc(c(cc1)OC)O)cc(cc2O)O
MOL005100	0.9131	0.0869	0.9366	Peucedani Radix	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	676152	TRUE	c12c(OC(CC1=O)c1cc(c(cc1)OC)O)cc(cc2O)O
MOL005100	0.9131	0.0869	0.9366	Asteris Radix Et Rhizoma	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	676152	TRUE	c12c(OC(CC1=O)c1cc(c(cc1)OC)O)cc(cc2O)O
MOL005100	0.9131	0.0869	0.9366	Citri Reticulatae Folium	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	676152	TRUE	c12c(OC(CC1=O)c1cc(c(cc1)OC)O)cc(cc2O)O

MOL005100	0.9131	0.0869	0.9366	Citri Reticulatae Pericarpium Viride	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	676152	TRUE	c12c(OC(CC1=O)c1cc(c(cc1)OC)O)cc(cc2O)O
MOL005100	0.9131	0.0869	0.9366	Euonymi Alati Ramulus	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	676152	TRUE	c12c(OC(CC1=O)c1cc(c(cc1)OC)O)cc(cc2O)O
MOL005100	0.9131	0.0869	0.9366	Aurantii Fructus Immaturus	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	676152	TRUE	c12c(OC(CC1=O)c1cc(c(cc1)OC)O)cc(cc2O)O
MOL005100	0.9131	0.0869	0.9366	Chrysanthemi Flos	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	676152	TRUE	c12c(OC(CC1=O)c1cc(c(cc1)OC)O)cc(cc2O)O
MOL005100	0.9131	0.0869	0.9366	Viticis Fructus	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	676152	TRUE	c12c(OC(CC1=O)c1cc(c(cc1)OC)O)cc(cc2O)O
MOL005100	0.9131	0.0869	0.9366	Hippophae Fructus	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	676152	TRUE	c12c(OC(CC1=O)c1cc(c(cc1)OC)O)cc(cc2O)O
MOL005100	0.9131	0.0869	0.9366	Zanthoxylum Nitidum	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	676152	TRUE	c12c(OC(CC1=O)c1cc(c(cc1)OC)O)cc(cc2O)O

MOL005100	0.9131	0.0869	0.9366	Portulacae Herba	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	676152	TRUE	c12c(OC(CC1=O)c1cc(c(cc1)OC)O)cc(cc2O)O
MOL005100	0.9131	0.0869	0.9366	Schizonepetae Herba	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	676152	TRUE	c12c(OC(CC1=O)c1cc(c(cc1)OC)O)cc(cc2O)O
MOL005100	0.9131	0.0869	0.9366	Citrus Reticulata	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	676152	TRUE	c12c(OC(CC1=O)c1cc(c(cc1)OC)O)cc(cc2O)O
MOL005100	0.9131	0.0869	0.9366	Citrus Aurantium	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	676152	TRUE	c12c(OC(CC1=O)c1cc(c(cc1)OC)O)cc(cc2O)O
MOL005100	0.9131	0.0869	0.9366	Sophorae Flavescentis Radix	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	676152	TRUE	c12c(OC(CC1=O)c1cc(c(cc1)OC)O)cc(cc2O)O
MOL005101	0.6833	0.3167	0.8336	Zanthoxylum Nitidum	nitidine	4501	FALSE	O1c2cc3c4[n+](cc5c(c4ccc3cc2OC1)cc(OC)c(OC)c5)C
MOL005101	0.6833	0.3167	0.8336	Broussonetiae Fructus	nitidine	4501	FALSE	O1c2cc3c4[n+](cc5c(c4ccc3cc2OC1)cc(OC)c(OC)c5)C
MOL005102	0.6935	0.3065	0.8062	Zanthoxylum Nitidum	OXYNITIDINE	97597	FALSE	O1c2cc3c4n(c(=O)c5c(c4ccc3cc2OC1)cc(OC)c(OC)c5)C
MOL005103	0.8872	0.1128	0.8148	Zanthoxylum Nitidum	6-[(2R)-2,3-dihydroxy-3-methyl-butyl]-5,7-dimethoxy-coumarin	160485	FALSE	OC(C(O)Cc1c(OC)c2c(oc(=O)cc2)cc1OC)(C)C
MOL005104	0.8120	0.1880	0.8079	Zanthoxylum Nitidum	Norchelerythrine	443719	FALSE	O1c2cc3c4ncc5c(c4ccc3cc2OC1)ccc(OC)c5OC

MOL005105	0.7159	0.2841	0.8407	Zanthoxylum Nitidum	Oxychelerythrine	147279	FALSE	O1c2cc3c4n(c(=O)c5c(c4ccc3cc2OC1)ccc(OC)c5OC)C
MOL005106	0.7105	0.2895	0.7571	Zanthoxylum Nitidum	oxyterihanine	13855597	FALSE	O1COc2c1cc1c3n(c(=O)c4c(c3ccc1c2)cc(c(c4)O)OC)C
MOL005107	0.4389	0.5611	0.7233	Zanthoxylum Nitidum	ethoxychelerythrine	25768645	FALSE	c12C(N(c3c(c1ccc(c2OC)OC)ccc1c3cc2c(c1)OCO2)C)OCC
MOL005108	0.7346	0.2654	0.7857	Zanthoxylum Nitidum	isofagaridine	177893	FALSE	O1c2cc3c4[n+](cc5c(c4ccc3cc2OC1)ccc(OC)c5O)C
MOL005109	0.9182	0.0818	0.8508	Zanthoxylum Nitidum	Capillarin	3083811	FALSE	c1(cc2c(c(=O)o1)cccc2)CC#CC
MOL005109	0.9182	0.0818	0.8508	Artemisiae Scopariae Herba	Capillarin	3083811	FALSE	c1(cc2c(c(=O)o1)cccc2)CC#CC
MOL005110	0.9065	0.0935	0.7042	Lysimachiae Foenigraeci Herba	.alpha.-Ionene	68057	FALSE	c12c(cc(cc2)C)CCCC1(C)C
MOL005110	0.9065	0.0935	0.7042	Chaenomeles Sinensis (Thouin) Koehne	.alpha.-Ionene	68057	FALSE	c12c(cc(cc2)C)CCCC1(C)C
MOL005110	0.9065	0.0935	0.7042	Ephedra Herba	.alpha.-Ionene	68057	FALSE	c12c(cc(cc2)C)CCCC1(C)C
MOL005111	0.5318	0.4682	0.6650	Chaenomeles Sinensis (Thouin) Koehne	Methyl 2,5-octadecadiynoate	42151	FALSE	C(=O)(C#CCC#CCCCCCCCCCCCC)OC
MOL005111	0.5318	0.4682	0.6650	Ginkgo Folium	Methyl 2,5-octadecadiynoate	42151	FALSE	C(=O)(C#CCC#CCCCCCCCCCCCC)OC
MOL005112	0.9286	0.0714	0.9368	Chaenomeles Sinensis (Thouin) Koehne	Ocimenol	5368785	FALSE	CC(CC/C=C(/C=C)\C)(O)C
MOL005113	0.8787	0.1213	0.8725	Chaenomeles Sinensis (Thouin) Koehne	2,3-Dihydrothiophene	136880	FALSE	C1CC=CS1
MOL005114	0.8907	0.1093	0.9689	Chaenomeles Sinensis (Thouin) Koehne	Pyrocinchonic anhydride	13010	FALSE	C1(=O)C(=C(C(=O)O1)C)C
MOL005114	0.8907	0.1093	0.9689	Mume Fructus	Pyrocinchonic anhydride	13010	FALSE	C1(=O)C(=C(C(=O)O1)C)C
MOL005114	0.8907	0.1093	0.9689	Ginkgo Folium	Pyrocinchonic anhydride	13010	FALSE	C1(=O)C(=C(C(=O)O1)C)C
MOL005115	0.9179	0.0821	0.9204	Capsici Fructus	2-methyl-butanoic acid	Not Available	FALSE	C(=O)(OCCCCCC)C(CC)C
MOL005115	0.9179	0.0821	0.9204	Chaenomeles Sinensis (Thouin) Koehne	2-methyl-butanoic acid	Not Available	FALSE	C(=O)(OCCCCCC)C(CC)C
MOL005116	0.9059	0.0941	0.9368	Chaenomeles Sinensis (Thouin) Koehne	Ethyl 3-(methylthio)propionate	61592	FALSE	C(=O)(CCSC)OCC
MOL005117	0.9430	0.0570	0.9724	Chaenomeles Sinensis (Thouin) Koehne	Anis alcohol	7738	FALSE	c1(ccc(cc1)OC)CO
MOL005118	0.9467	0.0533	0.8542	Flos Genkwa	Daphnetol	5280569	FALSE	o1c(=O)ccc2ccc(c(c12)O)O
MOL005118	0.9467	0.0533	0.8542	Chaenomeles Sinensis (Thouin) Koehne	Daphnetol	5280569	FALSE	o1c(=O)ccc2ccc(c(c12)O)O

MOL005118	0.9467	0.0533	0.8542	Semen Euphorbiae	Daphnetol	5280569	FALSE	o1c(=O)ccc2ccc(c(c12)O)O
MOL005119	0.9616	0.0384	0.9354	Chaenomeles Sinensis (Thouin) Koehne	p-Ethyltoluene	12160	FALSE	c1(ccc(cc1)CC)C
MOL005119	0.9616	0.0384	0.9354	Sojae Semen Nigrum	p-Ethyltoluene	12160	FALSE	c1(ccc(cc1)CC)C
MOL005120	0.7133	0.2867	0.6196	Gossampiniflos	PLY	984	FALSE	C(=O)CCCCCCCCCCCCCCC
MOL005120	0.7133	0.2867	0.6196	Hippophae Fructus	PLY	984	FALSE	C(=O)CCCCCCCCCCCCCCC
MOL005120	0.7133	0.2867	0.6196	Rose Rugosae Flos	PLY	984	FALSE	C(=O)CCCCCCCCCCCCCCC
MOL005120	0.7133	0.2867	0.6196	Chaenomeles Sinensis (Thouin) Koehne	PLY	984	FALSE	C(=O)CCCCCCCCCCCCCCC
MOL005120	0.7133	0.2867	0.6196	Morindae Officinalis Radix	PLY	984	FALSE	C(=O)CCCCCCCCCCCCCCC
MOL005120	0.7133	0.2867	0.6196	Maydis Seigma	PLY	984	FALSE	C(=O)CCCCCCCCCCCCCCC
MOL005120	0.7133	0.2867	0.6196	Raphani Semen	PLY	984	FALSE	C(=O)CCCCCCCCCCCCCCC
MOL005120	0.7133	0.2867	0.6196	Gnaphalii Affinis Herba	PLY	984	FALSE	C(=O)CCCCCCCCCCCCCCC
MOL005120	0.7133	0.2867	0.6196	Meliae Azedarach Fructus	PLY	984	FALSE	C(=O)CCCCCCCCCCCCCCC
MOL005122	0.9352	0.0648	0.9170	Flos Genkwa	FPR	7668	FALSE	c1(ccccc1)CCC
MOL005122	0.9352	0.0648	0.9170	Sojae Semen Nigrum	FPR	7668	FALSE	c1(ccccc1)CCC
MOL005122	0.9352	0.0648	0.9170	Chaenomeles Sinensis (Thouin) Koehne	FPR	7668	FALSE	c1(ccccc1)CCC
MOL005123	0.9263	0.0737	0.9298	Chaenomeles Sinensis (Thouin) Koehne	HEXYL BUTYRATE	17525	FALSE	C(=O)(OCCCCCC)CCC
MOL005124	0.8859	0.1141	0.8904	Chaenomeles Sinensis (Thouin) Koehne	Octyl butyrate	61030	FALSE	O(CCCCCCCC)C(=O)CCC
MOL005125	0.9483	0.0517	0.9709	Angelicae Sinensis Radix	ANN	7478	FALSE	c1(ccc(cc1)OC)C(=O)O
MOL005125	0.9483	0.0517	0.9709	Foeniculi Fructus	ANN	7478	FALSE	c1(ccc(cc1)OC)C(=O)O
MOL005125	0.9483	0.0517	0.9709	Linderae Radix	ANN	7478	FALSE	c1(ccc(cc1)OC)C(=O)O
MOL005125	0.9483	0.0517	0.9709	Arum Ternatum Thunb.	ANN	7478	FALSE	c1(ccc(cc1)OC)C(=O)O
MOL005125	0.9483	0.0517	0.9709	Rhododendri Daurici Folium	ANN	7478	FALSE	c1(ccc(cc1)OC)C(=O)O
MOL005125	0.9483	0.0517	0.9709	Viticis Fructus	ANN	7478	FALSE	c1(ccc(cc1)OC)C(=O)O
MOL005125	0.9483	0.0517	0.9709	Chaenomeles Sinensis (Thouin) Koehne	ANN	7478	FALSE	c1(ccc(cc1)OC)C(=O)O
MOL005126	0.9231	0.0769	0.8815	Chaenomeles Sinensis (Thouin) Koehne	1-Cyclohexene-1-propanol,a,2,6,6-tetramethyl	71553170	FALSE	C1(=C(CCCC1(C)C)C)CCC(O)C
MOL005127	0.9334	0.0666	0.9396	Capsici Fructus	Butyl caproate	12294	FALSE	C(C(=O)OCCCC)CCCC
MOL005127	0.9334	0.0666	0.9396	Chaenomeles Sinensis (Thouin) Koehne	Butyl caproate	12294	FALSE	C(C(=O)OCCCC)CCCC

MOL005127	0.9334	0.0666	0.9396	Momordicae Fructus	Butyl caproate	12294	FALSE	C(C(=O)OCCCC)CCCC
MOL005128	0.8807	0.1193	0.8899	Chaenomeles Sinensis (Thouin) Koehne	Hexyl hexoate	22873	FALSE	C(=O)(OCCCCCC)CCCCC
MOL005128	0.8807	0.1193	0.8899	Capsici Fructus	Hexyl hexoate	22873	FALSE	C(=O)(OCCCCCC)CCCCC
MOL005128	0.8807	0.1193	0.8899	Meliae Azedarach Fructus	Hexyl hexoate	22873	FALSE	C(=O)(OCCCCCC)CCCCC
MOL005131	0.9162	0.0838	0.9634	Chaenomeles Sinensis (Thouin) Koehne	KOJ	3840	FALSE	o1cc(O)c(=O)cc1CO
MOL005131	0.9162	0.0838	0.9634	Citri Sarcodactylis Fructus	KOJ	3840	FALSE	o1cc(O)c(=O)cc1CO
MOL005132	0.9243	0.0757	0.9580	Chaenomeles Sinensis (Thouin) Koehne	Paraldehyde	31264	FALSE	C1(OC(OC(O1)C)C)C
MOL005133	0.9102	0.0898	0.9201	Capsici Fructus	Hi-Dry	8200	FALSE	O(CCOCCO)CCOCCO
MOL005133	0.9102	0.0898	0.9201	Chaenomeles Sinensis (Thouin) Koehne	Hi-Dry	8200	FALSE	O(CCOCCO)CCOCCO
MOL005134	0.8458	0.1542	0.8172	Chaenomeles Sinensis (Thouin) Koehne	Hexyl octylate	14228	FALSE	C(=O)(CCCCCCC)OCCCCCC
MOL005136	0.7017	0.2983	0.7446	Rhododendronmolle	Andromedotoxin	Not Available	FALSE	C1(C2(C(CC1O)C(C1C3(CC2O)C(C(CC1)C(C3)(C)O)OC(=O)C)(C)O)O)(C)C
MOL005136	0.7017	0.2983	0.7446	Rhododendri Daurici Folium	Andromedotoxin	Not Available	FALSE	C1(C2(C(CC1O)C(C1C3(CC2O)C(C(CC1)C(C3)(C)O)OC(=O)C)(C)O)O)(C)C
MOL005138	0.5263	0.4737	0.6187	Rhododendronmolle	psi-Rhodomyrtoxin	Not Available	FALSE	c1(c(c(c2c(c1O)c1c(o2)c(c(c(c1O)C)O)C(=O)C(CC)C)C(=O)CC(C)C)O)C
MOL005139	0.7017	0.2983	0.7446	Rhododendronmolle	rhodotoxin II	Not Available	FALSE	O(C1C23C(C(O)(C4C(O)(C(O)C3)C(C(O)C4)(C)C)C)CCC1C(O)(C2)C)C(=O)C
MOL005140	0.9512	0.0488	0.9189	Sojae Semen Nigrum	Sparassol	596344	FALSE	O(c1cc(c(c(O)c1)C(=O)OC)C)C
MOL005140	0.9512	0.0488	0.9189	Rhododendronmolle	Sparassol	596344	FALSE	O(c1cc(c(c(O)c1)C(=O)OC)C)C
MOL005141	0.7682	0.2318	0.6957	Rhododendri Daurici Folium	graynotoxin III	Not Available	FALSE	OC1(C2C3(C(O)C(C(O)(C3)C)CC2)CC(O)C2(O)C1CC(O)C2(C)C)C
MOL005141	0.7682	0.2318	0.6957	Rhododendronmolle	graynotoxin III	Not Available	FALSE	OC1(C2C3(C(O)C(C(O)(C3)C)CC2)CC(O)C2(O)C1CC(O)C2(C)C)C
MOL005142	0.7925	0.2075	0.7665	Rhododendronmolle	rhodojaponinII	Not Available	FALSE	O1C2C3C(O)(C(C12)(C)C)C(O)CC12C(C3(O)C)CCC(C1O)C(O)(C2)C
MOL005143	0.8410	0.1590	0.8891	Dioscoreaebulbiferae	2-(3,4-dihydroxyphenyl)-7-hydroxy-3,5-dimethoxy-chromone	5489501	FALSE	o1c2c(c(=O)c(OC)c1c1cc(O)c(O)cc1)c(OC)cc(O)c2

MOL005143	0.8410	0.1590	0.8891	Rhododendronmolle	2-(3,4-dihydroxyphenyl)-7-hydroxy-3,5-dimethoxy-chromone	5489501	FALSE	o1c2c(c(=O)c(OC)c1c1cc(O)c(O)cc1)c(OC)cc(O)c2
MOL005144	0.7633	0.2367	0.7356	Rhododendronmolle	kalmanol	Not Available	FALSE	OC12C3C(C(O)(C4C(O)(C(C(O)C4)(C)C)C(O)C2)C)CCC3C(O)(C1)C
MOL005145	0.7744	0.2256	0.7797	Rhododendronmolle	rhodomolleinIII	Not Available	FALSE	OC1(C2C3(C(O)C(C(O)(C3)C)CC2)CC(OC(=O)C)C2(O)C1C(O)C(O)C2(C)C)C
MOL005147	0.6009	0.3991	0.6454	Fructus Ligustri Lucidi	LucidumosideD_qt	Not Available	FALSE	C1(/C(=C/C)/C(C(=CO1)C(=O)OC)CC(=O)OCCc1cc(c(cc1)OC)OC)O
MOL005148	0.8362	0.1638	0.7987	Fructus Ligustri Lucidi	mauritianin	Not Available	FALSE	O(C1C(O)C(O)C(OC1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)COC1OC(C(O)C(O)C1O)C)C1OC(C(O)C(O)C1O)C
MOL005151	0.9139	0.0861	0.9101	Rubi Fructus	[(3S)-3,7-dimethylocta-1,6-dien-3-yl] acetate	6999980	FALSE	O(C(CCC=C(C)C)(C)C=C)C(=O)C
MOL005151	0.9139	0.0861	0.9101	Fructus Ligustri Lucidi	[(3S)-3,7-dimethylocta-1,6-dien-3-yl] acetate	6999980	FALSE	O(C(CCC=C(C)C)(C)C=C)C(=O)C
MOL005151	0.9139	0.0861	0.9101	Mori Fructus	[(3S)-3,7-dimethylocta-1,6-dien-3-yl] acetate	6999980	FALSE	O(C(CCC=C(C)C)(C)C=C)C(=O)C
MOL005151	0.9139	0.0861	0.9101	Perillae Fructus	[(3S)-3,7-dimethylocta-1,6-dien-3-yl] acetate	6999980	FALSE	O(C(CCC=C(C)C)(C)C=C)C(=O)C
MOL005151	0.9139	0.0861	0.9101	Zingiber Officinale Roscoe	[(3S)-3,7-dimethylocta-1,6-dien-3-yl] acetate	6999980	FALSE	O(C(CCC=C(C)C)(C)C=C)C(=O)C
MOL005151	0.9139	0.0861	0.9101	Citri Fructus	[(3S)-3,7-dimethylocta-1,6-dien-3-yl] acetate	6999980	FALSE	O(C(CCC=C(C)C)(C)C=C)C(=O)C
MOL005151	0.9139	0.0861	0.9101	Prunellae Spica	[(3S)-3,7-dimethylocta-1,6-dien-3-yl] acetate	6999980	FALSE	O(C(CCC=C(C)C)(C)C=C)C(=O)C

MOL005152	0.8775	0.1225	0.6697	Fructus Ligustri Lucidi	[1R-(1a,4aa,8a,8aa)]-8-(b-D-glucopyranosyloxy)-4,4a,8,8a-tetrahydro-1-methyl-3-oxo-1H,3H-Pyrano[3,4-c]pyran-5-carboxylic acid, methyl ester	12304886	FALSE	C1(C2C(CC(=O)O1)C(=COC2OC1C(O)C(O)C(O)C(O1)CO)C(=O)OC)C
MOL005153	0.9317	0.0683	0.8117	Fructus Ligustri Lucidi	[1R-(1a,4aa,8a,8aa)]-8-(b-D-glucopyranosyloxy)-4,4a,8,8a-tetrahydro-1-methyl-3-oxo-1H,3H-Pyrano[3,4-c]pyran-5-carboxylic acid, methyl ester_qt	Not Available	FALSE	C1(C2C(CC(=O)O1)C(=COC2O)C(=O)OC)C
MOL005154	0.9214	0.0786	0.8194	Fructus Ligustri Lucidi	ligustrin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1OC1(OC)C(C(C1OC)/C=C/CO)CO
MOL005155	0.7553	0.2447	0.9079	Panacis Quinquefolii Radix	ginsenoside Ro_qt	7055468	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)OCCC(C)(C)CC4C3=CCC21C)O
MOL005155	0.7553	0.2447	0.9079	Fructus Ligustri Lucidi	ginsenoside Ro_qt	7055468	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)OCCC(C)(C)CC4C3=CCC21C)O
MOL005155	0.7553	0.2447	0.9079	Achyranthis Bidentatae Radix	ginsenoside Ro_qt	7055468	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)OCCC(C)(C)CC4C3=CCC21C)O
MOL005155	0.7553	0.2447	0.9079	Panax Ginseng C. A. Mey.	ginsenoside Ro_qt	7055468	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)OCCC(C)(C)CC4C3=CCC21C)O
MOL005155	0.7553	0.2447	0.9079	Panacis Japonici Rhizoma	ginsenoside Ro_qt	7055468	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)OCCC(C)(C)CC4C3=CCC21C)O
MOL005157	0.9593	0.0407	0.7975	Fructus Ligustri Lucidi	ZINC03847089	615080	FALSE	O(c1c(OC)c(OC)cc(OC)c1OC)C
MOL005158	0.9387	0.0613	0.9038	Fructus Ligustri Lucidi	Cimidahurinine	5315870	FALSE	C1(C(C(C(C(O1)CO)O)O)O)Oc1c(ccc(c1)CCO)O

MOL005159	0.9000	0.1000	0.7973	Fructus Ligustri Lucidi	ketologanin	12311348	FALSE	C1(C2C(C(=CO1)C(=O)OC)CC(=O)C2C)OC1C(O)C(O)C(O)C(O1)CO
MOL005160	0.9553	0.0447	0.8694	Fructus Ligustri Lucidi	ketologanin_qt	Not Available	FALSE	C1(C2C(C(=CO1)C(=O)OC)CC(=O)C2C)O
MOL005161	0.6690	0.3310	0.8266	Fructus Ligustri Lucidi	3-Acetylpomolic acid	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C)C(C)(C4C3=CCC21)O)C)OC(=O)C
MOL005162	0.9087	0.0913	0.8140	Fructus Ligustri Lucidi	nuzhenidic acid	Not Available	FALSE	C1(C(CCC(C1(O)CC(=O)O)OC1C(C(C(C(O1)CO)O)O)O)C(=O)OC)CC(=O)O
MOL005163	0.9238	0.0762	0.8193	Fructus Ligustri Lucidi	nuzhenidic acid_qt	Not Available	FALSE	C1(C(CCC(C1(O)CC(=O)O)O)C(=O)OC)CC(=O)O
MOL005164	0.9286	0.0714	0.8215	Fructus Ligustri Lucidi	Dihydrosyringin	71720642	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)c1c(cc(cc1OC)CCCO)OC
MOL005165	0.9269	0.0731	0.9262	Fructus Ligustri Lucidi	Dihydrosinapyl alcohol	529893	FALSE	Oc1c(cc(cc1OC)CCCO)OC
MOL005166	0.8890	0.1110	0.8057	Mori Cortex	QUOSP	5282166	FALSE	O(C1C(O)C(O)C(OC1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1)CO)C1OC(C(O)C(O)C1O)CO
MOL005166	0.8890	0.1110	0.8057	Fructus Ligustri Lucidi	QUOSP	5282166	FALSE	O(C1C(O)C(O)C(OC1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1)CO)C1OC(C(O)C(O)C1O)CO
MOL005166	0.8890	0.1110	0.8057	Eriobotryae Folium	QUOSP	5282166	FALSE	O(C1C(O)C(O)C(OC1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1)CO)C1OC(C(O)C(O)C1O)CO
MOL005167	0.8980	0.1020	0.6501	Fructus Ligustri Lucidi	Nuezhengalaside	Not Available	FALSE	C1(/C(=C\C)/C(C(=CO1)C(=O)OC)CCC)OC1C(O)C(O)C(O)C(O1)CO
MOL005168	0.9468	0.0532	0.8239	Fructus Ligustri Lucidi	Nuezhengalaside_qt	Not Available	FALSE	C1(/C(=C/C)/C(C(=CO1)C(=O)OC)CCC)O
MOL005169	0.1836	0.8164	0.7220	Fructus Ligustri Lucidi	(20S)-24-ene-3β,20-diol-3-acetate	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC(C(CCC=C(C)C)(C)O)C3CCC21)C)OC(=O)C
MOL005170	0.8775	0.1225	0.6697	Fructus Ligustri Lucidi	kingiside	Not Available	FALSE	C1(C2C(CC(=O)O1)C(=COC2OC1C(O)C(O)C(O)C(O1)CO)C(=O)OC)C
MOL005171	0.9317	0.0683	0.8117	Fructus Ligustri Lucidi	kingiside_qt	Not Available	FALSE	C1(C2C(CC(=O)O1)C(=COC2O)C(=O)OC)C

MOL005172	0.8925	0.1075	0.6163	Fructus Ligustri Lucidi	methyl (4S,5E,6S)-5-ethylidene-4-(2-methoxy-2-oxoethyl)-6-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4H-pyran-3-carboxylate	10788149	FALSE	C1(/C(=C/C)/C(C(=CO1)C(=O)OC)CC(=O)OC)OC1C(O)C(O)C(O)C(O1)CO
MOL005173	0.9303	0.0697	0.8745	Fructus Ligustri Lucidi	Oleoside dimethyl ester_qt	Not Available	FALSE	C1(/C(=C/C)/C(C(=CO1)C(=O)OC)CC(=O)OC)O
MOL005174	0.8780	0.1220	0.8132	Fructus Ligustri Lucidi	quercetin-3-O-rhamnoglucoside	14034832	FALSE	c1(c(c(=O)c2c(cc(cc2o1)O)O)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO)c1cc(c(cc1)O)O
MOL005175	0.8678	0.1322	0.8415	Fructus Ligustri Lucidi	kaempferol-3-O-α-L-rhamnosyl(1→2)-β-D-glucoside	12082378	FALSE	c1(c(c(=O)c2c(cc(cc2o1)O)O)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO)c1ccc(cc1)O
MOL005176	0.6733	0.3267	0.6169	Fructus Ligustri Lucidi	oleuropein	Not Available	FALSE	O1C(C(O)C(O)C(O)C1OC1OC=C(C(/C/1=C\C)CC(=O)OCCc1cc(O)c(O)cc1)C(=O)OC)CO
MOL005177	0.7649	0.2351	0.7652	Fructus Ligustri Lucidi	oleuropein_qt	56842347	FALSE	OC1OC=C(C(/C/1=C\C)CC(=O)OCCc1cc(O)c(O)cc1)C(=O)OC
MOL005179	0.7319	0.2681	0.7039	Fructus Ligustri Lucidi	Lucidumoside A_qt	Not Available	FALSE	OC1OC=C(C(C1CC)CC(=O)OCCc1ccc(O)cc1)C(=O)OC
MOL005180	0.9353	0.0647	0.9514	Fructus Ligustri Lucidi	AMG	76935	FALSE	O1C(C(O)C(O)C(O)C1OC)CO
MOL005180	0.9353	0.0647	0.9514	Perilla Frutescens	AMG	76935	FALSE	O1C(C(O)C(O)C(O)C1OC)CO
MOL005182	0.6835	0.3165	0.7010	Fructus Ligustri Lucidi	Lucidumoside C_qt	Not Available	FALSE	C1(/C(=C/C)/C(C(=CO1)C(=O)OC)CC(=O)OCC(OCC)c1cc(c(cc1)O)O)O
MOL005183	0.6862	0.3138	0.6780	Fructus Ligustri Lucidi	3b-(p-hydroxy-trans-cinnamoyloxy)-2a-hydroxy-oleanolic acid	Not Available	FALSE	C1(C(CC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C)(C)CC4C3=CCC21)C)O)OC(=O)/C=C\c1ccc(cc1)O

MOL005185	0.6727	0.3273	0.6912	Fructus Ligustri Lucidi	ligustroside_qt	Not Available	FALSE	OC1OC=C(C(/C/1=C\C)CC(=O)OCCc1ccc(O)cc1)C(=O)OC
MOL005186	0.6828	0.3172	0.6353	Fructus Ligustri Lucidi	10-hydroxyligstroside	Not Available	FALSE	C1(/C(=C/CO)/C(C(=CO1)C(=O)OC)CC(=O)OCCc1ccc(cc1)O)OC1C(O)C(O)C(O)C(O1)CO
MOL005187	0.7213	0.2787	0.6254	Fructus Ligustri Lucidi	10-hydroxyligstroside_qt	Not Available	FALSE	C1(/C(=C/CO)/C(C(=CO1)C(=O)OC)CC(=O)OCCc1ccc(cc1)O)O
MOL005189	0.8922	0.1078	0.7619	Fructus Ligustri Lucidi	nuezhenide_qt1	Not Available	FALSE	OC1OC=C(C(/C/1=C/C)CC(=O)OCC1OC(O)C(O)C(O)C1O)C(=O)OC
MOL005190	0.9326	0.0674	0.9041	Polygoni Orientalis Fructus	eriodictyol	440735	FALSE	O1C(CC(=O)c2c1cc(O)cc2O)c1cc(O)c(O)cc1
MOL005190	0.9326	0.0674	0.9041	Fructus Ligustri Lucidi	eriodictyol	440735	FALSE	O1C(CC(=O)c2c1cc(O)cc2O)c1cc(O)c(O)cc1
MOL005190	0.9326	0.0674	0.9041	Scutellariae Barbatae Herba	eriodictyol	440735	FALSE	O1C(CC(=O)c2c1cc(O)cc2O)c1cc(O)c(O)cc1
MOL005190	0.9326	0.0674	0.9041	Ephedrae Radix Et Rhizoma	eriodictyol	440735	FALSE	O1C(CC(=O)c2c1cc(O)cc2O)c1cc(O)c(O)cc1
MOL005190	0.9326	0.0674	0.9041	Drynariae Rhizoma	eriodictyol	440735	FALSE	O1C(CC(=O)c2c1cc(O)cc2O)c1cc(O)c(O)cc1
MOL005190	0.9326	0.0674	0.9041	Menthae Herba	eriodictyol	440735	FALSE	O1C(CC(=O)c2c1cc(O)cc2O)c1cc(O)c(O)cc1
MOL005191	0.6837	0.3163	0.8372	Fructus Ligustri Lucidi	3-O-acetyloleanolic acid	44583799	FALSE	OC(=O)C12C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)C(=O)OC)C)C)CC(CC2)(C)C
MOL005192	0.8693	0.1307	0.7995	Fructus Ligustri Lucidi	Manghaslin	Not Available	FALSE	O(C1C(O)C(O)C(OC1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1)COC1OC(C(O)C(O)C1O)C)C1OC(C(O)C(O)C1O)C
MOL005193	0.8362	0.1638	0.7987	Fructus Ligustri Lucidi	clitorin	Not Available	FALSE	O(C1C(O)C(O)C(OC1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)COC1OC(C(O)C(O)C1O)C)C1OC(C(O)C(O)C1O)C
MOL005194	0.7185	0.2815	0.7314	Fructus Ligustri Lucidi	syringaresinol diglucoside	Not Available	FALSE	C1(C(OC(C(C1O)O)Oc1c(c(c(c(c1)OC)OC1C(C(C(C(O1)O)O)O)O)OC)C1C2C(CO1)C(OC2)c1c(c(cc1OC1C(C(C(C(O1)CO)O)O)O)OC)OC1C(C(C(C(O1)CO)O)O)O)OC)CO)O
MOL005195	0.6786	0.3214	0.6088	Fructus Ligustri Lucidi	syringaresinol diglucoside_qt	Not Available	FALSE	Oc1c(c(c(c(c1)OC)O)OC)C1C2C(CO1)C(OC2)c1c(c(cc(cc1O)OC)O)OC
MOL005196	0.6338	0.3662	0.8148	Ilicis Cornutae Folium Immayuri	Ursolic acid deriv.	6475119	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3C)C)C(=O)O)C)(CC2)C)(CC1)C)(C)C)C(=O)C
MOL005196	0.6338	0.3662	0.8148	Fructus Ligustri Lucidi	Ursolic acid deriv.	6475119	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3C)C)C(=O)O)C)(CC2)C)(CC1)C)(C)C)C(=O)C
MOL005197	0.9137	0.0863	0.9235	Fructus Ligustri Lucidi	Butyl butyryllactate	24884216	FALSE	O(CCCC)C(=O)C(OC(=O)CCC)C

MOL005198	0.9341	0.0659	0.8846	Fructus Ligustri Lucidi	3,4-Dihydroxyphenylethyl alcohol glucoside	5316821	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)CCc1cc(c(cc1)O)O
MOL005199	0.7040	0.2960	0.7121	Fructus Ligustri Lucidi	olivil-4'-O-β-d-glucopyranoside	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)c1c(cc(cc1)CC1(COC(C1CO)c1cc(c(cc1)O)OC)O)OC
MOL005200	0.7753	0.2247	0.6797	Fructus Ligustri Lucidi	2H-Pyran-4-acetic acid, 2-(beta-D-glucopyranosyloxy)-3,4-dihydro-3-(2-hydroxyethylidene)-5-(methoxycarbonyl)-, 2-(3,4-dihydroxyphenyl)ethyl ester, (2S,3E,4S)-	6440747	FALSE	C1(/C(=C/CO)/C(C(=CO1)C(=O)OC)CC(=O)OCCc1cc(c(cc1)O)O)OC1C(O)C(O)C(O)C(O1)CO
MOL005201	0.8011	0.1989	0.7563	Fructus Ligustri Lucidi	10-hydroxyoleuropein_qt	Not Available	FALSE	C1(/C(=C/CO)/C(C(=CO1)C(=O)OC)CC(=O)OCCc1cc(c(cc1)O)O)O
MOL005202	0.7459	0.2541	0.6577	Fructus Ligustri Lucidi	Ligustaloside A	Not Available	FALSE	C1(C(C(C(=CO1)C(=O)OC)CC(=O)OCCc1cc(c(cc1)O)O)CC=O)OC1C(O)C(O)C(O)C(O1)CO
MOL005203	0.8142	0.1858	0.7566	Fructus Ligustri Lucidi	Ligustaloside A_qt	Not Available	FALSE	C1(C(C(C(=CO1)C(=O)OC)CC(=O)OCCc1cc(c(cc1)O)O)CC=O)O
MOL005204	0.2813	0.7187	0.7634	Fructus Ligustri Lucidi	(3a)-3-hydroxy-Urs-12-en-28-oic acid, methyl ester	40884488	FALSE	C12=CCC3C(C1(CCC1(C2C(C(CC1)C)C)C(=O)OC)C)(CCC1C3(CCC(C1(C)C)O)C)C

MOL005205	0.8925	0.1075	0.7229	Fructus Ligustri Lucidi	methyl (4S,5E,6S)-5-(2-hydroxyethylidene)-4-(2-methoxy-2-oxoethyl)-6-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4H-pyran-3-carboxylate	11351007	FALSE	C1(/C(=C/CO)/C(C(=CO1)C(=O)OC)CC(=O)OC)OC1C(O)C(O)C(O)C(O1)CO
MOL005206	0.9202	0.0798	0.8257	Fructus Ligustri Lucidi	10-Hydroxyoleoside dimethyl ester_qt	Not Available	FALSE	C1(/C(=C/CO)/C(C(=CO1)C(=O)OC)CC(=O)OC)O
MOL005207	0.6726	0.3274	0.6118	Fructus Ligustri Lucidi	Lucidumoside B	Not Available	FALSE	c1(c(ccc(c1)CCOC(=O)CC1C(C(OC=C1C(=O)OC)OC1OC(C(C(C1O)O)O)CO)CC)O)O
MOL005208	0.7906	0.2094	0.7812	Fructus Ligustri Lucidi	Lucidumoside B_qt	Not Available	FALSE	c1(c(ccc(c1)CCOC(=O)CC1C(C(OC=C1C(=O)OC)O)CC)O)O
MOL005209	0.4882	0.5118	0.8098	Fructus Ligustri Lucidi	Lucidusculine	Not Available	FALSE	C1CC2(C3C4(C1O)C1C5(C(C3)C4N(C2)CC)CC(C(C1)O)C(=C)C5OC(=O)C)C
MOL005210	0.0745	0.9255	0.7482	Fructus Ligustri Lucidi	Nuphleine	Not Available	FALSE	C1(CCC(N2C1CCC1(C2O)SCC2(C1)CCC1N(C2O)C(CCC1C)c1cocc1)c1ccoc1)C
MOL005211	0.6114	0.3886	0.8401	Fructus Ligustri Lucidi	Olitoriside	Not Available	FALSE	O1C(C(C(C(C1OC1C(CC(OC1C)OC1CC2(C(CC1)(C=O)C1C(CC2)C2(O)C(CC1)(C)C(CC2)C1=CC(=O)OC1)O)O)O)O)O)CO
MOL005212	0.6450	0.3550	0.7872	Fructus Ligustri Lucidi	Olitoriside_qt	Not Available	FALSE	OC1CC2(C(CC1)(C=O)C1C(CC2)C2(O)C(CC1)(C)C(CC2)C1=CC(=O)OC1)O
MOL005214	0.7370	0.2630	0.6055	Fructus Ligustri Lucidi	neonuezhenide	Not Available	FALSE	O1C(C(O)C(O)C(O)C1OC1OC=C(C(/C/1=C/C)CC(=O)OCC1OC(OCCc2cc(O)c(O)cc2)C(O)C(O)C1O)C(=O)OC)CO
MOL005215	0.6748	0.3252	0.6296	Fructus Ligustri Lucidi	neonuezhenide_qt	Not Available	FALSE	OC1OC=C(C(/C/1=C\C)CC(=O)OCC1OC(OCCc2cc(O)c(O)cc2)C(O)C(O)C1O)C(=O)OC
MOL005216	0.9071	0.0929	0.8938	Semen Euphorbiae	2-(Hexa-2,4-diyn-1-ylidene)-1,6-dioxa-spiro[4,4]non-3-ene	Not Available	FALSE	C12(CCCC1=O)C(=O)/C(=C/C#CC#CC)/C=C2

MOL005217	0.1987	0.8013	0.6312	Prunellae Spica	Δ7-stigmasterol	12303924	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(CC)C(C)C)C)C4(C)CCC23)C1)C)O
MOL005217	0.1987	0.8013	0.6312	Phellodendri Amurensis Cortex	Δ7-stigmasterol	12303924	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(CC)C(C)C)C)C4(C)CCC23)C1)C)O
MOL005217	0.1987	0.8013	0.6312	Semen Euphorbiae	Δ7-stigmasterol	12303924	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(CC)C(C)C)C)C4(C)CCC23)C1)C)O
MOL005218	0.7245	0.2755	0.6421	Semen Euphorbiae	cis-9-Hexadecenol	5367661	FALSE	C(/C=C\CCCCCC)CCCCCCCO
MOL005219	0.9250	0.0750	0.8711	Semen Euphorbiae	Daphnetin-8-glucoside	5316301	FALSE	c1(c(ccc2c1oc(=O)cc2)O)OC1OC(C(C(C1O)O)O)CO
MOL005221	0.0899	0.9101	0.7595	Semen Euphorbiae	Euphorbia factor Ti2	Not Available	FALSE	C12C(CC(=CC3C1(C(C(C1(C3C1(C)C)OC(=O)/C=C\C=C\C=C\CCC)OC(=O)C)C)O)CO)C(=O)C(=C2)C
MOL005223	0.4442	0.5558	0.7137	Semen Euphorbiae	DL-Laudanine	442304	FALSE	c12cc(c(cc1C(N(CC2)C)Cc1cc(c(cc1)OC)O)OC)OC
MOL005224	0.5743	0.4257	0.6182	Capsici Fructus	TETRATETRACONTANE	23494	FALSE	C(CCCCCCCCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCCCCC
MOL005224	0.5743	0.4257	0.6182	Calyx Seu Fructus Physalis	TETRATETRACONTANE	23494	FALSE	C(CCCCCCCCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCCCCC
MOL005224	0.5743	0.4257	0.6182	Flos Genkwa	TETRATETRACONTANE	23494	FALSE	C(CCCCCCCCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCCCCC
MOL005224	0.5743	0.4257	0.6182	Lycii Fructus	TETRATETRACONTANE	23494	FALSE	C(CCCCCCCCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCCCCC
MOL005224	0.5743	0.4257	0.6182	Microctis Folium	TETRATETRACONTANE	23494	FALSE	C(CCCCCCCCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCCCCC
MOL005224	0.5743	0.4257	0.6182	Semen Euphorbiae	TETRATETRACONTANE	23494	FALSE	C(CCCCCCCCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCCCCC
MOL005224	0.5743	0.4257	0.6182	Mori Fructus	TETRATETRACONTANE	23494	FALSE	C(CCCCCCCCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCCCCC
MOL005224	0.5743	0.4257	0.6182	Ranunculi Ternati Radix	TETRATETRACONTANE	23494	FALSE	C(CCCCCCCCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCCCCC
MOL005225	0.7963	0.2037	0.8217	Semen Euphorbiae	ingenol	Not Available	FALSE	C1(C2C1CC(C13C(=O)C2C=C(C(C1(C(C(=C3)C)O)O)O)CO)C)(C)C
MOL005226	0.7963	0.2037	0.8217	Semen Euphorbiae	ingenol	Not Available	FALSE	C123C(C(C(=CC(C1=O)C1C(CC2C)C1(C)C)CO)O)(C(C(=C3)C)O)O
MOL005227	0.7702	0.2298	0.8452	Semen Euphorbiae	casticin	5315263	FALSE	C12C(OC(C1=O)OC)C1CC(C(CC1)OC)O)CC(C2O)OC)OC
MOL005227	0.7702	0.2298	0.8452	Viticis Fructus	casticin	5315263	FALSE	C12C(OC(C1=O)OC)C1CC(C(CC1)OC)O)CC(C2O)OC)OC

MOL005227	0.7702	0.2298	0.8452	Viticis Cannabifoliae Fructus	casticin	5315263	FALSE	c12c(oc(c(c1=O)OC)c1cc(c(cc1)OC)O)cc(c(c2O)OC)OC
MOL005228	0.0454	0.9546	0.8072	Semen Euphorbiae	euphorbia steroid	Not Available	FALSE	C12(C(C(C3(OC3)CCC3C(C3(C)C)/C=C(/C1=O)\C)OC(=O)C)C(C(C2)C)OC(=O)Cc1ccccc1)OC(=O)C
MOL005229	0.7355	0.2645	0.7855	Viticis Fructus	Artemetin	5320351	FALSE	c12c(oc(c(c1=O)OC)c1cc(c(cc1)OC)OC)cc(c(c2O)OC)OC
MOL005229	0.7355	0.2645	0.7855	Semen Euphorbiae	Artemetin	5320351	FALSE	c12c(oc(c(c1=O)OC)c1cc(c(cc1)OC)OC)cc(c(c2O)OC)OC
MOL005229	0.7355	0.2645	0.7855	Artemisia Annua L.	Artemetin	5320351	FALSE	c12c(oc(c(c1=O)OC)c1cc(c(cc1)OC)OC)cc(c(c2O)OC)OC
MOL005229	0.7355	0.2645	0.7855	Verbenae Herb	Artemetin	5320351	FALSE	c12c(oc(c(c1=O)OC)c1cc(c(cc1)OC)OC)cc(c(c2O)OC)OC
MOL005230	0.3818	0.6182	0.7021	Semen Euphorbiae	lathyrol	Not Available	FALSE	OC12C(C(O)C(C1)C)C(O)C(=C)CCC1C(C1/C=C(/C2=O)\C)(C)C
MOL005231	0.8402	0.1598	0.7729	Semen Euphorbiae	isoeuphorbetin	71438018	FALSE	c1(c(c(c2c(c1)ccc(=O)o2)c1c2c(cc(c1O)O)oc(=O)cc2)O)O
MOL005232	0.9150	0.0850	0.9503	Semen Pharbitidis	cis-Hexahydro-o-xylene	16628	FALSE	C1(C(CCCC1)C)C
MOL005233	0.9083	0.0917	0.9516	Semen Pharbitidis	2-hydroxy-1-phenyl-1,4-pentadione	Not Available	FALSE	C(=O)(C(CC(=O)C)O)c1ccccc1
MOL005234	0.5362	0.4638	0.7239	Semen Pharbitidis	Chaohuoside A	Not Available	FALSE	C1(cc(c2c(c1CC=C(C)C)oc(c(c2=O)OC1OC(C(C(C1O)OC1OC(C(C(C1O)O)OC(=O)CC)COC(=O)C)OC(=O)C)C)c1ccc(cc1)OC)O)OC1OC(C(C(C1O)O)O)CO
MOL005235	0.8347	0.1653	0.8400	Paederiae Scandentis Herba	Embelin	3218	FALSE	C1(=CC(=O)C(=C(C1=O)CCCCCCCCCCC)O)O
MOL005235	0.8347	0.1653	0.8400	Radix Clematidis	Embelin	3218	FALSE	C1(=CC(=O)C(=C(C1=O)CCCCCCCCCCC)O)O
MOL005235	0.8347	0.1653	0.8400	Semen Pharbitidis	Embelin	3218	FALSE	C1(=CC(=O)C(=C(C1=O)CCCCCCCCCCC)O)O
MOL005235	0.8347	0.1653	0.8400	Ardisiae Japonicae Herba	Embelin	3218	FALSE	C1(=CC(=O)C(=C(C1=O)CCCCCCCCCCC)O)O
MOL005236	0.8658	0.1342	0.7870	Semen Pharbitidis	gibberellin	Not Available	FALSE	C1=CC23C(C(C1O)(C(=O)O3)C)C(C13C2CCC(C1)(C(=C)C3)O)C(=O)O
MOL005236	0.8658	0.1342	0.7870	Ginkgo Semen	gibberellin	Not Available	FALSE	C1=CC23C(C(C1O)(C(=O)O3)C)C(C13C2CCC(C1)(C(=C)C3)O)C(=O)O
MOL005237	0.8374	0.1626	0.7904	Semen Pharbitidis	gibberellin A5	Not Available	FALSE	C1=CC2(C3C(C1)(C1C4(C3C(=O)O)CC(CC1)(C(=C)C4)O)OC2=O)C
MOL005238	0.8944	0.1056	0.8738	Semen Pharbitidis	Gibberellin A8	Not Available	FALSE	C1(C(C2(C3C(C1)(C1C4(C3C(=O)O)CC(CC1)(C(=C)C4)O)OC2=O)C)O)O
MOL005239	0.7162	0.2838	0.8287	Semen Pharbitidis	Lysicamine	Not Available	FALSE	c1cc2c3c(n1)C(=O)c1c(c3c(c(c2)OC)OC)cccc1
MOL005239	0.7162	0.2838	0.8287	Jujubae Fructus	Lysicamine	Not Available	FALSE	c1cc2c3c(n1)C(=O)c1c(c3c(c(c2)OC)OC)cccc1
MOL005239	0.7162	0.2838	0.8287	Nelumbinis Plumula	Lysicamine	Not Available	FALSE	c1cc2c3c(n1)C(=O)c1c(c3c(c(c2)OC)OC)cccc1
MOL005240	0.0692	0.9308	0.7616	Semen Pharbitidis	Nimbolidin B	Not Available	FALSE	CC(=O)OC1CC(C2(C3C1(C(C(C(C3OC2)OC(=O)/C(=C/C)/C)(C)C1=C(C(CC1OC(=O)C)c1cocc1)C)COC(=O)C)C)C)OC(=O)C

MOL005241	0.3515	0.6485	0.7673	Semen Pharbitidis	Pennogenin	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC2C1(C(C1(O2)CCC(CO1)C)C)O)C)O
MOL005242	0.6156	0.3844	0.7290	Semen Pharbitidis	Pharbitic acid D	Not Available	FALSE	C1(C(C(C(C(O1)OC1C(C(C(OC1C)OCC1C(C(C(C(O1)OC(CCC)CCCCCCCC(CC(=O)O)O)OC1OC(C(C(C1OC1OCC(C(C1O)O)O)O)O)CO)O)O)O)O)O)OC1OC(C(C(C1O)O)O)C)O)C
MOL005243	0.9198	0.0802	0.8467	Semen Pharbitidis	pharbitic acid D_qt	Not Available	FALSE	OC(CCC)CCCCCCCC(CC(=O)O)O
MOL005244	0.9000	0.1000	0.9670	Semen Pharbitidis	SMB	448893	FALSE	CCC(C(=O)O)C
MOL005244	0.9000	0.1000	0.9670	Capsici Fructus	SMB	448893	FALSE	CCC(C(=O)O)C
MOL005244	0.9000	0.1000	0.9670	Farfarae Flos	SMB	448893	FALSE	CCC(C(=O)O)C
MOL005245	0.9234	0.0766	0.9459	Semen Pharbitidis	Propylcyclopentane	16270	FALSE	C1(CCC)CCCC1
MOL005245	0.9234	0.0766	0.9459	A. Dahurica (Fisch.) Benth. Et Hook	Propylcyclopentane	16270	FALSE	C1(CCC)CCCC1
MOL005246	0.8379	0.1621	0.7912	Semen Pharbitidis	gibberellin A20	Not Available	FALSE	O1C23C4C5(C(C2C(CCC3)(C1=O)C)C(=O)O)CC(O)(CC4)C(=C)C5
MOL005247	0.8890	0.1110	0.8282	Semen Pharbitidis	gibberellin A26	Not Available	FALSE	O1C23C4C5(C(C2C(C(O)C(C3)O)(C1=O)C)C(=O)O)CC(C(=O)C4)C(=C)C5
MOL005248	0.8670	0.1330	0.7867	Semen Pharbitidis	gibberellin A29	Not Available	FALSE	O1C23C4C5(C(C2C(CC(O)C3)(C1=O)C)C(=O)O)CC(O)(CC4)C(=C)C5
MOL005249	0.7915	0.2085	0.8297	Semen Pharbitidis	gibberellin A9	Not Available	FALSE	O1C23C4C5(C(C2C(CCC3)(C1=O)C)C(=O)O)CC(CC4)C(=C)C5
MOL005250	0.8380	0.1620	0.8467	Semen Pharbitidis	gibberellin glucoside I	Not Available	FALSE	O1C23C(C(C1=O)(C(OC1OC(C(O)C(O)C1O)CO)C=C3)C)C(C13C2CCC(O)(C1)C(=C)C3)C(=O)O
MOL005251	0.8658	0.1342	0.7870	Semen Pharbitidis	gibberellin glucoside I_qt	Not Available	FALSE	O1C23C(C(C1=O)(C(O)C=C3)C)C(C13C2CCC(O)(C1)C(=C)C3)C(=O)O
MOL005253	0.7863	0.2137	0.7794	Semen Pharbitidis	gibberellin glucosideII_qt	Not Available	FALSE	O1C23C(C(C1=O)(C(O)C=C3)C)C(C13C2CCC(O)(C1)C(=C)C3)C(=O)OC
MOL005254	0.8282	0.1718	0.8546	Semen Pharbitidis	gibberellin glucoside III	Not Available	FALSE	O(C1C(C2C(=C3C4(C2C(=O)O)CC(O)(C(=C)C4)CC3)C=C1)(C)C(=O)O)C1OC(C(O)C(O)C1O)CO
MOL005255	0.8681	0.1319	0.7557	Semen Pharbitidis	gibberellin glucoside III_qt	Not Available	FALSE	OC1C(C2C(=C3C4(C2C(=O)O)CC(O)(C(=C)C4)CC3)C=C1)(C)C(=O)O
MOL005256	0.9198	0.0802	0.8467	Semen Pharbitidis	ipurolic acid	Not Available	FALSE	OC(CCCCCCCC(O)CC(=O)O)CCC
MOL005257	0.8159	0.1841	0.7061	Semen Pharbitidis	Penniclavin	115247	FALSE	OC1(CN(C2C(=C1)c1c3c(C2)c[nH]c3ccc1)C)CO
MOL005259	0.9025	0.0975	0.9677	Semen Pharbitidis	(2R,3S)-3-hydroxy-2-methylbutanoic acid	11815846	FALSE	CC(C(C(=O)O)C)O
MOL005260	0.7933	0.2067	0.6084	Semen Pharbitidis	CHANOCLAVINE	5281381	FALSE	OC/C(=C/C1C(NC)Cc2c3c1cccc3[nH]c2)/C
MOL005261	0.7701	0.2299	0.6202	Semen Pharbitidis	LYSERGOL	14987	FALSE	c12c3C4=CC(CN(C4Cc1c[nH]c2ccc3)C)CO

MOL005262	0.5469	0.4531	0.7416	Semen Pharbitidis	(3S,11S)-11-[[(2R,3R,4S,5S,6R)-3-[[(2S,3R,4S,5S,6R)-3-[[(2S,3R,4S,5R,6S)-5-[[(2S,3R,4S,5R,6R)-3,5-dihydroxy-6-methyl-4-[[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-2-tetrahydropyranyl]oxy]-2-tetrahydropyranyl]oxy]-3,4-dihydroxy-6-methyl-2-tetrahydropyrany	21629994	FALSE	O1C(C(C(C(C1C)O)O)O)OC1C(C(OC(C1O)C)OC1C(C(C(OC1C)OC1C(C(C(OC1OC1C(OC(C(C1O)O)COC1OC(C(C(C1O)O)O)C)OC(CCCCCCCC(O)CC(=O)O)CCCCC)CO)O)O)O)O)O
MOL005263	0.9038	0.0962	0.7597	Semen Pharbitidis	pharbitic acid B_qt	Not Available	FALSE	OC(CCCCCCCC(O)CC(=O)O)CCCCC

MOL005264	0.6214	0.3786	0.7150	Semen Pharbitidis	(3S,11S)-11-[[(2R,3R,4S,5S,6R)-3-[[(2S,3R,4S,5S,6R)-3-[[(2S,3R,4S,5R,6S)-3,4-dihydroxy-6-methyl-5-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-methyl-2-tetrahydropyranyl]oxy]-2-tetrahydropyranyl]oxy]-4,5-dihydroxy-6-(hydroxymethyl)-2-tetrahydropyranyl]oxy]-4,5-d	21629992	FALSE	O1C(C(C(C(C1C)O)O)O)OCC1OC(C(C(C1O)O)OC1OC(C(C1OC1OC(C(C(C1O)O)OC1OC(C(C(C1O)O)O)C)C)O)O)CO)OC(CCCCCCCC(O)CC(=O)O)CCC

MOL005265	0.5971	0.4029	0.7385	Semen Pharbitidis	(3S,11S)-11-[[(2R,3R,4S,5S,6R)-3-[[(2S,3R,4S,5S,6R)-3-[[(2S,3R,4S,5R,6S)-5-[[(2S,3R,4S,5R,6R)-3,5-dihydroxy-6-methyl-4-[[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-2-tetrahydropyranyl]oxy]-2-tetrahydropyranyl]oxy]-3,4-dihydroxy-6-methyl-2-tetrahydropyrany	21629993	FALSE	O1C(C(C(C(C1C)O)O)O)OC1C(C(OC(C1O)C)OC1C(C(C(OC1C)OC1C(C(C(OC1OC1C(OC(C(C1O)O)COC1OC(C(C(C1O)O)O)C)OC(CCCCCCCC(O)CC(=O)O)CCC)CO)O)O)O)O)O)O
MOL005266	0.6887	0.3113	0.6700	Semen Pharbitidis	AGROCLAVIN	73484	FALSE	N1(C2C(c3c4c(C2)c[nH]c4ccc3)C=C(C1)C)C
MOL005268	0.9295	0.0705	0.9604	Semen Pharbitidis	Ethylcyclohexane	15504	FALSE	C1(CCCCC1)CC
MOL005268	0.9295	0.0705	0.9604	Eucommiae Folium	Ethylcyclohexane	15504	FALSE	C1(CCCCC1)CC
MOL005271	0.6582	0.3418	0.6063	Panax Ginseng C. A. Mey.	1-HEXADECYNE	12396	FALSE	C(CCCCCCC)CCCCCCC#C
MOL005272	0.7318	0.2682	0.6811	Allii Fistulost Bulbus	13-Tetradecenyl acetate	521718	FALSE	C(CCCCCCCCCCCC=C)OC(=O)C
MOL005272	0.7318	0.2682	0.6811	Panax Ginseng C. A. Mey.	13-Tetradecenyl acetate	521718	FALSE	C(CCCCCCCCCCCC=C)OC(=O)C
MOL005272	0.7318	0.2682	0.6811	Cornus Officinalis Sieb. Et Zucc.	13-Tetradecenyl acetate	521718	FALSE	C(CCCCCCCCCCCC=C)OC(=O)C

MOL005273	0.3636	0.6364	0.7949	Panax Ginseng C. A. Mey.	16-Oxoseratenediol	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(CC2=CC(=O)C3C(C2CC1)(CCC(C3(C)C)O)C)C)(C)C)C)(C)C)O
MOL005273	0.3636	0.6364	0.7949	Panacis Quinquefolii Radix	16-Oxoseratenediol	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(CC2=CC(=O)C3C(C2CC1)(CCC(C3(C)C)O)C)C)(C)C)C)(C)C)O
MOL005274	0.9127	0.0873	0.9508	Eriobotryae Folium	Neohexane	6403	FALSE	C(CC)(C)(C)C
MOL005274	0.9127	0.0873	0.9508	Panax Ginseng C. A. Mey.	Neohexane	6403	FALSE	C(CC)(C)(C)C
MOL005274	0.9127	0.0873	0.9508	Viticis Negundo Folium	Neohexane	6403	FALSE	C(CC)(C)(C)C
MOL005275	0.8985	0.1015	0.7186	Panax Ginseng C. A. Mey.	2,3,4-Trimethyldecane	Not Available	FALSE	C(C(CCCCCC)C)(C(C)C)C
MOL005276	0.8871	0.1129	0.7226	Panax Ginseng C. A. Mey.	2,3,8-Trimethyldecane	Not Available	FALSE	CC(C(CCCCC(CC)C)C)C
MOL005278	0.8078	0.1922	0.6385	Panax Ginseng C. A. Mey.	2-METHYLTRIDECANE	15269	FALSE	C(CCCCCCCC)CCC(C)C
MOL005278	0.8078	0.1922	0.6385	Capsici Fructus	2-METHYLTRIDECANE	15269	FALSE	C(CCCCCCCC)CCC(C)C
MOL005278	0.8078	0.1922	0.6385	Farfarae Flos	2-METHYLTRIDECANE	15269	FALSE	C(CCCCCCCC)CCC(C)C
MOL005278	0.8078	0.1922	0.6385	Maydis Seigma	2-METHYLTRIDECANE	15269	FALSE	C(CCCCCCCC)CCC(C)C
MOL005279	0.4038	0.5962	0.7568	Ginsen Radix Et Rhizoma Rubra	ginsenoside-Rh1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)O)C)C)C)C)C)O
MOL005279	0.4038	0.5962	0.7568	Panax Ginseng C. A. Mey.	ginsenoside-Rh1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)O)C)C)C)C)C)O
MOL005279	0.4038	0.5962	0.7568	Ginseng Folium	ginsenoside-Rh1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)O)C)C)C)C)C)O
MOL005280	0.2494	0.7506	0.7336	Panax Ginseng C. A. Mey.	ginsenoside-Rh1_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)O)C)C)(C)C)C)O
MOL005280	0.2494	0.7506	0.7336	Ginseng Folium	ginsenoside-Rh1_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)O)C)C)(C)C)C)O
MOL005280	0.2494	0.7506	0.7336	Ginsen Radix Et Rhizoma Rubra	ginsenoside-Rh1_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)O)C)C)(C)C)C)O
MOL005281	0.4038	0.5962	0.7568	Panax Ginseng C. A. Mey.	20(S)-Ginsenoside-Rh1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)C)C)O

MOL005282	0.2494	0.7506	0.7336	Panax Ginseng C. A. Mey.	20(S)-Ginsenoside-Rh1_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL005282	0.2494	0.7506	0.7336	Ginsen Radix Et Rhizoma Rubra	20(S)-Ginsenoside-Rh1_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL005283	0.6600	0.3400	0.8606	Panax Ginseng C. A. Mey.	20(S)-ginsenoside-Rg2	Not Available	FALSE	C12(C3(C(C(CC3)C(CCC=C(C)C)(C)O)C(CC1C1(C(C(C2)OC2C(OC3C(C(C(C(O3)C)O)O)O)C(C(C(O2)CO)O)O)C(C(CC1)O)(C)C)C)O)C)C
MOL005284	0.2494	0.7506	0.7336	Panacis Quinquefolii Radix	(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,6,12-triol	11468733	FALSE	C12(C3(C(C(CC3)C(CCC=C(C)C)(C)O)C(CC1C1(C(C(C2)O)C(C(CC1)O)(C)C)C)O)C)C
MOL005284	0.2494	0.7506	0.7336	Panax Ginseng C. A. Mey.	(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,6,12-triol	11468733	FALSE	C12(C3(C(C(CC3)C(CCC=C(C)C)(C)O)C(CC1C1(C(C(C2)O)C(C(CC1)O)(C)C)C)O)C)C

MOL005284	0.2494	0.7506	0.7336	Ginsen Radix Et Rhizoma Rubra	(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,6,12-triol	11468733	FALSE	C12(C3(C(C(CC3)C(CCC=C(C)C)(C)O)C(CC1C1(C(C(C2)O)C(C(CC1)O)(C)C)C)O)C)C
MOL005284	0.2494	0.7506	0.7336	Ginseng Folium	(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,6,12-triol	11468733	FALSE	C12(C3(C(C(CC3)C(CCC=C(C)C)(C)O)C(CC1C1(C(C(C2)O)C(C(CC1)O)(C)C)C)O)C)C

MOL005284	0.2494	0.7506	0.7336	Panacis Japonici Rhizoma	(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,6,12-triol	11468733	FALSE	C12(C3(C(C(CC3)C(CCC=C(C)C)(C)O)C(CC1C1(C(C(C2)O)C(C(CC1)O)(C)C)C)O)C)C
MOL005284	0.2494	0.7506	0.7336	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,6,12-triol	11468733	FALSE	C12(C3(C(C(CC3)C(CCC=C(C)C)(C)O)C(CC1C1(C(C(C2)O)C(C(CC1)O)(C)C)C)O)C)C

MOL005284	0.2494	0.7506	0.7336	Gynostemmae Pentaphylli Herba	(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,6,12-triol	11468733	FALSE	C12(C3(C(C(CC3)C(CCC=C(C)C)(C)O)C(CC1C1(C(C(C2)O)C(C(CC1)O)(C)C)C)O)C)C
MOL005285	0.2305	0.7695	0.7376	Panacis Quinquefolii Radix	20(s)-protopanaxadiol	9920281	FALSE	C12(C3(C(C(CC3)C(CCC=C(C)C)(O)C)C(CC1C1(C(CC2)C(C(CC1)O)(C)C)C)O)C)C
MOL005285	0.2305	0.7695	0.7376	Panax Ginseng C. A. Mey.	20(s)-protopanaxadiol	9920281	FALSE	C12(C3(C(C(CC3)C(CCC=C(C)C)(O)C)C(CC1C1(C(CC2)C(C(CC1)O)(C)C)C)O)C)C
MOL005286	0.6600	0.3400	0.8606	Panax Ginseng C. A. Mey.	20(R)-ginsenoside Rg2	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)OC2C(C(C(C(O2)C)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL005286	0.6600	0.3400	0.8606	Ginsen Radix Et Rhizoma Rubra	20(R)-ginsenoside Rg2	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)OC2C(C(C(C(O2)C)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL005287	0.6798	0.3202	0.8580	Panax Ginseng C. A. Mey.	20-(S)-Ginsenoside-Rg3	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)O)OC1C(C(C(C(O1)CO)O)O)O
MOL005288	0.2305	0.7695	0.7376	Panax Ginseng C. A. Mey.	20-(S)-Ginsenoside-Rg3_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL005289	0.9235	0.0765	0.9273	Panax Ginseng C. A. Mey.	3,4-Dimethylheptane	59954486	FALSE	C(C(CC)C)(CCC)C
MOL005290	0.9500	0.0500	0.8435	Panax Ginseng C. A. Mey.	3,5-Dimethyl-p-anisic acid	88944	FALSE	c1c(c(c(cc1C(=O)O)C)OC)C
MOL005290	0.9500	0.0500	0.8435	Polygoni Cuspidati Rhizoma Et Radix	3,5-Dimethyl-p-anisic acid	88944	FALSE	c1c(c(c(cc1C(=O)O)C)OC)C

MOL005291	0.6968	0.3032	0.7638	Panax Ginseng C. A. Mey.	3-O-beta-D-Glucuronopyranosyl gypsogenin	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(=O)O)CCC(C1)(C)C)C)C)C)(C)C=O)OC1OC(C(C(C1O)O)O)C(=O)O
MOL005292	0.7411	0.2589	0.8610	Panax Ginseng C. A. Mey.	3-O-beta-D-Glucuronopyranosyl gypsogenin_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(=O)O)CCC(C1)(C)C)C)C)C)(C)C=O)O
MOL005293	0.9288	0.0712	0.9028	Eriobotryae Folium	3-Ethyl-3-methylheptane	140213	FALSE	C(CCCC)(CC)(CC)C
MOL005293	0.9288	0.0712	0.9028	Panax Ginseng C. A. Mey.	3-Ethyl-3-methylheptane	140213	FALSE	C(CCCC)(CC)(CC)C
MOL005293	0.9288	0.0712	0.9028	Equiseti Hiemalis Herba	3-Ethyl-3-methylheptane	140213	FALSE	C(CCCC)(CC)(CC)C
MOL005294	0.9250	0.0750	0.9344	Eucommiae Folium	3-methylheptane	12263095	FALSE	C(CCCC)(CC)C
MOL005294	0.9250	0.0750	0.9344	Panax Ginseng C. A. Mey.	3-methylheptane	12263095	FALSE	C(CCCC)(CC)C
MOL005295	0.8958	0.1042	0.7959	Panax Ginseng C. A. Mey.	3-methylundecane	14656881	FALSE	C(CCCCCCCC)(CC)C
MOL005295	0.8958	0.1042	0.7959	Raphani Semen	3-methylundecane	14656881	FALSE	C(CCCCCCCC)(CC)C
MOL005296	0.8654	0.1346	0.7094	Sesami Nigrum Semen	4-Methyldodecane	Not Available	FALSE	C(CCCCCCCC)(CCC)C
MOL005296	0.8654	0.1346	0.7094	Panax Ginseng C. A. Mey.	4-Methyldodecane	Not Available	FALSE	C(CCCCCCCC)(CCC)C
MOL005297	0.8545	0.1455	0.6919	Panax Ginseng C. A. Mey.	5-Isobutylnonane	545936	FALSE	C(CC(C)C)(CCCC)CCCC
MOL005300	0.7323	0.2677	0.7999	Panax Ginseng C. A. Mey.	6'-Malonylginsenoside Rd1	Not Available	FALSE	O1C(C(C(C(C1OC1C(OC(C(C1O)O)CO)OC1C(C2C(CC1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)C)C)C)(C)C)O)O)O)COC(=O)CC(=O)O

MOL005301	0.2305	0.7695	0.7376	Panax Ginseng C. A. Mey.	6'-Malonylginsenoside Rd1_qt1	Not Available	FALSE	OC1C(C2C(CC1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C
MOL005302	0.5219	0.4781	0.8111	Panax Ginseng C. A. Mey.	7-(beta-Xylosyl)cephalomannine	Not Available	FALSE	C1(C(=O)C2(C(C(C3(C(C1=C(C(C3)OC(=C)C(C(c1ccccc1)NC(=O)/C(=C/C)/C)O)C)(C)C)O)OC(=O)c1ccccc1)C1(C(CC2OC2C(C(C(CO2)O)O)O)OC1)OC(=O)C)C)OC(=O)C
MOL005302	0.5219	0.4781	0.8111	Codonopsis Radix	7-(beta-Xylosyl)cephalomannine	Not Available	FALSE	C1(C(=O)C2(C(C(C3(C(C1=C(C(C3)OC(=C)C(C(c1ccccc1)NC(=O)/C(=C/C)/C)O)C)(C)C)O)OC(=O)c1ccccc1)C1(C(CC2OC2C(C(C(CO2)O)O)O)OC1)OC(=O)C)C)OC(=O)C
MOL005303	0.8063	0.1937	0.7316	Panax Ginseng C. A. Mey.	7-Tetradecyne	141979	FALSE	C(#CCCCCCC)CCCCCC
MOL005303	0.8063	0.1937	0.7316	Ardisiae Japonicae Herba	7-Tetradecyne	141979	FALSE	C(#CCCCCCC)CCCCCC
MOL005304	0.8497	0.1503	0.8163	Panax Ginseng C. A. Mey.	7alpha-L-Rhamnosyl-6-methoxylutcolin	Not Available	FALSE	c1(c(c(c2c(c1)oc(cc2=O)c1cc(c(cc1)O)O)O)OC)OC1C(C(C(C(O1)C)O)O)O
MOL005304	0.8497	0.1503	0.8163	Codonopsis Radix	7alpha-L-Rhamnosyl-6-methoxylutcolin	Not Available	FALSE	c1(c(c(c2c(c1)oc(cc2=O)c1cc(c(cc1)O)O)O)OC)OC1C(C(C(C(O1)C)O)O)O
MOL005305	0.9256	0.0744	0.8980	Panax Ginseng C. A. Mey.	Nepetin	5317284	FALSE	c1(c(c(c2c(c1)oc(cc2=O)c1cc(c(cc1)O)O)O)OC)O
MOL005305	0.9256	0.0744	0.8980	Oroxyli Semen	Nepetin	5317284	FALSE	c1(c(c(c2c(c1)oc(cc2=O)c1cc(c(cc1)O)O)O)OC)O
MOL005305	0.9256	0.0744	0.8980	Saussureae Involucratae Herba	Nepetin	5317284	FALSE	c1(c(c(c2c(c1)oc(cc2=O)c1cc(c(cc1)O)O)O)OC)O
MOL005305	0.9256	0.0744	0.8980	Inulae Herba	Nepetin	5317284	FALSE	c1(c(c(c2c(c1)oc(cc2=O)c1cc(c(cc1)O)O)O)OC)O
MOL005306	0.9311	0.0689	0.9602	Cornus Officinalis Sieb. Et Zucc.	Acetal	7765	FALSE	C(OCC)(OCC)C
MOL005306	0.9311	0.0689	0.9602	Rubi Fructus	Acetal	7765	FALSE	C(OCC)(OCC)C
MOL005306	0.9311	0.0689	0.9602	Panax Ginseng C. A. Mey.	Acetal	7765	FALSE	C(OCC)(OCC)C
MOL005306	0.9311	0.0689	0.9602	Litchi Semen	Acetal	7765	FALSE	C(OCC)(OCC)C
MOL005306	0.9311	0.0689	0.9602	Paederiae Scandentis Herba	Acetal	7765	FALSE	C(OCC)(OCC)C
MOL005308	0.8049	0.1951	0.8084	Panax Ginseng C. A. Mey.	Aposiopolamine	Not Available	FALSE	c1ccc(cc1)C(=C)C(=O)OC1CC2C3C(C(C1)N2)O3
MOL005309	0.7375	0.2625	0.8410	Panax Ginseng C. A. Mey.	Araloside A	Not Available	FALSE	C1(C(C(OC1CO)OC1C(C(C(OC1C(=O)O)OC1C(C2C(CC1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1OC(C(C(C1O)O)O)CO)C)C)(C)C)O)O)O)O

MOL005310	0.7553	0.2447	0.9079	Panax Ginseng C. A. Mey.	(4aS,6aR,6aS,6bR,8aR,10S,12aR,14bR)-10-hydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	7048528	FALSE	OC1C(C2C(CC1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)(C)C
MOL005310	0.7553	0.2447	0.9079	Caulis Akebiae	(4aS,6aR,6aS,6bR,8aR,10S,12aR,14bR)-10-hydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	7048528	FALSE	OC1C(C2C(CC1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)(C)C
MOL005311	0.8602	0.1398	0.7976	Panax Ginseng C. A. Mey.	Argininyl-fructosyl-glucose	Not Available	FALSE	O1CC(C(C(C1(CNC(C(=O)O)CCCNC(=N)N)O)O)OC1OC(C(C(C1O)O)O)CO)O
MOL005312	0.8799	0.1201	0.9097	Panax Ginseng C. A. Mey.	Argininyl-fructosyl-glucose_qt	Not Available	FALSE	O1CC(C(C(C1(CNC(C(=O)O)CCCNC(=N)N)O)O)O)O
MOL005313	0.9179	0.0821	0.8011	Panax Ginseng C. A. Mey.	5-[(3aS,6R,6aR)-2-keto-1,3,3a,4,6,6a-hexahydrothieno[3,4-d]imidazol-6-yl]valeric acid	5315463	FALSE	C1(SCC2C1NC(=O)N2)CCCCC(=O)O
MOL005314	0.0869	0.9131	0.6027	Panax Ginseng C. A. Mey.	Celabenzine	Not Available	FALSE	N1(CCCNC(=O)CC(NCCCC1)c1ccccc1)C(=O)c1ccccc1

MOL005315	0.9331	0.0669	0.9423	Stemonae Radix	(R)-()-Citronellal	75427	TRUE	CC(=CCCC(C)CC=O)C
MOL005315	0.9331	0.0669	0.9423	Lilii Bulbus	(R)-()-Citronellal	75427	TRUE	CC(=CCCC(C)CC=O)C
MOL005315	0.9331	0.0669	0.9423	Allii Fistulost Bulbus	(R)-()-Citronellal	75427	TRUE	CC(=CCCC(C)CC=O)C
MOL005315	0.9331	0.0669	0.9423	Myristicae Semen	(R)-()-Citronellal	75427	TRUE	CC(=CCCC(C)CC=O)C
MOL005315	0.9331	0.0669	0.9423	Panax Ginseng C. A. Mey.	(R)-()-Citronellal	75427	TRUE	CC(=CCCC(C)CC=O)C
MOL005316	0.9130	0.0870	0.9453	Panax Ginseng C. A. Mey.	MAV	657117	FALSE	C(=O)(C1OC(C(C(C1O)O)O)O)O
MOL005318	0.8914	0.1086	0.6890	Panax Ginseng C. A. Mey.	Dianthramine	441562	FALSE	c1(ccc(c(c1)Nc1c(ccc(c1)O)C(=O)O)C(=O)O)O
MOL005319	0.8496	0.1504	0.7676	Panax Ginseng C. A. Mey.	Ditertbutyl phthalate	121712	FALSE	c1ccc(c(c1)C(=O)OC(C)(C)C)C(=O)OC(C)(C)C
MOL005319	0.8496	0.1504	0.7676	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	Ditertbutyl phthalate	121712	FALSE	c1ccc(c(c1)C(=O)OC(C)(C)C)C(=O)OC(C)(C)C
MOL005319	0.8496	0.1504	0.7676	Panacis Quinquefolii Radix	Ditertbutyl phthalate	121712	FALSE	c1ccc(c(c1)C(=O)OC(C)(C)C)C(=O)OC(C)(C)C
MOL005320	0.7149	0.2851	0.6020	Panax Ginseng C. A. Mey.	arachidonate	5312542	FALSE	C(CC/C=C/C/C=C/C/C=C/C/C=C/CCCC(=O)O)CC
MOL005320	0.7149	0.2851	0.6020	Cistanches Herba	arachidonate	5312542	FALSE	C(CC/C=C/C/C=C/C/C=C/C/C=C/CCCC(=O)O)CC
MOL005321	0.7894	0.2106	0.7016	Codonopsis Radix	Frutinone A	441965	FALSE	c1ccc2c(c1)c(=O)c1c(o2)c2c(oc1=O)cccc2
MOL005321	0.7894	0.2106	0.7016	Panax Ginseng C. A. Mey.	Frutinone A	441965	FALSE	c1ccc2c(c1)c(=O)c1c(o2)c2c(oc1=O)cccc2
MOL005322	0.8264	0.1736	0.6799	Panax Ginseng C. A. Mey.	Gamma-Selinene	Not Available	FALSE	C1CC(=C)C2C(C1)(CCC(=C(C)C)C2)C
MOL005322	0.8264	0.1736	0.6799	Schisandrae Chinensis Fructus	Gamma-Selinene	Not Available	FALSE	C1CC(=C)C2C(C1)(CCC(=C(C)C)C2)C
MOL005323	0.6669	0.3331	0.7538	Ginseng Folium	ginsenoside La	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C)C2(CCC3C(OC4OC(C(C(C4O)O)O)CO)CC(OC(C1)C23)C=C(C)C)C)C)(C)C)(OC1OC(C(C(C1O)O)O)CO)C
MOL005323	0.6669	0.3331	0.7538	Panax Ginseng C. A. Mey.	ginsenoside La	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C)C2(CCC3C(OC4OC(C(C(C4O)O)O)CO)CC(OC(C1)C23)C=C(C)C)C)C)(C)C)(OC1OC(C(C(C1O)O)O)CO)C
MOL005324	0.3344	0.6656	0.7909	Panax Ginseng C. A. Mey.	ginsenoside La_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C)C2(CCC3C(O)CC(OC(C1)C23)C=C(C)C)C)C)(C)C)(O)C
MOL005324	0.3344	0.6656	0.7909	Ginseng Folium	ginsenoside La_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C)C2(CCC3C(O)CC(OC(C1)C23)C=C(C)C)C)C)(C)C)(O)C
MOL005325	0.7572	0.2428	0.8299	Panacis Japonici Rhizoma	ginsenoside Ro	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(C1)C)(C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)CO)C(=O)O
MOL005325	0.7572	0.2428	0.8299	Panacis Quinquefolii Radix	ginsenoside Ro	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(C1)C)(C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)CO)C(=O)O

MOL005325	0.7572	0.2428	0.8299	Achyranthis Bidentatae Radix	ginsenoside Ro	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)CO)C(=O)O
MOL005325	0.7572	0.2428	0.8299	Panax Ginseng C. A. Mey.	ginsenoside Ro	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)CO)C(=O)O
MOL005326	0.7794	0.2206	0.7964	Panax Ginseng C. A. Mey.	Ginsenoside-Ra0	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(CC(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1C(C(C(C(O1)CO)O)O)O)O)O)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O
MOL005327	0.2305	0.7695	0.7376	Nodus Nelumbinis Rhizomatis	Gypnoside V_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL005327	0.2305	0.7695	0.7376	Panacis Quinquefolii Radix	Gypnoside V_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL005327	0.2305	0.7695	0.7376	Ginseng Folium	Gypnoside V_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL005327	0.2305	0.7695	0.7376	Gynostemmae Pentaphylli Herba	Gypnoside V_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL005327	0.2305	0.7695	0.7376	Panax Ginseng C. A. Mey.	Gypnoside V_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL005328	0.7434	0.2566	0.7989	Panax Ginseng C. A. Mey.	Ginsenoside-Ra1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1OCC(C(C1O)O)OC1OCC(C(C1O)O)O)O)O)O)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O
MOL005328	0.7434	0.2566	0.7989	Panacis Quinquefolii Radix	Ginsenoside-Ra1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1OCC(C(C1O)O)OC1OCC(C(C1O)O)O)O)O)O)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O
MOL005329	0.7497	0.2503	0.8025	Panax Ginseng C. A. Mey.	Ginsenoside-Ra2	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1OC(C(C1OC1C(C(C(CO1)O)O)O)O)CO)O)O)O)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O)O
MOL005330	0.7559	0.2441	0.7973	Panax Ginseng C. A. Mey.	Ginsenoside-Ra3	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1C(C(C(C(O1)CO)O)OC1OCC(C(C1O)O)O)O)O)O)O)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O
MOL005331	0.7494	0.2506	0.8097	Panax Ginseng C. A. Mey.	ginsenoside Rb1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1C(C(C(C(O1)CO)O)O)O)O)O)O)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O

MOL005331	0.7494	0.2506	0.8097	Ginsen Radix Et Rhizoma Rubra	ginsenoside Rb1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1C(C(C(C(O1)CO)O)O)O)O)O)O)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O)O
MOL005331	0.7494	0.2506	0.8097	Panacis Japonici Rhizoma	ginsenoside Rb1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1C(C(C(C(O1)CO)O)O)O)O)O)O)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O
MOL005332	0.2305	0.7695	0.7376	Panax Ginseng C. A. Mey.	(3R,5R,8R,9R,10R,12R,13R,14R,17S)-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,12-diol	11048822	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL005332	0.2305	0.7695	0.7376	Panacis Japonici Rhizoma	(3R,5R,8R,9R,10R,12R,13R,14R,17S)-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,12-diol	11048822	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O

MOL005332	0.2305	0.7695	0.7376	Ginsen Radix Et Rhizoma Rubra	(3R,5R,8R,9R,10R,12R,13R,14R,17S)-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,12-diol	11048822	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL005333	0.7282	0.2718	0.8093	Panax Ginseng C. A. Mey.	ginsenoside-Rb2	Not Available	FALSE	C1CC2(C(C(C)(C1OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(O1)CO)O)O)O)C)CCC1(C2CC(C2C1(CCC2C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1C(C(C(CO1)O)O)O)O)O)O)C)O)C)C
MOL005333	0.7282	0.2718	0.8093	Ginseng Folium	ginsenoside-Rb2	Not Available	FALSE	C1CC2(C(C(C)(C1OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(O1)CO)O)O)O)C)CCC1(C2CC(C2C1(CCC2C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1C(C(C(CO1)O)O)O)O)O)O)C)O)C)C
MOL005333	0.7282	0.2718	0.8093	Gynostemmae Pentaphylli Herba	ginsenoside-Rb2	Not Available	FALSE	C1CC2(C(C(C)(C1OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(O1)CO)O)O)O)C)CCC1(C2CC(C2C1(CCC2C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1C(C(C(CO1)O)O)O)O)O)O)C)O)C)C
MOL005333	0.7282	0.2718	0.8093	Ginsen Radix Et Rhizoma Rubra	ginsenoside-Rb2	Not Available	FALSE	C1CC2(C(C(C)(C1OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(O1)CO)O)O)O)C)CCC1(C2CC(C2C1(CCC2C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1C(C(C(CO1)O)O)O)O)O)O)C)O)C)C

MOL005334	0.2305	0.7695	0.7376	Ginseng Folium	(3S,5R,8R,9R,10R,12R,13R,14R,17S)-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,12-diol	11213350	FALSE	C1CC2(C(C(C)(C1O)C)CCC1(C2CC(C2C1(CCC2C(CCC=C(C)C)(O)C)C)O)C)C
MOL005334	0.2305	0.7695	0.7376	Ginsen Radix Et Rhizoma Rubra	(3S,5R,8R,9R,10R,12R,13R,14R,17S)-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,12-diol	11213350	FALSE	C1CC2(C(C(C)(C1O)C)CCC1(C2CC(C2C1(CCC2C(CCC=C(C)C)(O)C)C)O)C)C

MOL005334	0.2305	0.7695	0.7376	Panacis Quinquefolii Radix	(3S,5R,8R,9R,10R,12R,13R,14R,17S)-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,12-diol	11213350	FALSE	C1CC2(C(C(C)(C1O)C)CCC1(C2CC(C2C1(CCC2C(CCC=C(C)C)(O)C)C)O)C)C
MOL005334	0.2305	0.7695	0.7376	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	(3S,5R,8R,9R,10R,12R,13R,14R,17S)-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,12-diol	11213350	FALSE	C1CC2(C(C(C)(C1O)C)CCC1(C2CC(C2C1(CCC2C(CCC=C(C)C)(O)C)C)O)C)C

MOL005334	0.2305	0.7695	0.7376	Panacis Japonici Rhizoma	(3S,5R,8R,9R,10R,12R,13R,14R,17S)-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,12-diol	11213350	FALSE	C1CC2(C(C(C)(C1O)C)CCC1(C2CC(C2C1(CCC2C(CCC=C(C)C)(O)C)C)O)C)C
MOL005334	0.2305	0.7695	0.7376	Gynostemmae Pentaphylli Herba	(3S,5R,8R,9R,10R,12R,13R,14R,17S)-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,12-diol	11213350	FALSE	C1CC2(C(C(C)(C1O)C)CCC1(C2CC(C2C1(CCC2C(CCC=C(C)C)(O)C)C)O)C)C

MOL005334	0.2305	0.7695	0.7376	Panax Ginseng C. A. Mey.	(3S,5R,8R,9R,10R,12R,13R,14R,17S)-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,12-diol	11213350	FALSE	C1CC2(C(C(C)(C1O)C)CCC1(C2CC(C2C1(CCC2C(CCC=C(C)C)(O)C)C)O)C)C
MOL005335	0.7282	0.2718	0.8093	Panax Ginseng C. A. Mey.	Gypenoside LXIX	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1OCC(C(C1O)O)O)O)O)O)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O)O
MOL005335	0.7282	0.2718	0.8093	Gynostemmae Pentaphylli Herba	Gypenoside LXIX	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1OCC(C(C1O)O)O)O)O)O)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O)O
MOL005336	0.7331	0.2669	0.8151	Panax Ginseng C. A. Mey.	ginsenoside-Rc	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1OC(C(C1O)O)CO)O)O)O)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O)O
MOL005336	0.7331	0.2669	0.8151	Ginseng Folium	ginsenoside-Rc	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1OC(C(C1O)O)CO)O)O)O)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O)O
MOL005336	0.7331	0.2669	0.8151	Ginsen Radix Et Rhizoma Rubra	ginsenoside-Rc	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1OC(C(C1O)O)CO)O)O)O)O)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O)O
MOL005336	0.7331	0.2669	0.8151	Panacis Japonici Rhizoma	ginsenoside-Rc	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1OC(C(C1O)O)CO)O)O)O)O)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O)O

MOL005337	0.7256	0.2744	0.8470	Ginsen Radix Et Rhizoma Rubra	(2S,3R,4S,5S,6R)-2-[(2S)-2-[(3S,5R,8R,9R,10R,12R,13R,14R,17S)-3-[(2R,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]oxy-12-hydroxy-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,1	11679800	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O)O

MOL005337	0.7256	0.2744	0.8470	Panax Ginseng C. A. Mey.	(2S,3R,4S,5S,6R)-2-[(2S)-2-[(3S,5R,8R,9R,10R,12R,13R,14R,17S)-3-[(2R,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]oxy-12-hydroxy-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,1	11679800	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O)O

MOL005337	0.7256	0.2744	0.8470	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	(2S,3R,4S,5S,6R)-2-[(2S)-2-[(3S,5R,8R,9R,10R,12R,13R,14R,17S)-3-[(2R,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]oxy-12-hydroxy-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,1	11679800	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O)O

MOL005337	0.7256	0.2744	0.8470	Ginseng Folium	(2S,3R,4S,5S,6R)-2-[(2S)-2-[(3S,5R,8R,9R,10R,12R,13R,14R,17S)-3-[(2R,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]oxy-12-hydroxy-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,1	11679800	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O)O

MOL005337	0.7256	0.2744	0.8470	Panacis Japonici Rhizoma	(2S,3R,4S,5S,6R)-2-[(2S)-2-[(3S,5R,8R,9R,10R,12R,13R,14R,17S)-3-[(2R,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]oxy-12-hydroxy-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,1	11679800	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O)O

MOL005337	0.7256	0.2744	0.8470	Panacis Quinquefolii Radix	(2S,3R,4S,5S,6R)-2-[(2S)-2-[(3S,5R,8R,9R,10R,12R,13R,14R,17S)-3-[(2R,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]oxy-12-hydroxy-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,1	11679800	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O
MOL005338	0.7489	0.2511	0.8340	Panacis Japonici Rhizoma	Ginsenoside Re	441921	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)OC2C(C(C(C(O2)C)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)(C)C)O
MOL005338	0.7489	0.2511	0.8340	Ginsen Radix Et Rhizoma Rubra	Ginsenoside Re	441921	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)OC2C(C(C(C(O2)C)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)(C)C)O
MOL005338	0.7489	0.2511	0.8340	Ginseng Folium	Ginsenoside Re	441921	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)OC2C(C(C(C(O2)C)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)(C)C)O
MOL005338	0.7489	0.2511	0.8340	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	Ginsenoside Re	441921	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)OC2C(C(C(C(O2)C)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)(C)C)O
MOL005338	0.7489	0.2511	0.8340	Gynostemmae Pentaphylli Herba	Ginsenoside Re	441921	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)OC2C(C(C(C(O2)C)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)(C)C)O
MOL005338	0.7489	0.2511	0.8340	Panax Ginseng C. A. Mey.	Ginsenoside Re	441921	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)OC2C(C(C(C(O2)C)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)(C)C)O

MOL005340	0.2494	0.7506	0.7336	Ginseng Folium	(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-17-[(2R)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,6,12-triol	9847853	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL005340	0.2494	0.7506	0.7336	Panax Ginseng C. A. Mey.	(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-17-[(2R)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,6,12-triol	9847853	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O

MOL005340	0.2494	0.7506	0.7336	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-17-[(2R)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,6,12-triol	9847853	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL005340	0.2494	0.7506	0.7336	Ginsen Radix Et Rhizoma Rubra	(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-17-[(2R)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,6,12-triol	9847853	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL005341	0.6724	0.3276	0.7238	Ginsen Radix Et Rhizoma Rubra	Sanchinoside C1	441923	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)C)(C)C)O
MOL005341	0.6724	0.3276	0.7238	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	Sanchinoside C1	441923	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)C)(C)C)O
MOL005341	0.6724	0.3276	0.7238	Panax Ginseng C. A. Mey.	Sanchinoside C1	441923	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)C)(C)C)O

MOL005341	0.6724	0.3276	0.7238	Panacis Japonici Rhizoma	Sanchinoside C1	441923	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)(C)C)O
MOL005341	0.6724	0.3276	0.7238	Ginseng Folium	Sanchinoside C1	441923	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)(C)C)O
MOL005342	0.6798	0.3202	0.8580	Panax Ginseng C. A. Mey.	Ginsenoside-Rg3	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL005343	0.2305	0.7695	0.7376	Panax Ginseng C. A. Mey.	Ginsenoside-Rg3_qt	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL005343	0.2305	0.7695	0.7376	Panacis Japonici Rhizoma	Ginsenoside-Rg3_qt	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL005344	0.2762	0.7238	0.8330	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	ginsenoside rh2	119307	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3O)CO)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL005344	0.2762	0.7238	0.8330	Ginseng Folium	ginsenoside rh2	119307	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3O)CO)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL005344	0.2762	0.7238	0.8330	Ginsen Radix Et Rhizoma Rubra	ginsenoside rh2	119307	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3O)CO)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL005344	0.2762	0.7238	0.8330	Panacis Quinquefolii Radix	ginsenoside rh2	119307	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3O)CO)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL005344	0.2762	0.7238	0.8330	Panax Ginseng C. A. Mey.	ginsenoside rh2	119307	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3O)CO)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C

MOL005345	0.2708	0.7292	0.7434	Panax Ginseng C. A. Mey.	(2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[[(3S,5R,8R,9R,10R,12R,13R,14R,17S)-12-hydroxy-4,4,8,10,14-pentamethyl-17-[(2Z)-6-methylhepta-2,5-dien-2-yl]-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-yl]oxy]oxane-3,4,5-triol	20839223	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)/C(=C\CC=C(C)C)/C)C)C)(C)C)OC1OC(C(C(C1O)O)O)CO
MOL005346	0.2146	0.7854	0.7288	Panax Ginseng C. A. Mey.	Ginsenoside-Rh3_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)/C(=C\CC=C(C)C)/C)C)C)(C)C)O
MOL005347	0.3220	0.6780	0.7810	Panax Ginseng C. A. Mey.	Ginsenoside-Rh4	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)O)(C2(C(C(C1)O)C(CC2)/C(=C\CC=C(C)C)/C)C)C)(C)C)O
MOL005348	0.2389	0.7611	0.7561	Panax Ginseng C. A. Mey.	Ginsenoside-Rh4_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)/C(=C\CC=C(C)C)/C)C)C)(C)C)O
MOL005349	0.6970	0.3030	0.8056	Panax Ginseng C. A. Mey.	Ginsenoside-Rs1	Not Available	FALSE	C1CC2(C(C(C1OC1C(C(C(C(O1)COC(=O)C)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)(C)C)CCC1(C2CC(C2C1(CCC2C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1C(C(C(CO1)O)O)O)O)O)O)C)O)C)C
MOL005350	0.6966	0.3034	0.8114	Panax Ginseng C. A. Mey.	Ginsenoside-Rs2	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)COC1OC(C(C1O)O)CO)O)O)O)C)C)(C)C)OC1C(C(C(C(O1)COC(=O)C)O)O)OC1C(C(C(C(O1)CO)O)O)O)O
MOL005351	0.6942	0.3058	0.6667	Panax Ginseng C. A. Mey.	Ginsenoyne A	Not Available	FALSE	OC(C=C)C#CC#CCC1C(CCCCCC=C)O1
MOL005353	0.7776	0.2224	0.7230	Panax Ginseng C. A. Mey.	Ginsenoyne C	Not Available	FALSE	OC(C=C)C#CC#CCC(C(CCCCCC=C)O)O
MOL005354	0.6821	0.3179	0.6912	Panax Ginseng C. A. Mey.	Ginsenoyne D	Not Available	FALSE	OC(CC)C#CC#CCC1C(CCCCCCC)O1
MOL005355	0.6855	0.3145	0.7265	Panax Ginseng C. A. Mey.	Ginsenoyne E	5317636	FALSE	O=C(C=C)C#CC#CCC1C(CCCCCCC)O1
MOL005356	0.7121	0.2879	0.7615	Panax Ginseng C. A. Mey.	Girinimbin	96943	FALSE	c1ccc2c(c1)c1c([nH]2)c2c(c(c1)C)OC(C=C2)(C)C

MOL005357	0.1675	0.8325	0.6096	Panax Ginseng C. A. Mey.	Gomisin B	Not Available	FALSE	C1(=C2C(=CC3=CC(C(C(c4c(C13)c(c(c(c4)OC)OC)OC)OC(=O)/C(=C\C)/C)(O)C)C)OCO2)OC
MOL005358	0.9162	0.0838	0.9720	Panax Ginseng C. A. Mey.	L-erythro-isocitric acid	439238	FALSE	C(C(=O)O)C(C(C(=O)O)O)C(=O)O
MOL005359	0.9162	0.0838	0.9720	Panax Ginseng C. A. Mey.	D-erythro-Isocitric acid	447805	FALSE	C(C(C(C(=O)O)O)C(=O)O)C(=O)O
MOL005361	0.7124	0.2876	0.8023	Panax Ginseng C. A. Mey.	Malonylginsenoside Rc	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(OC1C(O)C(C(C(O1)COC1OC(C(C1O)O)CO)O)O)C)C)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)COC(=O)CC(=O)O)O)O)CO
MOL005362	0.2305	0.7695	0.7376	Panax Ginseng C. A. Mey.	Malonylginsenoside Rc_qt1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL005363	0.6881	0.3119	0.8245	Panax Ginseng C. A. Mey.	Malonylginsenoside Rd	Not Available	FALSE	O1C(C(C(C(C1OC1C(OC(C(C1O)O)CO)OC1C(C2C(CC1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(OC1OC(C(C(C1O)O)O)CO)C)C)C)C)(C)C)O)O)O)COC(=O)CC(=O)O
MOL005363	0.6881	0.3119	0.8245	Gynostemmae Pentaphylli Herba	Malonylginsenoside Rd	Not Available	FALSE	O1C(C(C(C(C1OC1C(OC(C(C1O)O)CO)OC1C(C2C(CC1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(OC1OC(C(C(C1O)O)O)CO)C)C)C)C)(C)C)O)O)O)COC(=O)CC(=O)O
MOL005364	0.2305	0.7695	0.7376	Panax Ginseng C. A. Mey.	Malonylginsenoside Rd_qt	Not Available	FALSE	OC1C(C2C(CC1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C
MOL005364	0.2305	0.7695	0.7376	Gynostemmae Pentaphylli Herba	Malonylginsenoside Rd_qt	Not Available	FALSE	OC1C(C2C(CC1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C
MOL005365	0.9048	0.0952	0.8672	Panax Ginseng C. A. Mey.	MAL	6255	FALSE	C1(C(C(C(C(O1)OC1C(C(C(OC1CO)O)O)O)O)O)O)CO
MOL005366	0.8201	0.1799	0.6920	Semen Firmianae	Malvic acid	10416	FALSE	C(CCCCCC1=C(CCCCCCC(=O)O)C1)CC
MOL005366	0.8201	0.1799	0.6920	Panax Ginseng C. A. Mey.	Malvic acid	10416	FALSE	C(CCCCCC1=C(CCCCCCC(=O)O)C1)CC
MOL005366	0.8201	0.1799	0.6920	Cassiae Semen	Malvic acid	10416	FALSE	C(CCCCCC1=C(CCCCCCC(=O)O)C1)CC
MOL005367	0.9388	0.0612	0.9616	Rhizoma Dioscoreae	GUP	439680	FALSE	C(C1OC(C(C(C1O)O)O)O)O
MOL005367	0.9388	0.0612	0.9616	Panax Ginseng C. A. Mey.	GUP	439680	FALSE	C(C1OC(C(C(C1O)O)O)O)O
MOL005367	0.9388	0.0612	0.9616	Trichosanthis Radix	GUP	439680	FALSE	C(C1OC(C(C(C1O)O)O)O)O
MOL005367	0.9388	0.0612	0.9616	Commelinae Herba	GUP	439680	FALSE	C(C1OC(C(C(C1O)O)O)O)O
MOL005367	0.9388	0.0612	0.9616	Corayceps	GUP	439680	FALSE	C(C1OC(C(C(C1O)O)O)O)O
MOL005367	0.9388	0.0612	0.9616	Polygonati Rhizoma	GUP	439680	FALSE	C(C1OC(C(C(C1O)O)O)O)O
MOL005369	0.8660	0.1340	0.7494	Panax Ginseng C. A. Mey.	Mycosinol	Not Available	FALSE	CC#CC#C/C=C\1/OC2(C=C1)C(C=CO2)O
MOL005370	0.9124	0.0876	0.8748	Panax Ginseng C. A. Mey.	NN-Dimethyldecanamide	26690	FALSE	O=C(N(C)C)CCCCCCCCC
MOL005371	0.9238	0.0762	0.9278	Panax Ginseng C. A. Mey.	Nonacosanediol-6,8	Not Available	FALSE	CCCCCC(CC(O)CCC)O
MOL005371	0.9238	0.0762	0.9278	Eucommiae Cortex	Nonacosanediol-6,8	Not Available	FALSE	CCCCCC(CC(O)CCC)O

MOL005372	0.6552	0.3448	0.8570	Ginsen Radix Et Rhizoma Rubra	notoginsenoside R2	Not Available	FALSE	OC1C2C(CCC2C(CCC=C(C)C)(C)O)(C2(C(C1)C1(C(C(C2)OC2OC(C(C(C2OC2OCC(C(C2O)O)O)O)O)O)CO)C(C(CC1)O)(C)C)C)C)C
MOL005372	0.6552	0.3448	0.8570	Panacis Japonici Rhizoma	notoginsenoside R2	Not Available	FALSE	OC1C2C(CCC2C(CCC=C(C)C)(C)O)(C2(C(C1)C1(C(C(C2)OC2OC(C(C(C2OC2OCC(C(C2O)O)O)O)O)O)CO)C(C(CC1)O)(C)C)C)C)C
MOL005372	0.6552	0.3448	0.8570	Panax Ginseng C. A. Mey.	notoginsenoside R2	Not Available	FALSE	OC1C2C(CCC2C(CCC=C(C)C)(C)O)(C2(C(C1)C1(C(C(C2)OC2OC(C(C(C2OC2OCC(C(C2O)O)O)O)O)O)CO)C(C(CC1)O)(C)C)C)C)C
MOL005373	0.2494	0.7506	0.7336	Ginsen Radix Et Rhizoma Rubra	notoginsenoside R2_qt	Not Available	FALSE	OC1C2C(CCC2C(CCC=C(C)C)(C)O)(C2(C(C1)C1(C(C(C2)O)C(C(CC1)O)(C)C)C)C)C
MOL005373	0.2494	0.7506	0.7336	Panax Ginseng C. A. Mey.	notoginsenoside R2_qt	Not Available	FALSE	OC1C2C(CCC2C(CCC=C(C)C)(C)O)(C2(C(C1)C1(C(C(C2)O)C(C(CC1)O)(C)C)C)C)C
MOL005373	0.2494	0.7506	0.7336	Panacis Japonici Rhizoma	notoginsenoside R2_qt	Not Available	FALSE	OC1C2C(CCC2C(CCC=C(C)C)(C)O)(C2(C(C1)C1(C(C(C2)O)C(C(CC1)O)(C)C)C)C)C
MOL005374	0.7518	0.2482	0.8246	Panax Ginseng C. A. Mey.	Notoginsenoside R6	Not Available	FALSE	O1C(C(C(C(C1OC(CCC=C(C)C)(C1C2C(O)CC3C(C2(CC1)C)(CC(C1C3(CCC(C1(C)C)O)C)OC1OC(C(C(C1O)O)O)CO)C)C)O)O)O)COC1OC(C(C(C1O)O)O)CO
MOL005376	0.2167	0.7833	0.7442	Panax Ginseng C. A. Mey.	Panaxadiol	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C1(CCCC(O1)(C)C)C)C)C)(C)C)O
MOL005378	0.7893	0.2107	0.7333	Panax Ginseng C. A. Mey.	Panaxytriol	Not Available	FALSE	C=CC(O)C#CC#CCC(O)C(O)CCCCCCC
MOL005379	0.9202	0.0798	0.7618	Panax Ginseng C. A. Mey.	Pancratistatin	441597	FALSE	C12C(C(C3C(C1)C1C(NC3=O)C(C(C(C1O)O)O)O)O)OCO2
MOL005380	0.0553	0.9447	0.6282	Panax Ginseng C. A. Mey.	Pandamine	Not Available	FALSE	O1C(C(C(=O)NC(C(=O)NCC(c2ccc1cc2)O)Cc1ccccc1)NC(=O)C(N(C)C)C(CC)C)C(C)C
MOL005381	0.8517	0.1483	0.9255	Panax Ginseng C. A. Mey.	2-Formylpyrrole	13854	FALSE	c1c[nH]c(c1)C=O
MOL005381	0.8517	0.1483	0.9255	Campsis Flos	2-Formylpyrrole	13854	FALSE	c1c[nH]c(c1)C=O
MOL005381	0.8517	0.1483	0.9255	Momordicae Fructus	2-Formylpyrrole	13854	FALSE	c1c[nH]c(c1)C=O
MOL005382	0.9119	0.0881	0.7330	Panax Ginseng C. A. Mey.	Ramalic acid	5320886	FALSE	C1C(C(C(C1C)C(=O)OC1CC(C(C(C1)O)C(=O)O)C)O)OC
MOL005383	0.9041	0.0959	0.9002	Panax Ginseng C. A. Mey.	Methylselenocysteine	45266674	FALSE	C[Se]CC(C(=O)O)N
MOL005384	0.4023	0.5977	0.7423	Cistanches Herba	suchilactone	Not Available	FALSE	COc1c(OC)ccc(c1)CC1/C(=C/c2ccc3c(c2)OCO3)/C(=O)OC1
MOL005384	0.4023	0.5977	0.7423	Panax Ginseng C. A. Mey.	suchilactone	Not Available	FALSE	COc1c(OC)ccc(c1)CC1/C(=C/c2ccc3c(c2)OCO3)/C(=O)OC1
MOL005384	0.4023	0.5977	0.7423	Stemonae Radix	suchilactone	Not Available	FALSE	COc1c(OC)ccc(c1)CC1/C(=C/c2ccc3c(c2)OCO3)/C(=O)OC1

MOL005385	0.9028	0.0972	0.9139	Panax Ginseng C. A. Mey.	Suffruticoside A_qt1	Not Available	FALSE	c1(c(c(cc(c1)C(=O)OCC1(C(C(OC1)O)O)O)O)O)O
MOL005386	0.8696	0.1304	0.8112	Cornus Officinalis Sieb. Et Zucc.	Vulgarin	94253	FALSE	C1=CC(C2C(C1=O)(CCC1C2OC(=O)C1C)C)(C)O
MOL005386	0.8696	0.1304	0.8112	Folium Artemisiae Argyi	Vulgarin	94253	FALSE	C1=CC(C2C(C1=O)(CCC1C2OC(=O)C1C)C)(C)O
MOL005386	0.8696	0.1304	0.8112	Panax Ginseng C. A. Mey.	Vulgarin	94253	FALSE	C1=CC(C2C(C1=O)(CCC1C2OC(=O)C1C)C)(C)O
MOL005386	0.8696	0.1304	0.8112	Jujubae Fructus	Vulgarin	94253	FALSE	C1=CC(C2C(C1=O)(CCC1C2OC(=O)C1C)C)(C)O
MOL005386	0.8696	0.1304	0.8112	Eucommiae Cortex	Vulgarin	94253	FALSE	C1=CC(C2C(C1=O)(CCC1C2OC(=O)C1C)C)(C)O
MOL005388	0.8898	0.1102	0.7181	Panax Ginseng C. A. Mey.	Undecane, 3,6-dimethyl	Not Available	FALSE	CCC(CCC(CCCCC)C)C
MOL005389	0.8931	0.1069	0.6139	Panax Ginseng C. A. Mey.	PANGAMIC ACID	83182	FALSE	C(N(C(C)C)C(C)C)(N(C(C)C)C(C)C)C(=O)OCC(C(C(C(C(=O)O)O)O)O)O
MOL005390	0.9236	0.0764	0.9697	Jujubae Fructus	3-[[(2S)-2,4-dihydroxy-3,3-dimethylbutanoyl]amino]propanoic acid	5748353	FALSE	C(=O)(NCCC(=O)O)C(C(C)(C)CO)O
MOL005390	0.9236	0.0764	0.9697	Panax Ginseng C. A. Mey.	3-[[(2S)-2,4-dihydroxy-3,3-dimethylbutanoyl]amino]propanoic acid	5748353	FALSE	C(=O)(NCCC(=O)O)C(C(C)(C)CO)O
MOL005391	0.8363	0.1637	0.7550	Panacis Quinquefolii Radix	(Z,Z)-alpha-farnesene	5317320	FALSE	C(C/C(=C\C/C=C(\C=C)/C)/C)C=C(C)C
MOL005391	0.8363	0.1637	0.7550	Panax Ginseng C. A. Mey.	(Z,Z)-alpha-farnesene	5317320	FALSE	C(C/C(=C\C/C=C(\C=C)/C)/C)C=C(C)C
MOL005391	0.8363	0.1637	0.7550	Eriobotryae Folium	(Z,Z)-alpha-farnesene	5317320	FALSE	C(C/C(=C\C/C=C(\C=C)/C)/C)C=C(C)C
MOL005391	0.8363	0.1637	0.7550	Dichroae Radix	(Z,Z)-alpha-farnesene	5317320	FALSE	C(C/C(=C\C/C=C(\C=C)/C)/C)C=C(C)C
MOL005391	0.8363	0.1637	0.7550	Sesami Nigrum Semen	(Z,Z)-alpha-farnesene	5317320	FALSE	C(C/C(=C\C/C=C(\C=C)/C)/C)C=C(C)C
MOL005394	0.8943	0.1057	0.7320	Panax Ginseng C. A. Mey.	(Z)-2-methyl-5-[(1S,2R,4R)-2-methyl-3-methylene-2-norbornanyl]pent-2-en-1-ol	6857681	FALSE	C12C(CC/C=C(/C)\CO)(C)C(=C)C(CC1)C2

MOL005394	0.8943	0.1057	0.7320	Schisandrae Chinensis Fructus	(Z)-2-methyl-5-[(1S,2R,4R)-2-methyl-3-methylene-2-norbornanyl]pent-2-en-1-ol	6857681	FALSE	C12C(CC/C=C(/C)\CO)(C)C(=C)C(CC1)C2
MOL005394	0.8943	0.1057	0.7320	Santalum Album L.	(Z)-2-methyl-5-[(1S,2R,4R)-2-methyl-3-methylene-2-norbornanyl]pent-2-en-1-ol	6857681	FALSE	C12C(CC/C=C(/C)\CO)(C)C(=C)C(CC1)C2
MOL005396	0.7587	0.2413	0.7488	Panax Ginseng C. A. Mey.	cis-Widdrol alpha-epoxide	Not Available	FALSE	C1CC(C23C(C1)(CCC(CC2O3)(O)C)C)(C)C
MOL005397	0.3104	0.6896	0.6807	Panax Ginseng C. A. Mey.	Dammarane	3036917	FALSE	C12(C3(C(C(CC3)C(CCCC(C)C)C)CCC1C1(C(CC2)C(CCC1)(C)C)C)C)C
MOL005400	0.6425	0.3575	0.8411	Panax Ginseng C. A. Mey.	ginsenoside Rg5	Not Available	FALSE	OC1C2C(C3C(C4(C(CC3C)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)CC4)(C)C)C)C1)(CCC2/C(=C/CC=C(C)C)/C)C
MOL005401	0.1859	0.8141	0.7320	Panax Ginseng C. A. Mey.	ginsenoside Rg5_qt	Not Available	FALSE	OC1C2C(C3C(C4(C(CC3C)C(C(O)CC4)(C)C)C)C1)(CCC2/C(=C/CC=C(C)C)/C)C
MOL005402	0.5336	0.4664	0.6001	Panax Ginseng C. A. Mey.	Methyl margarate	15609	FALSE	O(C(=O)CCCCCCCCCCCCCCCC)C
MOL005402	0.5336	0.4664	0.6001	Sojae Semen Nigrum	Methyl margarate	15609	FALSE	O(C(=O)CCCCCCCCCCCCCCCC)C
MOL005402	0.5336	0.4664	0.6001	Broussonetiae Fructus	Methyl margarate	15609	FALSE	O(C(=O)CCCCCCCCCCCCCCCC)C
MOL005402	0.5336	0.4664	0.6001	Rose Rugosae Flos	Methyl margarate	15609	FALSE	O(C(=O)CCCCCCCCCCCCCCCC)C
MOL005402	0.5336	0.4664	0.6001	Platycladi Semen	Methyl margarate	15609	FALSE	O(C(=O)CCCCCCCCCCCCCCCC)C
MOL005402	0.5336	0.4664	0.6001	Hoveniae Dulcis Semen	Methyl margarate	15609	FALSE	O(C(=O)CCCCCCCCCCCCCCCC)C
MOL005402	0.5336	0.4664	0.6001	Morindae Officinalis Radix	Methyl margarate	15609	FALSE	O(C(=O)CCCCCCCCCCCCCCCC)C
MOL005403	0.4501	0.5499	0.6937	Panax Ginseng C. A. Mey.	oleanane	Not Available	FALSE	C12(C3(C(C4C(CC3)(CCC(C4)(C)C)C)CCC1C1(C(CC2)C(CCC1)(C)C)C)C)C
MOL005404	0.9240	0.0760	0.8436	Panax Ginseng C. A. Mey.	p-Glucosyloxymandelonitrile	Not Available	FALSE	C1(OC(C(C(C1O)O)O)CO)Cc1ccc(cc1)C(C)O

MOL005405	0.4605	0.5395	0.7648	Anisodus Acutangulus C. Y. Wu Et C .Chen Ex C. Che	Cusparine	442893	FALSE	c1ccc2c(c1)c(cc(n2)CCc1ccc2c(c1)OCO2)OC
MOL005406	0.8739	0.1261	0.9139	Daturae Flos	atropine	154417	FALSE	C1(CC2N(C(C1)CC2)C)OC(=O)C(c1ccccc1)CO
MOL005406	0.8739	0.1261	0.9139	Lycii Fructus	atropine	154417	FALSE	C1(CC2N(C(C1)CC2)C)OC(=O)C(c1ccccc1)CO
MOL005406	0.8739	0.1261	0.9139	Physochlainae Radix	atropine	154417	FALSE	C1(CC2N(C(C1)CC2)C)OC(=O)C(c1ccccc1)CO
MOL005406	0.8739	0.1261	0.9139	Anisodus Acutangulus C. Y. Wu Et C .Chen Ex C. Che	atropine	154417	FALSE	C1(CC2N(C(C1)CC2)C)OC(=O)C(c1ccccc1)CO
MOL005407	0.9298	0.0702	0.8903	Anisodus Acutangulus C. Y. Wu Et C .Chen Ex C. Che	1,3-bis[(2R)-1-methylpyrrolidin-2-yl]acetone	1201543	FALSE	N1(C(CC(=O)CC2N(CCC2)C)CCC1)C
MOL005408	0.8145	0.1855	0.8244	Anisodus Acutangulus C. Y. Wu Et C .Chen Ex C. Che	apoatropine	12306866	FALSE	C1(CC2N(C(C1)CC2)C)OC(=O)C(=C)c1ccccc1
MOL005408	0.8145	0.1855	0.8244	Daturae Flos	apoatropine	12306866	FALSE	C1(CC2N(C(C1)CC2)C)OC(=O)C(=C)c1ccccc1
MOL005409	0.8768	0.1232	0.7744	Anisodus Acutangulus C. Y. Wu Et C .Chen Ex C. Che	anisodamine	Not Available	FALSE	C12N(C(CC1O)CC(C2)OC(=O)C(c1ccccc1)CO)C
MOL005410	0.9471	0.0529	0.9452	Lignum Pini Nodi	1-Butyl-4-methoxybenzene	140362	FALSE	COc1ccc(cc1)CCCC
MOL005412	0.9625	0.0375	0.8120	Rhizome Of Whiteback Greenbrier	2,4,6-Trimethylanisole	77648	FALSE	c1(c(cc(cc1C)C)C)OC
MOL005414	0.6063	0.3937	0.7734	Rhizome Of Whiteback Greenbrier	Clavolonine	Not Available	FALSE	C1CN2C34C(C1)C(CC(=O)C3CCC2)C(C(C4)C)O
MOL005415	0.9101	0.0899	0.8495	Rhizome Of Whiteback Greenbrier	Clavorubin	5315956	FALSE	c1c(c(c2c(c1O)C(=O)c1c(C2=O)cc(c(c1O)C(=O)O)C)O)O
MOL005416	0.3924	0.6076	0.7236	Rhizome Of Whiteback Greenbrier	Japonicumins A	Not Available	FALSE	OC1C2C3(C(C(C(O)CC3)(C)C)C(=C)C=C2CC2(C(C3(C(C(CCC3)(CO)C)CC2)C)C1)C)C
MOL005417	0.4159	0.5841	0.7651	Rhizome Of Whiteback Greenbrier	Lycoclavanol	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C)CC2=CCC3C(C2CC1)(CCC(C3(C)C)O)C)C)(C)CO)O
MOL005418	0.6549	0.3451	0.8255	Rhizome Of Whiteback Greenbrier	Lycoctonine	Not Available	FALSE	C1(CCC2(C3C41C1C5C(CC(C(C5OC)C1)OC)(O)C(C3OC)(C4N(C2)CC)O)CO)OC

MOL005419	0.5107	0.4893	0.6239	Rhizome Of Whiteback Greenbrier	(6E,8E,10Z,12Z,14E,16E,18E,20Z,22Z,24E,26E)-2,6,10,14,19,23,27,31-octamethyldotriaconta-2,6,8,10,12,14,16,18,20,22,24,26,30-tridecaene	5319123	FALSE	CC(=CCC/C(=C/C=C/C(=C\C=C/C(=C/C=C/C=C(/C=C\C=C(/C=C/C=C(\C)/CCC=C(C)C)\C)\C)/C)/C)/C)C
MOL005420	0.8650	0.1350	0.7183	Rhizome Of Whiteback Greenbrier	Lycopose	Not Available	FALSE	C1(C(C(C(OC1CO)OC1C(C(C(OC1CO)OC1C(C(C(OC1CO)OC1C(C(C(OC1CO)OC1C(C(C(O1)CO)O)O)CO)O)O)O)O)O)O)O)O)O)O
MOL005422	0.9616	0.0384	0.7735	Rhizome Of Whiteback Greenbrier	beta-Fenchene	12309841	FALSE	C1(=C)CC2C(CC1C2)(C)C
MOL005423	0.8683	0.1317	0.6011	Rhizome Of Whiteback Greenbrier	(-)-Epicedrol	Not Available	FALSE	C123C(C(C(C1)C(CC2)(C)O)(C)C)CCC3C
MOL005423	0.8683	0.1317	0.6011	Radix Salviae	(-)-Epicedrol	Not Available	FALSE	C123C(C(C(C1)C(CC2)(C)O)(C)C)CCC3C
MOL005424	0.9355	0.0645	0.9489	Ginkgo Folium	pinitol	164619	FALSE	O(C1C(O)C(O)C(O)C(O)C1O)C
MOL005424	0.9355	0.0645	0.9489	Rhizome Of Whiteback Greenbrier	pinitol	164619	FALSE	O(C1C(O)C(O)C(O)C(O)C1O)C
MOL005425	0.9104	0.0896	0.9138	Rhizome Of Whiteback Greenbrier	Methyl caprate	8050	FALSE	C(CCCCCCCC)C(=O)OC
MOL005425	0.9104	0.0896	0.9138	Hoveniae Dulcis Semen	Methyl caprate	8050	FALSE	C(CCCCCCCC)C(=O)OC
MOL005425	0.9104	0.0896	0.9138	Perillae Fructus	Methyl caprate	8050	FALSE	C(CCCCCCCC)C(=O)OC
MOL005425	0.9104	0.0896	0.9138	Trollius Chinensis	Methyl caprate	8050	FALSE	C(CCCCCCCC)C(=O)OC
MOL005429	0.3193	0.6807	0.6125	Rhizoma Dioscoreae	hancinol	Not Available	FALSE	OC1(C2C(C(C(C2=O)(C=C1OC)CC=C)C)c1cc(OC)c(OC)cc1)C
MOL005430	0.3223	0.6777	0.6255	Rhizoma Dioscoreae	hancinone C	Not Available	FALSE	O(C1(/C(=C/c2cc(OC)c(OC)c(OC)c2)/C)C=C(C(=O)C=C1OC)CC=C)C
MOL005432	0.9284	0.0716	0.8333	Microctis Folium	ABK	5280896	FALSE	OC1(C(CC(=O)C=C1C)(C)C)/C=C/C(=C\C(=O)O)/C
MOL005432	0.9284	0.0716	0.8333	Rhizoma Dioscoreae	ABK	5280896	FALSE	OC1(C(CC(=O)C=C1C)(C)C)/C=C/C(=C\C(=O)O)/C

MOL005433	0.2214	0.7786	0.6091	Rhizoma Dioscoreae	(3S,8S,9S,10R,13R,14S,17R)-17-[(2R,5S)-5-ethyl-6-methylhept-6-en-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol	5283638	FALSE	OC1CC2=CCC3C4C(C(CC4)C(CCC(CC)C(=C)C)C)(CCC3C2(CC1)C)C
MOL005433	0.2214	0.7786	0.6091	Quisqualis Indica	(3S,8S,9S,10R,13R,14S,17R)-17-[(2R,5S)-5-ethyl-6-methylhept-6-en-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol	5283638	FALSE	OC1CC2=CCC3C4C(C(CC4)C(CCC(CC)C(=C)C)C)(CCC3C2(CC1)C)C
MOL005436	0.2032	0.7968	0.6108	Rhizoma Dioscoreae	24-Methylcholesta-5,7,22-trien-ebelta-ol	Not Available	FALSE	C1C(CC2=CC=C3C(C2(C1)C)CCC1(C3CCC1C(/C=C/C(C(C)C)C)C)C)O

MOL005437	0.3893	0.6107	0.8281	Rhizoma Dioscoreae	(2S,3S,3aR)-3a-allyl-2-(1,3-benzodioxol-5-yl)-5-methoxy-3-methyl-2,3-dihydrobenzofuran-6-one	10903924	FALSE	O1C(C(C2(C1=CC(=O)C(=C2)OC)CC=C)C)c1cc2OCOc2cc1
MOL005440	0.2167	0.7833	0.6060	Gynostemmae Pentaphylli Herba	Isofucosterol	5281326	FALSE	OC1CC2=CCC3C4C(C(CC4)C(CC/C(=C/C)/C(C)C)C)(CCC3C2(CC1)C)C
MOL005440	0.2167	0.7833	0.6060	Calendula Officinalis	Isofucosterol	5281326	FALSE	OC1CC2=CCC3C4C(C(CC4)C(CC/C(=C/C)/C(C)C)C)(CCC3C2(CC1)C)C
MOL005440	0.2167	0.7833	0.6060	Cuscutae Semen	Isofucosterol	5281326	FALSE	OC1CC2=CCC3C4C(C(CC4)C(CC/C(=C/C)/C(C)C)C)(CCC3C2(CC1)C)C
MOL005440	0.2167	0.7833	0.6060	Sargassum	Isofucosterol	5281326	FALSE	OC1CC2=CCC3C4C(C(CC4)C(CC/C(=C/C)/C(C)C)C)(CCC3C2(CC1)C)C
MOL005440	0.2167	0.7833	0.6060	Rhizoma Dioscoreae	Isofucosterol	5281326	FALSE	OC1CC2=CCC3C4C(C(CC4)C(CC/C(=C/C)/C(C)C)C)(CCC3C2(CC1)C)C
MOL005440	0.2167	0.7833	0.6060	Broussonetiae Fructus	Isofucosterol	5281326	FALSE	OC1CC2=CCC3C4C(C(CC4)C(CC/C(=C/C)/C(C)C)C)(CCC3C2(CC1)C)C
MOL005441	0.9388	0.0612	0.9616	Polygonati Rhizoma	BGC	64689	FALSE	O1C(C(O)C(O)C(O)C1O)CO
MOL005441	0.9388	0.0612	0.9616	Momordicae Fructus	BGC	64689	FALSE	O1C(C(O)C(O)C(O)C1O)CO
MOL005441	0.9388	0.0612	0.9616	Rhizoma Dioscoreae	BGC	64689	FALSE	O1C(C(O)C(O)C(O)C1O)CO
MOL005442	0.9498	0.0502	0.9626	Portulacae Herba	LDP	681	FALSE	Oc1cc(CCN)ccc1O
MOL005442	0.9498	0.0502	0.9626	Rhizoma Dioscoreae	LDP	681	FALSE	Oc1cc(CCN)ccc1O
MOL005443	0.5915	0.4085	0.7033	Rhizoma Dioscoreae	Batatasin I	442694	FALSE	O(c1c2c3c(ccc2cc(OC)c1)cc(OC)c(O)c3)C
MOL005444	0.9136	0.0864	0.9112	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	3-[2-(3-hydroxyphenyl)ethyl]-5-methoxyphenol	10466989	FALSE	C(Cc1cc(ccc1)O)c1cc(cc(c1)OC)O
MOL005444	0.9136	0.0864	0.9112	Rhizoma Dioscoreae	3-[2-(3-hydroxyphenyl)ethyl]-5-methoxyphenol	10466989	FALSE	C(Cc1cc(ccc1)O)c1cc(cc(c1)OC)O
MOL005446	0.8997	0.1003	0.7411	Rhizoma Dioscoreae	Batatasin IV	181271	FALSE	O(c1cc(CCc2c(O)cccc2)cc(O)c1)C
MOL005447	0.9429	0.0571	0.9672	Rhizoma Dioscoreae	L-Xyl	95259	FALSE	OC(C(O)CO)C(O)C=O
MOL005448	0.9127	0.0873	0.9711	Radix Salviae	Leucinum	7045798	FALSE	OC(=O)C(N)CC(C)C
MOL005448	0.9127	0.0873	0.9711	Jujubae Fructus	Leucinum	7045798	FALSE	OC(=O)C(N)CC(C)C
MOL005448	0.9127	0.0873	0.9711	Santalum Album L.	Leucinum	7045798	FALSE	OC(=O)C(N)CC(C)C
MOL005448	0.9127	0.0873	0.9711	Arum Ternatum Thunb.	Leucinum	7045798	FALSE	OC(=O)C(N)CC(C)C

MOL005448	0.9127	0.0873	0.9711	Trichosanthes Kirilowii Maxim	Leucinum	7045798	FALSE	OC(=O)C(N)CC(C)C
MOL005448	0.9127	0.0873	0.9711	Rhizoma Dioscoreae	Leucinum	7045798	FALSE	OC(=O)C(N)CC(C)C
MOL005449	0.8972	0.1028	0.9632	Cornus Officinalis Sieb. Et Zucc.	h-Met-h	6992087	FALSE	S(CCC(N)C(=O)O)C
MOL005449	0.8972	0.1028	0.9632	Ginkgo Folium	h-Met-h	6992087	FALSE	S(CCC(N)C(=O)O)C
MOL005449	0.8972	0.1028	0.9632	Angelicae Sinensis Radix	h-Met-h	6992087	FALSE	S(CCC(N)C(=O)O)C
MOL005449	0.8972	0.1028	0.9632	Vigna Radiata	h-Met-h	6992087	FALSE	S(CCC(N)C(=O)O)C
MOL005449	0.8972	0.1028	0.9632	Euryales Semen	h-Met-h	6992087	FALSE	S(CCC(N)C(=O)O)C
MOL005449	0.8972	0.1028	0.9632	Rhizoma Dioscoreae	h-Met-h	6992087	FALSE	S(CCC(N)C(=O)O)C
MOL005449	0.8972	0.1028	0.9632	Santalum Album L.	h-Met-h	6992087	FALSE	S(CCC(N)C(=O)O)C
MOL005449	0.8972	0.1028	0.9632	Radix Salviae	h-Met-h	6992087	FALSE	S(CCC(N)C(=O)O)C
MOL005449	0.8972	0.1028	0.9632	Bamusaeconcretiosilicea	h-Met-h	6992087	FALSE	S(CCC(N)C(=O)O)C
MOL005449	0.8972	0.1028	0.9632	Trichosanthes Kirilowii Maxim	h-Met-h	6992087	FALSE	S(CCC(N)C(=O)O)C
MOL005451	0.2113	0.7887	0.6437	Rhizoma Dioscoreae	holest-7-enol	Not Available	FALSE	OC1CC2C(C3C(=CC2)C2C(C(CC2)C(CCCC(C)C)C)(CC3)C)(CC1)C
MOL005454	0.8952	0.1048	0.8793	Rhizoma Dioscoreae	(S)-Allantoin	439714	FALSE	O=C1NC(=O)NC1NC(=O)N
MOL005455	0.9284	0.0716	0.8333	Rhizoma Dioscoreae	(-)-ABA	643732	FALSE	C1C(=O)C=C(C(C1(C)C)O)/C=C/C(=C\C(=O)O)/C
MOL005456	0.7463	0.2537	0.8211	Rhizoma Dioscoreae	Deltoside	Not Available	FALSE	C1(C(C(C(C(O1)OC1C(C(C(OC1CO)OC1CC2=CCC3C(C2(CC1)C)CCC1(C3CC2C1C(C1(O2)OC(C(CC1)C)OC1OC(C(C(C1O)O)O)CO)C)C)OC1OC(C(C(C1O)O)O)C)O)O)O)O)CO
MOL005457	0.3449	0.6551	0.7795	Rhizoma Dioscoreae	Deltoside_qt	Not Available	FALSE	OC1CC2=CCC3C(C2(CC1)C)CCC1(C2C(CC31)OC1(C2C)OC(O)C(CC1)C)C
MOL005458	0.2287	0.7713	0.7664	Rhizoma Dioscoreae	Dioscoreside C_qt	Not Available	FALSE	OC1CCC2(C(=CCC3C2CCC2(C4C(OC(=C4C)C(CC(CO)C)OC)CC32)C)C1)C
MOL005459	0.3326	0.6674	0.6585	Rhizoma Dioscoreae	Diosgenin-3-O-beta-D-glucopyranoside	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC2C1C(C1(O2)OCC(CC1)C)C)C)OC1OC(C(C(C1O)O)O)CO
MOL005460	0.2872	0.7128	0.7586	Rhizoma Dioscoreae	ophipogonin D_qt	Not Available	FALSE	OC1CCC2(C(=CCC3C2CCC2(C3CC3C2C(C2(O3)OCC(CC2)C)C)C)C1)C
MOL005460	0.2872	0.7128	0.7586	Dioscoreaebulbiferae	ophipogonin D_qt	Not Available	FALSE	OC1CCC2(C(=CCC3C2CCC2(C3CC3C2C(C2(O3)OCC(CC2)C)C)C)C1)C
MOL005460	0.2872	0.7128	0.7586	Polygonati Odorati Rhizoma	ophipogonin D_qt	Not Available	FALSE	OC1CCC2(C(=CCC3C2CCC2(C3CC3C2C(C2(O3)OCC(CC2)C)C)C)C1)C
MOL005460	0.2872	0.7128	0.7586	Lilii Bulbus	ophipogonin D_qt	Not Available	FALSE	OC1CCC2(C(=CCC3C2CCC2(C3CC3C2C(C2(O3)OCC(CC2)C)C)C)C1)C
MOL005462	0.4378	0.5622	0.6345	Rhizoma Dioscoreae	Methylcimicifugoside	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(C(C1)OC(=O)C)(C1C(C2)OC2(CC1C)OC(C1(OC21)C)OC)C)C)C3)(C)C)OC1C(C(C(CO1)O)O)O

MOL005463	0.3409	0.6591	0.7128	Rhizoma Dioscoreae	Methylcimicifugoside_qt	Not Available	FALSE	OC1CCC23C(C1(C)C)CC=C1C2(CC(OC(=O)C)C2(C1(C)CC1OC4(C5C(O5)(C)C(OC)O4)CC(C21)C)C)C3
MOL005464	0.3523	0.6477	0.7850	Rhizoma Dioscoreae	(3S,4aS,4bS,8R,8aS,10aR)-3-hydroxy-1,1,4a,8-tetramethyl-7-vinyl-3,4,4b,8,8a,9,10,10a-octahydrophenanthrene-2,5-dione	10313699	FALSE	C1(C(=O)C(C2C(C1)(C1C(CC2)C(C(=CC1=O)C=C)C)C)(C)C)O
MOL005465	0.5051	0.4949	0.7336	Rhizoma Dioscoreae	AIDS180907	5495928	FALSE	O1C(C=Cc2c3c(oc4c(c3=O)c(O)c(c(O)c4)CC=C(C)C)cc(O)c12)(C)C
MOL005466	0.4039	0.5961	0.6784	Rhizoma Dioscoreae	1,3,6-trihydroxy-8-(3-hydroxy-3-methyl-butyl)-7-methoxy-2-(3-methylbut-2-enyl)xanthone	5495926	FALSE	OC(CCc1c2c(oc3c(c2=O)c(O)c(c(O)c3)CC=C(C)C)cc(O)c1OC)(C)C
MOL005467	0.7959	0.2041	0.7516	Cornus Officinalis Sieb. Et Zucc.	Epicatechin gallate	65056	FALSE	C1(C(Cc2c(O)cc(O)cc2O1)OC(=O)c1cc(O)c(O)c(O)c1)c1cc(O)c(O)cc1
MOL005467	0.7959	0.2041	0.7516	Rhizoma Fagopyri Cymosi	Epicatechin gallate	65056	FALSE	C1(C(Cc2c(O)cc(O)cc2O1)OC(=O)c1cc(O)c(O)c(O)c1)c1cc(O)c(O)cc1
MOL005468	0.8605	0.1395	0.6915	Cornus Officinalis Sieb. Et Zucc.	1,2,3,6-tetra-O-galloyl-β-D-glucose	Not Available	FALSE	O1C(C(O)C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C1OC(=O)c1cc(O)c(O)c(O)c1)COC(=O)c1cc(O)c(O)c(O)c1
MOL005469	0.8778	0.1222	0.6737	Cornus Officinalis Sieb. Et Zucc.	1,2,3-tri-O-galloyl-β-D-glucose	Not Available	FALSE	O(C1C(OC(=O)c2cc(c(c(c2)O)O)O)C(OC(=O)c2cc(c(c(c2)O)O)O)C(O)C(O1)CO)C(=O)c1cc(c(c(c1)O)O)O
MOL005470	0.9616	0.0384	0.8773	Sesami Nigrum Semen	Durol	7269	FALSE	c1(c(cc(c(c1)C)C)C)C
MOL005470	0.9616	0.0384	0.8773	Cornus Officinalis Sieb. Et Zucc.	Durol	7269	FALSE	c1(c(cc(c(c1)C)C)C)C

MOL005471	0.8815	0.1185	0.6793	Cornus Officinalis Sieb. Et Zucc.	[(2R,3R,4S,5S,6R)-4,5-dihydroxy-2-(3,4,5-trihydroxybenzoyl)oxy-6-[(3,4,5-trihydroxybenzoyl)oxymethyl]oxan-3-yl] 3,4,5-trihydroxybenzoate	11969002	FALSE	c1(c(c(cc(c1)C(=O)OCC1C(C(C(C(O1)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O)O)O)O
MOL005472	0.9142	0.0858	0.9005	Cornus Officinalis Sieb. Et Zucc.	1,2-Benzenedicarboxylicacid, mono(2-ethyl)hexylester	Not Available	FALSE	c1(c(cccc1)C(=O)O)C(=O)OCC(CCCC)CC
MOL005472	0.9142	0.0858	0.9005	Mori Fructus	1,2-Benzenedicarboxylicacid, mono(2-ethyl)hexylester	Not Available	FALSE	c1(c(cccc1)C(=O)O)C(=O)OCC(CCCC)CC
MOL005473	0.8317	0.1683	0.8336	Cornus Officinalis Sieb. Et Zucc.	1,5-DIACETYLNAPHTHALENE	219219	FALSE	O=C(c1c2c(c(ccc2)C(=O)C)ccc1)C
MOL005474	0.7916	0.2084	0.8025	Cornus Officinalis Sieb. Et Zucc.	1-Acetyl-4,6,8-trimethylazulene	607590	FALSE	O=C(c1c2c(c(cc(cc2C)C)C)cc1)C
MOL005478	0.4768	0.5232	0.6437	Cornus Officinalis Sieb. Et Zucc.	11,14-Octadecadienoic acid, methyl ester	5365677	FALSE	C(=O)(CCCCCCCCC/C=C/C/C=C/CCC)OC
MOL005479	0.5674	0.4326	0.6249	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	pentatriacont-17-ene	5365022	FALSE	CCCCCCCCCCCCCCCCC/C=C/CCCCCCCCCCCCCCCCC
MOL005479	0.5674	0.4326	0.6249	Cornus Officinalis Sieb. Et Zucc.	pentatriacont-17-ene	5365022	FALSE	CCCCCCCCCCCCCCCCC/C=C/CCCCCCCCCCCCCCCCC
MOL005479	0.5674	0.4326	0.6249	Lycii Fructus	pentatriacont-17-ene	5365022	FALSE	CCCCCCCCCCCCCCCCC/C=C/CCCCCCCCCCCCCCCCC

MOL005480	0.9185	0.0815	0.9544	Capsici Fructus	Ucar AC	7996	FALSE	O(C(C)C)CCO
MOL005480	0.9185	0.0815	0.9544	Cornus Officinalis Sieb. Et Zucc.	Ucar AC	7996	FALSE	O(C(C)C)CCO
MOL005480	0.9185	0.0815	0.9544	Momordicae Fructus	Ucar AC	7996	FALSE	O(C(C)C)CCO
MOL005482	0.9039	0.0961	0.9629	Coriolus	FOA	6919	FALSE	c1(ccco1)C(=O)O
MOL005482	0.9039	0.0961	0.9629	Cornus Officinalis Sieb. Et Zucc.	FOA	6919	FALSE	c1(ccco1)C(=O)O
MOL005482	0.9039	0.0961	0.9629	Codonopsis Radix	FOA	6919	FALSE	c1(ccco1)C(=O)O
MOL005483	0.9253	0.0747	0.7293	Ranunculi Ternati Radix	2-Methylnaphthalene	7055	FALSE	c12c(ccc(c1)C)cccc2
MOL005483	0.9253	0.0747	0.7293	Cornus Officinalis Sieb. Et Zucc.	2-Methylnaphthalene	7055	FALSE	c12c(ccc(c1)C)cccc2
MOL005483	0.9253	0.0747	0.7293	Gossampiniflos	2-Methylnaphthalene	7055	FALSE	c12c(ccc(c1)C)cccc2
MOL005483	0.9253	0.0747	0.7293	Typhonii Rhizoma	2-Methylnaphthalene	7055	FALSE	c12c(ccc(c1)C)cccc2
MOL005483	0.9253	0.0747	0.7293	Radix Cynanchi Paniculati	2-Methylnaphthalene	7055	FALSE	c12c(ccc(c1)C)cccc2
MOL005483	0.9253	0.0747	0.7293	Mume Flos	2-Methylnaphthalene	7055	FALSE	c12c(ccc(c1)C)cccc2
MOL005484	0.9496	0.0504	0.9624	Cornus Officinalis Sieb. Et Zucc.	GRO	446626	FALSE	c1(C(C(=O)O)C)ccccc1
MOL005485	0.9098	0.0902	0.8058	Cornus Officinalis Sieb. Et Zucc.	3-dibenzofuransulfonic acid	3616629	FALSE	c12c3c(oc1cc(cc2)S(=O)(=O)O)cccc3
MOL005486	0.4946	0.5054	0.6075	Cornus Officinalis Sieb. Et Zucc.	3,4-Dehydrolycopen-16-al	5316458	FALSE	C(=C(\C)/C=O)\C=C/C(=C/C=C/C(=C\C=C/C(=C/C=C/C=C(/C=C\C=C(/C=C/C=C(/CCC=C(C)C)\C)\C)\C)/C)/C)/C
MOL005487	0.9279	0.0721	0.9390	Euphorbiae Helioscopiae Herba	5-Carboxyresorcinol	7424	FALSE	c1(cc(cc(c1)O)O)C(=O)O
MOL005487	0.9279	0.0721	0.9390	Cornus Officinalis Sieb. Et Zucc.	5-Carboxyresorcinol	7424	FALSE	c1(cc(cc(c1)O)O)C(=O)O

MOL005488	0.9081	0.0919	0.7333	Cornus Officinalis Sieb. Et Zucc.	3,5-Di-t-butyl-4-hydroxybenzaldehyde	73219	FALSE	Oc1c(C(C)(C)C)cc(cc1C(C)(C)C)C=O
MOL005488	0.9081	0.0919	0.7333	Gossampiniflos	3,5-Di-t-butyl-4-hydroxybenzaldehyde	73219	FALSE	Oc1c(C(C)(C)C)cc(cc1C(C)(C)C)C=O
MOL005489	0.9242	0.0758	0.7821	Cornus Officinalis Sieb. Et Zucc.	3,6-Digalloylglucose	Not Available	FALSE	O(C(=O)c1cc(c(c(c1)O)O)O)C1C(O)C(OC(C1O)O)COC(=O)c1cc(c(c(c1)O)O)O
MOL005490	0.9160	0.0840	0.7652	Cornus Officinalis Sieb. Et Zucc.	4-(4-ethylphenyl)benzoic acid	521801	FALSE	c1(ccc(cc1)C(=O)O)c1ccc(cc1)CC
MOL005491	0.9674	0.0326	0.9000	Cornus Officinalis Sieb. Et Zucc.	4-Ethyl-o-xylene	13629	FALSE	c1(cc(c(cc1)C)C)CC
MOL005491	0.9674	0.0326	0.9000	Citri Sarcodactylis Fructus	4-Ethyl-o-xylene	13629	FALSE	c1(cc(c(cc1)C)C)CC
MOL005492	0.9188	0.0812	0.8454	Caryophylliflos	4-Methoxy-1,2-benzodioxole	5319407	FALSE	O1OCc2c1cccc2OC
MOL005492	0.9188	0.0812	0.8454	Cornus Officinalis Sieb. Et Zucc.	4-Methoxy-1,2-benzodioxole	5319407	FALSE	O1OCc2c1cccc2OC
MOL005493	0.8418	0.1582	0.6667	Cornus Officinalis Sieb. Et Zucc.	6-Isopropyl-1,4-dimethylnaphthalene	603340	FALSE	C(c1cc2c(c(ccc2C)C)cc1)(C)C
MOL005495	0.9525	0.0475	0.8301	Cornus Officinalis Sieb. Et Zucc.	6-ethyl-2,5-dihydroxy-1,4-naphthoquinone	612788	FALSE	C1(=O)C(=CC(=O)c2c(c(ccc12)CC)O)O
MOL005496	0.9213	0.0787	0.8399	Cornus Officinalis Sieb. Et Zucc.	7,8-Dehydropenstemoside	Not Available	FALSE	C12(C(C(OC=C1C(=O)OC)OC1OC(C(C(C1O)O)O)CO)C(=CC2O)C)O
MOL005497	0.9400	0.0600	0.8419	Cornus Officinalis Sieb. Et Zucc.	7,8-Dehydropenstemoside_qt	Not Available	FALSE	C12(C(C(OC=C1C(=O)OC)O)C(=CC2O)C)O
MOL005498	0.8871	0.1129	0.7035	Cornus Officinalis Sieb. Et Zucc.	7-Hydroxycadalene	608115	FALSE	Oc1cc2c(c(C(C)C)ccc2C)cc1C
MOL005500	0.7659	0.2341	0.6499	Oroxyli Semen	linolenate	5282822	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/C/C=C/CC)O

MOL005500	0.7659	0.2341	0.6499	Cornus Officinalis Sieb. Et Zucc.	linolenate	5282822	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/C/C=C/CC)O
MOL005501	0.7537	0.2463	0.6093	Typhonii Rhizoma	Green Oil	8418	FALSE	c12c(cc3c(c1)cccc3)cccc2
MOL005501	0.7537	0.2463	0.6093	Oroxyli Semen	Green Oil	8418	FALSE	c12c(cc3c(c1)cccc3)cccc2
MOL005501	0.7537	0.2463	0.6093	Cinnamomi Ramulus	Green Oil	8418	FALSE	c12c(cc3c(c1)cccc3)cccc2
MOL005501	0.7537	0.2463	0.6093	Rhododendri Daurici Folium	Green Oil	8418	FALSE	c12c(cc3c(c1)cccc3)cccc2
MOL005501	0.7537	0.2463	0.6093	Radix Cynanchi Paniculati	Green Oil	8418	FALSE	c12c(cc3c(c1)cccc3)cccc2
MOL005501	0.7537	0.2463	0.6093	Cornus Officinalis Sieb. Et Zucc.	Green Oil	8418	FALSE	c12c(cc3c(c1)cccc3)cccc2
MOL005501	0.7537	0.2463	0.6093	Gossampiniflos	Green Oil	8418	FALSE	c12c(cc3c(c1)cccc3)cccc2
MOL005502	0.9037	0.0963	0.9584	Cornus Officinalis Sieb. Et Zucc.	Butoxysuccinic Acid	Not Available	FALSE	C(=O)(C(CC(=O)O)OCCCC)O
MOL005503	0.3419	0.6581	0.7930	Verbenae Herb	Cornudentanone	46191017	FALSE	C1(=CC(=O)C=C(C1=O)CC(OC(=O)C)CCCCCCCCCCCC)OC
MOL005503	0.3419	0.6581	0.7930	Cornus Officinalis Sieb. Et Zucc.	Cornudentanone	46191017	FALSE	C1(=CC(=O)C=C(C1=O)CC(OC(=O)C)CCCCCCCCCCCC)OC
MOL005504	0.7854	0.2146	0.7460	Cornus Officinalis Sieb. Et Zucc.	Cornusiin A	Not Available	FALSE	c1c(cc(c(c1O)O)O)C(=O)OCC1C(C(C(C(O1)O)OC(=O)c1c(c(c(c(c1)O)O)O)Oc1c(c(c2c(c1)C(=O)CC1C(OC(=O)c3c2c(c(c(c3)O)O)O)C(C(C(O1)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O
MOL005505	0.7569	0.2431	0.7401	Cornus Officinalis Sieb. Et Zucc.	Cornusiin B	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC1C(OC(=O)c3c2c(O)c(c(c3)O)O)C(C(C(O1)O)OC(=O)c1c(c(c(c(c1)O)O)O)Oc1c(c2c3c(c1)c(=O)oc1c3c(c(=O)o2)cc(c1O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O
MOL005506	0.8596	0.1404	0.7600	Cornus Officinalis Sieb. Et Zucc.	Cornusiin C	Not Available	FALSE	C1(C(C(C(C(O1)O)OC(=O)c1cc(c(c(c1Oc1c(c2c3c(c1)c(=O)oc1c3c(c(=O)o2)cc(c1O)O)O)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)CO
MOL005507	0.7786	0.2214	0.7224	Cornus Officinalis Sieb. Et Zucc.	Cornusiin G	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC1C(OC(=O)c3c2c(O)c(c(c3)Oc2cc(c(c(c2C(=O)OCC2C(C(C(C(O2)OC(=O)c2cc(c(c(c2)O)O)O)OC(=O)c2cc(c(c(c2)O)O)O)OC(=O)c2cc(c(c(c2)O)O)O)O)O)O)O)O)C(C(C(O1)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O
MOL005508	0.7472	0.2528	0.7763	Campsis Flos	Glucosol	6918774	FALSE	C12=CCC3C4(C(C(C(C(C4)O)O)(C)C)CCC3(C1(CCC1(C2C(C(CC1)C)C)C(=O)O)C)C)C
MOL005508	0.7472	0.2528	0.7763	Rubi Fructus	Glucosol	6918774	FALSE	C12=CCC3C4(C(C(C(C(C4)O)O)(C)C)CCC3(C1(CCC1(C2C(C(CC1)C)C)C(=O)O)C)C)C
MOL005508	0.7472	0.2528	0.7763	Radix Salviae	Glucosol	6918774	FALSE	C12=CCC3C4(C(C(C(C(C4)O)O)(C)C)CCC3(C1(CCC1(C2C(C(CC1)C)C)C(=O)O)C)C)C
MOL005508	0.7472	0.2528	0.7763	Chebulae Fructus	Glucosol	6918774	FALSE	C12=CCC3C4(C(C(C(C(C4)O)O)(C)C)CCC3(C1(CCC1(C2C(C(CC1)C)C)C(=O)O)C)C)C

MOL005508	0.7472	0.2528	0.7763	Rosae Laevigatae Fructus	Glucosol	6918774	FALSE	C12=CCC3C4(C(C(C(C(C4)O)O)(C)C)CCC3(C1(CCC1(C2C(C(CC1)C)C)C(=O)O)C)C)C
MOL005508	0.7472	0.2528	0.7763	Eriobotryae Folium	Glucosol	6918774	FALSE	C12=CCC3C4(C(C(C(C(C4)O)O)(C)C)CCC3(C1(CCC1(C2C(C(CC1)C)C)C(=O)O)C)C)C
MOL005508	0.7472	0.2528	0.7763	Potentillae Chinensis Herba	Glucosol	6918774	FALSE	C12=CCC3C4(C(C(C(C(C4)O)O)(C)C)CCC3(C1(CCC1(C2C(C(CC1)C)C)C(=O)O)C)C)C
MOL005508	0.7472	0.2528	0.7763	Cornus Officinalis Sieb. Et Zucc.	Glucosol	6918774	FALSE	C12=CCC3C4(C(C(C(C(C4)O)O)(C)C)CCC3(C1(CCC1(C2C(C(CC1)C)C)C(=O)O)C)C)C
MOL005510	0.9355	0.0645	0.9489	Cornus Officinalis Sieb. Et Zucc.	D-1-O-Methyl mucoinositol	5319730	FALSE	C1(C(C(C(C(C1O)O)O)O)O)OC
MOL005511	0.1225	0.8775	0.6292	Cornus Officinalis Sieb. Et Zucc.	D-delta-tocopherol	71257536	FALSE	O1C(CCCC(CCCC(CCCC(C)C)C)C)(CCc2c1c(cc(O)c2)C)C
MOL005512	0.9395	0.0605	0.7692	Cornus Officinalis Sieb. Et Zucc.	Dehydromorroniaglycone	Not Available	FALSE	O1C2OC3C(C1C)C(C(=CO3)C(=O)OC)C2
MOL005513	0.8490	0.1510	0.7174	Cornus Officinalis Sieb. Et Zucc.	DBF	568	FALSE	c12c3c(oc1cccc2)cccc3
MOL005513	0.8490	0.1510	0.7174	Ephedra Herba	DBF	568	FALSE	c12c3c(oc1cccc2)cccc3
MOL005514	0.8024	0.1976	0.7598	Cornus Officinalis Sieb. Et Zucc.	Ethyl,alpha-hydroxymyristate	Not Available	FALSE	C(=O)(C(CCCCCCCCCCCCC)O)OCC
MOL005515	0.9544	0.0456	0.7897	Cornus Officinalis Sieb. Et Zucc.	Eugenone	5317271	FALSE	c1c(c(c(cc1OC)OC)C(=O)CC(=O)C)OC
MOL005515	0.9544	0.0456	0.7897	Asari Radix Et Rhizoma	Eugenone	5317271	FALSE	c1c(c(c(cc1OC)OC)C(=O)CC(=O)C)OC
MOL005516	0.8429	0.1571	0.6701	Cornus Officinalis Sieb. Et Zucc.	Fluoren	6853	FALSE	c12c3c(Cc1cccc2)cccc3
MOL005516	0.8429	0.1571	0.6701	Bidentis Bipinnatae Herba	Fluoren	6853	FALSE	c12c3c(Cc1cccc2)cccc3
MOL005522	0.9276	0.0724	0.9664	Cornus Officinalis Sieb. Et Zucc.	LEN	7894	FALSE	CC(CCN)C
MOL005530	0.8982	0.1018	0.8953	Lobeliae Chinensis Herba	Hydroxygenkwanin	5318214	FALSE	c1c(c2c(cc1OC)oc(cc2=O)c1ccc(c(c1)O)O)O
MOL005530	0.8982	0.1018	0.8953	Swertiae Mileensis Herba	Hydroxygenkwanin	5318214	FALSE	c1c(c2c(cc1OC)oc(cc2=O)c1ccc(c(c1)O)O)O
MOL005530	0.8982	0.1018	0.8953	Cornus Officinalis Sieb. Et Zucc.	Hydroxygenkwanin	5318214	FALSE	c1c(c2c(cc1OC)oc(cc2=O)c1ccc(c(c1)O)O)O
MOL005530	0.8982	0.1018	0.8953	Flos Genkwa	Hydroxygenkwanin	5318214	FALSE	c1c(c2c(cc1OC)oc(cc2=O)c1ccc(c(c1)O)O)O
MOL005530	0.8982	0.1018	0.8953	Trichosanthes Kirilowii Maxim	Hydroxygenkwanin	5318214	FALSE	c1c(c2c(cc1OC)oc(cc2=O)c1ccc(c(c1)O)O)O
MOL005531	0.4279	0.5721	0.7645	Cornus Officinalis Sieb. Et Zucc.	Telocinobufagin	Not Available	FALSE	C1C(CC2(C(C1)(C1C(CC2)C2(C(CC1)(C(CC2)c1ccc(=O)oc1)C)O)C)O)O
MOL005534	0.9613	0.0387	0.8133	Cornus Officinalis Sieb. Et Zucc.	trans-Verbenol	88298	FALSE	C12C(C(C(C=C1C)O)C2)(C)C

MOL005535	0.9651	0.0349	0.8070	Cornus Officinalis Sieb. Et Zucc.	Vitamin B1.mol2	Not Available	FALSE	n1c(ncc(c1[NH3+])C[n+]1csc(c1C)CCO)C
MOL005536	0.5526	0.4474	0.6546	Cornus Officinalis Sieb. Et Zucc.	Z,Z-10,12-Hexadecadien-1-ol acetate	5363372	FALSE	C(CCCCCCCC/C=C\C=C/CCC)OC(=O)C
MOL005538	0.5873	0.4127	0.6432	Mori Cortex	Linolenyl alcohol	6436081	FALSE	C(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL005538	0.5873	0.4127	0.6432	Farfarae Flos	Linolenyl alcohol	6436081	FALSE	C(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL005538	0.5873	0.4127	0.6432	Cornus Officinalis Sieb. Et Zucc.	Linolenyl alcohol	6436081	FALSE	C(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL005538	0.5873	0.4127	0.6432	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	Linolenyl alcohol	6436081	FALSE	C(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL005538	0.5873	0.4127	0.6432	Eriobotryae Folium	Linolenyl alcohol	6436081	FALSE	C(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL005538	0.5873	0.4127	0.6432	Eucommiae Folium	Linolenyl alcohol	6436081	FALSE	C(CCCCCCC/C=C\C/C=C\C/C=C\CC)O
MOL005539	0.8578	0.1422	0.6306	Cornus Officinalis Sieb. Et Zucc.	Acenaphthylene	9161	FALSE	c12c3C=Cc1cccc2ccc3
MOL005540	0.8603	0.1397	0.6772	Cornus Officinalis Sieb. Et Zucc.	alpha-Corocalene	5316074	FALSE	c1cc(c2c(c1C)CCC(=C2)C)C(C)C
MOL005541	0.9010	0.0990	0.6610	Cornus Officinalis Sieb. Et Zucc.	TBU	6386	FALSE	C(C)(C)(C)O
MOL005542	0.7725	0.2275	0.7270	Cornus Officinalis Sieb. Et Zucc.	camptothin A	Not Available	FALSE	O1C(C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C=O)C(O)COC(=O)c2c(c3c(C1=O)cc(O)c(O)c3O)c(O)c(O)c(Oc1c(C(=O)OC(C(OC(=O)c3cc(O)c(O)c(O)c3)C3OC(=O)c4c(c5c(C(=O)OCC3O)cc(O)c(O)c5O)c(O)c(O)c(O)c4)C=O)cc(O)c(O)c1O)c2
MOL005543	0.7597	0.2403	0.7485	Cornus Officinalis Sieb. Et Zucc.	camptothin B	Not Available	FALSE	O1C(C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2c(Oc3c(O)c4oc(=O)c5c6c4c(c3)c(=O)oc6c(O)c(O)c5)c(O)c(O)c(O)c2)C=O)C(O)COC(=O)c2c(c3c(C1=O)cc(O)c(O)c3O)c(O)c(O)c(O)c2
MOL005544	0.9025	0.0975	0.7844	Verbenae Herb	Cornin	73467	FALSE	C12C(C(=COC1OC1OC(C(C(C1O)O)O)CO)C(=O)OC)C(=O)CC2C
MOL005544	0.9025	0.0975	0.7844	Cornus Officinalis Sieb. Et Zucc.	Cornin	73467	FALSE	C12C(C(=COC1OC1OC(C(C(C1O)O)O)CO)C(=O)OC)C(=O)CC2C
MOL005545	0.9343	0.0657	0.8496	Verbenae Herb	cornin_qt	12444745	FALSE	C12C(C(=COC1O)C(=O)OC)C(=O)CC2C
MOL005545	0.9343	0.0657	0.8496	Cornus Officinalis Sieb. Et Zucc.	cornin_qt	12444745	FALSE	C12C(C(=COC1O)C(=O)OC)C(=O)CC2C
MOL005547	0.8384	0.1616	0.7403	Cornus Officinalis Sieb. Et Zucc.	cornuside_qt	Not Available	FALSE	C1(C(OC=C(C1CCOC(=O)c1cc(c(c(c1)O)O)O)C(=O)OC)O)C=C

MOL005548	0.5145	0.4855	0.7233	Cornus Officinalis Sieb. Et Zucc.	cornusiin E	Not Available	FALSE	O1C2C(OC(=O)c3c(c4c(C(=O)OC2)cc(O)c(O)c4O)c(O)c(O)c(O)c3)C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(Oc3c(O)c4c(C(=O)OC5C(OC(=O)c6cc(O)c(O)c(O)c6)C(OC(=O)c6cc(O)c(O)c(O)c6)C(OC5COC(=O)c5c4c(O)c(O)c(O)c5)OC(=O)c4cc(O)c(O)c(O)c4)cc3O)c(O)c(O)c2)C1OC(=O)c1cc(O)c(O)c(O)c1
MOL005549	0.8861	0.1139	0.9722	Gossampiniflos	Dehydromevalonic lactone	557445	FALSE	O1CCC(=CC1=O)C
MOL005549	0.8861	0.1139	0.9722	Cornus Officinalis Sieb. Et Zucc.	Dehydromevalonic lactone	557445	FALSE	O1CCC(=CC1=O)C
MOL005550	0.9330	0.0670	0.9537	Cornus Officinalis Sieb. Et Zucc.	Vanirom	8467	FALSE	O(c1cc(ccc1O)C=O)CC
MOL005552	0.8637	0.1363	0.6846	Cornus Officinalis Sieb. Et Zucc.	gemin D	Not Available	FALSE	O1C(C(OC(=O)c2cc(O)c(O)c(O)c2)C(O)C=O)C(O)COC(=O)c2c(c3c(C1=O)cc(O)c(O)c3O)c(O)c(O)c(O)c2
MOL005553	0.5773	0.4227	0.7190	Cornus Officinalis Sieb. Et Zucc.	2-Monopalmitin	123409	FALSE	C(=O)(CCCCCCCCCCCCCCC)OC(CO)CO
MOL005554	0.9137	0.0863	0.9658	Campsis Flos	i-Butanol	6560	FALSE	C(C(C)C)O
MOL005554	0.9137	0.0863	0.9658	Sesami Nigrum Semen	i-Butanol	6560	FALSE	C(C(C)C)O
MOL005554	0.9137	0.0863	0.9658	Cornus Officinalis Sieb. Et Zucc.	i-Butanol	6560	FALSE	C(C(C)C)O
MOL005554	0.9137	0.0863	0.9658	Zingiber Officinale Roscoe	i-Butanol	6560	FALSE	C(C(C)C)O
MOL005555	0.8471	0.1529	0.7729	Cornus Officinalis Sieb. Et Zucc.	isoterchebin	Not Available	FALSE	O1C2(O)C(O)(O)C3c4c1c(O)c(O)cc4C(=O)OC1C(OC(=O)c4cc(O)c(O)c(O)c4)C(OC(=O)c4cc(O)c(O)c(O)c4)C(OC1COC(=O)C3=CC2=O)OC(=O)c1cc(O)c(O)c(O)c1
MOL005556	0.8828	0.1172	0.7121	Cornus Officinalis Sieb. Et Zucc.	1-tert-Butyl-7-methoxynaphthalene	608110	FALSE	c1(cccc2ccc(cc12)OC)C(C)(C)C
MOL005557	0.1643	0.8357	0.6971	Cornus Officinalis Sieb. Et Zucc.	lanosta-8,24-dien-3-ol,3-acetate	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1=C2CCC2(C1(C)CCC2C(CCC=C(C)C)C)C)C)OC(=O)C
MOL005558	0.9127	0.0873	0.9711	Cornus Officinalis Sieb. Et Zucc.	DLE	6950207	FALSE	OC(=O)C(N)CC(C)C
MOL005559	0.7451	0.2549	0.7902	Schizonepetae Herba	Maslinic acid	73659	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(C(C1)O)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL005559	0.7451	0.2549	0.7902	Actinidia Chinensis Planch	Maslinic acid	73659	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(C(C1)O)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL005559	0.7451	0.2549	0.7902	Rubi Fructus	Maslinic acid	73659	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(C(C1)O)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL005559	0.7451	0.2549	0.7902	Cornus Officinalis Sieb. Et Zucc.	Maslinic acid	73659	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(C(C1)O)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL005559	0.7451	0.2549	0.7902	Potentillae Chinensis Herba	Maslinic acid	73659	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(C(C1)O)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C

MOL005559	0.7451	0.2549	0.7902	Chebulae Fructus	Maslinic acid	73659	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(C(C1)O)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL005559	0.7451	0.2549	0.7902	Jujubae Fructus	Maslinic acid	73659	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(C(C1)O)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL005559	0.7451	0.2549	0.7902	Eriobotryae Folium	Maslinic acid	73659	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(C(C1)O)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL005559	0.7451	0.2549	0.7902	Rosae Laevigatae Fructus	Maslinic acid	73659	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(C(C1)O)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL005559	0.7451	0.2549	0.7902	Boehmeriae Rhizoma Et Radix	Maslinic acid	73659	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(C(C1)O)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL005559	0.7451	0.2549	0.7902	Crataegi Folium	Maslinic acid	73659	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(C(C1)O)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL005559	0.7451	0.2549	0.7902	Swertiae Mileensis Herba	Maslinic acid	73659	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(C(C1)O)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL005559	0.7451	0.2549	0.7902	Campsis Flos	Maslinic acid	73659	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(C(C1)O)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL005559	0.7451	0.2549	0.7902	Tamaricis Cacumen	Maslinic acid	73659	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(C(C1)O)O)(C)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL005560	0.3891	0.6109	0.6998	Cornus Officinalis Sieb. Et Zucc.	olean-13(18)-ene	Not Available	FALSE	C12(C(C3(C(CC2)C(CCC3)(C)C)C)CCC2=C3C(CCC12C)(CCC(C3)(C)C)C)C
MOL005561	0.9571	0.0429	0.9644	Cornus Officinalis Sieb. Et Zucc.	Anisylacetone	61007	FALSE	c1c(ccc(c1)CCC(=O)C)OC
MOL005561	0.9571	0.0429	0.9644	Linderae Radix	Anisylacetone	61007	FALSE	c1c(ccc(c1)CCC(=O)C)OC
MOL005563	0.9571	0.0429	0.9601	Schizonepetae Spica	(-)-Pulegone	638012	FALSE	O=C1CC(CCC1=C(C)C)C
MOL005563	0.9571	0.0429	0.9601	Glechomae Herba	(-)-Pulegone	638012	FALSE	O=C1CC(CCC1=C(C)C)C
MOL005563	0.9571	0.0429	0.9601	Cornus Officinalis Sieb. Et Zucc.	(-)-Pulegone	638012	FALSE	O=C1CC(CCC1=C(C)C)C
MOL005563	0.9571	0.0429	0.9601	Schizonepetae Herba	(-)-Pulegone	638012	FALSE	O=C1CC(CCC1=C(C)C)C
MOL005564	0.8418	0.1582	0.7151	Cornus Officinalis Sieb. Et Zucc.	tellimagrandin I	Not Available	FALSE	O1C(C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C=O)C(O)COC(=O)c2c(c3c(C1=O)cc(O)c(O)c3O)c(O)c(O)c(O)c2
MOL005565	0.9190	0.0810	0.9665	Cornus Officinalis Sieb. Et Zucc.	Uretan	5641	FALSE	O(C(=O)N)CC
MOL005566	0.3635	0.6365	0.7000	Cornus Officinalis Sieb. Et Zucc.	urs-12-en-28-al	Not Available	FALSE	O=CC12C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCCC1(C)C)C)C)C(C(CC2)C)C
MOL005567	0.4650	0.5350	0.7771	Capsici Fructus	vitamin a	445354	FALSE	C(/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)O
MOL005567	0.4650	0.5350	0.7771	Cornus Officinalis Sieb. Et Zucc.	vitamin a	445354	FALSE	C(/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)O
MOL005567	0.4650	0.5350	0.7771	Panacis Quinquefolii Radix	vitamin a	445354	FALSE	C(/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)O
MOL005567	0.4650	0.5350	0.7771	Vigna Radiata	vitamin a	445354	FALSE	C(/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)O
MOL005568	0.9233	0.0767	0.9271	Herba Clematidis Aethusaefoliae	WLN: QVR BM1	67069	FALSE	c1(c(cccc1)NC)C(=O)O

MOL005569	0.9699	0.0301	0.8240	Herba Clematidis Aethusaefoliae	4,6,7-trimethoxy-5-methyl-2H-chromen-2-one	54025699	FALSE	c12c(c(cc(=O)o1)OC)c(c(c(c2)OC)OC)C
MOL005570	0.9247	0.0753	0.9448	Typhonii Rhizoma	inositol	892	FALSE	C1(C(C(C(C(C1O)O)O)O)O)O
MOL005570	0.9247	0.0753	0.9448	Trollius Chinensis	inositol	892	FALSE	C1(C(C(C(C(C1O)O)O)O)O)O
MOL005570	0.9247	0.0753	0.9448	Canarii Fructus	inositol	892	FALSE	C1(C(C(C(C(C1O)O)O)O)O)O
MOL005570	0.9247	0.0753	0.9448	Amygdalus Communis Vas	inositol	892	FALSE	C1(C(C(C(C(C1O)O)O)O)O)O
MOL005570	0.9247	0.0753	0.9448	Maydis Seigma	inositol	892	FALSE	C1(C(C(C(C(C1O)O)O)O)O)O
MOL005570	0.9247	0.0753	0.9448	Herba Clematidis Aethusaefoliae	inositol	892	FALSE	C1(C(C(C(C(C1O)O)O)O)O)O
MOL005570	0.9247	0.0753	0.9448	Papaveris Pericarpium	inositol	892	FALSE	C1(C(C(C(C(C1O)O)O)O)O)O
MOL005571	0.9434	0.0566	0.9085	Flos Genkwa	Psi-cumene	7247	FALSE	c1(c(ccc(c1)C)C)C
MOL005572	0.5406	0.4594	0.6832	Flos Genkwa	12-benzoyoxy daphnetoxin	Not Available	FALSE	O1C2C3C4(OC5(OC3C(O5)(CC4C)C(=C)C)c3ccccc3)C3C(O)(C(O)C12CO)C(=O)C(=C3)C
MOL005573	0.9156	0.0844	0.8158	Menthae Herba	Genkwanin	5281617	FALSE	c12c(oc(cc1=O)c1ccc(cc1)O)cc(cc2O)OC
MOL005573	0.9156	0.0844	0.8158	Wikstroemiae Indicae Rasix	Genkwanin	5281617	FALSE	c12c(oc(cc1=O)c1ccc(cc1)O)cc(cc2O)OC
MOL005573	0.9156	0.0844	0.8158	Ginkgo Folium	Genkwanin	5281617	FALSE	c12c(oc(cc1=O)c1ccc(cc1)O)cc(cc2O)OC
MOL005573	0.9156	0.0844	0.8158	Artemisiae Scopariae Herba	Genkwanin	5281617	FALSE	c12c(oc(cc1=O)c1ccc(cc1)O)cc(cc2O)OC
MOL005573	0.9156	0.0844	0.8158	Flos Genkwa	Genkwanin	5281617	FALSE	c12c(oc(cc1=O)c1ccc(cc1)O)cc(cc2O)OC
MOL005573	0.9156	0.0844	0.8158	Swertiae Mileensis Herba	Genkwanin	5281617	FALSE	c12c(oc(cc1=O)c1ccc(cc1)O)cc(cc2O)OC
MOL005573	0.9156	0.0844	0.8158	Pogostemon Cablin (Blanco) Benth.	Genkwanin	5281617	FALSE	c12c(oc(cc1=O)c1ccc(cc1)O)cc(cc2O)OC
MOL005573	0.9156	0.0844	0.8158	Hydnocarpi Anthelminticae Semen	Genkwanin	5281617	FALSE	c12c(oc(cc1=O)c1ccc(cc1)O)cc(cc2O)OC
MOL005575	0.8343	0.1657	0.8270	Flos Genkwa	Gentiacaulein	5281634	FALSE	c1c(c(c2c(c1)oc1c(c2=O)c(cc(c1)OC)O)OC)O
MOL005575	0.8343	0.1657	0.8270	Hedysari Radix	Gentiacaulein	5281634	FALSE	c1c(c(c2c(c1)oc1c(c2=O)c(cc(c1)OC)O)OC)O
MOL005575	0.8343	0.1657	0.8270	Swertiae Mileensis Herba	Gentiacaulein	5281634	FALSE	c1c(c(c2c(c1)oc1c(c2=O)c(cc(c1)OC)O)OC)O

MOL005576	0.8397	0.1603	0.8039	Puerariae Flos	5-hydroxy-2-(4-hydroxyphenyl)-7-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxymethyl]tetrahydropyran-2-yl]oxy-chromone	21676297	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC1C(C(C(C(O1)C)O)O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1ccc(cc1)O

MOL005576	0.8397	0.1603	0.8039	Flos Genkwa	5-hydroxy-2-(4-hydroxyphenyl)-7-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxymethyl]tetrahydropyran-2-yl]oxy-chromone	21676297	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC1C(C(C(C(O1)C)O)O)O)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)c1ccc(cc1)O
MOL005577	0.9011	0.0989	0.8938	Hippophae Fructus	undecanal	8186	FALSE	C(CCCCC=O)CCCCC
MOL005577	0.9011	0.0989	0.8938	Lysimachiae Foenigraeci Herba	undecanal	8186	FALSE	C(CCCCC=O)CCCCC
MOL005577	0.9011	0.0989	0.8938	Campsis Flos	undecanal	8186	FALSE	C(CCCCC=O)CCCCC
MOL005577	0.9011	0.0989	0.8938	Ganoderma	undecanal	8186	FALSE	C(CCCCC=O)CCCCC
MOL005577	0.9011	0.0989	0.8938	Flos Genkwa	undecanal	8186	FALSE	C(CCCCC=O)CCCCC
MOL005577	0.9011	0.0989	0.8938	Citrus Reticulata	undecanal	8186	FALSE	C(CCCCC=O)CCCCC
MOL005578	0.4522	0.5478	0.7919	Flos Genkwa	7-hydroxy-3-(2-ketochromen-7-yl)-6-methoxy-coumarin	24721430	FALSE	c1(c2cc3c(oc2=O)cc(c(c3)OC)O)cc2c(cc1)ccc(=O)o2
MOL005580	0.8268	0.1732	0.7973	Flos Genkwa	yuenkanin	Not Available	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1ccc(cc1)O)OC1OC(C(C(C1O)O)O)O)COC1OCC(C(C1O)O)O)OC
MOL005581	0.4069	0.5931	0.7774	Flos Genkwa	genkwadaphnin	Not Available	FALSE	C123C(C4C(C(C3C)OC(=O)c3ccccc3)(OC(O2)(O4)c2ccccc2)C(=C)C)C2C(O2)(C(C2(C1C=C(C2=O)C)O)O)CO
MOL005582	0.5498	0.4502	0.6896	Flos Genkwa	yuanhuafin	Not Available	FALSE	O1C2C3C4(OC5(OC3C(O5)(C(OC(=O)C)C4C)C(=C)C)c3ccccc3)C3C(O)(C(O)C12CO)C(=O)C(=C3)C

MOL005583	0.3940	0.6060	0.7599	Flos Genkwa	yuanhuatin	Not Available	FALSE	O1C23C(C4OC4(C(O)C4(O)C2CC(C4=O)C)CO)C2OC1(OC2(C(OC(=O)c1ccccc1)C3C)C(=C)C)c1ccccc1
MOL005584	0.2222	0.7778	0.8339	Flos Genkwa	yuanhuacin	Not Available	FALSE	C123C(C4C(C(C3C)OC(=O)c3ccccc3)(OC(O2)(O4)/C=C/C=C/CCCCC)C(=C)C)C2C(O2)(C(C2(C1C=C(C2=O)C)O)O)CO
MOL005585	0.5511	0.4489	0.6760	Flos Genkwa	yuanhuapin	Not Available	FALSE	O1C2C3C4(OC5(OC3C(O5)(C(OC(=O)C)C4C)C(=C)C)c3ccccc3)C3C(O)(C(O)C12CO)C(=O)C(C3)C
MOL005586	0.3090	0.6910	0.7909	Flos Genkwa	yuanhuadine	Not Available	FALSE	C123C(C4C(C(C3C)OC(=O)C)(OC(O2)(O4)/C=C\C=C\CCCCC)C(=C)C)C2C(O2)(C(C2(C1C=C(C2=O)C)O)O)CO
MOL005587	0.9094	0.0906	0.8345	Radix Clematidis	1,2,4-TRIETHYLBENZENE	13415	FALSE	c1cc(cc(c1CC)CC)CC
MOL005588	0.9424	0.0576	0.8350	Radix Clematidis	2,3-Dihydro-4-hydroxy-2-indole-3-acetonitrile	Not Available	FALSE	c1(cccc2c1C(C(=O)N2)CC#N)O
MOL005589	0.9562	0.0438	0.9313	Radix Clematidis	3,4-DIMETHYLBENZALDEHYDE	22278	FALSE	c1c(cc(c(c1)C)C)C=O
MOL005589	0.9562	0.0438	0.9313	Angelicae Sinensis Radix	3,4-DIMETHYLBENZALDEHYDE	22278	FALSE	c1c(cc(c(c1)C)C)C=O
MOL005590	0.9578	0.0422	0.9500	Radix Clematidis	ETHYLBENZALDEHYDE	20861	FALSE	c1cc(ccc1C=O)CC
MOL005590	0.9578	0.0422	0.9500	Angelicae Sinensis Radix	ETHYLBENZALDEHYDE	20861	FALSE	c1cc(ccc1C=O)CC
MOL005590	0.9578	0.0422	0.9500	Capsici Fructus	ETHYLBENZALDEHYDE	20861	FALSE	c1cc(ccc1C=O)CC
MOL005591	0.7679	0.2321	0.8228	Radix Clematidis	Clematisprosapogenin,Cp7a	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)OC1OCC(C(C1O)O)OC1OC(C(C(C1O)O)O)CO)O)C)O)O
MOL005592	0.7553	0.2447	0.9079	Radix Clematidis	Clematisprosapogenin,Cp7a_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O
MOL005593	0.7498	0.2502	0.7956	Radix Clematidis	ClematosideA'	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(C)C)C1OC(C(OC2OCC(O)C(O)C2OC2OCC(O)C(O)C2OC2OCC(OC3OC(C(O)C(O)C3O)CO)C(O)C2O)C(O)C1O)C
MOL005594	0.7553	0.2447	0.9079	Panacis Japonici Rhizoma	ClematosideA'_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(C)C

MOL005594	0.7553	0.2447	0.9079	Radix Clematidis	ClematosideA'_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(C)C
MOL005595	0.4758	0.5242	0.7563	Radix Clematidis	ClematosideB	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)COC3OC(C(OC4OC(C(OC5OC(C(O)C(O)C5O)C)C(O)C4O)CO)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C)C1OC(C(OC2OCC(O)C(O)C2OC2OCC(O)C(O)C2OC2OCC(OC3OC(C(OC4OC(C(O)C(O)C4O)CO)C(O)C3O)CO)C(O)C2O)C(O)C1O)C
MOL005596	0.4778	0.5222	0.7535	Radix Clematidis	ClematosideC	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)COC3OC(C(OC4OC(C(OC5OC(C(O)C(O)C5O)C)C(O)C4O)CO)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C)C1OC(C(OC2OCC(O)C(O)C2OC2OCC(O)C(O)C2OC2OCC(OC3OC(C(OC4OC(C(O)C(O)C4O)COC4OC(C(O)C(O)C4O)C)C(O)C3O)CO)C(O)C2O)C(O)C1O)C
MOL005597	0.8852	0.1148	0.9723	Radix Clematidis	Cleomin	5315964	FALSE	C1NC(=S)OC1(C)CC
MOL005598	0.7211	0.2789	0.7714	Radix Clematidis	Embinin	21155963	FALSE	O1C(C(C(C(C1c1c(c2c(cc1OC)oc(cc2=O)c1ccc(cc1)OC)O)OC1OC(C(C(C1O)O)O)C)O)O)CO
MOL005599	0.6799	0.3201	0.7785	Radix Clematidis	Embinin_qt	14630648	FALSE	O1C(C(C(C(C1c1c(c2c(cc1OC)oc(cc2=O)c1ccc(cc1)OC)O)O)O)O)CO
MOL005600	0.4893	0.5107	0.7575	Radix Clematidis	clematosideA	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)COC3OC(C(OC4OC(C(OC5OC(C(O)C(O)C5O)C)C(O)C4O)CO)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C)C1OC(C(OC2OCC(O)C(O)C2OC2OCC(O)C(O)C2OC2OCC(OC3OC(C(O)C(O)C3O)CO)C(O)C2O)C(O)C1O)C
MOL005601	0.8874	0.1126	0.9669	Radix Clematidis	Protoanemonin	66948	FALSE	C1(=C)OC(=O)C=C1
MOL005601	0.8874	0.1126	0.9669	Ranunculi Ternati Radix	Protoanemonin	66948	FALSE	C1(=C)OC(=O)C=C1
MOL005602	0.9353	0.0647	0.9049	Radix Clematidis	ALLYLBENZENE	9309	FALSE	c1c(cccc1)CC=C
MOL005603	0.3482	0.6518	0.7267	Radix Clematidis	Heptyl phthalate	19284	FALSE	c1ccc(c(c1)C(=O)OCCCCCCC)C(=O)OCCCCCCC
MOL005605	0.9183	0.0817	0.6958	Radix Cynanchi Paniculati	1,6-Dimethylnaphthalene	11328	FALSE	c12c(cc(cc2)C)cccc1C
MOL005605	0.9183	0.0817	0.6958	Ginseng Folium	1,6-Dimethylnaphthalene	11328	FALSE	c12c(cc(cc2)C)cccc1C
MOL005606	0.9484	0.0516	0.8972	Radix Cynanchi Paniculati	p-Ethylcumene	20197	FALSE	c1(ccc(cc1)CC)C(C)C

MOL005607	0.9490	0.0510	0.9579	Radix Cynanchi Paniculati	2',4'-Dihydroxy-3'-methylacetophenone	592139	FALSE	c1(c(c(c(cc1)O)C)O)C(=O)C
MOL005608	0.9380	0.0620	0.9442	Radix Cynanchi Paniculati	TMHYDROP	12785	FALSE	c1(c(c(cc(c1O)C)O)C)C
MOL005608	0.9380	0.0620	0.9442	Angelicae Sinensis Radix	TMHYDROP	12785	FALSE	c1(c(c(cc(c1O)C)O)C)C
MOL005609	0.9362	0.0638	0.9717	Ephedra Herba	76897_FLUKA	2723683	FALSE	C(CC(C)O)(C)O
MOL005609	0.9362	0.0638	0.9717	Radix Cynanchi Paniculati	76897_FLUKA	2723683	FALSE	C(CC(C)O)(C)O
MOL005610	0.9229	0.0771	0.9591	Radix Cynanchi Paniculati	WLN: QR BV1	8375	FALSE	c1cccc(c1O)C(=O)C
MOL005611	0.8749	0.1251	0.9674	Radix Cynanchi Paniculati	2-Methylene cyclopentanol	Not Available	FALSE	OC1CCCC1=C
MOL005612	0.9276	0.0724	0.9616	Stemonae Radix	3,4-DIMETHOXYPHENOL	16251	FALSE	c1(c(cc(cc1)O)OC)OC
MOL005612	0.9276	0.0724	0.9616	Radix Cynanchi Paniculati	3,4-DIMETHOXYPHENOL	16251	FALSE	c1(c(cc(cc1)O)OC)OC
MOL005613	0.9424	0.0576	0.9540	Radix Cynanchi Paniculati	3-Acetylanisole	11460	FALSE	c1(cc(ccc1)OC)C(=O)C
MOL005614	0.9143	0.0857	0.9720	Radix Cynanchi Paniculati	m-Guaiacol	9007	FALSE	c1(cc(ccc1)O)OC
MOL005615	0.9258	0.0742	0.9597	Radix Cynanchi Paniculati	(3S)-3-methylhexan-1-ol	11228780	FALSE	C(CCC)(CCO)C
MOL005615	0.9258	0.0742	0.9597	Capsici Fructus	(3S)-3-methylhexan-1-ol	11228780	FALSE	C(CCC)(CCO)C
MOL005616	0.9164	0.0836	0.9368	Radix Cynanchi Paniculati	3-methyl-Cyclooctene	Not Available	FALSE	C1(CCCCCC=C1)C
MOL005617	0.9326	0.0674	0.9437	Nardostachyos Radix Et Rhizoma	(4R)-3,3,6-trimethylhepta-1,5-dien-4-ol	10898915	FALSE	OC(C(C)(C)C=C)C=C(C)C
MOL005617	0.9326	0.0674	0.9437	Radix Cynanchi Paniculati	(4R)-3,3,6-trimethylhepta-1,5-dien-4-ol	10898915	FALSE	OC(C(C)(C)C=C)C=C(C)C
MOL005619	0.1361	0.8639	0.6907	Radix Cynanchi Paniculati	Tomentolide A	Not Available	FALSE	C1(Oc2c(C=C1)c1c(c3c2C(=O)C(C(O3)C)C)c(cc(=O)o1)c1ccccc1)(C)C
MOL005620	0.9234	0.0766	0.9192	Nardostachyos Radix Et Rhizoma	Yomogi alcohol	5315406	FALSE	OC(/C=C/C(C)(C)C=C)(C)C

MOL005620	0.9234	0.0766	0.9192	Radix Cynanchi Paniculati	Yomogi alcohol	5315406	FALSE	OC(/C=C/C(C)(C)C=C)(C)C
MOL005621	0.6926	0.3074	0.7647	Radix Cynanchi Paniculati	lineolone	12311278	FALSE	OC12C(C(O)CC3C1(O)CC=C1C3(CCC(O)C1)C)(C(CC2)C(=O)C)C
MOL005622	0.7315	0.2685	0.7260	Radix Cynanchi Paniculati	tomentogenin	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C2(C(C(C1)O)(C(CC2)(O)C(C)O)C)O)C)O
MOL005623	0.7858	0.2142	0.7663	Radix Cynanchi Paniculati	sarcostin	Not Available	FALSE	C12(C3(C(C4(C(=CC3)CC(CC4)O)C)CC(C1(C(CC2)(C(C)O)O)C)O)O)O
MOL005625	0.6884	0.3116	0.6014	Radix Cynanchi Paniculati	cynapanoside C_qt	Not Available	FALSE	O1C2(OC=C3C2C(OC(=O)C2C(C4(C(=CC2O)CC(O)CC4)C)CC3)C1)C
MOL005626	0.3931	0.6069	0.7463	Radix Cynanchi Paniculati	cynapanoside B	Not Available	FALSE	O1C2(OC=C3C2C(OC(=O)C2C(C4(C(=CC2O)CC(OC2OC(C(OC5OC(C(OC6OC(C(O)C(OC)C6)C)C(O)C5)C)C(OC)C2)C)CC4)C)CC3)C1=O)C
MOL005627	0.7350	0.2650	0.6005	Radix Cynanchi Paniculati	cynapanoside B_qt	Not Available	FALSE	O1C2(OC=C3C2C(OC(=O)C2C(C4(C(=CC2O)CC(O)CC4)C)CC3)C1=O)C
MOL005628	0.3490	0.6510	0.7428	Radix Cynanchi Paniculati	cynapanoside C	Not Available	FALSE	O1C2(OC=C3C2C(OC(=O)C2C(C4(C(=CC2O)CC(OC2OC(C(OC5OC(C(OC6OC(C(O)C(OC)C6)C)C(O)C5)C)C(OC)C2)C)CC4)C)CC3)C1)C
MOL005630	0.2918	0.7082	0.7330	Radix Cynanchi Paniculati	cynatratoside B	Not Available	FALSE	O1CC2OC(=O)C3C(CCC4=COC1(C24)C)C1(C(=CC3)CC(CC1)OC1OC(C(C(C1)OC)OC1OC(C(C(C1)O)OC1OC(C(C(C1)OC)O)C)C)C)C
MOL005632	0.8084	0.1916	0.7906	Rhizoma Seu Herba Aristolochiae Mollissimae	6-Methoxy-aristololactam	Not Available	FALSE	O1c2c3c4c([nH]c(=O)c4cc2OC1)cc1c3cc(cc1OC)OC
MOL005633	0.8085	0.1915	0.8720	Rhizoma Seu Herba Aristolochiae Mollissimae	7-Methoxy-aromadendrin	Not Available	FALSE	c12c(cc(cc1O)C(=O)C)OC(C(C2=O)O)c1ccc(cc1)O
MOL005634	0.5060	0.4940	0.6944	Rhizoma Seu Herba Aristolochiae Mollissimae	8-beta-Ethoxy atractylenolide III	Not Available	FALSE	C1CC(=C)C2(C(C1)(CC1(C(=C(C(=O)O1)C)C2)OCC)C)C
MOL005635	0.7129	0.2871	0.7840	Rhizoma Seu Herba Aristolochiae Mollissimae	9-Ethoxyaristolactone	Not Available	FALSE	c12c(c3c4c(c1)C(=O)Oc4c(c1c3cccc1OC)OCC)OCO2
MOL005636	0.7215	0.2785	0.7762	Rhizoma Seu Herba Aristolochiae Mollissimae	9-Ethoxyaristololactam	Not Available	FALSE	O1c2c3c4c([nH]c(=O)c4cc2OC1)c(OCC)c1c3cccc1OC
MOL005637	0.4163	0.5837	0.6358	Rhizoma Seu Herba Aristolochiae Mollissimae	Aristoloterpenate	Not Available	FALSE	C1(C/C(=C/CC/C(=C/CC/C(=C/1)/C=O)/C)/C)OC(=O)c1c2c(cc3c(c2c2c(c1)OCO2)cccc3OC)[N+](=O)O
MOL005638	0.6295	0.3705	0.8807	Rubia Cordifolia	Mollugin	124219	FALSE	c1ccc2c(c1)c(c(c1c2OC(C=C1)(C)C)C(=O)OC)O
MOL005638	0.6295	0.3705	0.8807	Rhizoma Seu Herba Aristolochiae Mollissimae	Mollugin	124219	FALSE	c1ccc2c(c1)c(c(c1c2OC(C=C1)(C)C)C(=O)OC)O
MOL005639	0.8518	0.1482	0.7350	Rhizoma Seu Herba Aristolochiae Mollissimae	Neobavachalcone	5320052	FALSE	c1c(c(cc(c1C=O)OC)O)C(=O)/C=C/c1ccc(cc1)O

MOL005640	0.8783	0.1217	0.7927	Rhizoma Seu Herba Aristolochiae Mollissimae	(1R,2R,4E,6S,9R)-6-hydroxy-2-isopropenyl-5-methyl-11-oxabicyclo[7.2.1]dodec-4-en-10-one	23305215	FALSE	O1C2CC(CCC(O)/C(=C/CC2C(=C)C)/C)C1=O
MOL005641	0.9372	0.0628	0.7371	Rhizoma Seu Herba Aristolochiae Mollissimae	Mellitene	6908	FALSE	c1(c(c(c(c(c1C)C)C)C)C)C
MOL005642	0.8543	0.1457	0.8179	Rhizoma Seu Herba Aristolochiae Mollissimae	aristolactone	Not Available	FALSE	C12=CC(C(CC/C(=C\CC1)/C)C(=C)C)OC2=O
MOL005643	0.7467	0.2533	0.6988	Rhizoma Seu Herba Aristolochiae Mollissimae	mollislactone	Not Available	FALSE	O1C2CCC/C(=C\CC/C=C\2/C(=C/C)/C1=O)/C
MOL005645	0.4324	0.5676	0.8723	Cortex Periplocae Radicis	21-O-Methyl-5,14-pregndiene-3β,14β,17β,21-tetrol-20-one	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3=CCC1(O)C(COC)O)C)O
MOL005646	0.6064	0.3936	0.7472	Cortex Periplocae Radicis	21-O-Methyl-5-pregnene-3beta,14beta,17beta,20,21-pentol	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3(CCC1(O)C(O)COC)O)C)O
MOL005647	0.5228	0.4772	0.7624	Cortex Periplocae Radicis	21-O-Methyl-5-pregnene-3beta,17beta,20,21-tetrol	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3(CCC1(O)C(=O)COC)O)C)O
MOL005648	0.7657	0.2343	0.6559	Cortex Periplocae Radicis	3'-Methoxysecoisolariciresinol	Not Available	FALSE	COc1cc(ccc1O)CC(CO)C(Cc1cc(c(c(c1)OC)O)OC)CO
MOL005649	0.9504	0.0496	0.9731	Cortex Periplocae Radicis	4-Methoxysalicyaldehyde	69600	FALSE	O(c1cc(O)c(cc1)C=O)C
MOL005649	0.9504	0.0496	0.9731	Scutellariae Barbatae Herba	4-Methoxysalicyaldehyde	69600	FALSE	O(c1cc(O)c(cc1)C=O)C

MOL005650	0.2082	0.7918	0.7848	Cortex Periplocae Radicis	[(3S,8S,9S,10R,13S,14S,17S)-17-(1-hydroxyethyl)-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-yl] acetate	11783365	FALSE	C1(CCC2(C(=CCC3C4CCC(C(C)O)C4(C)CCC23)C1)C)OC(=O)C
MOL005651	0.6518	0.3482	0.7565	Cortex Periplocae Radicis	Glycoside H1	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CCC1C(OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)OC)O)C)C)OC1OC(C(C(C1)OC)OC1OC(C(C(C1OC(=O)C)OC)O)C)C
MOL005652	0.3529	0.6471	0.8877	Cortex Periplocae Radicis	Glycoside K_qt	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CCC1C(O)C)C)O
MOL005653	0.6468	0.3532	0.7540	Cortex Periplocae Radicis	Glycoside H2	Not Available	FALSE	O(C(C1C2(C(C3C(C4(C(=CC3)CC(OC3OC(C(OC5OC(C(O)C(OC)C5OC(=O)C)C)C(OC)C3)C)CC4)C)CC2)CC1O)C)C)C1OC(C(O)C(OC)C1OC1OC(C(O)C(O)C1O)COC1OC(C(O)C(O)C1O)CO)C
MOL005654	0.4974	0.5026	0.8859	Cortex Periplocae Radicis	Glycoside H2_qt	Not Available	FALSE	OC(C1C2(C(C3C(C4(C(=CC3)CC(O)CC4)C)CC2)CC1O)C)C
MOL005655	0.6517	0.3483	0.7967	Cortex Periplocae Radicis	Glycoside K	Not Available	FALSE	C1(OC(C(C(C1OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)OC)O)C)OC(C1C2(C(C3CC=C4CC(CCC4(C3CC2)C)O)CC1)C)C
MOL005656	0.8424	0.1576	0.8024	Cortex Periplocae Radicis	Glycozolidal	5317755	FALSE	c1c(cc2c(c1)c1c([nH]2)cc(c(c1)C=O)OC)OC
MOL005657	0.8419	0.1581	0.8719	Cortex Periplocae Radicis	Methyl-1propenyl thiosulfinate	Not Available	FALSE	C/C=C/S(=O)SC
MOL005658	0.5241	0.4759	0.7524	Cortex Periplocae Radicis	Periplogenin	10574	FALSE	OC12C3C(C4(C(O)(CC3)CC(O)CC4)C)CCC1(C(CC2)C1=CC(=O)OC1)C
MOL005659	0.5434	0.4566	0.6695	Cortex Periplocae Radicis	Periplogenin-3-O-alpha-L-rhamnopyranoside	Not Available	FALSE	C1(C(C(C(OC1C)OC1CC2(C(CC1)(C1C(CC2)C2(C(CC1)(C(CC2)C1=CC(=O)OC1)C)O)C)O)O)O)O
MOL005660	0.5241	0.4759	0.7524	Cortex Periplocae Radicis	Periplogenin-3-O-alpha-L-rhamnopyranoside_qt	12314105	FALSE	OC1CC2(C(CC1)(C1C(CC2)C2(C(CC1)(C(CC2)C1=CC(=O)OC1)C)O)C)O

MOL005662	0.3145	0.6855	0.7381	Cortex Periplocae Radicis	alpha-Amyrin acetate	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1C)C)C)C)C)(C)C)OC(=O)C
MOL005664	0.4481	0.5519	0.8424	Cortex Periplocae Radicis	glycoside E_qt	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CCC1(C(O)C)O)C)O
MOL005665	0.2145	0.7855	0.6624	Cortex Periplocae Radicis	Periplocoside M	Not Available	FALSE	O1C(CC(C(C1C)O)O)OC(C1(C2(C(C3C(CC2)C2(C(=CC3)CC(CC2)OC2OC(C=C(C2=O)OC)C)C)CC1)C)O)C
MOL005668	0.2800	0.7200	0.6134	Cortex Periplocae Radicis	periplocoside C_qt	Not Available	FALSE	OC1(C2(C(C3C(C4(C(=CC3)CC(OC3OC(C=C(OC)C3=O)C)CC4)C)CC2)CC1)C)C(OC1OC(C2OOC3(OC(C(O)C(OC)C3)C)COC2C1)C)C
MOL005670	0.2800	0.7200	0.6134	Cortex Periplocae Radicis	periplocoside B_qt	Not Available	FALSE	OC1(C2(C(C3C(C4(C(=CC3)CC(OC3OC(C=C(OC)C3=O)C)CC4)C)CC2)CC1)C)C(OC1OC(C2OOC3(OC(C(O)C(OC)C3)C)COC2C1)C)C
MOL005671	0.2850	0.7150	0.6302	Cortex Periplocae Radicis	periplocoside C	Not Available	FALSE	OC1(C2(C(C3C(C4(C(=CC3)CC(OC3OC(C=C(OC)C3=O)C)CC4)C)CC2)CC1)C)C(OC1OC(C2OOC3(OC(C(OC4OC(C(O)C(OC)C4)C)C(OC)C3)C)COC2C1)C)C
MOL005672	0.5001	0.4999	0.6266	Cortex Periplocae Radicis	periplocoside D	Not Available	FALSE	OC1(C2(C(C3C(C4(C(=CC3)CC(OC3OC(C=C(OC)C3=O)C)CC4)C)CC2)CC1)C)C(OC1OC(C2OOC3(OC(C(OC4OC(C(OC5OC(C(OC6OC(C(OC7OC(C(O)C(OC)C7O)C)C(OC)C6)C)C(OC)C5)C)C(OC)C4)C)C(OC)C3)C)COC2C1)C)C
MOL005673	0.2800	0.7200	0.6134	Cortex Periplocae Radicis	periplocoside D_qt	Not Available	FALSE	OC1(C2(C(C3C(C4(C(=CC3)CC(OC3OC(C=C(OC)C3=O)C)CC4)C)CC2)CC1)C)C(OC1OC(C2OOC3(OC(C(O)C(OC)C3)C)COC2C1)C)C
MOL005675	0.2404	0.7596	0.6248	Cortex Periplocae Radicis	periplocoside E_qt	Not Available	FALSE	OC1CC2=CCC3C4C(C(CC4)(C(C)OC4CC5C(C(O4)C)OOC4(CO5)OC(C(C(C4)OC)O)C)O)(CCC3C2(C)CC1)C
MOL005676	0.4187	0.5813	0.6354	Cortex Periplocae Radicis	periplocoside F	Not Available	FALSE	OC1(C2(C(C3C(C4(C(=CC3)CC(O)CC4)C)CC2)CC1)C)C(OC1OC(C2OOC3(OC(C(OC4OC(C(OC5OC(C(OC6OC(C(OC7OC(C(O)C(OC)C7O)C)C(OC)C6)C)C(OC)C5)C)C(OC)C4)C)C(OC)C3)C)COC2C1)C)C
MOL005677	0.2404	0.7596	0.6248	Cortex Periplocae Radicis	periplocoside F_qt	Not Available	FALSE	OC1(C2(C(C3C(C4(C(=CC3)CC(O)CC4)C)CC2)CC1)C)C(OC1OC(C2OOC3(OC(C(O)C(OC)C3)C)COC2C1)C)C
MOL005678	0.4371	0.5629	0.7003	Cortex Periplocae Radicis	periplocoside J	Not Available	FALSE	OC1(C2(C(C3C(C4(C(=CC3)CC(O)CC4)C)CC2)CC1)C)C(OC1OC(C2OOC3(OC(C(OC4OC(C(OC5OC(C(OC6OC(C(OC7OC(C(O)C(OC)C7O)C)C(OC)C6)C)C(O)C5)C)C(O)C4)C)C(OC)C3)C)COC2C1)C)C
MOL005679	0.2404	0.7596	0.6248	Cortex Periplocae Radicis	periplocoside J_qt	Not Available	FALSE	OC1(C2(C(C3C(C4(C(=CC3)CC(O)CC4)C)CC2)CC1)C)C(OC1OC(C2OOC3(OC(C(O)C(OC)C3)C)COC2C1)C)C
MOL005680	0.4839	0.5161	0.6811	Cortex Periplocae Radicis	periplocoside K	Not Available	FALSE	OC1(C2(C(C3C(C4(C(=CC3)CC(OC3OC(C=C(OC)C3=O)C)CC4)C)CC2)CC1)C)C(OC1OC(C2OOC3(OC(C(OC4OC(C(OC5OC(C(OC6OC(C(OC7OC(C(O)C(OC)C7O)C)C(OC)C6)C)C(O)C5)C)C(O)C4)C)C(OC)C3)C)COC2C1)C)C

MOL005681	0.2800	0.7200	0.6134	Cortex Periplocae Radicis	periplocoside K_qt	Not Available	FALSE	OC1(C2(C(C3C(C4(C(=CC3)CC(OC3OC(C=C(OC)C3=O)C)CC4)C)CC2)CC1)C)C(OC1OC(C2OOC3(OC(C(O)C(OC)C3)C)COC2C1)C)C
MOL005683	0.4481	0.5519	0.8424	Cortex Periplocae Radicis	delta 5-Pregnenetriol	150863	FALSE	OC1CCC2(C3C(C4C(C(CC4)(O)C(O)C)(CC3)C)CC=C2C1)C
MOL005685	0.1716	0.8284	0.6227	Cortex Periplocae Radicis	periplocoside O	Not Available	FALSE	OC1(C2(C(C3C(C4(C(=CC3)CC(OC3OC(C=C(OC)C3=O)C)CC4)C)CC2)CC1)C)C(OC1OC(C(O)C(OC)C1O)C)C
MOL005687	0.5221	0.4779	0.7829	Cortex Periplocae Radicis	periplocin	Not Available	FALSE	OC12C(C(CC2)C2=CC(=O)OC2)(CCC2C1CCC1(O)C2(CCC(OC2OC(C(O)C(OC)C2O)COC2C(OC(O)CC2O)C)C1)C)C
MOL005688	0.5241	0.4759	0.7524	Cortex Periplocae Radicis	periplocin_qt	Not Available	FALSE	OC12C(C(CC2)C2=CC(=O)OC2)(CCC2C1CCC1(O)C2(CCC(O)C1)C)C
MOL005689	0.2212	0.7788	0.6445	Cortex Periplocae Radicis	periplocymarin	Not Available	FALSE	OC12C3C(C4(C(O)(CC3)CC(OC3OC(C(O)C(OC)C3)C)CC4)C)CCC1(C(CC2)C1=CC(=O)OC1)C
MOL005690	0.5241	0.4759	0.7524	Cortex Periplocae Radicis	periplocymarin_qt	Not Available	FALSE	OC12C3C(C4(C(O)(CC3)CC(O)CC4)C)CCC1(C(CC2)C1=CC(=O)OC1)C
MOL005691	0.9150	0.0850	0.8239	Perilla Frutescens	Perilloside A	3086657	FALSE	O1C(C(O)C(O)C(O)C1OCC1=CCC(CC1)C(=C)C)CO
MOL005691	0.9150	0.0850	0.8239	Cortex Periplocae Radicis	Perilloside A	3086657	FALSE	O1C(C(O)C(O)C(O)C1OCC1=CCC(CC1)C(=C)C)CO
MOL005692	0.4471	0.5529	0.8433	Cortex Periplocae Radicis	NERIDIENONE A	100630	FALSE	OC1C2(C(C3C(C4(C(=CC(=O)CC4)C=C3)C)C1)CC=C2C(=O)C)C
MOL005693	0.3438	0.6562	0.8077	Cortex Periplocae Radicis	xysmalogenin	Not Available	FALSE	OC12C(C(CC2)C2=CC(=O)OC2)(CCC2C1CC=C1C2(CCC(O)C1)C)C
MOL005694	0.8419	0.1581	0.8262	Semen Pruni	Multiflorin A	5319939	FALSE	O(C1C(O)C(O)C(OC1C)Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)C1OC(C(O)C(O)C1O)COC(=O)C
MOL005694	0.8419	0.1581	0.8262	Gossampiniflos	Multiflorin A	5319939	FALSE	O(C1C(O)C(O)C(OC1C)Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)C1OC(C(O)C(O)C1O)COC(=O)C
MOL005695	0.8632	0.1368	0.8377	Semen Pruni	Multiflorin	5319938	FALSE	O(C1C(O)C(O)C(OC1C)Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)C1OC(C(O)C(O)C1O)CO
MOL005696	0.8694	0.1306	0.8098	Semen Pruni	Multinoside A	5319943	FALSE	O(C1C(O)C(O)C(OC1C)Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1)C1OC(C(O)C(O)C1O)CO
MOL005697	0.5765	0.4235	0.7881	Semen Lini	Cyclolinopeptide G	Not Available	FALSE	S(=O)(CCC1NC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C2N(CCC2)C1=O)Cc1ccccc1)Cc1ccccc1)Cc1c2c([nH]c1)cccc2)C(CC)C)CCS(=O)(=O)CC(C)C)C
MOL005698	0.5435	0.4565	0.7800	Semen Lini	Cyclolinopeptide H	Not Available	FALSE	S(CCC1NC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C2N(CCC2)C1=O)Cc1ccccc1)Cc1ccccc1)Cc1c2c([nH]c1)cccc2)C(CC)C)CCS(=O)(=O)CC(C)C
MOL005699	0.5774	0.4226	0.7773	Semen Lini	Cyclolinopeptide I	Not Available	FALSE	S(=O)(CCC1NC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C2N(CCC2)C1=O)Cc1ccccc1)Cc1ccccc1)Cc1c2c([nH]c1)cccc2)C(C)C)CCS(=O)(=O)CC(C)C
MOL005700	0.3559	0.6441	0.7213	Semen Lini	Cyclomahanimbine	Not Available	FALSE	c1ccc2c(c1)c1c([nH]2)c2c(c(c1)C)OC1(CC2C(CC1)C(=C)C)C

MOL005701	0.3670	0.6330	0.6556	Semen Lini	Linarin isovalerate	5319030	FALSE	C1(C(C(C(OC1C)OCC1CC(C(C(O1)Oc1cc2c(c(c1)O)c(=O)cc(o2)c1ccc(cc1)OC)O)O)O)OC(=O)CC(C)C)O
MOL005702	0.5923	0.4077	0.7873	Semen Lini	cyclolinopeptide F	Not Available	FALSE	S(=O)(CCC1NC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C2N(CCC2)C1=O)Cc1ccccc1)Cc1ccccc1)Cc1c2c([nH]c1)cccc2)C(C)C)CCS(=O)C)CC(C)C)C
MOL005703	0.4312	0.5688	0.6097	Semen Lini	Tetraprenol	5281365	FALSE	C(=C\CC/C(=C/CO)/C)(/CC/C=C(/CCC=C(C)C)\C)\C
MOL005706	0.9361	0.0639	0.9308	Semen Lini	Linamarin	11128	FALSE	C1(OC(C(C(C1O)O)O)CO)OC(C#N)(C)C
MOL005706	0.9361	0.0639	0.9308	Eriobotryae Folium	Linamarin	11128	FALSE	C1(OC(C(C(C1O)O)O)CO)OC(C#N)(C)C
MOL005707	0.9154	0.0846	0.8865	Eriobotryae Folium	CNH	6406	FALSE	OC(C#N)(C)C
MOL005707	0.9154	0.0846	0.8865	Semen Lini	CNH	6406	FALSE	OC(C#N)(C)C
MOL005708	0.9148	0.0852	0.8345	Semen Lini	Linustatin	119301	FALSE	C1(OC(C(C(C1O)O)O)OC(C#N)(C)C)COC1OC(C(C(C1O)O)O)CO
MOL005709	0.8846	0.1154	0.7956	Semen Lini	orientin-7-rhamnoside	Not Available	FALSE	o1c2c(C3OC(C(O)C(O)C3O)CO)c(OC3OC(C(C(C3O)O)O)C)cc(O)c2c(=O)cc1c1cc(O)c(O)cc1
MOL005710	0.9044	0.0956	0.8197	Semen Lini	orientin-7-rhamnoside_qt	Not Available	FALSE	o1c2c(C3OC(C(O)C(O)C3O)CO)c(O)cc(O)c2c(=O)cc1c1cc(O)c(O)cc1
MOL005711	0.8947	0.1053	0.8692	Folium Artemisiae Argyi	vinyl 2,2-dimethyl-3-phenyl-propionate	71438330	FALSE	c1(ccccc1)CC(C(=O)OC=C)(C)C
MOL005712	0.9579	0.0421	0.9565	Perillae Fructus	3-methyl-6-(1-methylethylidene)-cyclohexene	71385764	FALSE	C1=CC(CCC1=C(C)C)C
MOL005712	0.9579	0.0421	0.9565	Folium Artemisiae Argyi	3-methyl-6-(1-methylethylidene)-cyclohexene	71385764	FALSE	C1=CC(CCC1=C(C)C)C
MOL005713	0.9366	0.0634	0.9363	Folium Artemisiae Argyi	2,6,6-Trimethylcyclohexa-2,4-dienone	83528	FALSE	C1(C=CC=C(C1=O)C)(C)C
MOL005714	0.9299	0.0701	0.9722	Folium Artemisiae Argyi	cirsilneol	53754059	FALSE	O1CCON1CCC
MOL005715	0.8975	0.1025	0.6767	Folium Artemisiae Argyi	3,4-DIMETHYLBIPHENYL	20492	FALSE	c1(c2ccccc2)cc(c(cc1)C)C

MOL005717	0.9517	0.0483	0.7730	Folium Artemisiae Argyi	6,6-dimethyl-3-methylene bicyclo[3.1.1]-heptane	12180420	FALSE	C12CC(=C)CC(C1(C)C)C2
MOL005718	0.9241	0.0759	0.7246	Folium Artemisiae Argyi	6-Methoxy-7,8-methylenedioxy coumarin	5319474	FALSE	c1(=O)ccc2c(o1)c1c(c(c2)OC)OCO1
MOL005720	0.3223	0.6777	0.6966	Folium Artemisiae Argyi	24-methylenecycloartanone	Not Available	FALSE	C1C(=O)C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C(CC2)C(C)CCC(=C)C(C)C)C)C)C3)(C)C
MOL005721	0.3504	0.6496	0.7133	Folium Artemisiae Argyi	cycloart-25-en-3β,24-diol	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C4(C)CCC(C(CCC(C(=C)C)O)C)C4(C)CCC21C3)O
MOL005722	0.9172	0.0828	0.9733	Folium Artemisiae Argyi	ZINC00395662	6950811	FALSE	C1(CCCCO1)CO
MOL005723	0.9314	0.0686	0.7956	Euphorbiae Helioscopiae Herba	Phytodolor	5318565	FALSE	c12c(cc(c(c1OC)O)OC)ccc(=O)o2
MOL005723	0.9314	0.0686	0.7956	Folium Artemisiae Argyi	Phytodolor	5318565	FALSE	c12c(cc(c(c1OC)O)OC)ccc(=O)o2
MOL005723	0.9314	0.0686	0.7956	Apocyniveneti Folium	Phytodolor	5318565	FALSE	c12c(cc(c(c1OC)O)OC)ccc(=O)o2
MOL005723	0.9314	0.0686	0.7956	Lunulatae Herba	Phytodolor	5318565	FALSE	c12c(cc(c(c1OC)O)OC)ccc(=O)o2
MOL005723	0.9314	0.0686	0.7956	Morindae Officinalis Radix	Phytodolor	5318565	FALSE	c12c(cc(c(c1OC)O)OC)ccc(=O)o2
MOL005723	0.9314	0.0686	0.7956	Herba Sarcandrae	Phytodolor	5318565	FALSE	c12c(cc(c(c1OC)O)OC)ccc(=O)o2
MOL005723	0.9314	0.0686	0.7956	Artemisia Annua L.	Phytodolor	5318565	FALSE	c12c(cc(c(c1OC)O)OC)ccc(=O)o2
MOL005724	0.9082	0.0918	0.9606	Folium Artemisiae Argyi	Amylene	10553	FALSE	C(=CC)(C)C
MOL005725	0.9609	0.0391	0.9566	Folium Artemisiae Argyi	(-)-isoperitenone	439733	FALSE	C1(=O)C(CCC(=C1)C)C(=C)C
MOL005726	0.9322	0.0678	0.9349	Folium Artemisiae Argyi	Artemisia ketone	68346	FALSE	C(C(=O)C=C(C)C)(C=C)(C)C
MOL005726	0.9322	0.0678	0.9349	Artemisia Annua L.	Artemisia ketone	68346	FALSE	C(C(=O)C=C(C)C)(C=C)(C)C
MOL005727	0.9166	0.0834	0.9685	Santalum Album L.	MIPK	11251	FALSE	C(C(=O)C)(C)C
MOL005727	0.9166	0.0834	0.9685	Panacis Japonici Rhizoma	MIPK	11251	FALSE	C(C(=O)C)(C)C
MOL005727	0.9166	0.0834	0.9685	Pogostemon Cablin (Blanco) Benth.	MIPK	11251	FALSE	C(C(=O)C)(C)C
MOL005727	0.9166	0.0834	0.9685	Folium Artemisiae Argyi	MIPK	11251	FALSE	C(C(=O)C)(C)C
MOL005728	0.7871	0.2129	0.9303	Folium Artemisiae Argyi	Ayanin	5280682	TRUE	c1(c(OC)c(=O)c2c(O)cc(OC)cc2o1)c1cc(O)c(OC)cc1
MOL005728	0.7871	0.2129	0.9303	Viticis Fructus	Ayanin	5280682	TRUE	c1(c(OC)c(=O)c2c(O)cc(OC)cc2o1)c1cc(O)c(OC)cc1
MOL005730	0.9343	0.0657	0.9380	Folium Artemisiae Argyi	3-NONANONE	61235	FALSE	C(=O)(CCCCCC)CC
MOL005731	0.8792	0.1208	0.9591	Folium Artemisiae Argyi	Methylenecyclopentane	73714	FALSE	C1(=C)CCCC1
MOL005732	0.7737	0.2263	0.6778	Campsis Flos	Pentadecanal	17697	FALSE	O=CCCCCCCCCCCCCCC
MOL005732	0.7737	0.2263	0.6778	Hippophae Fructus	Pentadecanal	17697	FALSE	O=CCCCCCCCCCCCCCC

MOL005732	0.7737	0.2263	0.6778	Lysimachiae Foenigraeci Herba	Pentadecanal	17697	FALSE	O=CCCCCCCCCCCCCCC
MOL005732	0.7737	0.2263	0.6778	Folium Artemisiae Argyi	Pentadecanal	17697	FALSE	O=CCCCCCCCCCCCCCC
MOL005733	0.8976	0.1024	0.8717	Folium Artemisiae Argyi	(2S)-6-methyl-2-[(2S,5R)-5-methyl-5-vinyl-2-tetrahydrofuranyl]hept-5-en-3-one	88556	FALSE	CC(C(=O)CC=C(C)C)C1OC(CC1)(C=C)C
MOL005734	0.7812	0.2188	0.9075	Chrysanthemi Flos	eupatilin	5273755	FALSE	c1(c(cc2c(c1O)c(=O)cc(o2)c1ccc(c(c1)OC)OC)O)OC
MOL005734	0.7812	0.2188	0.9075	Schizonepetae Spica	eupatilin	5273755	FALSE	c1(c(cc2c(c1O)c(=O)cc(o2)c1ccc(c(c1)OC)OC)O)OC
MOL005734	0.7812	0.2188	0.9075	Folium Artemisiae Argyi	eupatilin	5273755	FALSE	c1(c(cc2c(c1O)c(=O)cc(o2)c1ccc(c(c1)OC)OC)O)OC
MOL005735	0.1603	0.8397	0.7003	Folium Artemisiae Argyi	dammaradienyl acetate	Not Available	FALSE	C(=O)(C)OC1=CCC2(C(=CCC3C4(C)CCC(C(CCCC(C)C)C)C4CCC23)C1(C)C)C
MOL005736	0.8254	0.1746	0.6165	Radix Cirsii Japonici	cyperene	Not Available	FALSE	C123C(C(CC2=C(CC3)C)CCC1C)(C)C
MOL005736	0.8254	0.1746	0.6165	Folium Artemisiae Argyi	cyperene	Not Available	FALSE	C123C(C(CC2=C(CC3)C)CCC1C)(C)C
MOL005736	0.8254	0.1746	0.6165	Broussonetiae Fructus	cyperene	Not Available	FALSE	C123C(C(CC2=C(CC3)C)CCC1C)(C)C
MOL005737	0.8672	0.1328	0.7325	Folium Artemisiae Argyi	vulgarole	Not Available	FALSE	O=C1C2C3(C(C2C(CCC3)(C)C)C(=C1)C)C
MOL005738	0.9487	0.0513	0.9312	Folium Artemisiae Argyi	2-benzylidenesuccinic acid	820629	FALSE	C(=O)(/C(=C/c1ccccc1)/CC(=O)O)O
MOL005739	0.8976	0.1024	0.8722	Ligustici Rhizoma Et Radix	Neryl butyrate	5352162	FALSE	C(CC=C(C)C)/C(=C\COC(=O)CCC)/C
MOL005739	0.8976	0.1024	0.8722	Folium Artemisiae Argyi	Neryl butyrate	5352162	FALSE	C(CC=C(C)C)/C(=C\COC(=O)CCC)/C
MOL005740	0.9218	0.0782	0.8966	Folium Artemisiae Argyi	artemisia alcohol	Not Available	FALSE	O(C(C(C)(C)C=C)C=C(C)C)C(=O)C
MOL005741	0.2872	0.7128	0.7151	Folium Artemisiae Argyi	cycloartenol acetate	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C4(C)CCC(C(CCC=C(C)C)C)C4(C)CCC21C3)OC(=O)C
MOL005742	0.7089	0.2911	0.7733	Folium Artemisiae Argyi	Chinova acid	120678	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3C)C)C(=O)O)C(=O)O)(CC2)C)(CC1)C)(C)C
MOL005743	0.8728	0.1272	0.7695	Folium Artemisiae Argyi	Proximadiol	165258	FALSE	OC1(C2C(CCC(C2)C(O)(C)C)(CCC1)C)C
MOL005744	0.9607	0.0393	0.8680	Folium Artemisiae Argyi	carvenone	Not Available	FALSE	O1C2(C1C(=O)C(CC2)C)C(C)C
MOL005745	0.3825	0.6175	0.7070	Folium Artemisiae Argyi	fernenol	Not Available	FALSE	OC1C(C2C(C3=CCC4(C(C3CC2)(CCC2(C4CCC2C(C)C)C)C)C)(CC1)C)(C)C
MOL005746	0.3938	0.6062	0.6582	Folium Artemisiae Argyi	fernenone	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=CCC3(C(C1CC2)(C)CCC1(C3CCC1(C)C)C)C)C)(C)C
MOL005747	0.9305	0.0695	0.9445	Folium Artemisiae Argyi	[(Z)-hex-1-enyl] acetate	10820631	FALSE	C(=C\CCCC)\OC(=O)C
MOL005748	0.3076	0.6924	0.7425	Folium Artemisiae Argyi	17020-04-1	177801	FALSE	O(C1C(C2C(C3C(=CC2)C2(C(C4C(CC2)(CCC(C4C)C)C)(CC3)C)C)(CC1)C)(C)C)C(=O)C

MOL005748	0.3076	0.6924	0.7425	Cichorii Radix	17020-04-1	177801	FALSE	O(C1C(C2C(C3C(=CC2)C2(C(C4C(CC2)(CCC(C4C)C)C)(CC3)C)C)(CC1)C)(C)C)C(=O)C
MOL005748	0.3076	0.6924	0.7425	Ardisiae Japonicae Herba	17020-04-1	177801	FALSE	O(C1C(C2C(C3C(=CC2)C2(C(C4C(CC2)(CCC(C4C)C)C)(CC3)C)C)(CC1)C)(C)C)C(=O)C
MOL005749	0.9588	0.0412	0.9571	Ardisiae Japonicae Herba	isopulegone	44163790	FALSE	C1(=O)CC(C)CCC1C(=C)C
MOL005749	0.9588	0.0412	0.9571	Folium Artemisiae Argyi	isopulegone	44163790	FALSE	C1(=O)CC(C)CCC1C(=C)C
MOL005750	0.9310	0.0690	0.8996	Folium Artemisiae Argyi	isoamylcyclohexane	521487	FALSE	C1(CCCCC1)CCC(C)C
MOL005751	0.3588	0.6412	0.7549	Maydis Seigma	(6aS,6aS,6bR,8aR,12aR,14aR,14bS)-4,4,6a,6b,8a,11,11,14a-octamethyl-2,6,6a,7,8,9,10,12,12a,13,14,14b-dodecahydro-1H-picen-3-one	10071029	FALSE	O=C1C(C2=CCC3C4(C(C5C(CC4)(CCC(C5)(C)C)C)(CCC3(C2CC1)C)C)C)(C)C
MOL005751	0.3588	0.6412	0.7549	Folium Artemisiae Argyi	(6aS,6aS,6bR,8aR,12aR,14aR,14bS)-4,4,6a,6b,8a,11,11,14a-octamethyl-2,6,6a,7,8,9,10,12,12a,13,14,14b-dodecahydro-1H-picen-3-one	10071029	FALSE	O=C1C(C2=CCC3C4(C(C5C(CC4)(CCC(C5)(C)C)C)(CCC3(C2CC1)C)C)C)(C)C
MOL005752	0.9527	0.0473	0.9767	Perillae Fructus	[(4R)-4-isopropenyl-1-cyclohexenyl]methanol	11788398	FALSE	C1(CCC(=CC1)CO)C(=C)C
MOL005752	0.9527	0.0473	0.9767	Folium Artemisiae Argyi	[(4R)-4-isopropenyl-1-cyclohexenyl]methanol	11788398	FALSE	C1(CCC(=CC1)CO)C(=C)C

MOL005752	0.9527	0.0473	0.9767	Campsis Flos	[(4R)-4-isopropenyl-1-cyclohexenyl] methanol	11788398	FALSE	C1(CCC(=CC1)CO)C(=C)C
MOL005755	0.4456	0.5544	0.6494	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	1-(4-hydroxybenzyl)-4-methoxy-9,10-dihydrophenanthrene-2,7-diol	11163864	FALSE	c1c(ccc(c1)O)Cc1c2c(c3ccc(cc3CC2)O)c(cc1O)OC
MOL005756	0.5670	0.4330	0.7694	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	2,3,4,7-tetramethoxyphenanthrene	11437978	FALSE	c1cc2c(cc1OC)ccc1c2c(c(c(c1)OC)OC)OC
MOL005757	0.5974	0.4026	0.8232	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	2,4,7-trimethoxy-9,10-dihydrophenanthrene	15693459	FALSE	c1cc2c(cc1OC)CCc1c2c(cc(c1)OC)OC
MOL005758	0.6370	0.3630	0.7389	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	2,4,7-trimethoxyphenanthrene	15693458	FALSE	c1c(cc(c2c3ccc(cc3ccc12)OC)OC)OC
MOL005759	0.9001	0.0999	0.6857	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	2,7-dihydroxy-4-methoxyphenanthrene-2,7-O-diglucoside	Not Available	FALSE	c1c(cc(c2c3ccc(cc3ccc12)OC1C(O)C(O)C(O)C(O1)CO)O)OC1C(O)C(O)C(O)C(O1)CO
MOL005760	0.8488	0.1512	0.6604	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	2,7-dihydroxy-4-methoxy-	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)c1cc2c(c(c1)OC)c1ccc(cc1cc2)O
MOL005761	0.4721	0.5279	0.6234	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	3-(p-hydroxybenzyl)-4-methoxy-9,10-dihydrophenanthrene	14630662	FALSE	c1c(ccc(c1)O)Cc1c(c2c3ccc(cc3CCc2cc1O)O)OC
MOL005762	0.8295	0.1705	0.9215	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	1,3-dimethoxy-5-[2-(3-methoxyphenyl)ethyl]benzene	15693460	FALSE	c1ccc(cc1OC)CCc1cc(cc(c1)OC)OC

MOL005764	0.8341	0.1659	0.8779	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	1,3-dimethoxy-5-(2-phenylethyl)benzene	10538117	FALSE	c1(cc(cc(c1)CCc1ccccc1)OC)OC
MOL005766	0.6161	0.3839	0.7257	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	3,7-dihydroxy-2,4-dimethoxyphenanthrene-3-O-glucoside	Not Available	FALSE	c1cc2c(cc1O)ccc1c2c(c(c(c1)OC)CC1CC(C(C(C1O)O)O)CO)OC
MOL005767	0.8854	0.1146	0.9243	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	3'-O-Methylbatatasin III	442711	FALSE	c1(cccc(c1)CCc1cc(cc(c1)OC)O)OC
MOL005768	0.4230	0.5770	0.7243	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	4,7-dihydroxy-1-p-hydroxybenzyl-2-methoxy-9,10-dihydrophenanthrene	44392570	FALSE	c1cc2c(cc1O)CCc1c2c(cc(c1Cc1ccc(cc1)O)OC)O
MOL005769	0.8479	0.1521	0.8418	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	7-methoxy-9,10-dihydrophenanthrene-2,5-diol	442702	FALSE	c1cc2c(cc1O)CCc1c2c(cc(c1)OC)O
MOL005770	0.6423	0.3577	0.6547	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	bletlol A	Not Available	FALSE	c1cc2c(cc1O)CCc1c2c(cc2c1C1C(CO2)C2C(=C(O1)C)C(C(C(C2)O)O)OC)OC
MOL005771	0.2936	0.7064	0.7477	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	bletlol B	Not Available	FALSE	c12c(C(C(CO1)c1cc(c(cc1)O)OC)OC(=O)C)c1c(c(c2)OC)c2ccc(cc2CC1)O
MOL005772	0.2811	0.7189	0.7395	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	bletlol C	Not Available	FALSE	c12c(C(C(CO1)c1cc(c(cc1)O)OC)OC(=O)C)cc1c3c(cc(cc3CCc1c2)O)OC
MOL005773	0.4964	0.5036	0.7630	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	blespirol	Not Available	FALSE	C12(CCc3cc(ccc13)O)c1c(OC2=O)cc(c2c3ccc(cc3ccc12)O)OC

MOL005774	0.4347	0.5653	0.7004	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	1-(2,7-dihydroxy-4-methoxy-9,10-dihydrophenanthren-1-yl)-4-methoxy-9,10-dihydrophenanthrene-2,7-diol	11317652	FALSE	c1(c(cc(c2c3ccc(cc3CCc12)O)OC)O)c1c(cc(c2c3ccc(cc3CCc12)O)OC)O
MOL005775	0.4533	0.5467	0.6962	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	Blestriarene B	442695	FALSE	c1(c(cc(c2c3ccc(cc3CCc12)O)OC)O)c1c(cc(c2c3ccc(cc3ccc12)O)OC)O
MOL005776	0.4692	0.5308	0.6951	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	1-(2,7-dihydroxy-4-methoxy-1-phenanthryl)-4-methoxyphenanthrene-2,7-diol	9982511	FALSE	c1(c(cc(c2c3ccc(cc3ccc12)O)OC)O)c1c(cc(c2c3ccc(cc3ccc12)O)OC)O
MOL005777	0.4603	0.5397	0.6882	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	blestrianol A	Not Available	FALSE	c1cc2c(cc1O)CCc1c2cc(c(c1c1c(c2c3ccc(cc3CCc2cc1O)O)OC)O)OC
MOL005778	0.5165	0.4835	0.6854	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	blestrianol C	14863077	FALSE	c1(c(cc(c2c3ccc(cc3ccc12)O)OC)O)c1c(cc2c(c1)c1c(cc(c(c1CC2)Cc1ccc(cc1)O)O)OC)O
MOL005779	0.2960	0.7040	0.6966	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	blestrin A	Not Available	FALSE	c1cc2c(c(c1O)Oc1cc3c(c(c1)OC)c1c(CC3)cc(cc1)O)CCc1c2c(cc(c1)O)OC
MOL005780	0.2916	0.7084	0.6915	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	blestrin B	14583572	FALSE	c1(c(cc(c2c3ccc(cc3CCc12)O)OC)O)Oc1cc2c(cc1)c1c(cc(cc1CC2)OC)O
MOL005781	0.3549	0.6451	0.6733	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	blestrin C	Not Available	FALSE	c1(c(cc(c2c3ccc(cc3ccc12)O)OC)O)Oc1cc2c(c(c1)OC)c1ccc(cc1CC2)O
MOL005782	0.3732	0.6268	0.6573	Bletilla Striata (Thunb.Ex A.Murray)Rchb.F.	blestrin D	Not Available	FALSE	c1(c(cc(c2c3ccc(cc3ccc12)O)OC)O)Oc1cc2c(cc1)c1ccc(c(c1CC2)OC)O
MOL005783	0.8765	0.1235	0.9114	A. Dahurica (Fisch.) Benth. Et Hook	Bisomer 2HEA	13165	FALSE	C(=O)(OCCO)C=C
MOL005785	0.9521	0.0479	0.7549	Notopterygii Rhizoma Et Radix	bergaptol	5280371	FALSE	c12c(c(c3c(c1)oc(=O)cc3)O)cco2
MOL005785	0.9521	0.0479	0.7549	A. Dahurica (Fisch.) Benth. Et Hook	bergaptol	5280371	FALSE	c12c(c(c3c(c1)oc(=O)cc3)O)cco2
MOL005786	0.8384	0.1616	0.7583	A. Dahurica (Fisch.) Benth. Et Hook	Byakangelicin	10211	FALSE	c12c(c3c(c(c1ccc(=O)o2)OC)cco3)OCC(C(C)(C)O)O
MOL005787	0.8822	0.1178	0.7110	A. Dahurica (Fisch.) Benth. Et Hook	CYCLODODECANE	9268	FALSE	C1CCCCCCCCCCC1

MOL005788	0.8874	0.1126	0.8831	A. Dahurica (Fisch.) Benth. Et Hook	Ethyl caprate	8048	FALSE	C(CCCCCCCC)C(=O)OCC
MOL005789	0.6941	0.3059	0.7360	A. Dahurica (Fisch.) Benth. Et Hook	neobyakangelicol	Not Available	FALSE	c12c(c(c3c(c1OCC(C(=C)C)O)occ3)OC)ccc(=O)o2
MOL005790	0.7717	0.2283	0.8320	A. Dahurica (Fisch.) Benth. Et Hook	5-[[(2S)-3,3-dimethyloxiran-2-yl]methoxy]-3,7-dihydropyrano[3,2-f]benzofuran-2-one	24721547	FALSE	c12c(cc3c(c2)CC(=O)O3)OCC=C1OCC1C(O1)(C)C
MOL005791	0.7891	0.2109	0.8077	A. Dahurica (Fisch.) Benth. Et Hook	oxypeucedanin	Not Available	FALSE	c12c(cc3c(c2)cco3)oc(=O)cc1OCC1C(O1)(C)C
MOL005792	0.7623	0.2377	0.7580	A. Dahurica (Fisch.) Benth. Et Hook	{5-[2'(R)-Hydroxy-3'-methyl-3'-butenyl-oxy]furocoumarin}	3009225	FALSE	c1c2c(c(c3c1occ3)OCC(C(=C)C)O)ccc(=O)o2
MOL005793	0.7550	0.2450	0.8045	A. Dahurica (Fisch.) Benth. Et Hook	9-[[(2R)-3,3-dimethyloxiran-2-yl]methoxy]furo[3,2-g]chromen-7-one	458010	FALSE	c1(=O)ccc2c(o1)c(c1c(c2)cco1)OCC1C(O1)(C)C
MOL005794	0.9648	0.0352	0.8073	A. Dahurica (Fisch.) Benth. Et Hook	sabinol	42626427	FALSE	C1(CC2(C(C)C)CC2C1=C)O
MOL005795	0.9115	0.0885	0.9224	Zanthoxyli Pericarpium	suberosin	68486	FALSE	c1(c(cc2c(c1)ccc(=O)o2)OC)CC=C(C)C
MOL005795	0.9115	0.0885	0.9224	A. Dahurica (Fisch.) Benth. Et Hook	suberosin	68486	FALSE	c1(c(cc2c(c1)ccc(=O)o2)OC)CC=C(C)C
MOL005797	0.8621	0.1379	0.8140	Coriandri Sativi Herba	TRIDECANAL	25311	FALSE	C(CCCCCC=O)CCCCCC
MOL005797	0.8621	0.1379	0.8140	Hippophae Fructus	TRIDECANAL	25311	FALSE	C(CCCCCC=O)CCCCCC
MOL005797	0.8621	0.1379	0.8140	Meliae Azedarach Fructus	TRIDECANAL	25311	FALSE	C(CCCCCC=O)CCCCCC
MOL005797	0.8621	0.1379	0.8140	Lysimachiae Foenigraeci Herba	TRIDECANAL	25311	FALSE	C(CCCCCC=O)CCCCCC
MOL005797	0.8621	0.1379	0.8140	A. Dahurica (Fisch.) Benth. Et Hook	TRIDECANAL	25311	FALSE	C(CCCCCC=O)CCCCCC

MOL005798	0.8776	0.1224	0.8482	A. Dahurica (Fisch.) Benth. Et Hook	Ethyl undecylate	12327	FALSE	C(CCCCCCCCC)C(=O)OCC
MOL005799	0.9321	0.0679	0.9608	A. Dahurica (Fisch.) Benth. Et Hook	ethyl but-2-enoate	429065	FALSE	C(=O)(/C=C/C)OCC
MOL005800	0.7655	0.2345	0.8012	A. Dahurica (Fisch.) Benth. Et Hook	Byakangelicol	3055167	FALSE	c12c(c(c3c(c1OCC1OC1(C)C)occ3)OC)ccc(=O)o2
MOL005801	0.6902	0.3098	0.8441	A. Dahurica (Fisch.) Benth. Et Hook	9-hydroxy-4-(3-methylbut-2-enoxy)furo[3,2-g]chromen-7-one	21826766	FALSE	c12c(c(c3c(c1OCC=C(C)C)ccc(=O)o3)O)occ2
MOL005802	0.4151	0.5849	0.6045	A. Dahurica (Fisch.) Benth. Et Hook	propyleneglycol monoleate	Not Available	FALSE	C(CC(=O)OCC(C)O)CCCCC/C=C\CCCCCCCC
MOL005803	0.9113	0.0887	0.8259	A. Dahurica (Fisch.) Benth. Et Hook	desmodimiine	Not Available	FALSE	O1C(C(C(c2n(CC1=O)c(cc2)C=O)O)C)C
MOL005806	0.8729	0.1271	0.7409	A. Dahurica (Fisch.) Benth. Et Hook	4-[(2S)-2,3-dihydroxy-3-methylbutoxy]furo[3,2-g]chromen-7-one	899657	FALSE	c12c(c(c3c(c1)oc(=O)cc3)OCC(O)C(C)(C)O)cco2
MOL005808	0.9235	0.0765	0.9239	A. Dahurica (Fisch.) Benth. Et Hook	[(3S)-octan-3-yl] acetate	11819488	FALSE	C(CCCCC)(OC(=O)C)CC
MOL005809	0.9296	0.0704	0.9472	A. Dahurica (Fisch.) Benth. Et Hook	(3E)-3,7-dimethylocta-3,6-dien-1-ol	6536347	FALSE	CC(=CC/C=C(/CCO)\C)C
MOL005812	0.8729	0.1271	0.9157	Aurantii Fructus	naringin	442428	FALSE	c12c(C(=O)CC(O1)c1ccc(cc1)O)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL005812	0.8729	0.1271	0.9157	licorice	naringin	442428	FALSE	c12c(C(=O)CC(O1)c1ccc(cc1)O)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL005812	0.8729	0.1271	0.9157	Citrus Reticulata	naringin	442428	FALSE	c12c(C(=O)CC(O1)c1ccc(cc1)O)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL005812	0.8729	0.1271	0.9157	Citrus Aurantium	naringin	442428	FALSE	c12c(C(=O)CC(O1)c1ccc(cc1)O)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL005812	0.8729	0.1271	0.9157	Citri Exocarpium Rubrum	naringin	442428	FALSE	c12c(C(=O)CC(O1)c1ccc(cc1)O)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL005812	0.8729	0.1271	0.9157	Canarii Fructus	naringin	442428	FALSE	c12c(C(=O)CC(O1)c1ccc(cc1)O)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL005812	0.8729	0.1271	0.9157	Citri Grandis Exocarpium	naringin	442428	FALSE	c12c(C(=O)CC(O1)c1ccc(cc1)O)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL005812	0.8729	0.1271	0.9157	Aurantii Fructus Immaturus	naringin	442428	FALSE	c12c(C(=O)CC(O1)c1ccc(cc1)O)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O

MOL005812	0.8729	0.1271	0.9157	Citri Reticulatae Pericarpium Viride	naringin	442428	FALSE	c12c(C(=O)CC(O1)c1ccc(cc1)O)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL005812	0.8729	0.1271	0.9157	Hedysari Radix	naringin	442428	FALSE	c12c(C(=O)CC(O1)c1ccc(cc1)O)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL005813	0.8480	0.1520	0.8200	Citrus Reticulata	Germacrene A	6440527	FALSE	C\1(=C\CC/C(=C\CC(CC1)C(=C)C)/C)/C
MOL005814	0.6089	0.3911	0.9058	Aurantii Fructus Immaturus	tangeretin	68077	TRUE	c12c(c(c(c(c1OC)OC)OC)OC)c(=O)cc(o2)c1ccc(cc1)OC
MOL005814	0.6089	0.3911	0.9058	Citri Grandis Exocarpium	tangeretin	68077	TRUE	c12c(c(c(c(c1OC)OC)OC)OC)c(=O)cc(o2)c1ccc(cc1)OC
MOL005814	0.6089	0.3911	0.9058	Citri Reticulatae Pericarpium Viride	tangeretin	68077	TRUE	c12c(c(c(c(c1OC)OC)OC)OC)c(=O)cc(o2)c1ccc(cc1)OC
MOL005814	0.6089	0.3911	0.9058	Citrus Reticulata	tangeretin	68077	TRUE	c12c(c(c(c(c1OC)OC)OC)OC)c(=O)cc(o2)c1ccc(cc1)OC
MOL005815	0.6529	0.3471	0.6859	Citrus Reticulata	Citromitin	Not Available	FALSE	c12c(c(c(c(c1OC)OC)OC)OC)OC(CC2=O)c1cc(c(cc1)OC)OC
MOL005816	0.8748	0.1252	0.8130	Citrus Reticulata	alpha-Sinensal	5281534	FALSE	C(=O)/C(=C/CC/C(=C/C/C=C(/C=C)\C)/C)/C
MOL005817	0.9504	0.0496	0.9664	Citrus Reticulata	2-(2-butynyl)-cyclohexanone	Not Available	FALSE	C1(=O)C(CCCC1)CC#CC
MOL005818	0.9218	0.0782	0.9175	Citrus Reticulata	2,5,5-trimethylhepta-1,6-diene	534952	FALSE	C=C(CCC(C=C)(C)C)C
MOL005820	0.9175	0.0825	0.9358	Citrus Reticulata	22410-74-8	5365825	FALSE	C(/C(=C/CCC=C(C)C)/C)O
MOL005821	0.9370	0.0630	0.9516	Panacis Japonici Rhizoma	(2S)-2-ethoxypentane	11804727	FALSE	C(CCC)(OCC)C
MOL005821	0.9370	0.0630	0.9516	Citrus Reticulata	(2S)-2-ethoxypentane	11804727	FALSE	C(CCC)(OCC)C
MOL005822	0.9045	0.0955	0.9013	Citrus Reticulata	3-decyn-2-ol	Not Available	FALSE	CC(C#CCCCCCC)O
MOL005823	0.9300	0.0700	0.9695	Citrus Reticulata	Isoprenol	12988	FALSE	C(C(=C)C)CO
MOL005824	0.9525	0.0475	0.9649	Citrus Reticulata	4-ACETYLBENZOIC ACID	11470	FALSE	c1(C(=O)C)ccc(cc1)C(=O)O
MOL005825	0.9340	0.0660	0.9499	Citrus Reticulata	6-Hepten-1-ol	543123	FALSE	C(CCCO)CC=C
MOL005826	0.9190	0.0810	0.9275	Citrus Reticulata	cis-2,6-Dimethyl-2,6-octadiene	5352478	FALSE	C(=C\C)(\CCC=C(C)C)/C
MOL005827	0.9155	0.0845	0.9718	Citrus Reticulata	Eufin	7766	FALSE	C(=O)(OCC)OCC
MOL005828	0.6593	0.3407	0.8218	Aurantii Fructus Immaturus	nobiletin	72344	TRUE	c12c(c(c(c(c1OC)OC)OC)OC)oc(cc2=O)c1cc(c(cc1)OC)OC
MOL005828	0.6593	0.3407	0.8218	Citri Grandis Exocarpium	nobiletin	72344	TRUE	c12c(c(c(c(c1OC)OC)OC)OC)oc(cc2=O)c1cc(c(cc1)OC)OC
MOL005828	0.6593	0.3407	0.8218	Citrus Reticulata	nobiletin	72344	TRUE	c12c(c(c(c(c1OC)OC)OC)OC)oc(cc2=O)c1cc(c(cc1)OC)OC

MOL005828	0.6593	0.3407	0.8218	Aurantii Fructus	nobiletin	72344	TRUE	c12c(c(c(c(c1OC)OC)OC)OC)oc(cc2=O)c1cc(c(cc1)OC)OC
MOL005828	0.6593	0.3407	0.8218	Citri Reticulatae Pericarpium Viride	nobiletin	72344	TRUE	c12c(c(c(c(c1OC)OC)OC)OC)oc(cc2=O)c1cc(c(cc1)OC)OC
MOL005828	0.6593	0.3407	0.8218	Centipedae Herba	nobiletin	72344	TRUE	c12c(c(c(c(c1OC)OC)OC)OC)oc(cc2=O)c1cc(c(cc1)OC)OC
MOL005829	0.8708	0.1292	0.8373	Citrus Reticulata	Undecyl acetate	15605	FALSE	C(CCCCCCCCC)COC(=O)C
MOL005830	0.8601	0.1399	0.7575	Ampelopsis Japonica	(-)-Gallocatechin gallate	5276890	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)OC(=O)c1cc(c(c(c1)O)O)O)c1cc(c(c(c1)O)O)O
MOL005830	0.8601	0.1399	0.7575	Areca Catechu L.	(-)-Gallocatechin gallate	5276890	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)OC(=O)c1cc(c(c(c1)O)O)O)c1cc(c(c(c1)O)O)O
MOL005830	0.8601	0.1399	0.7575	Ilicis Cornutae Folium Immayuri	(-)-Gallocatechin gallate	5276890	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)OC(=O)c1cc(c(c(c1)O)O)O)c1cc(c(c(c1)O)O)O
MOL005831	0.4206	0.5794	0.6825	Areca Catechu L.	Arborinol methy ether	Not Available	FALSE	C1C(C(C2C(C1)(C1=CCC3(C(C1CC2)(CCC1(C3CCC1C(C)C)C)C)C)(C)C)C
MOL005832	0.4001	0.5999	0.6642	Areca Catechu L.	Arborinol	Not Available	FALSE	C1CC(C2C(C1)(C1=CCC3(C(C1CC2)(CCC1(C3CCC1C(C)C)C)C)C)(C)C
MOL005833	0.9232	0.0768	0.9699	Areca Catechu L.	Arecaine	6971195	FALSE	C1C(=CCCN1C)C(=O)O
MOL005833	0.9232	0.0768	0.9699	Arecae Semen	Arecaine	6971195	FALSE	C1C(=CCCN1C)C(=O)O
MOL005834	0.9394	0.0606	0.9511	Areca Catechu L.	Arecolidine	Not Available	FALSE	C1=C(C(=CN(C1)C)OC)OC
MOL005835	0.9221	0.0779	0.9766	Arecae Semen	Guvacine	40468028	FALSE	C1CNCC(=C1)C(=O)O
MOL005835	0.9221	0.0779	0.9766	Areca Catechu L.	Guvacine	40468028	FALSE	C1CNCC(=C1)C(=O)O
MOL005836	0.9082	0.0918	0.7804	Areca Catechu L.	catechin	Not Available	FALSE	c1c(cc2c(c1O)CC(C(C2)c1cc(c(cc1)O)O)O)O)O
MOL005837	0.9347	0.0653	0.9856	Areca Catechu L.	arecoline	Not Available	FALSE	C1CC=C(CN1)C(=O)COC
MOL005838	0.9206	0.0794	0.9733	Arecae Semen	isoguvacine	7059534	FALSE	C1(=CCNCC1)C(=O)O
MOL005838	0.9206	0.0794	0.9733	Areca Catechu L.	isoguvacine	7059534	FALSE	C1(=CCNCC1)C(=O)O
MOL005839	0.7560	0.2440	0.7510	Areca Catechu L.	procyanidin A1	Not Available	FALSE	O1C2(Oc3c(C(c4c1cc(cc4O)O)C2O)c1c(CC(C(O1)c1cc(c(cc1)O)O)O)c(c3)O)c1cc(c(cc1)O)O
MOL005840	0.7873	0.2127	0.7969	Radix Cirsii Japonici	PANA	7013	TRUE	c1(c2c(ccc1)cccc2)Nc1ccccc1
MOL005840	0.7873	0.2127	0.7969	Pogostemon Cablin (Blanco) Benth.	PANA	7013	TRUE	c1(c2c(ccc1)cccc2)Nc1ccccc1
MOL005840	0.7873	0.2127	0.7969	Maydis Seigma	PANA	7013	TRUE	c1(c2c(ccc1)cccc2)Nc1ccccc1
MOL005840	0.7873	0.2127	0.7969	Morindae Officinalis Radix	PANA	7013	TRUE	c1(c2c(ccc1)cccc2)Nc1ccccc1
MOL005842	0.7789	0.2211	0.9433	Radix Cirsii Japonici	Pectolinarigenin	5320438	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)OC)O)c1ccc(cc1)OC
MOL005842	0.7789	0.2211	0.9433	Schizonepetae Spica	Pectolinarigenin	5320438	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)OC)O)c1ccc(cc1)OC
MOL005842	0.7789	0.2211	0.9433	Trollius Chinensis	Pectolinarigenin	5320438	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)OC)O)c1ccc(cc1)OC

MOL005843	0.9310	0.0690	0.9380	Radix Cirsii Japonici	1-Hydroxycumene	12053	FALSE	c1(ccccc1)C(C)(C)O
MOL005843	0.9310	0.0690	0.9380	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	1-Hydroxycumene	12053	FALSE	c1(ccccc1)C(C)(C)O
MOL005844	0.9281	0.0719	0.9290	Radix Cirsii Japonici	2,3,4-TRIMETHYLHEXANE	59954430	FALSE	C(C(CC)C)(C(C)C)C
MOL005845	0.9264	0.0736	0.9232	Radix Cirsii Japonici	3-METHYLOCTANE	25021965	FALSE	C(CCCCC)(CC)C
MOL005846	0.7644	0.2356	0.7827	Radix Cirsii Japonici	pectolinarin	Not Available	FALSE	c1(cc(=O)c2c(c(c(cc2o1)OC1OC(C(C(C1O)O)O)CO C1OC(C(C(C1O)O)O)C)OC)O)c1ccc(cc1)OC
MOL005847	0.7611	0.2389	0.8274	Herba Clinopodii Polycephali.	clinopodiside A	Not Available	FALSE	C12(C(=C3C(C(C2)O)(CCC(C3)(C)C)CO)C=CC2C1(CCC1C2(CCC(C1(CO)C)OC1C(C(C(OC2C(C(C(O2)CO)O)O)O)C(O1)COC1C(C(C(C(O1)CO)O)O)O)O)O)C)C
MOL005848	0.4733	0.5267	0.7713	Herba Clinopodii Polycephali.	NSC 258312	99651	FALSE	C12(C(=C3C(C(C2)O)(CCC(C3)(C)C)CO)C=CC2C1(CCC1C2(CCC(O)C1(CO)C)C)C)C
MOL005849	0.9045	0.0955	0.9143	Citri Grandis Exocarpium	didymin	1149877	FALSE	c12c(OC(CC1=O)c1ccc(cc1)OC)cc(cc2O)O
MOL005849	0.9045	0.0955	0.9143	Aurantii Fructus Immaturus	didymin	1149877	FALSE	c12c(OC(CC1=O)c1ccc(cc1)OC)cc(cc2O)O
MOL005849	0.9045	0.0955	0.9143	Herba Clinopodii Polycephali.	didymin	1149877	FALSE	c12c(OC(CC1=O)c1ccc(cc1)OC)cc(cc2O)O
MOL005849	0.9045	0.0955	0.9143	Citri Exocarpium Rubrum	didymin	1149877	FALSE	c12c(OC(CC1=O)c1ccc(cc1)OC)cc(cc2O)O
MOL005850	0.9024	0.0976	0.9431	Fructus Carotae	SPM	1103	FALSE	C(CCNCCCN)CNCCCN
MOL005850	0.9024	0.0976	0.9431	Hordei Fructus Germinatus	SPM	1103	FALSE	C(CCNCCCN)CNCCCN
MOL005850	0.9024	0.0976	0.9431	Herba Clinopodii Polycephali.	SPM	1103	FALSE	C(CCNCCCN)CNCCCN
MOL005851	0.7148	0.2852	0.8371	Radix Sanguisorbae	1,2,6-tri-O-galloyl-β-D-glucose	Not Available	FALSE	C1(C2C(CCC1C)(CCC1(C2=CCC2C1(CCC1C2(CCC(=O)C1(C)C)C)C)C)C(=O)O)(C)O
MOL005852	0.8658	0.1342	0.6807	Radix Sanguisorbae	1,2,6-tri-O-galloyl-β-D-glucopyranoside	Not Available	FALSE	C1(OC(C(C(C1O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)CC(=O)c1cc(c(c(c1)O)O)O)COC(=O)c1cc(c(c(c1)O)O)O
MOL005854	0.9396	0.0604	0.8437	Radix Sanguisorbae	1-(2,4-dihydroxy-6-methoxyphenyl)ethanone	10965145	FALSE	c1c(c(c(cc1O)O)C(=O)C)OC
MOL005855	0.7404	0.2596	0.7552	Rhapontici Radix	Tormentic acid	73193	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C

MOL005855	0.7404	0.2596	0.7552	Rosae Laevigatae Fructus	Tormentic acid	73193	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C
MOL005855	0.7404	0.2596	0.7552	Fructus Ligustri Lucidi	Tormentic acid	73193	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C
MOL005855	0.7404	0.2596	0.7552	Rubi Fructus	Tormentic acid	73193	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C
MOL005855	0.7404	0.2596	0.7552	Potentillae Discoloris Herba	Tormentic acid	73193	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C
MOL005855	0.7404	0.2596	0.7552	Boehmeriae Rhizoma Et Radix	Tormentic acid	73193	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C
MOL005855	0.7404	0.2596	0.7552	Verbenae Herb	Tormentic acid	73193	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C
MOL005855	0.7404	0.2596	0.7552	Lithospermum Erythrorhizon	Tormentic acid	73193	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C
MOL005855	0.7404	0.2596	0.7552	Potentillae Chinensis Herba	Tormentic acid	73193	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C
MOL005855	0.7404	0.2596	0.7552	Campsis Flos	Tormentic acid	73193	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C
MOL005855	0.7404	0.2596	0.7552	Sargentodoxae Caulis	Tormentic acid	73193	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C
MOL005855	0.7404	0.2596	0.7552	Eriobotryae Folium	Tormentic acid	73193	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C
MOL005855	0.7404	0.2596	0.7552	Ardisiae Japonicae Herba	Tormentic acid	73193	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C
MOL005855	0.7404	0.2596	0.7552	Radix Sanguisorbae	Tormentic acid	73193	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C
MOL005856	0.7404	0.2596	0.7552	Radix Sanguisorbae	2α-hydroxypomolic acid	Not Available	FALSE	C1(C2C(CCC1C)(CCC1(C2=CCC2C1(CCC1C2(CC(C(C1(C)C)O)O)C)C)C(=O)O)(C)O
MOL005857	0.8557	0.1443	0.6613	Radix Sanguisorbae	3,3',4-tri-O-methylellagic acid	Not Available	FALSE	o1c2c3c4c(c1=O)C=C(C(C4OC(=O)c3cc(c2O)OC)OC)OC
MOL005858	0.8500	0.1500	0.6651	Radix Sanguisorbae	3,7,8-Tri-O-methylellagic acid	Not Available	FALSE	c12c3c4c(oc1=O)c(c(cc4c(=O)oc3c(c(c2)OC)OC)O)OC
MOL005859	0.6686	0.3314	0.7741	Radix Sanguisorbae	3,11-dioxo-19α-hydroxyurs-12-en-28-oic acid	Not Available	FALSE	C1(C2C(CCC1C)(CCC1(C2=CC(=O)C2C1(CCC1C2(CCC(=O)C1(C)C)C)C)C)C(=O)O)(O)C
MOL005860	0.7048	0.2952	0.7592	Radix Sanguisorbae	3-O-galloylprocyanidin B-3	Not Available	FALSE	c1(cc(c2c(c1)OC(C(C2c1c(cc(c2c1OC(C(C2)O)c1ccc(c(c1)O)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)c1cc(c(cc1)O)O)O)O

MOL005861	0.8592	0.1408	0.6808	Radix Sanguisorbae	3-oxo-19α-hydroxyurs-12-en-28-oic acid	Not Available	FALSE	c1(c(c(cc(c1)C(=O)OCC1OC(C(C(C1O)O)OC(=C)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O)O
MOL005862	0.9214	0.0786	0.7658	Radix Sanguisorbae	Methyl 4,6-di-O-galloyl-beta-D-glucopyranoside	11972411	FALSE	O(C1C(O)C(O)C(C(O1)COC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)C
MOL005863	0.9022	0.0978	0.7698	Radix Sanguisorbae	methyl 6- O-digalloyl-β-glucopyranoside	Not Available	FALSE	c1(c(c(cc(c1)C(=O)Oc1c(c(ccc1O)C(=O)OCC1OC(C(C(C1O)O)O)OC)O)O)O)O
MOL005864	0.9243	0.0757	0.9060	Radix Sanguisorbae	methyl-6-O-galloyl-β-D-glucopyranoside	Not Available	FALSE	c1(c(c(cc(c1)C(=O)OCC1OC(C(C(C1O)O)O)OC)O)O)O
MOL005866	0.9495	0.0505	0.7923	Hoveniae Dulcis Semen	G6657_SIGMA	9882981	FALSE	C1(c2cc(c(c(c2)O)O)O)Oc2c(CC1O)c(cc(c2)O)O
MOL005866	0.9495	0.0505	0.7923	Ampelopsis Japonica	G6657_SIGMA	9882981	FALSE	C1(c2cc(c(c(c2)O)O)O)Oc2c(CC1O)c(cc(c2)O)O
MOL005866	0.9495	0.0505	0.7923	Radix Sanguisorbae	G6657_SIGMA	9882981	FALSE	C1(c2cc(c(c(c2)O)O)O)Oc2c(CC1O)c(cc(c2)O)O
MOL005867	0.7414	0.2586	0.8659	Radix Sanguisorbae	sanguisorbigenin	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(=C(C)C4C3=CCC21)C)C)O
MOL005870	0.8131	0.1869	0.7561	Radix Sanguisorbae	sanguiin H-2	Not Available	FALSE	O1C(C2OC(=O)c3c(c4c(C(=O)OC(C2O)C1OC(=O)c1cc2Oc5c(Oc2c(O)c1)c(O)c(c(c5Oc1c(O)c(O)cc(c1)C(=O)O)C(=O)O)c1c(cc(O)c(O)c1O)C(=O)O)cc(O)c(O)c4O)c(O)c(O)c(O)c3)CO
MOL005871	0.4323	0.5677	0.7394	Radix Sanguisorbae	sanguiin H-6	Not Available	FALSE	O1C2C(OC(=O)c3c(c4c(C(=O)OC2)cc(O)c(O)c4O)c(O)c(O)c(O)c3Oc2cc(C(=O)OC3OC4C(OC(=O)c5c(c6c(C(=O)OC4)cc(O)c(O)c6O)c(O)c(O)c(O)c5)C4OC(=O)c5c(c6c(C(=O)OC34)cc(O)c(O)c6O)c(O)c(O)c(O)c5)cc(O)c2O)C2OC(=O)c3c(c4c(C(=O)OC2C1OC(=O)c1cc(O)c(O)c(O)c1)cc(O)c(O)c4O)c(O)c(O)c(O)c3
MOL005872	0.8822	0.1178	0.7688	Radix Sanguisorbae	sanguisorbic acid dilactone	Not Available	FALSE	c12c3c4c(oc1=O)c(c(c(c4c(=O)oc3c(c(c2O)O)O)O)Oc1cc(cc(c1O)O)C(=O)O)O)O
MOL005873	0.6672	0.3328	0.6862	Radix Sanguisorbae	sanguisorbin B	Not Available	FALSE	C1(C2C(CCC1C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1OCC(C(C1O)O)O)C)C)C)C(=O)O)C
MOL005874	0.7574	0.2426	0.9071	Radix Sanguisorbae	sanguisorbin B _qt	Not Available	FALSE	C1(C2C(CCC1C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C)C(=O)O)C

MOL005875	0.5474	0.4526	0.6892	Radix Sanguisorbae	sanguisorbin E	Not Available	FALSE	C1(C2C(CCC1C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1OCC(C(C1O)O)O)C)C)C)C(=O)OC1OC(C(C(C1O)OC(=O)C)O)CO)C
MOL005876	0.3848	0.6152	0.7164	Radix Sanguisorbae	sanguisorbin E_qt	Not Available	FALSE	C1(C2C(CCC1C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C)C(=O)OC1OC(C(C(C1O)OC(=O)C)O)CO)C
MOL005877	0.9065	0.0935	0.7710	Radix Sanguisorbae	gallic acid 3-O-β-D-(6'-O-galloyl)glucopyranoside	Not Available	FALSE	c1(c(c(cc(c1)C(=O)OCC1OC(C(C(C1O)O)O)O)Cc1cc(cc(c1O)O)C(=O)O)O)O
MOL005878	0.4806	0.5194	0.7517	Radix Sanguisorbae	omolic acid-28-O-β-D-glucopyranoside	Not Available	FALSE	C1(C2C(CCC1C)C(CC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C)C(=C)OC1OC(C(C(C1O)O)O)CO)(C)O
MOL005879	0.3472	0.6528	0.8093	Radix Sanguisorbae	omolic acid-28-O-β-D-glucopyranoside_qt	Not Available	FALSE	C1(C2C(CCC1C)C(CC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C)C(=C)O)(C)O
MOL005880	0.7293	0.2707	0.8330	Radix Sanguisorbae	sauvissimoside R1	Not Available	FALSE	C1(C2C(CCC1C)(CCC1(C2=CCC2C1(CCC1C2(CC(C(C1(C(=O)O)C)O)O)C)C)C)C(=O)OOC1OC(C(C(C1O)O)O)CO)(C)O
MOL005881	0.7212	0.2788	0.6931	Radix Sanguisorbae	sauvissimoside R1_qt	Not Available	FALSE	C1(C2C(CCC1C)(CCC1(C2=CCC2C1(CCC1C2(CC(C(C1(C(=O)O)C)O)O)C)C)C)C(=O)OO)(C)O
MOL005882	0.6407	0.3593	0.6898	Radix Sanguisorbae	gambiriin A-1	Not Available	FALSE	c1(cc(c(c(c1)O)CC(C(c1ccc(c(c1)O)O)c1c(cc(c2c1OC(C(C2)O)c1cc(c(cc1)O)O)O)O)O)O)O
MOL005886	0.9127	0.0873	0.9675	Pogostemon Cablin (Blanco) Benth.	Methyl butenone	13143	FALSE	C(=C)(C(=O)C)C
MOL005887	0.8672	0.1328	0.6178	Pogostemon Cablin (Blanco) Benth.	seychellene	Not Available	FALSE	C12(C3(C(C(CC1)C)CC(C3)C2=C)C)C
MOL005888	0.8952	0.1048	0.8687	Pogostemon Cablin (Blanco) Benth.	Ombuin	5320287	FALSE	c12c(c(=O)c(c(o1)c1cc(c(cc1)OC)O)O)c(cc(c2)OC)O
MOL005888	0.8952	0.1048	0.8687	Eucommiae Cortex	Ombuin	5320287	FALSE	c12c(c(=O)c(c(o1)c1cc(c(cc1)OC)O)O)c(cc(c2)OC)O
MOL005888	0.8952	0.1048	0.8687	Gynostemmae Pentaphylli Herba	Ombuin	5320287	FALSE	c12c(c(=O)c(c(o1)c1cc(c(cc1)OC)O)O)c(cc(c2)OC)O
MOL005889	0.9206	0.0794	0.9008	Artemisia Annua L.	Rhamnetin	5281691	FALSE	c12c(c(=O)c(c(o1)c1cc(c(cc1)O)O)O)c(cc(c2)OC)O
MOL005889	0.9206	0.0794	0.9008	Mume Fructus	Rhamnetin	5281691	FALSE	c12c(c(=O)c(c(o1)c1cc(c(cc1)O)O)O)c(cc(c2)OC)O
MOL005889	0.9206	0.0794	0.9008	Potentillae Chinensis Herba	Rhamnetin	5281691	FALSE	c12c(c(=O)c(c(o1)c1cc(c(cc1)O)O)O)c(cc(c2)OC)O
MOL005889	0.9206	0.0794	0.9008	Caryophylliflos	Rhamnetin	5281691	FALSE	c12c(c(=O)c(c(o1)c1cc(c(cc1)O)O)O)c(cc(c2)OC)O
MOL005889	0.9206	0.0794	0.9008	Catechu	Rhamnetin	5281691	FALSE	c12c(c(=O)c(c(o1)c1cc(c(cc1)O)O)O)c(cc(c2)OC)O
MOL005889	0.9206	0.0794	0.9008	Pogostemon Cablin (Blanco) Benth.	Rhamnetin	5281691	FALSE	c12c(c(=O)c(c(o1)c1cc(c(cc1)O)O)O)c(cc(c2)OC)O
MOL005889	0.9206	0.0794	0.9008	Rhizoma Fagopyri Cymosi	Rhamnetin	5281691	FALSE	c12c(c(=O)c(c(o1)c1cc(c(cc1)O)O)O)c(cc(c2)OC)O

MOL005890	0.4914	0.5086	0.7588	Pogostemon Cablin (Blanco) Benth.	pachypodol	Not Available	FALSE	c1c(cc2c(c1OC)C(=O)C(=C(C2)c1cc(c(cc1)O)OC)OC)OC
MOL005891	0.7346	0.2654	0.6135	Pogostemon Cablin (Blanco) Benth.	β-bulnesene	Not Available	FALSE	C12=C(CCC(=C(C)C)CC1(C(CC2)C)C)C
MOL005895	0.9027	0.0973	0.7922	Pogostemon Cablin (Blanco) Benth.	Tricyclo[4.3.1.12,5]undec-3-en-10-ol, 3-(1-methylethyl)-, (1R,2S,5S,6S,10R)-rel-	Not Available	FALSE	C12C3C(=CC(C(CCC1)C2O)C3)C(C)C
MOL005896	0.8899	0.1101	0.6353	Pogostemon Cablin (Blanco) Benth.	Cedren-13-ol, 8-	Not Available	FALSE	C1(C)CCC2C(CO)(C)C3CC12CC=C3C
MOL005897	0.9405	0.0595	0.8703	Pogostemon Cablin (Blanco) Benth.	Labroda	3362	FALSE	c1(c(cc(cc1O)O)O)C(=O)CC
MOL005899	0.8416	0.1584	0.6557	Pogostemon Cablin (Blanco) Benth.	53111-25-4	6428535	FALSE	C12C(C(=CCCC1(C)C)C)CCC(=C2)C
MOL005899	0.8416	0.1584	0.6557	Ligustici Rhizoma Et Radix	53111-25-4	6428535	FALSE	C12C(C(=CCCC1(C)C)C)CCC(=C2)C
MOL005900	0.9403	0.0597	0.8766	Pogostemon Cablin (Blanco) Benth.	DHELWANGIN	54695756	FALSE	c1(c(=O)oc(cc1O)C)C(=O)CCC(C)C
MOL005901	0.8179	0.1821	0.7560	Pogostemon Cablin (Blanco) Benth.	6892-80-4	94334	FALSE	C12(C(=CCC(CC1)(O)C)C(CCC2)(C)C)C
MOL005902	0.9140	0.0860	0.6895	Pogostemon Cablin (Blanco) Benth.	2,2-Dimethylcyclopentylcyclohexane	Not Available	FALSE	C1(CCCCC1)C1C(CCC1)(C)C
MOL005903	0.8788	0.1212	0.7801	Pogostemon Cablin (Blanco) Benth.	WLN: RSR	8766	FALSE	c1(Sc2ccccc2)ccccc1
MOL005904	0.8704	0.1296	0.7113	Pogostemon Cablin (Blanco) Benth.	1,2,3,4,5,6-hexahydro-1,1,5,5-tetramethyl-7H-2,4a-methanonaphthalen-7-one	Not Available	FALSE	C1(C2CCC3(C(CC(=O)C=C13)(C)C)C2)(C)C

MOL005905	0.9317	0.0683	0.8315	Pogostemon Cablin (Blanco) Benth.	1-Oxaspiro[2.5] octan-4-one, 5,6,6-trimethyl-5-(3-oxo-1-butenyl)-, [3a,5b(Z)]-	Not Available	FALSE	O1CC21C(=O)C(C(CC2)(C)C)(/C=C/C(=O)C)C
MOL005906	0.9203	0.0797	0.9643	Pogostemon Cablin (Blanco) Benth.	(3S,4R)-2,5-dimethylhexane-3,4-diol	13072631	FALSE	CC(C(C(C(C)C)O)O)C
MOL005907	0.8866	0.1134	0.6325	Pogostemon Cablin (Blanco) Benth.	ZINC02090576	Not Available	FALSE	C123C4(C(CCC1(C)C)O)C2CC(C3)C4(C)C
MOL005908	0.8799	0.1201	0.9295	Pogostemon Cablin (Blanco) Benth.	3,5-Dihydroxy-4',7-dimethoxyflavone	5378823	FALSE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(cc1)OC)O)OC
MOL005908	0.8799	0.1201	0.9295	Tamaricis Cacumen	3,5-Dihydroxy-4',7-dimethoxyflavone	5378823	FALSE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(cc1)OC)O)OC
MOL005909	0.7778	0.2222	0.8898	Pogostemon Cablin (Blanco) Benth.	Pachypodol	5281677	FALSE	Oc1ccc(c2c(c(=O)c3c(cc(cc3o2)OC)O)OC)cc1OC
MOL005909	0.7778	0.2222	0.8898	Centipedae Herba	Pachypodol	5281677	FALSE	Oc1ccc(c2c(c(=O)c3c(cc(cc3o2)OC)O)OC)cc1OC
MOL005910	0.7869	0.2131	0.9589	Pogostemon Cablin (Blanco) Benth.	Retusin	5352005	TRUE	c1(cc(c2c(c1)oc(c(c2=O)OC)c1ccc(c(c1)OC)OC)O)OC
MOL005910	0.7869	0.2131	0.9589	Centipedae Herba	Retusin	5352005	TRUE	c1(cc(c2c(c1)oc(c(c2=O)OC)c1ccc(c(c1)OC)OC)O)OC
MOL005911	0.8335	0.1665	0.9218	Moslae Herba	5-Hydroxy-7,4'-dimethoxyflavanon	14057197	FALSE	c1(cc(c2c(c1)OC(CC2=O)c1ccc(cc1)OC)O)OC
MOL005911	0.8335	0.1665	0.9218	Pogostemon Cablin (Blanco) Benth.	5-Hydroxy-7,4'-dimethoxyflavanon	14057197	FALSE	c1(cc(c2c(c1)OC(CC2=O)c1ccc(cc1)OC)O)OC
MOL005912	0.7810	0.2190	0.8957	Pogostemon Cablin (Blanco) Benth.	5-Hydroxy-7·3‘,4'-trimethoxyflavanone	Not Available	FALSE	c1(cc(c2c(c1)OC(CC2=O)c1ccc(c(c1)OC)OC)O)OC
MOL005913	0.9403	0.0597	0.8766	Pogostemon Cablin (Blanco) Benth.	pogostone	Not Available	FALSE	C1=C(OC(=O)C(C1=O)C(=O)CCC(C)C)C

MOL005914	0.8701	0.1299	0.6067	Pogostemon Cablin (Blanco) Benth.	(β-maaliene)	Not Available	FALSE	C12C(CCC3(CCCC(=C13)C)C)C2(C)C
MOL005915	0.6499	0.3501	0.7277	Pogostemon Cablin (Blanco) Benth.	irisolidone-7-O-α-L-rhamnopyranoside	Not Available	FALSE	c1(c(c(c2c(c1)occ(c2=O)c1ccc(cc1)OC)O)OC)OC1OC(C(C(C1O)O)O)C
MOL005916	0.8090	0.1910	0.9065	Puerariae Flos	irisolidone	5281781	FALSE	c1(c(c(c2c(c1)occ(c2=O)c1ccc(cc1)OC)O)OC)O
MOL005916	0.8090	0.1910	0.9065	Iridis Tectori Rhizoma	irisolidone	5281781	FALSE	c1(c(c(c2c(c1)occ(c2=O)c1ccc(cc1)OC)O)OC)O
MOL005916	0.8090	0.1910	0.9065	Pogostemon Cablin (Blanco) Benth.	irisolidone	5281781	FALSE	c1(c(c(c2c(c1)occ(c2=O)c1ccc(cc1)OC)O)OC)O
MOL005917	0.8411	0.1589	0.7003	Pogostemon Cablin (Blanco) Benth.	Aciphyllene	Not Available	FALSE	C1(CCC(C2C(=C(CC2)C)C1)C)C(=C)C
MOL005918	0.7809	0.2191	0.7430	Pogostemon Cablin (Blanco) Benth.	phenanthrone	Not Available	FALSE	c1ccc2c(c1)C(=O)C1(c3c2ccc(c3)[N+](=O)O)CCCC1
MOL005919	0.7467	0.2533	0.7205	Pogostemon Cablin (Blanco) Benth.	campneoside	Not Available	FALSE	C1(C(C(C(C(O1)OCC(OC)c1ccc(c(c1)O)O)O)OC1OC(C(C(C1O)O)O)C)OC(=O)/C=C\c1cc(c(cc1)O)O)CO
MOL005920	0.8887	0.1113	0.7729	Pogostemon Cablin (Blanco) Benth.	quercetin 7-O-β-D-glucoside	Not Available	FALSE	C1(C(C(C(C(O1)Oc1cc(c2c(c1)CC(=C(C2=O)O)c1ccc(c(c1)O)O)O)O)O)O)CO
MOL005921	0.9240	0.0760	0.8597	Pogostemon Cablin (Blanco) Benth.	quercetin 7-O-β-D-glucoside	Not Available	FALSE	c1(cc(c2c(c1)CC(=C(C2=O)O)c1ccc(c(c1)O)O)O)O
MOL005924	0.5537	0.4463	0.8778	Pogostemon Cablin (Blanco) Benth.	3,23-dihydroxy-12-oleanen-28-oic acid	Not Available	FALSE	c1(cc(c2c(c1)CC(=C(C2=O)OC)c1ccc(c(c1)OC)OC)OC)O
MOL005925	0.7923	0.2077	0.7626	Pogostemon Cablin (Blanco) Benth.	orobanchoside	Not Available	FALSE	c1(c(ccc(c1)/C=C/C(=O)OC1C(C2C(OC1CO)OCC(c1ccc(c(c1)O)O)O2)OC1OC(C(C(C1O)O)O)C)O)O
MOL005926	0.9320	0.0680	0.9420	Rose Rugosae Flos	Geranyl formate	5282109	FALSE	C(=C\COC=O)(/CCC=C(C)C)\C
MOL005926	0.9320	0.0680	0.9420	Pogostemon Cablin (Blanco) Benth.	Geranyl formate	5282109	FALSE	C(=C\COC=O)(/CCC=C(C)C)\C
MOL005927	0.9057	0.0943	0.9105	Pogostemon Cablin (Blanco) Benth.	Acetate C-9	8918	FALSE	C(CCCCCC)CCOC(=O)C
MOL005928	0.9468	0.0532	0.9434	Lobeliae Chinensis Herba	isoferulic acid	736186	FALSE	c1(cc(c(cc1)OC)O)/C=C/C(=O)O
MOL005928	0.9468	0.0532	0.9434	Siphonostegiae Herba	isoferulic acid	736186	FALSE	c1(cc(c(cc1)OC)O)/C=C/C(=O)O
MOL005928	0.9468	0.0532	0.9434	Citri Sarcodactylis Fructus	isoferulic acid	736186	FALSE	c1(cc(c(cc1)OC)O)/C=C/C(=O)O
MOL005928	0.9468	0.0532	0.9434	Herbahypericiperforati	isoferulic acid	736186	FALSE	c1(cc(c(cc1)OC)O)/C=C/C(=O)O
MOL005928	0.9468	0.0532	0.9434	Hedysarum Multijugum Maxim.	isoferulic acid	736186	FALSE	c1(cc(c(cc1)OC)O)/C=C/C(=O)O
MOL005928	0.9468	0.0532	0.9434	Radix Salviae	isoferulic acid	736186	FALSE	c1(cc(c(cc1)OC)O)/C=C/C(=O)O
MOL005928	0.9468	0.0532	0.9434	Capsellae Herba	isoferulic acid	736186	FALSE	c1(cc(c(cc1)OC)O)/C=C/C(=O)O
MOL005928	0.9468	0.0532	0.9434	Schizonepetae Herba	isoferulic acid	736186	FALSE	c1(cc(c(cc1)OC)O)/C=C/C(=O)O
MOL005928	0.9468	0.0532	0.9434	Peucedani Radix	isoferulic acid	736186	FALSE	c1(cc(c(cc1)OC)O)/C=C/C(=O)O
MOL005928	0.9468	0.0532	0.9434	Hordei Fructus Germinatus	isoferulic acid	736186	FALSE	c1(cc(c(cc1)OC)O)/C=C/C(=O)O

MOL005928	0.9468	0.0532	0.9434	Cimicifugae Rhizoma	isoferulic acid	736186	FALSE	c1(cc(c(cc1)OC)O)/C=C/C(=O)O
MOL005929	0.9554	0.0446	0.7586	Herbahypericiperforati	(1S,2R,5S)-2,6,6-trimethylnorpinane	10969850	FALSE	C1(C)CCC2CC1C2(C)C
MOL005930	0.6985	0.3015	0.7534	Hippophae Fructus	procyanidin	Not Available	FALSE	C1(c2cc(c(cc2)O)O)(OC2C(c3cc(c(cc3)O)O)Oc3c(C2)c(cc(c3)O)O)Oc2c(C(C1O)O)c(cc(c2)O)O
MOL005930	0.6985	0.3015	0.7534	Herbahypericiperforati	procyanidin	Not Available	FALSE	C1(c2cc(c(cc2)O)O)(OC2C(c3cc(c(cc3)O)O)Oc3c(C2)c(cc(c3)O)O)Oc2c(C(C1O)O)c(cc(c2)O)O
MOL005930	0.6985	0.3015	0.7534	Receptaculum Nelumbinis	procyanidin	Not Available	FALSE	C1(c2cc(c(cc2)O)O)(OC2C(c3cc(c(cc3)O)O)Oc3c(C2)c(cc(c3)O)O)Oc2c(C(C1O)O)c(cc(c2)O)O
MOL005931	0.3642	0.6358	0.8027	Sophora Japonica L.	soyasponin I	Not Available	FALSE	C1C2C(C(CC1(C)C)O)(CC(C1(C2=CCC2C1CC(C1C2(CCC(C1)O)C)(CO)C)C)C)C
MOL005932	0.8542	0.1458	0.6634	Coicis Semen	Gaidic acid	5282743	FALSE	C(CCCCCCCCCC)CC/C=C/C(=O)O
MOL005932	0.8542	0.1458	0.6634	Sophora Japonica L.	Gaidic acid	5282743	FALSE	C(CCCCCCCCCC)CC/C=C/C(=O)O
MOL005932	0.8542	0.1458	0.6634	Spirodelae Herba	Gaidic acid	5282743	FALSE	C(CCCCCCCCCC)CC/C=C/C(=O)O
MOL005932	0.8542	0.1458	0.6634	Ardisiae Japonicae Herba	Gaidic acid	5282743	FALSE	C(CCCCCCCCCC)CC/C=C/C(=O)O
MOL005932	0.8542	0.1458	0.6634	Capsici Fructus	Gaidic acid	5282743	FALSE	C(CCCCCCCCCC)CC/C=C/C(=O)O
MOL005932	0.8542	0.1458	0.6634	Quisqualis Indica	Gaidic acid	5282743	FALSE	C(CCCCCCCCCC)CC/C=C/C(=O)O
MOL005932	0.8542	0.1458	0.6634	Allium Azureum Ledeb.	Gaidic acid	5282743	FALSE	C(CCCCCCCCCC)CC/C=C/C(=O)O
MOL005933	0.8946	0.1054	0.7835	Sophora Japonica L.	2E,4E-tetradecadienoic acid	5312404	FALSE	C(=O)(/C=C/C=C/CCCCCCCCC)O
MOL005934	0.8910	0.1090	0.7820	Linderae Radix	2-tetradecenoic acid	5282738	FALSE	C(=O)(/C=C/CCCCCCCCCCC)O
MOL005934	0.8910	0.1090	0.7820	Sophora Japonica L.	2-tetradecenoic acid	5282738	FALSE	C(=O)(/C=C/CCCCCCCCCCC)O
MOL005935	0.0907	0.9093	0.6332	Sophora Japonica L.	N-[6-(9-acridinylamino)hexyl]benzamide	146515	FALSE	C(=O)(c1ccccc1)NCCCCCCNc1c2c(nc3ccccc13)cccc2
MOL005936	0.4108	0.5892	0.7532	Sophora Japonica L.	kaikasaponinIII_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(O)CC(C3)(C)C)C)C)(CC2)C)(CC1)C)(C)C
MOL005937	0.7306	0.2694	0.8368	Sophora Japonica L.	kaikasaponinI	Not Available	FALSE	O(C1C(OC2C(O)C(O)C(O)C(O2)CO)C(O)C(O)C(O1)C(=O)O)C1CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)C(CC(C)(C)CC4C3=CCC21)O)C
MOL005938	0.4108	0.5892	0.7532	Sophora Japonica L.	kaikasaponinI_qt	Not Available	FALSE	OC1CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)C(CC(C)(C)CC4C3=CCC21)O)C
MOL005939	0.4261	0.5739	0.7644	Sophora Japonica L.	soyasponinIII	Not Available	FALSE	C1C2C(C(CC1(C)C)O)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)CO)O)C)C)C)C

MOL005940	0.8376	0.1624	0.8683	Sophora Japonica L.	quercetin-3'-methyl ether	Not Available	FALSE	c12c(c(cc(c1)O)O)oc(c(c2=O)O)c1c(c(ccc1)O)OC
MOL005941	0.4108	0.5892	0.7532	Sophora Japonica L.	azukisaponinI	Not Available	FALSE	C1C2C(C(CC1(C)C)O)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C)C
MOL005942	0.4800	0.5200	0.7116	Sophora Japonica L.	soyasaponinIII	Not Available	FALSE	C1C2C(C(C(C1(C)C)O)O)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)CO)O)C)C)C)C
MOL005943	0.8610	0.1390	0.8150	Fructussophorae	kaempferol-3,7-di-O-glucoside	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(cc1)O)O)CC1OC(C(C(C1O)O)O)CO
MOL005945	0.9556	0.0444	0.7242	Fructussophorae	Cytisine	Not Available	FALSE	c12n(CC3CC1CNC3)c(=O)ccc2
MOL005945	0.9556	0.0444	0.7242	Portulacae Herba	Cytisine	Not Available	FALSE	c12n(CC3CC1CNC3)c(=O)ccc2
MOL005945	0.9556	0.0444	0.7242	Trollius Chinensis	Cytisine	Not Available	FALSE	c12n(CC3CC1CNC3)c(=O)ccc2
MOL005946	0.8619	0.1381	0.8350	Fructussophorae	sophorabioside	Not Available	FALSE	O(C1C(O)C(O)C(OC1Oc1ccc(cc1)c1c(=O)c2c(oc1)cc(O)cc2O)CO)C1OC(C(O)C(O)C1O)C
MOL005947	0.8831	0.1169	0.8754	Fructussophorae	stizolamine	21780519	FALSE	N(C(=N)N)c1c(=O)n(c(cn1)CO)C
MOL005948	0.8829	0.1171	0.6140	Magnolia Officinalis Rehd Et Wils.	Triisopropylbenzene	12860	FALSE	c1(cc(cc(c1)C(C)C)C(C)C)C(C)C
MOL005949	0.7420	0.2580	0.6589	Magnolia Officinalis Rehd Et Wils.	1-Pentadecyne	69825	FALSE	C(CCCCCCC)CCCCCC#C
MOL005950	0.9611	0.0389	0.9007	Magnolia Officinalis Rehd Et Wils.	2,3,4,6-tetramethylphenol	76719	FALSE	c1(c(c(cc(c1O)C)C)C)C
MOL005951	0.7790	0.2210	0.7352	Magnolia Officinalis Rehd Et Wils.	2-Pentadecyn-1-ol	534429	FALSE	C(C#CCCCCCCCCCCCC)O
MOL005952	0.9064	0.0936	0.9413	Magnolia Officinalis Rehd Et Wils.	EP Solvent	17756	FALSE	O(CCC)CCO
MOL005953	0.9271	0.0729	0.9774	Magnolia Officinalis Rehd Et Wils.	EGMEA	8054	TRUE	O(CCOC)C(=O)C
MOL005954	0.9062	0.0938	0.9646	Magnolia Officinalis Rehd Et Wils.	Ethacrolein	70203	FALSE	C(=C)(CC)C=O
MOL005955	0.6891	0.3109	0.7437	Anisi Stellati Fructus	honokiol	72303	FALSE	c1(c2cc(c(cc2)O)CC=C)cc(ccc1O)CC=C
MOL005955	0.6891	0.3109	0.7437	Magnolia Officinalis Rehd Et Wils.	honokiol	72303	FALSE	c1(c2cc(c(cc2)O)CC=C)cc(ccc1O)CC=C
MOL005956	0.9179	0.0821	0.9684	Magnolia Officinalis Rehd Et Wils.	(2R)-3-methylbutan-2-ol	638099	FALSE	C(C(C)O)(C)C
MOL005957	0.9278	0.0722	0.9488	Ligustici Rhizoma Et Radix	(R)-Lavandulol	5464156	FALSE	C(CC=C(C)C)(C(=C)C)CO
MOL005957	0.9278	0.0722	0.9488	Magnolia Officinalis Rehd Et Wils.	(R)-Lavandulol	5464156	FALSE	C(CC=C(C)C)(C(=C)C)CO

MOL005958	0.9512	0.0488	0.9536	Magnolia Officinalis Rehd Et Wils.	4-Hydroxy-3-methylacetophenone	70135	FALSE	c1(cc(c(cc1)O)C)C(=O)C
MOL005959	0.9351	0.0649	0.9662	Magnolia Officinalis Rehd Et Wils.	BUQ	111509	FALSE	C(C(=O)C)CO
MOL005960	0.5795	0.4205	0.6007	Lycii Fructus	9-Octadecyne	141998	FALSE	C(#CCCCCCCCC)CCCCCCCC
MOL005960	0.5795	0.4205	0.6007	Magnolia Officinalis Rehd Et Wils.	9-Octadecyne	141998	FALSE	C(#CCCCCCCCC)CCCCCCCC
MOL005961	0.4772	0.5228	0.6398	Lycii Fructus	10,13-Octadecadienoic acid, methyl ester	5365678	FALSE	C(=O)(CCCCCCCC/C=C/C/C=C/CCCC)OC
MOL005961	0.4772	0.5228	0.6398	Broussonetiae Fructus	10,13-Octadecadienoic acid, methyl ester	5365678	FALSE	C(=O)(CCCCCCCC/C=C/C/C=C/CCCC)OC
MOL005961	0.4772	0.5228	0.6398	Lysimachiae Foenigraeci Herba	10,13-Octadecadienoic acid, methyl ester	5365678	FALSE	C(=O)(CCCCCCCC/C=C/C/C=C/CCCC)OC
MOL005961	0.4772	0.5228	0.6398	Magnolia Officinalis Rehd Et Wils.	10,13-Octadecadienoic acid, methyl ester	5365678	FALSE	C(=O)(CCCCCCCC/C=C/C/C=C/CCCC)OC
MOL005962	0.5912	0.4088	0.6116	Magnolia Officinalis Rehd Et Wils.	16-Heptadecenal	557527	FALSE	C(=O)CCCCCCCCCCCCCCC=C
MOL005963	0.8175	0.1825	0.7469	Pollen Typhae	BBV-029618	12225100	FALSE	S(=O)(=O)(CC(=O)OCC)Cl
MOL005963	0.8175	0.1825	0.7469	Magnolia Officinalis Rehd Et Wils.	BBV-029618	12225100	FALSE	S(=O)(=O)(CC(=O)OCC)Cl
MOL005965	0.9610	0.0390	0.9521	Magnolia Officinalis Rehd Et Wils.	()-p-Mentha-2,8-diene	78790	FALSE	C1(C(=C)C)CCC(C=C1)C
MOL005966	0.9543	0.0457	0.9488	Magnolia Officinalis Rehd Et Wils.	Cyclohexene	Not Available	FALSE	C1(=CCC(CC1)(C=C)C)C
MOL005967	0.8899	0.1101	0.9572	Magnolia Officinalis Rehd Et Wils.	Zyklohexen	8079	FALSE	C1CCC=CC1
MOL005968	0.9260	0.0740	0.9214	Magnolia Officinalis Rehd Et Wils.	D-Nerolidol	40488241	FALSE	C1(CC(CCC1C)C(=C)C)OC(=O)C
MOL005969	0.6718	0.3282	0.6602	Magnolia Officinalis Rehd Et Wils.	Elemol	Not Available	FALSE	C(CCCCCCC(/C=C/CCCC)C)OC(=O)C
MOL005970	0.7853	0.2147	0.8409	Magnolia Officinalis Rehd Et Wils.	Eucalyptol	34365085	FALSE	C12c3c(c4c(cc3)cc(cc4)O)CCC1(C(=O)CC2)C
MOL005972	0.6252	0.3748	0.6231	Magnolia Officinalis Rehd Et Wils.	OBOVATOL	100771	FALSE	c1(c(c(cc(c1)CC=C)Oc1ccc(cc1)CC=C)O)O

MOL005974	0.6583	0.3417	0.6174	Magnolia Officinalis Rehd Et Wils.	Phenol,2-methoxy	Not Available	FALSE	C(=O)(CCC(CCCCCCCCCCC)C)OC
MOL005975	0.9303	0.0697	0.9058	Magnolia Officinalis Rehd Et Wils.	(2R)-2-methyl-3-phenylpropanal	1549658	FALSE	C(=O)C(Cc1ccccc1)C
MOL005976	0.8302	0.1698	0.7579	Mori Cortex	Tetradecanal	31291	FALSE	C(CCCCCCC)CCCCCC=O
MOL005976	0.8302	0.1698	0.7579	Maydis Seigma	Tetradecanal	31291	FALSE	C(CCCCCCC)CCCCCC=O
MOL005976	0.8302	0.1698	0.7579	Meliae Azedarach Fructus	Tetradecanal	31291	FALSE	C(CCCCCCC)CCCCCC=O
MOL005976	0.8302	0.1698	0.7579	Magnolia Officinalis Rehd Et Wils.	Tetradecanal	31291	FALSE	C(CCCCCCC)CCCCCC=O
MOL005976	0.8302	0.1698	0.7579	Eucommiae Folium	Tetradecanal	31291	FALSE	C(CCCCCCC)CCCCCC=O
MOL005976	0.8302	0.1698	0.7579	Allii Fistulost Bulbus	Tetradecanal	31291	FALSE	C(CCCCCCC)CCCCCC=O
MOL005976	0.8302	0.1698	0.7579	Rose Rugosae Flos	Tetradecanal	31291	FALSE	C(CCCCCCC)CCCCCC=O
MOL005976	0.8302	0.1698	0.7579	Viticis Negundo Folium	Tetradecanal	31291	FALSE	C(CCCCCCC)CCCCCC=O
MOL005976	0.8302	0.1698	0.7579	Capsici Fructus	Tetradecanal	31291	FALSE	C(CCCCCCC)CCCCCC=O
MOL005976	0.8302	0.1698	0.7579	Hippophae Fructus	Tetradecanal	31291	FALSE	C(CCCCCCC)CCCCCC=O
MOL005977	0.8734	0.1266	0.8459	Magnolia Officinalis Rehd Et Wils.	Tridecanedial	544162	FALSE	C(=O)CCCCCCCCCCCC=O
MOL005978	0.9292	0.0708	0.9732	Magnolia Officinalis Rehd Et Wils.	Oxalic ether	7268	FALSE	C(=O)(C(=O)OCC)OCC
MOL005979	0.8859	0.1141	0.8863	Magnolia Officinalis Rehd Et Wils.	Papite	7847	FALSE	C(=C)C=O
MOL005980	0.9099	0.0901	0.8942	Magnolia Officinalis Rehd Et Wils.	Neohesperidin	Not Available	FALSE	c1c(c2c(cc1O)OC(CC2=O)c1cc(cc(c1)OC)O)O
MOL005981	0.9144	0.0856	0.7886	Carpesiumabrotanoidesl.	carabrone	Not Available	FALSE	C12(C(C1CCC(=O)C)CC1C(C2)OC(=O)C1=C)C
MOL005982	0.9437	0.0563	0.8038	Cassiae Semen	5,7-Dihydroxychromone	5281343	FALSE	c1cc(=O)c2c(cc(cc2o1)O)O
MOL005982	0.9437	0.0563	0.8038	Actinidia Chinensis Planch	5,7-Dihydroxychromone	5281343	FALSE	c1cc(=O)c2c(cc(cc2o1)O)O
MOL005982	0.9437	0.0563	0.8038	Mori Cortex	5,7-Dihydroxychromone	5281343	FALSE	c1cc(=O)c2c(cc(cc2o1)O)O
MOL005982	0.9437	0.0563	0.8038	Peanut Skin	5,7-Dihydroxychromone	5281343	FALSE	c1cc(=O)c2c(cc(cc2o1)O)O
MOL005982	0.9437	0.0563	0.8038	Polygoni Orientalis Fructus	5,7-Dihydroxychromone	5281343	FALSE	c1cc(=O)c2c(cc(cc2o1)O)O
MOL005983	0.9474	0.0526	0.8819	Phyllanthi Fructus	leucodelphinidin	Not Available	FALSE	c12c(C(C(C(O1)c1cc(c(c(c1)O)O)O)O)O)c(cc(c2)O)O

MOL005983	0.9474	0.0526	0.8819	Peanut Skin	leucodelphinidin	Not Available	FALSE	c12c(C(C(C(O1)c1cc(c(c(c1)O)O)O)O)O)c(cc(c2)O)O
MOL005987	0.9219	0.0781	0.7942	Herba Selaginellae Moellendorfii	sygringaresinol	71406631	FALSE	c1c(ccc(c1OC)OC(=O)CCc1cccc(c1)O)C(=O)O
MOL005988	0.9368	0.0632	0.7890	Herba Selaginellae Moellendorfii	4-hydroxymephenytion	40572060	FALSE	C1(c2ccc(cc2)O)(C(=O)N(C(=O)N1)C)CC
MOL005989	0.6429	0.3571	0.8363	Herba Selaginellae Moellendorfii	tamariscinaester	Not Available	FALSE	c12c(c(cc(c1)C(=O)C)OC)OC(c1cc(c(c(c1)OC)O)OC)C2
MOL005990	0.9211	0.0789	0.9512	Platycodon Grandiforus	1-methoxy-1,2-butadiene	57109763	FALSE	C(=C=CC)OC
MOL005991	0.9091	0.0909	0.9707	Platycodon Grandiforus	ISOPROPYL FORMATE	12257	FALSE	C(=O)OC(C)C
MOL005992	0.9180	0.0820	0.9501	Platycodon Grandiforus	2,3-dimethyl-1-pentene	12927329	FALSE	C=C(C(CC)C)C
MOL005992	0.9180	0.0820	0.9501	Ephedra Herba	2,3-dimethyl-1-pentene	12927329	FALSE	C=C(C(CC)C)C
MOL005993	0.8817	0.1183	0.7725	Platycodon Grandiforus	2-cyclopentene-1-undecanoic acid	Not Available	FALSE	C1(C=CCC1)CCCCCCCCCCC(=O)O
MOL005994	0.9035	0.0965	0.8517	Platycodon Grandiforus	2-hydroxybicyclo[3.1.1]heptan-6-one	Not Available	FALSE	C12C(CCC(C1=O)C2)O
MOL005995	0.7298	0.2702	0.7167	Platycodon Grandiforus	2'-O-acetylPlatycodin D2	Not Available	FALSE	OC1C(CC2(C(C1(CO)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)O)O)C)C)C)O
MOL005996	0.5692	0.4308	0.8366	Platycodon Grandiforus	2-O-methyl-3—O-β-D-glucopyranosyl platycogenate A	Not Available	FALSE	C1(C2(C(C3=CCC4C(C3(C1)C)(CCC1C4(CC(C(C1(C(=O)OOC)C)OC1C(C(C(C(O1)CO)O)O)O)OC)C)C)CC(CC2)(C)C)C(=O)OC)O
MOL005997	0.7514	0.2486	0.7999	Platycodon Grandiforus	2'-O-Polygalacin D	Not Available	FALSE	C1(C(OC(C(C1O)O)O)OC1C(CC2(C(C1(C)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)OC1OCC(C1O)(O)CO)O)O)OC(=O)C)O)C)C)C)O)O
MOL005998	0.6931	0.3069	0.7837	Platycodon Grandiforus	2'-O-polygalacin D2	Not Available	FALSE	C1(C(OC(C(C1O)O)OC1C(C(C(C(O1)O)O)O)O)OC1C(CC2(C(C1(C)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)OC1OCC(C1O)(O)CO)O)O)O)OC(=O)C)O)C)C)C)O)O

MOL005999	0.8993	0.1007	0.9630	Platycodon Grandiforus	crotonaldehyde	447466	FALSE	C/C=C/C=O
MOL005999	0.8993	0.1007	0.9630	Dichroae Radix	crotonaldehyde	447466	FALSE	C/C=C/C=O
MOL006000	0.8814	0.1186	0.8805	Platycodon Grandiforus	Cyclopentenone	13588	FALSE	C1C(=O)C=CC1
MOL006001	0.9106	0.0894	0.9659	Platycodon Grandiforus	Isobutenol	10557	FALSE	C(C(=C)C)O
MOL006002	0.8944	0.1056	0.8720	Platycodon Grandiforus	3,4-Heptadiene	556860	FALSE	CCC=C=CCC
MOL006003	0.9450	0.0550	0.7691	Platycodon Grandiforus	(1S,5R)-3,7,7-trimethylbicyclo[3.1.1]hept-3-ene	11240513	FALSE	C12C=C(CC(C1(C)C)C2)C
MOL006004	0.7525	0.2475	0.7992	Platycodon Grandiforus	3'-a-O-Polygalacin D	Not Available	FALSE	C1(C(OC(C(C1O)O)O)OC1C(CC2(C(C1(C)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)OC1OCC(C1O)(O)CO)O)OC(=O)C)O)O)C)C)O)O
MOL006005	0.9177	0.0823	0.9278	Platycodon Grandiforus	allyloxyethylene	221523	FALSE	C=CCOC=C
MOL006006	0.9090	0.0910	0.9144	Platycodon Grandiforus	3-ethyl-1,4-hexadiene	Not Available	FALSE	C=CC(/C=C/C)CC
MOL006007	0.9245	0.0755	0.9604	Platycodon Grandiforus	3-ethyl-cyclohexene	13077038	FALSE	C1=CC(CCC1)CC
MOL006008	0.7045	0.2955	0.7858	Platycodon Grandiforus	3'-O-acetylPlatycodin D2	Not Available	FALSE	C1(C(OC(C(C1O)O)OC1C(C(C(C(O1)O)O)O)O)OC1C(CC2(C(C1(CO)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)OC1OCC(C1O)(O)CO)O)OC(=O)C)O)O)C)C)O)O
MOL006009	0.7298	0.2702	0.7167	Platycodon Grandiforus	3'-O-acetylPlatycodin D2_qt	Not Available	FALSE	OC1C(CC2(C(C1(CO)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)O)O)C)C)C)O
MOL006010	0.6457	0.3543	0.8493	Platycodon Grandiforus	3-O-a-D-glucopyranosylplatycodigenin methyl ester	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)OC)C)C)C)(CO)CO)OC1C(C(C(C(O1)CO)O)O)O)O
MOL006011	0.5476	0.4524	0.7187	Platycodon Grandiforus	3-O-a-D-glucopyranosylplatycodigenin methyl ester_qt	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)OC)C)C)C)(CO)CO)O)O

MOL006012	0.7502	0.2498	0.8420	Platycodon Grandiforus	3-O-a-gentiobiosylplatycodigenin methyl ester	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)OC)C)C)(CO)CO)OC1C(C(C(C(O1)COC1C(C(C(C(O1)CO)O)O)O)O)O)O)O)O
MOL006013	0.6881	0.3119	0.8375	Platycodon Grandiforus	3-O-a-Laminaribiosylplatycodigenin methyl ester	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)OC)C)C)(CO)CO)OC1C(C(C(C(O1)CO)O)OC1C(C(C(C(O1)CO)O)O)O)O)O)O
MOL006014	0.7171	0.2829	0.8470	Platycodon Grandiforus	3-O-laminaribiosylplatycodigenin methyl ester	Not Available	FALSE	C1(C2(C(C3C(C1)(C1(C(CC3)C3(C(CC1)C(C(C(C3)O)OC1OC(C(C(C1O)O)OC1OC(C(C(C1O)O)O)CO)CO)(CO)CO)C)C)CC(CC2)(C)C)C(=O)OC)O
MOL006015	0.5340	0.4660	0.7289	Platycodon Grandiforus	3-O-laminaribiosylplatycodigenin methyl ester_qt	Not Available	FALSE	C1(C2(C(C3C(C1)(C1(C(CC3)C3(C(CC1)C(C(C(C3)O)O)(CO)CO)C)C)CC(CC2)(C)C)C(=O)OC)O
MOL006016	0.6949	0.3051	0.7831	Platycodon Grandiforus	3'-O-polygalacin D	Not Available	FALSE	C1(C(OC(C(C1O)O)OC1C(C(C(C(O1)O)O)O)O)OC1C(CC2(C(C1(C)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)OC1OCC(C1O)(O)CO)O)OC(=O)C)O)O)C)C)C)O)O
MOL006017	0.6457	0.3543	0.8493	Platycodon Grandiforus	3-O-β-D-glucopyranosyl platycodigenin methyl ester	Not Available	FALSE	C1(C2(C(C3=CCC4C(C3(C1)C)(CCC1C4(CC(C(C1(CO)CO)OC1OC(C(C(C1O)O)O)CO)O)C)C)CC(CC2)(C)C)C(=O)OC)O
MOL006018	0.7900	0.2100	0.8051	Platycodon Grandiforus	dimethyl 3-o-β-D glucopyranosylplatycogenate A	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)OC1OCC(C(C1OC1OC(C(C(C1O)O)CC1C(C(C(CO1)O)OC1OCC(C1O)(O)CO)O)C)O)O)C)C)(C=O)CO)OC1OC(C(C(C1O)O)O)CO)O
MOL006019	0.7502	0.2498	0.8420	Platycodon Grandiforus	3-O-β-gentiobiosyl platycodigenin methylester	Not Available	FALSE	C1(OC(C(C(C1O)O)O)OC1C(CC2(C(C1(CO)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC)O)C)C)C)O)COC1OC(C(C(C1O)O)O)CO
MOL006020	0.9069	0.0931	0.9616	Platycodon Grandiforus	5-HEXENOIC ACID	15308	FALSE	C=CCCCC(=O)O
MOL006021	0.7703	0.2297	0.8015	Platycodon Grandiforus	16-oxo-platycodin D	Not Available	FALSE	C1(C(OC(C(C1O)O)CO)OC1C(CC2(C(C1(CO)CO)CCC1(C2CC=C2C1(CC(=O)C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)OC1OCC(C1O)(O)CO)O)O)O)C)C)C)O)O

MOL006023	0.2168	0.7832	0.6260	Platycodon Grandiforus	α-Spinasterol-β-D-glucoside_qt	Not Available	FALSE	C12=CCC3C(C2CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C)(CCC(C3)O)C
MOL006024	0.7684	0.2316	0.8136	Platycodon Grandiforus	Deapio-Platycodin-D	Not Available	FALSE	C1(C(OC(C(C1O)O)CO)OC1C(CC2(C(C1(CO)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)O)O)O)O)O)C)C)C)O)O
MOL006025	0.7823	0.2177	0.8002	Platycodon Grandiforus	Deapio-Platycodin-D3	Not Available	FALSE	C1(C(OC(C(C1OC1C(C(C(C(O1)O)O)O)O)CO)OC1C(CC2(C(C1(CO)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)O)O)O)O)O)C)C)C)O)O
MOL006026	0.5721	0.4279	0.8519	Platycodon Grandiforus	dimethyl 2-O-methyl-3-O-a-D-glucopyranosyl platycogenate A	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)OC)C)C)(C(=O)OC)CO)OC1C(C(C(C(O1)CO)O)O)O)OC
MOL006027	0.6019	0.3981	0.8547	Platycodon Grandiforus	dimethyl 3-O-a-D-glucopyranosylplatycogenate A	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)OC)C)C)(CO)C(=O)OC)OC1C(C(C(C(O1)CO)O)O)O)O
MOL006028	0.6817	0.3183	0.7491	Platycodon Grandiforus	dimethyl 3-O-β-D-glucopyranosylplatycogenate A	Not Available	FALSE	C1(C2(C(C3=CCC4C(C3(C1)C)(CCC1C4(CC(C(C1(CC)C(=O)O)O)O)C)C)CC(CC2)(C)C)C(=O)OC)O
MOL006029	0.4686	0.5314	0.7187	Platycodon Grandiforus	dimethyl platyconate A	Not Available	FALSE	C1CC2(C(C3(C1C(C(C(C3)O)O)(C(=O)OC)CO)C)CC=C1C2(CC(C2(C1CC(CC2)(C)C)C(=O)OC)O)C)C
MOL006030	0.8909	0.1091	0.8448	Platycodon Grandiforus	Flavoplatycoside	Not Available	FALSE	C1(C(C(C(OC1C)OCC1C(C(C(C(O1)Oc1cc(c2c(c1)OC(C(C2=O)O)c1ccc(c(c1)O)O)O)O)O)O)O)O)O
MOL006031	0.9245	0.0755	0.8252	Platycodon Grandiforus	Grandoside	Not Available	FALSE	O1C(C(C(O)C(C1CO)O)OC1C(C(C(C(O1)CO)O)O)O)OCCC(C)C
MOL006032	0.8431	0.1569	0.6936	Platycodon Grandiforus	Inulin	Not Available	FALSE	C1(C(C(C(OC1CO)OC1C(C(OC(C1NC(=O)C)OC1C(C(C(OC1CO)OC1C(C(C(OC1CO)O)O)O)O)O)OC1CC(C(CO1)N(C(=O)C)C(CO)C(=O)C)O)CO)O)OC1C(C(C(C(O1)CO)O)O)O)O)O
MOL006033	0.7298	0.2702	0.7167	Platycodon Grandiforus	latycodigenin	Not Available	FALSE	C1(C(CC2(C(C1(CO)CO)CCC1(C)C3(C)CC(C4(C(=O)O)CCC(C)(C)CC4C3=CCC21)O)C)O)O
MOL006034	0.8044	0.1956	0.7783	Platycodon Grandiforus	lobetyol	Not Available	FALSE	C(CC/C=C/C(C(C#CC#C/C=C/C)O)O)O
MOL006035	0.8757	0.1243	0.7647	Platycodon Grandiforus	lobetyolin	Not Available	FALSE	C1(C(C(C(C(O1)CO)O)O)O)OC(/C=C/CCCO)C(C#CC#C/C=C/C)O

MOL006036	0.7386	0.2614	0.6942	Platycodon Grandiforus	lobetyolinin	Not Available	FALSE	C/C=C/C#CC#CC(C(OC1C(C(C(C(O1)COC1C(C(C(C(C1)CO)O)O)O)O)O)O)O)/C=C/CCCO)O
MOL006037	0.8044	0.1956	0.7783	Platycodon Grandiforus	lobetyolinin_qt	Not Available	FALSE	C/C=C/C#CC#CC(C(O)/C=C/CCCO)O
MOL006038	0.7520	0.2480	0.7942	Platycodon Grandiforus	Methy 2-O-methylPlatyconate A	Not Available	FALSE	C1(C(OC(C(C1O)O)CO)OC1C(CC2(C(C1(C(=O)OC)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)OC1OCC(C1O)(O)CO)O)O)O)O)C)C)C)O
MOL006039	0.9353	0.0647	0.9705	Platycodon Grandiforus	Methyl 3-methyl-2-pentenoate	5362896	FALSE	C(=O)(/C=C(/CC)\C)OC
MOL006040	0.6310	0.3690	0.8455	Platycodon Grandiforus	methyl 3-O-β-D-glucopyranosyl polygalacate	Not Available	FALSE	C1(C2(C(C3=CCC4C(C3(C1)C)(CCC1C4(CC(C(C1(CO)C)OC1OC(C(C(C1O)O)O)CO)O)C)C)CC(CC2)(C)C)C(=O)OC)O
MOL006041	0.4415	0.5585	0.7362	Platycodon Grandiforus	methyl 3-O-β-D-glucopyranosyl polygalacate qt	Not Available	FALSE	C1(C2(C(C3=CCC4C(C3(C1)C)(CCC1C4(CC(C(C1(CO)C)O)O)C)C)CC(CC2)(C)C)C(=O)OC)O
MOL006042	0.7406	0.2594	0.8601	Platycodon Grandiforus	methyl 3-O-β-laminaribiosyl polygalacate	Not Available	FALSE	C1(C2(C(C3C(C1)(C1(C(CC3)C3(C(CC1)C(C(C(C3)O)COC1OC(C(C(C1O)O)OC1OC(C(C(C1O)O)O)CO)O)CO)(CO)C)C)C)CC(CC2)(C)C)C(=O)OC)O
MOL006043	0.7380	0.2620	0.8107	Platycodon Grandiforus	methyl platyconate-A	Not Available	FALSE	C1(C2(C(C3=CCC4C(C3(C1)C)(CCC1C4(CC(C(C1(C(=O)OC)CO)OC1OC(C(C(C1O)O)O)CO)O)C)C)CC(CC2)(C)C)C(=O)OC1OC(C(C(C1O)O)OC1OCC(C(C1O)OC1OCC(C1O)(O)CO)O)C)O

MOL006044	0.4415	0.5585	0.7362	Platycodon Grandiforus	methyl (4aR,5R,6aR,6aS,6bR,8aR,9R,10R,11S,12aR,14bS)-5,10,11-trihydroxy-9-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylate	14543229	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)OC)C)C)C)(C)CO)O)O
MOL006045	0.6310	0.3690	0.8455	Platycodon Grandiforus	methyl3-O-a-D-Glucopyranosylpolygalacate	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)OC)C)C)C)(C)CO)OC1C(C(C(C(O1)CO)O)O)O)O
MOL006046	0.6810	0.3190	0.8482	Platycodon Grandiforus	methyl3-O-a-laminaribiosyl polygalacate	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)OC)C)C)C)(C)CO)OC1C(C(C(C(O1)CO)O)OC1C(C(C(C(O1)CO)O)O)O)O)O
MOL006047	0.9560	0.0440	0.8128	Platycodon Grandiforus	methylbutyl-1,2-benzenedicarboxylate	70153369	FALSE	c1(c(c(c(cc1)C)CCCC)C(=O)O)C(=O)O

MOL006048	0.5476	0.4524	0.7187	Platycodon Grandiforus	methyl (4aR,5R,6aR,6aS,6bR,8aR,10R,11S,12aR,14bS)-5,10,11-trihydroxy-9,9-bis(hydroxymethyl)-2,2,6a,6b,12a-pentamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylate	21594239	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)OC)C)C)(CO)CO)O)O
MOL006049	0.7277	0.2723	0.7130	Platycodon Grandiforus	Platycodigenin	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)O)C)C)(CO)CO)O)O
MOL006050	0.7363	0.2637	0.7852	Platycodon Grandiforus	Platycodin D2	Not Available	FALSE	C1(C(OC(C(C1O)O)OC1C(C(C(C(O1)O)O)O)O)OC1C(CC2(C(C1(CO)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)OC1OCC(C1O)(O)CO)O)O)O)O)C)C)O)O
MOL006051	0.7356	0.2644	0.7896	Platycodon Grandiforus	Platycodin-D3	Not Available	FALSE	C1(C(OC(C(C1OC1C(C(C(C(O1)O)O)O)O)O)CO)OC1C(CC2(C(C1(CO)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)OC1OCC(C1O)(O)CO)O)O)O)O)C)C)O)O
MOL006052	0.7217	0.2783	0.7133	Platycodon Grandiforus	Platycogenic acid A	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)O)C)C)(C(=O)O)CO)O)O
MOL006053	0.7154	0.2846	0.7119	Platycodon Grandiforus	Platycogenic acid B	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(C(C2)O)(CC(C(C1)(C)C)O)C(=O)O)C)C)(C)C(=O)O)O)O
MOL006054	0.7184	0.2816	0.7332	Platycodon Grandiforus	Platycogenic acid C	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(C(C2)O)(CC(C(C1)(C)C)O)C(=O)O)C)C)(C)C)O)O
MOL006055	0.7588	0.2412	0.7935	Platycodon Grandiforus	platyconate A	Not Available	FALSE	C1(C(OC(C(C1O)O)O)OC1C(CC2(C(C1(C(=O)OC)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)OC1OCC(C1O)(O)CO)O)O)O)O)C)C)C)O)O
MOL006056	0.7011	0.2989	0.7213	Platycodon Grandiforus	platyconate A_qt	Not Available	FALSE	OC1C(CC2(C(C1(C(=O)OC)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)O)O)C)C)C)O

MOL006057	0.7589	0.2411	0.7949	Platycodon Grandiforus	Platyconic acid-A Lactone	Not Available	FALSE	C1(C(OC(C(C1O)O)CO)OC1C(CC2(C(C1(CCC(=O)OCC)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)OC1OCC(C1O)(O)CO)O)O)O)O)O)O)O)O)O
MOL006058	0.7847	0.2153	0.7976	Platycodon Grandiforus	platycoside A	Not Available	FALSE	C1(C(OC(C(C1O)O)OC1C(C(C(C(O1)O)O)O)O)OC1C(CC2(C(C1(CO)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)O)O)O)O)O)C)C)O)O
MOL006059	0.7426	0.2574	0.8122	Platycodon Grandiforus	platycoside B	Not Available	FALSE	C1(C(OC(C(C1O)O)O)O)OC1C(CC2(C(C1(CO)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)O)O)O)OC(=O)C)O)C)C)O)O
MOL006060	0.7435	0.2565	0.8111	Platycodon Grandiforus	platycoside C	Not Available	FALSE	C1(C(OC(C(C1O)O)O)O)OC1C(CC2(C(C1(CO)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)O)O)O)OC(=O)C)O)C)C)O)O
MOL006061	0.6945	0.3055	0.8240	Platycodon Grandiforus	platycoside F	Not Available	FALSE	C1(C(OC(C(C1O)O)CO)OC1C(CC2(C(C1(CO)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)OC(=O)C)OC(=O)C)OC1C(C(C(C(O1)C)O)O)O)O)C)C)O)O
MOL006062	0.7528	0.2472	0.7929	Platycodon Grandiforus	platycoside G1	Not Available	FALSE	C1(C(OC(C(C1O)O)COC1C(C(C(C(O1)CO)O)O)O)OC1C(CC2(C(C1(CO)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)OC(=O)C)OC(=O)C)OC1C(C(C(C(O1)C)OC(=O)C(C(C(CO)O)O)O)O)O)C)C)O)O
MOL006063	0.7315	0.2685	0.7961	Platycodon Grandiforus	platycoside G3	Not Available	FALSE	C1(C(OC(C(C1O)O)CO)OC1C(CC2(C(C1(CO)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)OC(=O)C)OC(=O)C)OC1C(C(C(C(O1)C)OC(=O)C(C(C(CO)O)OC1C(C(CO1)(O)CO)O)O)O)O)O)C)C)O)O
MOL006064	0.6532	0.3468	0.7796	Platycodon Grandiforus	Platyeoside D	Not Available	FALSE	C1(C(OC(C(C1OC1C(C(C(O1)COC1C(C(C(O1)CO)O)O)O)O)O)O)O)CO)OC1C(CC2(C(C1(C)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)OC1OCC(C1O)(O)CO)O)O)O)O)C)C)O)O
MOL006065	0.6645	0.3355	0.7804	Platycodon Grandiforus	Platyeoside E	Not Available	FALSE	C1(C(OC(C(C1OC1C(C(C(O1)COC1C(C(C(O1)CO)O)O)O)O)O)O)O)CO)OC1C(CC2(C(C1(CO)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)OC1OCC(C1O)(O)CO)O)O)O)O)C)C)O)O
MOL006066	0.7205	0.2795	0.7345	Platycodon Grandiforus	Polygalacic acid	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)O)C)C)(C)CO)O)O

MOL006067	0.7695	0.2305	0.8027	Platycodon Grandiforus	Polygalacin D	Not Available	FALSE	C1(C(OC(C(C1O)O)O)OC1C(CC2(C(C1(C)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)OC1OCC(C1O)(O)CO)O)O)O)O)C)C)O)O
MOL006068	0.7275	0.2725	0.7861	Platycodon Grandiforus	polygalacin D2	Not Available	FALSE	C1(C(OC(C(C1O)O)OC1C(C(C(C(O1)O)O)O)O)OC1C(CC2(C(C1(C)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)OC1OCC(C1O)(O)CO)O)O)O)O)C)C)O)O
MOL006069	0.2168	0.7832	0.6260	Platycodon Grandiforus	stigmastenol	Not Available	FALSE	C12=CCC3C(C2CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C)(CCC(C3)O)C
MOL006070	0.7934	0.2066	0.8315	Platycodon Grandiforus	robinin	Not Available	FALSE	c1c(c2c(cc1OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O)O)oc(cc2=O)c1ccc(cc1)OC)O
MOL006071	0.8432	0.1568	0.7613	Platycodon Grandiforus	(1R,2R,3R,5R)-5-(((1R,2R,4R,5S)-5-hydroxy-4-(hydroxymethyl)-2-(isopentylperoxy)cyclohexyl)oxy)-3-(hydroxymethyl)cyclohexane-1,2-diol	Not Available	FALSE	C1C(C(CC(C1O)CO)OOCCC(C)C)OC1CC(C(C(C1)CO)O)O
MOL006072	0.6835	0.3165	0.8012	Platycodon Grandiforus	Platycodin A	Not Available	FALSE	C1(OC2C(CC3(C(C2(CO)CO)CCC2(C3CC=C3C2(CC(C2(C3(CC(CC2)(C)C)C)C(=O)OC2OCC(C(C2OC2OC(C(C(C2OC(=O)C)O)OC2OCC(C(C2O)C)C)C)O)O)O)C)C)O)C(C(C(C(O1)CO)O)O)O
MOL006073	0.6941	0.3059	0.8012	Platycodon Grandiforus	Platycodin C	Not Available	FALSE	C1(OC2C(CC3(C(C2(CO)CO)CCC2(C3CC=C3C2(CC(C2(C3(CC(CC2)(C)C)C)C(=O)OC2OCC(C(C2OC2OC(C(C(C2O)OC(=O)C)O)OC2OCC(C(C2O)C)C)C)O)O)O)C)C)O)C(C(C(C(O1)CO)O)O)O
MOL006074	0.7755	0.2245	0.8018	Platycodon Grandiforus	Platycodin D	Not Available	FALSE	C1(C(OC(C(C1O)O)CO)OC1C(CC2(C(C1(CO)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)OC1OCC(C1O)(O)CO)O)O)O)O)C)C)O)
MOL006075	0.7605	0.2395	0.8325	Platycodon Grandiforus	deapio platycoside F	Not Available	FALSE	C1(C(OC(C(C1O)O)CO)OC1C(CC2(C(C1(CO)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)O)O)O)O)O)C)C)O)O

MOL006076	0.7647	0.2353	0.7775	Platycodon Grandiforus	(deapio platycodin E	Not Available	FALSE	C1(C(OC(C(C1O)O)COC1C(C(C(C(O1)CCC1C(C(C(O1)CO)O)O)O)O)O)OC1C(CC2(C(C1(CO)CO)CCC1(C2CC=C2C1(CC(C1(C2CC(CC1)(C)C)C(=O)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)C)OC1OCC(C(C1O)O)O)O)O)C)C)O)O
MOL006077	0.9571	0.0429	0.7966	Platycodon Grandiforus	Thiamine	9543525	FALSE	[n+]1(c(c(sc1)CCO)C)Cc1c(nc(nc1)C)N
MOL006077	0.9571	0.0429	0.7966	Vigna Radiata	Thiamine	9543525	FALSE	[n+]1(c(c(sc1)CCO)C)Cc1c(nc(nc1)C)N
MOL006077	0.9571	0.0429	0.7966	Raphani Semen	Thiamine	9543525	FALSE	[n+]1(c(c(sc1)CCO)C)Cc1c(nc(nc1)C)N
MOL006077	0.9571	0.0429	0.7966	Gnaphalii Affinis Herba	Thiamine	9543525	FALSE	[n+]1(c(c(sc1)CCO)C)Cc1c(nc(nc1)C)N
MOL006077	0.9571	0.0429	0.7966	Portulacae Herba	Thiamine	9543525	FALSE	[n+]1(c(c(sc1)CCO)C)Cc1c(nc(nc1)C)N
MOL006077	0.9571	0.0429	0.7966	Capsici Fructus	Thiamine	9543525	FALSE	[n+]1(c(c(sc1)CCO)C)Cc1c(nc(nc1)C)N
MOL006077	0.9571	0.0429	0.7966	Corayceps	Thiamine	9543525	FALSE	[n+]1(c(c(sc1)CCO)C)Cc1c(nc(nc1)C)N
MOL006077	0.9571	0.0429	0.7966	Jujubae Fructus	Thiamine	9543525	FALSE	[n+]1(c(c(sc1)CCO)C)Cc1c(nc(nc1)C)N
MOL006077	0.9571	0.0429	0.7966	Humulus Scandens (Lour.) Merr.	Thiamine	9543525	FALSE	[n+]1(c(c(sc1)CCO)C)Cc1c(nc(nc1)C)N
MOL006077	0.9571	0.0429	0.7966	Hippophae Fructus	Thiamine	9543525	FALSE	[n+]1(c(c(sc1)CCO)C)Cc1c(nc(nc1)C)N
MOL006077	0.9571	0.0429	0.7966	Crataegi Folium	Thiamine	9543525	FALSE	[n+]1(c(c(sc1)CCO)C)Cc1c(nc(nc1)C)N
MOL006077	0.9571	0.0429	0.7966	Thalluslaminariae	Thiamine	9543525	FALSE	[n+]1(c(c(sc1)CCO)C)Cc1c(nc(nc1)C)N
MOL006077	0.9571	0.0429	0.7966	Typhonii Rhizoma	Thiamine	9543525	FALSE	[n+]1(c(c(sc1)CCO)C)Cc1c(nc(nc1)C)N
MOL006078	0.9305	0.0695	0.7978	Wikstroemiae Indicae Rasix	3,5-dihydroxy-2-(4-hydroxyphenyl)chromone	5393154	FALSE	c1(c(c(=O)c2c(o1)cccc2O)O)c1ccc(cc1)O
MOL006078	0.9305	0.0695	0.7978	Celosia Cristata L.	3,5-dihydroxy-2-(4-hydroxyphenyl)chromone	5393154	FALSE	c1(c(c(=O)c2c(o1)cccc2O)O)c1ccc(cc1)O
MOL006079	0.9355	0.0645	0.9489	Celosia Cristata L.	D-pintiol	164619	FALSE	C1(C(C(C(C(C1O)O)O)O)O)OC
MOL006080	0.8594	0.1406	0.7036	Celosia Cristata L.	amaranthin	Not Available	FALSE	N1(c2c(CC1C(=O)O)cc(OC1C(C(C(C(O1)CO)O)O)OC1OC(C(C(C1O)O)O)C(=O)O)c(c2)O)/C=C/C1=CC(=NC(C(=O)O)C1)C(=O)O
MOL006081	0.9402	0.0598	0.6223	Celosia Cristata L.	amaranthin_qt	Not Available	FALSE	N1(c2c(CC1C(=O)O)cc(O)c(c2)O)/C=C/C1=CC(=NC(C(=O)O)C1)C(=O)O
MOL006082	0.9389	0.0611	0.9701	Celosia Cristata L.	2-Hydroxyphenylethanol	82200	FALSE	c1(c(cccc1)O)CCO
MOL006084	0.8881	0.1119	0.7410	Sedum Aizoon L.	Myricetin-3-O-beta-D-(6'-O-galloyl)-glucopyranoside	5319986	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)COC(=O)c1cc(c(c(c1)O)O)O)c1cc(c(c(c1)O)O)O

MOL006085	0.8881	0.1119	0.7410	Sedum Aizoon L.	Myricetin-3-O-beta-D-(6'-O-galloyl)-galactopyranoside	5319985	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)COC(=O)c1cc(c(c(c1)O)O)O)c1cc(c(c(c1)O)O)O
MOL006086	0.9280	0.0720	0.7859	Dioscoreaebulbiferae	Isomyricitrin	5318606	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)c(O)c1)CO
MOL006086	0.9280	0.0720	0.7859	Sedum Aizoon L.	Isomyricitrin	5318606	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)c(O)c1)CO
MOL006087	0.8106	0.1894	0.6184	Sedum Aizoon L.	sedinine	Not Available	FALSE	C1=CCC(NC1C(CO)C)(C(c1ccccc1)CO)C
MOL006088	0.9325	0.0675	0.9424	Sedum Aizoon L.	D-sedoheptulose	5459879	FALSE	OCC(=O)C(O)C(O)C(O)C(O)CO
MOL006089	0.9134	0.0866	0.9224	Sedum Aizoon L.	(1R)-2-[(2S)-1-methyl-2-piperidyl]-1-phenyl-ethanol	11106868	FALSE	OC(CC1N(CCCC1)C)c1ccccc1
MOL006090	0.2190	0.7810	0.6457	Calendula Officinalis	4β-methylstigmasta-7,24(28)-diene-3β-ol	Not Available	FALSE	C1(CCC2(C(C1C)CC=C1C3CCC(C(CC/C(=C\C)/C(C)C)C)C3(C)CCC21)C)O
MOL006091	0.3938	0.6062	0.7615	Solidaginis Herba	Erythrodiol	101761	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(C)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)CO)C
MOL006091	0.3938	0.6062	0.7615	Chrysanthemi Flos	Erythrodiol	101761	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(C)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)CO)C
MOL006091	0.3938	0.6062	0.7615	Calendula Officinalis	Erythrodiol	101761	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(C)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)CO)C
MOL006091	0.3938	0.6062	0.7615	Borneolum Syntheticum	Erythrodiol	101761	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(C)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)CO)C
MOL006091	0.3938	0.6062	0.7615	Ilicis Cornutae Folium Immayuri	Erythrodiol	101761	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(C)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)CO)C
MOL006091	0.3938	0.6062	0.7615	Cortex Hibisci	Erythrodiol	101761	FALSE	C12(C(=CCC3C1(CCC1C3(CCC(C1(C)C)O)C)C)C1C(CC2)(CCC(C1)(C)C)CO)C
MOL006092	0.3996	0.6004	0.7624	Calendula Officinalis	arnidiol	Not Available	FALSE	C1CC(C(C2CCC3(C4(CC(C5(CCC(=C)C(C5C4CCC3C12C)C)C)O)C)C)(C)C)O
MOL006093	0.3827	0.6173	0.7344	Buddlejae Flos	δ-amyrin	12358447	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C)(C)CC4=C3CCC21)C)O
MOL006093	0.3827	0.6173	0.7344	Calendula Officinalis	δ-amyrin	12358447	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C)(C)CC4=C3CCC21)C)O
MOL006094	0.9261	0.0739	0.7925	Calendula Officinalis	quercetin glucoside	Not Available	FALSE	c1(c(c(=O)c2c(o1)cc(cc2OC1C(O)C(O)C(O)C(O1)CO)O)O)c1cc(c(cc1)O)O

MOL006096	0.8596	0.1404	0.8402	Calendula Officinalis	Isorhamnetin-3-O-neohesperidoside	11664505	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(OC2C(O)C(O)C(O)C(O2)C)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)OC
MOL006097	0.8499	0.1501	0.8548	Calendula Officinalis	calendoflaside	Not Available	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(OC2C(O)C(O)C(O)C(O2)C)C(O)C(O)C(O1)C)c1cc(c(cc1)O)OC
MOL006098	0.3932	0.6068	0.7541	Calendula Officinalis	faradiol	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CC(C4(C)CC=C(C)C(C)C4C3CCC21)O)C)O
MOL006099	0.3918	0.6082	0.7524	Calendula Officinalis	brein	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CC(C4(C)CCC(C)C(C)C4C3=CCC21)O)C)O
MOL006100	0.4041	0.5959	0.8150	Calendula Officinalis	Longispinogenin	489920	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(C(C4)CO)(CCC(C3)(C)C)CO)C)(CC2)C)(CC1)C)(C)C
MOL006101	0.4108	0.5892	0.7050	Calendula Officinalis	(3S,4aR,6aR,6aS,6bR,8aR,12S,12aS,14aR,14bR)-4,4,6a,6b,8a,12,14b-heptamethyl-11-methylene-1,2,3,4a,5,6,6a,7,8,9,10,12,12a,13,14,14a-hexadecahydropicen-3-ol	24721046	FALSE	C12(C3(C(C4C(CC3)(CCC(=C)C4C)C)CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C)C
MOL006101	0.4108	0.5892	0.7050	Centipedae Herba	(3S,4aR,6aR,6aS,6bR,8aR,12S,12aS,14aR,14bR)-4,4,6a,6b,8a,12,14b-heptamethyl-11-methylene-1,2,3,4a,5,6,6a,7,8,9,10,12,12a,13,14,14a-hexadecahydropicen-3-ol	24721046	FALSE	C12(C3(C(C4C(CC3)(CCC(=C)C4C)C)CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C)C

MOL006101	0.4108	0.5892	0.7050	Herba Cirsii	(3S,4aR,6aR,6aS,6bR,8aR,12S,12aS,14aR,14bR)-4,4,6a,6b,8a,12,14b-heptamethyl-11-methylene-1,2,3,4a,5,6,6a,7,8,9,10,12,12a,13,14,14a-hexadecahydropicen-3-ol	24721046	FALSE	C12(C3(C(C4C(CC3)(CCC(=C)C4C)C)CCC1C1(C(CC2)C(C(CC1)O)(C)C)C)C)C
MOL006102	0.3954	0.6046	0.6815	Calendula Officinalis	ursendiol	Not Available	FALSE	C1(C(CC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C)C(C)C4C3=CCC21)C)O)O
MOL006104	0.8369	0.1631	0.7088	Fructus Carotae	daucene	12309050	FALSE	C12(C(=C(CC1)C(C)C)CCC(=CC2)C)C
MOL006104	0.8369	0.1631	0.7088	Rose Rugosae Flos	daucene	12309050	FALSE	C12(C(=C(CC1)C(C)C)CCC(=CC2)C)C
MOL006105	0.7653	0.2347	0.6020	Fructus Carotae	Petroselinic acid	5281125	FALSE	C(=C\CCCCC(=O)O)\CCCCCCCCCC
MOL006105	0.7653	0.2347	0.6020	Foeniculi Fructus	Petroselinic acid	5281125	FALSE	C(=C\CCCCC(=O)O)\CCCCCCCCCC
MOL006105	0.7653	0.2347	0.6020	Ginkgo Folium	Petroselinic acid	5281125	FALSE	C(=C\CCCCC(=O)O)\CCCCCCCCCC
MOL006106	0.9435	0.0565	0.9586	Fructus Carotae	(6R)-6-pentyloxan-2-one	1714996	FALSE	C1(OC(=O)CCC1)CCCCC
MOL006108	0.9364	0.0636	0.9572	Pollen Typhae	Synthol	7043	FALSE	c1(c(cccc1)OC)OC
MOL006108	0.9364	0.0636	0.9572	Humulus Scandens (Lour.) Merr.	Synthol	7043	FALSE	c1(c(cccc1)OC)OC
MOL006109	0.8916	0.1084	0.9679	Capsici Fructus	PYR	1060	FALSE	C(=O)(C(=O)O)C
MOL006109	0.8916	0.1084	0.9679	Pollen Typhae	PYR	1060	FALSE	C(=O)(C(=O)O)C
MOL006109	0.8916	0.1084	0.9679	Capsellae Herba	PYR	1060	FALSE	C(=O)(C(=O)O)C
MOL006110	0.9091	0.0909	0.7179	Pollen Typhae	2,7-Dimethylnaphthalene	11396	FALSE	c12c(cc(cc1)C)cc(cc2)C
MOL006110	0.9091	0.0909	0.7179	Achyranthis Asperae Herba	2,7-Dimethylnaphthalene	11396	FALSE	c12c(cc(cc1)C)cc(cc2)C
MOL006110	0.9091	0.0909	0.7179	Gossampiniflos	2,7-Dimethylnaphthalene	11396	FALSE	c12c(cc(cc1)C)cc(cc2)C

MOL006114	0.8776	0.1224	0.8197	Pollen Typhae	kaempferol-3-O-α-L-rhamnosyl(1→2)-β-D-glucoside	Not Available	FALSE	c1(cc(c2c(c1)CC(=C(C2=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)O)O
MOL006115	0.9242	0.0758	0.7741	Pollen Typhae	kaempferol-3-O-α-L-rhamnosyl(1→2)-β-D-glucoside_qt	Not Available	FALSE	c1(cc(c2c(c1)CC(=C(C2=O)O)c1ccc(cc1)O)O)O
MOL006116	0.8738	0.1262	0.6843	Pollen Typhae	typhic acid	Not Available	FALSE	O(C(=O)C1=CC(Cc2c1cccc2/C(=C/C(=O)O)/O)C(=O)O)C(CC)C
MOL006119	0.8207	0.1793	0.6861	Zingiber Officinale Roscoe	2-methyltridec-1-ene	140334	FALSE	C(=C)(CCCCCCCCCCC)C
MOL006120	0.7435	0.2565	0.7747	Zingiber Officinale Roscoe	8-Gingerol	Not Available	FALSE	c1(cc(cc2c1CC(C(O2)c1cc2c(c(=O)c(c1)O)c(c(cc2C1Oc2c(CC1OC(=O)c1cc(c(c(c1)O)O)O)c(cc(c2)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O
MOL006122	0.9275	0.0725	0.9343	Zingiber Officinale Roscoe	HEPTENE	11610	FALSE	C(=C)CCCCC
MOL006123	0.8991	0.1009	0.8310	Zingiber Officinale Roscoe	zingiberol	Not Available	FALSE	C1(C=CC(CC1)(C)O)C(CCC=C(C)C)C
MOL006125	0.7642	0.2358	0.8446	Zingiber Officinale Roscoe	Gingerdione	162952	FALSE	C(CC(=O)CC(=O)CCCCC)c1cc(c(cc1)O)OC
MOL006126	0.5692	0.4308	0.7444	Schisandrae Chinensis Fructus	Hexahydrocurcumin	25763830	FALSE	C(CC(=O)CC(CCc1cc(c(cc1)O)OC)O)c1cc(c(cc1)O)OC
MOL006126	0.5692	0.4308	0.7444	Zingiber Officinale Roscoe	Hexahydrocurcumin	25763830	FALSE	C(CC(=O)CC(CCc1cc(c(cc1)O)OC)O)c1cc(c(cc1)O)OC
MOL006127	0.7342	0.2658	0.8258	Zingiber Officinale Roscoe	6-Dehydrogingerdione	5316449	FALSE	C(=C\C(=C\C(=O)CCCCC)\O)\c1cc(c(cc1)O)OC
MOL006128	0.5417	0.4583	0.6564	Zingiber Officinale Roscoe	gingerglycolipid)A	Not Available	FALSE	C1(C(C(C(C(O1)OCC(O)COC(=O)CCCCCCC/C=C\C/C=C\C/C=C\CC)O)O)O)COC1OC(C(C(C1O)O)O)CO
MOL006129	0.4070	0.5930	0.7563	Zingiber Officinale Roscoe	6-methylgingediacetate2	Not Available	FALSE	COc1cc(CCC(OC(=O)C)CC(CCCCC)OC(=O)C)ccc1OC
MOL006130	0.6252	0.3748	0.8156	Zingiber Officinale Roscoe	8-gingerdione	14440537	FALSE	c1c(c(cc(c1)CCC(=O)CC(=O)CCCCCCC)OC)O
MOL006131	0.7435	0.2565	0.7747	Zingiber Officinale Roscoe	8-gingerol	467320	FALSE	c12c(c(C3Oc4c(CC3OC(=O)c3cc(c(c(c3)O)O)O)c(cc(c4)O)O)cc(c2O)O)cc(C2Oc3c(CC2OC(=O)c2cc(c(c(c2)O)O)O)c(cc(c3)O)O)cc(c1=O)O
MOL006132	0.8677	0.1323	0.8807	Zingiber Officinale Roscoe	[5]-gingerol	Not Available	FALSE	c1c(c(cc(c1)CCC(=O)CC(CCCC)O)OC)O
MOL006133	0.5561	0.4439	0.7575	Zingiber Officinale Roscoe	(E)-1-(4-hydroxy-3-methoxyphenyl)dodec-4-en-3-one	6442560	FALSE	C(CCCC/C=C/C(=O)CCc1ccc(c(c1)OC)O)CC

MOL006134	0.8636	0.1364	0.8131	Rubia Cordifolia	1,3,6-trihydroxy-2-methylanthraquinone-3-O-(3'-O-acetyl)-α-rhamnosyl(1→2)-glucoside	Not Available	FALSE	c1c(cc2c(c1)C(=O)c1c(C2=O)cc(c(c1O)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)O)OC(=O)C)O)CO)O
MOL006135	0.9094	0.0906	0.7036	Rubia Cordifolia	2-Methyl-1,3,6-trihydroxyanthraquinone	5319801	FALSE	c1c(cc2c(c1)C(=O)c1c(C2=O)cc(c(c1O)C)O)O
MOL006136	0.8639	0.1361	0.7759	Rubia Cordifolia	1,3,6-trihydroxy-2-methylanthraquinone-3-O-(6'-O-acetyl)-α-rhamnosyl(1→2)-β-glucoside	Not Available	FALSE	c1c(cc2c(c1)C(=O)c1c(C2=O)cc(c(c1O)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)O)O)O)OC(=O)C)O
MOL006137	0.8710	0.1290	0.8179	Rubia Cordifolia	1,3,6-trihydroxy-2-methylanthraquinone-3-O-α-rhamnosyl-(1→2)-β-glucoside	57335470	FALSE	c1(c(c(cc2C(=O)c3cc(ccc3C(=O)c12)O)OC1C(OC2C(O)C(O)C(O)C(O2)C)C(O)C(O)C(O1)CO)C)O
MOL006138	0.8610	0.1390	0.8071	Rubia Cordifolia	2-Methyl-1,3,6-trihydroxy-9,10-anthraquinone-3-O-beta-D-xylosyl-(1-->2)-beta-D-(6'-O-acetyl) glucoside	5319802	FALSE	c1(c(c(cc2C(=O)c3cc(ccc3C(=O)c12)O)OC1C(OC2C(O)C(O)C(O)CO2)C(O)C(O)C(O1)COC(=O)C)C)O
MOL006139	0.8219	0.1781	0.8330	Rubia Cordifolia	1,3-dimethoxy-2-carboxyanthraquinone	Not Available	FALSE	c1ccc2c(c1)C(=O)c1c(C2=O)cc(c(c1OC)C(=O)O)OC

MOL006140	0.8718	0.1282	0.7779	Rubia Cordifolia	1,3-dihydroxy-2-hydroxymthyl anthraquinone-3-O-xylosyl(1→6)-glucoside	Not Available	FALSE	c1c(cc2c(c1)C(=O)c1c(C2=O)cc(c(c1O)CO)OC1OC(C(C(C1O)O)O)OC1OCC(C(C1O)O)O)C
MOL006141	0.8819	0.1181	0.7930	Rubia Cordifolia	1,3-dihydroxy-2-hydroxymthyl anthraquinone-3-O-xylosyl(1→6)-glucoside_qt	Not Available	FALSE	c1c(cc2c(c1)C(=O)c1c(C2=O)cc(c(c1O)CO)O)C
MOL006142	0.8071	0.1929	0.8017	Rubia Cordifolia	Ibericin	28578	FALSE	O(Cc1c(O)c2c(C(=O)c3c(C2=O)cccc3)cc1O)CC
MOL006143	0.8396	0.1604	0.8157	Rubia Cordifolia	1,3-dihydroxy-3-methylanthraquinone	Not Available	FALSE	c12c(C(=O)C3=C(C1=O)C(=CC(C3)(O)C)O)cccc2
MOL006144	0.8343	0.1657	0.8146	Rubia Cordifolia	1,4-dihydroxy-6-methyl-9,10-anthraquinone	11230545	FALSE	c1c(cc2c(c1)C(=O)c1c(C2=O)c(ccc1O)O)C
MOL006145	0.7805	0.2195	0.7331	Rubia Cordifolia	1-hydroxy-2-methyl-6-methoxyanthraquinone	Not Available	FALSE	c1(c(ccc2C(=O)c3cc(ccc3C(=O)c12)OC)C)O
MOL006146	0.8259	0.1741	0.8485	Rubia Cordifolia	Danthron methyl derivative	620286	FALSE	O(c1c2c(C(=O)c3c(C2=O)c(O)ccc3)ccc1)C
MOL006147	0.7073	0.2927	0.8186	Rubia Cordifolia	Alizarin-2-methylether	80103	FALSE	c1(c(ccc2C(=O)c3ccccc3C(=O)c12)OC)O
MOL006147	0.7073	0.2927	0.8186	Morindae Officinalis Radix	Alizarin-2-methylether	80103	FALSE	c1(c(ccc2C(=O)c3ccccc3C(=O)c12)OC)O
MOL006148	0.8509	0.1491	0.8010	Morindae Officinalis Radix	Deoxylucidin	32209	FALSE	Oc1c2c(C(=O)c3c(C2=O)cccc3)ccc1CO
MOL006148	0.8509	0.1491	0.8010	Rubia Cordifolia	Deoxylucidin	32209	FALSE	Oc1c2c(C(=O)c3c(C2=O)cccc3)ccc1CO

MOL006149	0.7576	0.2424	0.7786	Junci Medulla	7-hydroxy-8-methyl-4-vinyl-9,10-dihydrophenanthrene-1-carboxylic acid	9993796	FALSE	c1(c2c(c(cc1)C(=O)O)CCc1c2ccc(c1C)O)C=C
MOL006149	0.7576	0.2424	0.7786	Rubia Cordifolia	7-hydroxy-8-methyl-4-vinyl-9,10-dihydrophenanthrene-1-carboxylic acid	9993796	FALSE	c1(c2c(c(cc1)C(=O)O)CCc1c2ccc(c1C)O)C=C
MOL006150	0.6390	0.3610	0.7683	Rubia Cordifolia	1-acetoxy-6-hydroxy2-methylanthraquinone-3-O-α-rhamnosyl(1→4)-α-glucoside	Not Available	FALSE	c1c(cc2c(c1)C(=O)c1c(C2=O)cc(c(c1OC(=C)C)C)OC1OC(C(C(C1O)O)CC1OC(C(C(C1O)O)O)C)CO)O
MOL006151	0.6606	0.3394	0.6910	Rubia Cordifolia	1-acetoxy-6-hydroxy2-methylanthraquinone-3-O-α-rhamnosyl(1→4)-α-glucoside_qt	Not Available	FALSE	c1c(cc2c(c1)C(=O)c1c(C2=O)cc(c(c1OC(=C)C)C)O)O
MOL006152	0.9298	0.0702	0.8453	Rubia Cordifolia	2-carbamoyl-3-hydroxy-1,4-naphthoquinone	Not Available	FALSE	c1ccc2c(c1)C(=O)C(C(C2=O)O)C(=O)N
MOL006153	0.7412	0.2588	0.8385	Rubia Cordifolia	2'-hydroxymollugin	Not Available	FALSE	c1ccc2c(c1)c(c(c1c2OC(C(C1)O)(C)C)C(=O)OC)O

MOL006154	0.8383	0.1617	0.8272	Rubia Cordifolia	2-carboxymethyl-3-prenyl-2,3-epoxy-1,4-naphthoquinone	Not Available	FALSE	c1ccc2c(c1)C(=O)C1(C(C2=O)(O1)C=C(C)C)C(=O)OC
MOL006155	0.9055	0.0945	0.7991	Rubia Cordifolia	4-hydroxy-9,10-dioxoanthracene-2-carboxylic acid	179447	FALSE	c1ccc2c(c1)C(=O)c1c(C2=O)c(cc(c1)C(=O)O)O
MOL006156	0.9242	0.0758	0.8542	Rubia Cordifolia	6-methoxygeniposidic acid	Not Available	FALSE	C12C(C(CC=C1C(=O)O)O)C(=CC2OC)CO
MOL006157	0.9053	0.0947	0.7824	Rubia Cordifolia	Verantin	6683	FALSE	c12c(C(=O)c3c(C1=O)cccc3)c(cc(c2O)O)O
MOL006157	0.9053	0.0947	0.7824	Cassiae Semen	Verantin	6683	FALSE	c12c(C(=O)c3c(C1=O)cccc3)c(cc(c2O)O)O
MOL006158	0.8576	0.1424	0.7840	Rubia Cordifolia	Rubiadin	124062	FALSE	c12c(C(=O)c3c(C1=O)cccc3)cc(c(c2O)C)O
MOL006158	0.8576	0.1424	0.7840	Morindae Officinalis Radix	Rubiadin	124062	FALSE	c12c(C(=O)c3c(C1=O)cccc3)cc(c(c2O)C)O
MOL006159	0.8774	0.1226	0.7604	Rubia Cordifolia	Rubianic acid	92101	FALSE	c1(c(ccc2C(=O)c3ccccc3C(=O)c12)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)CO1)O
MOL006160	0.8615	0.1385	0.7770	Rubia Cordifolia	Alizarin	6293	FALSE	c1(c(ccc2C(=O)c3ccccc3C(=O)c12)O)O
MOL006161	0.8468	0.1532	0.8098	Rubia Cordifolia	2-Methyl-1,4-dihydroxyanthraquinone	99300	FALSE	c1(c(cc(c2C(=O)c3ccccc3C(=O)c12)O)C)O
MOL006162	0.9055	0.0945	0.7786	Rubia Cordifolia	Nordamnacanthal	160712	FALSE	c1(c(c(cc2C(=O)c3ccccc3C(=O)c12)O)C=O)O
MOL006163	0.7927	0.2073	0.8011	Rubia Cordifolia	1-Hydroxy-2-methylanthraquinone	160817	FALSE	c12c(C(=O)c3c(C1=O)cccc3)ccc(c2O)C
MOL006163	0.7927	0.2073	0.8011	Morindae Officinalis Radix	1-Hydroxy-2-methylanthraquinone	160817	FALSE	c12c(C(=O)c3c(C1=O)cccc3)ccc(c2O)C
MOL006164	0.2710	0.7290	0.6242	Rubia Cordifolia	Pallasone	5318483	FALSE	C1(=CC(=O)C=C(C1=O)OC)CCCCCCCCC/C=C\CCCCC
MOL006165	0.9040	0.0960	0.8446	Rubia Cordifolia	methyl 5-hydroxybenzo[g]benzofuran-4-carboxylate	10354359	FALSE	o1c2c(cc1)c(c(c1ccccc21)O)C(=O)OC
MOL006166	0.8327	0.1673	0.8306	Rubia Cordifolia	Lucidin omega-methyl ether	149782	FALSE	c1(c(c(cc2C(=O)c3ccccc3C(=O)c12)O)COC)O

MOL006167	0.6723	0.3277	0.8743	Rubia Cordifolia	methyl 6-hydroxy-2,2-dimethyl-3,4-dihydrobenzo[h]chromene-5-carboxylate	10779560	FALSE	O1C(CCc2c1c1c(c(O)c2C(=O)OC)cccc1)(C)C
MOL006168	0.6254	0.3746	0.6548	Rubia Cordifolia	rubioncolin B	Not Available	FALSE	C12C3(C(=COC3)C3C(O1)C1=CC=CC(C1C(=C3)O)C(=O)OC)Oc1c2cc(c2C(C(=O)CC(c12)(C)C)C(=O)OC)O
MOL006169	0.8834	0.1166	0.7813	Rubia Cordifolia	lucidin primeveroside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(c(O)c2c(c1)C(=O)c1c(C2=O)cccc1)CO)COC1OCC(O)C(O)C1O
MOL006170	0.9208	0.0792	0.7717	Rubia Cordifolia	Henine	10163	FALSE	Oc1c(c(O)c2c(c1)C(=O)c1c(C2=O)cccc1)CO
MOL006171	0.3190	0.6810	0.7466	Rubia Cordifolia	rubiprasin B	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2(C(=O)CC2C1(CCC1C2(CCC(C1(C)C)OC(=O)C)C)C)C)C)C
MOL006172	0.8659	0.1341	0.8620	Rubia Cordifolia	Rubilactone	132415	FALSE	o1c2c3c(c(O)c(c2ccc1=O)C(=O)OC)cccc3
MOL006173	0.3759	0.6241	0.7336	Rubia Cordifolia	Rubiatriol	183864	FALSE	OC1C2C3(C(C4C(=CC3)C3(C(CC4)C(C(O)CC3)(C)C)C)(CCC2(C(C1)C(C)C)C)C)C
MOL006174	0.7125	0.2875	0.8788	Rubia Cordifolia	Xyloidone	72734	FALSE	O1C(C=CC2=C1C(=O)c1c(C2=O)cccc1)(C)C
MOL006175	0.8880	0.1120	0.8148	Rubia Cordifolia	9-oxo-4-xanthenecarboxylic acid	410100	FALSE	o1c2c(c(=O)c3c1cccc3)cccc2C(=O)O
MOL006176	0.8574	0.1426	0.8126	Agrimonia Eupatoria	kaempferol-7-O-rhamnoside	Not Available	FALSE	c1(ccc(cc1)c1c(c(=O)c2c(o1)cc(cc2O)OC1OC(C(C(C1O)O)O)C)O)O
MOL006177	0.7290	0.2710	0.7293	Agrimonia Eupatoria	1β,2α,3β,19α-tetrahydroxyurs-12-en-28-oic acid	Not Available	FALSE	C1(C(C(C2C(C1O)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1(C)O)C)C(=O)O)C)C)(C)C)O)O
MOL006178	0.8878	0.1122	0.7990	Agrimonia Eupatoria	agrimoniin	14057208	FALSE	OC(=O)c1c(Oc2cc(C(=O)O)cc(O)c2O)c(O)c(O)c(O)c1
MOL006179	0.8837	0.1163	0.7770	Agrimonia Eupatoria	2-(6-carboxy-2,3,4-trihydroxyphenyl)-3,4,5-trihydroxybenzoic acid	10315050	FALSE	OC(=O)c1c(c2c(C(=O)O)cc(O)c(O)c2O)c(O)c(O)c(O)c1
MOL006179	0.8837	0.1163	0.7770	Radix Paeoniae Rubra	2-(6-carboxy-2,3,4-trihydroxyphenyl)-3,4,5-trihydroxybenzoic acid	10315050	FALSE	OC(=O)c1c(c2c(C(=O)O)cc(O)c(O)c2O)c(O)c(O)c(O)c1

MOL006179	0.8837	0.1163	0.7770	Quisqualis Indica	2-(6-carboxy-2,3,4-trihydroxyphenyl)-3,4,5-trihydroxybenzoic acid	10315050	FALSE	OC(=O)c1c(c2c(C(=O)O)cc(O)c(O)c2O)c(O)c(O)c(O)c1
MOL006179	0.8837	0.1163	0.7770	Rose Rugosae Flos	2-(6-carboxy-2,3,4-trihydroxyphenyl)-3,4,5-trihydroxybenzoic acid	10315050	FALSE	OC(=O)c1c(c2c(C(=O)O)cc(O)c(O)c2O)c(O)c(O)c(O)c1
MOL006181	0.8905	0.1095	0.8395	Agrimonia Eupatoria	(-)-alpha-Bisabolol	442343	FALSE	C1(C(CCC=C(C)C)(C)O)CCC(=CC1)C
MOL006184	0.9022	0.0978	0.9616	Agrimonia Eupatoria	3R-hydroxy-butanoic acid	92135	FALSE	C(=O)(CC(C)O)O
MOL006186	0.6765	0.3235	0.8193	Agrimonia Eupatoria	gdmonolide	Not Available	FALSE	O1C(Cc2c(C1=O)c(O)cc(O)c2)CCc1ccc(OC)cc1
MOL006189	0.9352	0.0648	0.9530	Perilla Frutescens	ZINC04521547	7269382	FALSE	C(CCCC)(C=C)O
MOL006189	0.9352	0.0648	0.9530	Aristolochiae Fructus	ZINC04521547	7269382	FALSE	C(CCCC)(C=C)O
MOL006190	0.8533	0.1467	0.8162	Perilla Frutescens	[(Z)-2-(3,5-dihydroxyphenyl)vinyl] (E)-3-(3,4-dihydroxyphenyl)prop-2-enoate	5316820	FALSE	c1(cc(cc(c1)/C=C\OC(=O)/C=C/c1cc(c(cc1)O)O)O)O
MOL006191	0.8636	0.1364	0.8299	Perilla Frutescens	[(Z)-2-(3,4-dihydroxyphenyl)vinyl] (E)-3-(3,4-dihydroxyphenyl)prop-2-enoate	5316819	FALSE	c1c(c(cc(c1)/C=C\OC(=O)/C=C/c1cc(c(cc1)O)O)O)O

MOL006192	0.7753	0.2247	0.6866	Perilla Frutescens	(R,E)-3-(3-ethoxy-4-hydroxyphenyl)-2-((3-(3-ethoxy-4-hydroxyphenyl)acryloyl)oxy)propanoic acid	Not Available	FALSE	c1(c(ccc(c1)CC(OC(=O)/C=C/c1cc(c(cc1)O)OCC)C(=O)O)O)OCC
MOL006193	0.9362	0.0638	0.9453	Perilla Frutescens	Citralva	1551246	FALSE	C(#N)/C=C(/CCC=C(C)C)\C
MOL006194	0.9303	0.0697	0.8157	Perilla Frutescens	3-β-D-glucopyranosyl-3-epi-2-isocucurbic acid	Not Available	FALSE	C1(C(C(C(C(O1)OC1C(C(CC1)C/C=C\CC)CC(=O)O)O)O)O)CO
MOL006195	0.9329	0.0671	0.9115	Perilla Frutescens	3-β-D-glucopyranosyl-3-epi-2-isocucurbic acid_qt	Not Available	FALSE	OC1C(C(CC1)C/C=C\CC)CC(=O)O
MOL006196	0.9420	0.0580	0.8865	Perilla Frutescens	3-β-D-glucopyranosyloxy-5-phenylvaleric acid	Not Available	FALSE	C1(C(C(C(C(O1)OC(CC(=O)O)CCc1ccccc1)O)O)O)CO
MOL006197	0.9554	0.0446	0.9600	Perilla Frutescens	(3R)-3-hydroxy-5-phenyl-valeric acid	9815528	FALSE	OC(CC(=O)O)CCc1ccccc1
MOL006198	0.9700	0.0300	0.7745	Maydis Seigma	APIOL	10659	FALSE	c12c(c(cc(c1OC)CC=C)OC)OCO2
MOL006198	0.9700	0.0300	0.7745	Perilla Frutescens	APIOL	10659	FALSE	c12c(c(cc(c1OC)CC=C)OC)OCO2
MOL006198	0.9700	0.0300	0.7745	Notopterygii Rhizoma Et Radix	APIOL	10659	FALSE	c12c(c(cc(c1OC)CC=C)OC)OCO2
MOL006198	0.9700	0.0300	0.7745	Foeniculi Fructus	APIOL	10659	FALSE	c12c(c(cc(c1OC)CC=C)OC)OCO2
MOL006199	0.9600	0.0400	0.9517	Perilla Frutescens	4-(2-Butyl)phenol	38989049	FALSE	c1(ccc(cc1)O)C(CC)C
MOL006200	0.9349	0.0651	0.7216	Perilla Frutescens	5'-β-D-glucopyranosyloxyjasmonic acid	Not Available	FALSE	C1(C(C(C(C(O1)OCC/C=C\CC1C(=O)CCC1CC(=O)O)O)O)O)CO
MOL006201	0.9509	0.0491	0.8701	Perilla Frutescens	Tuberonic acid	6443968	FALSE	OCC/C=C\CC1C(=O)CCC1CC(=O)O
MOL006202	0.7032	0.2968	0.6092	Perilla Frutescens	LAX	5280581	FALSE	C(=C\C/C=C\C/C=C\CCCCC)\CCCCCCC(=O)O

MOL006203	0.9025	0.0975	0.8998	Perilla Frutescens	SBB009008	76015	FALSE	C(CCCCCO)CCCC#C
MOL006205	0.9313	0.0687	0.9044	Perilla Frutescens	Benzyl alpha-D-mannopyranoside	10956572	FALSE	C1(C(C(C(C(O1)OCc1ccccc1)O)O)O)CO
MOL006207	0.6906	0.3094	0.7136	Perilla Frutescens	caffeylcyanin	Not Available	FALSE	c1(cc(c2c(c1)[o+]c(c(c2)OC1OC(C(C(C1)O)O)COC(=O)/C=C/c1ccc(c(c1)O)O)c1cc(c(cc1)O)O)OC1OC(C(C(C1O)O)O)CO)O
MOL006208	0.7739	0.2261	0.7299	Perilla Frutescens	caffeylmalonylcyanin	Not Available	FALSE	c1(cc(c2c(c1)[o+]c(c(c2)OC1OC(C(C(C1)O)O)COC(=O)/C=C/c1ccc(c(c1)O)O)c1cc(c(cc1)O)O)OC1OC(C(C(C1O)O)O)COC(=O)CC(=O)O)O
MOL006209	0.0384	0.9616	0.8145	Rose Rugosae Flos	cyanine	Not Available	FALSE	c12c(n(cc/c/1=C\c1c3c([n+](cc1)CCC(C)C)cccc3)CCC(C)C)cccc2
MOL006209	0.0384	0.9616	0.8145	Mori Fructus	cyanine	Not Available	FALSE	c12c(n(cc/c/1=C\c1c3c([n+](cc1)CCC(C)C)cccc3)CCC(C)C)cccc2
MOL006209	0.0384	0.9616	0.8145	Lycii Fructus	cyanine	Not Available	FALSE	c12c(n(cc/c/1=C\c1c3c([n+](cc1)CCC(C)C)cccc3)CCC(C)C)cccc2
MOL006209	0.0384	0.9616	0.8145	Perilla Frutescens	cyanine	Not Available	FALSE	c12c(n(cc/c/1=C\c1c3c([n+](cc1)CCC(C)C)cccc3)CCC(C)C)cccc2
MOL006210	0.9191	0.0809	0.8081	Perilla Frutescens	eugenyl-β-D-glucopyranoside(cirtrusinc)	Not Available	FALSE	c1(c(c(ccc1)CC=C)OC)OC1OC(C(C(C1O)O)O)CO
MOL006211	0.9268	0.0732	0.8824	Benzoinum	3-Allyl-2-methoxyphenol	596373	FALSE	c1(c(c(ccc1)CC=C)OC)O
MOL006211	0.9268	0.0732	0.8824	Perilla Frutescens	3-Allyl-2-methoxyphenol	596373	FALSE	c1(c(c(ccc1)CC=C)OC)O
MOL006212	0.9403	0.0597	0.9153	Perilla Frutescens	FERULIC ACID METHYL ESTER	10176654	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)OC)OC
MOL006213	0.9106	0.0894	0.8124	Perilla Frutescens	linaly-β-D-glucopyranoside	38358979	FALSE	C(CCC=C(C)C)(C=C)(OC1OC(C(C(C1O)O)O)CO)C
MOL006214	0.3247	0.6753	0.9535	Hippophae Fructus	progesterone	5994	TRUE	C12C(C3C(CC2)(C(CC3)C(=O)C)C)CCC2=CC(=O)CCC12C
MOL006214	0.3247	0.6753	0.9535	Perilla Frutescens	progesterone	5994	TRUE	C12C(C3C(CC2)(C(CC3)C(=O)C)C)CCC2=CC(=O)CCC12C
MOL006215	0.8944	0.1056	0.8177	Perilla Frutescens	luteolin-3,7-diglucoside	Not Available	FALSE	c12c(c(=O)c(co2)c2cc(OC3OC(C(C(C3O)O)O)CO)c(cc2)O)c(cc(c1)OC1OC(C(C(C1O)O)O)CO)O
MOL006216	0.9324	0.0676	0.8861	Perilla Frutescens	Santol	5281801	FALSE	c12c(c(=O)c(co2)c2cc(O)c(cc2)O)c(cc(c1)O)O

MOL006217	0.7413	0.2587	0.7177	Perilla Frutescens	malonylshisonin	Not Available	FALSE	c1(cc(c2c(c1)[o+]c(c(c2)OC1OC(C(C(C1O)O)O)O)CO C(=O)/C=C/c1ccc(cc1)O)c1cc(c(cc1)O)O)OC1OC(C (C(C1O)O)O)COC(=C)C(=O)O)O
MOL006218	0.8890	0.1110	0.9318	Ailanthi Cortex	Methyl caffeate	689075	FALSE	C(=C\c1cc(c(cc1)O)O)/C(=O)OC
MOL006218	0.8890	0.1110	0.9318	Lonicerae Japonicae Flos	Methyl caffeate	689075	FALSE	C(=C\c1cc(c(cc1)O)O)/C(=O)OC
MOL006218	0.8890	0.1110	0.9318	Cimicifugae Rhizoma	Methyl caffeate	689075	FALSE	C(=C\c1cc(c(cc1)O)O)/C(=O)OC
MOL006218	0.8890	0.1110	0.9318	Perilla Frutescens	Methyl caffeate	689075	FALSE	C(=C\c1cc(c(cc1)O)O)/C(=O)OC
MOL006218	0.8890	0.1110	0.9318	Plantaginis Herba	Methyl caffeate	689075	FALSE	C(=C\c1cc(c(cc1)O)O)/C(=O)OC
MOL006219	0.9165	0.0835	0.9288	Lilii Bulbus	Clorius	7150	FALSE	c1(C(=O)OC)ccccc1
MOL006219	0.9165	0.0835	0.9288	Trollius Chinensis	Clorius	7150	FALSE	c1(C(=O)OC)ccccc1
MOL006219	0.9165	0.0835	0.9288	Perilla Frutescens	Clorius	7150	FALSE	c1(C(=O)OC)ccccc1
MOL006219	0.9165	0.0835	0.9288	Ephedra Herba	Clorius	7150	FALSE	c1(C(=O)OC)ccccc1
MOL006219	0.9165	0.0835	0.9288	Puerariae Flos	Clorius	7150	FALSE	c1(C(=O)OC)ccccc1
MOL006219	0.9165	0.0835	0.9288	Benzoinum	Clorius	7150	FALSE	c1(C(=O)OC)ccccc1
MOL006219	0.9165	0.0835	0.9288	Menthae Herba	Clorius	7150	FALSE	c1(C(=O)OC)ccccc1
MOL006219	0.9165	0.0835	0.9288	Daturae Flos	Clorius	7150	FALSE	c1(C(=O)OC)ccccc1
MOL006219	0.9165	0.0835	0.9288	Caryophylliflos	Clorius	7150	FALSE	c1(C(=O)OC)ccccc1
MOL006221	0.9187	0.0813	0.8740	Perilla Frutescens	prunasin	Not Available	FALSE	C1(OC(c2ccccc2)C#N)OC(C(C(C1O)O)O)CO
MOL006221	0.9187	0.0813	0.8740	Amygdalus Communis Vas	prunasin	Not Available	FALSE	C1(OC(c2ccccc2)C#N)OC(C(C(C1O)O)O)CO
MOL006222	0.9187	0.0813	0.8740	Perilla Frutescens	Sambunigrin	Not Available	FALSE	C1(C(C(C(C(O1)OC(c1ccccc1)C#N)O)O)O)CO
MOL006225	0.9387	0.0613	0.9258	Perilla Frutescens	vinyl (E)-3-(3,4-dihydroxyphenyl)prop-2-enoate	11127419	FALSE	C(=C\c1cc(c(cc1)O)O)/C(=O)OC=C
MOL006227	0.9490	0.0510	0.8902	Moslae Herba	Elsholtziaketone	521240	FALSE	C(=O)(CC(C)C)c1occc1C
MOL006227	0.9490	0.0510	0.8902	Perilla Frutescens	Elsholtziaketone	521240	FALSE	C(=O)(CC(C)C)c1occc1C

MOL006228	0.9225	0.0775	0.8281	Perilla Frutescens	[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl] (4S)-4-prop-1-en-2-ylcyclohexene-1-carboxylate	21631012	FALSE	C1(C(C(OC(C1O)CO)OC(=O)C1=CCC(CC1)C(=C)C)O)O
MOL006229	0.9381	0.0619	0.8550	Perilla Frutescens	perilloside C	Not Available	FALSE	C1(CCC(CC1)COC1OC(C(C(C1O)O)O)O)C(=C)C
MOL006230	0.9552	0.0448	0.9745	Perilla Frutescens	perilloside c_qt	519954	FALSE	C1CC(CCC1C(=C)C)CO
MOL006231	0.9147	0.0853	0.8175	Perilla Frutescens	perilloside D	21631019	FALSE	C1(CCC(CC1)COC1OC(C(C(C1O)O)O)CO)C(=C)C
MOL006232	0.9318	0.0682	0.9542	Perilla Frutescens	Perilla ketone	68381	FALSE	c1(ccoc1)C(=O)CCC(C)C
MOL006233	0.9213	0.0787	0.9047	Dictamni Cortex	3'-O-methyl taxifolin	Not Available	FALSE	c1(cc2c(c(c1)O)C(=O)C(C(O2)c1cc(c(cc1)O)OC)O)O
MOL006234	0.8701	0.1299	0.6067	Caryophylliflos	β-maaliene	Not Available	FALSE	C12C(C1(C)C)CCC1(C2=C(CCC1)C)C
MOL006234	0.8701	0.1299	0.6067	Dictamni Cortex	β-maaliene	Not Available	FALSE	C12C(C1(C)C)CCC1(C2=C(CCC1)C)C
MOL006234	0.8701	0.1299	0.6067	Et Radix Patriniae Rhizoma	β-maaliene	Not Available	FALSE	C12C(C1(C)C)CCC1(C2=C(CCC1)C)C
MOL006235	0.7524	0.2476	0.8234	Wikstroemiae Indicae Rasix	Dasycarpamin	6325017	FALSE	c1(c(ccc2c1nc(c(c2OC)/C=C/C(C)C)O)OC)OC
MOL006235	0.7524	0.2476	0.8234	Dictamni Cortex	Dasycarpamin	6325017	FALSE	c1(c(ccc2c1nc(c(c2OC)/C=C/C(C)C)O)OC)OC
MOL006236	0.6798	0.3202	0.7061	Dictamni Cortex	Limonin diosphenol	Not Available	FALSE	O1C23C4(C(C56C(=C(O)C4=O)C(OC5CC(=O)OC6)(C)C)CCC2(C(OC(=O)C13)c1ccoc1)C)C
MOL006237	0.8332	0.1668	0.8639	Dictamni Cortex	O-ethylnor-γ-fagarine	71333996	FALSE	n1c2c(c(c3cccc(c13)OC)OCC)cco2
MOL006238	0.8443	0.1557	0.7805	Dictamni Cortex	O-ethylnordictamnine	45094326	FALSE	n1c2c(c(c3ccccc13)OCC)cco2
MOL006239	0.8869	0.1131	0.8349	Dictamni Cortex	Ptelein	159650	FALSE	o1c2nc3c(c(OC)c2cc1)cc(OC)cc3
MOL006240	0.9273	0.0727	0.8667	Arum Ternatum Thunb.	THM	5789	FALSE	O1C(n2cc(c(=O)[nH]c2=O)C)CC(O)C1CO
MOL006240	0.9273	0.0727	0.8667	Euphorbiae Helioscopiae Herba	THM	5789	FALSE	O1C(n2cc(c(=O)[nH]c2=O)C)CC(O)C1CO
MOL006240	0.9273	0.0727	0.8667	Sargassum	THM	5789	FALSE	O1C(n2cc(c(=O)[nH]c2=O)C)CC(O)C1CO
MOL006240	0.9273	0.0727	0.8667	Dictamni Cortex	THM	5789	FALSE	O1C(n2cc(c(=O)[nH]c2=O)C)CC(O)C1CO
MOL006240	0.9273	0.0727	0.8667	Allium Azureum Ledeb.	THM	5789	FALSE	O1C(n2cc(c(=O)[nH]c2=O)C)CC(O)C1CO
MOL006241	0.4845	0.5155	0.6593	Dictamni Cortex	azadirachtin	Not Available	FALSE	C1C(C2(C3(C4(C1OC(=O)/C(=C/C)/C)C(C(C(C3OC2)O)(C12C(C3CC1OC1C3(C=CO1)O)O2)C)C(OC4)(O)C(=O)OC)C)C(=O)OC)OC(=O)C
MOL006242	0.8707	0.1293	0.6294	Dictamni Cortex	beta-elemol	Not Available	FALSE	C1(C(CC(CC1)C(C)(O)C)C(C)C)(CC)C
MOL006243	0.8301	0.1699	0.8096	Dictamni Cortex	calodendrolid	478835	FALSE	C1C=C(C23C(C1)(C(OC(=O)C2O3)c1cocc1)C)C

MOL006244	0.8641	0.1359	0.8299	Dictamni Cortex	(1R,4R,6S,8aR)-1-(3-furyl)-4,6-dihydroxy-5,8a-dimethyl-4,6,7,8-tetrahydro-1H-isochromen-3-one	24799849	FALSE	C1C(C(=C2C(C1)(C(OC(=O)C2O)c1cocc1)C)C)O
MOL006245	0.9005	0.0995	0.7637	Dictamni Cortex	6beta-hydroxyfraxinellone	Not Available	FALSE	C1C(C(=C2C(C1)(C(OC2=O)C1COCC1)C)C)O
MOL006246	0.8641	0.1359	0.8299	Dictamni Cortex	(1R,4S,6R,8aR)-1-(3-furyl)-4,6-dihydroxy-5,8a-dimethyl-4,6,7,8-tetrahydro-1H-isochromen-3-one	24799852	FALSE	C1C(C(=C2C(C1)(C(OC(=O)C2O)c1cocc1)C)C)O
MOL006247	0.8641	0.1359	0.8299	Dictamni Cortex	dictamdiol	44448179	FALSE	C1C(C(=C2C(C1)(C(OC(=O)C2O)c1cocc1)C)C)O
MOL006248	0.9440	0.0560	0.8047	Dictamni Cortex	dictamnol	Not Available	FALSE	C1CC(C2C1C(CCCC2)C)(C)O
MOL006250	0.8392	0.1608	0.7040	Dictamni Cortex	dictamnoside, i	Not Available	FALSE	C1CC(C2C(C1O)(CCC(C2OOC1C(C(C(C(O1)(C)CO)O)O)O)O)C(C)(C)O)C)(O)C
MOL006251	0.8392	0.1608	0.7040	Dictamni Cortex	dictamnoside, j	Not Available	FALSE	C1CC(C2C(C1O)(CCC(C2OOC1C(C(C(C(O1)(C)CO)O)O)O)O)C(C)(C)O)C)(C)O
MOL006252	0.8790	0.1210	0.7118	Dictamni Cortex	dictamnoside, k	Not Available	FALSE	C1CC(C2C(C1O)(CCC(C2OOC1C(C(C(C(O1)(C)CO)O)O)O)O)C(C)(C)O)CO)(C)O
MOL006253	0.8679	0.1321	0.7160	Dictamni Cortex	dictamnoside, l	Not Available	FALSE	C1CC2(C3=CC(CCC3(C1O)O2)C(C)(C)OOC1C(C(C(C(O1)CO)O)O)O)O)C
MOL006254	0.6811	0.3189	0.6422	Dictamni Cortex	dictamnoside, n	Not Available	FALSE	C1(C(C(C(OC1(C)CO)OOC1(C2C(C(CC2)(O)CCC)C=CC(C1)O)CCC)O)O)O
MOL006255	0.3171	0.6829	0.7424	Dictamni Cortex	7alpha-acetyldihydronomilin	Not Available	FALSE	C1(=O)OC(C2C(C(C1)OC(=O)C)(C1C(C(C2)OC(=O)C)(C23C(CC1)(C(OC(=O)C2O3)c1cocc1)C)C)(C)C
MOL006256	0.7270	0.2730	0.6839	Dictamni Cortex	dictamnusine	Not Available	FALSE	C1(C(C(C(OC1CO)OC1CCC2(C(=C(C(=O)OC2c2occ2)O)C1C)C)O)O)O

MOL006257	0.8671	0.1329	0.8054	Dictamni Cortex	dictamnusine_qt	Not Available	FALSE	OC1CCC2(C(=C(C(=O)OC2c2cocc2)O)C1C)C
MOL006258	0.9172	0.0828	0.8238	Dictamni Cortex	Fraxinellone	124039	FALSE	O1C(C2(CCCC(=C2C1=O)C)C)c1ccoc1
MOL006258	0.9172	0.0828	0.8238	Meliae Cortex	Fraxinellone	124039	FALSE	O1C(C2(CCCC(=C2C1=O)C)C)c1ccoc1
MOL006259	0.9080	0.0920	0.7827	Dictamni Cortex	9alpha-Hydroxyfraxinellone	636856	FALSE	C1C(C(=C2C(C1)(C(OC2=O)c1cocc1)C)C)O
MOL006260	0.9134	0.0866	0.7905	Dictamni Cortex	isofraxinellone	Not Available	FALSE	C1C=C(C2C(C1)(C(OC2=O)C1COCC1)C)C
MOL006261	0.8871	0.1129	0.7854	Dictamni Cortex	Isomaculosidine	3083609	FALSE	o1c2n(c3c(c(=O)c2cc1)cc(OC)cc3OC)C
MOL006262	0.2916	0.7084	0.7456	Dictamni Cortex	7alpha-acetylobacunol	Not Available	FALSE	C1(=O)OC(C2C(C=C1)(C1C(C(C2)OC(=O)C)(C23C(CC1)(C(OC(=O)C2O3)c1cocc1)C)C)C)(C)C
MOL006263	0.6798	0.3202	0.7061	Dictamni Cortex	22318-10-1	Not Available	FALSE	C12OC(C3=C(C(=O)C4(C(C13COC(=O)C2)CCC1(C24C(C(=O)OC1c1cocc1)O2)C)C)O)(C)C
MOL006265	0.7727	0.2273	0.7145	Dictamni Cortex	meliartenin	Not Available	FALSE	C1C(C2(C3C(C1O)(C1C(C(C3)O)(C34C(C(=O)C1O)(C(CC3O4)c1cocc1)C)C)COC2O)C)OC(=O)C
MOL006267	0.3053	0.6947	0.8840	Dictamni Cortex	ELTANOLONE	31402	FALSE	C1C(CC2C(C1)(C1C(CC2)C2C(CC1)(C(CC2)C(=O)C)C)C)O
MOL006268	0.8099	0.1901	0.7994	Dictamni Cortex	preskimmianine	12305721	FALSE	O(c1c2c([nH]c(=O)c1CC=C(C)C)c(OC)c(OC)cc2)C
MOL006268	0.8099	0.1901	0.7994	Dichroae Radix	preskimmianine	12305721	FALSE	O(c1c2c([nH]c(=O)c1CC=C(C)C)c(OC)c(OC)cc2)C
MOL006270	0.2184	0.7816	0.7185	Dictamni Cortex	tirucallane	Not Available	FALSE	C1C(C(C2C(C1)(C1C(=CC2)C2(C(CC1)(C(CC2)C(C)CCC=C(C)C)C)C)C)(C)C)O
MOL006271	0.2868	0.7132	0.7959	Dictamni Cortex	trichirubine,b	Not Available	FALSE	C1=CC2(C3C(C1=O)(C14C(C(C3OC2)OC(=O)c2ccccc2)(C2C(CC1O4)(C(CC2)C1C(=C)OC(C1)O)C)C)C)C
MOL006272	0.7324	0.2676	0.7554	Dictamni Cortex	9alpha-hydroxyfraxinellone-9-o-beta-d-glucoside	Not Available	FALSE	C1(C(C(C(OC1CO)OC1C(CC2(C(=C1C)C(=O)OC2c1cocc1)C)C)O)O)O
MOL006273	0.8937	0.1063	0.7951	Dictamni Cortex	9alpha-hydroxyfraxinellone-9-o-beta-d-glucoside_qt	Not Available	FALSE	OC1C(CC2(C(=C1C)C(=O)OC2c1cocc1)C)C
MOL006274	0.8962	0.1038	0.8432	Dictamni Cortex	9beta-hydroxyfraxinellone	Not Available	FALSE	C1C(C(=C2C(C1)(C(OC2=O)c1cocc1)C)C)CO
MOL006276	0.2436	0.7564	0.6177	Ailanthi Cortex	SMR000232320	12004524	FALSE	O=C1C(C2C(C3C(=CC2)C2(C(C(CC2)C(CC(O)C(O)C(O)(C)C)C)(CC3)C)C)(CC1)C)(C)C

MOL006276	0.2436	0.7564	0.6177	Phellodendri Amurensis Cortex	SMR000232320	12004524	FALSE	O=C1C(C2C(C3C(=CC2)C2(C(C(CC2)C(CC(O)C(O)C(O)(C)C)C)(CC3)C)C)(CC1)C)(C)C
MOL006277	0.8970	0.1030	0.8047	Ailanthi Cortex	Shinjudilactone	Not Available	FALSE	O1C2C34C(C5(C(C2)C(=CC(=O)C5O)C)C)C(O)(C(C3CC1=O)C)C(=O)OC4
MOL006278	0.9140	0.0860	0.8335	Ailanthi Cortex	Shinjulactone A	Not Available	FALSE	O1C2(O)C3C4(C(OC(=O)CC4C(=C)C2O)CC2C3(C(O)C(O)C=C2C)C)C1
MOL006279	0.7144	0.2856	0.6528	Ailanthi Cortex	Shinjulactone B	Not Available	FALSE	O1C2C3(C(C(C(=O)C(=C3C(C2)(C2OC(=O)C=C2C)C)O)C)CC1=O)CO
MOL006280	0.8907	0.1093	0.7348	Ailanthi Cortex	Shinjulactone C	Not Available	FALSE	OC12C3(C45C(C(C6(C3CC(=O)OC6C4)CO)C2=O)(C1(O)C(=O)C=C5C)C)C
MOL006281	0.6716	0.3284	0.8364	Ailanthi Cortex	Shinjulactone K	Not Available	FALSE	O1C2C3(C(C4(C(C2)C(CC(O)C4=O)C)C)C(O)C(OC(=O)C)C(C3CC1=O)C)C
MOL006282	0.2904	0.7096	0.7131	Ailanthi Cortex	Vilmorrianine B	Not Available	FALSE	O(C12C3C4N(CC5(C(C4(C4C1C(OC(=O)c1ccc(OC)cc1)C(O)(C4)C(OC)C2)C(OC)CC5O)C3OC)COC)C)CC(=O)C
MOL006283	0.1805	0.8195	0.6361	Ailanthi Cortex	Vilmorrianine C	Not Available	FALSE	C123C4C(CN(C1C(C4OC)C1(C4C2CC(C4OC(=O)c2ccc(cc2)OC)C(C1)OC)OC(=O)C)CC)(CCC3OC)COC
MOL006284	0.9169	0.0831	0.8309	Ailanthi Cortex	Ailantone	Not Available	FALSE	O1C2(O)C3C4(C(OC(=O)CC4C(=C)C2O)CC2C3(C(O)C(=O)C=C2C)C)C1
MOL006285	0.7184	0.2816	0.7410	Ailanthi Cortex	ailantinol A	Not Available	FALSE	O1C2C3(C(C4(C(C2)C(=CC(=O)C4O)C)C)C(=O)OC3)C(CC1=O)C(C)C(=O)OC
MOL006286	0.8553	0.1447	0.6426	Rubi Fructus	alpha-amorphene	12306052	FALSE	C12C(CC=C(C1CCC(=C2)C)C)C(C)C
MOL006286	0.8553	0.1447	0.6426	Ailanthi Cortex	alpha-amorphene	12306052	FALSE	C12C(CC=C(C1CCC(=C2)C)C)C(C)C
MOL006287	0.8553	0.1447	0.6426	Benzoinum	α-muurolene	12306046	FALSE	C12C(CC=C(C1CCC(=C2)C)C)C(C)C
MOL006287	0.8553	0.1447	0.6426	Polygoni Orientalis Fructus	α-muurolene	12306046	FALSE	C12C(CC=C(C1CCC(=C2)C)C)C(C)C
MOL006287	0.8553	0.1447	0.6426	Ailanthi Cortex	α-muurolene	12306046	FALSE	C12C(CC=C(C1CCC(=C2)C)C)C(C)C
MOL006287	0.8553	0.1447	0.6426	Dichroae Radix	α-muurolene	12306046	FALSE	C12C(CC=C(C1CCC(=C2)C)C)C(C)C
MOL006288	0.8265	0.1735	0.6775	Ardisiae Japonicae Herba	α-cadinol	12302223	FALSE	OC1(C2C(C(CC1)C(C)C)C=C(CC2)C)C
MOL006288	0.8265	0.1735	0.6775	Ailanthi Cortex	α-cadinol	12302223	FALSE	OC1(C2C(C(CC1)C(C)C)C=C(CC2)C)C
MOL006288	0.8265	0.1735	0.6775	Eriobotryae Folium	α-cadinol	12302223	FALSE	OC1(C2C(C(CC1)C(C)C)C=C(CC2)C)C
MOL006289	0.8870	0.1130	0.8043	Rhododendri Daurici Folium	cis-Z-alpha-Bisabolene epoxide	Not Available	FALSE	O1C2(C1CC(CC2)/C(=C\CC=C(C)C)/C)C
MOL006289	0.8870	0.1130	0.8043	Perillae Fructus	cis-Z-alpha-Bisabolene epoxide	Not Available	FALSE	O1C2(C1CC(CC2)/C(=C\CC=C(C)C)/C)C
MOL006289	0.8870	0.1130	0.8043	Ailanthi Cortex	cis-Z-alpha-Bisabolene epoxide	Not Available	FALSE	O1C2(C1CC(CC2)/C(=C\CC=C(C)C)/C)C
MOL006290	0.8695	0.1305	0.9384	Ailanthi Cortex	IOM	59098743	FALSE	OC(=O)CN(C)C(=N)N
MOL006291	0.8789	0.1211	0.9429	Ailanthi Cortex	krebiozen	588	FALSE	O=C1N=C(N(C1)C)N

MOL006292	0.8291	0.1709	0.7593	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	δ-selinene	12308845	FALSE	C12(CCCC(=C2C=C(CC1)C(C)C)C)C
MOL006292	0.8291	0.1709	0.7593	Ligustici Rhizoma Et Radix	δ-selinene	12308845	FALSE	C12(CCCC(=C2C=C(CC1)C(C)C)C)C
MOL006292	0.8291	0.1709	0.7593	Solidaginis Herba	δ-selinene	12308845	FALSE	C12(CCCC(=C2C=C(CC1)C(C)C)C)C
MOL006292	0.8291	0.1709	0.7593	Ailanthi Cortex	δ-selinene	12308845	FALSE	C12(CCCC(=C2C=C(CC1)C(C)C)C)C
MOL006292	0.8291	0.1709	0.7593	Schisandrae Chinensis Fructus	δ-selinene	12308845	FALSE	C12(CCCC(=C2C=C(CC1)C(C)C)C)C
MOL006293	0.8981	0.1019	0.7396	Meliae Cortex	Thapsic acid	10459	FALSE	OC(=O)CCCCCCCCCCCCCCCC(=O)O
MOL006293	0.8981	0.1019	0.7396	Ailanthi Cortex	Thapsic acid	10459	FALSE	OC(=O)CCCCCCCCCCCCCCCC(=O)O
MOL006293	0.8981	0.1019	0.7396	Typhonii Rhizoma	Thapsic acid	10459	FALSE	OC(=O)CCCCCCCCCCCCCCCC(=O)O
MOL006294	0.2871	0.7129	0.6045	Ailanthi Cortex	(3S,4R,6S)-6-[(3S,5R,9R,10R,13S,14S,17S)-3-hydroxy-4,4,10,13,14-pentamethyl-2,3,5,6,9,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-17-yl]-2-methylheptane-2,3,4-triol	13967183	FALSE	C1(C2C(CCC1O)(C1C(=CC2)C2(C(C(CC2)C(CC(O)C(O)C(O)(C)C)C)(CC1)C)C)C)(C)C
MOL006295	0.2014	0.7986	0.7339	Ailanthi Cortex	ocotillol	12313665	FALSE	O1C(C2C3C(C4(C(C5(C(CC4)C(C(=O)CC5)(C)C)CC3)C)(CC2)C)(CCC1C(O)(C)C)C
MOL006295	0.2014	0.7986	0.7339	Panacis Quinquefolii Radix	ocotillol	12313665	FALSE	O1C(C2C3C(C4(C(C5(C(CC4)C(C(=O)CC5)(C)C)CC3)C)(CC2)C)(CCC1C(O)(C)C)C
MOL006296	0.2366	0.7634	0.6622	Ailanthi Cortex	stigmast-5-ene-3β,7α-diol	12309576	FALSE	OC1C2C3C(C(CC3)C(CCC(C(C)C)CC)C)(CCC2C2(C(=C1)CC(O)CC2)C)C
MOL006297	0.8597	0.1403	0.6921	Ailanthi Cortex	β-guaiene	Not Available	FALSE	C12=C(C(CC2)C)CC(=C(C)C)CCC1C
MOL006297	0.8597	0.1403	0.6921	Notoginseng Flos	β-guaiene	Not Available	FALSE	C12=C(C(CC2)C)CC(=C(C)C)CCC1C
MOL006297	0.8597	0.1403	0.6921	Ginsen Radix Et Rhizoma Rubra	β-guaiene	Not Available	FALSE	C12=C(C(CC2)C)CC(=C(C)C)CCC1C

MOL006298	0.2389	0.7611	0.6482	Ailanthi Cortex	(3S,6R,8S,9S,10R,13R,14S,17R)-17-[(1R,4S)-4-ethyl-1,5-dimethylhexyl]-10,13-dimethyl-2,3,6,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,6-diol	16053313	FALSE	OC1CC2C3C(C(CC3)C(CCC(C(C)C)CC)C)(CCC2C2(C1=CC(O)CC2)C)C
MOL006299	0.9275	0.0725	0.6928	Ailanthi Cortex	1,7,7-Trimethyl-2-vinylbicyclo[2.2.1]hept-2-ene	Not Available	FALSE	C1C2C=C(C(C1)(C2(C)C)C)C=C
MOL006300	0.8784	0.1216	0.6996	Ailanthi Cortex	1-hydroxy-canthin-6-one	Not Available	FALSE	n1cc(c2c3n(c(=O)ccc13)c1c2cccc1)O
MOL006301	0.8187	0.1813	0.6730	Ailanthi Cortex	1-Methoxycanthinone	Not Available	FALSE	n1cc(c2c3n(c(=O)ccc13)c1c2cccc1)OC
MOL006302	0.8780	0.1220	0.6983	Ailanthi Cortex	2-hydroxy-canthin-6-one	Not Available	FALSE	n1c(cc2c3n(c(=O)ccc13)c1c2cccc1)O
MOL006303	0.8734	0.1266	0.6269	Ailanthi Cortex	4,5-dihydrocanthin-6-one	Not Available	FALSE	n1ccc2c3n(C(=O)C(C(c13)O)O)c1c2cccc1
MOL006304	0.8676	0.1324	0.6620	Ailanthi Cortex	4-hydroxy-canthin-6-one	Not Available	FALSE	n1ccc2c3n(c(=O)cc(c13)O)c1c2cccc1
MOL006305	0.9621	0.0379	0.7091	Ailanthi Cortex	5,6,7,8-Tetramethoxy coumarin	151319	FALSE	o1c2c(c(OC)c(OC)c(OC)c2OC)ccc1=O
MOL006306	0.8191	0.1809	0.6535	Ailanthi Cortex	5-Methoxycanthin-6-one	Not Available	FALSE	O(c1c(=O)n2c3c(c4c2cccc4)ccnc3c1)C
MOL006307	0.9636	0.0364	0.8640	Ailanthi Cortex	7-methoxy-2H-chromene	5314753	FALSE	O1c2c(C=CC1)ccc(OC)c2
MOL006308	0.8729	0.1271	0.6816	Ailanthi Cortex	66762-19-4	Not Available	FALSE	n1ccc2c3n(c(=O)ccc13)c1c2cccc1O

MOL006309	0.6269	0.3731	0.8233	Ailanthi Cortex	Amarolide 11-acetate	Not Available	FALSE	O1C2C3(C(C4(C(C2)C(CC(O)C4=O)C)C)C(OC(=O)C)C(=O)C(C3CC1=O)C)C
MOL006310	0.8183	0.1817	0.8942	Ailanthi Cortex	Amarolide	Not Available	FALSE	O1C2C3(C(C4(C(C2)C(CC(O)C4=O)C)C)C(O)C(=O)C(C3CC1=O)C)C
MOL006311	0.8958	0.1042	0.7759	Ailanthi Cortex	Artelin	Not Available	FALSE	O1C2C(C(C1=O)C)C(O)CC(=C1C2C(=C(O)C1=O)C)C
MOL006312	0.8642	0.1358	0.6086	Litchi Semen	Azulol	3515	FALSE	Cc1c2c(cc1)c(C)ccc(c2)C(C)C
MOL006312	0.8642	0.1358	0.6086	Ardisiae Japonicae Herba	Azulol	3515	FALSE	Cc1c2c(cc1)c(C)ccc(c2)C(C)C
MOL006312	0.8642	0.1358	0.6086	Ephedra Herba	Azulol	3515	FALSE	Cc1c2c(cc1)c(C)ccc(c2)C(C)C
MOL006312	0.8642	0.1358	0.6086	Linderae Radix	Azulol	3515	FALSE	Cc1c2c(cc1)c(C)ccc(c2)C(C)C
MOL006312	0.8642	0.1358	0.6086	Ailanthi Cortex	Azulol	3515	FALSE	Cc1c2c(cc1)c(C)ccc(c2)C(C)C
MOL006313	0.8520	0.1480	0.6840	Ailanthi Cortex	Bicyclo[4.4.0]dec-1-ene, 2-isopropyl-5-methyl-9-methylene	Not Available	FALSE	CC(C)C1=C2CC(=C)CCC2C(CC1)C
MOL006314	0.8239	0.1761	0.6677	Ailanthi Cortex	Canthin-6-one	Not Available	FALSE	O=c1n2c3c(c4c2cccc4)ccnc3cc1
MOL006315	0.7125	0.2875	0.8323	Radix Stephaniae Cepharanthae.	Dehydrocreban ine	Not Available	FALSE	O1c2c3c4c(CCN(c4cc4c3ccc(OC)c4OC)C)cc2OC1
MOL006315	0.7125	0.2875	0.8323	Ailanthi Cortex	Dehydrocreban ine	Not Available	FALSE	O1c2c3c4c(CCN(c4cc4c3ccc(OC)c4OC)C)cc2OC1
MOL006316	0.8589	0.1411	0.7017	Ailanthi Cortex	(1R,8aS)-4-isopropyl-1,6-dimethyl-1,2,3,7,8,8a-hexahydronaphthalene	10987383	FALSE	C12C(CCC(=C1C=C(CC2)C)C(C)C)C
MOL006317	0.9200	0.0800	0.7887	Euphorbiae Humifusae Herba	(E)-4-[(1R,4R)-4-hydroxy-2,6,6-trimethyl-1-cyclohex-2-enyl]but-3-en-2-one	10889124	FALSE	C1C(C=C(C(C1(C)C)/C=C/C(=O)C)C)O
MOL006318	0.8532	0.1468	0.6858	Euphorbiae Humifusae Herba	1,3,4,6-tetra-O-galloyl-β-D-glucose	Not Available	FALSE	C1(C(O)C(C(C(O1)COC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O

MOL006319	0.3654	0.6346	0.6939	Euphorbiae Humifusae Herba	(2aR,3R,5aS,5bS,7aS,9S,11aR,12aS)-3-((S)-2,5-dimethyl-4-methylenehexyl)-2a,5a,8,8-tetramethylhexadecahydrocyclopenta[a]cyclopropa[e]phenanthren-9-ol	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C(CC2)CC(C)CC(=C)C(C)C)C)C)C3)(C)C)O
MOL006320	0.2557	0.7443	0.7704	Euphorbiae Humifusae Herba	3β-acetoxy-30-norlupan-20-one	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=O)C)C)C)C)C)(C)C)OC(=O)C
MOL006321	0.2263	0.7737	0.6713	Euphorbiae Humifusae Herba	(3S,4S,5R,10S,13R,14R,17R)-4,10,13,14-tetramethyl-17-((R)-6-methyl-5-methyleneheptan-2-yl)-2,3,4,5,6,10,12,13,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol	Not Available	FALSE	C12C(C3=CCC4(C(C3=CC1)(CCC4C(CCC(=C)C(C)C)C)C)C)(C)CCC(C2C)O
MOL006322	0.3063	0.6937	0.7418	Rhapontici Radix	Friedoolean-14-en-3-yl acetate	94225	FALSE	C12=CCC3(C(C2(CCC2C1(CCC1C2(CCC(C1(C)C)OC(=O)C)C)C)C)CC(CC3)(C)C)C
MOL006322	0.3063	0.6937	0.7418	Cichorii Radix	Friedoolean-14-en-3-yl acetate	94225	FALSE	C12=CCC3(C(C2(CCC2C1(CCC1C2(CCC(C1(C)C)OC(=O)C)C)C)C)CC(CC3)(C)C)C
MOL006322	0.3063	0.6937	0.7418	Echinopsis Radix	Friedoolean-14-en-3-yl acetate	94225	FALSE	C12=CCC3(C(C2(CCC2C1(CCC1C2(CCC(C1(C)C)OC(=O)C)C)C)C)CC(CC3)(C)C)C

MOL006322	0.3063	0.6937	0.7418	Euphorbiae Humifusae Herba	Friedoolean-14-en-3-yl acetate	94225	FALSE	C12=CCC3(C(C2(CCC2C1(CCC1C2(CCC(C1(C)C)OC(=O)C)C)C)C)CC(CC3)(C)C)C
MOL006322	0.3063	0.6937	0.7418	Codonopsis Radix	Friedoolean-14-en-3-yl acetate	94225	FALSE	C12=CCC3(C(C2(CCC2C1(CCC1C2(CCC(C1(C)C)OC(=O)C)C)C)C)CC(CC3)(C)C)C
MOL006323	0.6274	0.3726	0.7443	Euphorbiae Humifusae Herba	geraniin	Not Available	FALSE	C12(C(C3C(=CC2=O)C(=O)OC2C4C(C(OC2COC(=O)c2c(c5c(C(=O)O4)cc(c(c5O)O)O)c(c(c(c2)O)O)O)OC(=O)c2cc(c(c(c2)O)O)O)OC(=O)c2c3c(O1)c(c(c2)O)O)(O)O)O
MOL006324	0.3541	0.6459	0.6890	Euphorbiae Humifusae Herba	α-amyrenonol	Not Available	FALSE	O=C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3C)C)C)C)(CC2)C)(CC1)C)(C)C
MOL006325	0.9391	0.0609	0.7146	Euphorbiae Humifusae Herba	Ayapin	3083597	FALSE	O1c2c(OC1)cc1oc(=O)ccc1c2
MOL006326	0.0703	0.9297	0.8151	Euphorbiae Humifusae Herba	Ensaculin	208923	FALSE	O(CCCN1CCN(CC1)c1c(OC)cccc1)c1cc2c(oc(=O)c(c2C)C)cc1OC
MOL006327	0.3408	0.6592	0.7290	Sterculiae Lychnophorae Semen	sterculin A	Not Available	FALSE	C12C3(C4(C(CC1)C1(C(CC4)(C(CC1)C(C)C/C=C\C(C)(C)O)C)C)C3)CCC(C2(C)C)O
MOL006327	0.3408	0.6592	0.7290	Euphorbiae Humifusae Herba	sterculin A	Not Available	FALSE	C12C3(C4(C(CC1)C1(C(CC4)(C(CC1)C(C)C/C=C\C(C)(C)O)C)C)C3)CCC(C2(C)C)O
MOL006328	0.3504	0.6496	0.7133	Euphorbiae Humifusae Herba	(2aR,3R,5aS,5bS,7aS,9S,11aR,12aS)-3-((2S,5S)-5-hydroxy-6-methylhept-6-en-2-yl)-2a,5a,8,8-tetramethylhexadecahydrocyclopenta[a]cyclopropa[e]phenanthren-9-ol	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C(CC2)C(C)CCC(C(=C)C)O)C)C)C3)(C)C)O

MOL006329	0.8631	0.1369	0.7641	Euphorbiae Humifusae Herba	(2R,3S,4S,5R,6S)-2-((5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-3-yl)oxy)-4,5-dihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-3-yl 3,4,5-trihydroxybenzoate	Not Available	FALSE	C(=O)(c1cc(c(c(c1)O)O)O)OC1C(OC(C(C1O)O)CO)Oc1c(oc2c(c1=O)c(cc(c2)O)O)c1ccc(cc1)O
MOL006330	0.5552	0.4448	0.6034	Euphorbiae Humifusae Herba	3-((3R,4R,5R,8S,9R,10R,13R,14R,15R)-3-(3-hydroxyprop-1-en-2-yl)-4,9,10,13-tetramethyl-15-(prop-1-en-2-yl)hexadecahydro-1H-cyclopenta[a]phenanthren-4-yl)propanoic acid	Not Available	FALSE	C1(C(CCC2(C1CCC1C2(CCC2(C1C(CC2)C(=C)C)C)C)C)C(=C)CO)(C)CCC(=O)O
MOL006331	0.9201	0.0799	0.7919	Polygonati Rhizoma	4',5-Dihydroxyflavone	165521	FALSE	c1cc(c2c(c1)oc(cc2=O)c1ccc(cc1)O)O
MOL006331	0.9201	0.0799	0.7919	Microctis Folium	4',5-Dihydroxyflavone	165521	FALSE	c1cc(c2c(c1)oc(cc2=O)c1ccc(cc1)O)O
MOL006331	0.9201	0.0799	0.7919	Euphorbiae Humifusae Herba	4',5-Dihydroxyflavone	165521	FALSE	c1cc(c2c(c1)oc(cc2=O)c1ccc(cc1)O)O

MOL006332	0.1883	0.8117	0.7424	Euphorbiae Humifusae Herba	(3S,4S,5R,10S,13R,14R,17R)-3-hydroxy-4,10,13,14-tetramethyl-17-((R)-6-methyl-5-methyleneheptan-2-yl)-3,4,5,6,12,13,14,15,16,17-decahydro-1H-cyclopenta[a]phenanthrene-7,11(2H,10H)-dione	Not Available	FALSE	C12C(C3=C(C(=O)C1)C1(C(CC3=O)(C(CC1)C(CCC(=C)C(C)C)C)C)C)(C)CCC(C2C)O
MOL006333	0.3295	0.6705	0.7452	Euphorbiae Humifusae Herba	glut-5-en-3β-yl acetate	Not Available	FALSE	C1(CCC2C(=CCC3C4(C)CCC5(C)CCC(C)(C)CC5C4(CCC23C)C)C1(C)C)OC(=O)C
MOL006334	0.3645	0.6355	0.7910	Euphorbiae Humifusae Herba	(1R,3aR,5aR,5bR,7aS,9S,11aR,11bR,13aS,13bS)-1-(3-hydroxyprop-1-en-2-yl)-3a,5a,5b,8,8,11a-hexamethylicosahydro-1H-cyclopenta[a]chrysen-9-ol	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=C)CO)C)C)C)(C)C)O

MOL006335	0.2127	0.7873	0.7222	Euphorbiae Humifusae Herba	(3S,4S,5R,10S,13R,14R,17R)-3-hydroxy-4,10,13,14-tetramethyl-17-((R)-6-methyl-5-methyleneheptan-2-yl)-3,4,5,6,10,11,12,13,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-7(2H)-one	Not Available	FALSE	C12C(C3=C(C(=O)C1)C1(C(CC3)(C(CC1)C(CCC(=C)C(C)C)C)C)C)(C)CCC(C2C)O
MOL006336	0.2169	0.7831	0.7474	Euphorbiae Humifusae Herba	(3S,5S,9R,10R,13R,14R,17R)-17-((S,E)-6-hydroxy-6-methylhept-4-en-2-yl)-4,4,10,13,14-pentamethyl-2,3,4,5,6,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-ol	Not Available	FALSE	C12C(C3C(=CC1)C1(C(CC3)(C(CC1)C(C/C=C/C(C)(C)O)C)C)C)(C)CCC(C2(C)C)O

MOL006337	0.2366	0.7634	0.6622	Euphorbiae Humifusae Herba	(3S,7R,8S,9S,10R,13R,14R,17R)-17-((2R,5R)-5-ethyl-6-methylheptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthrene-3,7-diol	Not Available	FALSE	C1C(CC2=CC(C3C(C2(C1)C)CCC1(C3CCC1C(C)CCC(CC)C(C)C)C)O)O
MOL006338	0.3394	0.6606	0.6961	Euphorbiae Humifusae Herba	(2aR,3R,5aS,5bS,7aS,9S,11aR,12aS)-3-((S,Z)-6-ethoxy-2,6-dimethylhept-4-en-1-yl)-2a,5a,8,8-tetramethylhexadecahydrocyclopenta[a]cyclopropa[e]phenanthren-9-ol	Not Available	FALSE	C12C3(C4(C(CC1)C1(C(CC4)(C(CC1)CC(C/C=C\C(C)(C)OCC)C)C)C)C3)CCC(C2(C)C)O
MOL006339	0.9428	0.0572	0.9332	Potentillae Discoloris Herba	WLN: QVR CVQ	23461093	FALSE	c1(cc(ccc1)C(=O)O)C(=O)O
MOL006340	0.7041	0.2959	0.6948	Actinidia Chinensis Planch	Aurin	5100	FALSE	C(=C1C=CC(=O)C=C1)(c1ccc(cc1)O)c1ccc(cc1)O
MOL006340	0.7041	0.2959	0.6948	Potentillae Discoloris Herba	Aurin	5100	FALSE	C(=C1C=CC(=O)C=C1)(c1ccc(cc1)O)c1ccc(cc1)O
MOL006341	0.4320	0.5680	0.7393	Potentillae Discoloris Herba	agrimonine	Not Available	FALSE	C12C(C(OC3C1OC(=O)c1c(c4c(C(=O)OC3)cc(c(c4O)O)O)c(c(c(c1)O)O)O)OC(=O)c1c(Oc3cc(C(=O)OC4C5C(C6C(O4)COC(=O)c4c(c7c(C(=O)O6)cc(c(c7O)O)O)c(c(c(c4)O)O)O)OC(=O)c4c(c6c(C(=O)O5)cc(c(c6O)O)O)c(c(c(c4)O)O)O)cc(c3O)O)c(c(c(c1)O)O)OC(=O)c1c(c3c(C(=O)O2)cc(c(c3O)O)O)c(c(c(c1)O)O)O
MOL006344	0.5773	0.4227	0.6368	Pteridis Multifidae Herba	Creticoside C	Not Available	FALSE	C1(CC(C2C(C1)(C1(C3(CC2O)CC(CC1)C(C3)(C)O)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)O

MOL006345	0.5213	0.4787	0.7059	Pteridis Multifidae Herba	Creticoside C_qt	Not Available	FALSE	C1(CC(C2C(C1)(C1(C3(CC2O)CC(CC1)C(C3)(C)O)C)C)(C)C)O
MOL006346	0.0851	0.9149	0.9199	Pteridis Multifidae Herba	Itraconazole	56682298	FALSE	Clc1c(C2(OC(CO2)COc2ccc(N3CCN(CC3)c3ccc(n4c(=O)n(nc4)C(CC)C)cc3)cc2)Cn2ncnc2)ccc(Cl)c1
MOL006347	0.8789	0.1211	0.8953	Pteridis Multifidae Herba	(2R)-6-(2-hydroxyethyl)-2,5,7-trimethyl-1-indanone	115049	FALSE	O=C1C(Cc2c1c(c(c(c2)C)CCO)C)C
MOL006347	0.8789	0.1211	0.8953	Solanum Nigrum Linn.	(2R)-6-(2-hydroxyethyl)-2,5,7-trimethyl-1-indanone	115049	FALSE	O=C1C(Cc2c1c(c(c(c2)C)CCO)C)C
MOL006348	0.8576	0.1424	0.6909	Pteridis Multifidae Herba	pterosin C 3-O-glucoside	44201982	FALSE	O1C(C(O)C(O)C(O)C1OCCc1c(c2c(C(O)C(C2=O)C)cc1C)C)CO
MOL006349	0.9147	0.0853	0.7536	Pteridis Multifidae Herba	(2S,3S)-3-hydroxy-6-(2-hydroxyethyl)-2,5,7-trimethyl-1-indanone	186209	FALSE	OCCc1c(c2c(C(O)C(C2=O)C)cc1C)C
MOL006350	0.8681	0.1319	0.8810	Pteridis Multifidae Herba	Pterosin F	Not Available	FALSE	ClCCc1c(c2c(CC(C2=O)C)cc1C)C
MOL006351	0.8855	0.1145	0.8750	Pteridis Multifidae Herba	Pterosin O	135255	FALSE	O=C1C(Cc2c1c(c(c(c2)C)CCOC)C)C
MOL006352	0.9152	0.0848	0.7559	Pteridis Multifidae Herba	pterosin S	44201981	FALSE	OC1C(C(=O)c2c1cc(c(c2CO)CCO)C)C
MOL006353	0.2389	0.7611	0.6482	Ailanthi Altissimae Fructus	stigmast-4-ene-3,6a-diol	Not Available	FALSE	C1(CCC2(C(=C1)C(CC1C3CCC(C(CCC(CC)C(C)C)C)C3(C)CCC21)O)C)O
MOL006353	0.2389	0.7611	0.6482	Momordicae Semen	stigmast-4-ene-3,6a-diol	Not Available	FALSE	C1(CCC2(C(=C1)C(CC1C3CCC(C(CCC(CC)C(C)C)C)C3(C)CCC21)O)C)O
MOL006354	0.2081	0.7919	0.6542	Humulus Scandens (Lour.) Merr.	stigmastane—3,6—dione	Not Available	FALSE	C1(=O)CCC2(C(C1)C(=O)CC1C3CCC(C(CCC(CC)C(C)C)C)C3(C)CCC21)C
MOL006354	0.2081	0.7919	0.6542	Ailanthi Altissimae Fructus	stigmastane—3,6—dione	Not Available	FALSE	C1(=O)CCC2(C(C1)C(=O)CC1C3CCC(C(CCC(CC)C(C)C)C)C3(C)CCC21)C
MOL006355	0.7195	0.2805	0.7681	Ailanthi Altissimae Fructus	(+)-isolariciresinol 9-O-β-D-glucopyranoside	Not Available	FALSE	O1C(OC)(C2C(Cc3c(C2c2cc(OC)c(O)cc2)cc(O)c(OC)c3)CO)C(O)C(O)C(O)C1CO
MOL006356	0.9456	0.0544	0.9689	Ailanthi Altissimae Fructus	sorbitol	5780	FALSE	OC(C(O)C(O)CO)C(O)CO
MOL006356	0.9456	0.0544	0.9689	Veronicae Peregrinae Herba	sorbitol	5780	FALSE	OC(C(O)C(O)CO)C(O)CO
MOL006356	0.9456	0.0544	0.9689	Trollius Chinensis	sorbitol	5780	FALSE	OC(C(O)C(O)CO)C(O)CO
MOL006356	0.9456	0.0544	0.9689	Crataegi Folium	sorbitol	5780	FALSE	OC(C(O)C(O)CO)C(O)CO

MOL006358	0.1884	0.8116	0.6602	Gleditsiae Fructus	Stigmast-4-ene-3,6-dione	5490007	FALSE	O=C1CC2C3C(C(CC3)C(CCC(C(C)C)CC)C)(CCC2C2(C1=CC(=O)CC2)C)C
MOL006358	0.1884	0.8116	0.6602	Ailanthi Altissimae Fructus	Stigmast-4-ene-3,6-dione	5490007	FALSE	O=C1CC2C3C(C(CC3)C(CCC(C(C)C)CC)C)(CCC2C2(C1=CC(=O)CC2)C)C
MOL006358	0.1884	0.8116	0.6602	Tamaricis Cacumen	Stigmast-4-ene-3,6-dione	5490007	FALSE	O=C1CC2C3C(C(CC3)C(CCC(C(C)C)CC)C)(CCC2C2(C1=CC(=O)CC2)C)C
MOL006358	0.1884	0.8116	0.6602	Gleditsiae Spina	Stigmast-4-ene-3,6-dione	5490007	FALSE	O=C1CC2C3C(C(CC3)C(CCC(C(C)C)CC)C)(CCC2C2(C1=CC(=O)CC2)C)C
MOL006359	0.3500	0.6500	0.7900	Ailanthi Altissimae Fructus	22-hydroxyhopan-3-one	21582894	FALSE	C12(C3(C(C4(C(C(C(=O)CC4)(C)C)CC3)C)CCC1C1(C(C(CC1)C(O)(C)C)CC2)C)C)C
MOL006360	0.8659	0.1341	0.7719	Ailanthi Altissimae Fructus	3-O-α-L-arabinofuranosyl kaempferol 7-O-α-L-rhamnopyranoside	Not Available	FALSE	c1(c(OC2C(O)C(O)C(O2)CO)c(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)C)c1ccc(O)cc1
MOL006361	0.2127	0.7873	0.6657	Ailanthi Altissimae Fructus	3β-hydroxystigmast-5-en-7-one	Not Available	FALSE	C1(CCC2(C(=CC(=O)C3C4CCC(C(CCC(CC)C(C)C)C)C4(C)CCC23)C1)C)O
MOL006362	0.2151	0.7849	0.6516	Ailanthi Altissimae Fructus	(6S,8S,9S,10R,13R,14S,17R)-17-[(1R,4R)-4-ethyl-1,5-dimethylhexyl]-6-hydroxy-10,13-dimethyl-1,2,6,7,8,9,11,12,14,15,16,17-dodecahydrocyclopenta[a]phenanthren-3-one	9867274	FALSE	C1(=O)CCC2(C(=C1)C(CC1C3CCC(C(CCC(CC)C(C)C)C)C3(C)CCC21)O)C

MOL006364	0.6541	0.3459	0.6802	Phellodendri Amurensis Cortex	(2R,3R,4S)-4-(4-hydroxy-3,5-dimethoxy-phenyl)-5,7-dimethoxy-2,3-dimethylol-tetralin-6-ol	11711453	FALSE	c1(c(c(c2c(c1)CC(C(C2c1cc(c(c(c1)OC)O)OC)CO)CO)OC)O)OC
MOL006365	0.5399	0.4601	0.6553	Phellodendri Amurensis Cortex	(-)-oblongine	173713	FALSE	c1c(c(c2c(c1)CC[N+](C2Cc1ccc(cc1)O)(C)C)O)OC
MOL006368	0.8467	0.1533	0.7465	Phellodendri Amurensis Cortex	3,,5-dihydroxybenzoicacid-o-xylopyranosyl-glucopyranoside	Not Available	FALSE	c1c(cc(c(c1)OC1C(O)C(O)C(O)C(O1)COC1(C(C(C(C(O1)(C)C)(C)O)(C)O)(O)C)C)O)C(=O)O
MOL006369	0.7559	0.2441	0.7107	Phellodendri Amurensis Cortex	3-caffeoyl-5-feruoyl-quinic,acid	Not Available	FALSE	C1C(C(C(CC1(O)C(=O)O)OC(=O)/C=C/c1ccc(c(c1)OC)O)O)OC(=O)/C=C/c1ccc(c(c1)O)O
MOL006370	0.9497	0.0503	0.9440	Eucommiae Cortex	5-o-caffeoylquinic acid	5280633	FALSE	C1C(C(C(CC1(O)C(=O)O)O)O)OC(=O)/C=C/c1ccc(c(c1)O)O
MOL006370	0.9497	0.0503	0.9440	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	5-o-caffeoylquinic acid	5280633	FALSE	C1C(C(C(CC1(O)C(=O)O)O)O)OC(=O)/C=C/c1ccc(c(c1)O)O
MOL006370	0.9497	0.0503	0.9440	Phellodendri Amurensis Cortex	5-o-caffeoylquinic acid	5280633	FALSE	C1C(C(C(CC1(O)C(=O)O)O)O)OC(=O)/C=C/c1ccc(c(c1)O)O
MOL006371	0.7559	0.2441	0.7107	Phellodendri Amurensis Cortex	3-feruoyl-4-caff,eoylquinicacid	Not Available	FALSE	C1C(C(C(CC1(C(=O)O)O)OC(=O)/C=C/c1ccc(c(c1)O)O)O)OC(=O)/C=C/c1ccc(c(c1)OC)O
MOL006372	0.7559	0.2441	0.7107	Phellodendri Amurensis Cortex	3-feruoyl-5-caffeoyl-quinic,acid	Not Available	FALSE	C1C(C(C(CC1(O)C(=O)O)OC(=O)/C=C/c1ccc(c(c1)O)O)O)OC(=O)/C=C/c1ccc(c(c1)OC)O
MOL006373	0.9535	0.0465	0.8074	Phellodendri Amurensis Cortex	3-o-feruloylquinic,acid	Not Available	FALSE	C1C(C(C(CC1(C(=O)O)O)O)O)OC(=O)/C=C/c1ccc(c(c1)O)OC

MOL006374	0.8653	0.1347	0.8361	Phellodendri Amurensis Cortex	4,10-dimethylene-7-isopropyl-5(E)-cyclodecenol	Not Available	FALSE	C1(CCC(=C)/C=C/C(CCC1=C)C(C)C)O
MOL006375	0.9499	0.0501	0.8968	Phellodendri Amurensis Cortex	5-o-feruloylquinic,acid	Not Available	FALSE	c1(c(cc(cc1)/C=C/C(=O)OC1C(C(CC(C1)(C(=O)O)O)O)O)O)OC)O
MOL006375	0.9499	0.0501	0.8968	Artemisia Annua L.	5-o-feruloylquinic,acid	Not Available	FALSE	c1(c(cc(cc1)/C=C/C(=O)OC1C(C(CC(C1)(C(=O)O)O)O)O)O)OC)O
MOL006376	0.2400	0.7600	0.6133	Phellodendri Amurensis Cortex	7-Dehydrosigmasterol	Not Available	FALSE	C1(CC2C(CC1)(C1C(=CC2)C2C(CC1)(C)C(CC2)C(C)CCC(C(C)C)CC)C)O
MOL006376	0.2400	0.7600	0.6133	Chebulae Fructus	7-Dehydrosigmasterol	Not Available	FALSE	C1(CC2C(CC1)(C1C(=CC2)C2C(CC1)(C)C(CC2)C(C)CCC(C(C)C)CC)C)O
MOL006378	0.9497	0.0503	0.9440	Chrysanthemi Flos	STOCK1N-58770	12310830	FALSE	C1(C(CC(CC1OC(=O)/C=C/c1ccc(c(c1)O)O)(O)C(=O)O)O)O
MOL006378	0.9497	0.0503	0.9440	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	STOCK1N-58770	12310830	FALSE	C1(C(CC(CC1OC(=O)/C=C/c1ccc(c(c1)O)O)(O)C(=O)O)O)O
MOL006378	0.9497	0.0503	0.9440	Ginseng Folium	STOCK1N-58770	12310830	FALSE	C1(C(CC(CC1OC(=O)/C=C/c1ccc(c(c1)O)O)(O)C(=O)O)O)O
MOL006378	0.9497	0.0503	0.9440	Xanthii Fructus	STOCK1N-58770	12310830	FALSE	C1(C(CC(CC1OC(=O)/C=C/c1ccc(c(c1)O)O)(O)C(=O)O)O)O
MOL006378	0.9497	0.0503	0.9440	Phellodendri Amurensis Cortex	STOCK1N-58770	12310830	FALSE	C1(C(CC(CC1OC(=O)/C=C/c1ccc(c(c1)O)O)(O)C(=O)O)O)O
MOL006379	0.7898	0.2102	0.7491	Phellodendri Amurensis Cortex	Dihydrophelloside	Not Available	FALSE	c1(cc(c2c(c1CCC(OC1OC(C(C(C1O)O)O)CO)C)C)OC(C(C2=O)O)c1ccc(cc1)O)O)OC1OC(C(C(C1O)O)O)CO
MOL006380	0.7661	0.2339	0.7872	Phellodendri Amurensis Cortex	Dihydrophelloside_qt	Not Available	FALSE	c1(cc(c2c(c1CCC(O)(C)C)OC(C(C2=O)O)c1ccc(cc1)O)O)O
MOL006381	0.2713	0.7287	0.6638	Phellodendri Amurensis Cortex	51744-55-9	Not Available	FALSE	O1C(=O)C2=C3N=C(C(=C3C1=O)C)/C=c\1/[nH]/c(=C/c3[nH]c(/C=C\4/NC2=C(C4C)CCC(=O)OC)c(c3C=C)C)/c(c1CC)C
MOL006382	0.6522	0.3478	0.7571	Phellodendri Amurensis Cortex	THALPHENINE	Not Available	FALSE	O1c2c3c4C([N+](CCc4cc2OC)(C)C)Cc2c3c(C1)c1OCOc1c2
MOL006383	0.5932	0.4068	0.6751	Phellodendri Amurensis Cortex	a6+	Not Available	FALSE	c1(c(c(cc(c1)C1OCC2C1COC2c1cc(c(c(c1)OC)OC1C(O)C(O)C(O)C(O1)CO)OC)OC)OC1C(O)C(O)C(O)C(O1)CO)OC

MOL006384	0.5284	0.4716	0.6200	Polygonati Odorati Rhizoma	4-[(1R,3aS,4R,6aS)-4-(4-hydroxy-3,5-dimethoxyphenyl)-1,3,3a,4,6,6a-hexahydrofuro[4,3-c]furan-1-yl]-2,6-dimethoxyphenol	11604108	FALSE	c1(c(c(cc(c1)C1OCC2C1COC2c1cc(c(c(c1)OC)O)OC)OC)O)OC
MOL006384	0.5284	0.4716	0.6200	Polygonati Rhizoma	4-[(1R,3aS,4R,6aS)-4-(4-hydroxy-3,5-dimethoxyphenyl)-1,3,3a,4,6,6a-hexahydrofuro[4,3-c]furan-1-yl]-2,6-dimethoxyphenol	11604108	FALSE	c1(c(c(cc(c1)C1OCC2C1COC2c1cc(c(c(c1)OC)O)OC)OC)O)OC
MOL006384	0.5284	0.4716	0.6200	Phellodendri Amurensis Cortex	4-[(1R,3aS,4R,6aS)-4-(4-hydroxy-3,5-dimethoxyphenyl)-1,3,3a,4,6,6a-hexahydrofuro[4,3-c]furan-1-yl]-2,6-dimethoxyphenol	11604108	FALSE	c1(c(c(cc(c1)C1OCC2C1COC2c1cc(c(c(c1)OC)O)OC)OC)O)OC

MOL006384	0.5284	0.4716	0.6200	Lobeliae Chinensis Herba	4-[(1R,3aS,4R,6aS)-4-(4-hydroxy-3,5-dimethoxyphenyl)-1,3,3a,4,6,6a-hexahydrofuro[4,3-c]furan-1-yl]-2,6-dimethoxyphenol	11604108	FALSE	c1(c(c(cc(c1)C1OCC2C1COC2c1cc(c(c(c1)OC)O)OC)OC)O)OC
MOL006385	0.7376	0.2624	0.6968	Phellodendri Amurensis Cortex	Amurensine	Not Available	FALSE	O1c2cc3C4N(CC(c3cc2OC1)c1c(C4)cc(OC)c(O)c1)C
MOL006386	0.9515	0.0485	0.8543	Phellodendri Amurensis Cortex	candicine	23423071	FALSE	c1cc(ccc1O)C[N+](C)(C)C
MOL006387	0.9497	0.0503	0.9440	Phellodendri Amurensis Cortex	chlorogenic	Not Available	FALSE	c1(ccc(cc1O)/C=C/C(=O)OC1C(O)C(CC(C1)(O)C(=O)O)O)O
MOL006387	0.9497	0.0503	0.9440	Eucommiae Folium	chlorogenic	Not Available	FALSE	c1(ccc(cc1O)/C=C/C(=O)OC1C(O)C(CC(C1)(O)C(=O)O)O)O
MOL006387	0.9497	0.0503	0.9440	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	chlorogenic	Not Available	FALSE	c1(ccc(cc1O)/C=C/C(=O)OC1C(O)C(CC(C1)(O)C(=O)O)O)O
MOL006387	0.9497	0.0503	0.9440	Scutellariae Barbatae Herba	chlorogenic	Not Available	FALSE	c1(ccc(cc1O)/C=C/C(=O)OC1C(O)C(CC(C1)(O)C(=O)O)O)O
MOL006387	0.9497	0.0503	0.9440	Artemisia Annua L.	chlorogenic	Not Available	FALSE	c1(ccc(cc1O)/C=C/C(=O)OC1C(O)C(CC(C1)(O)C(=O)O)O)O
MOL006388	0.1822	0.8178	0.7614	Phellodendri Amurensis Cortex	cneorin-NP36	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CC=C1C3(C)CCC(C(C4C(C5C(C)(C)O5)O4)C)C3(C)CCC21)C
MOL006389	0.3134	0.6866	0.6070	Phellodendri Amurensis Cortex	columbamine	Not Available	FALSE	c1(c(cc2c(c1)CC[n+]1c2cc2c(c1)cc(c(c2)OCC)OCC)OCC)O
MOL006392	0.2022	0.7978	0.7354	Phellodendri Amurensis Cortex	dihydronilotic in	Not Available	FALSE	OC1C(C2C(C3C(=CC2)C2(C(C(CC2)C(CC(O)C2OC2(C)C)C)(CC3)C)C)(CC1)C)(C)C
MOL006393	0.7114	0.2886	0.7116	Phellodendri Amurensis Cortex	epiberberine	Not Available	FALSE	C123C(C(=O)C(C4(C1CCC1(C54C(C(=O)OC1c1cocc1)O5)C)C)O)C(OC2CCC(=O)O3)(C)C
MOL006394	0.8360	0.1640	0.6280	Phellodendri Amurensis Cortex	guanidine	3520	FALSE	NC(=N)N
MOL006396	0.5629	0.4371	0.7470	Phellodendri Amurensis Cortex	isomer-of-magnofl,orine	Not Available	FALSE	c1(c(c2c3c(c1)CC[N+](C3Cc1c2c(c(cc1)O)OCC)(C)C)O)OC
MOL006397	0.3456	0.6544	0.6241	Phellodendri Amurensis Cortex	jatrorrhizine	Not Available	FALSE	c1(c(cc2c(c1)CC[n+]1c2cc2c(c1)c(c(cc2)OCC)OCC)OCC)O
MOL006398	0.6759	0.3241	0.7091	Phellodendri Amurensis Cortex	litcubine	Not Available	FALSE	c1(c(cc2c(c1)CC[N+]1(C2Cc2c1cc(c(c2)OC)O)C)O)OC

MOL006399	0.5293	0.4707	0.6305	Phellodendri Amurensis Cortex	lotusine	Not Available	FALSE	c1(c(cc2c(c1)CC[N+](C2Cc1ccc(cc1)O)(C)C)OC)O
MOL006400	0.5327	0.4673	0.7539	Phellodendri Amurensis Cortex	magnofl,orinea	Not Available	FALSE	c1(c(c2c3c(c1)CC[N+](C3Cc1c2c(c(cc1)OCC)O)(C)C)O)OC
MOL006401	0.1938	0.8062	0.7828	Phellodendri Amurensis Cortex	melianone	44575793	FALSE	O1C(O)C(C2C3(C(C4=CCC5C(C4CC3)(CCC(=O)C5(C)C)C)(CC2)C)C)CC1C1OC1(C)C
MOL006403	0.9410	0.0590	0.8631	Phellodendri Amurensis Cortex	methyl,3-o-feruloylquinate	Not Available	FALSE	C1C(C(C(CC1(C(=O)O)C)O)O)OC(=O)/C=C/c1ccc(c(c1)OC)O
MOL006404	0.6927	0.3073	0.6294	Phellodendri Amurensis Cortex	n-methylhigenamine-7-o-beta-d-glucopyranoside	Not Available	FALSE	c1(c(cc2c(c1)CCN(C2Cc1ccc(cc1)O)C)OC1C(O)C(O)C(O)C(O1)CO)O
MOL006405	0.8386	0.1614	0.8393	Phellodendri Amurensis Cortex	(1S)-1-(4-hydroxybenzyl)-2-methyl-3,4-dihydro-1H-isoquinoline-6,7-diol	11426154	FALSE	c1(c(cc2c(c1)CCN(C2Cc1ccc(cc1)O)C)O)O
MOL006405	0.8386	0.1614	0.8393	Folium Nelumbinis	(1S)-1-(4-hydroxybenzyl)-2-methyl-3,4-dihydro-1H-isoquinoline-6,7-diol	11426154	FALSE	c1(c(cc2c(c1)CCN(C2Cc1ccc(cc1)O)C)O)O
MOL006407	0.9497	0.0503	0.9440	Phellodendri Amurensis Cortex	neochlorogenic acid	7067333	FALSE	C1C(C(C(CC1(C(=O)O)O)O)O)OC(=O)/C=C/c1ccc(c(c1)O)O
MOL006407	0.9497	0.0503	0.9440	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	neochlorogenic acid	7067333	FALSE	C1C(C(C(CC1(C(=O)O)O)O)O)OC(=O)/C=C/c1ccc(c(c1)O)O
MOL006407	0.9497	0.0503	0.9440	Chrysanthemi Flos	neochlorogenic acid	7067333	FALSE	C1C(C(C(CC1(C(=O)O)O)O)O)OC(=O)/C=C/c1ccc(c(c1)O)O
MOL006407	0.9497	0.0503	0.9440	Xanthii Fructus	neochlorogenic acid	7067333	FALSE	C1C(C(C(CC1(C(=O)O)O)O)O)OC(=O)/C=C/c1ccc(c(c1)O)O
MOL006408	0.8341	0.1659	0.7499	Phellodendri Amurensis Cortex	noricariside	Not Available	FALSE	c1(c(c(=O)c2c(o1)c(c(cc2O)O)C(CC(C)(C)OC1C(O)C(O)C(O)C(O1)CO)OC1C(O)C(O)C(O)C(O1)CO)O)c1ccc(cc1)O
MOL006409	0.8033	0.1967	0.6227	Phellodendri Amurensis Cortex	noricariside_qt	Not Available	FALSE	c1(c(c(=O)c2c(o1)c(c(cc2O)O)C(CC(C)(C)O)O)O)c1ccc(cc1)O

MOL006410	0.5024	0.4976	0.7330	Phellodendri Amurensis Cortex	obacunoic,acid	Not Available	FALSE	C12(C(CC(=O)C3(C1CCC1(C43C(C(=O)OC1c1cocc1)O4)C)C)C(OC2)(C)C)C(O)OC(=O)CCCCCCCC(=O)O
MOL006411	0.6347	0.3653	0.7342	Phellodendri Amurensis Cortex	obacunone	Not Available	FALSE	C123C(CC(=O)C4(C1CCC1(C54C(C(=O)OC1c1cocc1)O5)C)C)C(OC2CCC(=O)O3)(C)C
MOL006412	0.7545	0.2455	0.7910	Phellodendri Amurensis Cortex	phellavin_qt	Not Available	FALSE	C1(C(C(=O)c2c(O1)cc(c(c2O)CCC(C)(C)O)O)O)c1ccc(cc1)O
MOL006414	0.9539	0.0461	0.8358	Phellodendri Amurensis Cortex	7-hydroxy-6-(2-hydroxyethyl) coumarin	10910685	FALSE	c1(c(cc2c(c1)ccc(=O)o2)O)CCO
MOL006415	0.9585	0.0415	0.8203	Phellodendri Amurensis Cortex	7-hydroxy-8-(2-hydroxyethyl) coumarin	11745794	FALSE	c1c(c(c2c(c1)ccc(=O)o2)CCO)O
MOL006416	0.8976	0.1024	0.8063	Phellodendri Amurensis Cortex	phellodenol-c	Not Available	FALSE	c1(c(cc2c(c1)C=CC(=O)C2)O)C/C=C(/C)\CO
MOL006417	0.4920	0.5080	0.8223	Phellodendri Amurensis Cortex	(2R,3R,8R)-3,5-dihydroxy-2-(4-hydroxyphenyl)-8-isopropenyl-2,3,8,9-tetrahydrofuro[2,3-h]chromen-4-one	10937119	FALSE	c12cc(c3c(c1CC(O2)C(=C)C)OC(C(C3=O)O)c1ccc(cc1)O)O
MOL006418	0.6793	0.3207	0.8393	Phellodendri Amurensis Cortex	phellodensin-c	Not Available	FALSE	c12cc(c3c(c1CC(O2)C(C)(C)O)OC(C(C3=O)O)c1ccc(cc1)O)O
MOL006419	0.5073	0.4927	0.7415	Phellodendri Amurensis Cortex	(13aS)-2,3,10-trimethoxy-6,8,13,13a-tetrahydro-5H-isoquinolino[2,1-b]isoquinolin-9-ol	11282465	FALSE	c1(c(cc2c(c1)CCN1C2Cc2c(C1)c(c(cc2)OC)O)OC)OC
MOL006420	0.2356	0.7644	0.6901	Phellodendri Amurensis Cortex	tetrahydropalmatine	Not Available	FALSE	c1(c(cc2c(c1)CCN1C2Cc2c(C1)c(c(cc2)OC)OCC)OC)OC

MOL006421	0.5850	0.4150	0.7310	Phellodendri Amurensis Cortex	tetrahydroreticuline	440930	FALSE	c1(c(cc2c(c1)CC[N+](=C2Cc1ccc(c(c1)O)OC)C)O)OC
MOL006422	0.7723	0.2277	0.7942	Phellodendri Amurensis Cortex	thalifendine	Not Available	FALSE	O1c2cc3CC[n+]4c(c3cc2OC1)cc1c(c4)c(OC)c(O)cc1
MOL006422	0.7723	0.2277	0.7942	Thalictri Glandulosissimi Et	thalifendine	Not Available	FALSE	O1c2cc3CC[n+]4c(c3cc2OC1)cc1c(c4)c(OC)c(O)cc1
MOL006422	0.7723	0.2277	0.7942	Semiaquilegiae Radix	thalifendine	Not Available	FALSE	O1c2cc3CC[n+]4c(c3cc2OC1)cc1c(c4)c(OC)c(O)cc1
MOL006423	0.9335	0.0665	0.9003	Phellodendri Amurensis Cortex	vanilloloside	44577222	FALSE	c1(ccc(cc1OC)CO)OC1C(O)C(O)C(O)C(O1)CO
MOL006423	0.9335	0.0665	0.9003	Folium Nelumbinis	vanilloloside	44577222	FALSE	c1(ccc(cc1OC)CO)OC1C(O)C(O)C(O)C(O1)CO
MOL006425	0.5991	0.4009	0.8181	Eriocauli Flos	2-Benzo[1,3]dioxol-5-yl-5,7-dimethoxy-chroman	636811	FALSE	c1(cc(c2c(c1)OC(CC2)c1cc2c(cc1)OCO2)OC)OC
MOL006426	0.8530	0.1470	0.7410	Eriocauli Flos	1,3,6-trihydroxy-2,5,7-trimethoxyxanthone	Not Available	FALSE	c1(c(c(c2c(c1)OC1C(C2=O)C=C(C(=C1OC)O)OC)O)OC)O
MOL006427	0.8087	0.1913	0.7853	Eriocauli Flos	methyl farnesoate	5275508	FALSE	C(=C(\CC/C=C(/CCC=C(C)C)\C)/C)/C(=O)OC
MOL006428	0.7925	0.2075	0.8307	Eriocauli Flos	7,30-dihydroxy-5,40,50-trimethoxyisoflavone	Not Available	FALSE	c1(cc(c2c(c1)OCC(C2=O)c1cc(c(c(c1)O)OC)OC)OC)O
MOL006429	0.8584	0.1416	0.8331	Eriocauli Flos	Hispidulin 7-glucoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(OC)c(O)c2c(oc(cc2=O)c2ccc(O)cc2)c1)CO
MOL006430	0.4762	0.5238	0.6835	Eriocauli Flos	hispidulin,7-(6-e-p-coumaroyl-b-d-glucopyranoside)	Not Available	FALSE	c1(c(c(c2c(c1)OC(CC2=O)c1ccc(cc1)O)O)OC)OC1OC(C(C(C1O)O)O)COC(=O)/C=C/c1ccc(cc1)O
MOL006431	0.6673	0.3327	0.7682	Eriocauli Flos	patuletin-3-o-[2-o-e-feruloyl-b-d-glucopyranosyl-(1-6)-b-d-glucopyranoside]	Not Available	FALSE	c1(c(c(c2c(c1)oc(c(c2=O)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1CC(=O)/C=C/c1ccc(c(c1)OC)O)O)O)CO)c1ccc(c(c1)O)O)O)OC)O

MOL006432	0.7375	0.2625	0.7688	Eriocauli Flos	patuletin-3-o-[b-d-glucopyranosyl-(1-3)-2-o-e-caffeoyl-b-d-glucopyranosyl-(1-6)-b-d-glucopyranoside]	Not Available	FALSE	c1(c(c(c2c(c1)oc(c(c2=O)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1CC(=O)/C=C/c1ccc(c(c1)O)O)OC1OC(C(C(C1O)O)O)CO)O)CO)c1ccc(c(c1)O)O)O)OC)O
MOL006433	0.7231	0.2769	0.7518	Eriocauli Flos	patuletin-3-o-[b-d-glucopyranosyl-(1-3)-2-o-e-caffeoyl-b-d-glucopyranosyl-(1-6)-b-d-glucopyranoside_qt	Not Available	FALSE	c1(c(c(c2c(c1)oc(c(c2=O)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1CC(=O)/C=C\c1ccc(c(c1)O)O)O)O)CO)c1ccc(c(c1)O)O)O)OC)O
MOL006434	0.8939	0.1061	0.8547	Eriocauli Flos	toralac-tone-9-o-b-d-glucopyranoside	Not Available	FALSE	c1c(cc2c(c1OC1OC(C(C(C1O)O)O)CO)c(c1c(c2)cc(oc1=O)C)O)OC
MOL006436	0.9319	0.0681	0.8403	Bidentis Bipinnatae Herba	Okanin	5281294	FALSE	c1(c(c(c(cc1)O)O)O)C(=O)/C=C/c1cc(c(cc1)O)O
MOL006437	0.9094	0.0906	0.7937	Bidentis Bipinnatae Herba	maritimein	Not Available	FALSE	c12c(C(=O)/C(=C/c3cc(c(cc3)O)O)/O1)ccc(c2O)OC1OC(C(C(C1O)O)O)CO
MOL006438	0.9250	0.0750	0.8527	Bidentis Bipinnatae Herba	(2E)-2-(3,4-dihydroxybenzylidene)-6,7-dihydroxy-benzofuran-3-one	6123451	FALSE	c12c(C(=O)/C(=C\c3cc(c(cc3)O)O)/O1)ccc(c2O)O
MOL006440	0.8384	0.1616	0.7210	Bidentis Bipinnatae Herba	bicycloelemene	Not Available	FALSE	C12(C(=CC(=C(C)C)CC2)C(CCC1)C)C
MOL006440	0.8384	0.1616	0.7210	Viticis Fructus	bicycloelemene	Not Available	FALSE	C12(C(=CC(=C(C)C)CC2)C(CCC1)C)C
MOL006440	0.8384	0.1616	0.7210	Angelicae Sinensis Radix	bicycloelemene	Not Available	FALSE	C12(C(=CC(=C(C)C)CC2)C(CCC1)C)C
MOL006441	0.8776	0.1224	0.7445	Bidentis Bipinnatae Herba	bidenphenol glucoside	Not Available	FALSE	c1c(c(cc(c1)CC=C)OC)OC1OC(C(C(C1O)O)OC1OCC(C1O)(O)CO)CO

MOL006442	0.9526	0.0474	0.8593	Bidentis Bipinnatae Herba	(R)-2-(3,4-dihydroxyphenyl)-6,7-dihydroxybenzofuran-3(2H)-one	Not Available	FALSE	c1(ccc2c(c1O)OC(C2=O)c1ccc(c(c1)O)O)O
MOL006443	0.6678	0.3322	0.7972	Tinosporae Radix	stepharanine	10358881	FALSE	O(c1c2c[n+]3CCc4c(c3cc2ccc1O)cc(O)c(OC)c4)C
MOL006444	0.4252	0.5748	0.6598	Tinosporae Radix	S-trans-N-methyltetrahydrocolumbamine	5319782	FALSE	O(c1c2C[N+]3(C(Cc2ccc1OC)c1c(CC3)cc(OC)c(O)c1)C)C
MOL006445	0.5142	0.4858	0.6391	Tinosporae Radix	makisterone A	12312690	FALSE	OC12C(C(CC2)C(O)(C(O)CC(C(O)(C)C)C)C)(CCC2C3(C(CC(O)C(O)C3)C(=O)C=C12)C)C
MOL006447	0.6630	0.3370	0.7953	Thalictri Glandulosissimi Et	dehydrodiscretamine	157159	FALSE	c1(c(cc2c(c1)CC[n+]1c2cc2c(c1)c(c(cc2)O)OC)OC)O
MOL006447	0.6630	0.3370	0.7953	Tinosporae Radix	dehydrodiscretamine	157159	FALSE	c1(c(cc2c(c1)CC[n+]1c2cc2c(c1)c(c(cc2)O)OC)OC)O
MOL006448	0.6613	0.3387	0.8237	Tinosporae Radix	isocolumbin	Not Available	FALSE	O1C2C3C(CCC4C3(CC(OC4=O)c3ccoc3)C)(C(O)(C=C2)C1=O)C
MOL006449	0.7455	0.2545	0.8190	Tinosporae Radix	tinoside	Not Available	FALSE	C1(=O)C2C(CC(O1)c1cocc1)(C1C3OC(=O)C(C1(CC2)C)(C=C3)OC1C(O)C(O)C(O)C(O1)CO)C
MOL006450	0.6613	0.3387	0.8237	Tinosporae Radix	tinoside_qt	Not Available	FALSE	C1(=O)C2C(CC(O1)c1cocc1)(C1C3OC(=O)C(C1(CC2)C)(C=C3)O)C
MOL006451	0.9415	0.0585	0.7978	Cassiae Semen	WLN: L66J BQ DQ	8601	FALSE	c1c(cc2c(c1O)cccc2)O
MOL006452	0.8548	0.1452	0.8168	Radix Salviae	1,5-Dihydroxy-3-methylanthraquinone	5316800	FALSE	Oc1c2c(C(=O)c3c(C2=O)cccc3O)cc(c1)C
MOL006452	0.8548	0.1452	0.8168	Cassiae Semen	1,5-Dihydroxy-3-methylanthraquinone	5316800	FALSE	Oc1c2c(C(=O)c3c(C2=O)cccc3O)cc(c1)C
MOL006453	0.8848	0.1152	0.8454	Cassiae Semen	1,6,7-Trihydroxy-3-methoxy-anthraquinone	Not Available	FALSE	c1(c(cc2c(c1)C(=O)c1c(C2=O)cc(cc1O)OC)O)O
MOL006454	0.7471	0.2529	0.8493	Cassiae Semen	1-Hydroxy-7-methoxy-3-methyl-anthraquinone	12360346	FALSE	c1(ccc2c(c1)C(=O)c1c(C2=O)cc(cc1O)C)OC

MOL006455	0.8494	0.1506	0.7972	Cassiae Semen	1-[(beta-D-Glucopyranosyl-(1-3)-O-beta-D-glucopyranosyl-(1-6)-O-beta-D-glucopyranosyl)oxy]-8-hydroxy-3-methyl-9,10-anthraquinone	Not Available	FALSE	C1(OC(C(C(C1O)O)O)COC1OC(C(C(C1O)OC1OC(C(C(C1O)O)O)CO)O)CO)Oc1cc(cc2c1C(=O)c1c(C2=O)cccc1O)C
MOL006456	0.8217	0.1783	0.7815	Cassiae Semen	1-[(beta-D-Glucopyranosyl-(1-6)-O-beta-D-glucopyranosyl-(1-3)-O-beta-D-glucopyranosl(1-6)-O-beta-D-glucopyranosyl)oxy]-8-hydrox3-methyl-9,10-anthraquinone	Not Available	FALSE	C1(OC(C(C(C1O)O)O)COC1OC(C(C(C1O)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)O)CO)Oc1cc(cc2c1C(=O)c1c(C2=O)cccc1O)C
MOL006457	0.9114	0.0886	0.7942	Cassiae Semen	1-hydroxy-2-hydroxymethy-3-methoxyanthraquinine	Not Available	FALSE	c1cc(c2c(c1)C(=O)c1c(C2=O)cc(c(c1O)CO)OC)O
MOL006458	0.8306	0.1694	0.7960	Cassiae Semen	5-Hydroxyalizarin-methylether	5318136	FALSE	c1cc(c2c(c1)C(=O)c1c(C2=O)ccc(c1OC)O)O
MOL006460	0.7476	0.2524	0.8394	Hemerocallis Radix	Obtusifolin	3083575	FALSE	c1(c(c(c2c(c1)C(=O)c1c(C2=O)c(ccc1)O)OC)O)C
MOL006460	0.7476	0.2524	0.8394	Cassiae Semen	Obtusifolin	3083575	FALSE	c1(c(c(c2c(c1)C(=O)c1c(C2=O)c(ccc1)O)OC)O)C

MOL006461	0.9119	0.0881	0.8479	Cassiae Semen	2-benzyl-4,6-dihydroxy benzoic acid-6-O-β-D-glucopyranoside	Not Available	FALSE	c1c(c(c(cc1O)Cc1ccccc1)C(=O)O)OC1OC(C(C(C1O)O)O)CO
MOL006462	0.9408	0.0592	0.8986	Cassiae Semen	2-benzyl-4,6-dihydroxy benzoic acid-6-O-β-D-glucopyranoside_qt	Not Available	FALSE	c1c(c(c(cc1O)Cc1ccccc1)C(=O)O)O
MOL006463	0.9108	0.0892	0.7518	Cassiae Semen	6-hydroxymusizin,8-o-beta-d-glucoside	Not Available	FALSE	c1c(cc2c(c1OCCC(C(C(C(C=O)O)O)O)O)c(c(c(c2)C)C(=O)C)O)O
MOL006464	0.8785	0.1215	0.7926	Cassiae Semen	9-[(beta-D-Glucopyranosyl-(1-6)-O-D-glucopyranosyl)oxy]-10-hydroxy-7-methoxy-3-methy-1H-naphthol[2,3-c]pyran-1-one	Not Available	FALSE	C1(OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)Oc1c2c(c3c(=O)oc(cc3cc2cc(c1)OC)C)O
MOL006465	0.8662	0.1338	0.7785	Cassiae Semen	Rubrofusarin-6-beta-gentiobioside	Not Available	FALSE	c12c(cc3c(c1O)c(=O)cc(o3)C)cc(cc2OC1C(C(C(C(O1)COC1C(C(C(C(O1)CO)O)O)O)O)O)O)OC
MOL006466	0.9045	0.0955	0.8299	Cassiae Semen	Rubrofusarin	72537	FALSE	c12c(cc3c(c1O)c(=O)cc(o3)C)cc(cc2O)OC
MOL006468	0.8637	0.1363	0.8890	Cassiae Semen	Anthraglycoside A	5319323	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(cc(c1)C)C(=O)c1c(C2=O)c(O)cc(OC)c1)CO
MOL006468	0.8637	0.1363	0.8890	Polygoni Cuspidati Rhizoma Et Radix	Anthraglycoside A	5319323	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(cc(c1)C)C(=O)c1c(C2=O)c(O)cc(OC)c1)CO
MOL006469	0.7710	0.2290	0.7721	Hemerocallis Radix	Morkit	6780	FALSE	c1ccc2c(c1)C(=O)c1c(C2=O)cccc1
MOL006469	0.7710	0.2290	0.7721	Polygoni Cuspidati Rhizoma Et Radix	Morkit	6780	FALSE	c1ccc2c(c1)C(=O)c1c(C2=O)cccc1
MOL006469	0.7710	0.2290	0.7721	Cassiae Semen	Morkit	6780	FALSE	c1ccc2c(c1)C(=O)c1c(C2=O)cccc1
MOL006469	0.7710	0.2290	0.7721	Apocyniveneti Folium	Morkit	6780	FALSE	c1ccc2c(c1)C(=O)c1c(C2=O)cccc1
MOL006469	0.7710	0.2290	0.7721	Folium Ilicis Cornutae	Morkit	6780	FALSE	c1ccc2c(c1)C(=O)c1c(C2=O)cccc1

MOL006470	0.8731	0.1269	0.8144	Cassiae Semen	aurantio-obtusin,6-o-beta-d-glucoside	Not Available	FALSE	c1(c(cc2c(c1O)C(=O)C1C(C2=O)C=C(C(=C1OC)O)C)OC1C(O)C(O)C(O)C(O1)CO)OC
MOL006471	0.8439	0.1561	0.7572	Cassiae Semen	aurantio-obtusin,6-o-beta-d-glucoside_qt	Not Available	FALSE	c1(c(cc2c(c1O)C(=O)C1C(C2=O)C=C(C(=C1OC)O)C)O)OC
MOL006472	0.8563	0.1437	0.8317	Cassiae Semen	Aurantio-obtusin	155011	FALSE	c1(cc2c(c(c1OC)O)C(=O)c1c(C2=O)cc(c(c1OC)O)C)O
MOL006473	0.9033	0.0967	0.8788	Cassiae Semen	Cassiaside A	164146	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(cc3oc(cc(=O)c3c2O)C)ccc1)CO
MOL006474	0.9099	0.0901	0.8294	Cassiae Semen	cassiaside_qt	Not Available	FALSE	Oc1c2c(cc3oc(cc(=O)c3c2O)C)ccc1
MOL006475	0.7697	0.2303	0.7902	Cassiae Semen	Obtusin	155380	FALSE	c1(cc2c(c(c1OC)O)C(=O)c1c(C2=O)cc(c(c1OC)O)C)OC
MOL006476	0.8627	0.1373	0.6931	Cassiae Semen	chrysophanol, triglucoside	Not Available	FALSE	c1(cccc2c1C(=O)c1c(C2=O)cc(cc1O)C)OCC(C(C(C(C(=O)OCC(C(C(C(C=O)O)O)(O)OCC(C(C(C(C=O)O)O)O)O)O)O)O)O)O
MOL006477	0.9291	0.0709	0.7469	Cassiae Semen	chrysophanol-8-beta-d-glucoside	Not Available	FALSE	c1cc2c(c(c1)OOCC(C(C(C(C=O)O)O)O)O)C(=O)c1c(C2=O)cc(cc1O)C
MOL006478	0.9103	0.0897	0.7900	Cassiae Semen	LTAN	2950	FALSE	c1ccc2c(c1O)C(=O)c1c(C2=O)cccc1O
MOL006479	0.9293	0.0707	0.8114	Cassiae Semen	emodin-8-beta-dglucoside	Not Available	FALSE	c1(cc2c(c(c1)OOCC(C(C(C(C=O)O)O)O)O)C(=O)c1c(C2=O)cc(cc1O)C)O
MOL006480	0.8763	0.1237	0.7816	Corayceps	Galactomannan	439336	FALSE	O(C1C(OC(O)C(O)C1O)COC1OC(C(O)C(O)C1O)CO)C1OC(C(O)C(O)C1O)CO
MOL006480	0.8763	0.1237	0.7816	Cassiae Semen	Galactomannan	439336	FALSE	O(C1C(OC(O)C(O)C1O)COC1OC(C(O)C(O)C1O)CO)C1OC(C(O)C(O)C1O)CO
MOL006481	0.8570	0.1430	0.8831	Cassiae Semen	gluco-obtusifolin	Not Available	FALSE	O(c1c(OC)c2c(C(=O)c3c(C2=O)c(O)ccc3)cc1C)C1OC(C(O)C(O)C1O)CO
MOL006482	0.9024	0.0976	0.8282	Cassiae Semen	9,10-dihydroxy-7-methoxy-3-methylene-4H-benzo[g]isochromen-1-one	157661	FALSE	O1C(=C)Cc2c(c(O)c3c(c2)cc(OC)cc3O)C1=O
MOL006483	0.9381	0.0619	0.7650	Cassiae Semen	nor-rubrofusarin	Not Available	FALSE	c1c(cc2c(c1O)c(c1c(c2)oc(cc1=O)C)O)O
MOL006484	0.9348	0.0652	0.7510	Cassiae Semen	nor-toralactone	Not Available	FALSE	c1c(cc2c(c1O)c(c1c(c2)cc(oc1=O)C)O)O
MOL006485	0.8570	0.1430	0.8831	Cassiae Semen	Obtusifolin 2-glucoside	442761	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(OC)c2c(cc1C)C(=O)c1c(C2=O)c(O)ccc1)CO

MOL006486	0.7473	0.2527	0.8269	Cassiae Semen	obtusin	Not Available	FALSE	C1(CC2C(C(C1O)OC)C(=O)C1C(C2=O)CC(C(C1OC)O)C)OC
MOL006487	0.9320	0.0680	0.9367	Cassiae Semen	ononitol,monohydrate	Not Available	FALSE	C1(C(C(C(C(C1O)O)O)OCO)O)O
MOL006488	0.8412	0.1588	0.7335	Polygoni Cuspidati Rhizoma Et Radix	Questin	160717	FALSE	O(c1c2c(C(=O)c3c(C2=O)c(O)cc(c3)C)cc(O)c1)C
MOL006488	0.8412	0.1588	0.7335	Cassiae Semen	Questin	160717	FALSE	O(c1c2c(C(=O)c3c(C2=O)c(O)cc(c3)C)cc(O)c1)C
MOL006488	0.8412	0.1588	0.7335	Actinidia Chinensis Planch	Questin	160717	FALSE	O(c1c2c(C(=O)c3c(C2=O)c(O)cc(c3)C)cc(O)c1)C
MOL006489	0.9087	0.0913	0.7887	Cassiae Semen	Quinizarin	6688	FALSE	c1ccc2c(c1)C(=O)c1c(C2=O)c(ccc1O)O
MOL006490	0.8559	0.1441	0.6772	Cassiae Semen	rubrofusarin,triglucoside	Not Available	FALSE	c1(cc(cc2c1c(c1c(c2)oc(cc1=O)C)O)OC)OCC(C(C(C(C(=O)OCC(C(C(C(=O)O)O)(O)OCC(C(C(C(=O)O)O)O)O)O)O)O)O)O
MOL006491	0.7863	0.2137	0.6631	Cassiae Semen	Sterculic acid	12921	FALSE	OC(=O)CCCCCCCC1=C(C1)CCCCCCCC
MOL006491	0.7863	0.2137	0.6631	Semen Firmianae	Sterculic acid	12921	FALSE	OC(=O)CCCCCCCC1=C(C1)CCCCCCCC
MOL006492	0.8410	0.1590	0.7820	Cassiae Semen	torachrysone,8-o-[beta-d-glucopyranosyl(1-3)-o-beta-d-glucopyranosyl(1-6)-o-beta-d-glucopyranoside]	Not Available	FALSE	C1(C(C(C(OC1CO)OC1C(C(OC(C1O)OCC1C(C(C(C(O1)Oc1cc(cc2c1c(c(c(c2)C)C(=O)C)O)OC)O)O)O)CO)O)O)O)O
MOL006494	0.7011	0.2989	0.6351	Cassiae Semen	torachrysone,tetraglucoside	Not Available	FALSE	c1(cc(cc2c1c(c(c(c2)C)C(=O)C)O)OC)OCC(C(C(C(COCCC(C(C(C(C=O)OCC(C(C(C(C=O)O)O)O)O)O)O)O)OCCC(C(C(C(C=O)O)O)O)O)O)O)O
MOL006495	0.8600	0.1400	0.7864	Cassiae Semen	toralactone,9-o-[beta-d-glucopyranosyl-(1-3)-o-beta-d-glucopyranosyl-(1-6)-o-beta-dglucopyranoside]	Not Available	FALSE	C1(C(C(C(OC1CO)OC1C(C(OC(C1O)OCC1C(C(C(C(O1)Oc1cc(cc2c1c(c1c(c2)cc(oc1=O)C)O)OC)O)O)O)CO)O)O)O)O
MOL006496	0.4684	0.5316	0.6585	Cassiae Semen	toralactone,9-o-beta-d-gentiobioside	Not Available	FALSE	c1c(cc2c(c1OC1C(OC(C(C1O)O)OCC1C(C(C(C(O1)O)C)C)C)CO)c(c1c(c2)cc(oc1=O)C)O)OC
MOL006497	0.8995	0.1005	0.9385	Cassiae Semen	γ-hydroxyarginine	54162047	FALSE	OC(CC(N)C(=O)O)CN=C(N)N

MOL006498	0.7557	0.2443	0.8303	Ilicis Cornutae Folium Immayuri	23-hydroxyursolic acid	44568920	FALSE	C1(C2C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C(=O)O)C)C)(CCC1O)C)(C)CO
MOL006499	0.6728	0.3272	0.6730	Ilicis Cornutae Folium Immayuri	27-cis-p-coumaroyloxyursolic acid	Not Available	FALSE	C1(C2C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C(=O)O)COC(=O)/C=C\c2ccc(cc2)O)C)(CCC1O)C)(C)C
MOL006500	0.6703	0.3297	0.7161	Ilicis Cornutae Folium Immayuri	(1S,2R,4aS,6aS,6aR,6bR,8aR,10R,11R,12aR,14bS)-10,11-dihydroxy-1,2,6a,6b,12a-pentamethyl-9-methylene-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydro-1H-picene-4a-carboxylic acid	10647480	FALSE	OC1CC2(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3C)C)C(=O)O)C)(CCC2C(=C)C1O)C)C
MOL006501	0.8368	0.1632	0.7310	Ilicis Cornutae Folium Immayuri	Isochlorogenic acid b	5281780	FALSE	O(C1C(OC(=O)/C=C/c2cc(O)c(O)cc2)C(O)CC(O)(C1)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL006501	0.8368	0.1632	0.7310	Xanthii Fructus	Isochlorogenic acid b	5281780	FALSE	O(C1C(OC(=O)/C=C/c2cc(O)c(O)cc2)C(O)CC(O)(C1)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL006501	0.8368	0.1632	0.7310	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	Isochlorogenic acid b	5281780	FALSE	O(C1C(OC(=O)/C=C/c2cc(O)c(O)cc2)C(O)CC(O)(C1)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL006502	0.8390	0.1610	0.7279	Ilicis Cornutae Folium Immayuri	3,5-Di-O-caffeoylquinic acid	Not Available	FALSE	O(C1CC(O)(CC(OC(=O)/C=C/c2cc(O)c(O)cc2)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL006502	0.8390	0.1610	0.7279	Xanthii Fructus	3,5-Di-O-caffeoylquinic acid	Not Available	FALSE	O(C1CC(O)(CC(OC(=O)/C=C/c2cc(O)c(O)cc2)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL006503	0.9409	0.0591	0.9203	Ilicis Cornutae Folium Immayuri	4-Caffeoylquinic acid	Not Available	FALSE	O(C(=O)/C=C/c1ccc(c(c1)O)O)C1C(CC(CC1O)(O)C(=O)O)O
MOL006504	0.7959	0.2041	0.7516	Ampelopsis Japonica	(-)-Catechin gallate	5276454	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)OC(=O)c1cc(c(c(c1)O)O)O)c1cc(c(cc1)O)O
MOL006504	0.7959	0.2041	0.7516	Ilicis Cornutae Folium Immayuri	(-)-Catechin gallate	5276454	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)OC(=O)c1cc(c(c(c1)O)O)O)c1cc(c(cc1)O)O

MOL006504	0.7959	0.2041	0.7516	Rhizoma Fagopyri Cymosi	(-)-Catechin gallate	5276454	FALSE	C1(C(Cc2c(O1)cc(cc2O)O)OC(=O)c1cc(c(c(c1)O)O)O)c1cc(c(cc1)O)O
MOL006505	0.9402	0.0598	0.8161	Drynariae Rhizoma	(-)-epicatechin	72276	FALSE	O1C(C(O)Cc2c1cc(O)cc2O)c1cc(O)c(O)cc1
MOL006505	0.9402	0.0598	0.8161	Allii Fistulost Bulbus	(-)-epicatechin	72276	FALSE	O1C(C(O)Cc2c1cc(O)cc2O)c1cc(O)c(O)cc1
MOL006505	0.9402	0.0598	0.8161	Ginkgo Semen	(-)-epicatechin	72276	FALSE	O1C(C(O)Cc2c1cc(O)cc2O)c1cc(O)c(O)cc1
MOL006505	0.9402	0.0598	0.8161	Smilacis Glabrae Rhixoma	(-)-epicatechin	72276	FALSE	O1C(C(O)Cc2c1cc(O)cc2O)c1cc(O)c(O)cc1
MOL006505	0.9402	0.0598	0.8161	Ephedrae Radix Et Rhizoma	(-)-epicatechin	72276	FALSE	O1C(C(O)Cc2c1cc(O)cc2O)c1cc(O)c(O)cc1
MOL006505	0.9402	0.0598	0.8161	Ilicis Cornutae Folium Immayuri	(-)-epicatechin	72276	FALSE	O1C(C(O)Cc2c1cc(O)cc2O)c1cc(O)c(O)cc1
MOL006505	0.9402	0.0598	0.8161	Phyllanthi Fructus	(-)-epicatechin	72276	FALSE	O1C(C(O)Cc2c1cc(O)cc2O)c1cc(O)c(O)cc1
MOL006505	0.9402	0.0598	0.8161	Eriobotryae Folium	(-)-epicatechin	72276	FALSE	O1C(C(O)Cc2c1cc(O)cc2O)c1cc(O)c(O)cc1
MOL006506	0.7592	0.2408	0.7842	Ilicis Cornutae Folium Immayuri	Ilekudinoside F	Not Available	FALSE	O1CC(C(C(C1OC1C(C2C(C3C(CC2)(C2(C(=CC3)C3C(C(=C)CCC3(CC2)C(=O)OC2OC(C(C(C2OC2OC(C(C(C2O)O)O)C)O)O)CO)(O)C)C)(CC1)C)(C)C)OC1OC(C(C(C1O)O)O)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)O)CO)O
MOL006507	0.7554	0.2446	0.8338	Ilicis Cornutae Folium Immayuri	Ilekudinoside F_qt	Not Available	FALSE	OC1C(C2C(C3C(CC2)(C2(C(=CC3)C3C(C(=C)CCC3(CC2)C(=O)O)(O)C)C)(CC1)C)(C)C
MOL006508	0.7263	0.2737	0.8138	Ilicis Cornutae Folium Immayuri	Ilekudinoside H	Not Available	FALSE	O1CC(C(C(C1OC1C(C2C(C3C(CC2)(C2(C(=C4C5(CC2)CCC(OC5=O)(C4(C)O)C)CC3O)C)C)(CC1)C)(C)C)OC1OC(C(C(C1O)O)O)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO)O
MOL006509	0.5151	0.4849	0.6991	Ilicis Cornutae Folium Immayuri	Ilekudinoside H_qt	Not Available	FALSE	OC1C(C2C(C3C(CC2)(C2(C(=C4C5(CC2)CCC(OC5=O)(C4(C)O)C)CC3O)C)C)(CC1)C)(C)C
MOL006510	0.7314	0.2686	0.8509	Ilicis Cornutae Folium Immayuri	Ilekudinoside I	Not Available	FALSE	O1CC(C(C(C1OC1C(C2C(C3C(CC2)(C2(C(=C4C5(CC2)CCC(OC5=O)(C4(C)O)C)C(C3)O)C)C)(CC1)C)(C)C)OC1OC(C(C(C1O)O)O)CO)O)O
MOL006511	0.5073	0.4927	0.6823	Ilicis Cornutae Folium Immayuri	ilekudinoside J_qt	Not Available	FALSE	OC1C(C2C(C3C(CC2)(C2(C(=C4C5(CC2)CCC(OC5=O)(C4(C)O)C)C(C3)O)C)C)(CC1)C)(C)C
MOL006512	0.7172	0.2828	0.8357	Ilicis Cornutae Folium Immayuri	Kudinoside A	Not Available	FALSE	O1C2(C(O)(C3=C4C(C5(C(C6(C(CC5)C(C(OC5OCC(O)C(OC7OC(C(O)C(O)C7O)CO)C5OC5OC(C(O)C(O)C5O)C)CC6)(C)C)C)CC4O)C)(CCC3(CC2)C1=O)C)C)C
MOL006513	0.5073	0.4927	0.6823	Ilicis Cornutae Folium Immayuri	Kudinoside C_qt	Not Available	FALSE	O1C2(C(O)(C3=C4C(C5(C(C6(C(CC5)C(C(O)CC6)(C)C)C)CC4O)C)(CCC3(CC2)C1=O)C)C)C

MOL006514	0.7255	0.2745	0.8280	Ilicis Cornutae Folium Immayuri	Kudinoside B	Not Available	FALSE	O1C2(C(O)(C3=C4C(C5(C(C6(C(CC5)C(C(OC5OC C(O)C(OC7OC(C(O)C(O)C7OC7OC(C(O)C(O)C7O) CO)CO)C5O)CC6)(C)C)C)CC4O)C)(CCC3(CC2)C1 =O)C)C)C
MOL006515	0.7267	0.2733	0.8143	Ilicis Cornutae Folium Immayuri	Kudinoside C	Not Available	FALSE	O1C2(C(O)(C3=C4C(C5(C(C6(C(CC5)C(C(OC5OC C(O)C(OC7OC(C(O)C(O)C7OC7OC(C(O)C(O)C7O) CO)CO)C5OC5OC(C(O)C(O)C5O)C)CC6)(C)C)C)C C4O)C)(CCC3(CC2)C1=O)C)C)C
MOL006516	0.7383	0.2617	0.8248	Ilicis Cornutae Folium Immayuri	Kudinoside D	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=C5C(CC4)C(C(C(C5(O)C) C)C)C)C=C3)C)(CC2)C)(CC1)C)(C)C)C1OCC(O)C(OC2OC(C(O)C(O)C2O)CO)C1OC1OC(C(O)C(O)C1 O)C
MOL006517	0.3831	0.6169	0.6972	Ilicis Cornutae Folium Immayuri	Kudinoside J_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=C5C(CC4)C(C(C(C5(O)C) C)C)C)C=C3)C)(CC2)C)(CC1)C)(C)C
MOL006518	0.7474	0.2526	0.8080	Ilicis Cornutae Folium Immayuri	Kudinoside E	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=C5C(CC4)C(C(C(C5(O)C) C)C)C)C=C3)C)(CC2)C)(CC1)C)(C)C)C1OCC(O)C(OC2OC(C(O)C(O)C2OC2OC(C(O)C(O)C2O)CO)C O)C1OC1OC(C(O)C(O)C1O)C
MOL006519	0.7558	0.2442	0.8418	Ilicis Cornutae Folium Immayuri	Kudinoside F	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=C5C(CC4)C(C(C(C5(O)C) C)C)C)C(O)C3)C)(CC2)C)(CC1)C)(C)C)C1OCC(O) C(OC2OC(C(O)C(O)C2O)CO)C1OC1OC(C(O)C(O) C1O)C
MOL006520	0.4187	0.5813	0.7224	Ilicis Cornutae Folium Immayuri	Kudinoside F_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=C5C(CC4)C(C(C(C5(O)C) C)C)C)C(O)C3)C)(CC2)C)(CC1)C)(C)C
MOL006521	0.7497	0.2503	0.8193	Ilicis Cornutae Folium Immayuri	Kudinoside G	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCCC3C) C(=O)OC3OC(C(O)C(O)C3O)CO)C)CC2)(CC1)C)(C)C)C1OCC(O)C(OC2OC(C(O)C(O)C2O)CO)C1OC 1OC(C(O)C(O)C1O)C
MOL006522	0.4917	0.5083	0.7051	Ilicis Cornutae Folium Immayuri	Kudinoside G_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCCC3C) C(=O)OC3OC(C(O)C(O)C3O)CO)C)CC2)(CC1)C)(C)C
MOL006523	0.4111	0.5889	0.6727	Ilicis Cornutae Folium Immayuri	Kudinoside J	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=C5C(CC4)C(C(C(C5(O)C) C)C)C)C=C3)C)(CC2)C)(CC1)C)(C)C)C1OCC(O)C(O)C1O
MOL006524	0.6101	0.3899	0.7299	Ilicis Cornutae Folium Immayuri	Ligurobustosi de N	Not Available	FALSE	O(C1C(OC(=O)/C=C\c2cc(O)c(O)cc2)C(OC(OCCc2 ccc(O)cc2)C1O)CO)C1OC(C(OC2OC(C(O)C(O)C2 O)C)C(O)C1O)C
MOL006525	0.6774	0.3226	0.7208	Ilicis Cornutae Folium Immayuri	Ligurobustosi de N_qt	Not Available	FALSE	OC1C(OC(=O)/C=C\c2cc(O)c(O)cc2)C(OC(OCCc2c cc(O)cc2)C1O)CO
MOL006527	0.9224	0.0776	0.8768	Ilicis Cornutae Folium Immayuri	theobromine	5429	FALSE	c12c(c(=O)[nH]c(=O)n1C)n(cn2)C
MOL006528	0.4489	0.5511	0.6833	Ilicis Cornutae Folium Immayuri	ilekudinol A	Not Available	FALSE	O1C23C(C4(C(C5(C(CC4)C(=C)C(O)C(O)C5)C)C= C3)C)(CCC3(C2C(C(CC3)C)C)C1=O)C
MOL006529	0.3834	0.6166	0.8114	Ilicis Cornutae Folium Immayuri	ilekudinol C	10766328	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)C O)CC3)C)(CC2)C)(CC1)C)(CO)C

MOL006530	0.7646	0.2354	0.8150	Ilicis Cornutae Folium Immayuri	ilekudinoside A	Not Available	FALSE	O1CC(C(C(C1OC1C(C2C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3)(C)C)C(=O)OC2OC(C(C(C2O)O)O)CO)C)C)(CC1)C)(C)C)OC1OC(C(C(C1O)O)O)C)OC1OC(C(C(C1O)O)O)CO)O
MOL006531	0.4426	0.5574	0.7474	Ilicis Cornutae Folium Immayuri	[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl] (4aS,6aR,6aS,6bR,8aR,10S,12aR,14bS)-10-hydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylate	14189384	FALSE	OC1C(C2C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3)(C)C)C(=O)OC2OC(C(C(C2O)O)O)CO)C)C)(CC1)C)(C)C

MOL006532	0.7427	0.2573	0.7245	Ilicis Cornutae Folium Immayuri	(2S,3S,4S,5R,6R)-6-[[(3S,4aR,6aR,6bS,8aS,11R,12R,12aS,14aR,14bR)-12-hydroxy-4,4,6a,6b,11,12,14b-heptamethyl-8a-[oxo-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)-2-tetrahydropyranyl]oxy]methyl]-1,2,3,4a,5,6,7,8,9,10,11,12a,14,14a-tetradecahydropic	21635822	FALSE	O1C(C(C(C(C1CO)O)O)O)OC(=O)C12C(C(C(CC1)C)(O)C)C1=CCC3C(C1(CC2)C)(CCC1C3(CCC(C1(C)C)OC1OC(C(C(C1O)O)O)C(=O)O)C)C

MOL006533	0.7992	0.2008	0.8377	Ilicis Cornutae Folium Immayuri	[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydropyran-2-yl] (1S,2R,4aS,6aR,6aS,6bR,8aR,9R,10R,11R,12aR,14bS)-11-hydroxy-9-(hydroxymethyl)-1,2,6a,6b,9,12a-hexamethyl-10-[(2S,3R,4S,5S)-3,4,5-trihydroxytetrahydropyran-2-yl]oxy-2,3,4,5,6,6a,7,8,	21635823	FALSE	O1CC(C(C(C1OC1C(CC2(C(C1(C)CO)CCC1(C2CC=C2C1(CCC1(CCC(C(C21)C)C)C(=O)OC1OC(C(C(C1O)O)O)CO)C)C)C)O)O)O)O

MOL006534	0.6225	0.3775	0.7200	Ilicis Cornutae Folium Immayuri	[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl] (1S,2R,4aS,6aR,6aS,6bR,8aR,9R,10R,11R,12aR,14bS)-10,11-dihydroxy-9-(hydroxymethyl)-1,2,6a,6b,9,12a-hexamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydro-1H-picene-4a-carboxylate	10372074	FALSE	OC1C(CC2(C(C1(C)CO)CCC1(C2CC=C2C1(CCC1(CCC(C(C21)C)C)C(=O)OC1OC(C(C(C1O)O)O)CO)C)C)C)O

MOL006535	0.8009	0.1991	0.8121	Ilicis Cornutae Folium Immayuri	[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydropyran-2-yl] (1R,2R,4aS,6aR,6aS,6bR,8aR,9R,10S,12aR,14bS)-1-hydroxy-9-(hydroxymethyl)-1,2,6a,6b,9,12a-hexamethyl-10-[(2S,3R,4S,5S)-3,4,5-trihydroxytetrahydropyran-2-yl]oxy-2,3,4,5,6,6a,7,8,8a,10	21635824	FALSE	O1CC(C(C(C1OC1C(C2C(C3C(CC2)(C2(C(=CC3)C3C(C(CCC3(CC2)C(=O)OC2OC(C(C(C2O)O)O)CO)C)(O)C)C)C)(CC1)C)(CO)C)O)O)O

MOL006536	0.6252	0.3748	0.7540	Ilicis Cornutae Folium Immayuri	[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl] (1R,2R,4aS,6aR,6aS,6bR,8aR,9R,10S,12aR,14bS)-1,10-dihydroxy-9-(hydroxymethyl)-1,2,6a,6b,9,12a-hexamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylate	14286954	FALSE	OC1C(C2C(C3C(CC2)(C2(C(=CC3)C3C(C(CCC3(CC2)C(=O)OC2OC(C(C(C2O)O)O)CO)C)(O)C)C)C)(CC1)C)(CO)C
MOL006536	0.6252	0.3748	0.7540	Ilicis Purpureae Folium	[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl] (1R,2R,4aS,6aR,6aS,6bR,8aR,9R,10S,12aR,14bS)-1,10-dihydroxy-9-(hydroxymethyl)-1,2,6a,6b,9,12a-hexamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylate	14286954	FALSE	OC1C(C2C(C3C(CC2)(C2(C(=CC3)C3C(C(CCC3(CC2)C(=O)OC2OC(C(C(C2O)O)O)CO)C)(O)C)C)C)(CC1)C)(CO)C

MOL006537	0.7645	0.2355	0.8339	Ilicis Cornutae Folium Immayuri	[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydropyran-2-yl] (1R,2R,4aS,6aR,6aS,6bR,8aR,10S,12aR,14bS)-10-[(2S,3R,4S,5S)-3,5-dihydroxy-4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydropyran-2-yl]oxy-tetrahydropyran-2-yl]oxy-1-h	21635825	FALSE	O1CC(C(C(C1OC1C(C2C(C3C(CC2)(C2(C(=CC3)C3C(C(CCC3(CC2)C(=O)OC2OC(C(C(C2O)O)O)CO)C)(O)C)C)C)(CC1)C)(C)C)O)OC1OC(C(C(C1O)O)O)CO)O
MOL006538	0.5644	0.4356	0.7450	Ilicis Cornutae Folium Immayuri	ilekudinoside E_qt	Not Available	FALSE	OC1C(C2C(C3C(CC2)(C2(C(=CC3)C3C(C(CCC3(CC2)C(=O)OC2OC(C(C(C2O)O)O)CO)C)(O)C)C)C)(CC1)C)(C)C
MOL006539	0.7408	0.2592	0.8195	Ilicis Cornutae Folium Immayuri	ilekudinoside G	Not Available	FALSE	O1CC(C(C(C1OC1C(C2C(C3C(CC2)(C2(C(=CC3)C3C(C4(OC(=O)C3(CC2)CC4)C)(O)C)C)C)(CC1)C)(C)C)OC1OC(C(C(C1O)O)O)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO)O
MOL006540	0.4160	0.5840	0.7234	Ilicis Cornutae Folium Immayuri	ilekudinoside G_qt	Not Available	FALSE	OC1C(C2C(C3C(CC2)(C2(C(=CC3)C3C(C4(OC(=O)C3(CC2)CC4)C)(O)C)C)C)(CC1)C)(C)C
MOL006541	0.7333	0.2667	0.8482	Ilicis Cornutae Folium Immayuri	ilekudinoside J	Not Available	FALSE	O1C(C(C(C(C1CO)O)O)O)OC1C(C(C(OC1OC1C(C2C(C3C(CC2)(C2(C(=C4C5(CC2)CCC(OC5=O)(C4(C)O)C)C(C3)O)C)C)(CC1)C)(C)C)CO)O)O

MOL006542	0.7612	0.2388	0.8406	Ilicis Cornutae Folium Immayuri	(1R,2S,4aS,6aR,6aS,6bR,8aR,10S,12aR,14bS)-1,10-dihydroxy-1,2,6a,6b,9,9,12a-heptamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	21626432	FALSE	C1(C2C(C3C(CC2)(C2(C(=CC3)C3C(C(CCC3(CC2)C(=O)O)C)(O)C)C)C)(CCC1O)C)(C)C
MOL006543	0.7727	0.2273	0.8329	Ilicis Cornutae Folium Immayuri	latifoloside B	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C1OCC(O)C(O)C1OC1OC(C(O)C(O)C1O)C
MOL006544	0.4426	0.5574	0.7474	Ilicis Cornutae Folium Immayuri	latifoloside C_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C
MOL006545	0.7646	0.2354	0.8150	Ilicis Cornutae Folium Immayuri	latifoloside C	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C1OCC(O)C(OC2OC(C(O)C(O)C2O)CO)C1OC1OC(C(O)C(O)C1O)C
MOL006546	0.7811	0.2189	0.8415	Ilicis Cornutae Folium Immayuri	latifoloside D	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)CC2)(CC1)C)(C)C1OCC(O)C(O)C1OC1OC(C(O)C(O)C1O)C
MOL006547	0.7370	0.2630	0.8071	Ilicis Cornutae Folium Immayuri	latifoloside D_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C)C(=O)O)C)CC2)(CC1)C)(C)C
MOL006548	0.6550	0.3450	0.7333	Ilicis Cornutae Folium Immayuri	liguPurpurosi de A	Not Available	FALSE	O(C1C(OC(=O)/C=C\c2cc(O)c(O)cc2)C(OC(OCCc2cc(O)c(O)cc2)C1O)CO)C1OC(C(OC2OC(C(O)C(O)C2O)C)C(O)C1O)C
MOL006549	0.7728	0.2272	0.7308	Cistanches Herba	Acteoside_qt	Not Available	FALSE	OC1C(OC(=O)/C=C\c2cc(O)c(O)cc2)C(OC(OCCc2cc(O)c(O)cc2)C1O)CO
MOL006549	0.7728	0.2272	0.7308	Ilicis Cornutae Folium Immayuri	Acteoside_qt	Not Available	FALSE	OC1C(OC(=O)/C=C\c2cc(O)c(O)cc2)C(OC(OCCc2cc(O)c(O)cc2)C1O)CO
MOL006550	0.5485	0.4515	0.7156	Ilicis Cornutae Folium Immayuri	ligupurpurosi de B	Not Available	FALSE	O(C1C(OC(=O)/C=C\c2ccc(O)cc2)C(OC(OCCc2ccc(O)cc2)C1O)CO)C1OC(C(OC2OC(C(O)C(O)C2O)C)C(O)C1O)C
MOL006551	0.5705	0.4295	0.7091	Ilicis Cornutae Folium Immayuri	ligupurpurosi de B_qt	Not Available	FALSE	OC1C(OC(=O)/C=C\c2ccc(O)cc2)C(OC(OCCc2ccc(O)cc2)C1O)CO
MOL006552	0.5778	0.4222	0.6843	Ilicis Cornutae Folium Immayuri	osmanthuside B6	Not Available	FALSE	c1cc(ccc1O)/C=C\C(=O)OCC1C(C(C(C(O1)OCCc1ccc(cc1)O)O)OC1OC(C(C(C1O)O)O)C)O

MOL006553	0.5962	0.4038	0.6966	Ilicis Cornutae Folium Immayuri	osmanthuside B6_qt	Not Available	FALSE	c1cc(ccc1O)/C=C\C(=O)OCC1C(C(C(C(O1)OCCc1ccc(cc1)O)O)O)O
MOL006554	0.3614	0.6386	0.7222	Ilicis Cornutae Folium Immayuri	Taraxerol	92097	FALSE	OC1C(C2C(C3C(C4=CCC5(C(C4(CC3)C)CC(CC5)(C)C)C)(CC2)C)(CC1)C)(C)C
MOL006554	0.3614	0.6386	0.7222	Pseudostellariae Radix	Taraxerol	92097	FALSE	OC1C(C2C(C3C(C4=CCC5(C(C4(CC3)C)CC(CC5)(C)C)C)(CC2)C)(CC1)C)(C)C
MOL006554	0.3614	0.6386	0.7222	Codonopsis Radix	Taraxerol	92097	FALSE	OC1C(C2C(C3C(C4=CCC5(C(C4(CC3)C)CC(CC5)(C)C)C)(CC2)C)(CC1)C)(C)C
MOL006555	0.5654	0.4346	0.7130	Ilicis Cornutae Folium Immayuri	ulmoidol	Not Available	FALSE	O1C2C34OC(=O)C5(C4C(C(CC5)C)C)CCC3(C3(C(C12)C1(C(CC3)C(=C)C(O)C(O)C1)C)C)C
MOL006556	0.3953	0.6047	0.7329	Glechomae Herba	NSC 159627	92802	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3C)C)CO)C)(CC2)C)(CC1)C)(C)C
MOL006556	0.3953	0.6047	0.7329	Folium Ilicis Cornutae	NSC 159627	92802	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3C)C)CO)C)(CC2)C)(CC1)C)(C)C
MOL006556	0.3953	0.6047	0.7329	Solidaginis Herba	NSC 159627	92802	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3C)C)CO)C)(CC2)C)(CC1)C)(C)C
MOL006556	0.3953	0.6047	0.7329	Ilicis Cornutae Folium Immayuri	NSC 159627	92802	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3C)C)CO)C)(CC2)C)(CC1)C)(C)C
MOL006557	0.7523	0.2477	0.7411	Ilicis Cornutae Folium Immayuri	Ziyuglycoside I	Not Available	FALSE	C(=O)(OC1C(C(C(C(O1)CO)O)O)O)C12C(C(C(CC2)C)(C)O)C2=CCC3C4(C(C(C(CC4)OC4C(O)C(C(CO4)O)O)(C)C)CCC3(C2(CC1)C)C)C
MOL006557	0.7523	0.2477	0.7411	Ilicis Purpureae Folium	Ziyuglycoside I	Not Available	FALSE	C(=O)(OC1C(C(C(C(O1)CO)O)O)O)C12C(C(C(CC2)C)(C)O)C2=CCC3C4(C(C(C(CC4)OC4C(O)C(C(CO4)O)O)(C)C)CCC3(C2(CC1)C)C)C
MOL006558	0.4693	0.5307	0.7538	Ilicis Cornutae Folium Immayuri	zigu—glucoside I_qt	Not Available	FALSE	C(=O)(OC1C(C(C(C(O1)CO)O)O)O)C12C(C(C(CC2)C)(C)O)C2=CCC3C4(C(C(CCC4)(C)C)CCC3(C2(CC1)C)C)C
MOL006559	0.6942	0.3058	0.7150	Ilicis Cornutae Folium Immayuri	zigu—glucoside II	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)OCCC(C)C(C)(C4C3=CCC21O)C)OC1C(O)C(O)C(O)CO1
MOL006560	0.7612	0.2388	0.8406	Folium Ilicis Cornutae	ilexsideii_qt	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)OCCC(C)C(C)(C4C3=CCC21O)C)O)O
MOL006560	0.7612	0.2388	0.8406	Ilicis Cornutae Folium Immayuri	ilexsideii_qt	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)OCCC(C)C(C)(C4C3=CCC21O)C)O)O
MOL006574	0.8774	0.1226	0.8801	Sophorae Flavescentis Radix	2-Hydroxychalcone	5367146	FALSE	c1ccc(cc1)C(=O)/C=C/c1ccccc1O
MOL006581	0.0818	0.9182	0.6418	Sophorae Flavescentis Radix	2-n-tridecyl-5,7-dihydroxy-6,8-dimethyl chromone	Not Available	FALSE	c1(cc(=O)c2c(c(c(c(c2o1)C)O)C)O)CCCCCCCCCCCCC
MOL006591	0.5878	0.4122	0.7390	Sophorae Flavescentis Radix	Thc-9-cooh	98523	FALSE	c12c(cc(c(c1O)C(=O)O)CCCCC)OC(C1C2C=C(CC1)C)(C)C

MOL006592	0.9235	0.0765	0.8887	Sophorae Flavescentis Radix	7-Demethylsuberosin	5316525	FALSE	c1(c(cc2c(c1)ccc(=O)o2)O)CC=C(C)C
MOL006593	0.3439	0.6561	0.6426	Sophorae Flavescentis Radix	Deoxyhumulone	6450808	FALSE	c1(c(c(c(c(c1O)C(=O)CC(C)C)O)CC=C(C)C)O)CC=C(C)C
MOL006594	0.9549	0.0451	0.9732	Ephedra Herba	Eciphin	9294	FALSE	c1cccc(c1)C(C(C)NC)O
MOL006594	0.9549	0.0451	0.9732	Arum Ternatum Thunb.	Eciphin	9294	FALSE	c1cccc(c1)C(C(C)NC)O
MOL006594	0.9549	0.0451	0.9732	Sophorae Flavescentis Radix	Eciphin	9294	FALSE	c1cccc(c1)C(C(C)NC)O
MOL006594	0.9549	0.0451	0.9732	Ephedrae Radix Et Rhizoma	Eciphin	9294	FALSE	c1cccc(c1)C(C(C)NC)O
MOL006595	0.8797	0.1203	0.9002	Sophorae Flavescentis Radix	(2R)-flavanone	689010	FALSE	c1ccc2c(c1)OC(CC2=O)c1ccccc1
MOL006596	0.7264	0.2736	0.8037	Sophorae Flavescentis Radix	Glyceollin	Not Available	FALSE	c12ccc3c(c1C=CC(O2)(C)C)OCC1(C3Oc2c1ccc(c2)O)O
MOL006597	0.9517	0.0483	0.9467	Sophorae Flavescentis Radix	OMD	780	FALSE	c1cc(c(cc1O)CC(=O)O)O
MOL006597	0.9517	0.0483	0.9467	Arum Ternatum Thunb.	OMD	780	FALSE	c1cc(c(cc1O)CC(=O)O)O
MOL006599	0.3824	0.6176	0.6306	Sophorae Flavescentis Radix	3,4',5-Trihydroxy-7-methoxy-8-isopentenylflavone	5322079	FALSE	o1c2c(CC=C(C)C)c(OC)cc(O)c2c(=O)c(O)c1c1ccc(O)cc1
MOL006599	0.3824	0.6176	0.6306	Radix Euphorbiae Pekinensis	3,4',5-Trihydroxy-7-methoxy-8-isopentenylflavone	5322079	FALSE	o1c2c(CC=C(C)C)c(OC)cc(O)c2c(=O)c(O)c1c1ccc(O)cc1
MOL006600	0.5235	0.4765	0.7564	Sophorae Flavescentis Radix	1-[2,4-dihydroxy-3-(3-methylbut-2-enyl)phenyl]-3-phenylprop-2-en-1-one	6251270	FALSE	c1(ccc(c(c1CC=C(C)C)O)C(=O)/C=C/c1ccccc1)O
MOL006601	0.9466	0.0534	0.7515	Sophorae Flavescentis Radix	kuraranine	46187187	FALSE	OCC1CC(CN(C1)C)c1[nH]c(=O)ccc1

MOL006603	0.9134	0.0866	0.7946	Sophorae Flavescentis Radix	(E)-1-(2,6-dihydroxyphenyl)-3-(4-hydroxyphenyl)prop-2-en-1-one	12883590	FALSE	c1cc(c(c(c1)O)C(=O)/C=C/c1ccc(cc1)O)O
MOL006604	0.2766	0.7234	0.6475	Sophorae Flavescentis Radix	(2S)-7-hydroxy-2-(4-hydroxyphenyl)-5-methoxy-8-(3-methylbut-2-enyl)chroman-4-one	9928523	FALSE	c1(cc(c2c(c1CC=C(C)C)OC(CC2=O)c1ccc(cc1)O)OC)O
MOL006613	0.8321	0.1679	0.7595	Sophorae Flavescentis Radix	kushenin	Not Available	FALSE	O1C2C(c3c1cc(O)c(OC)c3)COc1c2ccc(O)c1
MOL006619	0.8110	0.1890	0.7775	Sophorae Flavescentis Radix	kushenol J	Not Available	FALSE	C1(C(C(=O)c2c(O1)cc(cc2)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)CO1)O)c1ccc(cc1)OC
MOL006620	0.8097	0.1903	0.8597	Sophorae Flavescentis Radix	kushenol J_qt	Not Available	FALSE	C1(C(C(=O)c2c(O1)cc(cc2)O)O)c1ccc(cc1)OC
MOL006621	0.2577	0.7423	0.6363	Sophorae Flavescentis Radix	(2R,3R)-2-(2,4-dihydroxyphenyl)-3,7-dihydroxy-8-[(2R)-2-isopropenyl-5-methylhex-4-enyl]-5-methoxy-4-chromanone	20832634	FALSE	O1C(C(O)C(=O)c2c1c(CC(CC=C(C)C)C(=C)C)c(O)cc2OC)c1c(O)cc(O)cc1
MOL006622	0.7520	0.2480	0.7112	Sophorae Flavescentis Radix	kushenol O	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2occ(c(=O)c2cc1)c1ccc(OC)cc1)COC1OCC(O)C(O)C1O
MOL006624	0.7237	0.2763	0.8027	Sophorae Flavescentis Radix	kushequinone A	Not Available	FALSE	C1(=O)C(=C(C(=O)C(=C1)OC)O)CC(CC=C(C)C)C(=C)C
MOL006626	0.7453	0.2547	0.6119	Sophorae Flavescentis Radix	leachianone,g	Not Available	FALSE	c1(cc(c2c(c1CC=C(C)C)OC(CC2=O)c1ccc(cc1O)O)O)O
MOL006630	0.9143	0.0857	0.7528	Sophorae Flavescentis Radix	Norartocarpetin	5481970	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1ccc(cc1O)O)O)O

MOL006632	0.1589	0.8411	0.6085	Sophorae Flavescentis Radix	(2S)-2-(3,4-dihydroxyphenyl)-6-[(2E)-3,7-dimethylocta-2,6-dienyl]-5,7-dihydroxychroman-4-one	639465	FALSE	c1(c(c(c2c(c1)OC(CC2=O)c1ccc(c(c1)O)O)O)C/C=C(/CCC=C(C)C)\C)O
MOL006633	0.9351	0.0649	0.9060	Sophorae Flavescentis Radix	DIMETHYLALLYLUMBELLIFERONE, 0-	320362	FALSE	c1c(cc2c(c1)ccc(=O)o2)OCC=C(C)C
MOL006637	0.9549	0.0451	0.9732	Sophorae Flavescentis Radix	Psi-ephedrin	7028	FALSE	c1cccc(c1)C(C(C)NC)O
MOL006637	0.9549	0.0451	0.9732	Ephedrae Radix Et Rhizoma	Psi-ephedrin	7028	FALSE	c1cccc(c1)C(C(C)NC)O
MOL006637	0.9549	0.0451	0.9732	Ephedra Herba	Psi-ephedrin	7028	FALSE	c1cccc(c1)C(C(C)NC)O
MOL006638	0.8605	0.1395	0.7294	Sophorae Flavescentis Radix	Pterocarpine	Not Available	FALSE	c1c(cc2c(c1)C1C(CO2)c2c(O1)cc1c(c2)OCO1)OC
MOL006642	0.7574	0.2426	0.8287	Sophorae Flavescentis Radix	sophoraflavoside II	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(O)CC(C3)(C)C(=O)O)C)C)(CC2)C)(CC1)C)(CO)C)C1OC(C(O)C(O)C1OC1C(O)C(O)C(OC1OC1C(O)C(O)C(OC1O)C)CO)C(=O)O
MOL006643	0.7098	0.2902	0.7774	Sophorae Flavescentis Radix	sophoraflavosideIII_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(O)CC(C3)(C)C(=O)O)C)C)(CC2)C)(CC1)C)(CO)C
MOL006644	0.7567	0.2433	0.7893	Sophorae Flavescentis Radix	sophoraflavoside IV	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(OC4OCC(O)C(O)C4OC4C(O)C(O)C(OC4O)CO)CC(C3)(C)C(=O)O)C)C)(CC2)C)(CC1)C)(CO)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)C)CO)C(=O)O
MOL006645	0.7098	0.2902	0.7774	Sophorae Flavescentis Radix	sophoraflavoside IV_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(O)CC(C3)(C)C(=O)O)C)C)(CC2)C)(CC1)C)(CO)C
MOL006646	0.7756	0.2244	0.8115	Sophorae Flavescentis Radix	sophoraflavosideIII	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(OC4OC(O)C(O)C(O)C4)CC(C3)(C)C(=O)O)C)C)(CC2)C)(CC1)C)(CO)C)C1OC(C(O)C(O)C1OC1C(O)C(O)C(OC1OC1C(O)C(O)C(OC1O)C)CO)C(=O)O
MOL006647	0.1946	0.8054	0.7548	Sophorae Flavescentis Radix	sophoraisoflavanone,a	Not Available	FALSE	c1(cc(c2c(c1)OCC(C2=O)c1c(c(cc1)O)C/C(=C/CC)/C)OCC)O)O
MOL006650	0.8350	0.1650	0.6919	Sophorae Flavescentis Radix	(-)-Maackiain-3-O-glucosyl-6'-O-malonate	Not Available	FALSE	O1C2C(c3c1cc1OCOc1c3)COc1c2ccc(OC2OC(C(O)C(O)C2O)COC(=O)CC(=O)O)c1

MOL006651	0.8866	0.1134	0.6191	Panax Ginseng C. A. Mey.	Trifolirhizin	Not Available	FALSE	O1C2C(c3c1cc1OCOc1c3)COc1c2ccc(OC2OC(C(O)C(O)C2O)CO)c1
MOL006651	0.8866	0.1134	0.6191	Pyrrosiae Folium	Trifolirhizin	Not Available	FALSE	O1C2C(c3c1cc1OCOc1c3)COc1c2ccc(OC2OC(C(O)C(O)C2O)CO)c1
MOL006651	0.8866	0.1134	0.6191	Sophorae Flavescentis Radix	Trifolirhizin	Not Available	FALSE	O1C2C(c3c1cc1OCOc1c3)COc1c2ccc(OC2OC(C(O)C(O)C2O)CO)c1
MOL006652	0.9008	0.0992	0.6047	Sophorae Flavescentis Radix	trifolrhizin	Not Available	FALSE	c1c(cc2c(c1)C1C(CO2)c2c(O1)cc1c(c2)OCO1)OOC1C(C(C(O1)CO)O)O)O
MOL006654	0.9371	0.0629	0.9471	Portulacae Herba	(-)-noradrenaline	439260	FALSE	Oc1cc(C(O)CN)ccc1O
MOL006655	0.9598	0.0402	0.9487	Portulacae Herba	Bethanid	2368	FALSE	c1(CN=C(NC)NC)ccccc1
MOL006656	0.9229	0.0771	0.9169	Portulacae Herba	Dopa D-form	6989908	FALSE	C(=O)(C(Cc1cc(c(cc1)O)O)N)O
MOL006657	0.9402	0.0598	0.6223	Portulacae Herba	isobetanidin	Not Available	FALSE	C1(CC(=CC(=N1)C(=O)O)/C=C/N1C(Cc2cc(c(cc12)O)O)C(=O)O)C(=O)O
MOL006658	0.8617	0.1383	0.7003	Portulacae Herba	betanin	Not Available	FALSE	c12c(CC(/[N+]/1=C/C=C/1\CC(NC(=C1)C(=O)O)C(=O)O)C(=O)O)cc(c(c2)O)OC1OC(C(C(C1O)O)O)CO
MOL006659	0.9369	0.0631	0.6193	Portulacae Herba	betanin_qt	Not Available	FALSE	c12c(CC(/[N+]/1=C\C=C/1\CC(NC(=C1)C(=O)O)C(=O)O)C(=O)O)cc(c(c2)O)O
MOL006660	0.2193	0.7807	0.7179	Portulacae Herba	parkeol	12313974	FALSE	OC1C(C2C(C3=CCC4(C(C3CC2)(CCC4C(CCC=C(C)C)C)C)C)(CC1)C)(C)C
MOL006661	0.8617	0.1383	0.7003	Portulacae Herba	isobetanin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2CC(/[N+](=C/C=C\3/CC(NC(=C3)C(=O)O)C(=O)O)/c2cc1O)C(=O)O)CO
MOL006662	0.9369	0.0631	0.6193	Portulacae Herba	isobetanin_qt	Not Available	FALSE	Oc1cc2CC(/[N+](=C/C=C\3/CC(NC(=C3)C(=O)O)C(=O)O)/c2cc1O)C(=O)O
MOL006663	0.8704	0.1296	0.6267	Buddlejae Flos	(s)-tryptophan-betaxanthin	Not Available	FALSE	c1cc2c(cc1)c(c[nH]2)CC(/N=C\C=C/1\C=C(NC(C1)C(=O)O)C(=O)O)C(=O)O
MOL006663	0.8704	0.1296	0.6267	Celosiae Semen	(s)-tryptophan-betaxanthin	Not Available	FALSE	c1cc2c(cc1)c(c[nH]2)CC(/N=C\C=C/1\C=C(NC(C1)C(=O)O)C(=O)O)C(=O)O
MOL006664	0.9388	0.0612	0.8913	Buddlejae Flos	(2R,3S,4S,5R,6S)-2-methylol-6-(2-phenylethoxy) tetrahydropyran-3,4,5-triol	11076951	FALSE	c1ccc(cc1)CCOC1C(O)C(O)C(O)C(O1)CO

MOL006665	0.9388	0.0612	0.8913	Buddlejae Flos	(2R,3S,4S,5R,6R)-2-methylol-6-(2-phenylethoxy) tetrahydropyran-3,4,5-triol	11289099	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)CCc1ccccc1
MOL006666	0.9276	0.0724	0.7015	Celosiae Semen	3-methoxytyramine-betaxanthin	Not Available	FALSE	C(/N=C\C=C/1\C=C(NC(C1)C(=O)O)C(=O)O)Cc1cc(c(cc1)O)OC
MOL006666	0.9276	0.0724	0.7015	Buddlejae Flos	3-methoxytyramine-betaxanthin	Not Available	FALSE	C(/N=C\C=C/1\C=C(NC(C1)C(=O)O)C(=O)O)Cc1cc(c(cc1)O)OC
MOL006668	0.6580	0.3420	0.7511	Buddlejae Flos	Neobudofficide	Not Available	FALSE	C1(C(C(C(OC1C)OCC1C(C(C(C(O1)Oc1cc(c2c(c1)oc(cc2=O)c1ccc(cc1)OC)O)OC1OC(C(C(C1O)O)O)C)O)O)O)O)O
MOL006669	0.8782	0.1218	0.8620	Buddlejae Flos	apigenin 7-O-beta-D-glucopyranoside	Not Available	FALSE	c12c(cc(cc1O)OC1C(O)C(O)C(O)C(O1)CO)oc(cc2=O)c1ccc(cc1)O
MOL006670	0.9512	0.0488	0.8524	Buddlejae Flos	aucubigenin	163040	FALSE	OC1OC=CC2C1C(=CC2O)CO
MOL006670	0.9512	0.0488	0.8524	Plantaginis Herba	aucubigenin	163040	FALSE	OC1OC=CC2C1C(=CC2O)CO
MOL006670	0.9512	0.0488	0.8524	Plantaginis Semen	aucubigenin	163040	FALSE	OC1OC=CC2C1C(=CC2O)CO
MOL006670	0.9512	0.0488	0.8524	Verbenae Herb	aucubigenin	163040	FALSE	OC1OC=CC2C1C(=CC2O)CO
MOL006670	0.9512	0.0488	0.8524	Figwort Root	aucubigenin	163040	FALSE	OC1OC=CC2C1C(=CC2O)CO
MOL006670	0.9512	0.0488	0.8524	Eucommiae Folium	aucubigenin	163040	FALSE	OC1OC=CC2C1C(=CC2O)CO
MOL006671	0.7467	0.2533	0.7205	Buddlejae Flos	beta-methoxylactecoside	Not Available	FALSE	C1(C(C(C(OC1CO)OCC(c1ccc(c(c1)O)O)OC)O)OC1C(C(C(C(O1)C)O)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O
MOL006672	0.7729	0.2271	0.7149	Buddlejae Flos	beta-methoxylactecoside_qt	Not Available	FALSE	C1(C(C(C(OC1CO)OCC(c1ccc(c(c1)O)O)OC)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O
MOL006673	0.1784	0.8216	0.6926	Buddlejae Flos	butyrospermyl acetate	Not Available	FALSE	O(C1C(C2C(C3C(=CC2)C2(C(C(CC2)C(CCC=C(C)C)C)(CC3)C)C)(CC1)C)(C)C)C(=O)C
MOL006674	0.7467	0.2533	0.7205	Buddlejae Flos	campneoside	Not Available	FALSE	CC1C(C(C(C(O1)OC1C(C(OC(C1OC(=O)/C=C/c1cc(c(cc1)O)O)CO)OCC(c1cc(c(cc1)O)O)OC)O)O)O)O
MOL006675	0.7729	0.2271	0.7150	Buddlejae Flos	campneoside_qt	Not Available	FALSE	OC1C(C(OC(C1OC(=O)/C=C/c1cc(c(cc1)O)O)CO)OCC(c1cc(c(cc1)O)O)OC)O
MOL006676	0.8729	0.1271	0.8037	Buddlejae Flos	Catalposide	93039	FALSE	O1C2(C1C(OC(=O)c1ccc(O)cc1)C1C2C(OC=C1)OC1OC(C(O)C(O)C1O)CO)CO
MOL006677	0.8374	0.1626	0.7574	Buddlejae Flos	catalposide_qt	Not Available	FALSE	O1C2(C1C(OC(=O)c1ccc(O)cc1)C1C2C(OC=C1)O)CO

MOL006678	0.6112	0.3888	0.7870	Celosiae Semen	celogenamide, a	Not Available	FALSE	c1ccc2c(c1)n1cc2CC(NC(=O)C(NC(=O)C(Cc2ccccc2)NC(=O)C(C(C)C)NC(=O)C1NC(=O)C(Cc1ccc(cc1)O)NC(=O)C1CCCN1C(=O)C1NC(=O)CC1)CO)C(=O)NC(CCCCN)C(=O)O
MOL006678	0.6112	0.3888	0.7870	Buddlejae Flos	celogenamide, a	Not Available	FALSE	c1ccc2c(c1)n1cc2CC(NC(=O)C(NC(=O)C(Cc2ccccc2)NC(=O)C(C(C)C)NC(=O)C1NC(=O)C(Cc1ccc(cc1)O)NC(=O)C1CCCN1C(=O)C1NC(=O)CC1)CO)C(=O)NC(CCCCN)C(=O)O
MOL006679	0.5617	0.4383	0.7843	Buddlejae Flos	celogentin,b	Not Available	FALSE	c1cc2c3cc1C(=C(C)C)C(NC(=O)C1NC(=O)CC1)C(=O)NC(C(=O)NC(=C(C)C)C(=O)NC1Cc2c([nH]3)n2cc(nc2)CC(NC(=O)C(NC1=O)CCCNC(=N)N)C(=O)NC(C(=O)O)Cc1c[nH]cn1)CC(C)C
MOL006679	0.5617	0.4383	0.7843	Celosiae Semen	celogentin,b	Not Available	FALSE	c1cc2c3cc1C(=C(C)C)C(NC(=O)C1NC(=O)CC1)C(=O)NC(C(=O)NC(=C(C)C)C(=O)NC1Cc2c([nH]3)n2cc(nc2)CC(NC(=O)C(NC1=O)CCCNC(=N)N)C(=O)NC(C(=O)O)Cc1c[nH]cn1)CC(C)C
MOL006680	0.4965	0.5035	0.7806	Buddlejae Flos	celogentin,c	Not Available	FALSE	c1cc2c3cc1C(=C(C)C)C(NC(=O)C1NC(=O)CC1)C(=O)NC(C(=O)NC(=C(C)C)C(=O)NC1Cc2c([nH]3)N2CC(=NC2)CC(NC(=O)C(CCCNC(=N)N)NC(=O)C2N(C1=O)CCC2)C(=O)O)CC(C)C
MOL006680	0.4965	0.5035	0.7806	Celosiae Semen	celogentin,c	Not Available	FALSE	c1cc2c3cc1C(=C(C)C)C(NC(=O)C1NC(=O)CC1)C(=O)NC(C(=O)NC(=C(C)C)C(=O)NC1Cc2c([nH]3)N2CC(=NC2)CC(NC(=O)C(CCCNC(=N)N)NC(=O)C2N(C1=O)CCC2)C(=O)O)CC(C)C
MOL006681	0.7264	0.2736	0.7281	Buddlejae Flos	echinacoside	Not Available	FALSE	CC1C(C(C(C(O1)OC1C(C(OC(C1OC(=O)/C=C/c1ccc(cc1)O)O)COC1C(C(C(C(O1)CO)O)O)O)OCCc1ccc(cc1)O)O)O)O)O
MOL006682	0.7728	0.2272	0.7308	Verbenae Herb	Calceolarioside A	5273566	FALSE	OC1C(OC(=O)/C=C/c2cc(O)c(O)cc2)C(OC(OCCc2cc(O)c(O)cc2)C1O)CO
MOL006682	0.7728	0.2272	0.7308	Plantaginis Semen	Calceolarioside A	5273566	FALSE	OC1C(OC(=O)/C=C/c2cc(O)c(O)cc2)C(OC(OCCc2cc(O)c(O)cc2)C1O)CO
MOL006682	0.7728	0.2272	0.7308	Buddlejae Flos	Calceolarioside A	5273566	FALSE	OC1C(OC(=O)/C=C/c2cc(O)c(O)cc2)C(OC(OCCc2cc(O)c(O)cc2)C1O)CO
MOL006682	0.7728	0.2272	0.7308	Plantaginis Herba	Calceolarioside A	5273566	FALSE	OC1C(OC(=O)/C=C/c2cc(O)c(O)cc2)C(OC(OCCc2cc(O)c(O)cc2)C1O)CO
MOL006682	0.7728	0.2272	0.7308	Campsis Flos	Calceolarioside A	5273566	FALSE	OC1C(OC(=O)/C=C/c2cc(O)c(O)cc2)C(OC(OCCc2cc(O)c(O)cc2)C1O)CO
MOL006683	0.7111	0.2889	0.7186	Buddlejae Flos	forsythoside,b	Not Available	FALSE	CC1C(C(C(C(O1)OC1C(C(OC(C1OC(=O)/C=C/c1ccc(cc1)O)O)COC1C(C(CO1)(CO)O)O)OCCc1cc(c(cc1)O)O)O)O)O)O
MOL006684	0.7728	0.2272	0.7308	Buddlejae Flos	jionoside D_qt	Not Available	FALSE	c1(c(ccc(c1)/C=C/C(=O)OC1C(C(C(OC1CO)OCCc1ccc(c(c1)O)O)O)O)O)O

MOL006685	0.7453	0.2547	0.8168	Buddlejae Flos	mimengoside B	Not Available	FALSE	O(C1C2C(C3(C(=C1)C1C(CC3)(CCC(C1)(C)C)CO)C)(CCC1C2(CCC(OC2OC(C(O)C(OC3OC(C(OC4OC(C(O)C(O)C4O)C)C(O)C3O)CO)C2OC2OC(C(O)C(O)C2O)CO)C)C1(CO)C)C)C)C
MOL006686	0.3678	0.6322	0.8126	Buddlejae Flos	mimengoside B_qt	Not Available	FALSE	O(C1C2C(C3(C(=C1)C1C(CC3)(CCC(C1)(C)C)CO)C)(CCC1C2(CCC(O)C1(CO)C)C)C)C
MOL006687	0.7678	0.2322	0.8124	Buddlejae Flos	mimengoside, c	Not Available	FALSE	C1C2=C3C(CC(C2(CCC1(C)C)CO)O)(C1(C(C=C3)C2(C(CC1)C(C(CC2)OC1C(C(C(C(O1)C)O)OC1OC(C(C(C1O)O)OC1C(O)C(O)C(O)C(O1)C)CO)OC1C(O)C(O)C(O)C(O1)CO)(C)CO)C)C)C
MOL006688	0.4733	0.5267	0.7713	Buddlejae Flos	mimengoside, d_qt	12315167	FALSE	C1C2=C3C(CC(C2(CCC1(C)C)CO)O)(C1(C(C=C3)C2(C(CC1)C(C(CC2)O)(C)CO)C)C)C
MOL006689	0.7522	0.2478	0.8375	Buddlejae Flos	mimengoside, d	Not Available	FALSE	C1C2=C3C(CC(C2(CCC1(C)C)CO)O)(C1(C(C=C3)C2(C(CC1)C(C(CC2)OC1C(O)C(OC2C(O)C(O)C(OC3C(O)C(O)C(O)CO3)C(O2)CO)C(O)C(O1)C)(C)CO)C)C)C
MOL006690	0.7733	0.2267	0.8129	Buddlejae Flos	mimengoside, e	Not Available	FALSE	C1C2C(CCC1(C)C)(C(CC1(C2=CC=C2C1(CCC1C2(CCC(C1(C)CO)OC1C(C(C(C(O1)C)O)OC1OC(C(C(C1O)O)OC1C(O)C(O)C(O)C(O1)C)CO)OC1C(O)C(O)C(O)C(O1)CO)C)C)C)O)CO
MOL006691	0.4802	0.5198	0.7723	Buddlejae Flos	mimengoside, e_qt	Not Available	FALSE	C1C2C(CCC1(C)C)(C(CC1(C2=CC=C2C1(CCC1C2(CCC(C1(C)CO)O)C)C)C)O)CO
MOL006692	0.7499	0.2501	0.8383	Buddlejae Flos	mimengoside, f	Not Available	FALSE	C1C2C(CCC1(C)C)(C(CC1(C2=CC=C2C1(CCC1C2(CCC(C1(C)CO)OC1C(O)C(OC2C(O)C(O)C(OC3C(O)C(O)C(O)CO3)C(O2)CO)C(O)C(O1)C)C)C)C)O)CO
MOL006693	0.4802	0.5198	0.7723	Buddlejae Flos	mimengoside, f_qt	Not Available	FALSE	C1C2C(CCC1(C)C)(C(CC1(C2=CC=C2C1(CCC1C2(CCC(C1(C)CO)O)C)C)C)O)CO
MOL006694	0.6743	0.3257	0.8460	Buddlejae Flos	mimengoside, g	Not Available	FALSE	C1C2C(CCC1(C)C)(C(CC1(C2=CC=C2C1(CCC1C2(CCC(C1(C)CO)OC1C(O)C(OC2C(O)C(O)C(O)C(O2)CO)C(O)C(O1)C)C)C)C)O)CO
MOL006695	0.4802	0.5198	0.7723	Buddlejae Flos	mimengoside, g_qt	Not Available	FALSE	C1C2C(CCC1(C)C)(C(CC1(C2=CC=C2C1(CCC1C2(CCC(C1(C)CO)O)C)C)C)O)CO
MOL006696	0.3145	0.6855	0.7381	Canarii Fructus	α-amyrin acetate	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3C)C)C)C)(CC2)C)(CC1)C)(C)C)C(=O)C
MOL006697	0.3619	0.6381	0.7333	Canarii Fructus	β-amyrenone	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C)(C)CC4C3=CCC21)C
MOL006698	0.7490	0.2510	0.7452	Canarii Fructus	naringin	Not Available	FALSE	C1(Oc2cc(cc(c2)O)/C=C\c2ccc(cc2)OC)OC(C(C(C1O)O)O)CO
MOL006699	0.9053	0.0947	0.9188	Canarii Fructus	5-[(Z)-2-(4-methoxyphenyl)vinyl]resorcinol	10399472	FALSE	Oc1cc(cc(c1)O)/C=C\c1ccc(cc1)OC
MOL006700	0.3918	0.6082	0.7524	Canarii Fructus	urs-12-ene-3β,16β-diol	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CC(C4(C)CCC(C)C(C)C4C3=CCC21)O)C)O

MOL006700	0.3918	0.6082	0.7524	Phyllanthi Fructus	urs-12-ene-3β,16β-diol	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CC(C4(C)CCC(C)C(C)C4C3=CCC21)O)C)O
MOL006701	0.9592	0.0408	0.7632	Canarii Fructus	Methylene-1-(1-methylethyl)bicyclo[3.1.0]hex-2-ene	Not Available	FALSE	C12(C=CC(=C)C1C2)C(C)C
MOL006702	0.9546	0.0454	0.7471	Canarii Fructus	(1R,3S,6S)-3,7,7-trimethylbicyclo[4.1.0]hept-4-ene	21674939	FALSE	C1(C2C1C=CC(C2)C)(C)C
MOL006702	0.9546	0.0454	0.7471	Rhododendri Daurici Folium	(1R,3S,6S)-3,7,7-trimethylbicyclo[4.1.0]hept-4-ene	21674939	FALSE	C1(C2C1C=CC(C2)C)(C)C
MOL006703	0.8947	0.1053	0.7365	Canarii Fructus	3-Methylene-1,5,5-trimethylcyclohexene	140110	FALSE	C1(CC(=CC(=C)C1)C)(C)C
MOL006705	0.8463	0.1537	0.8051	Canarii Fructus	METHYL TRIDECANOATE	15608	FALSE	O(C(=O)CCCCCCCCCCCC)C
MOL006705	0.8463	0.1537	0.8051	Rose Rugosae Flos	METHYL TRIDECANOATE	15608	FALSE	O(C(=O)CCCCCCCCCCCC)C
MOL006706	0.7114	0.2886	0.6528	Canarii Fructus	Chokegard	5364495	FALSE	C(CC/C=C\CCCC)CCCCCCC=O
MOL006707	0.3982	0.6018	0.7218	Canarii Fructus	3-epi-β-amyrin	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C)C)(CC2)C)(CC1)C)(C)C
MOL006707	0.3982	0.6018	0.7218	Phyllanthi Fructus	3-epi-β-amyrin	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C)C)(CC2)C)(CC1)C)(C)C

MOL006708	0.6635	0.3365	0.6966	Fraxini Cortex	(2S,3R,4S,5S,6R)-2-[4-[(1R,3aR,4S,6aS)-6a-hydroxy-4-(4-hydroxy-3-methoxyphenyl)-3,3a,4,6-tetrahydro-1H-furo[4,3-c]furan-1-yl]-2-methoxyphenoxy]-6-(hydroxymethyl)oxane-3,4,5-triol	14756314	FALSE	O1C(C2(O)C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(OC2OC(C(O)C(O)C2O)CO)cc1
MOL006708	0.6635	0.3365	0.6966	Eucommiae Cortex	(2S,3R,4S,5S,6R)-2-[4-[(1R,3aR,4S,6aS)-6a-hydroxy-4-(4-hydroxy-3-methoxyphenyl)-3,3a,4,6-tetrahydro-1H-furo[4,3-c]furan-1-yl]-2-methoxyphenoxy]-6-(hydroxymethyl)oxane-3,4,5-triol	14756314	FALSE	O1C(C2(O)C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(OC2OC(C(O)C(O)C2O)CO)cc1
MOL006709	0.6446	0.3554	0.7544	Eucommiae Cortex	AIDS214634	3010930	FALSE	O1C(C2(O)C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(O)cc1
MOL006709	0.6446	0.3554	0.7544	Fraxini Cortex	AIDS214634	3010930	FALSE	O1C(C2(O)C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(O)cc1

MOL006710	0.9196	0.0804	0.8342	Fraxini Cortex	8-(beta-D-Glucopyranosyloxy)-7-hydroxy-6-methoxy-2H-1-benzopyran-2-one	5273568	FALSE	c12c(OC3OC(C(C(C3O)O)O)CO)c(c(cc1ccc(=O)o2)OC)O
MOL006710	0.9196	0.0804	0.8342	Semen Aesculi	8-(beta-D-Glucopyranosyloxy)-7-hydroxy-6-methoxy-2H-1-benzopyran-2-one	5273568	FALSE	c12c(OC3OC(C(C(C3O)O)O)CO)c(c(cc1ccc(=O)o2)OC)O
MOL006711	0.9241	0.0759	0.8247	Fraxini Cortex	Osmanthuside H	192437	FALSE	O1C(C(O)C(O)C(O)C1OCCc1ccc(O)cc1)COC1OCC(O)(C1O)CO
MOL006712	0.9173	0.0827	0.8246	Fraxini Cortex	sinapaldehyde glucoside	25791064	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(OC)cc(cc1OC)/C=C/C=O)CO
MOL006713	0.7115	0.2885	0.8337	Celosiae Semen	Cristatain	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1C)(C)C)C(=O)O)C)C)(C)C=O)OC1OC(C(C(C1O)O)O)C(=O)O)O
MOL006714	0.7339	0.2661	0.7611	Celosiae Semen	Cristatain_qt	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1C)(C)C)C(=O)O)C)C)(C)C=O)O)O
MOL006715	0.7304	0.2696	0.8481	Celosiae Semen	celosin A	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C=O)OC1OC(C(C(C1OC1OCC(C(C1O)O)O)O)O)C(=O)O)O
MOL006716	0.7210	0.2790	0.7555	Celosiae Semen	celosin A_qt	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C=O)O)O
MOL006717	0.7439	0.2561	0.8380	Celosiae Semen	celosin B	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C(=O)O)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)C(=O)O)O
MOL006718	0.7229	0.2771	0.7402	Celosiae Semen	celosin B_qt	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C(=O)O)O)O
MOL006719	0.7647	0.2353	0.8161	Celosiae Semen	celosin D1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1OC(C(C(C1OC1C(C(C(C(O1)C)OC1OC(C(C(C1O)O)OC1OCC(C(C1O)O)O)CO)O)O)O)O)C)C)C(=O)O)(C)C(=O)O)O
MOL006720	0.7320	0.2680	0.7453	Celosiae Semen	celosin D1_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)C(=O)O)(C)C(=O)O)O

MOL006721	0.7234	0.2766	0.8452	Celosiae Semen	celosin E	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C)C)C(=O)O)(C)C(=O)O)OC1OC(C(C(C1O)O)O)C(=O)O)O
MOL006722	0.7202	0.2798	0.7405	Celosiae Semen	celosin E_qt	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C)C)C(=O)O)(C)C(=O)O)O)O
MOL006723	0.7046	0.2954	0.8388	Celosiae Semen	celosin F	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(=C)C1C)C(=O)O)C)C(=O)O)C)(C)C(=O)O)OC1OCC(C(C1O)O)O)O
MOL006724	0.7766	0.2234	0.8046	Celosiae Semen	celosin G	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1C)(C)C)C(=O)OC1OC(C(C(C1OC1C(C(C(O1)C)OC1OC(C(C(C1O)O)O)C(=O)O)O)O)O)O)C)C)C)C)(C)C(=O)O)OC1OC(C(C(C1O)O)O)CO)O
MOL006725	0.7297	0.2703	0.7332	Celosiae Semen	celosin G_qt	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1C)(C)C)C(=O)O)C)C)C)(C)C(=O)O)O)O
MOL006726	0.2167	0.7833	0.7442	Notoginseng Flos	panaxadiol	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)C)(CCC2C1(OC(CCC1)(C)C)C)C
MOL006727	0.7136	0.2864	0.8383	Notoginseng Flos	Notoginsenoside Fe	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O1)CO)C(C1CCC2(C3(CCC4C(C(CCC4(C3CC(C12)O)C)OC1C(O)C(O)C(O)C(O1)CO)(C)C)C)C)(CCC=C(C)C)C
MOL006728	0.2305	0.7695	0.7376	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	Gypenoside XIV_qt	Not Available	FALSE	OC(C1CCC2(C3(CCC4C(C(CCC4(C3CC(C12)O)C)O)(C)C)C)C)(CCC=C(C)C)C
MOL006728	0.2305	0.7695	0.7376	Notoginseng Flos	Gypenoside XIV_qt	Not Available	FALSE	OC(C1CCC2(C3(CCC4C(C(CCC4(C3CC(C12)O)C)O)(C)C)C)C)(CCC=C(C)C)C
MOL006728	0.2305	0.7695	0.7376	Gynostemmae Pentaphylli Herba	Gypenoside XIV_qt	Not Available	FALSE	OC(C1CCC2(C3(CCC4C(C(CCC4(C3CC(C12)O)C)O)(C)C)C)C)(CCC=C(C)C)C
MOL006729	0.7635	0.2365	0.7985	Panacis Japonici Rhizoma	Notoginsenoside Fc	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(OC1C(C(C(C(O1)COC1C(C(C(C(O1)CO)O)O)O)O)O)O)C)C)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(O)C(O)C(O)CO1
MOL006729	0.7635	0.2365	0.7985	Notoginseng Flos	Notoginsenoside Fc	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(OC1C(C(C(C(O1)COC1C(C(C(C(O1)CO)O)O)O)O)O)O)C)C)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)OC1C(O)C(O)C(O)CO1
MOL006730	0.2305	0.7695	0.7376	Notoginseng Flos	Notoginsenoside Fc_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)C)(C)C)O
MOL006730	0.2305	0.7695	0.7376	Panacis Japonici Rhizoma	Notoginsenoside Fc_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)C)(C)C)O
MOL006731	0.9026	0.0974	0.9637	Campsis Flos	Areginal	8025	FALSE	O(CC)C=O
MOL006731	0.9026	0.0974	0.9637	Panacis Japonici Rhizoma	Areginal	8025	FALSE	O(CC)C=O
MOL006731	0.9026	0.0974	0.9637	Notoginseng Flos	Areginal	8025	FALSE	O(CC)C=O
MOL006731	0.9026	0.0974	0.9637	Rubi Fructus	Areginal	8025	FALSE	O(CC)C=O

MOL006731	0.9026	0.0974	0.9637	Achyranthis Bidentatae Radix	Areginal	8025	FALSE	O(CC)C=O
MOL006731	0.9026	0.0974	0.9637	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Areginal	8025	FALSE	O(CC)C=O
MOL006732	0.9262	0.0738	0.9555	Notoginseng Flos	PROPYL FORMATE	8073	FALSE	O(CCC)C=O
MOL006733	0.5305	0.4695	0.7626	Ginseng Folium	ginsenoside-F2	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3O)CO)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(O)C(C(O)C1O)CO)(CCC=C(C)C)C)C
MOL006733	0.5305	0.4695	0.7626	Notoginseng Flos	ginsenoside-F2	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3O)CO)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(O)C(C(O)C1O)CO)(CCC=C(C)C)C)C
MOL006734	0.2305	0.7695	0.7376	Panacis Quinquefolii Radix	Gypenoside I_qt	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL006734	0.2305	0.7695	0.7376	Notoginseng Flos	Gypenoside I_qt	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL006734	0.2305	0.7695	0.7376	Ginseng Folium	Gypenoside I_qt	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL006734	0.2305	0.7695	0.7376	Panacis Japonici Rhizoma	Gypenoside I_qt	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL006734	0.2305	0.7695	0.7376	Gynostemmae Pentaphylli Herba	Gypenoside I_qt	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL006735	0.8773	0.1227	0.9657	Campsis Flos	Furfuranol	7361	FALSE	o1c(CO)ccc1
MOL006735	0.8773	0.1227	0.9657	Ginkgo Folium	Furfuranol	7361	FALSE	o1c(CO)ccc1
MOL006735	0.8773	0.1227	0.9657	Notoginseng Flos	Furfuranol	7361	FALSE	o1c(CO)ccc1
MOL006735	0.8773	0.1227	0.9657	Paederiae Scandentis Herba	Furfuranol	7361	FALSE	o1c(CO)ccc1
MOL006735	0.8773	0.1227	0.9657	Ardisiae Japonicae Herba	Furfuranol	7361	FALSE	o1c(CO)ccc1
MOL006735	0.8773	0.1227	0.9657	Cuscutae Semen	Furfuranol	7361	FALSE	o1c(CO)ccc1
MOL006735	0.8773	0.1227	0.9657	Apocyniveneti Folium	Furfuranol	7361	FALSE	o1c(CO)ccc1
MOL006735	0.8773	0.1227	0.9657	Litchi Semen	Furfuranol	7361	FALSE	o1c(CO)ccc1
MOL006735	0.8773	0.1227	0.9657	Pseudostellariae Radix	Furfuranol	7361	FALSE	o1c(CO)ccc1
MOL006735	0.8773	0.1227	0.9657	Caryophylliflos	Furfuranol	7361	FALSE	o1c(CO)ccc1
MOL006735	0.8773	0.1227	0.9657	Momordicae Fructus	Furfuranol	7361	FALSE	o1c(CO)ccc1
MOL006736	0.7494	0.2506	0.8097	Notoginseng Flos	gensenoside-Rb1	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(C(O)C(O)C1O)COC1OC(C(O)C(O)C1O)CO)(CCC=C(C)C)C)C
MOL006737	0.2305	0.7695	0.7376	Notoginseng Flos	gensenoside-Rb1_qt	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL006738	0.7118	0.2882	0.8238	Notoginseng Flos	gypenoside Ⅸ	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3O)CO)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(C(O)C(O)C1O)COC1OCC(O)C(O)C1O)(CCC=C(C)C)C)C

MOL006739	0.2305	0.7695	0.7376	Notoginseng Flos	gypenoside Ⅸ _qt	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL006740	0.7282	0.2718	0.8093	Notoginseng Flos	ginsenoside-Rb2	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(C(O)C(O)C1O)COC1OCC(O)C(O)C1O)(CCC=C(C)C)C)C
MOL006741	0.8836	0.1164	0.6061	Notoginseng Flos	α-Santalol	Not Available	FALSE	OC/C(=C/CCC1(C2(C3C2CC1C3)C)C)/C
MOL006742	0.7489	0.2511	0.8340	Notoginseng Flos	ginsenoside-Re	Not Available	FALSE	O(C1C2C(C3C(C4(C(C(CC4)C(OC4OC(C(O)C(O)C4O)CO)(CCC=C(C)C)C)C(O)C3)C)(C1)C)(CCC(O)C2(C)C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)CO)CO
MOL006743	0.7097	0.2903	0.8100	Notoginseng Flos	Gypenoside XV	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O)CO1)(CCC=C(C)C)C)C)C)(C)C)OC1C(OC2C(O)C(O)C(O)C(O2)CO)C(O)C(O)CO1
MOL006744	0.2305	0.7695	0.7376	Notoginseng Flos	Gypenoside XV_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(O)(CCC=C(C)C)C)C)C)(C)C)O
MOL006745	0.2494	0.7506	0.7336	Notoginseng Flos	ginsenoside-Re_qt	Not Available	FALSE	OC1C2C(C3C(C4(C(C(CC4)C(O)(CCC=C(C)C)C)C(O)C3)C)(C1)C)(CCC(O)C2(C)C)C
MOL006746	0.7331	0.2669	0.8151	Notoginseng Flos	ginsenoside-Rc	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(C(O)C(O)C1O)COC1OC(C(O)C1O)CO)(CCC=C(C)C)C)C
MOL006747	0.7496	0.2504	0.8413	Notoginseng Flos	gensenoside-Rd	Not Available	FALSE	O(C1C2C(C3C(C4(C(C(CC4)C(OC4OC(C(O)C(O)C4O)CO)(CCC=C(C)C)C)C(O)C3)C)(C1)C)(CCC(O)C2(C)C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)CO)CO
MOL006748	0.7083	0.2917	0.8460	Notoginseng Flos	gypenoside Ⅷ	Not Available	FALSE	OC1C2C(C3C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)CC4)(C)C)C)C1)(CCC2C(OC1OC(C(O)C(O)C1O)CO)(CC(C)C=C(C)C)C)C
MOL006749	0.2075	0.7925	0.7356	Panacis Quinquefolii Radix	gypenosideⅧ _qt	Not Available	FALSE	OC1C2C(C3C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)(CCC2C(O)(CC(C)C=C(C)C)C)C
MOL006749	0.2075	0.7925	0.7356	Notoginseng Flos	gypenosideⅧ _qt	Not Available	FALSE	OC1C2C(C3C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)(CCC2C(O)(CC(C)C=C(C)C)C)C
MOL006750	0.2214	0.7786	0.7352	Notoginseng Flos	dammar-20(22)-ene-3β,12β,26-triol	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC(/C(=C/CCC(CO)C)/C)C3C(CC21O)C)O
MOL006751	0.2592	0.7408	0.7049	Notoginseng Flos	20(R)-dammaran-3β,12β,20,25-tetrol	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC(C(CCCC(C)(C)O)(C)O)C3C(CC21O)C)O
MOL006752	0.7426	0.2574	0.8234	Panacis Quinquefolii Radix	gypenosideXVII	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3O)CO)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(C(O)C(O)C1O)COC1OC(C(O)C(O)C1O)CO)(CCC=C(C)C)C)C

MOL006752	0.7426	0.2574	0.8234	Notoginseng Flos	gypenosideXVII	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3O)CO)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(C(O)C(O)C1O)COC1OC(C(O)C(O)C1O)CO)(CCC=C(C)C)C
MOL006752	0.7426	0.2574	0.8234	Panacis Japonici Rhizoma	gypenosideXVII	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3O)CO)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(C(O)C(O)C1O)COC1OC(C(O)C(O)C1O)CO)(CCC=C(C)C)C)C
MOL006753	0.7335	0.2665	0.8072	Notoginseng Flos	ginsenoside Rb3	Not Available	FALSE	OC1C2C(C3C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)CC4)(C)C)C)C1)(CCC2C(OC1OC(C(O)C(O)C1O)COC1OCC(O)C(O)C1O)(CC/C=C(/CC)\C)C)C
MOL006753	0.7335	0.2665	0.8072	Gynostemmae Pentaphylli Herba	ginsenoside Rb3	Not Available	FALSE	OC1C2C(C3C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)CC4)(C)C)C)C1)(CCC2C(OC1OC(C(O)C(O)C1O)COC1OCC(O)C(O)C1O)(CC/C=C(/CC)\C)C)C
MOL006753	0.7335	0.2665	0.8072	Panacis Quinquefolii Radix	ginsenoside Rb3	Not Available	FALSE	OC1C2C(C3C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)CC4)(C)C)C)C1)(CCC2C(OC1OC(C(O)C(O)C1O)COC1OCC(O)C(O)C1O)(CC/C=C(/CC)\C)C)C
MOL006753	0.7335	0.2665	0.8072	Panacis Japonici Rhizoma	ginsenoside Rb3	Not Available	FALSE	OC1C2C(C3C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)CC4)(C)C)C)C1)(CCC2C(OC1OC(C(O)C(O)C1O)COC1OCC(O)C(O)C1O)(CC/C=C(/CC)\C)C)C
MOL006754	0.2288	0.7712	0.6902	Panacis Quinquefolii Radix	ginsenoside Rb3_qt	Not Available	FALSE	OC1C2C(C3C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)(CCC2C(O)(CC/C=C(/CC)\C)C)C
MOL006754	0.2288	0.7712	0.6902	Panacis Japonici Rhizoma	ginsenoside Rb3_qt	Not Available	FALSE	OC1C2C(C3C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)(CCC2C(O)(CC/C=C(/CC)\C)C)C
MOL006754	0.2288	0.7712	0.6902	Gynostemmae Pentaphylli Herba	ginsenoside Rb3_qt	Not Available	FALSE	OC1C2C(C3C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)(CCC2C(O)(CC/C=C(/CC)\C)C)C
MOL006754	0.2288	0.7712	0.6902	Notoginseng Flos	ginsenoside Rb3_qt	Not Available	FALSE	OC1C2C(C3C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)(CCC2C(O)(CC/C=C(/CC)\C)C)C
MOL006755	0.2813	0.7187	0.7215	Trichosanthis Radix	DIHYDROCUCURBITACIN B	267250	FALSE	C12C(=CCC3C2(C(=O)CC2(C3(CC(C2C(C(=O)CCC(OC(=O)C)(C)C)(C)O)O)C)C)C)C(C(=O)C(C1)O)(C)C
MOL006756	0.2400	0.7600	0.6133	Momordicae Semen	Schottenol	441837	FALSE	OC1CC2C(C3C(=CC2)C2C(C(CC2)C(CCC(C(C)C)CC)C)(CC3)C)(CC1)C
MOL006756	0.2400	0.7600	0.6133	Maydis Seigma	Schottenol	441837	FALSE	OC1CC2C(C3C(=CC2)C2C(C(CC2)C(CCC(C(C)C)CC)C)(CC3)C)(CC1)C
MOL006756	0.2400	0.7600	0.6133	Hippophae Fructus	Schottenol	441837	FALSE	OC1CC2C(C3C(=CC2)C2C(C(CC2)C(CCC(C(C)C)CC)C)(CC3)C)(CC1)C
MOL006756	0.2400	0.7600	0.6133	Trichosanthes Kirilowii Maxim	Schottenol	441837	FALSE	OC1CC2C(C3C(=CC2)C2C(C(CC2)C(CCC(C(C)C)CC)C)(CC3)C)(CC1)C
MOL006756	0.2400	0.7600	0.6133	Pseudostellariae Radix	Schottenol	441837	FALSE	OC1CC2C(C3C(=CC2)C2C(C(CC2)C(CCC(C(C)C)CC)C)(CC3)C)(CC1)C

MOL006756	0.2400	0.7600	0.6133	Trichosanthis Radix	Schottenol	441837	FALSE	OC1CC2C(C3C(=CC2)C2C(C(CC2)C(CCC(C(C)C)CC)C)(CC3)C)(CC1)C
MOL006757	0.7120	0.2880	0.8737	Trichosanthis Radix	Bryonolic acid	472768	FALSE	OC1C(C2C(C3=C(C4(C(C5C(CC4)(CCC(C5)(C)C(=O)O)C)(CC3)C)C)CC2)(CC1)C)(C)C
MOL006759	0.2400	0.7600	0.6133	Trichosanthis Radix	poriferast-7-en-3beta-ol	5283639	FALSE	C1C(CC2C(C1)(C1C(=CC2)C2C(CC1)(C(CC2)C(C)CCC(C(C)C)CC)C)C)O
MOL006759	0.2400	0.7600	0.6133	Benincasae Exocarpium	poriferast-7-en-3beta-ol	5283639	FALSE	C1C(CC2C(C1)(C1C(=CC2)C2C(CC1)(C(CC2)C(C)CCC(C(C)C)CC)C)C)O
MOL006760	0.9045	0.0955	0.9700	Trichosanthis Radix	(R)-ornithine	71082	FALSE	OC(=O)C(N)CCCN
MOL006762	0.9024	0.0976	0.9646	Trichosanthis Radix	2-Hydroxymethylserine	25201639	FALSE	C(=O)(C(N)(CO)CO)O
MOL006763	0.8395	0.1605	0.7286	Prunellae Spica	Malvidin-3,5-diglucoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2c(OC3OC(C(O)C(O)C3O)CO)cc(O)cc2[o+]c1c1cc(OC)c(O)c(OC)c1)CO
MOL006764	0.8531	0.1469	0.7564	Prunellae Spica	Peonin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2c(OC3OC(C(O)C(O)C3O)CO)cc(O)cc2[o+]c1c1cc(OC)c(O)cc1)CO
MOL006766	0.6783	0.3217	0.8034	Prunellae Spica	Vulgarsaponin B	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)O)C)C)(C)CO)OC1OC(C(C(C1O)O)O)COC(=O)CCC
MOL006767	0.9344	0.0656	0.7598	Prunellae Spica	Vulgaxanthin-I	5281217	FALSE	OC(=O)C(N/C=C/C1=CC(=NC(C1)C(=O)O)C(=O)O)CCC(=O)N
MOL006768	0.6762	0.3238	0.7560	Prunellae Spica	arjunglucoside I	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3O)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1O)C)(CO)C
MOL006769	0.9225	0.0775	0.7871	Prunellae Spica	isoquercetrin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1O)COc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1
MOL006769	0.9225	0.0775	0.7871	Mori Cortex	isoquercetrin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1O)COc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1
MOL006770	0.6680	0.3320	0.7469	Prunellae Spica	nigachigoside F1	Not Available	FALSE	C1(C(C2C(CC1)(CCC1(C2=CCC2C1(CCC1C2(CC(C(C1(C)CO)O)O)C)C)C)C(=O)OC1OC(C(C(C1O)O)O)CO)(C)O)C
MOL006773	0.6762	0.3238	0.7560	Prunellae Spica	sericoside	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3O)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1O)C)(CO)C
MOL006774	0.2400	0.7600	0.6133	Codonopsis Radix	stigmast-7-enol	12315384	FALSE	OC1CC2C(C3C(=CC2)C2C(C(CC2)C(CCC(C(C)C)CC)C)(CC3)C)(CC1)C
MOL006774	0.2400	0.7600	0.6133	Prunellae Spica	stigmast-7-enol	12315384	FALSE	OC1CC2C(C3C(=CC2)C2C(C(CC2)C(CCC(C(C)C)CC)C)(CC3)C)(CC1)C
MOL006774	0.2400	0.7600	0.6133	Panacis Quinquefolii Radix	stigmast-7-enol	12315384	FALSE	OC1CC2C(C3C(=CC2)C2C(C(CC2)C(CCC(C(C)C)CC)C)(CC3)C)(CC1)C
MOL006775	0.9260	0.0740	0.8495	Ephedrae Radix Et Rhizoma	epi-Afzelechin	443639	FALSE	O1C(C(O)Cc2c1cc(O)cc2O)c1ccc(O)cc1

MOL006775	0.9260	0.0740	0.8495	Drynariae Rhizoma	epi-Afzelechin	443639	FALSE	O1C(C(O)Cc2c1cc(O)cc2O)c1ccc(O)cc1
MOL006775	0.9260	0.0740	0.8495	Phyllanthi Fructus	epi-Afzelechin	443639	FALSE	O1C(C(O)Cc2c1cc(O)cc2O)c1ccc(O)cc1
MOL006776	0.9318	0.0682	0.8544	Phyllanthi Fructus	(2S,3R,4S,5S,6R)-2-[4-(2-hydroxyethyl)-2,6-dimethoxy-phenoxy]-6-methylol-tetrahydropyran-3,4,5-triol	10959332	FALSE	c1(c(cc(cc1OC)CCO)OC)OC1C(O)C(O)C(O)C(O1)CO
MOL006777	0.9434	0.0566	0.9381	Phyllanthi Fructus	2,6-dimethoxy-4-(2-hydroxyethyl) phenol 1-O-beta-D-glucopyranoside_qt	14151162	FALSE	c1(c(cc(cc1OC)CCO)OC)O
MOL006778	0.9449	0.0551	0.9042	Phyllanthi Fructus	2-[2-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl] acetic acid	10979933	FALSE	c1(c(cccc1)CC(=O)O)OC1C(O)C(O)C(O)C(O1)CO
MOL006779	0.9483	0.0517	0.9641	Phyllanthi Fructus	OHP	11970	FALSE	c1(c(cccc1)CC(=O)O)O
MOL006780	0.9167	0.0833	0.7717	Phyllanthi Fructus	3,6-digallylglucose	Not Available	FALSE	O=CC(O)C(O)(C(O)C(O)C(O)Cc1cc(O)c(O)c(O)c1)Cc1cc(O)c(O)c(O)c1
MOL006781	0.9403	0.0597	0.9171	Phyllanthi Fructus	3-ethoxy-4,5-dihy-droxy-benzoic acid	Not Available	FALSE	C(=O)(c1cc(c(c(c1)O)O)OCC)O
MOL006782	0.8528	0.1472	0.7656	Phyllanthi Fructus	4′-hydroxyphyllaemblicin B	Not Available	FALSE	O1C2C(O)(C(O)CC(C2)C(=O)OC2OC(C(O)C(O)C2OC2OC(C(O)C(O)C2O)CO)CO)C(=O)C21OCC(C(OC(=O)c1ccc(O)cc1)C2)C
MOL006783	0.7510	0.2490	0.7707	Phyllanthi Fructus	apigenin-7-O-(6'-butyryl-beta-glucopyranoside)	Not Available	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)C(O)C(=O)CCC)c1ccc(O)cc1

MOL006785	0.8364	0.1636	0.7193	Phyllanthi Fructus	emblicanin A	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC1C(OC(=O)c3c2c(c(c(c3)O)O)O)C(=C(C(=O)O1)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O
MOL006786	0.7368	0.2632	0.7001	Phyllanthi Fructus	emblicanin B	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC1C(OC(=O)c3c2c(c(c(c3)O)O)O)c2c(C(=O)O1)oc(=O)c1c(c3c(c(=O)o2)cc(c(c3O)O)O)c(c(c(c1)O)O)O)O)O
MOL006787	0.8892	0.1108	0.7194	Phyllanthi Fructus	furosin	Not Available	FALSE	O1C2(O)C3c4c1c(O)c(O)cc4C(=O)OC1C(O)C(OC(=O)C3=CC(=O)C2(O)O)C(OC1OC(=O)c1cc(O)c(O)c(O)c1)CO
MOL006787	0.8892	0.1108	0.7194	Euphorbiae Helioscopiae Herba	furosin	Not Available	FALSE	O1C2(O)C3c4c1c(O)c(O)cc4C(=O)OC1C(O)C(OC(=O)C3=CC(=O)C2(O)O)C(OC1OC(=O)c1cc(O)c(O)c(O)c1)CO
MOL006788	0.8930	0.1070	0.8875	Phyllanthi Fructus	gallic acid 3-O-β-D-glucoside	Not Available	FALSE	C(=O)(c1cc(c(O)c(O)c1)OC1C(O)C(O)C(O)C(O1)CO)O
MOL006789	0.9067	0.0933	0.7973	Granati Pericarpium	Gallic acid-3-O-(6'-O-galloyl)glucoside	11972353	FALSE	C(=O)(c1cc(c(O)c(O)c1)OC1C(O)C(O)C(O)C(O1)COC(=O)c1cc(O)c(O)c(O)c1)O
MOL006789	0.9067	0.0933	0.7973	Chebulae Fructus	Gallic acid-3-O-(6'-O-galloyl)glucoside	11972353	FALSE	C(=O)(c1cc(c(O)c(O)c1)OC1C(O)C(O)C(O)C(O1)COC(=O)c1cc(O)c(O)c(O)c1)O
MOL006789	0.9067	0.0933	0.7973	Phyllanthi Fructus	Gallic acid-3-O-(6'-O-galloyl)glucoside	11972353	FALSE	C(=O)(c1cc(c(O)c(O)c1)OC1C(O)C(O)C(O)C(O1)COC(=O)c1cc(O)c(O)c(O)c1)O
MOL006790	0.8710	0.1290	0.6776	Phyllanthi Fructus	isocorilagin	Not Available	FALSE	C1(C(C2C(CC1O)C(=O)OC1C(C(COC(=O)c3c2c(c(c(c3)O)O)O)OC(C1O)OC(=O)c1cc(O)c(O)c(O)c1)O)O)O
MOL006791	0.9495	0.0505	0.7923	Ginkgo Folium	epigallocatechin	72277	FALSE	O1C(C(O)Cc2c1cc(O)cc2O)c1cc(O)c(O)c(O)c1
MOL006791	0.9495	0.0505	0.7923	Phyllanthi Fructus	epigallocatechin	72277	FALSE	O1C(C(O)Cc2c1cc(O)cc2O)c1cc(O)c(O)c(O)c1
MOL006791	0.9495	0.0505	0.7923	Apocyniveneti Folium	epigallocatechin	72277	FALSE	O1C(C(O)Cc2c1cc(O)cc2O)c1cc(O)c(O)c(O)c1
MOL006791	0.9495	0.0505	0.7923	Phaseoli Semen	epigallocatechin	72277	FALSE	O1C(C(O)Cc2c1cc(O)cc2O)c1cc(O)c(O)c(O)c1
MOL006791	0.9495	0.0505	0.7923	Polygoni Orientalis Fructus	epigallocatechin	72277	FALSE	O1C(C(O)Cc2c1cc(O)cc2O)c1cc(O)c(O)c(O)c1
MOL006792	0.9076	0.0924	0.8863	Phyllanthi Fructus	L-malic acid 2-0-gallate	Not Available	FALSE	C(=O)(C(CC(=O)O)OC(=O)c1c(C)cc(c(c1O)O)O)O
MOL006793	0.9018	0.0982	0.8888	Phyllanthi Fructus	mucic acid 1,4-lactone 2-0-gallate	Not Available	FALSE	C1(=O)C(C(O)C(C(O)C(=O)O)O1)OC(=O)c1c(C)cc(c(c1O)O)O

MOL006794	0.8992	0.1008	0.7396	Phyllanthi Fructus	mucic acid 1,4-lactone 3,5-di-0-gallate	Not Available	FALSE	C1(=O)C(O)C(C(C(C(=O)O)OC(=O)c2cc(O)c(O)c(O)c2)O1)OC(=O)c1cc(O)c(O)c(O)c1
MOL006795	0.9017	0.0983	0.8504	Phyllanthi Fructus	mucic acid 1,4-lactone 3-0-gallate	Not Available	FALSE	C1(=O)C(O)C(C(C(O)C(=O)O)O1)OC(=O)c1cc(O)c(O)c(O)c1
MOL006796	0.8946	0.1054	0.8646	Phyllanthi Fructus	mucic acid 1,4-lactone 5-0-gallate	Not Available	FALSE	C1(=O)C(O)C(O)C(C(C(=O)O)OC(=O)c2cc(O)c(O)c(O)c2)O1
MOL006797	0.8989	0.1011	0.8760	Phyllanthi Fructus	mucic acid-2-O-gallate	Not Available	FALSE	C(=O)(C(C(O)C(O)C(O)C(=O)O)OC(=O)c1c(C)cc(c(c1O)O)O)O
MOL006798	0.7473	0.2527	0.7092	Phyllanthi Fructus	pedunculagin	Not Available	FALSE	O1C2C(OC(=O)c3c(c4c(C(=O)OC2)cc(O)c(O)c4O)c(O)c(O)c(O)c3)C2OC(=O)c3c(c4c(C(=O)OC2C1O)cc(O)c(O)c4O)c(O)c(O)c(O)c3
MOL006798	0.7473	0.2527	0.7092	Radix Paeoniae Rubra	pedunculagin	Not Available	FALSE	O1C2C(OC(=O)c3c(c4c(C(=O)OC2)cc(O)c(O)c4O)c(O)c(O)c(O)c3)C2OC(=O)c3c(c4c(C(=O)OC2C1O)cc(O)c(O)c4O)c(O)c(O)c(O)c3
MOL006799	0.9162	0.0838	0.8274	Phyllanthi Fructus	(2S,3R,3aS,4R,4'S,5'R,6S,7aR)-3,4,4'-trihydroxy-3,5'-bis(hydroxymethyl)spiro[3a,4,5,6,7,7a-hexahydrobenzofuran-2,2'-tetrahydropyran]-6-carboxylic acid	11057167	FALSE	O1C2(OCC(C(O)C2)CO)C(O)(C2C1CC(CC2O)C(=O)O)CO

MOL006800	0.9197	0.0803	0.8403	Phyllanthi Fructus	(2S,3R,3aS,4'S,5'R,6S,7aR)-3,4'-dihydroxy-3,5'-dimethylol-spiro[3a,4,5,6,7,7a-hexahydrobenzofuran-2,2'-tetrahydropyran]-6-carboxylic acid	10914547	FALSE	O1C2(OCC(C(O)C2)CO)C(O)(C2C1CC(CC2)C(=O)O)CO
MOL006802	0.7858	0.2142	0.7228	Phyllanthi Fructus	phyllaemblicin A	Not Available	FALSE	O1C2C(O)(C(O)CC(C2)C(=O)OC2OC(C(O)C(O)C2O)CO)C(=O)C21OCC(C(OC(=O)c1ccccc1)C2)C
MOL006803	0.8096	0.1904	0.7519	Phyllanthi Fructus	phyllaemblicin B	Not Available	FALSE	O1C2C(O)(C(O)CC(C2)C(=O)OC2OC(C(O)C(O)C2OC2OC(C(O)C(O)C2O)CO)CO)C(=O)C21OCC(C(OC(=O)c1ccccc1)C2)C
MOL006804	0.7644	0.2356	0.7490	Phyllanthi Fructus	phyllaemblicin C	Not Available	FALSE	O1C2C(O)(C(O)CC(C2)C(=O)OC2OC(C(O)C(O)C2OC2OC(C(O)C(O)C2OC2OCC(O)C(O)C2O)CO)CO)C(=O)C21OCC(C(OC(=O)c1ccccc1)C2)C
MOL006805	0.8899	0.1101	0.7902	Phyllanthi Fructus	(2S,3R,3aS,4'S,5'R,6S,7aR)-3,4'-dihydroxy-3-methylol-5'-[[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]oxymethyl]spiro[3a,4,5,6,7,7a-hexahydrobenzofuran-2,2'-tetrahydropyran]-6-carboxylic acid	11049298	FALSE	O1C2(OCC(C(O)C2)COC2OC(C(O)C(O)C2O)CO)C(O)(C2C1CC(CC2)C(=O)O)CO

MOL006806	0.8516	0.1484	0.7103	Phyllanthi Fructus	Phyllanemblin A	Not Available	FALSE	C1(C2C(C(C(O1)OC(=O)c1cc(c(c(c1O)O)O)OC(=O)c1c3c4c(C(=O)O2)cc(c(c4oc3c(c(c1)O)O)O)O)O)OC
MOL006807	0.8734	0.1266	0.6886	Phyllanthi Fructus	Phyllanemblin B	Not Available	FALSE	C1(C2C(C(C(O1)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1c(c3c(C(=O)O2)cc(c(c3O)O)O)c(c(c(c1)O)O)O)O)
MOL006808	0.8199	0.1801	0.7534	Phyllanthi Fructus	Phyllanemblin C	Not Available	FALSE	C12C(C(C(C(O1)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)C(CC(=O)O)C1C(C(=O)Oc3c1c(c(c(c3)O)O)O)O)OC(=O)c1c(c3c(C(=O)OC2)cc(c(c3O)O)O)c(O)c(O)c(c1)O)OC(=O)C(CC(=O)O)C1C(C(=O)Oc2c1c(c(c(c2)O)O)O)O
MOL006809	0.8776	0.1224	0.7912	Phyllanthi Fructus	Phyllanemblin D	Not Available	FALSE	C1(C(C(C(C(O1)O)OC(=O)C(CC(=O)O)C1C(OC(=O)c2c1c(c(c(c2)O)O)O)O)C(=O)O)O)O)CO
MOL006810	0.8746	0.1254	0.7874	Phyllanthi Fructus	Phyllanemblin E	Not Available	FALSE	C1(C(C(C(C(O1)O)O)O)OC(=O)C(CC(=O)O)C1C(OC(=O)c2c1c(c(c(c2)O)O)O)C(=O)O)CO
MOL006811	0.8827	0.1173	0.7815	Phyllanthi Fructus	Phyllanemblin F	Not Available	FALSE	C1(C(C(C(C(O1)O)O)O)O)COC(=O)C(CC(=O)O)C1C(OC(=O)c2c1c(c(c(c2)O)O)O)C(=O)O
MOL006813	0.7436	0.2564	0.7581	Phyllanthi Fructus	prodelphinidin B-2 3-O-gallate	Not Available	FALSE	c1(C2c3c(OC(C2O)c2cc(c(c(c2)O)O)O)cc(cc3O)O)c2c(CC(C(O2)c2cc(c(c(c2)O)O)O)O)OC(=O)c2cc(c(c(c2)O)O)O)c(cc1O)O
MOL006814	0.8205	0.1795	0.7430	Phyllanthi Fructus	punicafolin	Not Available	FALSE	O1C2C(OC(=O)c3cc(O)c(O)c(O)c3)C(OC(=O)c3c(c4c(C(=O)OC2)cc(O)c(O)c4O)c(O)c(O)c(O)c3)C(OC(=O)c2cc(O)c(O)c(O)c2)C1OC(=O)c1cc(O)c(O)c(O)c1
MOL006815	0.8633	0.1367	0.7136	Phyllanthi Fructus	Punigluconin	Not Available	FALSE	O1C(C(COC(=O)c2c(c(c(c(c2)O)O)O)O)c2c(C1=O)cc(c(c2O)O)O)O)C(OC(=O)c1cc(c(c(c1)O)O)O)C(OC(=O)c1cc(c(c(c1)O)O)O)C(=O)O
MOL006817	0.8489	0.1511	0.7222	Phyllanthi Fructus	tercatain	Not Available	FALSE	O(C1C(O)C2OC(=O)c3c(c(c(c(c3)O)O)O)O)c3c(c(c(cc3C(=O)OCC(C2OC(=O)c2cc(O)c(O)c(O)c2)O1)O)O)O)C(=O)c1cc(O)c(O)c(O)c1
MOL006818	0.8769	0.1231	0.8650	Phyllanthi Fructus	uteolin-4'-O-neohesperiodoside	Not Available	FALSE	O(C1C(O)C(O)C(OC1Oc1c(O)cc(cc1)c1oc2c(c(=O)c1)c(O)cc(O)c2)CO)C1OC(C(O)C(O)C1O)C
MOL006819	0.3619	0.6381	0.7333	Phyllanthi Fructus	beta-Amyrone	Not Available	FALSE	O=C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C)C)(CC2)C)(CC1)C)(C)C
MOL006820	0.7959	0.2041	0.7516	Phyllanthi Fructus	L-Epicatechin gallate	107905	FALSE	O1C(C(OC(=O)c2cc(O)c(O)c(O)c2)Cc2c1cc(O)cc2O)c1cc(O)c(O)cc1
MOL006821	0.8601	0.1399	0.7575	Phyllanthi Fructus	(-)-epigallocatechin-3-gallate	65064	FALSE	O1C(C(OC(=O)c2cc(O)c(O)c(O)c2)Cc2c1cc(O)cc2O)c1cc(O)c(O)c(O)c1
MOL006821	0.8601	0.1399	0.7575	Ginkgo Semen	(-)-epigallocatechin-3-gallate	65064	FALSE	O1C(C(OC(=O)c2cc(O)c(O)c(O)c2)Cc2c1cc(O)cc2O)c1cc(O)c(O)c(O)c1
MOL006822	0.9319	0.0681	0.7900	Phyllanthi Fructus	1,6-Di-O-galloyl-glucose	440221	FALSE	O(C1C(O)C(O)C(O)C(O1)COC(=O)c1cc(O)c(O)c(O)c1)C(=O)c1cc(O)c(O)c(O)c1

MOL006823	0.9193	0.0807	0.7162	Phyllanthi Fructus	3,6-digalloyl glucose	Not Available	FALSE	O=CC(O)C(O)(C(O)C(O)C(O)C(=O)c1cc(O)c(O)c(O)c1)C(=O)c1cc(O)c(O)c(O)c1
MOL006824	0.4015	0.5985	0.6981	Phyllanthi Fructus	α-amyrin	12358389	FALSE	C1(C2C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)(CCC1O)C)(C)C
MOL006824	0.4015	0.5985	0.6981	Radix Salviae	α-amyrin	12358389	FALSE	C1(C2C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3C)C)C)C)(CCC1O)C)(C)C
MOL006825	0.7024	0.2976	0.7332	Phyllanthi Fructus	chebulagic acid	Not Available	FALSE	O1C2C3OC(=O)C(C4C5C(C(=O)OC(C3OC(=O)c3c(c6c(C(=O)OC2)cc(O)c(O)c6O)c(O)c(O)c(O)c3)C1OC(=O)c1cc(O)c(O)c(O)c1)cc(O)c(O)c5OC(=O)C4O)CC(=O)O
MOL006826	0.8675	0.1325	0.8396	Chebulae Fructus	chebulic acid	71308174	FALSE	c12c(C(=O)OC(C1C(C(=O)O)CC(=O)O)C(=O)O)cc(c(c2O)O)O
MOL006826	0.8675	0.1325	0.8396	Phyllanthi Fructus	chebulic acid	71308174	FALSE	c12c(C(=O)OC(C1C(C(=O)O)CC(=O)O)C(=O)O)cc(c(c2O)O)O
MOL006828	0.9266	0.0734	0.7931	Phyllanthi Fructus	1,6-di-o-galloyl-β-D-glucose	Not Available	FALSE	O(C1C(O)C(O)C(OC(=O)c2cc(O)c(O)c(O)c2)C(O1)CO)C(=O)c1cc(O)c(O)c(O)c1
MOL006829	0.9062	0.0938	0.9136	Phyllanthi Fructus	glucogallin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1O)COC(=O)c1cc(O)c(O)c(O)c1
MOL006830	0.9125	0.0875	0.9561	Phyllanthi Fructus	Mucinsaeure	3037582	FALSE	OC(C(O)C(O)C(=O)O)C(O)C(=O)O
MOL006831	0.8487	0.1513	0.7728	Phyllanthi Fructus	terchebin	Not Available	FALSE	O1C2(O)C3C4C1C(O)C(O)CC4C(=O)OC1C(OC(=O)c4cc(O)c(O)c(O)c4)C(OC(=O)C3=CC(=O)C2(O)O)C(OC1OC(=O)c1cc(O)c(O)c(O)c1)COC(=O)c1cc(O)c(O)c(O)c1
MOL006832	0.9130	0.0870	0.8979	Radix Rhei Et Rhizome	beta-Glucogallin	124021	FALSE	O1C(C(O)C(O)C(O)C1OC(=O)c1cc(O)c(O)c(O)c1)CO
MOL006832	0.9130	0.0870	0.8979	Euphorbiae Helioscopiae Herba	beta-Glucogallin	124021	FALSE	O1C(C(O)C(O)C(O)C1OC(=O)c1cc(O)c(O)c(O)c1)CO
MOL006832	0.9130	0.0870	0.8979	Phyllanthi Fructus	beta-Glucogallin	124021	FALSE	O1C(C(O)C(O)C(O)C1OC(=O)c1cc(O)c(O)c(O)c1)CO
MOL006833	0.8976	0.1024	0.7833	Commelinae Herba	Kumujan B	597266	FALSE	O(C(=O)c1nccc2c3c([nH]c12)cccc3)C
MOL006834	0.8371	0.1629	0.7809	Commelinae Herba	3-(4-hydroxy-3-methoxyphenyl)-N-[2-(4-hydroxyphenyl)ethyl]propanamide	16119667	FALSE	c1(ccc(cc1OC)CCC(=O)NCCc1ccc(cc1)O)O
MOL006836	0.8412	0.1588	0.7346	Commelinae Herba	Flavocommelin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c2c(oc(cc2=O)c2ccc(OC3OC(C(O)C(O)C3O)CO)cc2)cc1OC
MOL006837	0.7963	0.2037	0.8488	Jujubae Fructus	spinosin_qt	Not Available	FALSE	O1C(C(O)C(O)C(C1CO)O)c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1OC
MOL006837	0.7963	0.2037	0.8488	Commelinae Herba	spinosin_qt	Not Available	FALSE	O1C(C(O)C(O)C(C1CO)O)c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1OC

MOL006839	0.7440	0.2560	0.7225	Commelinae Herba	awobanin	Not Available	FALSE	c1(c2c(cc(c1)O)[o+]c(c(c2)OC1C(O)C(C(C(O1)COC(=O)/C=C/c1ccc(cc1)O)O)O)c1cc(c(c(c1)O)O)O)OC1OC(C(C(C1O)O)O)CO
MOL006841	0.8930	0.1070	0.8016	Tribulifructus	Harman	5281404	FALSE	[nH]1c2c(c3c1cccc3)ccnc2C
MOL006841	0.8930	0.1070	0.8016	Commelinae Herba	Harman	5281404	FALSE	[nH]1c2c(c3c1cccc3)ccnc2C
MOL006841	0.8930	0.1070	0.8016	Uncariae Ramulus Cumuncis	Harman	5281404	FALSE	[nH]1c2c(c3c1cccc3)ccnc2C
MOL006842	0.8047	0.1953	0.7312	Commelinae Herba	malonyl awobanin	Not Available	FALSE	[o+]1c(c(OC2OC(C(O)C(O)C2O)COC(=O)/C=C/c2ccc(O)cc2)cc2c1cc(O)cc2OC1OC(C(O)C(O)C1O)COC(=O)CC(=O)O)c1cc(O)c(O)c(O)c1
MOL006843	0.6289	0.3711	0.7254	Commelinae Herba	malonylawobanin	Not Available	FALSE	c1(c2c(cc(c1)O)O/C(=C/1\C=C(C(=O)C(=C1)O)O)/C(=C2)OC1C(O)C(C(C(O1)CC(=O)/C=C/c1ccc(cc1)O)O)O)OC1OC(CC(C1O)O)C(=O)CC=O
MOL006844	0.9026	0.0974	0.7340	Daturae Flos	Norharman	64961	FALSE	[nH]1c2c(c3c1cncc3)cccc2
MOL006844	0.9026	0.0974	0.7340	Farfarae Flos	Norharman	64961	FALSE	[nH]1c2c(c3c1cncc3)cccc2
MOL006844	0.9026	0.0974	0.7340	Tribulifructus	Norharman	64961	FALSE	[nH]1c2c(c3c1cncc3)cccc2
MOL006844	0.9026	0.0974	0.7340	Codonopsis Radix	Norharman	64961	FALSE	[nH]1c2c(c3c1cncc3)cccc2
MOL006844	0.9026	0.0974	0.7340	Commelinae Herba	Norharman	64961	FALSE	[nH]1c2c(c3c1cncc3)cccc2
MOL006844	0.9026	0.0974	0.7340	Arisaematis Rhizoma	Norharman	64961	FALSE	[nH]1c2c(c3c1cncc3)cccc2
MOL006844	0.9026	0.0974	0.7340	Hoveniae Dulcis Semen	Norharman	64961	FALSE	[nH]1c2c(c3c1cncc3)cccc2
MOL006844	0.9026	0.0974	0.7340	Arum Ternatum Thunb.	Norharman	64961	FALSE	[nH]1c2c(c3c1cncc3)cccc2
MOL006845	0.6789	0.3211	0.7368	Ampelopsis Japonica	schizandriside	14521043	FALSE	c1(cc2c(cc1OC)CC(C(C2c1ccc(c(c1)OC)O)COC1OCC(C(C1O)O)O)CO)O
MOL006846	0.7418	0.2582	0.7111	Ampelopsis Japonica	1,2,3,4,6-penta-o-galloyl-β-d-glucose	Not Available	FALSE	C1(C(C(C(C(O1)COC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O
MOL006847	0.8465	0.1535	0.6982	Ampelopsis Japonica	2,3,4,6-tetra-o-galloyl-d-glucopyranoside	Not Available	FALSE	O(C1C(C(C(C(O1)COC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)C
MOL006848	0.8815	0.1185	0.6793	Ampelopsis Japonica	1,2,6-tri-o-galloyl-β-d-glucopyranoside	Not Available	FALSE	C1(C(C(O)C(O)C(O1)COC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O

MOL006849	0.8723	0.1277	0.6682	Ampelopsis Japonica	[(2R,3S,4R,5R,6S)-4,5-dihydroxy-6-(3,4,5-trihydroxybenzoyl)oxy-2-[(3,4,5-trihydroxybenzoyl)oxymethyl]oxan-3-yl] 3,4,5-trihydroxybenzoate	10077822	FALSE	C1(C(O)C(O)C(C(O1)COC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O
MOL006850	0.3243	0.6757	0.7531	Solanum Nigrum Linn.	C10822	Not Available	FALSE	C12(C(C3C(O1)CC1C3(CCC3C1CC=C1C3(CCC(C1)O)C)C)C)CCC(CN2)C
MOL006850	0.3243	0.6757	0.7531	Herba Solani Lyrati	C10822	Not Available	FALSE	C12(C(C3C(O1)CC1C3(CCC3C1CC=C1C3(CCC(C1)O)C)C)C)CCC(CN2)C
MOL006851	0.3564	0.6436	0.6114	Solanum Nigrum Linn.	solamargine	Not Available	FALSE	C1(CCC2(C(C1)CCC1C3CC4OC5(C(C4C3(C)CCC21)C)NCC(CC5)C)C)OC1C(O)C(O)C(O)C(O1)CO
MOL006851	0.3564	0.6436	0.6114	Herba Solani Lyrati	solamargine	Not Available	FALSE	C1(CCC2(C(C1)CCC1C3CC4OC5(C(C4C3(C)CCC21)C)NCC(CC5)C)C)OC1C(O)C(O)C(O)C(O1)CO
MOL006852	0.3526	0.6474	0.7206	Solanum Nigrum Linn.	solamargine_qt	Not Available	FALSE	C1(CCC2(C(C1)CCC1C3CC4OC5(C(C4C3(C)CCC21)C)NCC(CC5)C)C)O
MOL006852	0.3526	0.6474	0.7206	Herba Solani Lyrati	solamargine_qt	Not Available	FALSE	C1(CCC2(C(C1)CCC1C3CC4OC5(C(C4C3(C)CCC21)C)NCC(CC5)C)C)O
MOL006853	0.7031	0.2969	0.8530	Herba Solani Lyrati	solasonine	Not Available	FALSE	C12(C3C(CC1C1C(CC2)C2(C(=CC1)CC(CC2)OC1C(C(OC2OC(C(C(C2O)O)O)CO)C(C(O1)CO)O)OC1C(C(C(C(O1)C)O)O)O)C)OC1(C3C)CCC(CN1)C)C
MOL006853	0.7031	0.2969	0.8530	Solanum Nigrum Linn.	solasonine	Not Available	FALSE	C12(C3C(CC1C1C(CC2)C2(C(=CC1)CC(CC2)OC1C(C(OC2OC(C(C(C2O)O)O)CO)C(C(O1)CO)O)OC1C(C(C(C(O1)C)O)O)O)C)OC1(C3C)CCC(CN1)C)C
MOL006854	0.3243	0.6757	0.7531	Solanum Nigrum Linn.	solasonine_qt	Not Available	FALSE	C12(C3C(CC1C1C(CC2)C2(C(=CC1)CC(CC2)O)C)OC1(C3C)CCC(CN1)C)C
MOL006854	0.3243	0.6757	0.7531	Herba Solani Lyrati	solasonine_qt	Not Available	FALSE	C12(C3C(CC1C1C(CC2)C2(C(=CC1)CC(CC2)O)C)OC1(C3C)CCC(CN1)C)C
MOL006855	0.6875	0.3125	0.8546	Herba Solani Lyrati	solamargine	Not Available	FALSE	O1C2C(C3(C(C4C(CC3)C3(C(=CC4)CC(OC4OC(C(OC5OC(C(O)C(O)C5O)C)C(O)C4OC4OC(C(O)C(O)C4O)C)CO)CC3)C)C2)C)C(C21NCC(CC2)C)C
MOL006857	0.3341	0.6659	0.7485	Solanum Nigrum Linn.	tomatidenol	Not Available	FALSE	C1(=CCC2(C(C1)CCC1C3CC4OC5(C(C4C3(C)CCC21)C)NCC(CC5)C)C)O
MOL006857	0.3341	0.6659	0.7485	Herba Solani Lyrati	tomatidenol	Not Available	FALSE	C1(=CCC2(C(C1)CCC1C3CC4OC5(C(C4C3(C)CCC21)C)NCC(CC5)C)C)O

MOL006858	0.3526	0.6474	0.7206	Herba Solani Lyrati	Soladulcidin	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(O)CC5)C)CC3)C2)C)C(C21NCC(CC2)C)C
MOL006858	0.3526	0.6474	0.7206	Siegesbeckiae Herba	Soladulcidin	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(O)CC5)C)CC3)C2)C)C(C21NCC(CC2)C)C
MOL006859	0.9089	0.0911	0.9307	Herba Solani Lyrati	Volon	31307	FALSE	FC12C(C3C(C(O)(C(O)C3)C(=O)CO)(CC1O)C)CCC1=CC(=O)C=CC21C
MOL006860	0.3795	0.6205	0.7532	Herba Solani Lyrati	15a-hydroxysoladulcidine	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(O)CC5)C)CC3)C2O)C)C(C21NCC(CC2)C)C
MOL006861	0.7493	0.2507	0.7698	Borneolum Syntheticum	asiatic acid	51340198	FALSE	C1(CC(C2(C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1C)C)C(=O)O)C)C)O)(C)CO)O
MOL006865	0.1945	0.8055	0.7268	Borneolum Syntheticum	dipterocarpol	Not Available	FALSE	CC12C(C3(C)C(CC2)C(C)(C)C(=O)CC3)CCC2C1(C)CCC2C(CCC=C(C)C)(C)O
MOL006866	0.9591	0.0409	0.8313	Borneolum Syntheticum	Isosafrole	637796	FALSE	C(=C\C)/c1cc2c(cc1)OCO2
MOL006866	0.9591	0.0409	0.8313	Myristicae Semen	Isosafrole	637796	FALSE	C(=C\C)/c1cc2c(cc1)OCO2
MOL006867	0.9267	0.0733	0.9555	Borneolum Syntheticum	α-pinenepinene	Not Available	FALSE	C1(C(=CCC(C1)C)C)C
MOL006868	0.9523	0.0477	0.9704	Borneolum Syntheticum	β-terpineol	8748	FALSE	C1CC(CCC1(C)O)C(=C)C
MOL006868	0.9523	0.0477	0.9704	Smilacis Glabrae Rhixoma	β-terpineol	8748	FALSE	C1CC(CCC1(C)O)C(=C)C
MOL006868	0.9523	0.0477	0.9704	Aristolochiae Fructus	β-terpineol	8748	FALSE	C1CC(CCC1(C)O)C(=C)C
MOL006869	0.9322	0.0678	0.9424	Radix Cynanchi	WLN: QR CQ DV1	6990	FALSE	c1(c(cc(cc1)O)O)C(=O)C
MOL006869	0.9322	0.0678	0.9424	Angelicae Sinensis Radix	WLN: QR CQ DV1	6990	FALSE	c1(c(cc(cc1)O)O)C(=O)C
MOL006869	0.9322	0.0678	0.9424	Cortex Moutan	WLN: QR CQ DV1	6990	FALSE	c1(c(cc(cc1)O)O)C(=O)C
MOL006870	0.2506	0.7494	0.6250	Radix Cynanchi	cynanchoside c2	Not Available	FALSE	OC12C(C(OC(=O)/C=C(/C(C)C)\C)CC3C1(O)CC=C1C3(CCC(OC3OC(C(OC4OC(C(OC5OC(C(O)C(OC)C5)C)C(OC)C4)C)C(OC)C3)C)C1)C)(C(CC2)C(=O)C)C
MOL006871	0.3223	0.6777	0.6140	Radix Cynanchi	cynanchoside c2_qt	Not Available	FALSE	OC12C(C(OC(=O)/C=C(/C(C)C)\C)CC3C1(O)CC=C1C3(CCC(O)C1)C)(C(C(=O)C)CC2)C
MOL006872	0.3339	0.6661	0.7248	Radix Cynanchi	atratoglaucoside b	Not Available	FALSE	O(C1CC2=CCC3C(C2(CC1)C)C/C=C/1\C2C(OC3=O)COC2(OC1=O)C)C1OC(C(OC2OC(C(OC3OC(C(O)C(OC)C3)C)C(OC)C2)C)C(OC)C1O)C
MOL006874	0.2522	0.7478	0.6975	Radix Cynanchi	atratoglaucoside,a	Not Available	FALSE	C1(C(OC(CC1OC)OC1C(C(C(OC1C)OC1CC2=CCC3C(C2(CC1)C)CCC1=COC2(C1C(CO2)OC3=O)C)O)OC)C)O
MOL006876	0.4153	0.5847	0.7415	Radix Cynanchi	atratoglaucoside,b	Not Available	FALSE	C1(CC2=CCC3C(C2(CC1)C)C/C=C/1\C2C(OC1=O)(OCC2OC3=O)C)OC1C(C(C(C(O1)C)OC1OC(C(C(C1)OC)OC1C(C(C(C(O1)C)O)OC)O)C)OC)O
MOL006878	0.1905	0.8095	0.6764	Radix Cynanchi	atratoside,a	Not Available	FALSE	C1(C(CC(OC1C)OC1C(CC(OC1C)OC1C(CC(OC1C)OC1C(CC2(C(=CCC3C2CCC(C3=O)(c2ccoc2C)C)C1)C)O)OC)OC)OC)O

MOL006879	0.3542	0.6458	0.7680	Radix Cynanchi	atratoside,a_qt	Not Available	FALSE	OC1C(O)CC2(C(=CCC3C2CCC(C3=O)(c2ccoc2C)C)C1)C
MOL006880	0.8137	0.1863	0.7789	Radix Cynanchi	cynanogenin,a	Not Available	FALSE	C1(C(CC2=CCC(C(C2(C1)C)CCC(=O)c1ccoc1C)C(=O)O)O)O
MOL006881	0.5333	0.4667	0.7892	Radix Cynanchi	cynanogenin,b	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CC=C(OC3=O)c1ccoc1C)O)O
MOL006882	0.4124	0.5876	0.6417	Radix Cynanchi	cynanoside,a	Not Available	FALSE	C1(C(CC2=CCC(C(C2(C1)C)CCC(=O)c1ccoc1C)C(=O)O)OC1OC(C(OC2CC(C(OC3CC(C(C(O3)C)O)OC)C(O2)C)OC)C(C1)OC)C)O
MOL006883	0.8137	0.1863	0.7789	Radix Cynanchi	cynanoside,c_qt	Not Available	FALSE	C1(C(CC2=CCC(C(C2(C1)C)CCC(=O)c1ccoc1C)C(=O)O)O)O
MOL006884	0.4732	0.5268	0.7333	Radix Cynanchi	cynanoside,b	Not Available	FALSE	C1(C(CC2=CCC(C(C2(C1)C)CCC(=O)c1ccoc1C)C(=O)O)OC1OC(C(OC2CC(C(OC3CC(C(C(O3)C)OC3OC(C(C(C3O)O)O)CO)OC)C(O2)C)OC)C(C1)OC)C)O
MOL006885	0.3997	0.6003	0.6621	Radix Cynanchi	cynanoside,c	Not Available	FALSE	C1(C(CC2=CCC(C(C2(C1)C)CCC(=O)c1ccoc1C)C(=O)O)OC1OC(C(OC2CC(C(C(O2)C)OC2CC(C(C(O2)C)O)OC)O)C(C1)OC)C)O
MOL006886	0.3643	0.6357	0.7515	Radix Cynanchi	cynanoside,d	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CC=C(OC3=O)c1ccoc1C)OC1OC(C(OC2CC(C(OC3CC(C(C(O3)C)OC3OC(C(C(C3O)O)O)CO)OC)C(O2)C)OC)C(C1)OC)C)O
MOL006887	0.5333	0.4667	0.7892	Radix Cynanchi	cynanoside,d_qt	Not Available	FALSE	C1(CC2(C3C(CC=C2CC1O)C(=O)OC(=CC3)c1ccoc1C)C)O
MOL006888	0.3441	0.6559	0.7165	Radix Cynanchi	cynanoside,e	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC1=COC2(C1(C(OC3=O)CO2)O)C)OC1OC(C(OC2CC(C(OC3CC(C(C(O3)C)O)OC)C(O2)C)OC)C(C1)OC)C)O
MOL006889	0.8660	0.1340	0.7671	Radix Cynanchi	cynanoside,f_qt	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC1=COC2(C1(C(OC3=O)CO2)O)C)O)O
MOL006890	0.5160	0.4840	0.7614	Radix Cynanchi	cynanoside,f	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC1=COC2(C1(C(OC3=O)CO2)O)C)OC1OC(C(OC2CC(C(OC3CC(C(C(O3)C)OC3OC(C(C(C3O)O)O)CO)OC)C(O2)C)OC)C(C1)OC)C)O
MOL006891	0.4272	0.5728	0.7509	Radix Cynanchi	cynanoside,g	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC1=COC2(C1(C(OC3=O)CO2)O)C)OC1OC(C(OC2CC(C(C(O2)C)OC2CC(C(C(O2)C)O)OC)O)C(C1)OC)C)O
MOL006892	0.8660	0.1340	0.7671	Radix Cynanchi	cynanoside,g_qt	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC1=COC2(C1(C(OC3=O)CO2)O)C)O)O
MOL006893	0.4491	0.5509	0.7625	Radix Cynanchi	cynanoside,i	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC1=COC2(C1C(OC3=O)CO2)C)OC1OC(C(OC2CC(C(OC3CC(C(C(O3)C)OC3OC(C(C(C3O)O)O)CO)OC)C(O2)C)OC)C(C1)OC)C)O
MOL006894	0.7316	0.2684	0.7409	Radix Cynanchi	glaucoside,d_qt	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC1=COC2(C1C(OC3=O)CO2)C)O)O
MOL006895	0.3441	0.6559	0.7454	Radix Cynanchi	glaucoside,d	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC1=COC2(C1C(OC3=O)CO2)C)OC1OC(C(OC2CC(C(C(O2)C)OC2CC(C(C(O2)C)O)OC)O)C(C1)OC)C)O

MOL006896	0.3728	0.6272	0.7531	Radix Cynanchi	cynanoside,k	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC(C3=O)c1ccoc1C)OC1OC(C(OC2CC(C(OC3CC(C(C(O3)C)OC3OC(C(C(C3O)O)O)CO)OC)C(O2)C)OC)C(C1)OC)C)O
MOL006897	0.5262	0.4738	0.7804	Radix Cynanchi	cynanoside,l_qt	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC(C3=O)c1ccoc1C)O)O
MOL006898	0.5905	0.4095	0.7671	Radix Cynanchi	cynanoside,l	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC(C3=O)c1ccoc1C)OC1OC(C(OC2CC(C(C(O2)C)OC2CC(C(C(O2)C)OC2OC(C(C(C2O)O)O)COC2OC(C(C(C2O)O)O)CO)OC)O)C(C1)OC)C)O
MOL006899	0.1851	0.8149	0.6797	Radix Cynanchi	cynanoside,m	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC(C3=O)c1ccoc1C)OC1OC(C(OC2CC(C(OC3CC(C(C(O3)C)O)OC)C(O2)C)OC)C(C1)OC)C)O
MOL006900	0.3599	0.6401	0.7573	Radix Cynanchi	cynanoside,n	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC(C3=O)(c1ccoc1C)C)OC1OC(C(OC2CC(C(OC3CC(C(C(O3)C)OC3OC(C(C(C3O)O)O)CO)OC)C(O2)C)OC)C(C1)OC)C
MOL006901	0.4267	0.5733	0.7573	Radix Cynanchi	cynanoside,o	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1O)C)CCC(C3=O)(c1ccoc1C)C)OC1OC(C(OC2CC(C(OC3CC(C(C(O3)C)OC3OC(C(C(C3O)O)O)CO)OC)C(O2)C)OC)C(C1)OC)C)O
MOL006902	0.2063	0.7937	0.7029	Radix Cynanchi	cynanoside,p3	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC(C3=O)(C1=CC(=O)OC1C)C)OC1OC(C(OC2CC(C(OC3CC(C(C(O3)C)O)OC)C(O2)C)OC)C(C1)OC)C)O
MOL006903	0.3933	0.6067	0.7560	Radix Cynanchi	cynanoside,p4	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC(C3=O)(C1=CC(=O)OC1C)C)OC1OC(C(OC2CC(C(OC3CC(C(C(O3)C)OC3OC(C(C(C3O)O)O)CO)OC)C(O2)C)OC)C(C1)OC)C)O
MOL006904	0.3816	0.6184	0.7529	Radix Cynanchi	cynanoside,p5	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC(C3=O)(C1=CC(=O)OC1(C)OC)C)OC1OC(C(OC2CC(C(OC3CC(C(C(O3)C)OC3OC(C(C(C3O)O)O)CO)OC)C(O2)C)OC)C(C1)OC)C)O
MOL006905	0.4305	0.5695	0.7602	Radix Cynanchi	cynanoside,q1	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC(C3=O)(c1ccoc1C)O)OC1OC(C(OC2CC(C(OC3CC(C(C(O3)C)OC3OC(C(C(C3O)O)O)CO)OC)C(O2)C)OC)C(C1)OC)C)O
MOL006906	0.2826	0.7174	0.7521	Radix Cynanchi	cynatroside,c	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC(C3=O)(c1ccoc1C)O)OC1OC(C(OC2CC(C(C(O2)C)OC2CC(C(C(O2)C)O)OC)O)C(C1)OC)C)O
MOL006907	0.4949	0.5051	0.7782	Radix Cynanchi	cynanoside,q3	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC(C3=O)(c1ccoc1C)O)OC1OC(C(OC2CC(C(C(O2)C)OC2CC(C(C(O2)C)OC2OC(C(C(C2O)O)O)CO)OC)O)C(C1)OC)C)O
MOL006908	0.1884	0.8116	0.6751	Radix Cynanchi	cynanoside,r1	Not Available	FALSE	C1(=O)C(CC2=CCC3C(C2(C1)C)CCC(C3=O)(c1ccoc1C)C)OC1OC(C(OC2CC(C(OC3CC(C(C(O3)C)O)OC)C(O2)C)OC)C(C1)OC)C
MOL006909	0.2098	0.7902	0.7075	Radix Cynanchi	cynanoside,r2	Not Available	FALSE	C1(=O)C(CC2=CCC3C(C2(C1O)C)CCC(C3=O)(c1ccoc1C)C)OC1OC(C(OC2CC(C(OC3CC(C(C(O3)C)O)OC)C(O2)C)OC)C(C1)OC)C

MOL006910	0.4154	0.5846	0.7547	Radix Cynanchi	cynanoside,r3	Not Available	FALSE	C1(=O)C(CC2=CCC3C(C2(C1O)C)CCC(C3=O)(C1Ccoc1C)C)OC1OC(C(OC2CC(C(OC3CC(C(C(O3)C)OC3OC(C(C(C3O)O)O)CO)OC)C(O2)C)OC)C(C1)OC)C
MOL006911	0.4101	0.5899	0.6425	Radix Cynanchi	cynanoside,s	Not Available	FALSE	C1(C(CC2=CCC(C(C2(C1)C)CC(=O)O)OC(=O)c1ccoc1C)OC1OC(C(OC2CC(C(OC3CC(C(C(O3)C)O)O)C)C(O2)C)OC)C(C1)OC)C)O
MOL006912	0.8669	0.1331	0.8047	Radix Cynanchi	cynanoside,s_qt	Not Available	FALSE	C1(C(CC2=CCC(C(C2(C1)C)CC(=O)O)OC(=O)c1ccoc1C)O)O
MOL006913	0.2850	0.7150	0.7398	Radix Cynanchi	cynanversicoside g	Not Available	FALSE	C1(C(CC(OC1C)OC1C(CC(OC1C)OC1C(C(O)C(OC1C)OC1CC2=CCC3=C4OC5C6C4(CCC3C2(CC1)C)COC6(OC5)C)OC)OC)OC)O
MOL006914	0.9000	0.1000	0.9613	Radix Cynanchi	cynanversicoside g_qt 1	44208031	FALSE	C1(C(CC(OC1C)O)OC)O
MOL006915	0.6938	0.3062	0.7668	Radix Cynanchi	cynanversicoside g_qt 2	Not Available	FALSE	OC1CCC2(C)C(=CCC3=C4OC5COC6(OCC4(CCC23)C56)C)C1
MOL006916	0.2218	0.7782	0.7317	Radix Cynanchi	cynatroside,a	Not Available	FALSE	C1(C(OC(CC1OC)OC1C(CC(OC1C)OC1C(OC(CC1OC)OC1C(CC2(C(=CCC3C2CCC(C3=O)c2ccoc2C)C1)C)O)C)O)C)O
MOL006917	0.2998	0.7002	0.7246	Radix Cynanchi	cynatratoside,f	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC1=COC2(C1C(OC3=O)CO2)C)OC1OC(C(OC2CC(C(OC3CC(C(C(O3)C)O)OC)C(O2)C)OC)C(C1)OC)C)O
MOL006918	0.2192	0.7808	0.7210	Radix Cynanchi	cynatroside,b	Not Available	FALSE	C1(C(CC(OC1C)OC1C(CC(OC1C)OC1C(CC(OC1C)OC1C(CC2(C(=CCC3C2CCC(C3=O)(c2ccoc2C)O)C1)C)O)OC)OC)OC)O
MOL006919	0.7316	0.2684	0.7409	Cynanchistauntonii Rhizoma Et Radix	glaucogenin,a	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC1=COC2(C1C(OC3=O)CO2)C)O)O
MOL006919	0.7316	0.2684	0.7409	Radix Cynanchi	glaucogenin,a	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC1=COC2(C1C(OC3=O)CO2)C)O)O
MOL006920	0.3536	0.6464	0.7418	Radix Cynanchi	glaucogenin,c,3-o-beta-d-cymaropyranosyl-(1-4)-alpha-l-diginopyranosyl-(1-4)-,beta-d-thevetopyranoside	Not Available	FALSE	C1(CC2=CCC3C(C2(CC1)C)CCC1=COC2(C1C(CO2)OC3=O)C)OC1C(C(C(C(O1)C)OC1OC(C(C(C1)OC)OC1C(C(C(C(O1)C)O)OC)O)C)OC)O
MOL006922	0.3441	0.6559	0.7454	Radix Cynanchi	glaucoside,c	Not Available	FALSE	C1(C(OC(CC1OC)OC1C(CC(OC1C)OC1C(OC(CC1OC)OC1C(CC2(C(=CCC3C2CCC2=COC4(C2C(OC3=O)CO4)C)C1)C)O)C)O)C)O
MOL006923	0.7316	0.2684	0.7409	Radix Cynanchi	glaucoside,c_qt	Not Available	FALSE	OC1CC2=CCC3C(=O)OC4C5C(=COC5(OC4)C)CCC3C2(C)CC1O

MOL006924	0.8660	0.1340	0.7671	Radix Cynanchi	hancopregnane	Not Available	FALSE	C1(C(CC2=CCC3C(C2(C1)C)CCC1=COC2(C1(C(OC3=O)CO2)O)C)O)O
MOL006925	0.8700	0.1300	0.8590	Radix Cynanchi	2h-pyran-2-one, tetrahydro-6-nonyl	15663978	FALSE	C1(OC(=O)CCC1)CCCCCCCCC
MOL006926	0.9265	0.0735	0.9626	Semiaquilegiae Radix	Cork acid	22494956	FALSE	C(=O)(CCCCCCC(=O)O)O
MOL006926	0.9265	0.0735	0.9626	Radix Cynanchi	Cork acid	22494956	FALSE	C(=O)(CCCCCCC(=O)O)O
MOL006926	0.9265	0.0735	0.9626	Cortex Hibisci	Cork acid	22494956	FALSE	C(=O)(CCCCCCC(=O)O)O
MOL006926	0.9265	0.0735	0.9626	Ranunculi Ternati Radix	Cork acid	22494956	FALSE	C(=O)(CCCCCCC(=O)O)O
MOL006927	0.9054	0.0946	0.9657	Pseudobulbus Cremastrae Seu Pleiones	4-hydroxybenzyl alcohol	125	FALSE	c1(ccc(cc1)O)CO
MOL006927	0.9054	0.0946	0.9657	Radix Cynanchi	4-hydroxybenzyl alcohol	125	FALSE	c1(ccc(cc1)O)CO
MOL006929	0.9258	0.0742	0.9093	Radix Cynanchi	2-Acetylresorcinol	69687	FALSE	c1(c(cccc1O)O)C(=O)C
MOL006930	0.7143	0.2857	0.7629	Arum Ternatum Thunb.	(+) isolariciresinol 9-o-β-d-glucopyranoside	Not Available	FALSE	c1(cc(ccc1O)C1C(C(Cc2c1cc(O)c(OC)c2)CO)COC1OC(C(C(C1O)O)O)CO)OC
MOL006931	0.6905	0.3095	0.7091	Cimicifugae Rhizoma	isolariciresino	Not Available	FALSE	c1(cc(ccc1O)C1C(C(Cc2c1cc(O)c(OC)c2)CO)COC1OC(C(C(C1O)O)O)CO)OC
MOL006931	0.6905	0.3095	0.7091	Arum Ternatum Thunb.	isolariciresino	Not Available	FALSE	c1(cc(ccc1O)C1C(C(Cc2c1cc(O)c(OC)c2)CO)COC1OC(C(C(C1O)O)O)CO)OC
MOL006932	0.9549	0.0451	0.9732	Arum Ternatum Thunb.	l-Pseudoephedrine	62946	FALSE	c1(C(C(NC)C)O)ccccc1
MOL006933	0.7418	0.2582	0.7111	Arum Ternatum Thunb.	1,2,3,4,6-penta-o-galloyl-β-d-glucose	Not Available	FALSE	C1(C(C(C(C(O1)COC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1OC(=O)c1cc(c(c(c1)O)O)O)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O
MOL006934	0.9339	0.0661	0.9707	Arum Ternatum Thunb.	WLN: Q5Q	8105	FALSE	C(CCCCO)O
MOL006934	0.9339	0.0661	0.9707	Raphani Semen	WLN: Q5Q	8105	FALSE	C(CCCCO)O
MOL006935	0.9260	0.0740	0.9220	Arum Ternatum Thunb.	Octylene	8125	FALSE	C=CCCCCCC
MOL006935	0.9260	0.0740	0.9220	Farfarae Flos	Octylene	8125	FALSE	C=CCCCCCC
MOL006935	0.9260	0.0740	0.9220	Allii Tuberosi Semen	Octylene	8125	FALSE	C=CCCCCCC
MOL006937	0.8244	0.1756	0.7279	Arum Ternatum Thunb.	12,13-epoxy-9-hydroxynonadeca-7,10-dienoic acid	Not Available	FALSE	C(=O)(CCCCC/C=C/C(/C=C/C1C(CCCCCC)O1)O)O

MOL006938	0.9286	0.0714	0.8851	Arum Ternatum Thunb.	DUR	13712	FALSE	OCC1C(O)CC(O1)n1c(=O)[nH]c(=O)cc1
MOL006938	0.9286	0.0714	0.8851	Euphorbiae Helioscopiae Herba	DUR	13712	FALSE	OCC1C(O)CC(O1)n1c(=O)[nH]c(=O)cc1
MOL006939	0.8915	0.1085	0.9613	Sesami Nigrum Semen	Methylpyrazine	7976	FALSE	c1nccnc1C
MOL006939	0.8915	0.1085	0.9613	Arum Ternatum Thunb.	Methylpyrazine	7976	FALSE	c1nccnc1C
MOL006939	0.8915	0.1085	0.9613	Benincasae Exocarpium	Methylpyrazine	7976	FALSE	c1nccnc1C
MOL006940	0.9034	0.0966	0.9684	Arum Ternatum Thunb.	D-2-Aminobutyrate	6971251	FALSE	C(=O)(C(CC)N)O
MOL006940	0.9034	0.0966	0.9684	Silybum Marianum	D-2-Aminobutyrate	6971251	FALSE	C(=O)(C(CC)N)O
MOL006942	0.8620	0.1380	0.9505	Arum Ternatum Thunb.	N-(5-methylisoxazol-3-yl)acetamide	538625	FALSE	o1nc(cc1C)NC(=O)C
MOL006943	0.2819	0.7181	0.7257	Arum Ternatum Thunb.	5,8-epidioxyergosta-6,22-dien-3-ol	Not Available	FALSE	C1(CCC2(C3(C1)OOC1(C2CCC2(C1CCC2C(C)/C=C/C(C)C(C)C)C)C=C3)C)O
MOL006944	0.7657	0.2343	0.6084	Arum Ternatum Thunb.	8-Octadecenoic acid	5282758	FALSE	C(=O)(CCCCCC/C=C/CCCCCCCCC)O
MOL006946	0.8985	0.1015	0.8385	Trichosanthes Kirilowii Maxim	adenosine	Not Available	FALSE	C1(OC(C(C1O)O)n1c2c(nc1)C(NC=N2)N)O
MOL006946	0.8985	0.1015	0.8385	Arum Ternatum Thunb.	adenosine	Not Available	FALSE	C1(OC(C(C1O)O)n1c2c(nc1)C(NC=N2)N)O
MOL006948	0.9208	0.0792	0.8633	Fritiliariae Irrhosae Bulbus	inosine	1260558	FALSE	n1(c2c(nc1)c(=O)[nH]cn2)C1OC(C(C1O)O)CO
MOL006948	0.9208	0.0792	0.8633	Arum Ternatum Thunb.	inosine	1260558	FALSE	n1(c2c(nc1)c(=O)[nH]cn2)C1OC(C(C1O)O)CO
MOL006949	0.9464	0.0536	0.9717	Arum Ternatum Thunb.	6-Deoxy-gulose	151257	FALSE	O=CC(O)C(O)C(O)C(O)C
MOL006950	0.9156	0.0844	0.9614	Prinsepiae Nux	(2R)-2-acetamidoglutaric acid	1560015	FALSE	C(CCC(=O)O)(NC(=O)C)C(=O)O
MOL006950	0.9156	0.0844	0.9614	Arum Ternatum Thunb.	(2R)-2-acetamidoglutaric acid	1560015	FALSE	C(CCC(=O)O)(NC(=O)C)C(=O)O
MOL006951	0.9503	0.0497	0.8222	Arum Ternatum Thunb.	pedatisectine a	Not Available	FALSE	c1c(ccc(n1)Cn1cnc2c1ncnc2N)O
MOL006952	0.9290	0.0710	0.9367	Arum Ternatum Thunb.	pedatisectine f	Not Available	FALSE	c1c(nc(cn1)C(C(O)C(O)O)O)C

MOL006953	0.8799	0.1201	0.9710	Fritillariaeussuriensis Bulbus	Thy	1135	FALSE	c1(=O)[nH]c(=O)c(c[nH]1)C
MOL006953	0.8799	0.1201	0.9710	Arum Ternatum Thunb.	Thy	1135	FALSE	c1(=O)[nH]c(=O)c(c[nH]1)C
MOL006953	0.8799	0.1201	0.9710	Arisaematis Rhizoma	Thy	1135	FALSE	c1(=O)[nH]c(=O)c(c[nH]1)C
MOL006953	0.8799	0.1201	0.9710	Sargassum	Thy	1135	FALSE	c1(=O)[nH]c(=O)c(c[nH]1)C
MOL006953	0.8799	0.1201	0.9710	Fritiliariae Irrhosae Bulbus	Thy	1135	FALSE	c1(=O)[nH]c(=O)c(c[nH]1)C
MOL006954	0.9282	0.0718	0.9564	Arum Ternatum Thunb.	BVE	8108	FALSE	O(C=C)CCCC
MOL006956	0.9402	0.0598	0.8572	Arum Ternatum Thunb.	cyclo-(leu-tyr)	15550385	FALSE	c1cc(ccc1O)CC1NC(=O)C(NC1=O)CC(C)C
MOL006957	0.8801	0.1199	0.7297	Arum Ternatum Thunb.	(3S,6S)-3-(benzyl)-6-(4-hydroxybenzyl)piperazine-2,5-quinone	11438306	FALSE	c1cc(ccc1)CC1NC(=O)C(NC1=O)Cc1ccc(cc1)O
MOL006958	0.9465	0.0535	0.8805	Arum Ternatum Thunb.	cyclo-(val-tyr)	56929107	FALSE	c1c(ccc(c1)CC1NC(=O)C(NC1=O)C(C)C)O
MOL006960	0.4574	0.5426	0.7432	Arum Ternatum Thunb.	(5R)-5-hydroxy-1-(4-hydroxy-3-methoxyphenyl)tetradecan-3-one	23786427	FALSE	C(CC(=O)CC(CCCCCCCCC)O)c1cc(c(cc1)O)OC
MOL006961	0.8910	0.1090	0.8303	Arum Ternatum Thunb.	GR	6802	FALSE	OCC1C(O)C(O)C(O1)n1cnc2c(=O)[nH]c(N)nc12
MOL006962	0.8542	0.1458	0.6634	Arum Ternatum Thunb.	2Z-hexadecenoic acid	5312417	FALSE	C(=O)(/C=C\CCCCCCCCCCCCC)O
MOL006963	0.4321	0.5679	0.6275	Arum Ternatum Thunb.	Ethyl linolelaidate	5365672	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)OCC
MOL006963	0.4321	0.5679	0.6275	Citri Sarcodactylis Fructus	Ethyl linolelaidate	5365672	FALSE	C(=O)(CCCCCCC/C=C/C/C=C/CCCCC)OCC
MOL006964	0.9317	0.0683	0.9736	Arum Ternatum Thunb.	valeraldoxime	9601699	FALSE	C(=N\O)/CCCC
MOL006965	0.4439	0.5561	0.6039	Arum Ternatum Thunb.	soya-cerebroside ii	Not Available	FALSE	C(=O)(C(CCCCCCCCCCCCCCC)O)NC(COC1OC(C(C(C1O)O)O)CO)C(/C=C/CC/C=C\CCCCCCCCC)O
MOL006965	0.4439	0.5561	0.6039	Humulus Scandens (Lour.) Merr.	soya-cerebroside ii	Not Available	FALSE	C(=O)(C(CCCCCCCCCCCCCCC)O)NC(COC1OC(C(C(C1O)O)O)CO)C(/C=C/CC/C=C\CCCCCCCCC)O
MOL006967	0.8873	0.1127	0.8367	Arum Ternatum Thunb.	beta-D-Ribofuranoside, xanthine-9	64959	FALSE	OCC1C(O)C(O)C(O1)n1cnc2c(O)nc(O)nc12

MOL006968	0.2431	0.7569	0.8342	Radix Stephaniae Cepharanthae.	(S)-(6-methoxy-4-quinolyl)-[(2S,4S,5S)-5-vinylquinuclidin-2-yl]methanol	667448	FALSE	c12c(C(C3N4CC(C(C3)CC4)C=C)O)ccnc1ccc(c2)OC
MOL006969	0.8534	0.1466	0.8741	Radix Stephaniae Cepharanthae.	cepharamine	Not Available	FALSE	C1(C(=O)N2CCCSC12)N
MOL006970	0.2072	0.7928	0.6831	Radix Stephaniae Cepharanthae.	homoaromoline	Not Available	FALSE	c12c3Oc4c5C(Cc6cc(Oc7ccc(CC1N(CCc2cc(c3O)OC)C)cc7)c(cc6)OC)N(CCc5cc(c4)OC)C
MOL006971	0.7131	0.2869	0.8656	Radix Stephaniae Cepharanthae.	CREBANINE	Not Available	FALSE	c12c3C(Cc4c1ccc(c4OC)OC)N(CCc3cc1c2OCO1)C
MOL006972	0.2098	0.7902	0.7029	Radix Stephaniae Cepharanthae.	Pycnamine	Not Available	FALSE	c12c3c(c(cc1CCN(C2Cc1cc(Oc2ccc(CC4c5cc(O3)c(cc5CCN4C)OC)cc2)c(cc1)O)C)OC)OC
MOL006973	0.1963	0.8037	0.7123	Radix Stephaniae Cepharanthae.	cepharanthine	Not Available	FALSE	c12c3c(cc4c1OCO4)CCN(C3Cc1ccc(cc1)Oc1cc(CC3c4cc(O2)c(cc4CCN3C)OC)ccc1OC)C
MOL006974	0.2236	0.7764	0.7294	Radix Stephaniae Cepharanthae.	cycleanine	Not Available	FALSE	C12N(CCc3cc(c(c(c13)Oc1ccc(CC3N(CCc4cc(c(c(c34)Oc3ccc(C2)cc3)OC)OC)C)cc1)OC)OC)C
MOL006975	0.7402	0.2598	0.8011	Radix Stephaniae Cepharanthae.	Cepharanone B	Not Available	FALSE	[nH]1c(=O)c2c3c(c4c(cc13)cccc4)c(c(c2)OC)OC
MOL006976	0.8634	0.1366	0.7382	Aristolochiae Fructus	Cepharanone A	Not Available	FALSE	c12cc3c(c4c5ccccc5cc(c14)[nH]c2=O)OCO3
MOL006976	0.8634	0.1366	0.7382	Radix Stephaniae Cepharanthae.	Cepharanone A	Not Available	FALSE	c12cc3c(c4c5ccccc5cc(c14)[nH]c2=O)OCO3
MOL006977	0.7989	0.2011	0.7770	Radix Stephaniae Cepharanthae.	Cepharadione A	Not Available	FALSE	n1(c(=O)c(=O)c2c3c(c4c(cc13)cccc4)c1OCOc1c2)C
MOL006978	0.6847	0.3153	0.8324	Radix Stephaniae Cepharanthae.	Cepharadione B	Not Available	FALSE	n1(c(=O)c(=O)c2c3c(c4c(cc13)cccc4)c(c(c2)OC)OC)C
MOL006979	0.8634	0.1366	0.9230	Papaveris Pericarpium	morphine	5288826	TRUE	C123c4c5OC2C(C=CC1C(Cc4ccc5O)N(CC3)C)O
MOL006979	0.8634	0.1366	0.9230	Radix Stephaniae Cepharanthae.	morphine	5288826	TRUE	C123c4c5OC2C(C=CC1C(Cc4ccc5O)N(CC3)C)O
MOL006980	0.5409	0.4591	0.9018	Papaveris Pericarpium	papaverine	4680	TRUE	c12c(cc(c(c2)OC)OC)ccnc1Cc1cc(c(cc1)OC)OC
MOL006980	0.5409	0.4591	0.9018	Panacis Quinquefolii Radix	papaverine	4680	TRUE	c12c(cc(c(c2)OC)OC)ccnc1Cc1cc(c(cc1)OC)OC
MOL006980	0.5409	0.4591	0.9018	Radix Stephaniae Cepharanthae.	papaverine	4680	TRUE	c12c(cc(c(c2)OC)OC)ccnc1Cc1cc(c(cc1)OC)OC
MOL006981	0.2048	0.7952	0.6918	Radix Stephaniae Cepharanthae.	Trilobine	Not Available	FALSE	O1c2c3C4NCCc3cc(OC)c2Oc2c1cc1C(N(CCc1c2)C)Cc1cc(Oc2ccc(C4)cc2)c(OC)cc1
MOL006982	0.7277	0.2723	0.8919	Radix Stephaniae Cepharanthae.	codeine	5284371	FALSE	C123c4c5OC2C(C=CC1C(Cc4ccc5OC)N(CC3)C)O
MOL006982	0.7277	0.2723	0.8919	Papaveris Pericarpium	codeine	5284371	FALSE	C123c4c5OC2C(C=CC1C(Cc4ccc5OC)N(CC3)C)O
MOL006983	0.7420	0.2580	0.8185	Radix Stephaniae Cepharanthae.	Dehydrostephanine	Not Available	FALSE	N1(CCc2c3c(c4c(cc13)c(ccc4)OC)c1OCOc1c2)C

MOL006984	0.7409	0.2591	0.7623	Radix Stephaniae Cepharanthae.	stesakine	Not Available	FALSE	N1(CCc2c3c(c4c(CC13)c(c(cc4)O)OC)c1OCOc1c2)C
MOL006985	0.7339	0.2661	0.8494	Stemonae Radix	Stephanine	Not Available	FALSE	c12c3C(Cc4c1cccc4OC)N(CCc3cc1c2OCO1)C
MOL006985	0.7339	0.2661	0.8494	Radix Stephaniae Cepharanthae.	Stephanine	Not Available	FALSE	c12c3C(Cc4c1cccc4OC)N(CCc3cc1c2OCO1)C
MOL006986	0.7248	0.2752	0.8317	Jujubae Fructus	Nornuciferine	41169	FALSE	O(c1c2c3C(NCCc3cc1OC)Cc1c2cccc1)C
MOL006986	0.7248	0.2752	0.8317	Radix Stephaniae Cepharanthae.	Nornuciferine	41169	FALSE	O(c1c2c3C(NCCc3cc1OC)Cc1c2cccc1)C
MOL006987	0.2063	0.7937	0.6819	Radix Stephaniae Cepharanthae.	Cepharanoline	Not Available	FALSE	O1c2c3C(N(CCc3cc3OCOc23)C)Cc2ccc(Oc3cc(CC4N(CCc5c4cc1c(OC)c5)C)ccc3O)cc2
MOL006989	0.7265	0.2735	0.6847	Cortex Hibisci	mucilage	72042	FALSE	O(C1C(OC(=O)C)C(O)C(OC1CO)OC1C(OC(=O)C)C(O)C(OC1CO)OC1C(OC(=O)C)C(O)C(OC1CO)OC)C1OC(C(OC2OC(C(OC3OC(C(OC4OC(C(OC5OC(C(OC)C(OC(=O)C)C5O)CO)C(OC(=O)C)C4O)CO)C(OC(=O)C)C3O)C(=O)O)C(OC(=O)C)C2O)CO)C(O)C1NC(=O)C)CO
MOL006990	0.9267	0.0733	0.8229	Radix Paeoniae Rubra	(1S,2S,4R)-trans-2-hydroxy-1,8-cineole-B-D-glucopyranoside	Not Available	FALSE	C1C2(C(CC(C1)C(O2)(C)C)OC1OC(C(C(C1O)O)O)CO)C
MOL006991	0.9446	0.0554	0.8642	Radix Paeoniae Rubra	60761-00-4	109010	FALSE	C1C2(C(CC(C1)C(O2)(C)C)O)C
MOL006991	0.9446	0.0554	0.8642	Morindae Officinalis Radix	60761-00-4	109010	FALSE	C1C2(C(CC(C1)C(O2)(C)C)O)C
MOL006992	0.9197	0.0803	0.9070	Radix Paeoniae Rubra	(2R,3R)-4-methoxyl-distylin	Not Available	FALSE	c1(cc(c2c(c1)OC(C(C2=O)OC)c1ccc(c(c1)O)O)O)O
MOL006993	0.8063	0.1937	0.8217	Radix Paeoniae Rubra	1-o-beta-d-glucopyranosyl-8-o-benzoylpaeonisuffrone	Not Available	FALSE	c1(ccccc1)C(=O)OCC12C3(CC1C(=O)CC3(OC2)C)OC1OC(C(C(C1O)O)O)CO
MOL006994	0.8471	0.1529	0.7625	Radix Paeoniae Rubra	1-o-beta-d-glucopyranosyl-8-o-benzoylpaeonisuffrone_qt	Not Available	FALSE	c1(ccccc1)C(=O)OCC12C3(CC1C(=O)CC3(OC2)C)O
MOL006995	0.7675	0.2325	0.7476	Radix Paeoniae Rubra	1-o-beta-d-glucopyranosylpaeonisuffrone	Not Available	FALSE	c1(ccccc1)C(=O)OCC12C3(CC1C(=O)CC3(OC2OC)C)OC1OC(C(C(C1O)O)O)CO

MOL006996	0.7688	0.2312	0.7446	Radix Paeoniae Rubra	1-o-beta-d-glucopyranosylpaeonisuffrone_qt	Not Available	FALSE	c1(ccccc1)C(=O)OCC12C3(CC1C(=O)CC3(OC2OC)C)O
MOL006997	0.8323	0.1677	0.7140	Linderae Radix	2-[(2R,5R,6R)-6,10-dimethylspiro[4.5]dec-9-en-2-yl]propan-2-ol	21675005	FALSE	CC(C)(O)C1CC2(CC1)C(CCC=C2C)C
MOL006997	0.8323	0.1677	0.7140	Radix Paeoniae Rubra	2-[(2R,5R,6R)-6,10-dimethylspiro[4.5]dec-9-en-2-yl]propan-2-ol	21675005	FALSE	CC(C)(O)C1CC2(CC1)C(CCC=C2C)C
MOL006999	0.2400	0.7600	0.6133	Radix Paeoniae Rubra	stigmast-7-en-3-ol	Not Available	FALSE	C1(CCC2(C(C1)CC=C1C3CCC(C(CCC(CC)C(C)C)C)C3(C)CCC21)C)O
MOL007000	0.8455	0.1545	0.7187	Radix Paeoniae Rubra	2-methoxy-5-(e)-propenyl-phenol-beta-vicianoside	Not Available	FALSE	C1(C(C(C(OC1)OCC1C(C(C(C(O1)Oc1cc(ccc1OC)/C=C/C)O)O)O)O)O)O
MOL007001	0.9496	0.0504	0.9448	Radix Paeoniae Rubra	2-methoxy-5-[(Z)-prop-1-enyl]phenol	1781945	FALSE	Oc1cc(ccc1OC)/C=C\C
MOL007002	0.8609	0.1391	0.8300	Figwort Root	paeonioflorin	Not Available	FALSE	C12(C3(C4(OC2OC(C1C3)(C4)O)C)OC1OC(C(C(C1O)O)O)CO)COC(=O)c1ccccc1
MOL007002	0.8609	0.1391	0.8300	Radix Paeoniae Rubra	paeonioflorin	Not Available	FALSE	C12(C3(C4(OC2OC(C1C3)(C4)O)C)OC1OC(C(C(C1O)O)O)CO)COC(=O)c1ccccc1
MOL007002	0.8609	0.1391	0.8300	Cortex Moutan	paeonioflorin	Not Available	FALSE	C12(C3(C4(OC2OC(C1C3)(C4)O)C)OC1OC(C(C(C1O)O)O)CO)COC(=O)c1ccccc1
MOL007003	0.5219	0.4781	0.7609	Cortex Moutan	benzoyl paeoniflorin	Not Available	FALSE	C12(C3(C4(OC2OC(C1C3)(C4)O)C)OC1OC(C(C(C1O)O)O)COC(=O)c1ccccc1)COC(=O)c1ccccc1
MOL007003	0.5219	0.4781	0.7609	Radix Paeoniae Rubra	benzoyl paeoniflorin	Not Available	FALSE	C12(C3(C4(OC2OC(C1C3)(C4)O)C)OC1OC(C(C(C1O)O)O)COC(=O)c1ccccc1)COC(=O)c1ccccc1
MOL007004	0.8571	0.1429	0.8299	Radix Paeoniae Rubra	Albiflorin	Not Available	FALSE	C12(C3(C(C2)C(CC1(OC3=O)C)O)COC(=O)c1ccccc1)OC1OC(C(C(C1O)O)O)CO
MOL007005	0.8788	0.1212	0.7799	Radix Paeoniae Rubra	Albiflorin_qt	Not Available	FALSE	C12(C3(C(C2)C(CC1(OC3=O)C)O)COC(=O)c1ccccc1)O
MOL007006	0.8857	0.1143	0.8322	Cortex Moutan	oxypaeoniflorin	Not Available	FALSE	C12(C3(C4(OC2OC(C1C3)(C4)O)C)OC1OC(C(C(C1O)O)O)CO)COC(=O)c1ccc(cc1)O

MOL007006	0.8857	0.1143	0.8322	Radix Paeoniae Rubra	oxypaeoniflorin	Not Available	FALSE	C12(C3(C4(OC2OC(C1C3)(C4)O)C)OC1OC(C(C(C1O)O)O)CO)COC(=O)c1ccc(cc1)O
MOL007007	0.7717	0.2283	0.7589	Radix Paeoniae Rubra	4-ethyl-paeoniflorin	Not Available	FALSE	c1ccc(cc1)C(=O)OCC12C3(CC1C1(CC3OC2O1)OCC)OC1OC(C(C(C1O)O)O)CO
MOL007008	0.7353	0.2647	0.7525	Radix Paeoniae Rubra	4-ethyl-paeoniflorin_qt	Not Available	FALSE	c1ccc(cc1)C(=O)OCC12C3(CC1C1(CC3OC2O1)OCC)O
MOL007009	0.7878	0.2122	0.7932	Radix Paeoniae Rubra	4-o-galloylalbiflorin	Not Available	FALSE	c1(ccccc1)C(=O)OCC12C3(CC1C(CC3(OC2=O)C)OC(=O)c1cc(c(c(c1)O)O)O)OC1OC(C(C(C1O)O)O)CO
MOL007010	0.6944	0.3056	0.7376	Radix Paeoniae Rubra	4-o-galloylalbiflorin_qt	Not Available	FALSE	c1(ccccc1)C(=O)OCC12C3(CC1C(CC3(OC2=O)C)OC(=O)c1cc(c(c(c1)O)O)O)O
MOL007011	0.7740	0.2260	0.7461	Radix Paeoniae Rubra	4-o-methyl-paeoniflorin	Not Available	FALSE	C12(C3(OC4C1(C(C(C3)(O4)OC)C2)COC(=O)c1ccccc1)C)OC1C(C(C(C(O1)CO)O)O)O
MOL007012	0.7639	0.2361	0.7424	Radix Paeoniae Rubra	4-o-methyl-paeoniflorin_qt	Not Available	FALSE	C12(C3(OC4C1(C(C(C3)(O4)OC)C2)COC(=O)c1ccccc1)C)O
MOL007014	0.9066	0.0934	0.8008	Radix Paeoniae Rubra	8-debenzoylpaeonidanin	Not Available	FALSE	C12(CC3C(=O)CC1(OC(C23CO)OC)C)OC1C(C(C(C(O1)CO)O)O)O
MOL007015	0.9318	0.0682	0.8023	Radix Paeoniae Rubra	8-debenzoylpaeonidanin_qt	Not Available	FALSE	C12(CC3C(=O)CC1(OC(C23CO)OC)C)O
MOL007016	0.7783	0.2217	0.6849	Radix Paeoniae Rubra	Paeoniflorigenone	Not Available	FALSE	c1(ccccc1)C(=O)OCC1C2CC3(C(CC2=O)(OC1O3)C)O
MOL007017	0.7756	0.2244	0.6633	Radix Paeoniae Rubra	9-ethyl-neo-paeoniaflorin A	Not Available	FALSE	c1ccc(cc1)C(=O)OCC1(C2C(=O)CC(CC2)OC1OCC)OC1C(C(C(C(O1)CO)O)O)O
MOL007018	0.7700	0.2300	0.6507	Radix Paeoniae Rubra	9-ethyl-neo-paeoniaflorin A_qt	Not Available	FALSE	c1ccc(cc1)C(=O)OCC1(C2C(=O)CC(CC2)OC1OCC)O
MOL007019	0.8205	0.1795	0.7430	Quisqualis Indica	Eugeniin	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC1OC(C(C(C1OC(=O)c1cc(c(c(c21)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O
MOL007019	0.8205	0.1795	0.7430	Juglandis Semen	Eugeniin	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC1OC(C(C(C1OC(=O)c1cc(c(c(c21)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O
MOL007019	0.8205	0.1795	0.7430	Cornus Officinalis Sieb. Et Zucc.	Eugeniin	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC1OC(C(C(C1OC(=O)c1cc(c(c(c21)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O

MOL007019	0.8205	0.1795	0.7430	Radix Paeoniae Rubra	Eugeniin	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC1OC(C(C(C1OC(=O)c1cc(c(c(c21)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O
MOL007019	0.8205	0.1795	0.7430	Caryophylliflos	Eugeniin	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC1OC(C(C(C1OC(=O)c1cc(c(c(c21)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O
MOL007020	0.8633	0.1367	0.7920	Radix Paeoniae Rubra	Lactiflorin_qt	Not Available	FALSE	OC12C3(C(C1)C(OC3=O)(CC2O)C)COC(=O)c1ccc[illegible]cc1
MOL007021	0.7964	0.2036	0.8387	Radix Paeoniae Rubra	trans-.beta.-Terpinyl benzoate	570530	FALSE	O(C(C1CCC(=C)CC1)(C)C)C(=O)c1ccccc1
MOL007022	0.8253	0.1747	0.8160	Radix Paeoniae Rubra	evofolinB	Not Available	FALSE	OCC(c1cc(OC)c(O)cc1)C(=O)c1cc(OC)c(O)cc1
MOL007022	0.8253	0.1747	0.8160	Hydnocarpi Anthelminticae Semen	evofolinB	Not Available	FALSE	OCC(c1cc(OC)c(O)cc1)C(=O)c1cc(OC)c(O)cc1
MOL007023	0.8069	0.1931	0.8074	Radix Paeoniae Rubra	galloylpaeoniflorine	Not Available	FALSE	CC12CC3(C4CC1(C4(C(O2)O3)COC(=O)c1ccccc1)OC1C(C(C(C(O1)COC(=O)c1cc(c(c(c1)O)O)O)O)O)O)O
MOL007024	0.8886	0.1114	0.7846	Radix Paeoniae Rubra	galloylpaeoniflorine_qt 2	Not Available	FALSE	CC12CC3(C4CC1(C4(C(O2)O3)COC(=O)c1ccccc1)O)O
MOL007025	0.5219	0.4781	0.7609	Radix Paeoniae Rubra	isobenzoylpaeoniflorin	Not Available	FALSE	C12(C3(OC4C1(C(C(C3)(O4)O)C2)COC(=O)c1ccccc1)C)OC1C(C(C(C(O1)COC(=O)c1ccccc1)O)O)O
MOL007026	0.9195	0.0805	0.7825	Radix Paeoniae Rubra	paeonin,a	Not Available	FALSE	O(C12OC=C(C(C1)C(=O)C=C2C)COC)C1OC(C(O)C(O)C1O)CO
MOL007027	0.9316	0.0684	0.8877	Radix Paeoniae Rubra	paeonin,a_qt	Not Available	FALSE	OC12OC=C(C(C1)C(=O)C=C2C)COC
MOL007028	0.9254	0.0746	0.8728	Radix Paeoniae Rubra	paeonin,b	Not Available	FALSE	O(C12OC=C(C(C1)C(=O)C=C2C)CO)C1OC(C(O)C(O)C1O)CO
MOL007029	0.9444	0.0556	0.8811	Radix Paeoniae Rubra	paeonin,b_qt	Not Available	FALSE	OC12OC=C(C(C1)C(=O)C=C2C)CO
MOL007030	0.9183	0.0817	0.8055	Radix Paeoniae Rubra	paeonin,c	Not Available	FALSE	C12(CC(C(=O)C=C1C)C(=C)C(O2)OC)OC1C(C(C(C(O1)CO)O)O)O
MOL007031	0.9473	0.0527	0.8696	Radix Paeoniae Rubra	paeonin,c_qt	Not Available	FALSE	C12(CC(C(=O)C=C1C)C(=C)C(O2)OC)O
MOL007034	0.2774	0.7226	0.7376	Radix Aconiti Kusnezoffii	Deoxyaconitine	Not Available	FALSE	O(C12C3C4N(CC5(C(C4(C4C1C(OC(=O)c1ccccc1)C(O)(C4)C(OC)C2O)C(OC)CC5)C3OC)COC)CC)C(=O)C
MOL007035	0.9427	0.0573	0.8868	Radix Salviae	(E)-3-(3-hydroxy-4,5-dimethoxy-phenyl)acrylic acid	10998653	FALSE	c1(c(c(cc(c1)/C=C/C(=O)O)O)OC)OC
MOL007036	0.6310	0.3690	0.7184	Radix Salviae	5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthren-4-one	11011966	FALSE	C1CC(c2c(C1=O)c1c(cc2)cc(c(c1O)O)C(C)C)(C)C
MOL007037	0.7280	0.2720	0.7954	Radix Salviae	1,2-DT-Quinone	105119	FALSE	c12c(c3c(C(=O)C1=O)c1c(cc3)C(=CCC1)C)occ2C

MOL007038	0.3313	0.6687	0.8144	Radix Salviae	Dehydromiltirone	3082765	FALSE	c12c(ccc3c1C(=O)C(=O)C(=C3)C(C)C)C(CC=C2)(C)C
MOL007040	0.7133	0.2867	0.8587	Radix Salviae	1-ketoisocryptotanshinone	Not Available	FALSE	C1(CCC(=O)c2c1ccc1c2C(=O)C2=C(C1=O)C(CO2)C)(C)C
MOL007041	0.5706	0.4294	0.7754	Radix Salviae	2-isopropyl-8-methylphenanthrene-3,4-dione	135872	FALSE	c1ccc(c2c1c1c(cc2)C=C(C(=O)C1=O)C(C)C)C
MOL007042	0.7472	0.2528	0.7763	Campsis Flos	3-epicorosolic,acid	15917998	FALSE	C12=CCC3C4(C(C(C(C(C4)O)O)(C)C)CCC3(C1(CCC1(C2C(C(CC1)C)C)C(=O)O)C)C)C
MOL007042	0.7472	0.2528	0.7763	Radix Salviae	3-epicorosolic,acid	15917998	FALSE	C12=CCC3C4(C(C(C(C(C4)O)O)(C)C)CCC3(C1(CCC1(C2C(C(CC1)C)C)C(=O)O)C)C)C
MOL007043	0.9305	0.0695	0.9570	Radix Salviae	1-(3,4-dihydroxyphenyl)-2-hydroxyethanone	22134444	FALSE	c1(ccc(cc1O)C(=O)CO)O
MOL007044	0.8770	0.1230	0.9320	Radix Salviae	3,7-dimethylocta-2,6-dien-1-yl formate	Not Available	FALSE	C(=O)C(O)/C=C(\C)/CCC=C(C)C
MOL007045	0.7665	0.2335	0.8371	Radix Salviae	3α-hydroxytanshinone Ⅱa	14626764	FALSE	c12c(c3c(cc1)c1c(C(=O)C3=O)c(co1)C)C(CCC2(C)C)O
MOL007046	0.7964	0.2036	0.7401	Radix Salviae	3beta-Hydroxytanshinone IIA	5318350	FALSE	c12c(c3c(cc1)c1c(C(=O)C3=O)c(co1)C)CCC(C2(C)C)O
MOL007047	0.9580	0.0420	0.7912	Radix Salviae	(1R,4R,5S)-1-isopropyl-4-methyl-4-bicyclo[3.1.0]hexanol	11744854	FALSE	C1CC2(CC2C1(O)C)C(C)C
MOL007048	0.8618	0.1382	0.7420	Radix Salviae	(E)-3-[2-(3,4-dihydroxyphenyl)-7-hydroxy-benzofuran-4-yl]acrylic acid	10403222	FALSE	c1(ccc(cc1O)c1oc2c(c1)c(ccc2O)/C=C/C(=O)O)O

MOL007049	0.4803	0.5197	0.8168	Radix Salviae	4-methylenemiltirone	14609851	FALSE	c12c(ccc3c1C(=O)C(=O)C(=C3)C(C)C)C(=C)CCC2
MOL007050	0.5751	0.4249	0.7038	Radix Salviae	2-(4-hydroxy-3-methoxyphenyl)-5-(3-hydroxypropyl)-7-methoxy-3-benzofurancarboxaldehyde	6709746	FALSE	c1c(c(cc(c1)c1c(c2c(c(cc(c2)CCCO)OC)o1)C=O)OC)O
MOL007053	0.3813	0.6187	0.7715	Radix Salviae	7-oxoroyleanone2	2751800	FALSE	C1CC(C2C(C1)(C1=C(C(=O)C2)C(=O)C(=C(C1=O)O)C(C)C)C)(C)C
MOL007054	0.3055	0.6945	0.7914	Radix Salviae	(4bS,8aS,10S)-10-hydroxy-2-isopropyl-4b,8,8-trimethyl-5,6,7,8a,9,10-hexahydrophenanthrene-3,4-dione	14609850	FALSE	C1CC(C2C(C1)(C1=C(C(C2)O)C=C(C(=O)C1=O)C(C)C)C)(C)C
MOL007055	0.6085	0.3915	0.6767	Radix Salviae	9-methyl lithospermateb	Not Available	FALSE	c1(cc(ccc1O)C1C(c2c(O1)c(ccc2/C=C/C(=O)OC(Cc1ccc(c(c1)O)O)C(=O)OC)O)C(=O)OC(Cc1ccc(c(c1)O)O)C(=O)O)O
MOL007056	0.8035	0.1965	0.6474	Radix Salviae	TNP00297	Not Available	FALSE	C12(CCC3C(C(=C)CCC1O2)CC3(C)C)C
MOL007058	0.7774	0.2226	0.7455	Radix Salviae	formyltanshinone	14609847	FALSE	c1cc(c2c(c1)c1c(cc2)c2c(C(=O)C1=O)c(co2)C)C=O
MOL007059	0.8151	0.1849	0.7018	Radix Salviae	3-beta-Hydroxymethylenetanshiquinone	5318290	FALSE	C1C(C(=C)c2c(C1)c1c(cc2)c2c(C(=O)C1=O)c(co2)C)O
MOL007059	0.8151	0.1849	0.7018	Eucommiae Cortex	3-beta-Hydroxymethylenetanshiquinone	5318290	FALSE	C1C(C(=C)c2c(C1)c1c(cc2)c2c(C(=O)C1=O)c(co2)C)O
MOL007059	0.8151	0.1849	0.7018	Codonopsis Radix	3-beta-Hydroxymethylenetanshiquinone	5318290	FALSE	C1C(C(=C)c2c(C1)c1c(cc2)c2c(C(=O)C1=O)c(co2)C)O

MOL007060	0.6979	0.3021	0.6748	Radix Salviae	Lithospermic acid B	6451084	FALSE	c1cc(cc(c1O)O)CC(C(=O)O)OC(=O)/C=C/c1ccc(c2c1C(C(O2)c1cc(c(cc1)O)O)C(=O)OC(C(=O)O)Cc1cc(c(cc1)O)O)O
MOL007060	0.6979	0.3021	0.6748	Lithospermum Erythrorhizon	Lithospermic acid B	6451084	FALSE	c1cc(cc(c1O)O)CC(C(=O)O)OC(=O)/C=C/c1ccc(c2c1C(C(O2)c1cc(c(cc1)O)O)C(=O)OC(C(=O)O)Cc1cc(c(cc1)O)O)O
MOL007060	0.6979	0.3021	0.6748	Panacis Quinquefolii Radix	Lithospermic acid B	6451084	FALSE	c1cc(cc(c1O)O)CC(C(=O)O)OC(=O)/C=C/c1ccc(c2c1C(C(O2)c1cc(c(cc1)O)O)C(=O)OC(C(=O)O)Cc1cc(c(cc1)O)O)O
MOL007061	0.6958	0.3042	0.8018	Radix Salviae	Methylenetanshinquinone	105118	FALSE	C1CC(=C)c2c(C1)c1c(cc2)c2c(C(=O)C1=O)c(co2)C
MOL007062	0.3339	0.6661	0.6418	Radix Salviae	neo-przewaquinone a	Not Available	FALSE	c12C(=O)C(=O)c3c(c1occ2C)ccc1c3CCCC(=C)c2ccc3c(c2CC/C=C/1\C)C(=O)C(=O)c1c3occ1C
MOL007063	0.4369	0.5631	0.7872	Radix Salviae	przewalskin a	Not Available	FALSE	C1CC(C2C3(C1)c1c(C(C2=O)OC3=O)cc(c(c(c1=O)C(=O)C)O)C(C)C)(C)C
MOL007064	0.6056	0.3944	0.8700	Radix Salviae	przewalskin b	Not Available	FALSE	C1CC(C2C(=C1)C1C3(CC2)C(C(=O)O1)(C(=O)C(=C3)C(C)C)O)(C)C
MOL007065	0.1982	0.8018	0.7065	Radix Salviae	przewalskin c	Not Available	FALSE	C1CC(C2C(=C1)C1C3(C(C2)OC)cc(c(c1O)O)C(C)C)(C)C
MOL007066	0.3148	0.6852	0.6787	Radix Salviae	przewalskin d	Not Available	FALSE	C1=CC2=Cc3c(CCC2C(C1)(C)C)cc(c(c3O)O)C(C)C
MOL007067	0.7673	0.2327	0.8371	Radix Salviae	Przewaquinone A	619402	FALSE	o1c2c(c(c1)CO)C(=O)C(=O)c1c3CCCC(c3ccc21)(C)C
MOL007068	0.7890	0.2110	0.7765	Radix Salviae	Przewaquinone B	622085	FALSE	c1cc(c2c(c1)c1c(cc2)c2c(C(=O)C1=O)c(co2)CO)C
MOL007069	0.8183	0.1817	0.8290	Radix Salviae	przewaquinone c	Not Available	FALSE	C1CC(c2c(C1)c1c(cc2)c2c(C(=O)C1=O)c(co2)C)(O)C
MOL007070	0.8383	0.1617	0.8244	Radix Salviae	(6S,7R)-6,7-dihydroxy-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	10470747	FALSE	C1C(C(c2c(C1)c1c(cc2)c2c(C(=O)C1=O)c(co2)C)(O)C)O
MOL007071	0.8748	0.1252	0.7077	Radix Salviae	przewaquinone f	Not Available	FALSE	C1C(C(c2c(C1)c1c(cc2)c2c(C(=O)C1=O)c(co2)C)CO)O
MOL007072	0.9395	0.0605	0.9414	Radix Salviae	(2S)-3-(3,4-dihydroxyphenyl)-2-hydroxypropanoic acid	179536	FALSE	c1(ccc(cc1O)CC(C(=O)O)O)O
MOL007073	0.3272	0.6728	0.7962	Radix Salviae	saloilenone	Not Available	FALSE	c12ccc3c4c1C(C(C(=O)c4ccc3C)C(C)C)OCC2(C)C

MOL007074	0.6979	0.3021	0.6748	Radix Salviae	salvianolic acid b	51066555	FALSE	c1cc(cc(c1O)O)CC(C(=O)O)OC(=O)/C=C/c1ccc(c2c1C(C(O2)c1cc(c(cc1)O)O)C(=O)OC(C(=O)O)Cc1cc(c(cc1)O)O)O
MOL007075	0.7823	0.2177	0.6296	Radix Salviae	salvianolic acid n	Not Available	FALSE	C1=C(C=C(C2C1C=Cc1c(O2)cc(c(c1)O)O)O)/C=C/C(=O)OC(C(=O)O)Cc1cc(c(cc1)O)O
MOL007076	0.2714	0.7286	0.7873	Radix Salviae	Saprothoquinone	372741	FALSE	C1(=O)C(=O)C(=Cc2ccc(c(c12)CCC=C(C)C)C)C(C)C
MOL007077	0.3493	0.6507	0.6168	Radix Salviae	sclareol	7060889	FALSE	C1CC(C2C(C1)(CCCC2(C)O)CCC(=C)C)O)C)(C)C
MOL007079	0.7615	0.2385	0.8229	Radix Salviae	tanshinaldehyde	Not Available	FALSE	C1CC(c2c(C1)c1c(cc2)c2c(C(=O)C1=O)c(co2)C)(C=O)C
MOL007080	0.7992	0.2008	0.6960	Radix Salviae	Tanshinol A	5321622	FALSE	c1cc(c2c(c1)c1c(cc2)c2c(C(=O)C1=O)c(co2)C)CO
MOL007081	0.3703	0.6297	0.8431	Radix Salviae	Danshenol B	3083515	FALSE	C1CC(c2c(C1)c1c(cc2)C2=C(C(=O)C1(O)CC(=O)C)C(CO2)C)(C)C
MOL007082	0.5400	0.4600	0.8104	Radix Salviae	Danshenol A	3083514	FALSE	c1cc(c2c(c1)c1c(cc2)C2=C(C(=O)C1(O)CC(=O)C)C(CO2)C)C
MOL007083	0.5472	0.4528	0.6216	Radix Salviae	Z-8-Hexadecen-1-ol acetate	5363535	FALSE	C(CCCCCC/C=C\CCCCCCC)OC(=O)C
MOL007084	0.2708	0.7292	0.8038	Radix Salviae	Aethiopinone	157301	FALSE	C1(C(CCC2C1C(=O)C(=O)C(=C2)C(C)C)CCCC(=C)C
MOL007085	0.4842	0.5158	0.7829	Radix Salviae	Salvilenone	Not Available	FALSE	c12c(ccc3c1c1C(=C(C3=O)C(C)C)OC(c1cc2)(C)C)C
MOL007087	0.6058	0.3942	0.8172	Radix Salviae	carnosol	Not Available	FALSE	O1C(=O)C23c4c(C1CC2C(CCC3)(C)C)cc(c(c4O)O)C(C)C
MOL007088	0.5790	0.4210	0.8872	Radix Salviae	cryptotanshinone	160254	FALSE	c12c(ccc3c1C(=O)C(=O)C1=C3OCC1C)C(CCC2)(C)C
MOL007088	0.5790	0.4210	0.8872	Nardostachyos Radix Et Rhizoma	cryptotanshinone	160254	FALSE	c12c(ccc3c1C(=O)C(=O)C1=C3OCC1C)C(CCC2)(C)C
MOL007090	0.7255	0.2745	0.7690	Radix Salviae	dan-shexinkum a	Not Available	FALSE	c12c(c3c(cc1)C(=O)C(=C(C3=O)O)C(C)CO)cccc2C
MOL007091	0.6744	0.3256	0.7992	Radix Salviae	dan-shexinkum b	5320113	FALSE	c12c(c3c(cc1)C(=O)C(=C(C3=O)O)C(C)C)cccc2C
MOL007092	0.7374	0.2626	0.8202	Radix Salviae	dan-shexinkum c	5320114	FALSE	c12c(c3c(cc1)C(=O)C(=C(C3=O)O)C)cccc2C
MOL007093	0.5927	0.4073	0.8332	Radix Salviae	dan-shexinkum d	Not Available	FALSE	C1C(C(C2=C(O1)C(=O)c1c(C2=O)ccc2c1cccc2C)(CO)C)C
MOL007094	0.5766	0.4234	0.8432	Radix Salviae	danshenspirok etallactone	Not Available	FALSE	c1ccc(c2c1c1c(cc2)C2(OCC1=O)CC(CO2)C)C
MOL007095	0.5340	0.4660	0.8110	Radix Salviae	danshenspirok etallactoneii	Not Available	FALSE	O1C2(CC(C1)C)OC(=O)c1c2ccc2C(CCCc12)(C)C
MOL007097	0.3904	0.6096	0.7584	Radix Salviae	dehydrouvaol	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(CO)CCC(=C)C(C)C4C3=CCC21)C)O
MOL007098	0.4538	0.5462	0.8039	Radix Salviae	deoxyneocryptotanshinone	15690458	FALSE	C1(=O)C(=C(C(=O)c2c1c1c(cc2)C(CCC1)(C)C)C(C)C)O

MOL007099	0.7410	0.2590	0.8199	Radix Salviae	dihydroisotanshinone Ⅰ	11778300	FALSE	c1c(c2c(cc1)c1c(cc2)C(=O)C2=C(C1=O)OCC2C)C
MOL007100	0.7122	0.2878	0.8268	Radix Salviae	dihydrotanshinlactone	Not Available	FALSE	c1cc(c2c(c1)c1c(cc2)c2c(oc1=O)C(CO2)C)C
MOL007101	0.7220	0.2780	0.8067	Radix Salviae	dihydrotanshinone Ⅰ	40785034	FALSE	c1ccc(c2c1c1c(cc2)C2=C(C(=O)C1=O)C(CO2)C)C
MOL007103	0.4536	0.5464	0.6694	Radix Salviae	dimetbyl lithosper-mate b	Not Available	FALSE	c1(cc(ccc1O)C1C(c2c(O1)c(ccc2/C=C/C(=O)OC(Cc1ccc(c(c1)O)O)C(=O)OC)O)C(=O)OC(Cc1ccc(c(c1)O)O)C(=O)OC)O
MOL007104	0.4943	0.5057	0.6144	Radix Salviae	dimethyllithospermate	Not Available	FALSE	c1c(c(cc(c1)C1Oc2c(C1C(=O)OC)c(ccc2O)/C=C/C(=O)OC(C(=O)OC)Cc1ccc(c(c1)O)O)O)O
MOL007105	0.5034	0.4966	0.8499	Radix Salviae	epidanshenspiroketallactone	Not Available	FALSE	c1ccc(c2c1C1C(C=C2)C2(OCC1=O)CC(CO2)C)C
MOL007107	0.2364	0.7636	0.7221	Radix Salviae	C09092	442027	FALSE	C1CC(C2C(C1)(c1c(CC2)cc(c(c1)O)C(C)C)C)(C)C
MOL007107	0.2364	0.7636	0.7221	Viticis Fructus	C09092	442027	FALSE	C1CC(C2C(C1)(c1c(CC2)cc(c(c1)O)C(C)C)C)(C)C
MOL007108	0.6302	0.3698	0.8869	Radix Salviae	isocryptotanshi-none	Not Available	FALSE	C1CCC(c2c1c1c(cc2)C(=O)C2=C(C1=O)OCC2C)(C)C
MOL007110	0.7815	0.2185	0.7530	Radix Salviae	isotanshinone iib	Not Available	FALSE	c12c(c3c(cc1)C(=O)c1c(C3=O)occ1C)CCCC2(C)CO
MOL007111	0.6345	0.3655	0.8781	Radix Salviae	Isotanshinone II	626354	FALSE	C1CCC(c2c1c1c(cc2)C(=O)c2c(C1=O)occ2C)(C)C
MOL007112	0.7396	0.2604	0.8054	Radix Salviae	Isotanshinone I	623940	FALSE	c1c(c2c(cc1)c1c(cc2)C(=O)c2c(C1=O)occ2C)C
MOL007113	0.7805	0.2195	0.6952	Radix Salviae	lithospermic acid	6441498	FALSE	c1c(c(cc(c1)CC(C(=O)O)OC(=O)/C=C/c1ccc(c2c1C(C(O2)c1ccc(c(c1)O)O)C(=O)O)O)O)O
MOL007116	0.8729	0.1271	0.7690	Glechomae Herba	methylrosmarinate	Not Available	FALSE	c1(ccc(cc1O)CC(OC(=O)/C=C\c1ccc(c(c1)O)O)C(=O)OC)O
MOL007116	0.8729	0.1271	0.7690	Radix Salviae	methylrosmarinate	Not Available	FALSE	c1(ccc(cc1O)CC(OC(=O)/C=C\c1ccc(c(c1)O)O)C(=O)OC)O
MOL007117	0.6347	0.3653	0.8334	Radix Salviae	methyltanshinonate	14610613	FALSE	c12c(c3c(cc1)c1c(C(=O)C3=O)c(co1)C)CCCC2(C)C(=O)OC
MOL007118	0.2962	0.7038	0.7589	Radix Salviae	microstegiol	Not Available	FALSE	c12c(ccc3c1C(C(=O)C(=C3)C(C)C)(CCCC2)C)C)OC
MOL007119	0.5769	0.4231	0.7955	Radix Salviae	miltionone Ⅰ	5319835	FALSE	c12c(c3c(cc1)C(=O)C(=C(C3=O)O)C(C)C)C(=O)CCC2(C)C
MOL007120	0.6458	0.3542	0.8318	Radix Salviae	miltionone Ⅱ	5319836	FALSE	C12=C(C3=C(C(=O)C4=C(C3=CC1=O)OCC4C)O)CCCC2(C)C
MOL007121	0.4654	0.5346	0.8505	Radix Salviae	miltipolone	Not Available	FALSE	C1CC(C2C3(C1)C1C(C(C2)OC3)CC(C(C(=O)C1)O)C)(C)C
MOL007122	0.3346	0.6654	0.7970	Radix Salviae	Miltirone	160142	FALSE	C12C(CCC3C1C(=O)C(=C3)C(C)C)C(CCC2)(C)C
MOL007123	0.7551	0.2449	0.8244	Radix Salviae	miltirone Ⅱ	Not Available	FALSE	C12C(=CCC3C1C(=O)C(=CCC3=O)O)C(CCC2=O)(C)C
MOL007124	0.6525	0.3475	0.8395	Radix Salviae	neocryptotanshinone ii	5320066	FALSE	C1C(c2c(CC1)c1c(cc2)C(=O)C(=C(C1=O)O)C)(C)C
MOL007125	0.5872	0.4128	0.7888	Radix Salviae	neocryptotanshinone	44425165	FALSE	C1(=O)C(=O)C(=C(c2c1c1c(cc2)C(CCC1)(C)C)O)C(C)CO

MOL007126	0.5590	0.4410	0.7768	Radix Salviae	przewalskin	Not Available	FALSE	C1(CCCC23c4cc(c(cc4C(CC12)OC3)C)O)(C)C
MOL007127	0.7765	0.2235	0.7796	Radix Salviae	1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	10062187	FALSE	C1(=O)C(=O)c2c(c3c1c1c(cc3)C(=O)CCC1)occ2C
MOL007128	0.7793	0.2207	0.7535	Radix Salviae	paramiltioic acid	Not Available	FALSE	C123C(CC(C4(C=C1C(=O)O)OC(=O)C(=C4)C)OC3)C(CCC2)(C)C
MOL007129	0.9051	0.0949	0.7593	Radix Salviae	potassium salvianolate d	Not Available	FALSE	c1(c(ccc(c1CC(=O)O)/C=C\C(=O)OC(Cc1cc(c(cc1)O)O)C(=O)O)O)O
MOL007130	0.8624	0.1376	0.8030	Radix Salviae	prolithospermic acid	Not Available	FALSE	c1(ccc(cc1O)C1Cc2c(c(ccc2/C=C/C(=O)O)O)O1)O
MOL007131	0.8484	0.1516	0.7836	Radix Salviae	(2S,3S)-2-(3,4-dihydroxyphenyl)-7-hydroxy-4-[(E)-3-hydroxy-3-oxoprop-1-enyl]-2,3-dihydrobenzofuran-3-carboxylic acid	9841711	FALSE	c1(cc(ccc1O)C1C(c2c(c(ccc2/C=C/C(=O)O)O)O1)C(=O)O)O
MOL007132	0.9136	0.0864	0.8056	Herba Sarcandrae	(2R)-3-(3,4-dihydroxyphenyl)-2-[(Z)-3-(3,4-dihydroxyphenyl)acryloyl]oxy-propionic acid	9841799	FALSE	c1(ccc(cc1O)CC(OC(=O)/C=C\c1ccc(c(c1)O)O)C(=O)O)O
MOL007132	0.9136	0.0864	0.8056	Radix Salviae	(2R)-3-(3,4-dihydroxyphenyl)-2-[(Z)-3-(3,4-dihydroxyphenyl)acryloyl]oxy-propionic acid	9841799	FALSE	c1(ccc(cc1O)CC(OC(=O)/C=C\c1ccc(c(c1)O)O)C(=O)O)O

MOL007133	0.7213	0.2787	0.8301	Radix Salviae	salviacoccin	Not Available	FALSE	C1(=O)C2=CCC34C(C=CCC3(C2(CC(O1)c1cocc1)C)O)C(=O)OC4
MOL007134	0.9395	0.0605	0.9414	Salviae Chinensis Herba	danshensu	11600642	FALSE	c1(c(cc(cc1)CC(C(=O)O)O)O)O
MOL007134	0.9395	0.0605	0.9414	Radix Salviae	danshensu	11600642	FALSE	c1(c(cc(cc1)CC(C(=O)O)O)O)O
MOL007135	0.9156	0.0844	0.8116	Radix Salviae	salvianic acid c	Not Available	FALSE	c1(c(ccc(c1)CC(O)C(=O)OC(Cc1cc(c(cc1)O)O)C(=O)O)O)O
MOL007138	0.9051	0.0949	0.7593	Radix Salviae	salvianolic acid d	Not Available	FALSE	c1(c(ccc(c1CC(=O)O)/C=C/C(=O)OC(Cc1cc(c(cc1)O)O)C(=O)O)O)O
MOL007139	0.7088	0.2912	0.6079	Radix Salviae	salvianolic acid e	Not Available	FALSE	c1(ccc(cc1O)/C=C(\C(=O)OC(Cc1cc(c(cc1)O)O)C(=O)O)/c1c(c(ccc1/C=C/C(=O)OC(Cc1cc(c(cc1)O)O)C(=O)O)O)O)O
MOL007140	0.8782	0.1218	0.7447	Radix Salviae	(Z)-3-[2-[(E)-2-(3,4-dihydroxyphenyl)vinyl]-3,4-dihydroxy-phenyl]acrylic acid	11602092	FALSE	c1(c(ccc(c1/C=C/c1ccc(c(c1)O)O)/C=C/C(=O)O)O)O
MOL007141	0.8287	0.1713	0.7945	Radix Salviae	salvianolic acid g	Not Available	FALSE	c1c(c(c2c(c1)C=C1c3c(O2)c(ccc3CC(C1=O)C(=O)O)O)O)O
MOL007142	0.7800	0.2200	0.6321	Radix Salviae	salvianolic acid j	Not Available	FALSE	O1C(C(Oc2c1cc(cc2)/C=C/C(=O)OC(Cc1cc(c(cc1)O)O)C(=O)O)c1cc(c(cc1)O)O)C(=O)O
MOL007143	0.4827	0.5173	0.7964	Radix Salviae	salvilenone Ⅰ	Not Available	FALSE	C1CC(C2=C(C1)C1C(C=C2)C=C(C(=C1)O)C(=O)C)C)C
MOL007144	0.2621	0.7379	0.7586	Radix Salviae	salviol	13966147	FALSE	C1(CC(C2C(C1)(c1c(CC2)cc(c(c1)O)C(C)C)C)C)C)O
MOL007145	0.4614	0.5386	0.8076	Radix Salviae	salviolone	10355691	FALSE	c12c(ccc3C(CCCc13)(C)C)cc(c(=O)c(c2)O)C
MOL007146	0.3096	0.6904	0.8006	Radix Salviae	salvipisone	821448	FALSE	c1(c(ccc2c1C(=O)C(=C(C2=O)C(C)C)O)C)CCCC(=C)C

MOL007147	0.9158	0.0842	0.8335	Radix Salviae	methyl (1S,4aS,5R,7S,7aS)-5,7-dihydroxy-7-methyl-1-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4a,5,6,7a-tetrahydro-1H-cyclopenta[d]pyran-4-carboxylate	13892722	FALSE	C12C(C(=COC1OC1OC(C(C(C1O)O)O)CO)C(=O)OC)C(CC2(C)O)O
MOL007148	0.9469	0.0531	0.8078	Radix Salviae	shanzhiside methyl ester_qt	25026345	FALSE	C12C(C(=COC1O)C(=O)OC)C(CC2(C)O)O
MOL007149	0.2931	0.7069	0.7743	Radix Salviae	NSC 122421	94162	FALSE	C1CC(C2C(C1)(C1C(C(=O)C2)CC(C1)O)C(C)C)C(C)C
MOL007150	0.8239	0.1761	0.8399	Radix Salviae	(6S)-6-hydroxy-1-methyl-6-methylol-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-quinone	16730071	FALSE	C1(=O)C(=O)c2c(c3c1c1c(cc3)C(CCC1)(CO)O)occ2C
MOL007151	0.8383	0.1617	0.8244	Radix Salviae	Tanshindiol B	5321620	FALSE	C1C(C(c2c(C1)c1c(cc2)c2c(C(=O)C1=O)c(co2)C)(O)C)O
MOL007152	0.8383	0.1617	0.8244	Radix Salviae	Przewaquinone E	126072	FALSE	C1C(C(c2c(C1)c1c(cc2)c2c(C(=O)C1=O)c(co2)C)(O)C)O
MOL007153	0.7381	0.2619	0.7783	Radix Salviae	Tanshilactone	Not Available	FALSE	c1cc(c2c(c1)c1c(cc2)c2c(oc1=O)c(co2)C)C
MOL007154	0.6571	0.3429	0.8414	Peucedani Radix	tanshinone iia	164676	FALSE	c12c(c3c(cc1)c1c(C(=O)C3=O)c(co1)C)CCCC2(C)C
MOL007154	0.6571	0.3429	0.8414	Radix Salviae	tanshinone iia	164676	FALSE	c12c(c3c(cc1)c1c(C(=O)C3=O)c(co1)C)CCCC2(C)C
MOL007155	0.7925	0.2075	0.7335	Radix Salviae	(6S)-6-(hydroxymethyl)-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	9926694	FALSE	c12c(c3c(cc1)c1c(C(=O)C3=O)c(co1)C)CCCC2(C)CO

MOL007156	0.7255	0.2745	0.7690	Radix Salviae	tanshinone Ⅵ	Not Available	FALSE	C(CO)(C1=C(O)c2c(C(=O)C1=O)c1c(cc2)c(ccc1)C)C
MOL007157	0.7483	0.2517	0.7677	Radix Salviae	tanshinone i	114917	FALSE	c1c(c2c(cc1)c1c(cc2)c2c(C(=O)C1=O)c(co2)C)C
MOL007157	0.7483	0.2517	0.7677	Peucedani Radix	tanshinone i	114917	FALSE	c1c(c2c(cc1)c1c(cc2)c2c(C(=O)C1=O)c(co2)C)C
MOL007158	0.3012	0.6988	0.7449	Radix Salviae	Spirostan-3-ol, (3beta,5alpha, 25S)-	Not Available	FALSE	C1CC2(C(CC1O)CCC1C2CCC2(C1CC1C2C(C2(O1)CCC(CO2)C)C)C)C
MOL007158	0.3012	0.6988	0.7449	Solanum Nigrum Linn.	Spirostan-3-ol, (3beta,5alpha, 25S)-	Not Available	FALSE	C1CC2(C(CC1O)CCC1C2CCC2(C1CC1C2C(C2(O1)CCC(CO2)C)C)C)C
MOL007159	0.3953	0.6047	0.7329	Radix Salviae	uvaol	40469789	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(CO)CCC(C)C(C)C4C3=CCC21)C)O
MOL007159	0.3953	0.6047	0.7329	Folium Ilicis Cornutae	uvaol	40469789	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(CO)CCC(C)C(C)C4C3=CCC21)C)O
MOL007160	0.8268	0.1732	0.6586	Radix Salviae	β-cadinol	Not Available	FALSE	C1(C2C(C(CC1)C(C)C)CC(=C)CC2)(O)C
MOL007165	0.2228	0.7772	0.7144	Trichosanthes Kirilowii Maxim	10α-cucurbita-5,24-diene-3β-ol	Not Available	FALSE	C1CC(C(C2=CCC3C4(CCC(C(CCC=C(C)C)C)C4(C)CCC3(C12)C)C)(C)C)O
MOL007167	0.9211	0.0789	0.8324	Trichosanthes Kirilowii Maxim	2,2'bioxazolidine-3,3'-diethanol	Not Available	FALSE	C1OC(N(C1)CCO)C1OCCN1CCO
MOL007168	0.8978	0.1022	0.9319	Trichosanthes Kirilowii Maxim	Odhpca	69113	FALSE	c1(c(ccnc1)O)C(=O)O
MOL007169	0.9426	0.0574	0.9105	Trichosanthes Kirilowii Maxim	4-hydroxy-2-methoxybenzoic acid	12695575	FALSE	C(=O)(c1c(cc(cc1)O)OC)O
MOL007170	0.9517	0.0483	0.8746	Semiaquilegiae Radix	cirsiumaldehyde	12366272	FALSE	O(Cc1ccc(C=O)o1)Cc1ccc(C=O)o1
MOL007170	0.9517	0.0483	0.8746	Trichosanthes Kirilowii Maxim	cirsiumaldehyde	12366272	FALSE	O(Cc1ccc(C=O)o1)Cc1ccc(C=O)o1
MOL007170	0.9517	0.0483	0.8746	Lobeliae Chinensis Herba	cirsiumaldehyde	12366272	FALSE	O(Cc1ccc(C=O)o1)Cc1ccc(C=O)o1
MOL007170	0.9517	0.0483	0.8746	Momordicae Fructus	cirsiumaldehyde	12366272	FALSE	O(Cc1ccc(C=O)o1)Cc1ccc(C=O)o1
MOL007171	0.3557	0.6443	0.7786	Trichosanthes Kirilowii Maxim	5-dehydrokarounidiol	Not Available	FALSE	C1(CCC2(C(=CC=C3C4(C)CCC5(C)CCC(C)(CO)CC5C4(CC=C23)C)C1(C)C)C)O
MOL007172	0.3819	0.6181	0.8127	Trichosanthes Kirilowii Maxim	7-oxo-dihydrokaro-unidiol	Not Available	FALSE	C12(C(C3C(CC2)(CCC(C3)(CO)C)C)(CCC2=C1C(=O)CC1C2(CCC(C1(C)C)O)C)C)C

MOL007173	0.9346	0.0654	0.9639	Gynostemmae Pentaphylli Herba	beta-D-arabinopyranose	444173	FALSE	OC1C(O)C(O)C(O)CO1
MOL007173	0.9346	0.0654	0.9639	Trichosanthes Kirilowii Maxim	beta-D-arabinopyranose	444173	FALSE	OC1C(O)C(O)C(O)CO1
MOL007174	0.8243	0.1757	0.8434	Trichosanthes Kirilowii Maxim	5-hydroxy-2-(3-hydroxy-4-methoxyphenyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	11016019	FALSE	C1(C(C(OC(C1O)Oc1cc(c2c(c1)oc(cc2=O)c1ccc(c(c1)O)OC)O)CO)O)O
MOL007175	0.3831	0.6169	0.7153	Trichosanthes Kirilowii Maxim	karounidiol 3-o-benzoate	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC=C1C3(C)CCC4(C)CCC(C)(CO)CC4C3(CC=C21)C)C)OC(=O)c1ccccc1
MOL007176	0.9346	0.0654	0.9639	Trichosanthes Kirilowii Maxim	ARA	439731	FALSE	OC1C(O)C(O)C(O)CO1
MOL007177	0.9011	0.0989	0.9677	Silybum Marianum	FCY	6419722	FALSE	C(=O)(C(N)CS)O
MOL007177	0.9011	0.0989	0.9677	Trichosanthes Kirilowii Maxim	FCY	6419722	FALSE	C(=O)(C(N)CS)O
MOL007177	0.9011	0.0989	0.9677	Bamusaeconcretiosilicea	FCY	6419722	FALSE	C(=O)(C(N)CS)O
MOL007178	0.9339	0.0661	0.9658	Trichosanthes Kirilowii Maxim	1,4-D-Galactonolactone	97165	FALSE	C1(=O)C(O)C(O)C(C(O)CO)O1
MOL007179	0.4112	0.5888	0.6385	Ginkgo Folium	Linolenic acid ethyl ester	5367460	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)OCC
MOL007179	0.4112	0.5888	0.6385	Campsis Flos	Linolenic acid ethyl ester	5367460	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)OCC
MOL007179	0.4112	0.5888	0.6385	Trichosanthes Kirilowii Maxim	Linolenic acid ethyl ester	5367460	FALSE	C(=O)(CCCCCCC/C=C\C/C=C\C/C=C\CC)OCC
MOL007181	0.7672	0.2328	0.6482	Trichosanthes Kirilowii Maxim	Punicic acid	5281126	FALSE	C(=O)(CCCCCCC/C=C\C=C\C=C/CCCC)O

MOL007182	0.8642	0.1358	0.8234	Trichosanthes Kirilowii Maxim	5-hydroxy-2-[4-hydroxy-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]-7-methoxychromen-4-one	10479460	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)O)OC1C(O)C(O)C(O)C(O1)CO)O)OC
MOL007183	0.9043	0.0957	0.9005	Trichosanthes Kirilowii Maxim	dibutyl (2R)-2-hydroxybutanedioate	10467092	FALSE	C(C(=O)OCCCC)C(O)C(=O)OCCCC
MOL007184	0.9188	0.0812	0.9747	Trichosanthes Kirilowii Maxim	[(2R,5S)-5-(hydroxymethyl)oxolan-2-yl]methanol	12886254	FALSE	C1(OC(CC1)CO)CO
MOL007185	0.3821	0.6179	0.7822	Trichosanthes Kirilowii Maxim	isokarounidiol	Not Available	FALSE	C1(CCC2(C(C1(C)C)C=CC1=C2CCC2(C1(C)CCC1(C)CCC(C)(CO)CC21)C)C)O
MOL007186	0.3799	0.6201	0.7894	Momordicae Semen	Karounidiol	159490	FALSE	C12(C(C3C(CC2)(CCC(C3)(CO)C)C)(CC=C2C1=CCC1C2(CCC(C1(C)C)O)C)C)C
MOL007186	0.3799	0.6201	0.7894	Trichosanthes Kirilowii Maxim	Karounidiol	159490	FALSE	C12(C(C3C(CC2)(CCC(C3)(CO)C)C)(CC=C2C1=CCC1C2(CCC(C1(C)C)O)C)C)C
MOL007188	0.9261	0.0739	0.7925	Saxifraga Stolonifera	quercetin-5-o-β-d-glucoside	52946987	FALSE	c1(c(O)c(=O)c2c(cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL007189	0.9076	0.0924	0.9719	Saxifraga Stolonifera	MESACONATE	638129	FALSE	C(=C\C(=O)O)(/C(=O)O)\C
MOL007192	0.9072	0.0928	0.8001	Folium Nelumbinis	quercetin-3-o-beta-d-glucuronide	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1C(C(C(C(O1)C(=O)O)O)O)O)c1ccc(c(c1)O)O)O)O
MOL007192	0.9072	0.0928	0.8001	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	quercetin-3-o-beta-d-glucuronide	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1C(C(C(C(O1)C(=O)O)O)O)O)c1ccc(c(c1)O)O)O)O
MOL007193	0.9072	0.0928	0.8001	Folium Nelumbinis	quercetin,3-o-b-d-glucuronide	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)C(=O)O)c1cc(O)c(O)cc1
MOL007193	0.9072	0.0928	0.8001	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	quercetin,3-o-b-d-glucuronide	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)C(=O)O)c1cc(O)c(O)cc1
MOL007194	0.9140	0.0860	0.8280	Folium Nelumbinis	kaempferol,3-glucoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1

MOL007196	0.9140	0.0860	0.8280	Folium Nelumbinis	kaempferol,3-galactoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL007197	0.8967	0.1033	0.8608	Linderae Radix	DFA	11487	FALSE	c1(Nc2ccccc2)ccccc1
MOL007197	0.8967	0.1033	0.8608	Typhonii Rhizoma	DFA	11487	FALSE	c1(Nc2ccccc2)ccccc1
MOL007197	0.8967	0.1033	0.8608	Folium Nelumbinis	DFA	11487	FALSE	c1(Nc2ccccc2)ccccc1
MOL007198	0.9136	0.0864	0.9606	Folium Nelumbinis	GCO	10690	FALSE	C(C(C(CO)O)O)(C(C(=O)O)O)O
MOL007199	0.9223	0.0777	0.9631	Folium Nelumbinis	Pentenal	5364752	FALSE	C(=C\C=O)/CC
MOL007200	0.6964	0.3036	0.6145	Folium Nelumbinis	Decylcyclohexane	15713	FALSE	C1(CCCCCCCCCC)CCCCC1
MOL007201	0.7414	0.2586	0.7281	Folium Nelumbinis	brahmic acid	51531966	FALSE	C1(C(CC2(C(C1(CO)C)C(CC1(C)C3(C)CCC4(C(=O)O)CCC(C)C(C)C4C3=CCC21)O)C)O)O
MOL007201	0.7414	0.2586	0.7281	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	brahmic acid	51531966	FALSE	C1(C(CC2(C(C1(CO)C)C(CC1(C)C3(C)CCC4(C(=O)O)CCC(C)C(C)C4C3=CCC21)O)C)O)O
MOL007202	0.9250	0.0750	0.9341	Folium Nelumbinis	2-Nonynoic acid	74611	FALSE	C(CCCCC)C#CC(=O)O
MOL007206	0.5692	0.4308	0.7435	Nelumbinis Plumula	Armepavine	442169	FALSE	O(C)c1c(OC)cc2c(c1)CCN(C2Cc1ccc(cc1)O)C
MOL007206	0.5692	0.4308	0.7435	Folium Nelumbinis	Armepavine	442169	FALSE	O(C)c1c(OC)cc2c(c1)CCN(C2Cc1ccc(cc1)O)C
MOL007207	0.8117	0.1883	0.8275	Folium Nelumbinis	Machiline	440989	FALSE	C1(NCCc2cc(c(cc12)O)OC)Cc1ccc(cc1)O
MOL007208	0.8787	0.1213	0.8887	Folium Nelumbinis	3-Decyne	75425	FALSE	C(CC#CCC)CCCC
MOL007209	0.9644	0.0356	0.8360	Folium Nelumbinis	adamantane	9238	FALSE	C12CC3CC(C1)CC(C2)C3
MOL007209	0.9644	0.0356	0.8360	Litchi Semen	adamantane	9238	FALSE	C12CC3CC(C1)CC(C2)C3
MOL007210	0.6987	0.3013	0.7929	Folium Nelumbinis	o-Nornuciferine	197017	FALSE	N1(CCc2c3c(c4c(CC13)cccc4)c(c(c2)O)OC)C
MOL007211	0.9136	0.0864	0.9606	Sinapis Semen	(2S,3S,4S,5R)-2,3,4,5,6-pentahydroxyhexanoic acid	3246058	FALSE	C(C(C(C(C(C(C(=O)O)O)O)O)O)O)O
MOL007211	0.9136	0.0864	0.9606	Folium Nelumbinis	(2S,3S,4S,5R)-2,3,4,5,6-pentahydroxyhexanoic acid	3246058	FALSE	C(C(C(C(C(C(C(=O)O)O)O)O)O)O)O
MOL007212	0.8229	0.1771	0.8044	Folium Nelumbinis	dehydroroemerine	Not Available	FALSE	N1CCc2c3c(c4c(cc13)cccc4)c1c(c2)OCO1
MOL007213	0.5920	0.4080	0.7436	Jujubae Fructus	Nuciferin	10146	FALSE	c12c3C(Cc4c1cccc4)N(CCc3cc(c2OC)OC)C
MOL007213	0.5920	0.4080	0.7436	Nelumbinis Plumula	Nuciferin	10146	FALSE	c12c3C(Cc4c1cccc4)N(CCc3cc(c2OC)OC)C
MOL007213	0.5920	0.4080	0.7436	Folium Nelumbinis	Nuciferin	10146	FALSE	c12c3C(Cc4c1cccc4)N(CCc3cc(c2OC)OC)C
MOL007214	0.9461	0.0539	0.8873	Folium Nelumbinis	(+)-Leucocyanidin	155206	FALSE	C1(C(C(c2c(O1)cc(cc2O)O)O)O)c1cc(c(cc1)O)O
MOL007215	0.9292	0.0708	0.8289	Folium Nelumbinis	5'-o-methyladenosine	Not Available	FALSE	c1(ncnc2c1ncn2C1C(C(C(O1)COC)O)O)N

MOL007216	0.7248	0.2752	0.8317	Folium Nelumbinis	n-nornuciferine	12313579	FALSE	N1CCc2c3c(c4c(CC13)cccc4)c(c(c2)OC)OC
MOL007217	0.9474	0.0526	0.8819	Folium Nelumbinis	leucodelphinidin	44563331	FALSE	C1(C(C(c2c(O1)cc(cc2O)O)O)O)c1cc(c(c(c1)O)O)O
MOL007218	0.7947	0.2053	0.8909	Folium Nelumbinis	Remerin	Not Available	FALSE	c12c3C(Cc4c2cccc4)N(CCc3cc2c1OCO2)C
MOL007219	0.9140	0.0860	0.8280	Folium Nelumbinis	kaempferol 3-o-bata-d-galactopyranoside	Not Available	FALSE	c1c(c2c(cc1O)oc(c(c2=O)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)O)O
MOL007220	0.8533	0.1467	0.6768	Folium Nelumbinis	beta -cyclogeraniol diglycoside	Not Available	FALSE	C1(C(C(C(OC1CO)OCC1C(C(C(C(O1)OCC1=C(C)CCCC1(C)C)O)O)O)O)O)O
MOL007221	0.9597	0.0403	0.9262	Folium Nelumbinis	.beta.-Cyclogeraniol	111664	FALSE	OCC1=C(C)CCCC1(C)C
MOL007222	0.8914	0.1086	0.9469	Folium Nelumbinis	RNG	241	FALSE	c1ccccc1
MOL007222	0.8914	0.1086	0.9469	Benzoinum	RNG	241	FALSE	c1ccccc1
MOL007223	0.9072	0.0928	0.8001	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	quercetin-3-o-glucuronide	Not Available	FALSE	Oc1cc(c2c(c1)oc(c(c2=O)OC1C(C(C(C(O1)C(=O)O)O)O)O)c1ccc(c(c1)O)O)O
MOL007223	0.9072	0.0928	0.8001	Folium Nelumbinis	quercetin-3-o-glucuronide	Not Available	FALSE	Oc1cc(c2c(c1)oc(c(c2=O)OC1C(C(C(C(O1)C(=O)O)O)O)O)c1ccc(c(c1)O)O)O
MOL007224	0.9280	0.0720	0.7859	Folium Nelumbinis	myricetin-3-o-glucopyranoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(c(c(c1)O)O)O
MOL007226	0.6370	0.3630	0.7518	Folium Nelumbinis	dehydronuciferine	Not Available	FALSE	N1(CCc2c3c(c4c(cc13)cccc4)c(c(c2)OC)OC)C
MOL007227	0.9280	0.0720	0.7859	Folium Nelumbinis	myricetin-3-o-beta-d-glucopyranoside	Not Available	FALSE	c1c(cc(c2c1oc(c(c2=O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(c(c1)O)O)O)O)O
MOL007227	0.9280	0.0720	0.7859	Astragali Cpmplanatisemen	myricetin-3-o-beta-d-glucopyranoside	Not Available	FALSE	c1c(cc(c2c1oc(c(c2=O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(c(c1)O)O)O)O)O
MOL007228	0.9140	0.0860	0.8280	Astragali Cpmplanatisemen	kaempferol-3-o-beta-d-glucoside	Not Available	FALSE	c1c(cc(c2c1oc(c(c2=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)O)O
MOL007228	0.9140	0.0860	0.8280	Cuscutae Semen	kaempferol-3-o-beta-d-glucoside	Not Available	FALSE	c1c(cc(c2c1oc(c(c2=O)OC1OC(C(C(C1O)O)O)CO)c1ccc(cc1)O)O)O

MOL007228	0.9140	0.0860	0.8280	Folium Nelumbinis	kaempferol-3-o-beta-d-glucoside	Not Available	FALSE	c1c(cc(c2c1oc(c(c2=O)OC1OC(C(C(C1O)O)O)O)CO)c1ccc(cc1)O)O)O
MOL007229	0.8923	0.1077	0.9451	Folium Nelumbinis	Cyclooctene	638079	FALSE	C1=CCCCCCC1
MOL007230	0.9242	0.0758	0.9441	Calyx Seu Fructus Physalis	Malonic ester	7761	FALSE	C(=O)(CC(=O)OCC)OCC
MOL007231	0.2106	0.7894	0.6090	Calyx Seu Fructus Physalis	gramisterol	Not Available	FALSE	C1CC(C(C2C1(C1C(=CC2)C2C(CC1)(C(CC2)C(CCC(=C)C(C)C)C)C)C)C)O
MOL007233	0.9302	0.0698	0.9332	Calyx Seu Fructus Physalis	Methyl nonylate	15606	FALSE	C(CCC(=O)OC)CCCCC
MOL007233	0.9302	0.0698	0.9332	Perillae Fructus	Methyl nonylate	15606	FALSE	C(CCC(=O)OC)CCCCC
MOL007233	0.9302	0.0698	0.9332	Broussonetiae Fructus	Methyl nonylate	15606	FALSE	C(CCC(=O)OC)CCCCC
MOL007233	0.9302	0.0698	0.9332	Platycladi Semen	Methyl nonylate	15606	FALSE	C(CCC(=O)OC)CCCCC
MOL007233	0.9302	0.0698	0.9332	Sterculiae Lychnophorae Semen	Methyl nonylate	15606	FALSE	C(CCC(=O)OC)CCCCC
MOL007233	0.9302	0.0698	0.9332	Hoveniae Dulcis Semen	Methyl nonylate	15606	FALSE	C(CCC(=O)OC)CCCCC
MOL007234	0.8701	0.1299	0.8398	Calyx Seu Fructus Physalis	Isopropyl caprate	16833	FALSE	C(=O)(CCCCCCCCC)OC(C)C
MOL007235	0.8331	0.1669	0.6789	Calyx Seu Fructus Physalis	physalin a	Not Available	FALSE	O1C23C4C5(CC(OC(=O)C5=C)C2(OC(=O)C3(O)CCC2C(C1(O)C4=O)C(O)C=C1C2(C)C(=O)C=CC1)C
MOL007236	0.8761	0.1239	0.6195	Calyx Seu Fructus Physalis	physalin d	Not Available	FALSE	O1C23C4C5(CC6OC(=O)C5COC1(C1C(C5(C(O)(C(O)C1)CC=CC5=O)C)CCC3(O)C(=O)OC26C)C4=O
MOL007237	0.8421	0.1579	0.6679	Calyx Seu Fructus Physalis	physalin o	Not Available	FALSE	O1C23C4C5(CC(OC(=O)C5C)C2(OC(=O)C3(O)CCC2C(C1(O)C4=O)C(O)C=C1C2(C)C(=O)C=CC1)C)
MOL007238	0.7817	0.2183	0.6419	Calyx Seu Fructus Physalis	physalin b	Not Available	FALSE	O1C23C4C5(CC6OC(=O)C5COC1(C4=O)C1C(CCC3(O)C(=O)OC26C)C2(C(=CC1)CC=CC2=O)C)C
MOL007239	0.7528	0.2472	0.7106	Folium Ilicis Cornutae	cornutaside c	Not Available	FALSE	C1C(CCC2(CCC3(C4(CCC5C(C(CCC5(C4CC=C3C12)C)OC1C(C(C(CO1)O)O)O)(C)C)C)C)C(=O)OC1C(C(C(C(O1)CO)O)O)O)(C)CO
MOL007240	0.7470	0.2530	0.8231	Folium Ilicis Cornutae	cornutaside c_qt	Not Available	FALSE	C1C(CCC2(CCC3(C4(CCC5C(C(CCC5(C4CC=C3C12)C)O)(C)C)C)C)C(=O)O)(C)CO
MOL007241	0.6685	0.3315	0.7340	Folium Ilicis Cornutae	cornutaside a	Not Available	FALSE	C1(C(CCC2(CCC3(C4(CCC5C(C(CCC5(C4CC=C3C12)C)OC1C(C(C(CO1)O)O)OC(=O)C)(C)C)C)C)C(=O)OC1C(C(C(C(O1)CO)O)O)O)C)(C)O
MOL007242	0.6291	0.3709	0.7240	Folium Ilicis Cornutae	cornutaside a	Not Available	FALSE	C1(C(CCC2(CCC3(C4(CCC5C(C(CCC5(C4CC=C3C12)C)OC1C(C(C(CO1)O)O)OC(=O)C)(C)C)C)C)C(=O)O)C)(C)O
MOL007243	0.8943	0.1057	0.7320	Linderae Radix	santalol	12315259	FALSE	C1(C2CC(C1=C)CC2)(CC/C=C(/CO)\C)C
MOL007243	0.8943	0.1057	0.7320	Cayratiae Japonicae Herba	santalol	12315259	FALSE	C1(C2CC(C1=C)CC2)(CC/C=C(/CO)\C)C
MOL007243	0.8943	0.1057	0.7320	Folium Ilicis Cornutae	santalol	12315259	FALSE	C1(C2CC(C1=C)CC2)(CC/C=C(/CO)\C)C

MOL007243	0.8943	0.1057	0.7320	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	santalol	12315259	FALSE	C1(C2CC(C1=C)CC2)(CC/C=C(/CO)\C)C
MOL007243	0.8943	0.1057	0.7320	Santalum Album L.	santalol	12315259	FALSE	C1(C2CC(C1=C)CC2)(CC/C=C(/CO)\C)C
MOL007244	0.8343	0.1657	0.7250	Folium Ilicis Cornutae	3,4-di-o-caffeoylquinic acid	Not Available	FALSE	C1(CC(C(C(C1)O)OC(=O)/C=C\c1cc(cc(c1)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)(C(=O)O)O
MOL007245	0.9147	0.0853	0.8193	Folium Ilicis Cornutae	3-Methylkempferol	5280862	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC)c1ccc(cc1)O
MOL007245	0.9147	0.0853	0.8193	Gossampiniflos	3-Methylkempferol	5280862	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC)c1ccc(cc1)O
MOL007246	0.7472	0.2528	0.7763	Folium Ilicis Cornutae	2-hydroxy ursolicacid	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(O)C(CC5(C4CC=C3C2C(C(CC1)C)C)C)O)(C)C)C)C)O
MOL007247	0.7557	0.2443	0.8303	Folium Ilicis Cornutae	23-hydroxyursolic acid	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(O)CCC5(C4CC=C3C2C(C(CC1)C)C)C)(CO)C)C)C)O
MOL007247	0.7557	0.2443	0.8303	Campsis Flos	23-hydroxyursolic acid	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(O)CCC5(C4CC=C3C2C(C(CC1)C)C)C)(CO)C)C)C)O
MOL007248	0.6915	0.3085	0.7559	Folium Ilicis Cornutae	27-o-(z)-coumaroyloxy ursolicacid	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(O)CCC5(C4CC=C3C2C(C(CC1)C)C)C)(C)C)C)C)COC(=O)/C=C/c1c(cccc1)O)O
MOL007249	0.3424	0.6576	0.7567	Folium Ilicis Cornutae	3-Hydroxynorlupen-2-one	490365	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C(=O)C)C4C3CCC21)C)O
MOL007250	0.3394	0.6606	0.8099	Folium Ilicis Cornutae	3-beta-hydroxylup-20(29)-en-30-al	10071968	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C(=C)C=O)C4C3CCC21)C)O
MOL007251	0.6252	0.3748	0.7540	Folium Ilicis Cornutae	pedunculoside	Not Available	FALSE	C1(CCC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C(=O)OC5C(O)C(O)C(O)C(O5)CO)CCC(C)(C)(C4C3=CCC21)O)C)O
MOL007252	0.7552	0.2448	0.7883	Folium Ilicis Cornutae	pedunculoside_qt	Not Available	FALSE	C1(CCC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C)(C)(C4C3=CCC21)O)C)O
MOL007253	0.7423	0.2577	0.7468	Peucedani Radix	Asiatic acid	119034	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(C(C1)O)O)(CO)C)C)C1C(CC3)(CCC(C1C)C)C(=O)O)C)C
MOL007253	0.7423	0.2577	0.7468	Folium Ilicis Cornutae	Asiatic acid	119034	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(C(C1)O)O)(CO)C)C)C1C(CC3)(CCC(C1C)C)C(=O)O)C)C
MOL007253	0.7423	0.2577	0.7468	Humulus Scandens (Lour.) Merr.	Asiatic acid	119034	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(C(C1)O)O)(CO)C)C)C1C(CC3)(CCC(C1C)C)C(=O)O)C)C
MOL007253	0.7423	0.2577	0.7468	Potentillae Chinensis Herba	Asiatic acid	119034	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(C(C1)O)O)(CO)C)C)C1C(CC3)(CCC(C1C)C)C(=O)O)C)C

MOL007253	0.7423	0.2577	0.7468	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	Asiatic acid	119034	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(C(C1)O)O)(CO)C)C)C1C(CC3)(CCC(C1C)C)C(=O)O)C)C
MOL007254	0.7408	0.2592	0.7565	Campsis Flos	Arjunolic acid	73641	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(CO)C)O)O
MOL007254	0.7408	0.2592	0.7565	Akebiae Frucyus	Arjunolic acid	73641	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(CO)C)O)O
MOL007254	0.7408	0.2592	0.7565	Folium Ilicis Cornutae	Arjunolic acid	73641	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(CO)C)O)O
MOL007254	0.7408	0.2592	0.7565	Chebulae Fructus	Arjunolic acid	73641	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(CO)C)O)O
MOL007255	0.8330	0.1670	0.6860	Folium Ilicis Cornutae	(-)-Drimenol	3080551	FALSE	C12(C(CC=C(C1CO)C)C(CCC2)(C)C)C
MOL007255	0.8330	0.1670	0.6860	Ganoderma	(-)-Drimenol	3080551	FALSE	C12(C(CC=C(C1CO)C)C(CCC2)(C)C)C
MOL007256	0.8443	0.1557	0.7858	Folium Ilicis Cornutae	Myristamide	69492	FALSE	C(CCCCCCCC)CCCCC(=O)N
MOL007257	0.7674	0.2326	0.8339	Folium Ilicis Cornutae	ilexsideii	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)OC5C(O)C(O)C(O)C(O5)CO)CCC(C)C(C)(C4C3=CCC21)O)C)OC1C(OC2C(O)C(O)C(O)C(O2)CO)C(O)CO)CO1
MOL007258	0.7645	0.2355	0.8339	Folium Ilicis Cornutae	ilexoside ii	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C)C1OCC(O)C(OC2OC(C(O)C(O)C2O)CO)C1O
MOL007259	0.7612	0.2388	0.8406	Folium Ilicis Cornutae	ilexoside ii_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(C(=O)O)(CC4)CCC(C3(O)C)C)C)(CC2)C)(CC1)C)(C)C
MOL007260	0.8977	0.1023	0.8170	Viscum Angulatum Heyne	Isorhamnetin-3-mono-beta-D-glucoside	5318645	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(OC)c(O)cc1)CO
MOL007260	0.8977	0.1023	0.8170	Radix Bupleuri	Isorhamnetin-3-mono-beta-D-glucoside	5318645	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(OC)c(O)cc1)CO
MOL007260	0.8977	0.1023	0.8170	Artemisiae Scopariae Herba	Isorhamnetin-3-mono-beta-D-glucoside	5318645	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(OC)c(O)cc1)CO
MOL007260	0.8977	0.1023	0.8170	Ginkgo Folium	Isorhamnetin-3-mono-beta-D-glucoside	5318645	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(OC)c(O)cc1)CO
MOL007260	0.8977	0.1023	0.8170	Chrysanthemi Flos	Isorhamnetin-3-mono-beta-D-glucoside	5318645	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(OC)c(O)cc1)CO
MOL007260	0.8977	0.1023	0.8170	Hippophae Fructus	Isorhamnetin-3-mono-beta-D-glucoside	5318645	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(OC)c(O)cc1)CO
MOL007260	0.8977	0.1023	0.8170	Folium Ilicis Cornutae	Isorhamnetin-3-mono-beta-D-glucoside	5318645	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(OC)c(O)cc1)CO

MOL007260	0.8977	0.1023	0.8170	Calendula Officinalis	Isorhamnetin-3-mono-beta-D-glucoside	5318645	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(OC)c(O)cc1)CO
MOL007261	0.5303	0.4697	0.6409	Folium Ilicis Cornutae	neolignan	Not Available	FALSE	o1c(c(c2c1c(cc(c2)/C=C/C(=O)OC)OC)CO)c1cc(c(cc1)O)OC
MOL007262	0.9435	0.0565	0.9699	Trollius Chinensis	Methyl phenylacetate	7559	FALSE	c1(CC(=O)OC)ccccc1
MOL007262	0.9435	0.0565	0.9699	Caryophylliflos	Methyl phenylacetate	7559	FALSE	c1(CC(=O)OC)ccccc1
MOL007262	0.9435	0.0565	0.9699	Perillae Fructus	Methyl phenylacetate	7559	FALSE	c1(CC(=O)OC)ccccc1
MOL007262	0.9435	0.0565	0.9699	Sterculiae Lychnophorae Semen	Methyl phenylacetate	7559	FALSE	c1(CC(=O)OC)ccccc1
MOL007263	0.9379	0.0621	0.9665	Ranunculi Ternati Radix	Methyl succinate	7820	FALSE	C(=O)(CCC(=O)OC)OC
MOL007263	0.9379	0.0621	0.9665	Trollius Chinensis	Methyl succinate	7820	FALSE	C(=O)(CCC(=O)OC)OC
MOL007264	0.8238	0.1762	0.7629	Trollius Chinensis	agnuside	Not Available	FALSE	C12C(OC3OC(C(C(C3O)O)O)CO)OC=CC1C(C=C2COC(=O)c1ccc(cc1)O)O
MOL007264	0.8238	0.1762	0.7629	Viticis Fructus	agnuside	Not Available	FALSE	C12C(OC3OC(C(C(C3O)O)O)CO)OC=CC1C(C=C2COC(=O)c1ccc(cc1)O)O
MOL007265	0.8676	0.1324	0.7793	Viticis Fructus	agnusid_qt	Not Available	FALSE	C12C(O)OC=CC1C(C=C2COC(=O)c1ccc(cc1)O)O
MOL007265	0.8676	0.1324	0.7793	Trollius Chinensis	agnusid_qt	Not Available	FALSE	C12C(O)OC=CC1C(C=C2COC(=O)c1ccc(cc1)O)O
MOL007266	0.7523	0.2477	0.6700	Trollius Chinensis	C10328	Not Available	FALSE	C12C3CCN1CC=C2COC(=O)C(C(C/C(=C\C)/C(=O)O3)C)(C)O
MOL007267	0.9193	0.0807	0.8449	Trollius Chinensis	methyl 3,4-dihydroxy-5-(3,4,5-trihydroxybenzoyl)oxybenzoate	10131824	FALSE	COC(=O)c1cc(OC(=O)c2cc(c(c(c2)O)O)O)c(c(c1)O)O
MOL007268	0.9391	0.0609	0.9003	Trollius Chinensis	Proglobeflowery acid	132759	FALSE	O(c1c(O)c(CC=C(C)C)cc(c1)C(=O)O)C
MOL007269	0.9490	0.0510	0.9605	Trollius Chinensis	Veratramide	73705	FALSE	c1(c(ccc(c1)C(=O)N)OC)OC
MOL007270	0.9364	0.0636	0.9444	Perillae Fructus	DIMETHYL SUBERATE	15611	FALSE	C(=O)(CCCCCCC(=O)OC)OC
MOL007270	0.9364	0.0636	0.9444	Trollius Chinensis	DIMETHYL SUBERATE	15611	FALSE	C(=O)(CCCCCCC(=O)OC)OC
MOL007271	0.9654	0.0346	0.9382	Trollius Chinensis	Methyl veratrate	16522	FALSE	c1(c(ccc(c1)C(=O)OC)OC)OC
MOL007272	0.9503	0.0497	0.9724	Figwort Root	Homovanillyl alcohol	16928	FALSE	c1(cc(ccc1O)CCO)OC

MOL007272	0.9503	0.0497	0.9724	Trollius Chinensis	Homovanillyl alcohol	16928	FALSE	c1(cc(ccc1O)CCO)OC
MOL007273	0.9523	0.0477	0.9057	Trollius Chinensis	Globeflowery acid	6451636	FALSE	O1C(CCc2c1c(OC)cc(c2)C(=O)O)(C)C
MOL007274	0.8121	0.1879	0.9002	Artemisiae Scopariae Herba	Skrofulein	188323	FALSE	c12c(c(c(c(c2)OC)OC)O)c(=O)cc(o1)c1ccc(cc1)O
MOL007274	0.8121	0.1879	0.9002	Abrus Precatorius L.	Skrofulein	188323	FALSE	c12c(c(c(c(c2)OC)OC)O)c(=O)cc(o1)c1ccc(cc1)O
MOL007274	0.8121	0.1879	0.9002	Trollius Chinensis	Skrofulein	188323	FALSE	c12c(c(c(c(c2)OC)OC)O)c(=O)cc(o1)c1ccc(cc1)O
MOL007274	0.8121	0.1879	0.9002	Viticis Fructus	Skrofulein	188323	FALSE	c12c(c(c(c(c2)OC)OC)O)c(=O)cc(o1)c1ccc(cc1)O
MOL007274	0.8121	0.1879	0.9002	Artemisia Annua L.	Skrofulein	188323	FALSE	c12c(c(c(c(c2)OC)OC)O)c(=O)cc(o1)c1ccc(cc1)O
MOL007275	0.9426	0.0574	0.9606	Vigna Radiata	BDF	24310	FALSE	C1(C(C(C(CO1)O)O)O)(CO)O
MOL007275	0.9426	0.0574	0.9606	Trollius Chinensis	BDF	24310	FALSE	C1(C(C(C(CO1)O)O)O)(CO)O
MOL007276	0.9461	0.0539	0.9466	Ardisiae Japonicae Herba	VERATRIC ACID	7121	FALSE	c1(c(ccc(c1)C(=O)O)OC)OC
MOL007276	0.9461	0.0539	0.9466	Trollius Chinensis	VERATRIC ACID	7121	FALSE	c1(c(ccc(c1)C(=O)O)OC)OC
MOL007277	0.9088	0.0912	0.9694	Trollius Chinensis	salicylaldoxime	Not Available	FALSE	c1(c(cccc1)O)/C=N/O
MOL007279	0.7022	0.2978	0.7572	Rhizoma Fagopyri Cymosi	procyanidin,b	13269088	FALSE	c1(cc(c2c(c1)OC(C(C2c1c(cc(c2c1OC(C(C2)O)c1cc(c(cc1)O)O)O)O)O)c1cc(c(cc1)O)O)O)O
MOL007280	0.8986	0.1014	0.9053	Rhizoma Fagopyri Cymosi	3-methylquercetin	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC)c1cc(O)c(O)cc1
MOL007281	0.8777	0.1223	0.6887	Rhizoma Fagopyri Cymosi	1,3-dimethoxy-2-o-beta-xylo-pyranosyl-5-o-beta-glucopyranosyl-benzene	Not Available	FALSE	C1(C(C(C(C(O1)Oc1cc(c(c(c1)OC)OC1C(OCC(C1O)O)OC)OC)O)O)O)CO
MOL007282	0.9312	0.0688	0.7724	Rhizoma Fagopyri Cymosi	1,3-dimethoxy-2-o-beta-xylo-pyranosyl-5-o-beta-glucopyranosyl-benzene_qt	Not Available	FALSE	Oc1cc(c(c(c1)OC)OC1C(OCC(C1O)O)OC)OC
MOL007283	0.7022	0.2978	0.7572	Rhizoma Fagopyri Cymosi	procyanidin b2	122738	FALSE	c1(cc(c2c(c1)OC(C(C2c1c(cc(c2c1OC(C(C2)O)c1cc(c(cc1)O)O)O)O)O)c1cc(c(cc1)O)O)O)O
MOL007283	0.7022	0.2978	0.7572	Eriobotryae Folium	procyanidin b2	122738	FALSE	c1(cc(c2c(c1)OC(C(C2c1c(cc(c2c1OC(C(C2)O)c1cc(c(cc1)O)O)O)O)O)c1cc(c(cc1)O)O)O)O
MOL007283	0.7022	0.2978	0.7572	Drynariae Rhizoma	procyanidin b2	122738	FALSE	c1(cc(c2c(c1)OC(C(C2c1c(cc(c2c1OC(C(C2)O)c1cc(c(cc1)O)O)O)O)O)c1cc(c(cc1)O)O)O)O

MOL007284	0.7022	0.2978	0.7572	Rhizoma Fagopyri Cymosi	Procyanidin B4	147299	FALSE	c1(cc(c2c(c1)OC(C(C2c1c(cc(c2c1OC(C(C2)O)c1ccc(c(c1)O)O)O)O)O)c1ccc(c(c1)O)O)O)O
MOL007285	0.7347	0.2653	0.7970	Rhizoma Fagopyri Cymosi	Procyanidol C1	169853	FALSE	c1(cc(c2c(c1)OC(C(C2c1c(cc(c2c1OC(C(C2c1c(cc(c2c1OC(C(C2)O)c1ccc(c(c1)O)O)O)O)O)c1ccc(c(c1)O)O)O)O)O)c1ccc(c(c1)O)O)O)O
MOL007286	0.7347	0.2653	0.7970	Rhizoma Fagopyri Cymosi	(2R,3S,4R)-2-(3,4-dihydroxyphenyl)-4-[(2R,3R)-2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxychroman-8-yl]-8-[(2R,3S,4S)-2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxychroman-4-yl]chroman-3,5,7-triol	21676343	FALSE	c1(cc(c2c(c1)OC(C(C2c1c(cc(c2c1OC(C(C2c1c(cc(c2c1OC(C(C2)O)c1ccc(c(c1)O)O)O)O)O)c1ccc(c(c1)O)O)O)O)O)c1ccc(c(c1)O)O)O)O
MOL007287	0.8828	0.1172	0.8683	Rhizoma Fagopyri Cymosi	emodin-8-o-beta-d-glucopyranoside	Not Available	FALSE	c1(c(cc2c(c1)C(=O)c1c(C2=O)cc(cc1O)C)O)OC1C(O)C(O)C(O)C(O1)CO
MOL007288	0.8566	0.1434	0.8479	Rhizoma Fagopyri Cymosi	emodin-8-o-beta-d-glucopyranoside_qt	Not Available	FALSE	c1(c(cc2c(c1)C(=O)c1c(C2=O)cc(cc1O)C)O)O
MOL007289	0.8953	0.1047	0.7932	Rhizoma Fagopyri Cymosi	3-methyl-gossypetin,8-o-beta-d-glucopyranoside	Not Available	FALSE	c1(cc(c2c(c1OC1OC(C(C(C1O)O)O)CO)oc(c(c2=O)OC)c1cc(c(cc1)O)O)O)O
MOL007290	0.9220	0.0780	0.8954	Rhizoma Fagopyri Cymosi	2-(3,4-dihydroxyphenyl)-5,7,8-trihydroxy-3-methoxy-chromone	5386958	FALSE	c1(cc(c2c(c1O)oc(c(c2=O)OC)c1cc(c(cc1)O)O)O)O

MOL007291	0.3383	0.6617	0.6951	Rhizoma Fagopyri Cymosi	Hecogenin	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C2C(C(=O)C1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)O
MOL007291	0.3383	0.6617	0.6951	Tribulifructus	Hecogenin	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C2C(C(=O)C1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)O
MOL007292	0.3425	0.6575	0.7122	Rhizoma Fagopyri Cymosi	lapathoside,a	Not Available	FALSE	C1(C(C(C(OC1COC(=O)/C=C/c1ccc(cc1)O)OC1(CC(C(O1)COC(=O)/C=C/c1cc(OC)c(O)cc1)O)OC(=O)/C=C/c1ccc(cc1)O)COC(=O)/C=C/c1cc(OC)c(O)cc1)O)O)O
MOL007293	0.8410	0.1590	0.8891	Rhizoma Fagopyri Cymosi	3,5-dimethylquercetin	Not Available	FALSE	c1(c(c(=O)c2c(cc(O)cc2o1)OC)OC)c1cc(O)c(O)cc1
MOL007294	0.7560	0.2440	0.7510	Litchi Semen	procyanidin A2	Not Available	FALSE	c1(cc(c2C3c4c(OC(Oc2c1)(C3O)c1cc(c(cc1)O)O)cc(c1c4OC(C(C1)O)c1ccc(c(c1)O)O)O)O)O
MOL007294	0.7560	0.2440	0.7510	Semen Aesculi	procyanidin A2	Not Available	FALSE	c1(cc(c2C3c4c(OC(Oc2c1)(C3O)c1cc(c(cc1)O)O)cc(c1c4OC(C(C1)O)c1ccc(c(c1)O)O)O)O)O
MOL007294	0.7560	0.2440	0.7510	Rhizoma Fagopyri Cymosi	procyanidin A2	Not Available	FALSE	c1(cc(c2C3c4c(OC(Oc2c1)(C3O)c1cc(c(cc1)O)O)cc(c1c4OC(C(C1)O)c1ccc(c(c1)O)O)O)O)O
MOL007295	0.7955	0.2045	0.9060	Rhizoma Fagopyri Cymosi	2-(4-methoxyphenyl)-7-methyl-chromone	784791	FALSE	c12c(oc(cc1=O)c1ccc(cc1)OC)cc(cc2)C
MOL007296	0.3588	0.6412	0.7549	Rhizoma Fagopyri Cymosi	glucose ,d-glucose	Not Available	FALSE	C1C(CCC2(C1C1(C(CC2)(C2C(CC1)(C1C(=CC2)C(C(=O)CC1)(C)C)C)C)C)C)(C)C
MOL007297	0.7482	0.2518	0.7320	Rhizoma Fagopyri Cymosi	tannin	Not Available	FALSE	C1(C(C(C(C(O1)COC(=O)c1cc(c(c(c1)OC(=O)c1cc(c(c(c1)O)O)O)O)O)OC(=O)c1cc(c(c(c1)OC(=O)c1cc(c(c(c1)O)O)O)O)O)OC(=O)c1cc(c(c(c1)OC(=O)c1cc(c(c(c1)O)O)O)O)O)OC(=O)c1cc(c(c(c1)OC(=O)c1cc(c(c(c1)O)O)O)O)O)OC(=O)c1cc(c(c(c1)OC(=O)c1cc(c(c(c1)O)O)O)O)O)O
MOL007298	0.9203	0.0797	0.9437	Rhizoma Fagopyri Cymosi	3,4-Dihydroxybenzamide	148675	FALSE	c1(cc(c(cc1)O)O)C(=O)N
MOL007299	0.3934	0.6066	0.7363	Rhizoma Fagopyri Cymosi	glutinol	Not Available	FALSE	C1(CCC2C(=CCC3C4(C)CCC5(C)CCC(C)(C)CC5C4(CCC23C)C)C1(C)C)O
MOL007300	0.9369	0.0631	0.8943	Rhizoma Fagopyri Cymosi	6-o-galloyl-d-glucose	Not Available	FALSE	c1(c(c(cc(c1)C(=O)OCC1C(C(C(C(C1)O)O)O)O)O)O)O)O
MOL007301	0.8936	0.1064	0.6417	Rhizoma Fagopyri Cymosi	3,,8-dihydroxy-10-methoxy-5-h-isochromeno[4,,3-b]chromen-7-one	Not Available	FALSE	c1(cc(c2c(c1)oc1c(c2=O)OCc2c1ccc(c2)O)O)OC

MOL007302	0.8071	0.1929	0.8298	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	madecassoside	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2O)(C2(C(=CC1)C1C(CC2)(CCC(C1C)C)C(=O)OC1C(C(C(C(O1)COC1C(C(C(C(O1)CO)OOC1C(C(C(C(O1)C)O)O)O)O)O)O)O)O)C)C)C)(C)CO)O)O
MOL007303	0.7414	0.2586	0.7281	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	madecassoside_qt	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2O)(C2(C(=CC1)C1C(CC2)(CCC(C1C)C)C(=O)O)C)C)(C)CO)O)O
MOL007304	0.7776	0.2224	0.6900	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	3,4-di-o-caffeoylquinic,acid	Not Available	FALSE	C1C(C(C(CC1(C(=O)O)O)OOc1c(ccc(c1)/C=C/C(=O)C)O)OOc1c(ccc(c1)/C=C/C(=O)C)O)O
MOL007305	0.8368	0.1632	0.7310	Xanthii Fructus	(1S,3S,4R,5S)-3,4-bis[[(E)-3-(3,4-dihydroxyphenyl)acryloyl]oxy]-1,5-dihydroxy-cyclohexane-1-carboxylic acid	10324242	FALSE	C1(CC(CC(C1OC(=O)/C=C/c1cc(c(cc1)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)(O)C(=O)O)O
MOL007305	0.8368	0.1632	0.7310	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	(1S,3S,4R,5S)-3,4-bis[[(E)-3-(3,4-dihydroxyphenyl)acryloyl]oxy]-1,5-dihydroxy-cyclohexane-1-carboxylic acid	10324242	FALSE	C1(CC(CC(C1OC(=O)/C=C/c1cc(c(cc1)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)(O)C(=O)O)O
MOL007305	0.8368	0.1632	0.7310	Dipsaci Radix	(1S,3S,4R,5S)-3,4-bis[[(E)-3-(3,4-dihydroxyphenyl)acryloyl]oxy]-1,5-dihydroxy-cyclohexane-1-carboxylic acid	10324242	FALSE	C1(CC(CC(C1OC(=O)/C=C/c1cc(c(cc1)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)(O)C(=O)O)O

MOL007306	0.8042	0.1958	0.6964	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	3,5-dicaffeoyl-4-malonylquinic,acid	Not Available	FALSE	C1C(CC(C(C1OC(=O)/C=C/c1cc(c(cc1)O)O)OC(=O)CC(=O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)(O)C(=O)O
MOL007307	0.6982	0.3018	0.6930	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	castillicetin	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC(=O)/C=C\c1cc(c(cc1)O)O)c1ccc(c(c1)O)O)O)O
MOL007309	0.7918	0.2082	0.8224	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	asiaticoside,c	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2C)C(CC(C1C)C)C(=O)OC1CC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)OC1C(C(C(C(O1)C)O)O)O)CO)C)C)(CO)C)O)O
MOL007310	0.7216	0.2784	0.7181	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	asiaticoside,c_qt	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2C)C(CC(C1C)C)C(=O)O)C)C)C)(CO)C)O)O
MOL007311	0.8124	0.1876	0.8313	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	asiaticoside-b	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2O)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1C(C(C(C(O1)COC1C(C(C(C(O1)CO)OOC1C(C(C(C(O1)C)O)O)O)O)O)O)O)O)O)C)C)C)(C)CO)O)O
MOL007312	0.7415	0.2585	0.7373	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	asiaticoside-b_qt	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2O)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)C)(C)CO)O)O
MOL007313	0.8430	0.1570	0.8031	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	Xanthanoic acid	65736	FALSE	C1(c2ccccc2Oc2ccccc12)C(=O)O
MOL007314	0.9043	0.0957	0.8155	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	kaempferol,3-o-b-d-glucuronide	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O)C(O1)C(=O)O)c1ccc(O)cc1
MOL007315	0.7776	0.2224	0.6950	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	3,5-di-o-caffeoylquinic,acid	Not Available	FALSE	C1C(C(C(CC1(C(=O)O)O)OOc1c(ccc(c1)/C=C/C(=O)C)O)O)OOc1c(ccc(c1)/C=C/C(=O)C)O
MOL007316	0.8390	0.1610	0.7279	Chrysanthemi Flos	3,5-di-o-caffeoylquinic acid	Not Available	FALSE	C1C(C(C(CC1(O)C(=O)O)OC(=O)/C=C/c1ccc(c(c1)O)O)O)OC(=O)/C=C/c1ccc(c(c1)O)O
MOL007316	0.8390	0.1610	0.7279	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	3,5-di-o-caffeoylquinic acid	Not Available	FALSE	C1C(C(C(CC1(O)C(=O)O)OC(=O)/C=C/c1ccc(c(c1)O)O)O)OC(=O)/C=C/c1ccc(c(c1)O)O
MOL007317	0.7530	0.2470	0.8032	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	asiaticoside,f	Not Available	FALSE	C1(C(C(C2C(C1)(C1C3(CC2)C2(C(=CC1)C1C(CC2)(CCC(C1C)C)C(=O)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)OC1C(C(C(C(O1)C)O)O)O)O)CO)C3)C)C)(CO)C)O)O
MOL007318	0.7453	0.2547	0.6870	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	asiaticoside,f_qt	Not Available	FALSE	C1(C(C(C2C(C1)(C1C3(CC2)C2(C(=CC1)C1C(CC2)(CCC(C1C)C)C(=O)O)C3)C)(C)CO)O)O

MOL007319	0.7414	0.2586	0.7281	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	madecassoside,acid	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2O)(C2(C(=CC1)C1C(CC2)(CCC(C1C)C)C(=O)O)C)C)(C)CO)O)O
MOL007320	0.7068	0.2932	0.6693	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	8-acetoxycentellynol	Not Available	FALSE	C=CC(C#CC#CC(/C=C\CCCCC)OC(=O)C)O
MOL007321	0.7701	0.2299	0.8266	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	[(2S,3R,4S,5S,6R)-6-[[(2R,3R,4R,5S,6R)-3,4-dihydroxy-6-(hydroxymethyl)-5-[(2S,3R,4R,5R,6R)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]oxymethyl]-3,4,5-trihydroxyoxan-2-yl] (1S,2R,4aS,6aR,6aS,6bR,8aR,9R,10R,11R,12aR,14bR)-10,11-dihydroxy-9-(hydroxymet	24721205	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CC(C(C1(CO)C)O)O)C)C)C(C(CC2)C)C)C(=O)OC1OC(COC2OC(C(C(C2O)O)OC2C(C(C(C(O2)C)O)O)O)CO)C(C(C1O)O)O
MOL007322	0.9612	0.0388	0.8272	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	(1R,2R,5S)-2,6,6-trimethylnorpinan-3-one	10329459	FALSE	C12C(C(=O)CC(C1(C)C)C2)C
MOL007323	0.7333	0.2667	0.7357	Sargentodoxae Caulis	madasiatic acid	Not Available	FALSE	C1(C(CC2(C(C1(C)C)C(CC1(C)C3(C)CCC4(C(=O)O)CCC(C)C(C)C4C3=CCC21)O)C)O)O
MOL007323	0.7333	0.2667	0.7357	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	madasiatic acid	Not Available	FALSE	C1(C(CC2(C(C1(C)C)C(CC1(C)C3(C)CCC4(C(=O)O)CCC(C)C(C)C4C3=CCC21)O)C)O)O
MOL007324	0.7736	0.2264	0.8296	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	madecassoside	45356919	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CC(C(C1(CO)C)O)O)C)C)C(C(CC2)C)C)C(=O)OC1OC(COC2OC(C(C(C2O)O)OC2C(C(C(C(O2)C)O)O)O)CO)C(C(C1O)O)O

MOL007325	0.9612	0.0388	0.8272	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	30469-22-8	84532	FALSE	C12C(C(=O)CC(C1(C)C)C2)C
MOL007326	0.8498	0.1502	0.7183	Xanthii Fructus	Cynarin(e)	5281769	FALSE	C1C(CC(C(C1O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)(OC(=O)/C=C/c1cc(c(cc1)O)O)C(=O)O
MOL007326	0.8498	0.1502	0.7183	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	Cynarin(e)	5281769	FALSE	C1C(CC(C(C1O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)(OC(=O)/C=C/c1cc(c(cc1)O)O)C(=O)O
MOL007327	0.9356	0.0644	0.7515	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	Uregit	3278	FALSE	c1(c(ccc(c1Cl)OCC(=O)O)C(=O)C(=C)CC)Cl
MOL007328	0.7911	0.2089	0.8241	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	asiaticoside	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1C)C)C(=O)OC1C(C(C(C(O1)COC1C(C(C(C(O1)CO)OOC1C(C(C(C(O1)C)O)O)O)O)O)O)O)O)C)C)(C)CO)O)O
MOL007329	0.7423	0.2577	0.7468	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	asiaticoside_qt	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1C)C)C(=O)O)C)C)C)(C)CO)O)O
MOL007330	0.9543	0.0457	0.9542	Glechomae Herba	MENTHOL	16666	FALSE	C1(C(CCC(C1)C)C(C)C)O
MOL007330	0.9543	0.0457	0.9542	Mahoniae Caulis	MENTHOL	16666	FALSE	C1(C(CCC(C1)C)C(C)C)O
MOL007330	0.9543	0.0457	0.9542	Centella Asiatica (L.) Urban[Hydro-Cotyle Asiatica L.]	MENTHOL	16666	FALSE	C1(C(CCC(C1)C)C(C)C)O
MOL007330	0.9543	0.0457	0.9542	Rhododendri Daurici Folium	MENTHOL	16666	FALSE	C1(C(CCC(C1)C)C(C)C)O
MOL007330	0.9543	0.0457	0.9542	Cistanches Herba	MENTHOL	16666	FALSE	C1(C(CCC(C1)C)C(C)C)O
MOL007331	0.9545	0.0455	0.8682	Hedysari Radix	2-Butyl-4-hydroxyanisole	8456	FALSE	c1(cc(ccc1O)OC)C(C)(C)C
MOL007331	0.9545	0.0455	0.8682	Panacis Quinquefolii Radix	2-Butyl-4-hydroxyanisole	8456	FALSE	c1(cc(ccc1O)OC)C(C)(C)C
MOL007331	0.9545	0.0455	0.8682	Oroxyli Semen	2-Butyl-4-hydroxyanisole	8456	FALSE	c1(cc(ccc1O)OC)C(C)(C)C
MOL007331	0.9545	0.0455	0.8682	Humulus Scandens (Lour.) Merr.	2-Butyl-4-hydroxyanisole	8456	FALSE	c1(cc(ccc1O)OC)C(C)(C)C
MOL007332	0.9030	0.0970	0.8555	Humulus Scandens (Lour.) Merr.	3-methyldecane	25021915	FALSE	C(CC(CC)C)CCCCC
MOL007333	0.8223	0.1777	0.7160	Humulus Scandens (Lour.) Merr.	9-Thiafluorene	3023	FALSE	c12c3c(sc1cccc2)cccc3

MOL007334	0.9078	0.0922	0.9434	Humulus Scandens (Lour.) Merr.	3-bromoisonicotinic acid	817972	FALSE	c1(c(cncc1)Br)C(=O)O
MOL007336	0.9138	0.0862	0.7992	Humulus Scandens (Lour.) Merr.	vitexin_qt	45157620	FALSE	c12c(C)c(cc(c1c(=O)cc(o2)c1ccc(cc1)O)O)O
MOL007336	0.9138	0.0862	0.7992	Vigna Radiata	vitexin_qt	45157620	FALSE	c12c(C)c(cc(c1c(=O)cc(o2)c1ccc(cc1)O)O)O
MOL007338	0.9257	0.0743	0.8391	Gynostemmae Pentaphylli Herba	Acetylthymol	68252	FALSE	c1(cc(C)ccc1C(C)C)OC(=O)C
MOL007338	0.9257	0.0743	0.8391	Moslae Herba	Acetylthymol	68252	FALSE	c1(cc(C)ccc1C(C)C)OC(=O)C
MOL007338	0.9257	0.0743	0.8391	Humulus Scandens (Lour.) Merr.	Acetylthymol	68252	FALSE	c1(cc(C)ccc1C(C)C)OC(=O)C
MOL007339	0.9068	0.0932	0.6717	Humulus Scandens (Lour.) Merr.	2,5-ditert-butylphenol	79983	FALSE	c1(cc(c(cc1)C(C)(C)C)O)C(C)(C)C
MOL007340	0.9546	0.0454	0.9258	Nardostachyos Radix Et Rhizoma	Methyl carvacrol	80790	FALSE	c1(cc(ccc1C)C(C)C)OC
MOL007340	0.9546	0.0454	0.9258	Ephedra Herba	Methyl carvacrol	80790	FALSE	c1(cc(ccc1C)C(C)C)OC
MOL007340	0.9546	0.0454	0.9258	Humulus Scandens (Lour.) Merr.	Methyl carvacrol	80790	FALSE	c1(cc(ccc1C)C(C)C)OC
MOL007341	0.6885	0.3115	0.7662	Jujubae Fructus	alphitotic acid	44584080	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC3C(=C)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C
MOL007341	0.6885	0.3115	0.7662	Humulus Scandens (Lour.) Merr.	alphitotic acid	44584080	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC3C(=C)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C
MOL007342	0.4439	0.5561	0.6039	Humulus Scandens (Lour.) Merr.	soya-cerebroside i	Not Available	FALSE	O1C(C(O)C(O)C(O)C1OCC(NC(=O)C(O)CCCCCCCCCCCCCCC)C(O)/C=C/CC/C=C/CCCCCCCCC)CO
MOL007345	0.9491	0.0509	0.7594	Vigna Radiata	Boc-D-Trp-OH	111050	FALSE	c12c(CC(NC(=O)OC(C)(C)C)C(=O)O)c[nH]c1cccc2
MOL007347	0.9319	0.0681	0.8897	Vigna Radiata	Boc-D-Tyr-OH	1549481	FALSE	C(OC(=O)NC(C(=O)O)Cc1ccc(cc1)O)(C)(C)C
MOL007347	0.9319	0.0681	0.8897	Euryales Semen	Boc-D-Tyr-OH	1549481	FALSE	C(OC(=O)NC(C(=O)O)Cc1ccc(cc1)O)(C)(C)C
MOL007351	0.4402	0.5598	0.7146	Solanum Nigrum Linn.	12β,27-dihydroxysolasodine	Not Available	FALSE	C1(CCC2(C(=CCC3C4CC5OC6(C(C5C4(C)C(CC23)O)C)NCC(CC6)CO)C1)C)O
MOL007352	0.3220	0.6780	0.7142	Solanum Nigrum Linn.	23-o-acetyl-12β-hydroxysolasodine	Not Available	FALSE	C1(CCC2(C(=CCC3C4CC5OC6(C(C5C4(C)C(CC23)O)C)NCC(CC6OC(=O)C)C)C1)C)O
MOL007353	0.7048	0.2952	0.8553	Solanum Nigrum Linn.	solamargine	Not Available	FALSE	C12(C(C3C(O1)CC1C3(CCC3C1CC=C1C3(CCC(C1)OC1OC(C(C(C1O)O)OC1C(OC3C(C(C(C(O3)C)O)O)O)C(C(C(O1)C)O)O)CO)C)C)CCC(CN2)C

MOL007354	0.7063	0.2937	0.8303	Solanum Nigrum Linn.	Uttronin A	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(OC4OC(C(OC6OC(C(O)C(OC7OCC(O)C(O)C7O)C6OC6OC(C(O)C(O)C6O)CO)CO)C(O)C4O)CO)CC5)C)CC3)C2)C)C(C21OCC(CC2)C)C
MOL007355	0.9353	0.0647	0.9295	Capsellae Herba	acetylcholine	187	FALSE	[N+](C)(C)(C)CCOC(=O)C
MOL007355	0.9353	0.0647	0.9295	Solanum Nigrum Linn.	acetylcholine	187	FALSE	[N+](C)(C)(C)CCOC(=O)C
MOL007357	0.8657	0.1343	0.7477	Asteris Radix Et Rhizoma	Ac-Shanz-ME	162823	FALSE	O(C1(C2C(C(O)C1)C(=COC2OC1OC(C(O)C(O)C1O)CO)C(=O)OC)C)C(=O)C
MOL007357	0.8657	0.1343	0.7477	Solanum Nigrum Linn.	Ac-Shanz-ME	162823	FALSE	O(C1(C2C(C(O)C1)C(=COC2OC1OC(C(O)C(O)C1O)CO)C(=O)OC)C)C(=O)C
MOL007358	0.9120	0.0880	0.7030	Solanum Nigrum Linn.	uttroside a_qt	Not Available	FALSE	O(C1(C2C(C(O)C1)C(=COC2OC(=O)OC)C)C(=O)C
MOL007358	0.9120	0.0880	0.7030	Asteris Radix Et Rhizoma	uttroside a_qt	Not Available	FALSE	O(C1(C2C(C(O)C1)C(=COC2OC(=O)OC)C)C(=O)C
MOL007359	0.8001	0.1999	0.6487	Solanum Nigrum Linn.	Pterosin B glucoside	134279	FALSE	O1C(C(O)C(O)C(O)C1OCCc1c(c2c(CC(C2=O)C)cc1C)C)CO
MOL007360	0.8986	0.1014	0.8187	Solanum Nigrum Linn.	quercetin-3-gentiobioside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1)COC1OC(C(O)C(O)C1O)CO
MOL007361	0.7063	0.2937	0.8303	Solanum Nigrum Linn.	desgalactotigonin	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(OC4OC(C(OC6OC(C(O)C(OC7OCC(O)C(O)C7O)C6OC6OC(C(O)C(O)C6O)CO)CO)C(O)C4O)CO)CC5)C)CC3)C2)C)C(C21OCC(CC2)C)C
MOL007362	0.3012	0.6988	0.7449	Solanum Nigrum Linn.	Spirostan-3-ol, (3alpha,5alpha,25S)-	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(O)CC5)C)CC3)C2)C)C(C21OCC(CC2)C)C
MOL007363	0.6965	0.3035	0.6668	Solanum Nigrum Linn.	solanaviol	Not Available	FALSE	O1C2(C3(C4(C(OC2C(O)C3OC(=O)C)C=C(C(O)C4)C)COC(=O)C)C)C1
MOL007364	0.8936	0.1064	0.7615	Cortex Moutan	apiopaeonoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(ccc(OC)c1)C(=O)C)COC1OCC(O)(C1O)CO
MOL007365	0.8532	0.1468	0.8093	Cortex Moutan	galloyl-oxypaeoniflorin	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)COC(=O)c1cc(c(c(c1)O)O)O)C12C3(OC4C1(C(C(O4)(C3)O)C2)COC(=O)c1ccc(cc1)O)C
MOL007366	0.9090	0.0910	0.7962	Cortex Moutan	galloyl-oxypaeoniflorin_qt 2	Not Available	FALSE	OC12CC3C2(C2OC1(C)CC3(O2)O)COC(=O)c1ccc(cc1)O
MOL007367	0.9281	0.0719	0.8696	Cortex Moutan	paeonoside	57375575	FALSE	C(=O)(C)c1c(cc(cc1)OC)OC1OC(C(C(C1O)O)O)CO
MOL007368	0.7740	0.2260	0.7461	Cortex Moutan	4-O-methylpaeoniflorin	Not Available	FALSE	c1cc(ccc1)C(=O)OCC12C3(CC1C1(OC2OC3(C1)C)OC)OC1OC(C(C(C1O)O)O)CO
MOL007369	0.7639	0.2361	0.7424	Cortex Moutan	4-O-methylpaeoniflorin_qt	Not Available	FALSE	c1cc(ccc1)C(=O)OCC12C3(CC1C1(OC2OC3(C1)C)OC)O

MOL007370	0.6083	0.3917	0.7207	Cortex Moutan	6-o-vanillyoxypaeoniflorin	Not Available	FALSE	c1cc(cc(c1O)OC)C(=O)OCC1C(C(C(C(O1)OC12CC3C(CC1OC)(OCC23COC(=O)c1ccc(cc1)O)O)O)O)O
MOL007371	0.8916	0.1084	0.7716	Cortex Moutan	6-o-vanillyoxypaeoniflorin_qt 2	Not Available	FALSE	OC12CC3C(CC1OC)(OCC23COC(=O)c1ccc(cc1)O)O
MOL007372	0.9413	0.0587	0.9634	Cortex Moutan	3-Hydroxy-4-methoxyacetophenone	95693	FALSE	c1(cc(c(cc1)OC)O)C(=O)C
MOL007373	0.9455	0.0545	0.9316	Cortex Moutan	1-(2,3-dihydroxy-4-methoxyphenyl)ethanone	12820	FALSE	c1(c(c(c(cc1)OC)O)O)C(=O)C
MOL007374	0.9200	0.0800	0.7181	Cortex Moutan	5-[[5-(4-methoxyphenyl)-2-furyl]methylene]barbituric acid	2177166	FALSE	C1(=O)NC(=O)NC(=O)C1=Cc1ccc(o1)c1ccc(cc1)OC
MOL007377	0.9249	0.0751	0.8825	Cortex Moutan	mudanoside A	Not Available	FALSE	c1(c(ccc(c1)C(=O)OCC1C(C(C(C(O1)O)O)O)O)O)OC(=O)C
MOL007378	0.9489	0.0511	0.8982	Cortex Moutan	3-acetyl-4-hydroxybenzoic acid	9179245	FALSE	c1(c(ccc(c1)C(=O)O)O)C(=O)C
MOL007379	0.8976	0.1024	0.8380	Cortex Moutan	3-[(2S,3R,4S,5S,6R)-6-[[(2R,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxymethyl]-3,4,5-trihydroxyoxan-2-yl]oxy-4,5-dihydroxybenzoic acid	21604164	FALSE	C1(C(C(OC1)OCC1C(C(C(C(O1)Oc1cc(cc(c1O)O)C(=O)O)O)O)O)O)(CO)O
MOL007380	0.7466	0.2534	0.7992	Cortex Moutan	mudanpinoic, acid,a	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2=CCC3(C(C42C(C1)C4)CC(CC3)(C)C)C(=O)O)C)C)(C)C)O
MOL007381	0.6476	0.3524	0.7498	Cortex Moutan	mudanpioside-h	Not Available	FALSE	c1cc(ccc1O)C(=O)OCC1C(C(C(C(O1)OC12CC3C(CC1OC)(OCC23COC(=O)c1ccc(cc1)O)O)O)O)O

MOL007382	0.8916	0.1084	0.7716	Cortex Moutan	mudanpioside-h_qt 2	Not Available	FALSE	OC12CC3C(CC1OC)(OCC23COC(=O)c1ccc(cc1)O)O
MOL007383	0.7151	0.2849	0.7468	Cortex Moutan	paeonidanin	Not Available	FALSE	O(C12C3(C(C2)C(=O)CC1(CC3OC)C)COC(=O)c1ccccc1)C1OC(C(O)C(O)C1O)CO
MOL007384	0.6942	0.3058	0.6955	Cortex Moutan	paeonidanin_qt	Not Available	FALSE	OC12C3(C(C2)C(=O)CC1(CC3OC)C)COC(=O)c1ccccc1
MOL007386	0.9214	0.0786	0.9100	Polygoni Cuspidati Rhizoma Et Radix	(2S,3R,4S,5S,6R)-2-(4-hydroxy-3-methoxyphenoxy)-6-(hydroxymethyl)oxane-3,4,5-triol	11962143	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc(OC)c(O)cc1)CO
MOL007386	0.9214	0.0786	0.9100	Actinidia Chinensis Planch	(2S,3R,4S,5S,6R)-2-(4-hydroxy-3-methoxyphenoxy)-6-(hydroxymethyl)oxane-3,4,5-triol	11962143	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc(OC)c(O)cc1)CO
MOL007386	0.9214	0.0786	0.9100	Polygoni Avicularis Herba	(2S,3R,4S,5S,6R)-2-(4-hydroxy-3-methoxyphenoxy)-6-(hydroxymethyl)oxane-3,4,5-triol	11962143	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc(OC)c(O)cc1)CO
MOL007387	0.9056	0.0944	0.9678	Polygoni Avicularis Herba	2-MOHYDROP	69988	FALSE	Oc1cc(OC)c(O)cc1
MOL007387	0.9056	0.0944	0.9678	Actinidia Chinensis Planch	2-MOHYDROP	69988	FALSE	Oc1cc(OC)c(O)cc1
MOL007387	0.9056	0.0944	0.9678	Polygoni Cuspidati Rhizoma Et Radix	2-MOHYDROP	69988	FALSE	Oc1cc(OC)c(O)cc1

MOL007388	0.7472	0.2528	0.7763	Actinidia Chinensis Planch	(1S,2R,4aS,6aR,6aS,6bR,8aR,10R,11S,12aR,14bS)-10,11-dihydroxy-1,2,6a,6b,9,9,12a-heptamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydro-1H-picene-4a-carboxylic acid	24721200	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3C)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C
MOL007389	0.8876	0.1124	0.6787	Artemisia Annua L.	artemisitene	Not Available	FALSE	O1OC2(CCC3C41C(CCC3C)C(=C)C(=O)OC4O2)C
MOL007390	0.7960	0.2040	0.6939	Artemisia Annua L.	annulide	Not Available	FALSE	C12C3C(C(=C)C(=O)O1)CCC(C3CCC2=C)C
MOL007391	0.8334	0.1666	0.7328	Artemisia Annua L.	dihydroepideoxyarteannuin b	13918039	FALSE	O1C23C(C(C1=O)C)CCC(C2CCC(=C3)C)C
MOL007392	0.8212	0.1788	0.7448	Artemisia Annua L.	Deoxyarteannuin B	636625	FALSE	O1C23C(C(=C)C1=O)CCC(C2CCC(=C3)C)C
MOL007395	0.8767	0.1233	0.8479	Artemisia Annua L.	chrysosplenol	Not Available	FALSE	c1(c(c(c2c(c1)oc(c(c2=O)OC)c1ccc(c(c1)O)O)O)OC)OC
MOL007396	0.9374	0.0626	0.8693	Artemisia Annua L.	norannulic acid	71355939	FALSE	C1(CCC(C2CCC(=C)C(C12)O)C)C(=O)O
MOL007397	0.9583	0.0417	0.8247	Artemisia Annua L.	(1R,5R)-6,6-dimethyl-2-methylene-3-norpinanone	10012081	FALSE	C12C(=C)C(=O)CC(C1)C2(C)C
MOL007400	0.9294	0.0706	0.8169	Artemisia Annua L.	vicenin-2_qt	Not Available	FALSE	c1c(cc2c(c1O)C(=O)CC(=[O+]2)c1ccc(cc1)O)O
MOL007401	0.8927	0.1073	0.8728	Artemisia Annua L.	Cirsiliol	160237	FALSE	c1(cc(=O)c2c(c(c(cc2o1)OC)OC)O)c1cc(c(cc1)O)O
MOL007402	0.8578	0.1422	0.7972	Artemisia Annua L.	ponticaepoxide	Not Available	FALSE	O1C(C1C=C)/C=C\C#CC#CC#CC
MOL007405	0.7739	0.2261	0.8903	Artemisiae Scopariae Herba	Cirsilineol	162464	FALSE	c1(cc(=O)c2c(c(c(cc2o1)OC)OC)O)c1cc(c(cc1)O)OC
MOL007405	0.7739	0.2261	0.8903	Artemisia Annua L.	Cirsilineol	162464	FALSE	c1(cc(=O)c2c(c(c(cc2o1)OC)OC)O)c1cc(c(cc1)O)OC
MOL007406	0.9419	0.0581	0.7963	Artemisia Annua L.	Umckalin	5316862	FALSE	o1c(=O)ccc2c(c(c(cc12)O)OC)OC
MOL007407	0.8973	0.1027	0.8899	Artemisia Annua L.	5,7,8,3'-Tetrahydroxy-3,4'-dimethoxy flavone	5321861	FALSE	c1(c(c(=O)c2c(cc(c(c2o1)O)O)O)OC)c1cc(c(cc1)OC)O

MOL007408	0.7338	0.2662	0.9056	Artemisia Annua L.	4'-methylpenduletin	5318355	FALSE	c1(c(c(=O)c2c(c(c(cc2o1)OC)OC)O)OC)c1ccc(cc1)OC
MOL007410	0.9286	0.0714	0.8466	Artemisia Annua L.	Artemisinin B	126891	FALSE	OC12C(C(CCC1C(=C)C(=O)O)C)CC=C(C2O)C
MOL007411	0.9396	0.0604	0.9409	Artemisia Annua L.	isoartemisia ketone	12308603	FALSE	C=C(CC(=O)C(C=C)(C)C)C
MOL007412	0.9126	0.0874	0.8826	Artemisia Annua L.	DMQT	5281603	FALSE	c1(c(c(=O)c2c(c(c(cc2o1)OC)OC)O)OC)c1cc(c(cc1)O)O
MOL007413	0.8801	0.1199	0.7792	Artemisia Annua L.	schaftoside	Not Available	FALSE	c12c(c(c(c(c1O)C1OC(C(C(C1O)O)O)CO)O)C1OCC(C(C1O)O)O)oc(cc2=O)c1ccc(cc1)O
MOL007414	0.8801	0.1199	0.7779	Artemisia Annua L.	isoschaftoside	Not Available	FALSE	c12c(c(c(c(c1O)C1OCC(C(C1O)O)O)O)C1OC(C(C(C1O)O)O)CO)oc(cc2=O)c1ccc(cc1)O
MOL007416	0.8399	0.1601	0.9192	Artemisia Annua L.	Penduletin	5320462	TRUE	c1(c(c(=O)c2c(c(c(cc2o1)OC)OC)O)OC)c1ccc(cc1)O
MOL007416	0.8399	0.1601	0.9192	Viticis Fructus	Penduletin	5320462	TRUE	c1(c(c(=O)c2c(c(c(cc2o1)OC)OC)O)OC)c1ccc(cc1)O
MOL007417	0.7868	0.2132	0.8088	Artemisia Annua L.	3,5-Dihydroxy-6,7,3',4'-tetramethoxyflavone	5316832	FALSE	c1(c(c(=O)c2c(c(c(cc2o1)OC)OC)O)O)c1cc(c(cc1)OC)OC
MOL007418	0.7082	0.2918	0.8244	Artemisia Annua L.	eupatorin	Not Available	FALSE	C123C(C4(C(CC3)C(CCC4)(C(=O)OC3OC(C(C(C3O)O)O)CO)C)C)CCC(C1)(C(=C)C2)OC1C(OC2OC(C(C(C2O)O)O)CO)C(C(C(O1)CO)O)O
MOL007419	0.6600	0.3400	0.8397	Artemisia Annua L.	eupatorin_qt	Not Available	FALSE	C123C(C4(C(CC3)C(C(=O)O)(CCC4)C)C)CCC(C1)(C(=C)C2)O
MOL007420	0.9517	0.0483	0.9719	Chrysanthemi Flos	gamma-Terpineol	11467	FALSE	C1(CCC(=C(C)C)CC1)(C)O
MOL007420	0.9517	0.0483	0.9719	Artemisia Annua L.	gamma-Terpineol	11467	FALSE	C1(CCC(=C(C)C)CC1)(C)O
MOL007420	0.9517	0.0483	0.9719	Capsici Fructus	gamma-Terpineol	11467	FALSE	C1(CCC(=C(C)C)CC1)(C)O
MOL007421	0.9235	0.0765	0.8269	Artemisia Annua L.	Quercetagetin-3,4'-dimethyl ether	5320823	FALSE	c1(c(c(=O)c2c(o1)cc(c(c2O)O)O)OC)c1cc(c(cc1)OC)O
MOL007422	0.8728	0.1272	0.7911	Artemisia Annua L.	6,8-di-c-glucosylapigenin	Not Available	FALSE	c1(cc(=O)c2c(O)c(c(O)c(c2o1)C1C(O)C(O)C(O)C(O1)CO)C1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL007424	0.8779	0.1221	0.6664	Artemisia Annua L.	artemisinin	Not Available	FALSE	C123C4OC(OO3)(CCC2C(CCC1C(C(=O)O4)C)C)C
MOL007425	0.8621	0.1379	0.6550	Artemisia Annua L.	dihydroartemisinin	Not Available	FALSE	C12OC(C(C3C41C(C(CC3)C)CCC(O2)(OO4)C)C)O
MOL007426	0.8422	0.1578	0.6712	Artemisia Annua L.	deoxyartemisinin	Not Available	FALSE	O1C2(CCC3C4(C1OC(=O)C(C4CCC3C)C)O2)C
MOL007427	0.8750	0.1250	0.6912	Artemisia Annua L.	bornyl isovalerate	36690486	FALSE	C12(C(CC(C1(C)C)CC2)OC(=O)CC(C)C)C

MOL007428	0.9080	0.0920	0.8396	Artemisia Annua L.	nchembio875-comp6	10922465	FALSE	C(=O)(C(=C)C1CCC(C2CCC(=CC12)C)C)O
MOL007429	0.8420	0.1580	0.7220	Artemisia Annua L.	qinghaosu v	Not Available	FALSE	C12C3C(C(=C)C(=O)O1)CCC(C3CCC2(C)O)C
MOL007430	0.8752	0.1248	0.6924	Artemisia Annua L.	qinghaosu iv	Not Available	FALSE	O1C2(C(CC3C4(C1OC(=O)C(C4CCC3C)C)O2)O)C
MOL007431	0.9153	0.0847	0.7569	Artemisia Annua L.	qinghaosu i	Not Available	FALSE	C1=C(C2C3C(C1)C(CCC3C(=O)O2)C)C
MOL007432	0.7929	0.2071	0.8634	Artemisia Annua L.	methyl 2-[(1R,4R,4aS,8aR)-4,7-dimethyl-1,2,3,4,4a,5,6,8a-octahydronaphthalen-1-yl]prop-2-enoate	11139489	FALSE	C1(CCC(C2CCC(=CC12)C)C)C(=C)C(=O)OC
MOL007433	0.8212	0.1788	0.7448	Artemisia Annua L.	deoxyisoartemisinin b	13969118	FALSE	O1C23C(C(=C)C1=O)CCC(C2CCC(=C3)C)C
MOL007434	0.8655	0.1345	0.7976	Artemisia Annua L.	artesunate	Not Available	FALSE	C12OC(C(C3C41C(C(CC3)C)CCC(O2)(OO4)C)C)OC(=O)CCC(=O)O
MOL007435	0.8801	0.1199	0.7779	Artemisia Annua L.	apigenin 6-c-beta-arabinopyranosyl-8-c-beta-galactopyranoside	Not Available	FALSE	c1(cc(=O)c2c(O)c(c(O)c(c2o1)C1C(O)C(O)C(O)C(O)C(O1)CO)C1C(O)C(O)C(O)CO1)c1ccc(O)cc1
MOL007436	0.8729	0.1271	0.7978	Artemisia Annua L.	apigenin 6-c-beta-chinovopyranosyl-8-c-beta-galactopyranoside	Not Available	FALSE	C1(C(O)C(C(OC1C)c1c(c2c(c(c1O)C1OC(C(C(C1O)O)O)CO)oc(cc2=O)c1ccc(cc1)O)O)O)O
MOL007437	0.8801	0.1199	0.7779	Artemisia Annua L.	apigenin 6-c-beta-xylopyranosyl-8-c-beta-galactopyranoside	Not Available	FALSE	c1(cc(=O)c2c(O)c(c(O)c(c2o1)C1C(O)C(O)C(O)C(O)C(O1)CO)C1C(O)C(O)C(O)CO1)c1ccc(O)cc1
MOL007438	0.8729	0.1271	0.7979	Artemisia Annua L.	apigenin-6-c-glu-8-c-rha	Not Available	FALSE	c1(c(c(c2c(c1C1C(C(C(C(O1)C)O)O)O)oc(cc2=O)c1ccc(cc1)O)O)C1C(C(C(C(O1)CO)O)O)O)O
MOL007439	0.8729	0.1271	0.7980	Artemisia Annua L.	apigenin-6-c-rha-8-c-glu	Not Available	FALSE	c1(c(c(c2c(c1C1C(C(C(C(O1)CO)O)O)O)oc(cc2=O)c1ccc(cc1)O)O)C1C(C(C(C(O1)C)O)O)O)O

MOL007441	0.9076	0.0924	0.8350	Artemisia Annua L.	(2S)-2-[(1R,4R,4aS,8aS)-4,7-dimethyl-1,2,3,4,4a,5,6,8a-octahydronaphthalen-1-yl]propionic acid	5325616	FALSE	OC(=O)C(C1C2C(C(CC1)C)CCC(=C2)C)C
MOL007443	0.8977	0.1023	0.8170	Artemisia Annua L.	isorhamnetin, 3-glucoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)c(c1)OC
MOL007445	0.8977	0.1023	0.8170	Artemisia Annua L.	isorhamnetin-glu	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1C(C(C(C(O1)CO)O)O)O)c1ccc(c(c1)OC)O)O)O
MOL007446	0.8721	0.1279	0.7875	Artemisia Annua L.	mearnsetin-di-glu	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)CO)O)O)O)O)O)c1cc(c(c(c1)O)OC)O)O)O
MOL007447	0.8797	0.1203	0.8528	Artemisia Annua L.	2-(3,5-dihydroxy-4-methoxy-phenyl)-3,5,7-trihydroxy-chromone	10359384	FALSE	c1(cc(c2c(c1)oc(c(c2=O)O)c1cc(c(c(c1)O)OC)O)O)O
MOL007448	0.9598	0.0402	0.8104	Artemisia Annua L.	trans-Pinocarveyl acetate	162395	FALSE	C1C(C(=C)C2C(C1C2)(C)C)OC(=O)C
MOL007449	0.2106	0.7894	0.6090	Lycii Fructus	24-methylidenelophenol	5283640	FALSE	C1(CCC2(C(C1C)CC=C1C3CCC(C(CCC(=C)C(C)C)C)C3(C)CCC21)C)O
MOL007449	0.2106	0.7894	0.6090	Perillae Fructus	24-methylidenelophenol	5283640	FALSE	C1(CCC2(C(C1C)CC=C1C3CCC(C(CCC(=C)C(C)C)C)C3(C)CCC21)C)O
MOL007449	0.2106	0.7894	0.6090	Silybum Marianum	24-methylidenelophenol	5283640	FALSE	C1(CCC2(C(C1C)CC=C1C3CCC(C(CCC(=C)C(C)C)C)C3(C)CCC21)C)O
MOL007450	0.4974	0.5026	0.8860	Silybum Marianum	SILYBIN	31553	FALSE	C1(c2cc(c(cc2)O)OC)C(Oc2c(O1)cc(cc2)C1Oc2c(C(=O)C1O)c(cc(c2)O)O)CO
MOL007451	0.7681	0.2319	0.9035	Silybum Marianum	silydianin	Not Available	FALSE	C12C3C(C(C=C1C1Oc4c(C(=O)C1O)c(cc(c4)O)O)C(=O)C2(OC3)O)c1cc(c(cc1)O)OC
MOL007452	0.6893	0.3107	0.8693	Silybum Marianum	silychristin	Not Available	FALSE	c12c(OC(C1CO)c1cc(c(cc1)O)OC)c(cc(c2)C1Oc2c(C(=O)C1O)c(cc(c2)O)O)O

MOL007453	0.9491	0.0509	0.8080	Silybum Marianum	5,7-Dihydroxychromone	Not Available	FALSE	c1(cc2c(c(c1)O)C(=O)CC=[O+]2)O
MOL007454	0.6494	0.3506	0.8974	Silybum Marianum	silymonin	Not Available	FALSE	C12C3C(C(C=C1C1Oc4c(C(=O)C1)c(cc(c4)O)O)C(=O)C2(OC3)O)c1cc(c(cc1)O)OC
MOL007455	0.3393	0.6607	0.8245	Silybum Marianum	silandrin	Not Available	FALSE	c12c(C(=O)CC(O1)c1cc3c(cc1)OC(C(O3)CO)c1cc(c(cc1)O)OC)c(cc(c2)O)O
MOL007456	0.5257	0.4743	0.8718	Silybum Marianum	Isosilybin	Not Available	FALSE	C1(c2cc(c(cc2)O)OC)C(Oc2c(O1)ccc(c2)C1Oc2c(C(=O)C1O)c(cc(c2)O)O)CO
MOL007457	0.0622	0.9378	0.7976	Silybum Marianum	isosilychristin	Not Available	FALSE	C(=O)(C)OCC1C(Oc2c1cc(cc2OC(=O)C)C1C(C(=O)c2c(cc(cc2O1)OC(=O)C)OC(=O)C)OC(=O)C)c1cc(c(cc1)OC(=O)C)OC
MOL007458	0.9034	0.0966	0.9684	Silybum Marianum	(S)-2-Aminobutanoate	6971252	FALSE	C(=O)(C(CC)N)O
MOL007459	0.9501	0.0499	0.9630	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	[(1R)-1-methoxyethyl]benzene	10776403	FALSE	c1(ccccc1)C(C)OC
MOL007460	0.8909	0.1091	0.9442	Aucklandiae Radix	Cyclooctadiene	299882	FALSE	C1=CCCCCC=C1
MOL007460	0.8909	0.1091	0.9442	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	Cyclooctadiene	299882	FALSE	C1=CCCCCC=C1
MOL007461	0.9212	0.0788	0.7653	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	1,2-DIHYDRO-1,5,8-TRIMETHYLNAPHTHALENE	Not Available	FALSE	c12c(ccc(c1C(CC=C2)C)C)C
MOL007461	0.9212	0.0788	0.7653	Ginkgo Folium	1,2-DIHYDRO-1,5,8-TRIMETHYLNAPHTHALENE	Not Available	FALSE	c12c(ccc(c1C(CC=C2)C)C)C
MOL007461	0.9212	0.0788	0.7653	Junci Medulla	1,2-DIHYDRO-1,5,8-TRIMETHYLNAPHTHALENE	Not Available	FALSE	c12c(ccc(c1C(CC=C2)C)C)C

MOL007462	0.9178	0.0822	0.7268	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	1,4,6-trimethyl-1,2,3,4-tetralin	Not Available	FALSE	C1C(c2c(C(C1)C)ccc(c2)C)C
MOL007463	0.8968	0.1032	0.9485	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	(1R,2S)-1-ethyl-2-methylcyclopropane	21572745	FALSE	C1C(C1C)CC
MOL007464	0.9430	0.0570	0.9549	Coriandri Sativi Herba	1-methyl-5-isopropenyl cyclohexene	12304570	FALSE	C1CC=C(CC1C(=C)C)C
MOL007464	0.9430	0.0570	0.9549	Gynostemmae Pentaphylli Herba	1-methyl-5-isopropenyl cyclohexene	12304570	FALSE	C1CC=C(CC1C(=C)C)C
MOL007464	0.9430	0.0570	0.9549	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	1-methyl-5-isopropenyl cyclohexene	12304570	FALSE	C1CC=C(CC1C(=C)C)C
MOL007466	0.9271	0.0729	0.9433	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	DICHLOROANILINE	11844	FALSE	c1cc(c(c(c1)Cl)Cl)N
MOL007467	0.9080	0.0920	0.9727	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	2,6-dimethyl-cyclohexanol	6992792	FALSE	C1(CCCC(C1O)C)C
MOL007468	0.9669	0.0331	0.9625	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	3,5-Dimethoxyacetophenone	95997	FALSE	c1c(cc(cc1OC)C(=O)C)OC
MOL007469	0.9456	0.0544	0.9764	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	3,4-dichloroaniline	Not Available	FALSE	C1(=C)C=CC(C(=C1)Cl)Cl
MOL007470	0.9173	0.0827	0.9559	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	(2E)-3-ethylpenta-2,4-dien-1-ol	5364723	FALSE	C=C/C(=C/CO)/CC
MOL007472	0.4777	0.5223	0.6406	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	(9Z,12E)-octadeca-9,12-dienoic acid methyl ester	6149093	FALSE	C(/C=C\CCCCCCCC(=O)OC)/C=C/CCCCC
MOL007473	0.8882	0.1118	0.9442	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	N3-Oxalyl-L-2,3-diaminopropanoate	440259	FALSE	C(=O)(C(N)CNC(=O)C(=O)O)O

MOL007474	0.3560	0.6440	0.7297	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	(2R,3S,4S,5R,6S)-2-(hydroxymethyl)-6-[(2S)-6-methyl-2-[(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-3,6,12-trihydroxy-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-17-yl]hept-5-en-2-yl]oxyoxane-3,4,5-triol	9809542	FALSE	C12(C3(C(C(CC1C1(C(C(C(CC1)O)(C)C)C(C2)O)C)O)C(C(OC1C(C(C(C(O1)CO)O)O)O)(CCC=C(C)C)C)CC3)C)C
MOL007475	0.5928	0.4072	0.7475	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	ginsenoside f2	Not Available	FALSE	C12(C3(C(C4(C(C(C(OC5C(C(C(C(O5)CO)O)O)O)CC4)(C)C)CC3)C)CC(C1C(C(OC1C(C(C(C(O1)CO)O)O)O)(CCC=C(C)C)C)CC2)O)C)C
MOL007475	0.5928	0.4072	0.7475	Gynostemmae Pentaphylli Herba	ginsenoside f2	Not Available	FALSE	C12(C3(C(C4(C(C(C(OC5C(C(C(C(O5)CO)O)O)O)CC4)(C)C)CC3)C)CC(C1C(C(OC1C(C(C(C(O1)CO)O)O)O)(CCC=C(C)C)C)CC2)O)C)C
MOL007476	0.7494	0.2506	0.8097	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	ginsenoside rb1	Not Available	FALSE	O(C1C(OC(C(C1O)O)CO)OC1C(C2C(CC1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)CO)O)O)O)(C)CCC=C(C)C)C)C)(C)C)C1C(C(C(C(O1)CO)O)O)O
MOL007476	0.7494	0.2506	0.8097	Gynostemmae Pentaphylli Herba	ginsenoside rb1	Not Available	FALSE	O(C1C(OC(C(C1O)O)CO)OC1C(C2C(CC1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)CO)O)O)O)(C)CCC=C(C)C)C)C)(C)C)C1C(C(C(C(O1)CO)O)O)O

MOL007477	0.7282	0.2718	0.8093	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	(2S,3R,4S,5S,6R)-2-[(2S)-2-[(3S,5R,8R,9R,10R,12R,13R,14R,17S)-3-[(2R,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]oxy-12-hydroxy-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,1	6917976	FALSE	C12(C3(C(C(CC3)C(OC3OC(COC4C(C(C(CO4)O)O)O)C(C(C3O)O)O)(CCC=C(C)C)C)C(CC1C1(C(CC2)C(C(CC1)OC1C(OC2OC(C(C(C2O)O)O)CO)C(C(C(O1)CO)O)O)(C)C)C)O)C)C
MOL007478	0.7282	0.2718	0.8093	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	ginsenoside rb3	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)CO1)C(C1CCC2(C3(CCC4C(C(CCC4(C3CC(C12)O)C)OC1C(OC2C(O)C(O)C(O)C(O2)CO)C(O)C(O)C(O1)CO)(C)C)C)C)(CCC=C(C)C)C
MOL007479	0.7331	0.2669	0.8151	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	ginsenoside rc	Not Available	FALSE	C12C(C3(C(C(C2)O)C(CC3)C(OC2OC(C(C(C2O)O)O)COC2OC(C(C2O)O)CO)(CCC=C(C)C)C)C)(CCC2C1(CCC(C2(C)C)OC1C(OC2OC(C(C(C2O)O)O)CO)C(C(C(O1)CO)O)O)C)C
MOL007480	0.2305	0.7695	0.7376	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	ginsenoside rd_qt	Not Available	FALSE	C1(CCC2(C(CCC3(C4(C(C(CC23)O)C(CC4)C(O)(CCC=C(C)C)C)C)C)C1(C)C)C)O
MOL007480	0.2305	0.7695	0.7376	Panacis Quinquefolii Radix	ginsenoside rd_qt	Not Available	FALSE	C1(CCC2(C(CCC3(C4(C(C(CC23)O)C(CC4)C(O)(CCC=C(C)C)C)C)C)C1(C)C)C)O
MOL007480	0.2305	0.7695	0.7376	Gynostemmae Pentaphylli Herba	ginsenoside rd_qt	Not Available	FALSE	C1(CCC2(C(CCC3(C4(C(C(CC23)O)C(CC4)C(O)(CCC=C(C)C)C)C)C)C1(C)C)C)O
MOL007481	0.6702	0.3298	0.8663	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	ginsenoside rf	Not Available	FALSE	C12(C(C3(C(C(C2)OC2C(OC4OC(C(C(C4O)O)O)CO)C(C(C(O2)CO)O)O)C(C(CC3)O)(C)C)C)CC(C2C1(CCC2C(CCC=C(C)C)(C)O)C)O)C

MOL007482	0.6600	0.3400	0.8606	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	(2S,3R,4R,5R,6S)-2-[[(2R,3R,4S,5S,6R)-2-[[(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-3,12-dihydroxy-17-[(1S)-1-hydroxy-1,5-dimethylhex-4-enyl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-6-yl]oxy]-4,5-dihydroxy-	21599924	FALSE	OC1C(C2C(CC1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)OC2C(C(C(C(O2)C)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C
MOL007483	0.7279	0.2721	0.8093	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	ginsenoside rg3	51346142	FALSE	C12C(C3(C(C(C2)O)C(CC3)C(OC2C(OC3OC(C(C(C3O)O)O)CO)C(C(C(O2)CO)O)O)(CCC=C(C)C)C)C)(CCC2C1(CCC(C2(C)C)OC1OC(C(C(C1O)O)O)COC1C(C(C(CO1)O)O)O)C)C

MOL007484	0.4038	0.5962	0.7568	Ginsen Radix Et Rhizoma Rubra	(2R,3R,4S,5S,6R)-2-[[(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-3,12-dihydroxy-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-6-yl]oxy]-6-(hydroxymethyl)oxane-3,4,5-triol	12855920	FALSE	OC1C(C2C(CC1)(C1C(CC2OC2OC(C(C(C2O)O)O)CO)C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C

MOL007484	0.4038	0.5962	0.7568	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	(2R,3R,4S,5S,6R)-2-[[(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-3,12-dihydroxy-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-6-yl]oxy]-6-(hydroxymethyl)oxane-3,4,5-triol	12855920	FALSE	OC1C(C2C(CC1)(C1C(CC2OC2OC(C(C(C2O)O)O)CO)C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C

MOL007485	0.7572	0.2428	0.8299	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	(2S,3S,4S,5R,6R)-6-[[(3S,4aR,6aR,6bS,8aS,12aS,14aR,14bR)-4,4,6a,6b,11,11,14b-heptamethyl-8a-[oxo-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)-2-tetrahydropyranyl]oxy]methyl]-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydropicen-3-yl]oxy]-3,4-di	11815492	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)OC1C(OC3OC(C(C(C3O)O)O)CO)C(C(C(O1)C(=O)O)O)O)C)C)CC(CC2)(C)C)C(=O)OC1OC(C(C(C1O)O)O)CO

MOL007485	0.7572	0.2428	0.8299	Achyranthis Bidentatae Radix	(2S,3S,4S,5R,6R)-6-[[(3S,4aR,6aR,6bS,8aS,12aS,14aR,14bR)-4,4,6a,6b,11,11,14b-heptamethyl-8a-[oxo-[[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)-2-tetrahydropyranyl]oxy]methyl]-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydropicen-3-yl]oxy]-3,4-di	11815492	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)OC1C(OC3OC(C(C(C3O)O)O)CO)C(C(C(O1)C(=O)O)O)O)C)C)CC(CC2)(C)C)C(=O)OC1OC(C(C(C1O)O)O)CO
MOL007486	0.9529	0.0471	0.7478	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	ZINC01532096	1549061	FALSE	c1c(cc(cc1Cl)N1C(=O)C2(C(C1=O)(C2)C)C)Cl
MOL007487	0.7341	0.2659	0.8385	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	notoginsenoside1	Not Available	FALSE	OC1C(C2C(CC1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)OC2C(C(C(CO2)O)O)O)(C2(C(C(C1)O)C(CC2)C(OC1OC(C(C(C1O)O)O)CO)(C)CCC=C(C)C)C)C)(C)C
MOL007488	0.6552	0.3448	0.8570	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	notoginsenoside2	Not Available	FALSE	OC1C(C2C(CC1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)OC2C(C(C(CO2)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C
MOL007489	0.7494	0.2506	0.8097	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	notoginsenoside3	Not Available	FALSE	O(C1C(OC2C(O)C(O)C(O)C(O2)CO)C(O)C(O)C(O1)CO)C1CCC2(C(C1(C)C)CCC1(C)C3(C)CCC(C(CCC=C(C)C)(C)OC4C(O)C(O)C(O)C(O4)COC4C(O)C(O)C(O)C(O4)CO)C3C(CC21)O)C
MOL007490	0.2305	0.7695	0.7376	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	notoginsenoside3_qt	Not Available	FALSE	OC1CCC2(C(C1(C)C)CCC1(C)C2CC(O)C2C(CCC12C)C(CCC=C(C)C)(O)C)C
MOL007491	0.7622	0.2378	0.7951	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	notoginsenoside4	Not Available	FALSE	O(C1C(OC(C(C1O)O)CO)OC1C(C2C(CC1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)COC1OCC(C(C1O)O)O)O)O)O)(C)CCC=C(C)C)C)C)(C)C)C1C(C(C(C(O1)CO)O)O)O

MOL007492	0.8963	0.1037	0.9341	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	Butylcyclobutane	544591	FALSE	CCCCC1CCC1
MOL007494	0.7118	0.2882	0.8238	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	gypenosideix	46887681	FALSE	C1(C2C(CCC1OC1OC(C(C(C1O)O)O)CO)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)C)C)(C)
MOL007495	0.7426	0.2574	0.8234	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	gypenosidexvii	44584555	FALSE	C1(C2C(CCC1OC1OC(C(C(C1O)O)O)CO)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)C)C)C)(C)C
MOL007496	0.9448	0.0552	0.9754	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	isopulegone	Not Available	FALSE	C1(=O)C(CCC(C1)C)C(=O)C
MOL007497	0.9458	0.0542	0.9269	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	NaPst	7406	FALSE	c1(ccccc1)C(C)C
MOL007497	0.9458	0.0542	0.9269	Saussureae Involucratae Herba	NaPst	7406	FALSE	c1(ccccc1)C(C)C
MOL007498	0.7326	0.2674	0.6140	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	10Z,13Z-nonadecadienoic acid	5282804	FALSE	C(/C=C\CCCCCCCCC(=O)O)/C=C\CCCCC
MOL007500	0.2170	0.7830	0.7636	Panax Ginseng C. A. Mey.	panaxatriol	73599	FALSE	C12(C3(C(C(CC3)C3(OC(CCC3)(C)C)C)C(CC1C1(C(C(C2)O)C(C(CC1)O)(C)C)C)O)C)C
MOL007500	0.2170	0.7830	0.7636	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	panaxatriol	73599	FALSE	C12(C3(C(C(CC3)C3(OC(CCC3)(C)C)C)C(CC1C1(C(C(C2)O)C(C(CC1)O)(C)C)C)O)C)C
MOL007501	0.6692	0.3308	0.6865	Ginsen Radix Et Rhizoma Rubra	panaxydol	126312	FALSE	C=CC(C#CC#CCC1OC1CCCCCCC)O
MOL007501	0.6692	0.3308	0.6865	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	panaxydol	126312	FALSE	C=CC(C#CC#CCC1OC1CCCCCCC)O
MOL007501	0.6692	0.3308	0.6865	Panacis Quinquefolii Radix	panaxydol	126312	FALSE	C=CC(C#CC#CCC1OC1CCCCCCC)O
MOL007502	0.6294	0.3706	0.6584	Saposhnikoviae Radix	NSC692928	5469789	FALSE	C=CC(C#CC#CC/C=C\CCCCCCC)O
MOL007502	0.6294	0.3706	0.6584	Ginsen Radix Et Rhizoma Rubra	NSC692928	5469789	FALSE	C=CC(C#CC#CC/C=C\CCCCCCC)O
MOL007502	0.6294	0.3706	0.6584	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	NSC692928	5469789	FALSE	C=CC(C#CC#CC/C=C\CCCCCCC)O
MOL007503	0.7893	0.2107	0.7333	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	panaxytriol	Not Available	FALSE	C=CC(C#CC#CCC(C(CCCCCCC)O)O)O
MOL007504	0.2167	0.7833	0.7442	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	NSC 308879	73498	FALSE	C12(C3(C(C(CC3)C3(OC(CCC3)(C)C)C)C(CC1C1(C(CC2)C(C(CC1)O)(C)C)C)O)C)C

MOL007504	0.2167	0.7833	0.7442	Gynostemmae Pentaphylli Herba	NSC 308879	73498	FALSE	C12(C3(C(C(CC3)C3(OC(CCC3)(C)C)C)C(CC1C1(C(CC2)C(C(CC1)O)(C)C)C)O)C)C
MOL007505	0.8945	0.1055	0.9682	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	WLN: QR DG	4684	FALSE	c1c(ccc(c1)O)Cl
MOL007506	0.2206	0.7794	0.7111	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	protopanoxadiol	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1C3(C)CCC(C(CCC=C(C)C)(C)O)C3C(CC21O)C)C)O
MOL007507	0.8731	0.1269	0.7171	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	sanchinan-a	Not Available	FALSE	O(C1C(O)C(OC(OC2C(O)C(OC(O)C2O)CO)C1O)COC1OC(C(O)C(OC2OC(C(O)C(O)C2O)COC2OC(C(O)C2O)CO)C1O)CO)C1OC(C(O)C(O)C1O)COC1OC(C(O)C(OC2OC(C(O)C(O)C2O)COC2OC(C(O)C(O)C2O)CO)C1O)CO
MOL007508	0.8254	0.1746	0.6165	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	α-cyperene	Not Available	FALSE	C1C2CC3=C(CCC3(C(C1)C)C2(C)C)C
MOL007509	0.8331	0.1669	0.6734	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	(4aS,9aR)-2,9,9-trimethyl-5-methylene-4,4a,6,7,8,9a-hexahydro-3H-benzo[7]annulene	11769623	FALSE	C12C(C(=C)CCCC1(C)C)CCC(=C2)C
MOL007510	0.8140	0.1860	0.6026	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	α-copaene	Not Available	FALSE	C1=C(CC2(C(C1)CC(CC2)C(C)C)C)C
MOL007511	0.9214	0.0786	0.9739	Amygdalus Communis Vas	(5S)-5-ethyloxolan-2-one	5325911	FALSE	C1CC(=O)OC1CC
MOL007511	0.9214	0.0786	0.9739	Panax Notoginseng (Burk.) F. H. Chen Ex C. Chow	(5S)-5-ethyloxolan-2-one	5325911	FALSE	C1CC(=O)OC1CC
MOL007512	0.9205	0.0795	0.7028	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	1-methyl-6-isopropylienebicyclo[3.1.0]hexane	Not Available	FALSE	C12(CCCC1C2=C(C)C)C
MOL007515	0.8663	0.1337	0.7368	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	14-pentadecenoic acid	543854	FALSE	C(=O)(CCCCCCCCCCCCC=C)O
MOL007516	0.9288	0.0712	0.9706	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	L-()-2,3-Butanediol	439888	FALSE	CC(C(C)O)O

MOL007517	0.9461	0.0539	0.8079	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(1S)-bornane-2,5-dione	6971265	FALSE	C1(=O)CC2C(=O)CC1(C2(C)C)C
MOL007518	0.9017	0.0983	0.8836	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Rikacid SA	7922	FALSE	O1C(=O)CCC1=O
MOL007519	0.8396	0.1604	0.6091	Santalum Album L.	(1S,2S,4R)-2-methyl-3-methylene-2-(4-methylpent-3-enyl)norbornane	11106484	FALSE	C1(C(=C)C2CCC1C2)(CCC=C(C)C)C
MOL007519	0.8396	0.1604	0.6091	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(1S,2S,4R)-2-methyl-3-methylene-2-(4-methylpent-3-enyl)norbornane	11106484	FALSE	C1(C(=C)C2CCC1C2)(CCC=C(C)C)C
MOL007519	0.8396	0.1604	0.6091	Panacis Japonici Rhizoma	(1S,2S,4R)-2-methyl-3-methylene-2-(4-methylpent-3-enyl)norbornane	11106484	FALSE	C1(C(=C)C2CCC1C2)(CCC=C(C)C)C
MOL007519	0.8396	0.1604	0.6091	Echinopsis Radix	(1S,2S,4R)-2-methyl-3-methylene-2-(4-methylpent-3-enyl)norbornane	11106484	FALSE	C1(C(=C)C2CCC1C2)(CCC=C(C)C)C
MOL007520	0.8943	0.1057	0.7320	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	trans-beta-Santalol	6450269	FALSE	C(/C(=C/CCC1(C2CCC(C1=C)C2)C)/C)O
MOL007521	0.9446	0.0554	0.8579	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	2-ethenyl-1,1-dimethyl-3-methylene-cyclohexane	Not Available	FALSE	C1(C(C(=C)CCC1)C=C)(C)C

MOL007522	0.9231	0.0769	0.9651	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	2-methyl-3-butene-1-ol	12454408	FALSE	C(C=C)(CO)C
MOL007523	0.9052	0.0948	0.9730	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	AKG	51	FALSE	C(=O)(CCC(=O)O)C(=O)O
MOL007524	0.8817	0.1183	0.8429	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(E)-dodec-3-en-1-yne	5367346	FALSE	C#C/C=C/CCCCCCCC
MOL007526	0.6779	0.3221	0.7094	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	7,10,13-Hexadecatrienoic acid, methyl ester	5367325	FALSE	C(=O)(CCCCC/C=C/C/C=C/C/C=C/CC)OC
MOL007527	0.8799	0.1201	0.6163	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	9-cedranone	Not Available	FALSE	C123C(CCC1C(C(C(C(=O)C2)C)C3)(C)C)C
MOL007528	0.8406	0.1594	0.7115	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	cubenol	Not Available	FALSE	C1(CCC(C2(CCC(=CC12)C)O)C)C(C)C
MOL007531	0.9034	0.0966	0.8692	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	isopulegyl acetate	14038452	FALSE	C1(C(CC(CC1)C)OC(=O)C)C(=C)C
MOL007532	0.8939	0.1061	0.9621	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	L-Milchsaeure	107689	FALSE	C(=O)(C(O)C)O
MOL007533	0.7349	0.2651	0.6950	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	santalyl acetate	24832104	FALSE	C(=O)(C)OC/C(=C\CCC1(C(=C)C2CCC1C2)C)/C
MOL007534	0.8260	0.1740	0.6868	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	sesquicineole	Not Available	FALSE	C12C(CC(CO1)(CC2)C)(CCC=C(C)C)C
MOL007535	0.2081	0.7919	0.6542	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(5S,8S,9S,10R,13R,14S,17R)-17-[(1R,4R)-4-ethyl-1,5-dimethylhexyl]-10,13-dimethyl-2,4,5,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,6-dione	13992092	FALSE	C1(=O)CCC2(C(C1)C(=O)CC1C3CCC(C(CCC(CC)C(C)C)C)C3(C)CCC21)C
MOL007536	0.1892	0.8108	0.6375	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	Stigmasta-5,22-dien-3-beta-yl acetate	6437330	FALSE	C12C(C3(C(=CC2)CC(CC3)OC(=O)C)C)CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C

MOL007536	0.1892	0.8108	0.6375	Lysimachiae Foenigraeci Herba	Stigmasta-5,22-dien-3-beta-yl acetate	6437330	FALSE	C12C(C3(C(=CC2)CC(CC3)OC(=O)C)C)CCC2(C1CCC2C(/C=C/C(C(C)C)CC)C)C
MOL007537	0.9473	0.0527	0.8073	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	viridiflorine	7565610	FALSE	C(=O)(C(C(C)O)(C(C)C)O)OCC1C2N(CCC2)CC1
MOL007538	0.8323	0.1677	0.7140	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	agarospirol	Not Available	FALSE	CC(C)(O)C1CCC2(C1)C(CCC=C2C)C
MOL007539	0.9331	0.0669	0.8194	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	amomumoside	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)C1C2(CC(C(C1)C2(C)C)O)C
MOL007540	0.9636	0.0364	0.8239	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	amomumoside_qt	7140312	FALSE	OC1CC2C(CC1(C2(C)C)C)O
MOL007541	0.9583	0.0417	0.9014	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	cis-isoascaridole	6430795	FALSE	C12(C(C)C)CCC(C=C1)(OO2)C
MOL007542	0.4235	0.5765	0.6649	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	camphorene	Not Available	FALSE	C1(C(=C)CCC=C(C)C)CCC(=CC1)CCC=C(C)C
MOL007543	0.7090	0.2910	0.6525	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	cis-9-Hexadecenal	5364643	FALSE	C(/C=C\CCCCCC)CCCCCCC=O
MOL007544	0.8895	0.1105	0.6520	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	isospathulenol	71590568	FALSE	C1CC(C2C3C(CCC(=C)C12)C3(C)C)(O)C
MOL007545	0.9022	0.0978	0.8489	Santalum Album L.	lanceol	15560069	FALSE	C(/C(=C/CCC(=C)C1CC=C(CC1)C)/C)O
MOL007545	0.9022	0.0978	0.8489	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	lanceol	15560069	FALSE	C(/C(=C/CCC(=C)C1CC=C(CC1)C)/C)O
MOL007546	0.8929	0.1071	0.9691	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	2H-pyran	186148	FALSE	C1C=CC=CO1
MOL007547	0.8942	0.1058	0.8976	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	2-Pyrol	12025	FALSE	N1C(=O)CCC1
MOL007548	0.8346	0.1654	0.7356	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(1S,4aS,8aS)-7-isopropyl-1,4a-dimethyl-2,3,4,5,6,8a-hexahydronaphthalen-1-ol	10966105	FALSE	C1(CCCC2(CCC(=CC12)C(C)C)C)(O)C
MOL007549	0.9273	0.0727	0.8667	Fritiliariae Irrhosae Bulbus	alpha-Thymidine	5270603	FALSE	OCC1C(O)CC(O1)n1c(=O)[nH]c(=O)c(C)c1
MOL007549	0.9273	0.0727	0.8667	Fritillariaeussuriensis Bulbus	alpha-Thymidine	5270603	FALSE	OCC1C(O)CC(O1)n1c(=O)[nH]c(=O)c(C)c1
MOL007549	0.9273	0.0727	0.8667	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	alpha-Thymidine	5270603	FALSE	OCC1C(O)CC(O1)n1c(=O)[nH]c(=O)c(C)c1
MOL007550	0.9626	0.0374	0.8817	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	trans-limonene oxide	Not Available	FALSE	C12(C(O1)CC(CC2)C(=C)C)C

MOL007552	0.8596	0.1404	0.6650	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	β-calacorene	Not Available	FALSE	C1CC(c2c(C1=C)ccc(c2)C)C(C)C
MOL007553	0.9487	0.0513	0.8045	Paederiae Scandentis Herba	(-)-beta-Fenchol	61123	FALSE	C12C(C(C(CC1)(C2)C)O)(C)C
MOL007553	0.9487	0.0513	0.8045	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(-)-beta-Fenchol	61123	FALSE	C12C(C(C(CC1)(C2)C)O)(C)C
MOL007554	0.8396	0.1604	0.6091	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(1S,2R,4R)-2-methyl-3-methylene-2-(4-methylpent-3-enyl)norbornane	10889018	FALSE	C12C(C(=C)C(CC1)C2)(CCC=C(C)C)C
MOL007555	0.9660	0.0340	0.8024	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	(1R,4R,5S)-1-isopropyl-4-methyl-3-bicyclo[3.1.0]hexanone	6553876	FALSE	C12(CC(=O)C(C1C2)C)C(C)C
MOL007556	0.9372	0.0628	0.9186	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	gamma-Terpinyl acetate	82480	FALSE	C(=O)(C)OC1(CCC(=C(C)C)CC1)C
MOL007557	0.8517	0.1483	0.6995	Amomum Aurantiacum H. T. Tsai Et S. W. Zhao	γ-gurjunene	Not Available	FALSE	C1(CCC2C(CCC(C=C12)C(=C)C)C)C
MOL007559	0.9608	0.0392	0.9751	Hordei Fructus Germinatus	Hordenine	68313	FALSE	Oc1ccc(cc1)CCN(C)C
MOL007559	0.9608	0.0392	0.9751	Selaginella Doederleinii Hieron	Hordenine	68313	FALSE	Oc1ccc(cc1)CCN(C)C
MOL007560	0.9563	0.0437	0.8349	Selaginella Doederleinii Hieron	(2R,3R,4R,5R,6S)-2-methyl-6-[4-(2-methylaminoethyl)phenoxy]tetrahydropyran-3,4,5-triol	20407216	FALSE	O(C1C(O)C(O)C(O)C(O1)C)c1ccc(cc1)CCNC
MOL007561	0.9528	0.0472	0.9783	Aurantii Fructus Immaturus	N-Methyltyramine	9727	FALSE	Oc1ccc(cc1)CCNC
MOL007561	0.9528	0.0472	0.9783	Citri Fructus	N-Methyltyramine	9727	FALSE	Oc1ccc(cc1)CCNC

MOL007561	0.9528	0.0472	0.9783	Selaginella Doederleinii Hieron	N-Methyltyramine	9727	FALSE	Oc1ccc(cc1)CCNC
MOL007561	0.9528	0.0472	0.9783	Aurantii Fructus	N-Methyltyramine	9727	FALSE	Oc1ccc(cc1)CCNC
MOL007565	0.9303	0.0697	0.8593	Selaginella Doederleinii Hieron	Doederleinic acid	5316957	FALSE	O1C2C1CC(=CC2O)C(=O)O
MOL007566	0.2244	0.7756	0.6963	Selaginella Doederleinii Hieron	2,2',3,3'-tetrahydrorobustaflavone	25112482	FALSE	c1(cc(cc2c1C(=O)CC(O2)c1ccc(c(c1)c1c(c2c(OC(CC2=O)c2ccc(cc2)O)cc1OC)O)OC)OC)O
MOL007567	0.1209	0.8791	0.7261	Selaginella Doederleinii Hieron	5-hydroxy-8-[5-(5-hydroxy-4-keto-7-methoxy-chromen-2-yl)-2-methoxy-phenyl]-7-methoxy-2-(4-methoxyphenyl)chromone	5490003	FALSE	c1(cc(=O)c2c(o1)c(c(cc2O)OC)c1c(ccc(c1)c1cc(=O)c2c(o1)cc(cc2O)OC)OC)c1ccc(cc1)OC
MOL007568	0.1804	0.8196	0.6896	Selaginella Doederleinii Hieron	heveaflavone	15559724	FALSE	c1(cc(=O)c2c(o1)c(c(cc2O)OC)c1c(ccc(c1)c1cc(=O)c2c(o1)cc(cc2O)OC)O)c1ccc(cc1)OC
MOL007569	0.9039	0.0961	0.9048	Selaginella Doederleinii Hieron	3-hydroxy-1-(3,5-dimethoxy-4-hydroxyphenyl)propan-1-one	54353627	FALSE	c1c(c(c(cc1C(=O)CCO)OC)O)OC
MOL007570	0.9287	0.0713	0.9268	Hydnocarpi Anthelminticae Semen	beta-Hydroxypropiovanillone	75142	FALSE	c1cc(c(cc1C(=O)CCO)OC)O
MOL007570	0.9287	0.0713	0.9268	Selaginella Doederleinii Hieron	beta-Hydroxypropiovanillone	75142	FALSE	c1cc(c(cc1C(=O)CCO)OC)O
MOL007573	0.9485	0.0515	0.7587	Selaginella Doederleinii Hieron	Hordenine-O-a-L-rhamnopyranoside	13877701	FALSE	C1(C(C(C(C(O1)Oc1ccc(cc1)CCN(C)C)O)O)O)C

MOL007575	0.6279	0.3721	0.6439	Selaginella Doederleinii Hieron	notracheloside	Not Available	FALSE	O1C(C(C(C(C1Oc1c(cc(cc1)CC1(C(=O)OCC1Cc1ccc(O)c(c1)OC)O)OC)O)O)O)O)CO
MOL007576	0.4258	0.5742	0.6140	Selaginella Doederleinii Hieron	6-[5-(5,7-dihydroxy-4-keto-chromen-2-yl)-2-methoxy-phenyl]-5,7-dihydroxy-2-(4-hydroxyphenyl)chromone	11757331	FALSE	c1c(cc(c2c1oc(cc2=O)c1cc(c(cc1)OC)c1c(cc2c(c1O)c(=O)cc(o2)c1ccc(cc1)O)O)O)O
MOL007577	0.9142	0.0858	0.9125	Perillae Fructus	2,4-Dimethylpentane	7907	FALSE	C(CC(C)C)(C)C
MOL007577	0.9142	0.0858	0.9125	Santalum Album L.	2,4-Dimethylpentane	7907	FALSE	C(CC(C)C)(C)C
MOL007578	0.9331	0.0669	0.9613	Ephedra Herba	2-Methylpentan-3-one	11265	FALSE	C(=O)(C(C)C)CC
MOL007578	0.9331	0.0669	0.9613	Santalum Album L.	2-Methylpentan-3-one	11265	FALSE	C(=O)(C(C)C)CC
MOL007579	0.9132	0.0868	0.9675	Santalum Album L.	cis-4-Hydroxy-L-proline	6971054	FALSE	C(=O)(C1NCC(C1)O)O
MOL007580	0.9005	0.0995	0.9314	Santalum Album L.	m-Picoline	7970	FALSE	c1(cccnc1)C
MOL007580	0.9005	0.0995	0.9314	Ginkgo Folium	m-Picoline	7970	FALSE	c1(cccnc1)C
MOL007581	0.7871	0.2129	0.9378	Santalum Album L.	Pymadin	1727	FALSE	c1(ccncc1)N
MOL007582	0.9255	0.0745	0.9517	Santalum Album L.	MIK	7909	FALSE	C(CC(=O)C)(C)C
MOL007582	0.9255	0.0745	0.9517	Ephedra Herba	MIK	7909	FALSE	C(CC(=O)C)(C)C
MOL007583	0.8821	0.1179	0.7128	Santalum Album L.	bergamotol, z-.alpha.-trans	Not Available	FALSE	C(/C(=C\CCC1(C2C(=CCC1C2)C)C)/C)O
MOL007584	0.9160	0.0840	0.8045	Santalum Album L.	e-nuciferol	Not Available	FALSE	C(/C(=C/CCC(C)c1ccc(cc1)C)/C)O
MOL007585	0.8971	0.1029	0.9289	Santalum Album L.	N-Ethylpyrrole	185226	FALSE	n1(cccc1)CC
MOL007586	0.8779	0.1221	0.9262	Santalum Album L.	Methylpyrrole	7304	FALSE	n1(cccc1)C
MOL007587	0.8765	0.1235	0.8384	Pseudostellariae Radix	Azole	8027	FALSE	c1cc[nH]c1
MOL007587	0.8765	0.1235	0.8384	Santalum Album L.	Azole	8027	FALSE	c1cc[nH]c1

MOL007588	0.9216	0.0784	0.7964	Santalum Album L.	10(E)-beta-Santalic acid	11673107	FALSE	C(=O)(/C(=C/CCC1(C(=C)C2CCC1C2)C)/C)O
MOL007589	0.8989	0.1011	0.9110	Santalum Album L.	2-Methylpenta-1,3-diene	638070	FALSE	C=C(/C=C/C)C
MOL007594	0.8474	0.1526	0.8175	Santalum Album L.	SANTALIN	246331	FALSE	c12c(C(=O)C3=C(C1=O)CCCC3)cc(c(c2O)OC)O
MOL007595	0.9483	0.0517	0.8418	Santalum Album L.	santenone	12663337	FALSE	C12(C(=O)CC(CC1)C2C)C
MOL007596	0.9256	0.0744	0.9133	Santalum Album L.	(Z)-3-(4-hydroxy-3,5-dimethoxy-phenyl)acrolein	5352903	FALSE	C(=O)/C=C\c1cc(c(c(c1)OC)O)OC
MOL007598	0.9494	0.0506	0.8884	Cotyledon Fimbriata Turcz.	2,2-dimethylchroman-6-carboxylic acid	222064	FALSE	C1(CCc2c(O1)ccc(c2)C(=O)O)(C)C
MOL007599	0.4429	0.5571	0.7028	Cotyledon Fimbriata Turcz.	Friedelanol	101341	FALSE	C12(C(C3C(CC2)(CCC(C3)(C)C)C)(CCC2(C1CCC1(C2CCC(C1C)O)C)C)C)C
MOL007600	0.9192	0.0808	0.7797	Cotyledon Fimbriata Turcz.	herbacetin-8-O-α-D-lyxopyranoside	Not Available	FALSE	c1(c(c(=O)c2c(o1)c(c(cc2O)O)OC1OCC(C(C1O)O)O)O)c1ccc(cc1)O
MOL007601	0.9227	0.0773	0.9566	Allium Azureum Ledeb.	(+)-L-Alliin	51380903	FALSE	C(=O)(C(N)CS(=O)CC=C)O
MOL007601	0.9227	0.0773	0.9566	Allii Sativi Bulbus	(+)-L-Alliin	51380903	FALSE	C(=O)(C(N)CS(=O)CC=C)O
MOL007602	0.8557	0.1443	0.8517	Allium Azureum Ledeb.	(E)-CH3SCH=CHSCH3	5370886	FALSE	C(=C\SC)/SC
MOL007603	0.9069	0.0931	0.9347	Allium Azureum Ledeb.	1,3-Propanedithiol	8013	FALSE	C(CS)CS
MOL007604	0.8804	0.1196	0.9410	Capsici Fructus	m-DITHIANE	10451	FALSE	S1CSCCC1
MOL007604	0.8804	0.1196	0.9410	Allium Azureum Ledeb.	m-DITHIANE	10451	FALSE	S1CSCCC1
MOL007604	0.8804	0.1196	0.9410	Allii Tuberosi Semen	m-DITHIANE	10451	FALSE	S1CSCCC1
MOL007605	0.8936	0.1064	0.8897	Allium Azureum Ledeb.	2,2-bis(methylthio)propane	525428	FALSE	CC(C)(SC)SC

MOL007606	0.8923	0.1077	0.7988	Allium Azureum Ledeb.	(1R,3R)-1-methyl-2,3,4,9-tetrahydro-1H-$b-carboline-3-carboxylic acid	6920042	FALSE	[nH]1c2c(c3ccccc13)CC(NC2C)C(=O)O
MOL007607	0.9168	0.0832	0.7846	Cichorii Radix	(3R)-2,3,4,9-tetrahydro-1H-$b-carboline-3-carboxylic acid	6920043	FALSE	[nH]1c2c(c3ccccc13)CC(NC2)C(=O)O
MOL007607	0.9168	0.0832	0.7846	Allium Azureum Ledeb.	(3R)-2,3,4,9-tetrahydro-1H-$b-carboline-3-carboxylic acid	6920043	FALSE	[nH]1c2c(c3ccccc13)CC(NC2)C(=O)O
MOL007608	0.9031	0.0969	0.8291	Allium Azureum Ledeb.	2,4-Dimethylthiophene	34296	FALSE	c1(cc(cs1)C)C
MOL007609	0.8383	0.1617	0.6270	Allium Azureum Ledeb.	allyl propyl trisulfide	525330	FALSE	S(SCCC)SCC=C
MOL007611	0.8545	0.1455	0.8693	Allium Azureum Ledeb.	3',5-dihydroxy-4'-methoxyflavone 7-o-α-rhamnosesyl(1.6)-β-d-glucoside	Not Available	FALSE	C1(C(O)C(O)C(O)C(O1)C)OCC1C(C(C(C(Oc2cc(c3c(c2)OC(CC3=O)c2cc(c(cc2)OC)O)O)O1)O)O)O
MOL007612	0.8494	0.1506	0.8684	Allium Azureum Ledeb.	3',5-dihydroxy-4'-methoxyflavone 7-o-β-glucosyl (1.2)-α-d-rhamnoseside	Not Available	FALSE	C1(C(OC2C(O)C(O)C(O)C(O2)CO)C(O)C(O)C(O1)C)Oc1cc(c2c(c1)OC(CC2=O)c1cc(c(cc1)OC)O)O
MOL007613	0.8249	0.1751	0.7430	Allium Azureum Ledeb.	3,5-dimethyl-1,2,4-trithiane	Not Available	FALSE	S1SC(SC(C1)C)C

MOL007614	0.8999	0.1001	0.9317	Allium Azureum Ledeb.	Allyl isopropyl sulfide	521309	FALSE	C=CCSC(C)C
MOL007615	0.9230	0.0770	0.9455	Allium Azureum Ledeb.	(3S)-3-methylhexane	638046	FALSE	CCC(CCC)C
MOL007616	0.8613	0.1387	0.9063	Allium Azureum Ledeb.	4',5-dihydroxy flavonoids-7-o-α- glucosyl (1.2)- β-d-rhamnoseside	Not Available	FALSE	C1(C(OC2C(O)C(O)C(O)C(O2)CO)C(O)C(O)C(O1)C)Oc1cc(c2c(c1)OC(CC2=O)c1ccc(cc1)O)O
MOL007617	0.8596	0.1404	0.8563	Allium Azureum Ledeb.	4-methyl-1,2,3-trithiane	Not Available	FALSE	S1SSC(CC1)C
MOL007618	0.7878	0.2122	0.7148	Allium Azureum Ledeb.	5-methyl-1,2,3,4-tetrathiane	Not Available	FALSE	S1SSSC(C1)C
MOL007619	0.9159	0.0841	0.9342	Allii Tuberosi Semen	Methyl allyl sulfide	66282	FALSE	C(C=C)SC
MOL007619	0.9159	0.0841	0.9342	Allii Sativi Bulbus	Methyl allyl sulfide	66282	FALSE	C(C=C)SC
MOL007619	0.9159	0.0841	0.9342	Allium Azureum Ledeb.	Methyl allyl sulfide	66282	FALSE	C(C=C)SC
MOL007620	0.8433	0.1567	0.6607	Allii Sativi Bulbus	Allitridin	16315	FALSE	S(SCC=C)SCC=C
MOL007620	0.8433	0.1567	0.6607	Allium Azureum Ledeb.	Allitridin	16315	FALSE	S(SCC=C)SCC=C
MOL007621	0.8971	0.1029	0.9547	Allium Azureum Ledeb.	DMDS	12232	FALSE	S(SC)C
MOL007621	0.8971	0.1029	0.9547	Raphani Semen	DMDS	12232	FALSE	S(SC)C
MOL007621	0.8971	0.1029	0.9547	Allii Sativi Bulbus	DMDS	12232	FALSE	S(SC)C
MOL007621	0.8971	0.1029	0.9547	Allii Tuberosi Semen	DMDS	12232	FALSE	S(SC)C
MOL007621	0.8971	0.1029	0.9547	Paederiae Scandentis Herba	DMDS	12232	FALSE	S(SC)C
MOL007622	0.9105	0.0895	0.9300	Allium Azureum Ledeb.	methyldisulfanylethane	123388	FALSE	S(CC)SC
MOL007624	0.8756	0.1244	0.8358	Allium Azureum Ledeb.	Thiole	8030	TRUE	c1ccsc1
MOL007625	0.7079	0.2921	0.8248	Allium Azureum Ledeb.	desgalactotigonin7	Not Available	FALSE	C1(C(C(C(C(O1)OC1C(OC(C(C1OC1OCC(O)C(C1O)O)O)O)CO)OC1C(C(C(OC1CO)OC1CCC2(C(C1)CCC1C2CCC2C1CC1OC3(OCC(CC3)C)C(C21C)C)C)O)O)O)O)O)CO
MOL007626	0.3251	0.6749	0.7474	Allium Azureum Ledeb.	desgalactotigonin_qt	Not Available	FALSE	OC1CCC2(C(C1)CCC1C2CCC2C1CC1OC3(OCC(CC3)C)C(C21C)C)C
MOL007627	0.8540	0.1460	0.7936	Allium Azureum Ledeb.	diAllS2	16590	FALSE	S(SCC=C)CC=C
MOL007627	0.8540	0.1460	0.7936	Allii Tuberosi Semen	diAllS2	16590	FALSE	S(SCC=C)CC=C
MOL007627	0.8540	0.1460	0.7936	Allii Sativi Bulbus	diAllS2	16590	FALSE	S(SCC=C)CC=C
MOL007627	0.8540	0.1460	0.7936	Capsici Fructus	diAllS2	16590	FALSE	S(SCC=C)CC=C

MOL007628	0.8401	0.1599	0.7934	Allium Azureum Ledeb.	Methyl trisulfide	19310	FALSE	S(SC)SC
MOL007628	0.8401	0.1599	0.7934	Raphani Semen	Methyl trisulfide	19310	FALSE	S(SC)SC
MOL007628	0.8401	0.1599	0.7934	Allii Sativi Bulbus	Methyl trisulfide	19310	FALSE	S(SC)SC
MOL007628	0.8401	0.1599	0.7934	Capsellae Herba	Methyl trisulfide	19310	FALSE	S(SC)SC
MOL007628	0.8401	0.1599	0.7934	Momordicae Fructus	Methyl trisulfide	19310	FALSE	S(SC)SC
MOL007629	0.8613	0.1387	0.7424	Allium Azureum Ledeb.	SSP-SSP	12377	FALSE	S(SCCC)CCC
MOL007630	0.8261	0.1739	0.6015	Allium Azureum Ledeb.	PROPYL TRISULFIDE	22383	FALSE	S(SCCC)SCCC
MOL007630	0.8261	0.1739	0.6015	Allii Fistulost Bulbus	PROPYL TRISULFIDE	22383	FALSE	S(SCCC)SCCC
MOL007631	0.8170	0.1830	0.6163	Allium Azureum Ledeb.	Heptadecenoic acid	5282747	FALSE	C(=O)(/C=C/CCCCCCCCCCCCCC)O
MOL007632	0.8584	0.1416	0.8258	Allium Azureum Ledeb.	2-methyldisulfanylpropane	123494	FALSE	S(SC)C(C)C
MOL007632	0.8584	0.1416	0.8258	Allii Tuberosi Semen	2-methyldisulfanylpropane	123494	FALSE	S(SC)C(C)C
MOL007633	0.8399	0.1601	0.7520	Allium Azureum Ledeb.	(E)-1-isopropyldisulfanylprop-1-ene	Not Available	FALSE	S(S/C=C/C)C(C)C
MOL007634	0.3159	0.6841	0.7723	Allium Azureum Ledeb.	laxogenin	Not Available	FALSE	C1(CCC2(C(C1)C(=O)CC1C3CC4OC5(C(C4C3(C)CCC21)C)OCC(CC5)C)C)O
MOL007635	0.9476	0.0524	0.8584	Allium Azureum Ledeb.	Lunularic acid	161413	FALSE	C(=O)(c1c(cccc1CCc1ccc(cc1)O)O)O
MOL007636	0.7229	0.2771	0.8405	Allium Azureum Ledeb.	macrostemonoside a	Not Available	FALSE	C1(CCC2(OC1)OC1C(C2C)(C)C2C(C1)C1C(CC2)C2(C(CC1)CC(CC2)C1(OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)OC1OC(C(C(C1O)O)O)CO)O)CO)OC1OC(C(C(C1O)O)O)CO)C)C
MOL007637	0.3204	0.6796	0.6678	Allium Azureum Ledeb.	macrostemonoside d_qt	Not Available	FALSE	C1(CCC2(OC1)OC1C(C2C)(C)C2C(C1)C1C(CC2)C2(C(CC1)CCCC2)C)C
MOL007638	0.6805	0.3195	0.8342	Allium Azureum Ledeb.	macrostemonoside d	Not Available	FALSE	C1(CCC2(OC1)OC1C(C2C)(C)C2C(C1)C1C(CC2)C2(C(CC1)CC(CC2)C1(OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)OC1OC(C(C(C1O)O)O)CO)O)CO)OC1OC(C(C(C1O)O)O)COC(=O)C)C)C

MOL007639	0.7651	0.2349	0.8010	Allium Azureum Ledeb.	macrostemonoside e	Not Available	FALSE	C12(C(C3CCC4CC(C5OC(C(C(C5OC5OC(C(C(C5O)O)O)CO)OC5OC(C(C(C5O)O)O)CO)O)CO)(OC5OC(C(C(C5O)O)O)CO)CCC4(C)C3CC1)CC1C2C(=C(O1)CCC(COC1OC(C(C(C1O)O)O)CO)C)C)C
MOL007640	0.2792	0.7208	0.7661	Allium Azureum Ledeb.	macrostemonoside e_qt	Not Available	FALSE	C12(C(C3CCC4C(CCC(O)C4)(C)C3CC1)CC1OC(=C(C21)C)CCC(CO)C)C
MOL007641	0.7688	0.2312	0.8184	Allium Azureum Ledeb.	macrostemonoside f	Not Available	FALSE	O(C1C(OC2C(O)C(O)C(O)C(O2)CO)C(O)C(O)C(O1)CO)C1CCC2(C(C1)CCC1C3CC4OC(=C(C4C3(C)CCC21)C)CCC(COC1C(O)C(O)C(O)C(O1)CO)C)C
MOL007642	0.2792	0.7208	0.7661	Allium Azureum Ledeb.	macrostemonoside f_qt	Not Available	FALSE	OC1CCC2(C(C1)CCC1C3C(C)(CCC21)C1C(OC(=C1C)CCC(C)CO)C3)C
MOL007643	0.8971	0.1029	0.8947	Capsici Fructus	methylallyl disulphide	62434	FALSE	S(SC)CC=C
MOL007643	0.8971	0.1029	0.8947	Allium Azureum Ledeb.	methylallyl disulphide	62434	FALSE	S(SC)CC=C
MOL007643	0.8971	0.1029	0.8947	Allii Sativi Bulbus	methylallyl disulphide	62434	FALSE	S(SC)CC=C
MOL007644	0.8662	0.1338	0.8414	Allii Sativi Bulbus	Methyldithio-1-propene	5366552	FALSE	S(SC)/C=C/C
MOL007644	0.8662	0.1338	0.8414	Allii Tuberosi Semen	Methyldithio-1-propene	5366552	FALSE	S(SC)/C=C/C
MOL007644	0.8662	0.1338	0.8414	Capsici Fructus	Methyldithio-1-propene	5366552	FALSE	S(SC)/C=C/C
MOL007644	0.8662	0.1338	0.8414	Allium Azureum Ledeb.	Methyldithio-1-propene	5366552	FALSE	S(SC)/C=C/C
MOL007645	0.8478	0.1522	0.7395	Allium Azureum Ledeb.	Methyl 1-propenyl trisulfide	5352690	FALSE	S(S/C=C/C)SC
MOL007646	0.8555	0.1445	0.8444	Allium Azureum Ledeb.	2,3-Dithiahexane	16592	FALSE	S(SC)CCC
MOL007646	0.8555	0.1445	0.8444	Gynostemmae Pentaphylli Herba	2,3-Dithiahexane	16592	FALSE	S(SC)CCC
MOL007647	0.8299	0.1701	0.6955	Allium Azureum Ledeb.	Propyl methyl trisulfide	5319765	FALSE	S(SCCC)SC
MOL007647	0.8299	0.1701	0.6955	Cistanches Herba	Propyl methyl trisulfide	5319765	FALSE	S(SCCC)SC
MOL007648	0.8575	0.1425	0.7629	Allium Azureum Ledeb.	APDS	16591	FALSE	S(SCCC)CC=C
MOL007649	0.8472	0.1528	0.7359	Allium Azureum Ledeb.	2-propyldisulfanylpropane	118529	FALSE	S(SCCC)C(C)C
MOL007650	0.8219	0.1781	0.7466	Allium Azureum Ledeb.	PGA(sup 1)	5281912	FALSE	C1(C(C=CC1=O)/C=C/C(CCCCC)O)CCCCCCC(=O)O

MOL007651	0.8268	0.1732	0.7182	Allium Azureum Ledeb.	Prostaglandin B1	5280388	FALSE	C1(=C(CCC1=O)/C=C/C(CCCCC)O)CCCCCCC(=O)O
MOL007655	0.5397	0.4603	0.6991	Figwort Root	angroside C	Not Available	FALSE	C1(C(C(OC(C1O)OCCc1cc(c(cc1)OC)O)COC1C(C(C(CO1)O)O)O)OC(=O)/C=C\c1cc(c(cc1)O)OC)OC1C(C(C(C(O1)C)O)O)O
MOL007656	0.5149	0.4851	0.6514	Figwort Root	scropolioside A	10557021	FALSE	O1C2(C1C(OC1OC(C(OC(=O)C)C(OC(=O)/C=C\c3ccc(OC)cc3)C1OC(=O)C)C)C1C2C(OC=C1)OC1OC(C(O)C(O)C1O)CO)CO
MOL007659	0.5209	0.4791	0.6758	Figwort Root	scropolioside D	Not Available	FALSE	O1C2(C1C(OC1OC(C(OC(=O)C)C(OC(=O)/C=C\c3ccccc3)C1OC(=O)C)C)C1C2C(OC=C1)OC1OC(C(O)C(O)C1O)CO)CO
MOL007662	0.7834	0.2166	0.7509	Figwort Root	harpagoside_qt	Not Available	FALSE	C12C(C(CC1(OC(=O)/C=C/c1ccccc1)C)O)(C=COC2O)O
MOL007663	0.9229	0.0771	0.8448	Figwort Root	catapol	11810558	FALSE	C12(C3C(C(C1O2)O)C=COC3OC1OC(C(C(C1O)O)O)CO)CO
MOL007665	0.9559	0.0441	0.8681	Paederiae Scandentis Herba	geniposide_qt	Not Available	FALSE	C12C(C(=COC1O)C(=O)OC)CC=C2CO
MOL007665	0.9559	0.0441	0.8681	Figwort Root	geniposide_qt	Not Available	FALSE	C12C(C(=COC1O)C(=O)OC)CC=C2CO
MOL007666	0.8966	0.1034	0.9428	Figwort Root	5-(methylthio)valeronitrile	93320	FALSE	C(#N)CCCCSC
MOL007667	0.6839	0.3161	0.7286	Figwort Root	6'-O-cinnamoylharpagirle	Not Available	FALSE	c1cccc(c1)/C=C\C(=O)OCC1C(C(C(C(O1)OC1C2C(C=CC1)(C(CC2(O)C)O)O)O)O)O
MOL007668	0.9322	0.0678	0.8340	Figwort Root	6'-O-cinnamoylharpagirle_qt 2	Not Available	FALSE	OC1C2C(C=CC1)(C(CC2(O)C)O)O
MOL007669	0.9025	0.0975	0.8107	Figwort Root	6-O-methylcatalpol	44144291	FALSE	O1C2(C1C(OC)C1C2C(OC=C1)OC1OC(C(O)C(O)C1O)CO)CO
MOL007670	0.9255	0.0745	0.7725	Figwort Root	6-O-methylcatalpol_qt	Not Available	FALSE	O1C2(C1C(OC)C1C2C(OC=C1)O)CO
MOL007671	0.9346	0.0654	0.8555	Figwort Root	harpagide	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)(CO)O)C1C2C(C=CO1)(CCC2(C)O)O
MOL007672	0.9519	0.0481	0.8781	Figwort Root	7-hydroxy-9-hydroxymethyl-3-oxo-	Not Available	FALSE	C12CC(=O)CCC1C(C=C2CO)O
MOL007673	0.5425	0.4575	0.6605	Figwort Root	cistanoside D	5315930	FALSE	O(C1C(OC(=O)/C=C/c2cc(OC)c(O)cc2)C(OC(OCCc2cc(OC)c(O)cc2)C1O)CO)C1OC(C(O)C(O)C1O)C
MOL007673	0.5425	0.4575	0.6605	Cistanches Herba	cistanoside D	5315930	FALSE	O(C1C(OC(=O)/C=C/c2cc(OC)c(O)cc2)C(OC(OCCc2cc(OC)c(O)cc2)C1O)CO)C1OC(C(O)C(O)C1O)C
MOL007674	0.8056	0.1944	0.8194	Abrus Precatorius L.	abrusin	Not Available	FALSE	c1(cc(=O)c2c(o1)c(c(c(c2O)OC)OC)C1C(O)C(O)C(O)C(O1)CO)c1ccc(cc1)O

MOL007675	0.8168	0.1832	0.8119	Abrus Precatorius L.	abrusin-2'-O-apioside	Not Available	FALSE	O(C1C(O)C(O)C(OC1c1c2oc(cc(=O)c2c(O)c(OC)c1OC)c1ccc(O)cc1)CO)C1OCC(O)(C1O)CO
MOL007676	0.3918	0.6082	0.8096	Abrus Precatorius L.	(4R,4aR,6aR,6aS,6bR,8aR,10S,12aS)-4,10-dihydroxy-2,2,4a,6a,6b,9,9,12a-octamethyl-3,4,5,6,6a,7,8,8a,10,11,12,14-dodecahydro-1H-picen-13-one	21594179	FALSE	C1C(CC(C2(CCC3(C4(CCC5C(C(CCC5(C4C(=O)CC3=C12)C)O)(C)C)C)C)C)O)(C)C
MOL007677	0.9429	0.0571	0.9672	Abrus Precatorius L.	aldehydo-L-arabinose	5460291	FALSE	C(C(CO)O)(C(C=O)O)O
MOL007677	0.9429	0.0571	0.9672	Rosae Laevigatae Fructus	aldehydo-L-arabinose	5460291	FALSE	C(C(CO)O)(C(C=O)O)O
MOL007678	0.9132	0.0868	0.8193	Abrus Precatorius L.	precatorine	193241	FALSE	O(c1c(O)cc(cc1O)C(=O)O)C(=O)c1c[n+](ccc1)C
MOL007679	0.9365	0.0635	0.7697	Abrus Precatorius L.	hypaphorine	160489	FALSE	C(=O)(C(Cc1c[nH]c2c1cccc2)[N+](C)(C)C)O
MOL007679	0.9365	0.0635	0.7697	Vaccariae Semen	hypaphorine	160489	FALSE	C(=O)(C(Cc1c[nH]c2c1cccc2)[N+](C)(C)C)O
MOL007680	0.9524	0.0476	0.8732	Abri Herba	Abrine	6921653	FALSE	c12c(CC(C(=O)O)NC)c[nH]c1cccc2
MOL007680	0.9524	0.0476	0.8732	Abrus Precatorius L.	Abrine	6921653	FALSE	c12c(CC(C(=O)O)NC)c[nH]c1cccc2
MOL007681	0.4108	0.5892	0.7532	Abrus Precatorius L.	sophoradiol	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)C(CC(C)(C)CC4C3=CCC21)O)C)O
MOL007682	0.2075	0.7925	0.6415	Abrus Precatorius L.	abricin	Not Available	FALSE	C1CCCC2=CC(=O)C3C4CCC(C4(CCC3C12C)C)C(C)CCCC(CO)C
MOL007683	0.1740	0.8260	0.7190	Abrus Precatorius L.	abridin	Not Available	FALSE	C1(=O)CCC2(C(=C1)CCC1C3CCC(C(/C=C/C(=O)C)C)C3(C)CCC21)C
MOL007684	0.7710	0.2290	0.9264	Abrus Precatorius L.	abrectorin	44257585	FALSE	c1(cc(=O)c2c(o1)cc(c(c2)OC)O)c1cc(c(cc1)OC)O
MOL007685	0.9442	0.0558	0.9405	Pseudostellariae Radix	Hydroferulic	14340	FALSE	c1(cc(c(cc1)O)OC)CCC(=O)O
MOL007685	0.9442	0.0558	0.9405	Gypsophila Licentiana Hand.-Mazz.	Hydroferulic	14340	FALSE	c1(cc(c(cc1)O)OC)CCC(=O)O
MOL007687	0.9550	0.0450	0.8963	Gypsophila Licentiana Hand.-Mazz.	Dimethylcaffeic acid	717531	FALSE	C(=O)(/C=C/c1cc(c(cc1)OC)OC)O
MOL007688	0.7607	0.2393	0.7346	Gypsophila Licentiana Hand.-Mazz.	desacetylanguidine	Not Available	FALSE	C12(C3(C4(C(OC1C(C3O)O)C=C(CC4)C)COC(=O)C)C)CC2
MOL007689	0.1987	0.8013	0.6312	Gypsophila Licentiana Hand.-Mazz.	stigmast-7-enol	Not Available	FALSE	C1(CCC2(C(=CC=C3C4CCC(C(/C=C/C(CC)C(C)C)C)C4(C)CCC23)C1)C)O

MOL007691	0.2400	0.7600	0.6133	Gypsophila Licentiana Hand.-Mazz.	stigmast-7-enol-glucoside_qt	Not Available	FALSE	OC1CCC2(C(C1)CC=C1C3CCC(C(CCC(C(C)C)CC)C)C3(C)CCC21)C
MOL007693	0.7533	0.2467	0.6375	Gypsophila Licentiana Hand.-Mazz.	dichotomide,ii	Not Available	FALSE	c1cccc2c1[nH]c1c2cc(nc1C(C)O)C(=O)N/C=C\C(=O)OC
MOL007694	0.4506	0.5494	0.8545	Gypsophila Licentiana Hand.-Mazz.	dichotomin,h	Not Available	FALSE	N12C(CCC1)C(=O)NC(C(C)O)C(=O)NC(Cc1ccccc1)C(=O)NC(C(=O)N1C(CCC1)C(=O)CC(C(=O)NC(C(=O)NC(C2=O)C)C(CC)C)CC(C)C)Cc1ccc(cc1)O
MOL007695	0.3676	0.6324	0.8595	Gypsophila Licentiana Hand.-Mazz.	dichotomin,i	Not Available	FALSE	N12C(CCC1)C(=O)NC(C(C)O)C(=O)NC(Cc1ccccc1)C(=O)NC(C(=O)N1C(CCC1)C(=O)CC(C(=O)NC(C(=O)NC(C2=O)CC(C)C)C(CC)C)CC(C)C)Cc1ccc(cc1)O
MOL007696	0.4629	0.5371	0.6754	Gypsophila Licentiana Hand.-Mazz.	dichotomin,j	44566559	FALSE	c1(ccc(cc1)O)CC1C(=O)NC(C)C(=O)NCC(=O)NC(C(C)CC)C(=O)NC(C(=O)NC(C(=O)N1)CC(C)C)Cc1ccccc1
MOL007697	0.4515	0.5485	0.8850	Gypsophila Licentiana Hand.-Mazz.	dichotomin,k	Not Available	FALSE	c1(ccc(cc1)CC1C(=O)NC(C(=O)NC(C(=O)NC(C(=O)N2C(CCC2)C(=O)NC(C(=O)NC(C(=O)NC(C(=O)N2C(C(=O)N1)CCC2)C(CC)C)C(C)C)C(C)CC)C(C)C)Cc1ccc(cc1)O)O
MOL007698	0.9078	0.0922	0.8099	Gypsophila Licentiana Hand.-Mazz.	dichotomine,a	Not Available	FALSE	c1cccc2c1[nH]c1c2cc(nc1C(C)O)C(=O)O
MOL007699	0.9013	0.0987	0.7306	Gypsophila Licentiana Hand.-Mazz.	dichotomine,b	Not Available	FALSE	c1cccc2c1[nH]c1c2cc(nc1C(CO)O)C(=O)O
MOL007700	0.8867	0.1133	0.7175	Gypsophila Licentiana Hand.-Mazz.	dichotomine,c	Not Available	FALSE	c1cccc2c1[nH]c1c2cc(nc1C(CO)O)C(=O)OC
MOL007701	0.7330	0.2670	0.6711	Gypsophila Licentiana Hand.-Mazz.	dichotomine,d	Not Available	FALSE	c1cccc2c1[nH]c1c2cc(nc1C(CO)O)C(=O)OCCCC
MOL007702	0.7913	0.2087	0.7138	Gypsophila Licentiana Hand.-Mazz.	3-[3-[5-(2-carboxyethyl)-2-hydroxy-3-methoxyphenyl]-5-methoxy-4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]propanoic acid	11203673	FALSE	c1(cc(cc(c1O)c1cc(cc(c1OC1C(C(C(C(O1)CO)O)O)O)OC)CCC(=O)O)CCC(=O)O)OC

MOL007703	0.8558	0.1442	0.6421	Gypsophila Licentiana Hand.-Mazz.	3-[3-[5-(2-carboxyethyl)-2-hydroxy-3-methoxyphenyl]-4-hydroxy-5-methoxyphenyl]propanoic acid	11223011	FALSE	c1(cc(cc(c1O)c1cc(cc(c1O)OC)CCC(=O)O)CCC(=O)O)OC
MOL007704	0.6671	0.3329	0.6050	Gypsophila Licentiana Hand.-Mazz.	dichotomoside,b	Not Available	FALSE	c1(cc(cc(c1O)c1cc(cc(c1OC1C(C(C(C(O1)CO)O)O)O)OC)CCC(=O)OCCCO)CCC(=O)O)OC
MOL007706	0.6740	0.3260	0.6038	Gypsophila Licentiana Hand.-Mazz.	dichotomoside,c	Not Available	FALSE	c1(cc(cc(c1O)c1cc(cc(c1OC1C(C(C(C(O1)CO)O)O)O)OC)CCC(=O)O)CCC(=O)OCCCO)OC
MOL007709	0.7849	0.2151	0.7205	Gypsophila Licentiana Hand.-Mazz.	butyl 3-[3-methoxy-4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl] propanoate	11327449	FALSE	c1cc(cc(c1OC1C(C(C(C(O1)CO)O)O)O)OC)CCC(=O)OCCCC
MOL007710	0.9369	0.0631	0.8985	Gypsophila Licentiana Hand.-Mazz.	dichotomoside,e_qt	Not Available	FALSE	c1cc(cc(c1O)OC)CCC(=O)OCCCC
MOL007711	0.8936	0.1064	0.7463	Gypsophila Licentiana Hand.-Mazz.	glucodichotomine,b	Not Available	FALSE	c1cccc2c1[nH]c1c2cc(nc1C(CO)OC1C(C(C(C(O1)CO)O)O)O)C(=O)O
MOL007712	0.9203	0.0797	0.7230	Gypsophila Licentiana Hand.-Mazz.	glucodichotomine,b_qt	Not Available	FALSE	c1cccc2c1[NH+]=C1C2=CC(=NC1C(CO)O)C(=O)O
MOL007714	0.5012	0.4988	0.8376	Lithospermum Erythrorhizon	1-methoxyacetylshikonin	Not Available	FALSE	C1(=O)C=CC(=O)c2c(c(cc(c12)O)C(CC=C(C)C)OC(=O)C)OC
MOL007715	0.6154	0.3846	0.6232	Lithospermum Erythrorhizon	[(1R)-1-(5,8-dihydroxy-1,4-dioxo-2-naphthyl)-4-methyl-pent-3-enyl] propanoate	153984	FALSE	C1(=O)C(=CC(=O)c2c(ccc(c12)O)O)C(CC=C(C)C)OC(=O)CC
MOL007716	0.7212	0.2788	0.6998	Lithospermum Erythrorhizon	acetylshikonin	9967285	FALSE	c12c(C(=O)C=C(C1=O)C(CC=C(C)C)OC(=O)C)c(ccc2O)O
MOL007719	0.8675	0.1325	0.8280	Lithospermum Erythrorhizon	Arnebin 7	98914	FALSE	c12c(C(=O)C=C(C1=O)CCC=C(C)C)c(ccc2O)O

MOL007719	0.8675	0.1325	0.8280	Schisandrae Chinensis Fructus	Arnebin 7	98914	FALSE	c12c(C(=O)C=C(C1=O)CCC=C(C)C)c(ccc2O)O
MOL007720	0.9490	0.0510	0.9297	Lithospermum Erythrorhizon	(2R)-3-oxo-2-phenylbutane nitrile	700649	FALSE	C(#N)C(C(=O)C)c1ccccc1
MOL007721	0.2336	0.7664	0.7228	Lithospermum Erythrorhizon	Totarol	92783	FALSE	C12(c3c(c(c(cc3)O)C(C)C)CCC1C(CCC2)(C)C)C
MOL007722	0.8983	0.1017	0.8053	Lithospermum Erythrorhizon	Isoarnebin 4	479503	FALSE	CC(=CCC(O)C1=CC(=O)c2c(C1=O)c(O)ccc2O)C
MOL007723	0.8684	0.1316	0.8439	Lithospermum Erythrorhizon	Alkannan	5317321	FALSE	C1(=O)C(=CC(=O)c2c(ccc(c12)O)O)CCCC(C)C
MOL007724	0.9038	0.0962	0.9704	Lithospermum Erythrorhizon	SENECIC ACID	10931	FALSE	C(=CC(=O)O)(C)C
MOL007725	0.9453	0.0547	0.8501	Lithospermum Erythrorhizon	5-Methylphthalide	41013	FALSE	c1c(cc2c(c1)C(=O)OC2)C
MOL007727	0.9302	0.0698	0.9691	Lithospermum Erythrorhizon	Ethyl senecioate	12516	FALSE	C(=C(C)C)C(=O)OCC
MOL007732	0.7422	0.2578	0.7845	Lithospermum Erythrorhizon	arnebinone	Not Available	FALSE	C1(=O)C(=C(C(=O)C2=C1C(CCC2C(=C)C)(C=C)C)OC)OC
MOL007733	0.8760	0.1240	0.7681	Lithospermum Erythrorhizon	Butyric acid, 3-hydroxy-3-methyl-	Not Available	FALSE	C(=O)(C(C(C)(C)O)c1ccc(cc1)C1CCCCC1)O
MOL007734	0.7830	0.2170	0.8136	Lithospermum Erythrorhizon	5-[(E)-5-(3-furyl)-2-methyl-pent-2-enyl]-2,3-dimethoxy-p-benzoquinone	6505036	FALSE	C1(=O)C(=C(C(=O)C(=C1)C/C(=C/CCc1cocc1)/C)OC)OC
MOL007741	0.5737	0.4263	0.7560	Herba Sarcandrae	epimedin c	Not Available	FALSE	c12c(c(=O)c(c(o2)c2ccc(cc2)OC)OC2C(OC3C(C(C(C(O3)C)O)O)O)C(C(C(O2)C)O)O)c(cc(c1CC=C(C)C)OC1OC(C(C(C1O)O)O)CO)O
MOL007742	0.8762	0.1238	0.7857	Herba Sarcandrae	Istanbulin-A	3082428	FALSE	O1C2(O)CC3C(C(CCC3=O)C)(CC2=C(C1=O)C)C
MOL007743	0.8884	0.1116	0.9200	Herba Sarcandrae	ZINC00391893	6950539	FALSE	c12c(OC(CC1=O)c1ccccc1)cc(cc2O)OC
MOL007744	0.7920	0.2080	0.7744	Herba Sarcandrae	CHLORANTHALACTONE A	Not Available	FALSE	O1C2=CC3(C4C(C4)C(=C)C3CC2=C(C1=O)C)C
MOL007745	0.9386	0.0614	0.9144	Meliae Cortex	WLN: QVR BVQ	18183610	FALSE	C(=O)(c1c(C(=O)O)cccc1)O
MOL007745	0.9386	0.0614	0.9144	Angelicae Sinensis Radix	WLN: QVR BVQ	18183610	FALSE	C(=O)(c1c(C(=O)O)cccc1)O

MOL007745	0.9386	0.0614	0.9144	Sojae Semen Nigrum	WLN: QVR BVQ	18183610	FALSE	C(=O)(c1c(C(=O)O)cccc1)O
MOL007745	0.9386	0.0614	0.9144	Herba Sarcandrae	WLN: QVR BVQ	18183610	FALSE	C(=O)(c1c(C(=O)O)cccc1)O
MOL007746	0.8974	0.1026	0.8442	Herba Sarcandrae	chloranoside a	Not Available	FALSE	OC1(C2C(C3(C1CC1=C(C(=O)OC1=C3)C)C)C2)COC1OC(C(O)C(O)C1O)CO
MOL007747	0.8904	0.1096	0.8009	Herba Sarcandrae	chloranoside a_qt	Not Available	FALSE	OC1(C2C(C3(C1CC1=C(C(=O)OC1=C3)C)C)C2)CO
MOL007748	0.9052	0.0948	0.8890	Herba Sarcandrae	Uvangoletin	6483649	FALSE	O(c1c(C(=O)CCc2ccccc2)c(O)cc(O)c1)C
MOL007749	0.9086	0.0914	0.8108	Eucommiae Cortex	[(1S,4aS,5R,7S,7aS)-4a,5-dihydroxy-7-methyl-1-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-1,5,6,7a-tetrahydrocyclopenta[c]pyran-7-yl] ethanoate	9978650	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)C1C2C(C=CO1)(C(CC2(C)OC(=O)C)O)O
MOL007749	0.9086	0.0914	0.8108	Ajugae Decumbentis Herba	[(1S,4aS,5R,7S,7aS)-4a,5-dihydroxy-7-methyl-1-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-1,5,6,7a-tetrahydrocyclopenta[c]pyran-7-yl] ethanoate	9978650	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)C1C2C(C=CO1)(C(CC2(C)OC(=O)C)O)O
MOL007750	0.9373	0.0627	0.8045	Ajugae Decumbentis Herba	Harpagide 7-acetate_qt	Not Available	FALSE	OC1C2C(C=CO1)(C(CC2(C)OC(=O)C)O)O
MOL007750	0.9373	0.0627	0.8045	Eucommiae Cortex	Harpagide 7-acetate_qt	Not Available	FALSE	OC1C2C(C=CO1)(C(CC2(C)OC(=O)C)O)O

MOL007751	0.5677	0.4323	0.6933	Ajugae Decumbentis Herba	Ajugasterone C	441826	FALSE	C1(C(CC2(C(C1)C(=O)C=C1C3(CCC(C(C(CCC(C)C)O)(C)O)C3(C)CC(C21)O)O)C)O)O
MOL007755	0.7751	0.2249	0.7339	Ajugae Decumbentis Herba	decumbeside B	Not Available	FALSE	c1(ccc(cc1)/C=C/C(=O)OC1C(C(C(OC1OC1C2C(C=CO1)(CC1C2(O1)C)O)CO)O)O)O
MOL007756	0.7313	0.2687	0.6930	Ajugae Decumbentis Herba	decumbeside C	Not Available	FALSE	O(C1C(O)C(C(O)C(O1)CO)OC(=O)/C=C/c1ccc(cc1)O)C1C2C(C=CO1)(C(CC2(C)OC(=O)C)O)O
MOL007757	0.7313	0.2687	0.6930	Ajugae Decumbentis Herba	decumbeside D	Not Available	FALSE	O(C1C(O)C(C(O)C(O1)CO)OC(=O)/C=C/c1ccc(cc1)O)C1C2C(C=CO1)(C(CC2(C)OC(=O)C)O)O
MOL007761	0.7751	0.2249	0.7339	Ajugae Decumbentis Herba	decumbeside A	Not Available	FALSE	c1(ccc(cc1)/C=C/C(=O)OC1C(C(C(OC1OC1C2C(C=CO1)(CC1C2(O1)C)O)CO)O)O)O
MOL007769	0.9029	0.0971	0.8226	Ajugae Decumbentis Herba	reptoside	44584096	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)C1C2C(C=CO1)(CCC2(C)OC(=O)C)O
MOL007769	0.9029	0.0971	0.8226	Eucommiae Cortex	reptoside	44584096	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)C1C2C(C=CO1)(CCC2(C)OC(=O)C)O
MOL007769	0.9029	0.0971	0.8226	Eucommiae Folium	reptoside	44584096	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)C1C2C(C=CO1)(CCC2(C)OC(=O)C)O
MOL007770	0.9551	0.0449	0.8166	Eucommiae Cortex	reptoside_qt	Not Available	FALSE	OC1C2C(C=CO1)(CCC2(C)OC(=O)C)O
MOL007770	0.9551	0.0449	0.8166	Eucommiae Folium	reptoside_qt	Not Available	FALSE	OC1C2C(C=CO1)(CCC2(C)OC(=O)C)O
MOL007770	0.9551	0.0449	0.8166	Ajugae Decumbentis Herba	reptoside_qt	Not Available	FALSE	OC1C2C(C=CO1)(CCC2(C)OC(=O)C)O
MOL007771	0.5220	0.4780	0.7349	Ajugae Decumbentis Herba	Ajugalactone	181744	FALSE	C1(C(CC2(C(C1)C(=O)C=C1C3(CCC(C(C4CC(=C(C(=O)O4)C)CC)(C)O)C3(C)C(=O)CC21)O)C)O)O
MOL007772	0.4693	0.5307	0.6501	Ajugae Decumbentis Herba	ajugasterone B	Not Available	FALSE	CCC(CC(C(C)(C1CCC2(C1(CCC1C2=CC(=O)C2C1(CC(C(C2)O)O)C)C)O)O)O)C(=C)CO
MOL007773	0.7273	0.2727	0.8457	Clematidis Armandii Caulis	clemontanoside C	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(OC2OCC(O)C(O)C2O)C1OC1OC(C(O)C(O)C1O)C
MOL007774	0.7815	0.2185	0.8065	Clematidis Armandii Caulis	clemontanoside A	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1C(C(C(C(O1)CO)O)O)O)C)C)C(=O)OC1C(C(C(C(O1)COC1C(C(C(C(O1)CO)O)O)O)O)O)O)OC1C(C(C(C(O1)C)O)O)O)O
MOL007775	0.7553	0.2447	0.9079	Clematidis Armandii Caulis	clemontanoside B_qt	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C)C(=O)O
MOL007776	0.7556	0.2444	0.8414	Clematidis Armandii Caulis	clemontanoside B	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C)C(=O)OC1C(C(C(C(O1)COC1C(C(C(C(O1)C)O)O)O)O)O)OC1C(C(C(C(O1)CO)O)O)O
MOL007778	0.9119	0.0881	0.8176	Plantaginis Herba	Plantaginin	5320623	FALSE	c12c(oc(cc2=O)c2ccc(cc2)O)cc(c(c1O)O)OC1OC(C(C(C1O)O)O)CO
MOL007778	0.9119	0.0881	0.8176	Plantaginis Semen	Plantaginin	5320623	FALSE	c12c(oc(cc2=O)c2ccc(cc2)O)cc(c(c1O)O)OC1OC(C(C(C1O)O)O)CO
MOL007779	0.7728	0.2272	0.7308	Plantaginis Herba	kusaginin _qt	Not Available	FALSE	C(=O)(/C=C/c1cc(c(cc1)O)O)OC1C(OC(C(C1O)O)O)OCCc1cc(c(cc1)O)O)CO
MOL007780	0.9242	0.0758	0.8536	Plantaginis Herba	Yuheinoside	155882	FALSE	C12C(C(=COC1OC1OC(C(C(C1O)O)O)CO)C=O)(CCC2C)O

MOL007781	0.9545	0.0455	0.8475	Plantaginis Herba	plantarenaloside_qt	Not Available	FALSE	C12C(C(=COC1O)C=O)(CCC2C)O
MOL007782	0.8236	0.1764	0.7456	Plantaginis Herba	plantamajoside	Not Available	FALSE	c1cc(c(cc1CCOC1C(C(C(C(O1)CO)OC(=O)/C=C/c1cc(c(cc1)O)O)OC1C(C(C(C(O1)CO)O)O)O)O)O)O)O
MOL007782	0.8236	0.1764	0.7456	Plantaginis Semen	plantamajoside	Not Available	FALSE	c1cc(c(cc1CCOC1C(C(C(C(O1)CO)OC(=O)/C=C/c1cc(c(cc1)O)O)OC1C(C(C(C(O1)CO)O)O)O)O)O)O
MOL007783	0.7428	0.2572	0.6192	Plantaginis Herba	melampyroside	Not Available	FALSE	O(C1OC=CC2C1C(=CC2)COC(=O)c1ccccc1)C1OC(O)(C(O)C(O)C1O)CO
MOL007784	0.8389	0.1611	0.8379	Plantaginis Herba	melampyroside_qt	Not Available	FALSE	OC1OC=CC2C1C(=CC2)COC(=O)c1ccccc1
MOL007785	0.8628	0.1372	0.7153	Plantaginis Herba	asperuloside	Not Available	FALSE	C12C3C(C=C2COC(=O)C)OC(=O)C3=COC1OC1OC(C(C(C1O)O)O)CO
MOL007785	0.8628	0.1372	0.7153	Paederiae Scandentis Herba	asperuloside	Not Available	FALSE	C12C3C(C=C2COC(=O)C)OC(=O)C3=COC1OC1OC(C(C(C1O)O)O)CO
MOL007785	0.8628	0.1372	0.7153	Morindae Officinalis Radix	asperuloside	Not Available	FALSE	C12C3C(C=C2COC(=O)C)OC(=O)C3=COC1OC1OC(C(C(C1O)O)O)CO
MOL007786	0.9246	0.0754	0.7598	Paederiae Scandentis Herba	asperuloside_qt	Not Available	FALSE	C12C3C(C=C2COC(=O)C)OC(=O)C3=COC1O
MOL007786	0.9246	0.0754	0.7598	Morindae Officinalis Radix	asperuloside_qt	Not Available	FALSE	C12C3C(C=C2COC(=O)C)OC(=O)C3=COC1O
MOL007786	0.9246	0.0754	0.7598	Plantaginis Herba	asperuloside_qt	Not Available	FALSE	C12C3C(C=C2COC(=O)C)OC(=O)C3=COC1O
MOL007787	0.9116	0.0884	0.8394	Plantaginis Semen	majoroside	Not Available	FALSE	CC1=C2C(CC1O)C(=COC2OC1C(C(C(C(O1)CO)O)O)O)C(=O)OC
MOL007787	0.9116	0.0884	0.8394	Plantaginis Herba	majoroside	Not Available	FALSE	CC1=C2C(CC1O)C(=COC2OC1C(C(C(C(O1)CO)O)O)O)C(=O)OC
MOL007788	0.9549	0.0451	0.8576	Plantaginis Herba	majoroside_qt	Not Available	FALSE	CC1=C2C(CC1O)C(=COC2O)C(=O)OC
MOL007788	0.9549	0.0451	0.8576	Plantaginis Semen	majoroside_qt	Not Available	FALSE	CC1=C2C(CC1O)C(=COC2O)C(=O)OC
MOL007789	0.9264	0.0736	0.9436	Momordicae Fructus	FRU	439709	FALSE	OC1(OC(C(O)C1O)CO)CO
MOL007789	0.9264	0.0736	0.9436	Plantaginis Herba	FRU	439709	FALSE	OC1(OC(C(O)C1O)CO)CO
MOL007791	0.9482	0.0518	0.8177	Plantaginis Herba	4-hydroxycinnamic acid _qt	Not Available	FALSE	OC1OC=C(C2C1C(O)(CC2O)C)C=O
MOL007792	0.5187	0.4813	0.6440	Plantaginis Herba	Isomartynoside	6476337	FALSE	O(C1C(O)C(OC(OCCc2cc(OC)c(O)cc2)C1O)COC(=O)/C=C/c1cc(O)c(OC)cc1)C1OC(C(O)C(O)C1O)C
MOL007792	0.5187	0.4813	0.6440	Clerodendrum Trichotomum Thunb	Isomartynoside	6476337	FALSE	O(C1C(O)C(OC(OCCc2cc(OC)c(O)cc2)C1O)COC(=O)/C=C/c1cc(O)c(OC)cc1)C1OC(C(O)C(O)C1O)C

MOL007794	0.7667	0.2333	0.7239	Plantaginis Herba	beta-D-Glucopyranoside, 2-(3,4-dihydroxyphenyl)ethyl 3-O-(6-deoxy-alpha-L-mannopyranosyl)-, 6-(3-(3,4-dihydroxyphenyl)-2-propenoate), (E)-	6438553	FALSE	O(C1C(O)(C(OC(C1O)COC(=O)/C=C/c1cc(O)c(O)cc1)OCC)c1cc(O)c(O)cc1)C1OC(C(O)C(O)C1O)C
MOL007795	0.8389	0.1611	0.7224	Plantaginis Herba	isoacteoside_qt	Not Available	FALSE	OC1C(O)(C(OC(C1O)COC(=O)/C=C/c1cc(O)c(O)cc1)OCC)c1cc(O)c(O)cc1
MOL007797	0.6629	0.3371	0.7044	Plantaginis Herba	leucosceptoside A	Not Available	FALSE	C1(C(C(C(C(O1)OCCc1cc(c(cc1)O)O)O)OC1OC(C(C(C1O)O)O)C)OC(=O)/C=C\c1cc(c(cc1)O)OC)CO
MOL007798	0.6615	0.3385	0.6937	Plantaginis Herba	leucosceptoside A_qt	Not Available	FALSE	C1(C(C(C(C(O1)OCCc1cc(c(cc1)O)O)O)O)OC(=O)/C=C\c1cc(c(cc1)O)OC)CO
MOL007800	0.5423	0.4577	0.6599	Plantaginis Herba	Martynoside	5319292	FALSE	O(C1C(OC(=O)/C=C/c2cc(OC)c(O)cc2)C(OC(OCCc2cc(O)c(OC)cc2)C1O)CO)C1OC(C(O)C(O)C1O)C
MOL007800	0.5423	0.4577	0.6599	Clerodendrum Trichotomum Thunb	Martynoside	5319292	FALSE	O(C1C(OC(=O)/C=C/c2cc(OC)c(O)cc2)C(OC(OCCc2cc(O)c(OC)cc2)C1O)CO)C1OC(C(O)C(O)C1O)C
MOL007800	0.5423	0.4577	0.6599	Plantaginis Semen	Martynoside	5319292	FALSE	O(C1C(OC(=O)/C=C/c2cc(OC)c(O)cc2)C(OC(OCCc2cc(O)c(OC)cc2)C1O)CO)C1OC(C(O)C(O)C1O)C
MOL007801	0.5141	0.4859	0.6476	Plantaginis Herba	martynoside_qt	Not Available	FALSE	OC1C(OC(=O)/C=C/c2cc(OC)c(O)cc2)C(OC(OCCc2cc(O)c(OC)cc2)C1O)CO
MOL007803	0.8584	0.1416	0.8331	Plantaginis Semen	homoplantaginin	Not Available	FALSE	COc1c(cc2c(c1O)c(=O)cc(o2)c1ccc(cc1)O)OC1C(C(C(C(O1)CO)O)O)O
MOL007803	0.8584	0.1416	0.8331	Plantaginis Herba	homoplantaginin	Not Available	FALSE	COc1c(cc2c(c1O)c(=O)cc(o2)c1ccc(cc1)O)OC1C(C(C(C(O1)CO)O)O)O
MOL007804	0.8386	0.1614	0.7389	Plantaginis Herba	hellicoside	Not Available	FALSE	c1(ccc(cc1O)/C=C/C(=O)OC1C(OC(C(C1OC1C(C(C(C(O1)CO)O)O)O)O)OCC(c1cc(c(cc1)O)O)O)CO)O
MOL007804	0.8386	0.1614	0.7389	Plantaginis Semen	hellicoside	Not Available	FALSE	c1(ccc(cc1O)/C=C/C(=O)OC1C(OC(C(C1OC1C(C(C(C(O1)CO)O)O)O)O)OCC(c1cc(c(cc1)O)O)O)CO)O
MOL007805	0.8620	0.1380	0.7431	Plantaginis Semen	hellicoside_qt	Not Available	FALSE	c1(ccc(cc1O)/C=C/C(=O)OC1C(OC(C(C1O)O)OCC(c1cc(c(cc1)O)O)O)CO)O
MOL007805	0.8620	0.1380	0.7431	Plantaginis Herba	hellicoside_qt	Not Available	FALSE	c1(ccc(cc1O)/C=C/C(=O)OC1C(OC(C(C1O)O)OCC(c1cc(c(cc1)O)O)O)CO)O

MOL007806	0.9236	0.0764	0.7912	Plantaginis Herba	2-(3,4-dihydroxyphenyl)-5,6-dihydroxy-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	185766	FALSE	c1(cc(=O)c2c(O)c(c(cc2o1)OC1OC(C(C(O)C1O)O)CO)O)c1cc(O)c(O)cc1
MOL007807	0.6531	0.3469	0.6875	Clerodendrum Trichotomum Thunb	Plantainoside C	6476335	FALSE	O(C1C(O)C(OC(OCCc2cc(O)c(O)cc2)C1O)COC(=O)/C=C/c1cc(O)c(OC)cc1)C1OC(C(O)C(O)C1O)C
MOL007807	0.6531	0.3469	0.6875	Plantaginis Herba	Plantainoside C	6476335	FALSE	O(C1C(O)C(OC(OCCc2cc(O)c(O)cc2)C1O)COC(=O)/C=C/c1cc(O)c(OC)cc1)C1OC(C(O)C(O)C1O)C
MOL007808	0.5860	0.4140	0.6690	Plantaginis Herba	plantainoside C_qt	Not Available	FALSE	OC1C(O)C(OC(OCCc2cc(O)c(O)cc2)C1O)COC(=O)/C=C/c1cc(O)c(OC)cc1
MOL007810	0.8233	0.1767	0.7404	Plantaginis Herba	[(2R,3R,4S,5R,6R)-6-[2-(3,4-dihydroxyphenyl)ethoxy]-3,5-dihydroxy-4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]methyl (E)-3-(3,4-dihydroxyphenyl)prop-2-enoate	9986606	FALSE	O(C1C(O)C(OC(OCCc2cc(O)c(O)cc2)C1O)COC(=O)/C=C/c1cc(O)c(O)cc1)C1OC(C(O)C(O)C1O)CO
MOL007812	0.9197	0.0803	0.8208	Plantaginis Semen	2'-O-beta-Glucopyranosyl-5,7,4',5'-tetrahydroxyflavanone	174157	FALSE	C1(C(C(C(C(O1)Oc1cc(cc(c1O)O)C1CC(=O)c2c(O1)cc(cc2O)O)O)O)O)CO
MOL007813	0.9471	0.0529	0.9170	Plantaginis Semen	Dihydrotricetin	440836	FALSE	Oc1cc(cc(c1O)O)C1CC(=O)c2c(O1)cc(cc2O)O

MOL007814	0.8233	0.1767	0.7404	Plantaginis Semen	plantainoside D	Not Available	FALSE	C(C1C(C(C(C(O1)OC1C(C(OC(C1O)OCCc1cc(c(cc1)O)O)COC(=O)/C=C/c1cc(c(cc1)O)O)O)O)O)O)O
MOL007815	0.7854	0.2146	0.7148	Plantaginis Semen	plantainoside D_qt	Not Available	FALSE	OC1C(C(OC(C1O)OCCc1cc(c(cc1)O)O)COC(=O)/C=C\c1cc(c(cc1)O)O)O
MOL007816	0.7948	0.2052	0.7119	Plantaginis Semen	plantasioside	44423103	FALSE	C1C(OC2C(C(C(OC2O1)COC(=O)/C=C/c1cc(c(cc1)O)O)O)O)c1cc(c(cc1)O)O
MOL007817	0.8328	0.1672	0.8309	Plantaginis Semen	7H-purin-3-ium-6-amine	57461989	FALSE	c1(ncnc2c1nc[nH]2)N
MOL007818	0.9133	0.0867	0.8135	Plantaginis Semen	Hypolaetin-8-glucoside	5318255	FALSE	c1c(c(c2c(c1O)c(=O)cc(o2)c1cc(c(cc1)O)O)OC1OC(C(C(C1O)O)O)CO)O
MOL007819	0.9267	0.0733	0.8817	Plantaginis Semen	Hypolaetin	5281648	FALSE	c1c(c(c2c(c1O)c(=O)cc(o2)c1cc(c(cc1)O)O)O)O
MOL007820	0.7420	0.2580	0.8437	Plantaginis Semen	plantenolic acid	Not Available	FALSE	O1C2(O)C(C3C(C4C(C5(C(=CC4)C4C(CC5)(CCC(C4)(C)C)C(=O)O)C)(CC3)C)(CC2)C1)(C)C
MOL007822	0.9188	0.0812	0.7906	Plantaginis Semen	catalpol_qt	Not Available	FALSE	C12C(C(OC=C1)O)C1(C(C2O)O1)CO
MOL007824	0.6637	0.3363	0.7288	Plantaginis Semen	3,4-Dihydroxy-beta-phenethyl-O-beta-D-glucopyranosyl-(1-3)-O-alpha-L-rhmnopyranosyl-(1-6)-4-O-caffeoyl-beta-D-glucopyranoside	Not Available	FALSE	c1(c(ccc(c1)/C=C/C(=O)OC1C(C(C(CC1COC1OC(C(C(C1O)O)O)C)OCCc1cc(c(cc1)O)O)O)OC1C(C(C(C(CO)O1)O)O)O)O)O
MOL007825	0.6746	0.3254	0.7091	Plantaginis Semen	3,4-Dihydroxy-beta-phenethyl-O-beta-D-glucopyranosyl-(1-3)-O-alpha-L-rhmnopyranosyl-(1-6)-4-O-caffeoyl-beta-D-glucopyranoside_qt	Not Available	FALSE	c1(c(ccc(c1)/C=C/C(=O)OC1C(C(C(CC1CO)OCCc1cc(c(cc1)O)O)O)O)O)O

MOL007828	0.9358	0.0642	0.8810	Plantaginis Semen	3,4-dihydroaucubin	Not Available	FALSE	C12C(C(OCC1)OC1C(O)C(O)C(O)C(O1)CO)C(=CC2O)CO
MOL007829	0.9497	0.0503	0.8508	Plantaginis Semen	3,4-dihydroaucubin_qt	Not Available	FALSE	C12C(C(OCC1)O)C(=CC2O)CO
MOL007830	0.7923	0.2077	0.7628	Plantaginis Semen	crenatoside	Not Available	FALSE	c1(c(ccc(c1)/C=C/C(=O)OC1C(C2C(OC1CO)OCC(O2)c1cc(c(cc1)O)O)OC1OC(C(C(C1O)O)O)C)O)O
MOL007831	0.7995	0.2005	0.7218	Plantaginis Semen	crenatoside_qt	Not Available	FALSE	c1(c(ccc(c1)/C=C\C(=O)OC1C(C2C(OC1CO)OCC(O2)c1cc(c(cc1)O)O)O)O)O
MOL007833	0.9559	0.0441	0.8681	Plantaginis Semen	geniposide_qt	Not Available	FALSE	COC(=O)C1=COC(C2C1CC=C2CO)O
MOL007834	0.7923	0.2077	0.7627	Plantaginis Semen	orobanchoside	Not Available	FALSE	C1(C2C(OC(C1OC(=O)/C=C/c1ccc(c(c1)O)O)CO)OCC(O2)c1ccc(c(c1)O)O)OC1C(O)C(O)C(O)C(O1)C
MOL007835	0.7995	0.2005	0.7218	Plantaginis Semen	orobanchoside_qt	Not Available	FALSE	C1(C2C(OC(C1OC(=O)/C=C\c1ccc(c(c1)O)O)CO)OCC(O2)c1ccc(c(c1)O)O)O
MOL007836	0.9182	0.0818	0.8446	Plantaginis Semen	plantaginin_qt	Not Available	FALSE	c1cc(ccc1C1=CC(=O)C2=C(C(=C(CC2O1)O)O)O)O
MOL007837	0.9273	0.0727	0.9560	Plantaginis Semen	plantagoguanidinic,acid	Not Available	FALSE	C1(N=C(NC1)N)C(CCC=C(C)C)C(=O)O
MOL007838	0.8809	0.1191	0.8023	Phaseoli Semen	catechin-7-O-β-D-glucopyranoside	Not Available	FALSE	C1(C(C(C(C(O1)Oc1cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)O)O)O)CO
MOL007839	0.7306	0.2694	0.8368	Phaseoli Semen	azukisaponin	Not Available	FALSE	C1(OC(C(C(C1O)O)O)CO)OC1C(C(C(OC1OC1C(C2C(CC1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C)C(O)CC(C1)(C)C)C)C)(C)C)C(=O)O)O)O
MOL007840	0.4108	0.5892	0.7532	Phaseoli Semen	azukisaponin_qt	Not Available	FALSE	C1(C(C)(C2C(CC1)(C1CC=C3C(CCC4(C3CC(CC4O)(C)C)C)(C1(CC2)C)C)C)C)O
MOL007841	0.7476	0.2524	0.8562	Phaseoli Semen	3-O[β-D-glucopyranosyl(1→2)-β-D-glucuronopyranosyl]soyasapogenol B	Not Available	FALSE	C1(OC(C(C(C1O)O)O)CO)OC1C(C(C(OC1OC1C(C2C(CC1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)C(O)CC(C1)(C)C)C)C)(C)CO)C(=O)O)O)O
MOL007842	0.4231	0.5769	0.7463	Phaseoli Semen	3-O[β-D-glucopyranosyl(1→2)-β-D-glucuronopyranosyl]soyasapogenol B_qt	Not Available	FALSE	OC1C(C2C(CC1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)C(O)CC(C1)(C)C)C)C)(C)CO

MOL007843	0.7746	0.2254	0.8365	Phaseoli Semen	3-O-[a-L-rhamnopyranosyl(1→2)-β-D-glucopyra-nosyl(l→2)-β-D-glucuronopyranosyl]-soyasapogenol B	Not Available	FALSE	C1(C(C(C(OC1C)OC1C(C(C(OC1OC1C(OC(C(C1O)O)C(=O)O)OC1C(C2C(CC1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(CC(C1)(C)C)O)C)C)C)(CO)C)CO)O)O)O)O)O
MOL007844	0.4261	0.5739	0.7644	Phaseoli Semen	3-O-[a-L-rhamnopyranosyl(1→2)-β-D-glucopyra-nosyl(l→2)-β-D-glucuronopyranosyl]-soyasapogenol B_qt	Not Available	FALSE	OC1C(C2C(CC1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(CC(C1)(C)C)O)C)C)C)(CO)C
MOL007845	0.7368	0.2632	0.8516	Phaseoli Semen	3-O-[β-D-glucopyranosyl(1→2)-β-D-glucuronopyranosyl]-soyasapogenol B	Not Available	FALSE	C1(C(C(C(OC1CO)OC1C(OC(C(C1O)O)C(=O)O)OC1C(C2C(CC1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(CC(C1)(C)C)O)C)C)C)(CO)C)O)O)O
MOL007846	0.4261	0.5739	0.7644	Phaseoli Semen	3-O-[β-D-glucopyranosyl(1→2)-β-D-glucuronopyranosyl]-soyasapogenol B_qt	Not Available	FALSE	OC1C(C2C(CC1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(CC(C1)(C)C)O)C)C)C)(CO)C
MOL007847	0.7507	0.2493	0.8515	Phaseoli Semen	Azukisaponin III	441909	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C(=O)O)C)C)(CC2)C)(CC1)C)(CO)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)CO)C(=O)O

MOL007848	0.6962	0.3038	0.8140	Phaseoli Semen	(2R,4aS,6aR,6aS,6bR,8aR,9S,10S,12aR,14bR)-10-hydroxy-2,4a,6a,6b,9,12a-hexamethyl-9-methylol-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-2-carboxylic acid	21594159	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C(=O)O)C)C)(CC2)C)(CC1)C)(CO)C
MOL007849	0.7507	0.2493	0.8515	Phaseoli Semen	3-O-[β-D-glucopyranosyl(1→2)-β-D-glucuronopyranosyl]-azukisapogenol	Not Available	FALSE	O(C1C(OC2OC(C(O)C(O)C2O)CO)C(O)C(C(O1)C(=O)O)O)C1CCC2(C(CCC3(C)C4(C)CCC5(C)CCC(C)(C(=O)O)CC5C4=CCC23)C1(C)CO)C
MOL007850	0.6962	0.3038	0.8140	Phaseoli Semen	3-O-[β-D-glucopyranosyl(1→2)-β-D-glucuronopyranosyl]-azukisapogenol_qt	Not Available	FALSE	OC1CCC2(C(CCC3(C)C4(C)CCC5(C)CCC(C)(C(=O)O)CC5C4=CCC23)C1(C)CO)C
MOL007851	0.7607	0.2393	0.8182	Phaseoli Semen	3-O-(β-D-glucopyranosyl)28-D-glucopyranosyl(1→6)-β-D-glucopyranosyl] gypsogenic acid	Not Available	FALSE	C1(C(C(C(C(O1)OC(=O)C12CCC3(C(=CCC4C3(CCC3C4(CCC(C3(C)C(=O)O)OC3C(C(C(C(O3)CO)O)O)O)C)C)C1CC(CC2)(C)C)C)O)O)O)COC1C(C(C(C(O1)CO)O)O)O

MOL007852	0.7344	0.2656	0.8125	Phaseoli Semen	3-O-(β-D-glucopyranosyl)28-D-glucopyranosyl(1→6)-β-D-glucopyranosyl] gypsogenic acid_qt	Not Available	FALSE	C12=CCC3C(C1(CCC1(C2CC(CC1)(C)C)C(=O)O)C)(CCC1C3(CCC(C1(C)C(=O)O)O)C)C
MOL007853	0.7834	0.2166	0.7901	Phaseoli Semen	3-O-[β-D-glucopyranosyl(1→2)β-D-glucuropyranosyl]-29-O-[β-D-glucopyranosyl(1→6)-β-D-glucopyranosyl]azukisapogenol	Not Available	FALSE	C1(C(C(C(C(O1)OCC1OC(C(C(C1O)O)O)OC(=O)C1(CC2C(CC1)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)CO)OC1C(C(C(C(O1)C(=O)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)C)C)C)C)O)O)O)CO
MOL007854	0.6962	0.3038	0.8140	Phaseoli Semen	3-O-[β-D-glucopyranosyl(1→2)β-D-glucuropyranosyl]-29-O-[β-D-glucopyranosyl(1→6)-β-D-glucopyranosyl]azukisapogenol_qt	Not Available	FALSE	OC(=O)C1(CC2C(CC1)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)CO)OC1C(C(C(C(O1)C(=O)O)O)O)C)C)C)C)C
MOL007855	0.9253	0.0747	0.9016	Phaseoli Semen	3-furanmethanol-β-D-glucopyranoside	Not Available	FALSE	o1cc(cc1)COC1C(C(C(C(O1)CO)O)O)O
MOL007856	0.8884	0.1116	0.9693	Phaseoli Semen	3-Furylmethanol	20449	FALSE	o1cc(cc1)CO
MOL007856	0.8884	0.1116	0.9693	Paederiae Scandentis Herba	3-Furylmethanol	20449	FALSE	o1cc(cc1)CO

MOL007856	0.8884	0.1116	0.9693	Physochlainae Radix	3-Furylmethanol	20449	FALSE	o1cc(cc1)CO
MOL007856	0.8884	0.1116	0.9693	Sojae Semen Nigrum	3-Furylmethanol	20449	FALSE	o1cc(cc1)CO
MOL007857	0.7266	0.2734	0.8625	Phaseoli Semen	triterpenoidsaponin	Not Available	FALSE	C1(C(C(C(OC1CO)OC1C(C(C(OC1CO)OC1CCC2(C(C1(C)CO)CCC1(C2CC=C2C1CCC1(C2CC(CC1)(C)C)C=O)C)C)O)O)O)O)O
MOL007858	0.3622	0.6378	0.8006	Phaseoli Semen	triterpenoidsaponin_qt	Not Available	FALSE	OC1CCC2(C(C1(C)CO)CCC1(C2CC=C2C1CCC1(C2CC(CC1)(C)C)C=O)C)C
MOL007859	0.8809	0.1191	0.8023	Phaseoli Semen	catechin-7-O-β-D-glucopyranoside	Not Available	FALSE	C1(C(OC(C(C1O)O)Oc1cc(c2c(c1)OC(C(C2)O)c1ccc(c(c1)O)O)O)CO)O
MOL007860	0.8949	0.1051	0.7916	Hyperici Japonici Herber	quercetin-7-rhamnoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2oc(c(O)c(=O)c2c(O)c1)c1cc(O)c(O)cc1)C
MOL007872	0.8949	0.1051	0.7916	Hyperici Japonici Herber	quercetin-7-O-rhamnoside	Not Available	FALSE	c1(c(O)c(=O)c2c(cc(cc2o1)OC1C(O)C(O)C(O)C(O1)C)O)c1cc(O)c(O)cc1
MOL007873	0.6453	0.3547	0.6342	Hyperici Japonici Herber	Isoamyl laurate	61386	FALSE	C(=O)(CCCCCCCCCCC)OCCC(C)C
MOL007875	0.8416	0.1584	0.6472	Hyperici Japonici Herber	mesylmethane	6213	FALSE	S(=O)(=O)(C)C
MOL007875	0.8416	0.1584	0.6472	Capsellae Herba	mesylmethane	6213	FALSE	S(=O)(=O)(C)C
MOL007875	0.8416	0.1584	0.6472	Equiseti Hiemalis Herba	mesylmethane	6213	FALSE	S(=O)(=O)(C)C
MOL007876	0.9011	0.0989	0.8890	Sesami Nigrum Semen	2,4-dimethylheptane	24884352	FALSE	C(C(CCC)C)C(C)C
MOL007876	0.9011	0.0989	0.8890	Equiseti Hiemalis Herba	2,4-dimethylheptane	24884352	FALSE	C(C(CCC)C)C(C)C
MOL007876	0.9011	0.0989	0.8890	Hyperici Japonici Herber	2,4-dimethylheptane	24884352	FALSE	C(C(CCC)C)C(C)C
MOL007878	0.9265	0.0735	0.8040	Hyperici Japonici Herber	4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-(alpha-D-galactopyranosyloxy)-5,7-dihydroxy-	6455156	FALSE	c1(c(oc2c(c1=O)c(cc(O)c2)O)c1cc(O)c(O)cc1)OC1C(O)C(O)C(O)C(O1)CO

MOL007879	0.6793	0.3207	0.9478	Aurantii Fructus Immaturus	Tetramethoxyluteolin	631170	FALSE	c12c(c(cc(c2)OC)OC)c(=O)cc(o1)c1cc(c(cc1)OC)OC
MOL007879	0.6793	0.3207	0.9478	Hyperici Japonici Herber	Tetramethoxyluteolin	631170	FALSE	c12c(c(cc(c2)OC)OC)c(=O)cc(o1)c1cc(c(cc1)OC)OC
MOL007880	0.9396	0.0604	0.7888	Hyperici Japonici Herber	3,5,7,3′,5′pentahydroxyflavonol	Not Available	FALSE	O1C(CC(c2c1cc(O)cc2O)O)c1cc(O)cc(O)c1
MOL007881	0.8986	0.1014	0.8425	Hyperici Japonici Herber	1,3,5,6-tetrahydroxyxanthone	5479774	FALSE	c1(=O)c2c(cc(cc2oc2c1ccc(O)c2O)O)O
MOL007882	0.8911	0.1089	0.7775	Hyperici Japonici Herber	Xanthone der.	5281663	FALSE	c1(=O)c2c(cc(cc2oc2c1cccc2O)O)O
MOL007883	0.9220	0.0780	0.9678	Benincasae Exocarpium	2-Methyl-5-ethylpyrazine	25915	FALSE	c1c(ncc(n1)C)CC
MOL007883	0.9220	0.0780	0.9678	Sesami Nigrum Semen	2-Methyl-5-ethylpyrazine	25915	FALSE	c1c(ncc(n1)C)CC
MOL007884	0.8952	0.1048	0.9574	Campsis Flos	2,5-Dimethylpiazine	31252	FALSE	c1(cnc(cn1)C)C
MOL007884	0.8952	0.1048	0.9574	Benincasae Exocarpium	2,5-Dimethylpiazine	31252	FALSE	c1(cnc(cn1)C)C
MOL007884	0.8952	0.1048	0.9574	Sesami Nigrum Semen	2,5-Dimethylpiazine	31252	FALSE	c1(cnc(cn1)C)C
MOL007885	0.2075	0.7925	0.6293	Benincasae Exocarpium	(3S,5S,9R,10S,13R,14R,17R)-17-[(2R,3E,5S)-5-ethyl-6-methylhepta-3,6-dien-2-yl]-10,13-dimethyl-2,3,4,5,6,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol	16058081	FALSE	C1(CCC2(C(C1)CC=C1C3CCC(C(/C=C/C(C(=C)C)CC)C)C3(C)CCC21)C)O

MOL007886	0.2151	0.7849	0.6233	Benincasae Exocarpium	(3S,5S,9R,10S,13R,14R,17R)-17-[(2R,5S)-5-ethyl-6-methylhept-6-en-2-yl]-10,13-dimethyl-2,3,4,5,6,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol	5283655	FALSE	C1(CCC2(C(C1)CC=C1C3CCC(C(CCC(C(=C)C)CC)C)C3(C)CCC21)C)O
MOL007887	0.9399	0.0601	0.9625	Benincasae Exocarpium	Hexyl formate	61177	FALSE	C(CCCC)COC=O
MOL007887	0.9399	0.0601	0.9625	Polygonati Odorati Rhizoma	Hexyl formate	61177	FALSE	C(CCCC)COC=O
MOL007888	0.9112	0.0888	0.9407	Campsis Flos	TRIMETHYL PYRAZINE	26808	FALSE	c1(c(nc(cn1)C)C)C
MOL007888	0.9112	0.0888	0.9407	Sesami Nigrum Semen	TRIMETHYL PYRAZINE	26808	FALSE	c1(c(nc(cn1)C)C)C
MOL007888	0.9112	0.0888	0.9407	Benincasae Exocarpium	TRIMETHYL PYRAZINE	26808	FALSE	c1(c(nc(cn1)C)C)C
MOL007889	0.3934	0.6066	0.7363	Benincasae Exocarpium	(3S,6aS,6aS,6bR,8aR,12aR,14aR,14bS)-4,4,6a,6b,8a,11,11,14a-octamethyl-1,2,3,6,6a,7,8,9,10,12,12a,13,14,14b-tetradecahydropicen-3-ol	9932254	FALSE	C1C(C(C2=CCC3C(C2C1)(CCC1(C3(CCC2(C1CC(CC2)(C)C)C)C)C)C)(C)C)O
MOL007890	0.3103	0.6897	0.7425	Benincasae Exocarpium	isomultifloreny l acetate	Not Available	FALSE	C1C(C(C2C(C1)(C1=C(CC2)C2(C(CC1)(C)C1C(CC2)(CCC(C)(C1)C)C)C)C)C)OC(=O)C
MOL007891	0.8719	0.1281	0.8219	Benincasae Exocarpium	2,6-Dimethylpiazine	7938	FALSE	c1(cncc(n1)C)C

MOL007891	0.8719	0.1281	0.8219	Sesami Nigrum Semen	2,6-Dimethylpiazine	7938	FALSE	c1(cncc(n1)C)C
MOL007891	0.8719	0.1281	0.8219	Achyranthis Bidentatae Radix	2,6-Dimethylpiazine	7938	FALSE	c1(cncc(n1)C)C
MOL007892	0.2573	0.7427	0.6837	Benincasae Exocarpium	cucurbita-5,24-dienol	Not Available	FALSE	C1C(C(C2=CCC3C(C2C1)(CCC1(C3(CCC1(C)C(C)CCC=C(C)C)C)C)(C)C)O
MOL007893	0.3892	0.6108	0.7792	Benincasae Exocarpium	glut-5-en-3β,28-diol	Not Available	FALSE	C1C(C(C2=CCC3C(C2C1)(CCC1(C3(CCC2(C1CC(CC2)(C)C)CO)C)C)(C)C)O
MOL007894	0.3934	0.6066	0.7363	Benincasae Exocarpium	glutenol	Not Available	FALSE	C1C(C(C2=CCC3C(C2C1)(CCC1(C3(CCC2(C1CC(CC2)(C)C)C)C)C)(C)C)O
MOL007895	0.6048	0.3952	0.7364	Junci Medulla	2,8-dihydroxy-1,7-dimethyl-6-ethenyl-10,11-dihydrodibenz[b,f]-oxepin	Not Available	FALSE	O1c2c(CCc3c1c(c(c(c3)O)C)C=C)c(c(cc2)O)C
MOL007896	0.5702	0.4298	0.6726	Junci Medulla	1,7-dimethyl-5-vinyl-9,10-dihydrophenanthrene-2,3-diol	10264910	FALSE	c1(c(c(cc2c3c(cc(cc3CCc12)C)C=C)O)O)C
MOL007897	0.6490	0.3510	0.6291	Junci Medulla	1,7-dimethyl-5-vinyl-9,10-dihydrophenanthrene-2,6-diol	10038555	FALSE	c1(c(ccc2c3c(c(c(cc3CCc12)C)O)C=C)O)C
MOL007898	0.6680	0.3320	0.7562	Junci Medulla	1,8-dimethyl-4-vinyl-9,10-dihydrophenanthrene-2,7-diol	10038556	FALSE	c1(c(ccc2c3c(cc(c(c3CCc12)C)O)C=C)O)C
MOL007899	0.6862	0.3138	0.6364	Junci Medulla	2,8-dihydroxy-1,6-dimethyl-5-ethenyl-9,10-dihydrophenanthrene	71345525	FALSE	c1(c(ccc2c3c(c(cc(c3CCc12)O)C)C=C)O)C
MOL007901	0.9053	0.0947	0.9733	Junci Medulla	RON	6950514	FALSE	C(=O)(C(N)CCC)O
MOL007902	0.8759	0.1241	0.7403	Lasiosphaera Seu Calvatia	105013-74-9	Not Available	FALSE	O1C23C(CCC(C2)C1(C)C)(CCC=C3CO)C

MOL007902	0.8759	0.1241	0.7403	Linderae Radix	105013-74-9	Not Available	FALSE	O1C23C(CCC(C2)C1(C)C)(CCC=C3CO)C
MOL007902	0.8759	0.1241	0.7403	Junci Medulla	105013-74-9	Not Available	FALSE	O1C23C(CCC(C2)C1(C)C)(CCC=C3CO)C
MOL007903	0.7160	0.2840	0.7577	Junci Medulla	1-methyl-5-vinylphenanthrene-2,7-diol	5316810	FALSE	c1(c(ccc2c3c(cc(cc3C=C)O)ccc12)O)C
MOL007904	0.7661	0.2339	0.7135	Junci Medulla	dehydroeffusal	Not Available	FALSE	c1(c(c2c(cc1)c1c(cc2)cc(cc1C=O)O)C)O
MOL007906	0.6683	0.3317	0.7715	Junci Medulla	JUNCUSOL	72740	FALSE	c1(c(c2c(cc1)c1c(cc(c(c1C=C)C)O)CC2)C)O
MOL007907	0.7719	0.2281	0.6468	Junci Medulla	3,7-dihydroxy-2,8-dimethyl-9,10-dihydrophenanthrene-4-carbaldehyde	10107070	FALSE	c1(c(c2c(cc1)c1c(cc(c(c1C=O)O)C)CC2)C)O
MOL007908	0.6726	0.3274	0.6835	Junci Medulla	7-hydroxy-2-methoxy-1,8-dimethyl-9,10-dihydrophenanthrene-4-carbaldehyde	10062303	FALSE	c1(c(c2c(cc1)c1c(c(cc1C=O)OC)C)CC2)C)O
MOL007909	0.9513	0.0487	0.9506	Ardisiae Japonicae Herba	p-menth-4-en-3-one	12088058	FALSE	C1(=O)C(=CCC(C1)C)C(C)C
MOL007909	0.9513	0.0487	0.9506	Junci Medulla	p-menth-4-en-3-one	12088058	FALSE	C1(=O)C(=CCC(C1)C)C(C)C
MOL007910	0.7173	0.2827	0.7950	Junci Medulla	1-methyl-5-vinyl-9,10-dihydrophenanthrene-2,7-diol	100801	FALSE	c1(c(ccc2c3c(cc(cc3CCc12)O)C=C)O)C
MOL007911	0.5318	0.4682	0.6577	Junci Medulla	juncunol	Not Available	FALSE	c1(c(ccc2c3cc(c(cc3CCc12)C=C)C)O)C
MOL007912	0.7148	0.2852	0.6623	Junci Medulla	1-(3,7-dihydroxy-2,8-dimethyl-9,10-dihydrophenanthren-4-yl)ethanone	21728333	FALSE	C(=O)(C)c1c(c(cc2c1c1ccc(c(c1CC2)C)O)C)O
MOL007913	0.8841	0.1159	0.9066	Junci Medulla	mono-p-coumaroyl glyceride	Not Available	FALSE	C(=O)(/C=C\c1ccc(cc1)O)OCC(CO)O
MOL007914	0.8516	0.1484	0.8132	Aucklandiae Radix	473-08-5	6452086	FALSE	C1(=C2C(CCC1=O)(CCC(C2)C(=C)C)C)C
MOL007914	0.8516	0.1484	0.8132	Centipedae Herba	473-08-5	6452086	FALSE	C1(=C2C(CCC1=O)(CCC(C2)C(=C)C)C)C

MOL007914	0.8516	0.1484	0.8132	Nardostachyos Radix Et Rhizoma	473-08-5	6452086	FALSE	C1(=C2C(CCC1=O)(CCC(C2)C(=C)C)C)C
MOL007914	0.8516	0.1484	0.8132	Junci Medulla	473-08-5	6452086	FALSE	C1(=C2C(CCC1=O)(CCC(C2)C(=C)C)C)C
MOL007914	0.8516	0.1484	0.8132	Fritillariaeussuriensis Bulbus	473-08-5	6452086	FALSE	C1(=C2C(CCC1=O)(CCC(C2)C(=C)C)C)C
MOL007915	0.6969	0.3031	0.6697	Junci Medulla	1-hydroxyethyl)-2,6-dihydroxy-1,7-dimethyl-9,10-dihydrophenanthrene	Not Available	FALSE	c1(c(ccc2c3c(c(c(cc3CCc12)C)O)C(C)O)O)C
MOL007916	0.6841	0.3159	0.6561	Junci Medulla	5-(1-hydroxyethyl)-2,8-dihydroxy-1,7-dimethyl-9,10-dihydrophenanthrene	Not Available	FALSE	c1(c(ccc2c3c(cc(c(c3CCc12)O)C)C(C)O)O)C
MOL007917	0.4128	0.5872	0.6991	Junci Medulla	8-hydroxy-2-methoxy-1,6-dimethyl-5-ethenyl-9,10-dihydrophenanthrene	Not Available	FALSE	c1(c(ccc2c3c(c(cc(c3CCc12)O)C)C=C)OC)C
MOL007918	0.3985	0.6015	0.7894	Junci Medulla	2-hydroxy-7-methoxy-1,8-dimethyl-5-ethenyl-9,10-dihydrophenanthrene	Not Available	FALSE	c1(c(ccc2c3c(cc(c(c3CCc12)C)OC)C=C)O)C
MOL007919	0.7261	0.2739	0.7689	Junci Medulla	2-hydroxy-7-carboxy-1-methyl-5-ethenyl-9,10-dihydrophenanthrene	Not Available	FALSE	c1(c(ccc2c3c(cc(cc3CCc12)C(=O)O)C=C)O)C

MOL007920	0.5845	0.4155	0.7860	Myristicae Semen	meso-1,4-Bis-(4-hydroxy-3-methoxyphenyl)-2,3-dimethylbutane	476856	FALSE	O(c1cc(CC(C(Cc2cc(OC)c(O)cc2)C)C)ccc1O)C
MOL007920	0.5845	0.4155	0.7860	Sargentodoxae Caulis	meso-1,4-Bis-(4-hydroxy-3-methoxyphenyl)-2,3-dimethylbutane	476856	FALSE	O(c1cc(CC(C(Cc2cc(OC)c(O)cc2)C)C)ccc1O)C
MOL007921	0.5551	0.4449	0.6410	Paederiae Scandentis Herba	syringaresnol diglucoside	15126926	FALSE	c1(C2C3C(C(c4c(cc(OC5C(C(C(C(O5)CO)O)O)O)cc4OC)OC)OC3)CO2)c(cc(OC2C(C(C(C(O2)CO)O)O)O)cc1OC)OC
MOL007921	0.5551	0.4449	0.6410	Sargentodoxae Caulis	syringaresnol diglucoside	15126926	FALSE	c1(C2C3C(C(c4c(cc(OC5C(C(C(C(O5)CO)O)O)O)cc4OC)OC)OC3)CO2)c(cc(OC2C(C(C(C(O2)CO)O)O)O)cc1OC)OC
MOL007923	0.8398	0.1602	0.7249	Polygoni Orientalis Fructus	2-(4-hydroxyphenyl)ethyl (E)-3-(4-hydroxyphenyl)prop-2-enoate	16119626	FALSE	c1(ccc(cc1)/C=C/C(=O)OCCc1ccc(cc1)O)O
MOL007923	0.8398	0.1602	0.7249	Sargentodoxae Caulis	2-(4-hydroxyphenyl)ethyl (E)-3-(4-hydroxyphenyl)prop-2-enoate	16119626	FALSE	c1(ccc(cc1)/C=C/C(=O)OCCc1ccc(cc1)O)O
MOL007923	0.8398	0.1602	0.7249	Daturae Flos	2-(4-hydroxyphenyl)ethyl (E)-3-(4-hydroxyphenyl)prop-2-enoate	16119626	FALSE	c1(ccc(cc1)/C=C/C(=O)OCCc1ccc(cc1)O)O

MOL007924	0.9341	0.0659	0.8846	Sargentodoxae Caulis	(2R,3R,4R,5S,6R)-2-[2-(3,4-dihydroxyphenyl)ethoxy]-6-methylol-tetrahydropyran-3,4,5-triol	6915839	FALSE	O1C(C(O)C(O)C(O)C1OCCc1cc(O)c(O)cc1)CO
MOL007925	0.9377	0.0623	0.8776	Sargentodoxae Caulis	3,5-dimethoxy-4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybenzoic acid	10383888	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(OC)cc(cc1OC)C(=O)O)CO
MOL007926	0.6334	0.3666	0.7476	Sargentodoxae Caulis	[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl] (1R,2R,4aS,6aR,6aS,6bR,8aR,10R,11R,12aR,14bS)-1,10,11-trihydroxy-1,2,6a,6b,9,9,12a-heptamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylate	21122581	FALSE	C12=CCC3C4(C(C(C(C(C4)O)O)(C)C)CCC3(C1(CCC1(C2C(C(CC1)C)(O)C)C(=O)OC1C(C(C(C(O1)CO)O)O)O)C)C)C
MOL007927	0.5932	0.4068	0.6751	Cistanches Herba	Liriodendrin	Not Available	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(OC3OC(C(O)C(O)C3O)CO)c(OC)c2)C1)c1cc(OC)c(OC2OC(C(O)C(O)C2O)CO)c(OC)c1
MOL007927	0.5932	0.4068	0.6751	Sargentodoxae Caulis	Liriodendrin	Not Available	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(OC3OC(C(O)C(O)C3O)CO)c(OC)c2)C1)c1cc(OC)c(OC2OC(C(O)C(O)C2O)CO)c(OC)c1

MOL007928	0.5284	0.4716	0.6200	Sargentodoxae Caulis	liriodendrin_qt	Not Available	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)c(OC)c2)C1)c1cc(OC)c(O)c(OC)c1
MOL007928	0.5284	0.4716	0.6200	Polygonati Odorati Rhizoma	liriodendrin_qt	Not Available	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)c(OC)c2)C1)c1cc(OC)c(O)c(OC)c1
MOL007928	0.5284	0.4716	0.6200	Eucommiae Folium	liriodendrin_qt	Not Available	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)c(OC)c2)C1)c1cc(OC)c(O)c(OC)c1
MOL007928	0.5284	0.4716	0.6200	Cistanches Herba	liriodendrin_qt	Not Available	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)c(OC)c2)C1)c1cc(OC)c(O)c(OC)c1
MOL007930	0.8545	0.1455	0.8693	Echinopsis Radix	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Citri Reticulatae Folium	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Gossampiniflos	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Asteris Radix Et Rhizoma	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Citrus Reticulata	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Euonymi Alati Ramulus	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Chrysanthemi Flos	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Citri Fructus	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Hippophae Fructus	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Citrus Aurantium	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Viticis Fructus	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Schizonepetae Spica	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Portulacae Herba	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Aurantii Fructus Immaturus	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Schizonepetae Herba	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Lobeliae Chinensis Herba	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Citri Fructus Retinervus	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C

MOL007930	0.8545	0.1455	0.8693	Stephaniae Tetrandrae Radix	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Citri Reticulatae Pericarpium Viride	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Aurantii Fructus	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Peucedani Radix	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Zanthoxylum Nitidum	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007930	0.8545	0.1455	0.8693	Lysimachiae Herba	hesperidin	10621	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL007931	0.8764	0.1236	0.8492	Lysimachiae Herba	iso-Rhamnetin 3-O-robinobioside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(OC)c(O)cc1)COC1OC(C(O)C(O)C1O)C
MOL007932	0.8807	0.1193	0.8493	Daturae Flos	5,7-dihydroxy-2-(4-hydroxyphenyl)-3-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-[[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxymethyl]tetrahydropyran-2-yl]oxy-chromone	15944778	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)C)c1ccc(cc1)O

MOL007932	0.8807	0.1193	0.8493	Lysimachiae Herba	5,7-dihydroxy-2-(4-hydroxyphenyl)-3-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-[[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxymethyl]tetrahydropyran-2-yl]oxy-chromone	15944778	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O)C(O1)C)c1ccc(cc1)O
MOL007932	0.8807	0.1193	0.8493	Glechomae Herba	5,7-dihydroxy-2-(4-hydroxyphenyl)-3-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-[[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxymethyl]tetrahydropyran-2-yl]oxy-chromone	15944778	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O)C(O1)C)c1ccc(cc1)O
MOL007934	0.9473	0.0527	0.9622	Lysimachiae Herba	2-Hexanoylfuran	61738	FALSE	C(=O)(c1occc1)CCCCC
MOL007934	0.9473	0.0527	0.9622	Eriobotryae Folium	2-Hexanoylfuran	61738	FALSE	C(=O)(c1occc1)CCCCC

MOL007936	0.8649	0.1351	0.8310	Lysimachiae Herba	rhamnocitrin-3,4'-diglucOside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(OC)c2)c1ccc(OC2OC(C(O)C(O)C2O)CO)cc1)CO
MOL007937	0.8890	0.1110	0.6576	Rhapontici Radix	Arctic acid	182071	FALSE	c1(ccc(s1)c1ccc(s1)C#CC)C(=O)O
MOL007938	0.6373	0.3627	0.7061	Rhapontici Radix	(2S,3R,5R,9R,10R,11R,13R,14S,17S)-2,3,11,14-tetrahydroxy-10,13-dimethyl-17-[(1R,2R)-1,2,5-trihydroxy-1,5-dimethylhexyl]-2,3,4,5,9,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-6-one	14376672	FALSE	C12=CC(=O)C3C(C2C(CC2(C1(CCC2C(C(CCC(O)(C)C)O)(O)C)O)C)O)(CC(C(C3)O)O)C
MOL007939	0.6563	0.3437	0.7921	Dioscoreaebulbiferae	diosbulbin B	Not Available	FALSE	O1C23C(C4C(C(OC3=O)C2)C2CC(OC2=O)C4)(CC1c1ccoc1)C
MOL007939	0.6563	0.3437	0.7921	Rhapontici Radix	diosbulbin B	Not Available	FALSE	O1C23C(C4C(C(OC3=O)C2)C2CC(OC2=O)C4)(CC1c1ccoc1)C
MOL007940	0.8575	0.1425	0.9072	Rhapontici Radix	Rubrosterone	Not Available	FALSE	C1(C(CC2(C(C1)C(=O)C=C1C3(CCC(=O)C3(C)CCC21)O)C)O)O

MOL007941	0.3982	0.6018	0.7030	Rhapontici Radix	[(4R,5R)-4,5-dihydroxy-1,1-dimethyl-5-[(2S,3R,5R,9R,10R,13R,14S,17S)-2,3,14-trihydroxy-10,13-dimethyl-6-oxo-2,3,4,5,9,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-17-yl]hexyl] acetate	11226211	FALSE	C1(O)C(O)CC2(C(C1)C(=O)C=C1C3(O)CCC(C(C(O)CCC(C)(C)OC(=O)C)(C)O)C3(C)CCC21)C
MOL007943	0.6401	0.3599	0.7128	Rhapontici Radix	(2S,3R,5R,9R,10R,11R,13R,14S,17S)-2,3,11,14-tetrahydroxy-10,13-dimethyl-17-[(1R,2R,4S)-1,2,4-trihydroxy-1,5-dimethylhexyl]-2,3,4,5,9,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-6-one	11799446	FALSE	C12=CC(=O)C3C(C2C(CC2(C1(CCC2C(C(CC(C(C)C)O)O)(O)C)O)C)O)(CC(C(C3)O)O)C
MOL007944	0.7373	0.2627	0.7540	Rhapontici Radix	arjunic acid	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1O)CO)(C)C
MOL007945	0.8683	0.1317	0.6153	Rhapontici Radix	Arctinol b	Not Available	FALSE	c1(ccc(s1)C(CO)O)c1sc(cc1)C#CC

MOL007946	0.8265	0.1735	0.6775	Et Radix Patriniae Rhizoma	19435-97-3	3084311	FALSE	OC1(C2C(C(CC1)C(C)C)C=C(CC2)C)C
MOL007946	0.8265	0.1735	0.6775	Tamaricis Cacumen	19435-97-3	3084311	FALSE	OC1(C2C(C(CC1)C(C)C)C=C(CC2)C)C
MOL007946	0.8265	0.1735	0.6775	Viticis Negundo Folium	19435-97-3	3084311	FALSE	OC1(C2C(C(CC1)C(C)C)C=C(CC2)C)C
MOL007946	0.8265	0.1735	0.6775	Lycii Fructus	19435-97-3	3084311	FALSE	OC1(C2C(C(CC1)C(C)C)C=C(CC2)C)C
MOL007947	0.8347	0.1653	0.6547	Et Radix Patriniae Rhizoma	β-guaiene	Not Available	FALSE	C12C(CC(CCC1C)C(=C)C)C(=C)CC2
MOL007948	0.8614	0.1386	0.8269	Farfarae Flos	Limene	3033866	FALSE	C\1(=C(\CCC=C(C)C)/C)/CCC(=CC1)C
MOL007948	0.8614	0.1386	0.8269	Et Radix Patriniae Rhizoma	Limene	3033866	FALSE	C\1(=C(\CCC=C(C)C)/C)/CCC(=CC1)C
MOL007949	0.9315	0.0685	0.9387	Et Radix Patriniae Rhizoma	Isodihydroavandulyl aldehyde	5362661	FALSE	C(=C\CC(C)C)(\C(C)C)/C=O
MOL007950	0.9238	0.0762	0.7793	Bistortae Rhizoma	[(2R,3S,4R,5R)-2,4,5-trihydroxy-1-oxo-6-(3,4,5-trihydroxyphenyl)carbonyloxy-hexan-3-yl] 3,4,5-trihydroxybenzoate	20836500	FALSE	O=CC(O)C(C(O)C(O)COC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O
MOL007951	0.9179	0.0821	0.9128	Quisqualis Indica	ϐ-Ս-Galloylglucos	128839	FALSE	O=CC(O)C(O)C(O)C(O)COC(=O)c1cc(O)c(O)c(O)c1
MOL007951	0.9179	0.0821	0.9128	Bistortae Rhizoma	ϐ-Ֆ-Galloylglucos	128839	FALSE	O=CC(O)C(O)C(O)C(O)COC(=O)c1cc(O)c(O)c(O)c1
MOL007953	0.9465	0.0535	0.9065	Bistortae Rhizoma	hyperin _qt	Not Available	FALSE	OC1=C(Oc2c(C1O)c(O)cc(O)c2)c1cc(O)c(O)cc1
MOL007953	0.9465	0.0535	0.9065	Bruceae Fructus	hyperin _qt	Not Available	FALSE	OC1=C(Oc2c(C1O)c(O)cc(O)c2)c1cc(O)c(O)cc1
MOL007954	0.9293	0.0707	0.9186	Bistortae Rhizoma	GRE	9338	FALSE	Oc1c(c(O)ccc1)C(=O)O
MOL007954	0.9293	0.0707	0.9186	Polygoni Cuspidati Rhizoma Et Radix	GRE	9338	FALSE	Oc1c(c(O)ccc1)C(=O)O
MOL007955	0.3223	0.6777	0.6966	Bistortae Rhizoma	24-Methylenecycloartanone	Not Available	FALSE	O=C1C(C2C3(C4(C3)C(C3(C(CC4)(C(CC3)C(CCC(=C)C(C)C)C)C)C)CC2)CC1)(C)C
MOL007956	0.9064	0.0936	0.7424	Swertiae Mileensis Herba	Swerchirin	5281660	FALSE	c1(=O)c2c(cc(cc2oc2c(ccc(c12)O)OC)OC)O
MOL007956	0.9064	0.0936	0.7424	Vaccariae Semen	Swerchirin	5281660	FALSE	c1(=O)c2c(cc(cc2oc2c(ccc(c12)O)OC)OC)O
MOL007957	0.8478	0.1522	0.7770	Swertiae Mileensis Herba	Swertiaperennin	5281653	FALSE	c1(=O)c2c(cc(cc2oc2ccc(c(c12)O)OC)OC)O
MOL007958	0.9500	0.0500	0.8452	Swertiae Mileensis Herba	Erythrocentaurin	191120	FALSE	O1CCc2c(C1=O)cccc2C=O
MOL007959	0.9577	0.0423	0.7735	Swertiae Mileensis Herba	swermirin	Not Available	FALSE	O1CCC(=C(C1=O)C(=O)C)/C(=C/C)/C(=O)C

MOL007960	0.8214	0.1786	0.8403	Swertiae Mileensis Herba	8-hydroxy-1,2,6-trimethoxy-xanthone	5378284	FALSE	c1(=O)c2c(cc(cc2oc2ccc(c(c12)OC)OC)OC)O
MOL007961	0.8213	0.1787	0.7093	Swertiae Mileensis Herba	1-Hydroxy-2,3,4,5-tetramethoxyxanthone	5318357	FALSE	c1(=O)c2c(c(c(c(c2oc2c(cccc12)OC)OC)OC)OC)O
MOL007962	0.9015	0.0985	0.8115	Swertiae Mileensis Herba	1,7-dihydroxy-3,5-dimethoxy xanthone	14860621	FALSE	c1(=O)c2c(cc(cc2oc2c(cc(cc12)O)OC)OC)O
MOL007963	0.8035	0.1965	0.8047	Swertiae Mileensis Herba	1-hydroxy-2,3,5-trimethoxy-xanthone	5318372	FALSE	c1(=O)c2c(c(c(cc2oc2c(cccc12)OC)OC)OC)O
MOL007964	0.8600	0.1400	0.6536	Swertiae Mileensis Herba	1,8-dihydroxy-2,3,4,5-tetramethoxyxanthone	Not Available	FALSE	c1(=O)c2c(c(c(c(c2oc2c(ccc(c12)O)OC)OC)OC)OC)O
MOL007965	0.8187	0.1813	0.6745	Swertiae Mileensis Herba	1-hydroxy-2,3,4,6-tetramethoxy-xanthone	11522801	FALSE	c1(=O)c2c(c(c(c(c2oc2cc(ccc12)OC)OC)OC)OC)O
MOL007966	0.8180	0.1820	0.7176	Swertiae Mileensis Herba	1-Hydroxy-2,3,4,7-tetramethoxyxanthone	5318358	FALSE	c1(=O)c2c(c(c(c(c2oc2ccc(cc12)OC)OC)OC)OC)O
MOL007967	0.8157	0.1843	0.7234	Swertiae Mileensis Herba	1-hydroxy-2,3,5,7-tetramethoxyxanthone	Not Available	FALSE	c1(=O)c2c(c(c(cc2oc2c(cc(cc12)OC)OC)OC)OC)O
MOL007968	0.8896	0.1104	0.7780	Swertiae Mileensis Herba	norbellidifolin	Not Available	FALSE	c1cc(c2c(c1O)C(=O)C1C(O2)C=C(C=C1O)O)O
MOL007969	0.8956	0.1044	0.7885	Swertiae Mileensis Herba	Bellidofolin	5281623	FALSE	c1cc(c2c(c1O)c(=O)c1c(o2)cc(cc1O)OC)O
MOL007970	0.8072	0.1928	0.8187	Swertiae Mileensis Herba	5,8-Dimethylbellidifolin	5378285	FALSE	c1cc(c2c(c1OC)c(=O)c1c(o2)cc(cc1O)OC)OC
MOL007971	0.2867	0.7133	0.6996	Swertiae Mileensis Herba	balanophonin	Not Available	FALSE	c1(c(cc(cc1)C1C(c2c(c(cc(c2)/C=C/C=C)OC)O1)CO)OC)O

MOL007972	0.6446	0.3554	0.7544	Swertiae Mileensis Herba	8-hydroxypinoresinal	Not Available	FALSE	c1(c(cc(cc1)C1C2C(CO1)(C(OC2)c1ccc(c(c1)OC)O)O)OC)O
MOL007973	0.7616	0.2384	0.8365	Benzoinum	sumaresinolic acid	51892378	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O
MOL007973	0.7616	0.2384	0.8365	Swertiae Mileensis Herba	sumaresinolic acid	51892378	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O
MOL007974	0.3614	0.6386	0.7222	Swertiae Mileensis Herba	3-epitaraxerol	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2=CCC3(C(C2(CC1)C)CC(CC3)(C)C)C)C)(C)C)O
MOL007975	0.3475	0.6525	0.7554	Swertiae Mileensis Herba	3α,6β-dihydroxy-taraxer-14-en	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2=CCC3(C(C2(CC1)C)CC(CC3)(C)C)C)C)(C)C)O
MOL007976	0.3475	0.6525	0.7554	Swertiae Mileensis Herba	3β,6β-dihydroxytaraxer-14-en-28-oic acid	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2=CCC3(C(C2(CC1)C)CC(CC3)(C)C)C)C)(C)C)O
MOL007977	0.3776	0.6224	0.7256	Swertiae Mileensis Herba	2α,3β,6α-trihydroxytaraxer-14-en	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2O)(C2=CCC3(C(C2(CC1)C)CC(CC3)(C)C)C)C)(C)C)O)O
MOL007978	0.8275	0.1725	0.7976	Saururi Herba	quercitrin-2'-gallate	Not Available	FALSE	c1(cc(c2oc3c(c(=O)c2O)c(cc(c3)O)O)ccc1O)OC(=O)c1c(C)cc(c(c1O)O)O
MOL007979	0.9213	0.0787	0.8064	Mori Cortex	Avicularin	5490064	FALSE	c1(ccc(cc1O)c1c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C1O)O)CO)O
MOL007979	0.9213	0.0787	0.8064	Astragali Cpmplanatisemen	Avicularin	5490064	FALSE	c1(ccc(cc1O)c1c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C1O)O)CO)O
MOL007979	0.9213	0.0787	0.8064	Rhododendri Daurici Folium	Avicularin	5490064	FALSE	c1(ccc(cc1O)c1c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C1O)O)CO)O
MOL007979	0.9213	0.0787	0.8064	Polygoni Avicularis Herba	Avicularin	5490064	FALSE	c1(ccc(cc1O)c1c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C1O)O)CO)O
MOL007979	0.9213	0.0787	0.8064	Saururi Herba	Avicularin	5490064	FALSE	c1(ccc(cc1O)c1c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C1O)O)CO)O
MOL007980	0.1175	0.8825	0.6647	Saururi Herba	saucernelignan-8	Not Available	FALSE	C1(OC(C(C1C)C)c1cc(c(cc1)OC(C)C(O)c1ccc(c(cc1)OC)OC)OC)c1ccc(c(c1)OC)OC(C)C(O)c1ccc(c(c1)O)OC
MOL007981	0.1106	0.8894	0.6713	Saururi Herba	saucernelignan-7	Not Available	FALSE	C1(OC(C(C1C)C)c1cc(c(cc1)OC(C)C(O)c1cc2c(cc1)OCO2)OC)c1ccc(c(c1)OC)OC(C)C(O)c1ccc(c(c1)O)OC
MOL007982	0.9213	0.0787	0.8064	Saururi Herba	Polystachoside	11968848	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL007983	0.7862	0.2138	0.7644	Saururi Herba	SAUCHINONE	Not Available	FALSE	O1C23OCOC3=CC(=O)C3C2C(C(C(C3)C)C)c2c1cc1OCOc1c2
MOL007985	0.4066	0.5934	0.7105	Saururi Herba	austrobailignan-5	Not Available	FALSE	c12c(ccc(c1)CC(CCc1cc3c(cc1)OCO3)C)OCO2
MOL007986	0.9289	0.0711	0.9052	Pseudobulbus Cremastrae Seu Pleiones	Gastrodin	115067	FALSE	O1C(C(O)C(O)C(O)C1Oc1ccc(cc1)CO)CO

MOL007988	0.7041	0.2959	0.7253	Pseudobulbus Cremastrae Seu Pleiones	loroglossin_qt	Not Available	FALSE	Oc1ccc(COC(=O)C(O)(CC(C)C)C(O)C(=O)OCc2ccc(O)cc2)cc1
MOL007990	0.5621	0.4379	0.7212	Pseudobulbus Cremastrae Seu Pleiones	Militarin_qt	Not Available	FALSE	Oc1ccc(COC(=O)C(O)(CC(C)C)CC(=O)OCc2ccc(O)cc2)cc1
MOL007991	0.8188	0.1812	0.8494	Pseudobulbus Cremastrae Seu Pleiones	2-methoxy-9,10-dihydrophenanthrene-4,5-diol	11506999	FALSE	c1c(cc(c2c3c(cccc3CCc12)O)O)OC
MOL007992	0.7640	0.2360	0.8253	Pseudobulbus Cremastrae Seu Pleiones	flavanthrinin	14777892	FALSE	O(c1c2c3c(ccc2cc(O)c1)cc(O)cc3)C
MOL007993	0.7080	0.2920	0.7204	Ilicis Purpureae Folium	(1S,4aR,6aR,6aS,6bR,8aR,10S,12aR,14bS)-1-hydroxy-2,2,6a,6b,9,9,12a-heptamethyl-10-[(2S,3R,4S,5R)-3,4,5-trihydroxyoxan-2-yl]oxy-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	21770233	FALSE	O1CC(C(C(C1OC1C(C2C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3O)(C)C)C(=O)O)C)C)(CC1)C)(C)C)O)O)O
MOL007994	0.7614	0.2386	0.8330	Ilicis Purpureae Folium	ilexoside A_qt	12315525	FALSE	OC1C(C2C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3O)(C)C)C(=O)O)C)C)(CC1)C)(C)C
MOL007995	0.3773	0.6227	0.6820	Ilicis Purpureae Folium	3β-O-(β-D-xylopyranosyl)pomolic acid methyl ester	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)OC)CCC(C)C(C)(C4C3=CCC21)O)C)OC1C(O)C(O)C(O)CO1
MOL007996	0.3078	0.6922	0.8123	Ilicis Purpureae Folium	Pomolic acid acetate	457300	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)OC)CCC(C)C(C)(C4C3=CCC21)O)C)O
MOL007997	0.7552	0.2448	0.7883	Ilicis Purpureae Folium	Rotundic acid	12315075	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C
MOL007998	0.9043	0.0957	0.8155	Ilicis Purpureae Folium	kaempferol-3-O-glucuronide	Not Available	FALSE	O1C(Oc2c(oc3c(c2=O)c(O)cc(O)c3)c2ccc(O)cc2)C(O)C(O)C(O)C1C(=O)O

MOL007999	0.9257	0.0743	0.9634	Ginkgo Folium	ZINC02038914	6560259	FALSE	C(C(=C)C)(CC)O
MOL007999	0.9257	0.0743	0.9634	Ilicis Purpureae Folium	ZINC02038914	6560259	FALSE	C(C(=C)C)(CC)O
MOL008001	0.9172	0.0828	0.9475	Ilicis Purpureae Folium	3-hexenal	643139	FALSE	C(=C\CC)/CC=O
MOL008002	0.9351	0.0649	0.8886	Ilicis Purpureae Folium	4-Formyl-2,6-xylenol	75222	FALSE	c1(cc(c(c(c1)C)O)C)C=O
MOL008003	0.6372	0.3628	0.7983	Stachyurimedulla Helwingiaemedulla	propapyriogeninA1	Not Available	FALSE	C1C(C(=O)CC2(CCC3(C4(CCC5C(C(=O)CCC5(C4C(C=C3C12)OC)C)(C)C)C)C(=O)O)(C)C
MOL008003	0.6372	0.3628	0.7983	Tetrapanacis Medulla	propapyriogeninA1	Not Available	FALSE	C1C(C(=O)CC2(CCC3(C4(CCC5C(C(=O)CCC5(C4C(C=C3C12)OC)C)(C)C)C)C(=O)O)(C)C
MOL008004	0.7076	0.2924	0.8296	Tetrapanacis Medulla	papyrioside L-IIa	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(OC2C(O)C(O)C(O)C(O2)C)C(O1)CO)C(=O)C12CCC3(C4(CCC5C(C(=O)CCC5(C4C(C=C3C2CC(C(=O)C1)(C)C)OC)C)(C)C)C
MOL008005	0.6372	0.3628	0.7983	Tetrapanacis Medulla	papyrioside L-IIa_qt	Not Available	FALSE	OC(=O)C12CCC3(C4(CCC5C(C(=O)CCC5(C4C(C=C3C2CC(C(=O)C1)(C)C)OC)C)(C)C)C)C
MOL008006	0.6261	0.3739	0.7773	Stachyurimedulla Helwingiaemedulla	paryriogenin A	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C2C=CC2=C3C(CC(C12)C)(CC(=O)C(C3)(C)C)C(=O)O)C)C
MOL008006	0.6261	0.3739	0.7773	Tetrapanacis Medulla	paryriogenin A	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C2C=CC2=C3C(CC(C12)C)(CC(=O)C(C3)(C)C)C(=O)O)C)C
MOL008007	0.6849	0.3151	0.7816	Tetrapanacis Medulla	propapyriogeninA2	Not Available	FALSE	C1C(C(=O)CC2(CCC3(C4(CCC5C(C(=O)CCC5(C4C(C=C3C12)O)C)(C)C)C)C(=O)O)(C)C
MOL008007	0.6849	0.3151	0.7816	Stachyurimedulla Helwingiaemedulla	propapyriogeninA2	Not Available	FALSE	C1C(C(=O)CC2(CCC3(C4(CCC5C(C(=O)CCC5(C4C(C=C3C12)O)C)(C)C)C)C(=O)O)(C)C
MOL008008	0.7260	0.2740	0.8322	Stachyurimedulla Helwingiaemedulla	papyrioside L-Ⅱb	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(OC2C(O)C(O)C(O)C(O2)C)C(O1)CO)C(=O)C12CCC3(C4(CCC5C(C(CCC5(C4C(C=C3C2CC(C(=O)C1)(C)C)OC)C)O)(C)C)C)C
MOL008008	0.7260	0.2740	0.8322	Tetrapanacis Medulla	papyrioside L-Ⅱb	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(OC2C(O)C(O)C(O)C(O2)C)C(O1)CO)C(=O)C12CCC3(C4(CCC5C(C(CCC5(C4C(C=C3C2CC(C(=O)C1)(C)C)OC)C)O)(C)C)C)C
MOL008009	0.6874	0.3126	0.8107	Tetrapanacis Medulla	papyrioside L-Ⅱb_qt	Not Available	FALSE	OC(=O)C12CCC3(C4(CCC5C(C(CCC5(C4C(C=C3C2CC(C(=O)C1)(C)C)OC)C)O)(C)C)C)C
MOL008009	0.6874	0.3126	0.8107	Stachyurimedulla Helwingiaemedulla	papyrioside L-Ⅱb_qt	Not Available	FALSE	OC(=O)C12CCC3(C4(CCC5C(C(CCC5(C4C(C=C3C2CC(C(=O)C1)(C)C)OC)C)O)(C)C)C)C
MOL008010	0.7467	0.2533	0.8358	Stachyurimedulla Helwingiaemedulla	papyrioside L-Ⅱc	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(OC2C(O)C(O)C(O)C(O2)C)C(O1)CO)C(=O)C12CCC3(C4(CCC5C(C)(C)C(=O)CCC5(C4C(C=C3C2CC(C(=O)C1)(C)C)O)C)C
MOL008010	0.7467	0.2533	0.8358	Tetrapanacis Medulla	papyrioside L-Ⅱc	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(OC2C(O)C(O)C(O)C(O2)C)C(O1)CO)C(=O)C12CCC3(C4(CCC5C(C)(C)C(=O)CCC5(C4C(C=C3C2CC(C(=O)C1)(C)C)O)C)C

MOL008011	0.6849	0.3151	0.7816	Tetrapanacis Medulla	papyrioside L-Ⅱc_qt	Not Available	FALSE	OC(=O)C12CCC3(C4(CCC5C(C)(C)C(=O)CCC5(C4C(C=C3C2CC(C(=O)C1)(C)C)O)C)C)C
MOL008011	0.6849	0.3151	0.7816	Stachyurimedulla Helwingiaemedulla	papyrioside L-Ⅱc_qt	Not Available	FALSE	OC(=O)C12CCC3(C4(CCC5C(C)(C)C(=O)CCC5(C4C(C=C3C2CC(C(=O)C1)(C)C)O)C)C)C
MOL008012	0.7623	0.2377	0.8321	Tetrapanacis Medulla	papyrioside L-Ⅱd	Not Available	FALSE	O(C(=O)C12CCC3(C4(CCC5C(C)(C)C(CCC5(C4C(C=C3C2CC(C(=O)C1)(C)C)O)C)O)C)C1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(OC2C(O)C(O)C(O)C(O2)CO)O)CO
MOL008012	0.7623	0.2377	0.8321	Stachyurimedulla Helwingiaemedulla	papyrioside L-Ⅱd	Not Available	FALSE	O(C(=O)C12CCC3(C4(CCC5C(C)(C)C(CCC5(C4C(C=C3C2CC(C(=O)C1)(C)C)O)C)O)C)C1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(OC2C(O)C(O)C(O)C(O2)CO)O)CO
MOL008013	0.7314	0.2686	0.7914	Stachyurimedulla Helwingiaemedulla	papyrioside L-Ⅱd_qt	Not Available	FALSE	OC(=O)C12CCC3(C4(CCC5C(C)(C)C(CCC5(C4C(C=C3C2CC(C(=O)C1)(C)C)O)C)O)C)C
MOL008013	0.7314	0.2686	0.7914	Tetrapanacis Medulla	papyrioside L-Ⅱd_qt	Not Available	FALSE	OC(=O)C12CCC3(C4(CCC5C(C)(C)C(CCC5(C4C(C=C3C2CC(C(=O)C1)(C)C)O)C)O)C)C
MOL008014	0.6088	0.3912	0.7809	Stachyurimedulla Helwingiaemedulla	paryriogenin B	Not Available	FALSE	C1(=O)CCC2(C(C1)CCC1(C2=CC=C2C1(CCC1(C2CC(C(=O)C1)(C)C)C(=O)O)C)C)C
MOL008014	0.6088	0.3912	0.7809	Tetrapanacis Medulla	paryriogenin B	Not Available	FALSE	C1(=O)CCC2(C(C1)CCC1(C2=CC=C2C1(CCC1(C2CC(C(=O)C1)(C)C)C(=O)O)C)C)C
MOL008015	0.6753	0.3247	0.8053	Stachyurimedulla Helwingiaemedulla	paryriogenin C	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C2=CCC2=C3C(CCC12C)(CC(=O)C(C3)(C)C)C(=O)O)C)C)O
MOL008015	0.6753	0.3247	0.8053	Tetrapanacis Medulla	paryriogenin C	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C2=CCC2=C3C(CCC12C)(CC(=O)C(C3)(C)C)C(=O)O)C)C)O
MOL008016	0.6798	0.3202	0.8142	Tetrapanacis Medulla	paryriogenin D	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C2C=CC2=C3C(CCC12C)(CC(C(C3)(C)C)O)C(=O)O)C)C
MOL008016	0.6798	0.3202	0.8142	Stachyurimedulla Helwingiaemedulla	paryriogenin D	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C2C=CC2=C3C(CCC12C)(CC(C(C3)(C)C)O)C(=O)O)C)C
MOL008017	0.7211	0.2789	0.8122	Stachyurimedulla Helwingiaemedulla	paryriogenin E	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C2C=CC2=C3C(CCC12C)(CC(C(C3)(C)C)O)C(=O)O)C)C)O
MOL008017	0.7211	0.2789	0.8122	Tetrapanacis Medulla	paryriogenin E	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C2C=CC2=C3C(CCC12C)(CC(C(C3)(C)C)O)C(=O)O)C)C)O
MOL008018	0.4599	0.5401	0.7603	Tetrapanacis Medulla	paryriogenin G	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C2C=CC2=C3C4(CCC12C)C(C(C(C3)(C)C)O)OC4=O)C)C)O
MOL008018	0.4599	0.5401	0.7603	Stachyurimedulla Helwingiaemedulla	paryriogenin G	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C2C=CC2=C3C4(CCC12C)C(C(C(C3)(C)C)O)OC4=O)C)C)O
MOL008019	0.3088	0.6912	0.7193	Tetrapanacis Medulla	paryriogenin H	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C2C=CC2=C3C(=CC(=O)C(C3)(C)C)CCC12C)C)C
MOL008019	0.3088	0.6912	0.7193	Stachyurimedulla Helwingiaemedulla	paryriogenin H	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C2C=CC2=C3C(=CC(=O)C(C3)(C)C)CCC12C)C)C
MOL008020	0.3248	0.6752	0.7202	Tetrapanacis Medulla	paryriogenin I	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C2C=CC2=C3C(=CC(=O)C(C3)(C)C)CCC12C)C)C)O
MOL008020	0.3248	0.6752	0.7202	Stachyurimedulla Helwingiaemedulla	paryriogenin I	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C2C=CC2=C3C(=CC(=O)C(C3)(C)C)CCC12C)C)C)O

MOL008021	0.3689	0.6311	0.7348	Stachyurimedulla Helwingiaemedulla	paryriogenin J	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C2C=CC2=C3C4(CCC12C)CC(C(C3)(C)C)OC4=O)C)C)O
MOL008021	0.3689	0.6311	0.7348	Tetrapanacis Medulla	paryriogenin J	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C2C=CC2=C3C4(CCC12C)CC(C(C3)(C)C)OC4=O)C)C)O
MOL008022	0.2445	0.7555	0.6007	Tetrapanacis Medulla	Tetrapanoside A	Not Available	FALSE	C1C(CC2=CC(=O)C3C(C2(C1)C)CCC1(C3CCC1C(C)/C=C/C(CC)C(C)C)C)OC1C(C(C(C(O1)CO)O)O)O
MOL008023	0.1950	0.8050	0.6843	Tetrapanacis Medulla	Tetrapanoside A_qt	Not Available	FALSE	C1C(CC2=CC(=O)C3C(C2(C1)C)CCC1(C3CCC1C(C)/C=C/C(CC)C(C)C)C)O
MOL008025	0.2127	0.7873	0.6657	Tetrapanacis Medulla	Tetrapanoside B_qt	Not Available	FALSE	C1C(CC2=CC(=O)C3C(C2(C1)C)CCC1(C3CCC1C(C)CCC(CC)C(C)C)C)O
MOL008031	0.7394	0.2606	0.7373	Rosae Laevigatae Fructus	65669-84-3	182497	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C)C(=O)O)C)(CC2)C)(CC1O)C)(CO)C
MOL008031	0.7394	0.2606	0.7373	Potentillae Chinensis Herba	65669-84-3	182497	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C)C(=O)O)C)(CC2)C)(CC1O)C)(CO)C
MOL008032	0.6993	0.3007	0.8590	Potentillae Chinensis Herba	(1S,2R,4aS,6aR,6aS,6bR,8aR,12aR,14bS)-1,2,6a,6b,9,9,12a-heptamethyl-10-oxo-1,2,3,4,5,6,6a,7,8,8a,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	9890209	FALSE	C12=CCC3C(C1(CCC1(C2C(C(CC1)C)C)C(=O)O)C)(CCC1C3(CCC(=O)C1(C)C)C)C
MOL008032	0.6993	0.3007	0.8590	Jujubae Fructus	(1S,2R,4aS,6aR,6aS,6bR,8aR,12aR,14bS)-1,2,6a,6b,9,9,12a-heptamethyl-10-oxo-1,2,3,4,5,6,6a,7,8,8a,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	9890209	FALSE	C12=CCC3C(C1(CCC1(C2C(C(CC1)C)C)C(=O)O)C)(CCC1C3(CCC(=O)C1(C)C)C)C

MOL008034	0.7038	0.2962	0.7941	Cayratiae Japonicae Herba	21302-79-4	Not Available	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)C(=O)O)CC3)C)(CC2)C)(C1C(=O)O)C)(C)C
MOL008034	0.7038	0.2962	0.7941	Jujubae Fructus	21302-79-4	Not Available	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)C(=O)O)CC3)C)(CC2)C)(C1C(=O)O)C)(C)C
MOL008034	0.7038	0.2962	0.7941	Hoveniae Dulcis Semen	21302-79-4	Not Available	FALSE	OC1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)C(=O)O)CC3)C)(CC2)C)(C1C(=O)O)C)(C)C
MOL008036	0.9285	0.0715	0.7495	Cayratiae Japonicae Herba	DIMETHYL QUINOLINE	34222	FALSE	n1c2c(c(cc1)C)cccc2C
MOL008038	0.8464	0.1536	0.8003	Stachyurimedulla Helwingiaemedulla	ADA-ADA-ADA	5287609	FALSE	C1(C(OC(C(C1O)O)OC1C(OC(C(C1O)O)O)C(=O)O)C(=O)O)OC1OC(C(C(C1O)O)O)C(=O)O
MOL008038	0.8464	0.1536	0.8003	Sterculiae Lychnophorae Semen	ADA-ADA-ADA	5287609	FALSE	C1(C(OC(C(C1O)O)OC1C(OC(C(C1O)O)O)C(=O)O)C(=O)O)OC1OC(C(C(C1O)O)O)C(=O)O
MOL008039	0.8574	0.1426	0.8313	Artemisiae Scopariae Herba	Isoarcapillin	5318508	FALSE	o1c(c2c(OC)cc(O)c(OC)c2)cc(=O)c2c1cc(OC)c(O)c2O
MOL008040	0.8909	0.1091	0.8556	Artemisiae Scopariae Herba	Eupalitin	5748611	FALSE	c12c(=O)c(c(oc1cc(c(c2O)OC)OC)c1ccc(cc1)O)O
MOL008041	0.9161	0.0839	0.8785	Artemisiae Scopariae Herba	Eupatolitin	5317291	FALSE	o1c2c(c(O)c(OC)c(OC)c2)c(=O)c(O)c1c1cc(O)c(O)cc1
MOL008042	0.9006	0.0994	0.9033	Artemisiae Scopariae Herba	(2R,3R)-3,5-dihydroxy-2-(4-hydroxyphenyl)-7-methoxychroman-4-one	181132	FALSE	O1C(C(O)C(=O)c2c1cc(OC)cc2O)c1ccc(O)cc1
MOL008043	0.8942	0.1058	0.8385	Artemisiae Scopariae Herba	capillarisin	5281342	FALSE	c12c(c(c(c(c2)O)OC)O)c(=O)cc(o1)Oc1ccc(cc1)O
MOL008044	0.8914	0.1086	0.8532	Artemisiae Scopariae Herba	7-Methylcapillarisin	5319541	FALSE	o1c2c(c(O)c(OC)c(OC)c2)c(=O)cc1Oc1ccc(O)cc1
MOL008045	0.8569	0.1431	0.8372	Artemisiae Scopariae Herba	4'-Methylcapillarisin	5319540	FALSE	o1c2c(c(O)c(OC)c(O)c2)c(=O)cc1Oc1ccc(OC)cc1
MOL008046	0.9411	0.0589	0.8371	Artemisiae Scopariae Herba	Demethoxycapillarisin	5316511	FALSE	o1c2c(c(O)cc(O)c2)c(=O)cc1Oc1ccc(O)cc1
MOL008046	0.9411	0.0589	0.8371	Rose Rugosae Flos	Demethoxycapillarisin	5316511	FALSE	o1c2c(c(O)cc(O)c2)c(=O)cc1Oc1ccc(O)cc1
MOL008047	0.8322	0.1678	0.6743	Artemisiae Scopariae Herba	Artepillin A	Not Available	FALSE	O1C(Cc2c1c(cc(c2)/C=C\C(=O)O)CC=C(C)C)C(CO)C
MOL008050	0.9373	0.0627	0.9298	Artemisiae Scopariae Herba	5-Hydroxyferulate	446834	FALSE	O(c1cc(cc(O)c1O)/C=C/C(=O)O)C

MOL008051	0.8728	0.1272	0.8049	Artemisiae Scopariae Herba	Neocapillene	5320055	FALSE	C(#CC#CCC)c1ccccc1
MOL008052	0.8854	0.1146	0.8369	Artemisiae Scopariae Herba	Capillene	3083613	FALSE	c1(CC#CC#CC)ccccc1
MOL008053	0.8812	0.1188	0.8154	Artemisiae Scopariae Herba	penta-1,3-diynylbenzene	10983572	FALSE	c1(ccccc1)C#CC#CC
MOL008054	0.8836	0.1164	0.8878	Artemisiae Scopariae Herba	Capillanol	Not Available	FALSE	CC(CC#CCc1ccccc1)O
MOL008055	0.8790	0.1210	0.8609	Artemisiae Scopariae Herba	Norcapillene	587245	FALSE	c1(CC#CC#C)ccccc1
MOL008056	0.8691	0.1309	0.7595	Artemisiae Scopariae Herba	Capillarol	Not Available	FALSE	C(=O)(/C=C\c1cc(c(cc1)O)C(=O)C=C(C)C)OC
MOL008057	0.8880	0.1120	0.8423	Artemisiae Scopariae Herba	Capillin	10321	FALSE	C(=O)(C#CC#CC)c1ccccc1
MOL008058	0.8318	0.1682	0.7018	Artemisiae Scopariae Herba	α-humulene	50987499	FALSE	C\1=C(/C/C=C\C(C/C=C(\CC1)/C)(C)C)\C
MOL008059	0.9517	0.0483	0.8290	Bruceae Fructus	4-Ethoxycarbonyl-2-quinolone	160782	FALSE	[nH]1c(=O)cc(c2ccccc12)C(=O)OCC
MOL008060	0.8077	0.1923	0.8074	Bruceae Fructus	dehydrobruceine A	Not Available	FALSE	C1=C(C(=O)C(=C2CC3OC(=O)C(C4C53OCC4(C(=O)OC)C(C(C5C12C)O)O)OC(=O)CC(C)C)C)O
MOL008061	0.8205	0.1795	0.8210	Bruceae Fructus	dehydrobrussatol	Not Available	FALSE	C123C4C(OC3)(C(C(C1C1(C(=C(C(=O)C(=C1)O)C)CC2OC(=O)C4OC(=O)C=C(C)C)C)O)O)C(=O)OC
MOL008062	0.7658	0.2342	0.8160	Bruceae Fructus	dehydrobruceantinol	Not Available	FALSE	O1C2(C3C4(C(C5(C(=C(C(=O)C(=C5)O)C)CC4OC(=O)C3OC(=O)C(=C(C)C)C(O)C)C(O)C2O)C1)C(=O)OC
MOL008063	0.8827	0.1173	0.8011	Bruceae Fructus	javanicin	10149	FALSE	C1(=O)C(=C(C(=O)c2c(cccc12)O)OC)O)CC(=O)C)C
MOL008064	0.7461	0.2539	0.8003	Bruceae Fructus	yadanzioside A	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)CC(C)C)C(C(=O)C(=C5)OC3OC(C(O)C(O)C3O)CO)C)C)C(O)C2O)C1)C(=O)OC
MOL008065	0.7915	0.2085	0.7967	Bruceae Fructus	yadanzioside A_qt	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)CC(C)C)C(C(=O)C(=C5)O)C)C)C(O)C2O)C1)C(=O)OC
MOL008066	0.9335	0.0665	0.8394	Bruceae Fructus	yadanziolide A	Not Available	FALSE	O1C2(CO)C3(C4(C(C5(C(CC4OC(=O)C3O)C(=CC(=O)C5O)C)C)C(O)C2O)C1)O
MOL008067	0.7476	0.2524	0.8013	Bruceae Fructus	bruceoside A	Not Available	FALSE	C123C4C(OC3)(C(C(C1C1(C(CC2OC(=O)C4OC(=O)C=C(C)C)C(C(=O)C(=C1)OC1OC(C(C(C1O)O)O)CO)C)C)O)O)C(=O)OC
MOL008068	0.7952	0.2048	0.8058	Bruceae Fructus	bruceoside A_qt	Not Available	FALSE	C123C4C(OC3)(C(C(C1C1(C(CC2OC(=O)C4OC(=O)C=C(C)C)C(C(=O)C(=C1)O)C)C)O)O)C(=O)OC
MOL008069	0.7982	0.2018	0.8513	Bruceae Fructus	Isobruceine A	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)CC(C)C)C(=C(O)C(=O)C5)C)C)C(O)C2O)C1)C(=O)OC
MOL008070	0.9398	0.0602	0.8227	Bruceae Fructus	Bruceine D	Not Available	FALSE	O1C2(C3(O)C4(C(C5(C(CC4OC(=O)C3O)C(=CC(=O)C5O)C)C)C(O)C2O)C1)C

MOL008071	0.9035	0.0965	0.8142	Bruceae Fructus	yadanzigan	Not Available	FALSE	O1C2(C3(O)C4(C(C5(C(CC4OC(=O)C3O)C(=CC(OC3OC(C(C(C3O)O)O)CO)C5O)C)C)C(O)C2O)C1)C
MOL008072	0.9458	0.0542	0.8393	Bruceae Fructus	yadanzigan_qt	Not Available	FALSE	O1C2(C3(O)C4(C(C5(C(CC4OC(=O)C3O)C(=CC(O)C5O)C)C)C(O)C2O)C1)C
MOL008073	0.7994	0.2006	0.8575	Bruceae Fructus	brusatol	Not Available	FALSE	C123C4C(OC3)(C(C(C1C1(C(CC2OC(=O)C4OC(=O)C=C(C)C)C(=C(C(=O)C1)O)C)C)O)O)C(=O)OC
MOL008074	0.8194	0.1806	0.7043	Bruceae Fructus	bruceaketolic acid	Not Available	FALSE	C1(=O)C(OC(=O)C)C2C34C(O1)CC(C(C3C(C(C2(OC4)C(=O)OC)O)O)(CC(=O)O)C)C(=C)C
MOL008075	0.6402	0.3598	0.8224	Bruceae Fructus	bruceantin	Not Available	FALSE	C123C4C(OC3)(C(C(C1C1(C(CC2OC(=O)C4OC(=O)/C=C(/C(C)C)\C)C(=C(C(=O)C1)O)C)C)O)O)C(=O)OC
MOL008076	0.5841	0.4159	0.7892	Bruceae Fructus	Bruceantinol	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)/C=C(/C(OC(=O)C)(C)C)\C)C(=C(O)C(=O)C5)C)C)C(O)C2O)C1)C(=O)OC
MOL008077	0.8005	0.1995	0.8178	Bruceae Fructus	yadanzioside B	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)CC(C)C)C(=C(OC3OC(C(O)C(O)C3O)CO)C(=O)C5O)C)C)C(O)C2O)C1)C(=O)OC
MOL008078	0.8425	0.1575	0.8358	Bruceae Fructus	yadanzioside B_qt	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)CC(C)C)C(=C(O)C(=O)C5O)C)C)C(O)C2O)C1)C(=O)OC
MOL008079	0.7145	0.2855	0.8192	Bruceae Fructus	yadanzioside C	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)/C=C(/C(O)(C)C)\C)C(C(=O)C(=C5)OC3OC(C(O)C(O)C3O)CO)C)C)C(O)C2O)C1)C(=O)OC
MOL008080	0.7388	0.2612	0.8244	Bruceae Fructus	yadanzioside C_qt	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)/C=C(/C(O)(C)C)\C)C(C(=O)C(=C5)O)C)C)C(O)C2O)C1)C(=O)OC
MOL008081	0.8637	0.1363	0.7767	Bruceae Fructus	yadanzioside D	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)C)C(=CC(OC3OC(C(O)C(O)C3O)CO)C5O)C)C)C(O)C2O)C1)C(=O)OC
MOL008082	0.8959	0.1041	0.7865	Bruceae Fructus	yadanzioside D_qt	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)C)C(=CC(O)C5O)C)C)C(O)C2O)C1)C(=O)OC
MOL008083	0.7562	0.2438	0.7905	Bruceae Fructus	yadanzioside E	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)C=C(C)C)C(=CC(OC3OC(C(O)C(O)C3O)CO)C5O)C)C)C(O)C2O)C1)C(=O)OC
MOL008084	0.8177	0.1823	0.8143	Bruceae Fructus	yadanzioside E_qt	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)C=C(C)C)C(=CC(O)C5O)C)C)C(O)C2O)C1)C(=O)OC
MOL008085	0.8695	0.1305	0.7859	Bruceae Fructus	yadanzioside F	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)C)C(C(=O)C(=C5)OC3OC(C(O)C(O)C3O)CO)C)C)C(O)C2O)C1)C(=O)OC
MOL008086	0.9005	0.0995	0.7700	Bruceae Fructus	yadanzioside F_qt	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)C)C(C(=O)C(=C5)O)C)C)C(O)C2O)C1)C(=O)OC
MOL008087	0.5921	0.4079	0.7784	Bruceae Fructus	yadanzioside G	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)/C=C(/C(OC(=O)C)(C)C)\C)C(C(=O)C(=C5)OC3OC(C(O)C(O)C3O)CO)C)C)C(O)C2O)C1)C(=O)OC

MOL008088	0.5715	0.4285	0.7152	Bruceae Fructus	yadanzioside G_qt	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)/C=C(/C(OC(=O)C)(C)C)\C)C(C(=O)C(=C5)O)C)C)C(O)C2O)C1)C(=O)OC
MOL008089	0.7506	0.2494	0.7869	Bruceae Fructus	yadanzioside H	Not Available	FALSE	C1(C=C(C2C(C1O)(C1C34C(C2)OC(=O)C(C3C(C(C1O)O)(C(=O)OC)OC4)OC(=O)CC(C)C)C)C)OC1C(C(C(C(O1)CO)O)O)O
MOL008090	0.8121	0.1879	0.7948	Bruceae Fructus	yadanzioside H_qt	Not Available	FALSE	C1(C=C(C2C(C1O)(C1C34C(C2)OC(=O)C(C3C(C(C1O)O)(C(=O)OC)OC4)OC(=O)CC(C)C)C)C)O
MOL008091	0.8721	0.1279	0.7865	Bruceae Fructus	yadanzioside I	Not Available	FALSE	O1C(C(C(C(C1CO)O)O)O)OC1=C(C2C(CC1=O)(C1C34C(OC(=O)C(C3C(OC4)(C(C1O)O)C(=O)OC)OC(=O)C)C2)C)C
MOL008092	0.8960	0.1040	0.8168	Bruceae Fructus	Bruceine B	Not Available	FALSE	OC1=C(C2C(CC1=O)(C1C34C(OC(=O)C(C3C(OC4)(C(C1O)O)C(=O)OC)OC(=O)C)C2)C)C
MOL008093	0.8035	0.1965	0.8115	Bruceae Fructus	yadanzioside J	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)CC(O)(C)C)C(C(=O)C(=C5)OC3OC(C(O)C(O)C3O)CO)C)C)C(O)C2O)C1)C(=O)OC
MOL008094	0.8459	0.1541	0.8104	Bruceae Fructus	yadanzioside J_qt	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)CC(O)(C)C)C(C(=O)C(=C5)O)C)C)C(O)C2O)C1)C(=O)OC
MOL008095	0.5880	0.4120	0.7811	Bruceae Fructus	yadanzioside K	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)/C=C(/C(OC(=O)C)(C)C)\C)C(=C(OC3OC(C(O)C(O)C3O)CO)C(=O)C5)C)C)C(O)C2O)C1)C(=O)OC
MOL008096	0.5841	0.4159	0.7892	Bruceae Fructus	yadanzioside K_qt	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)/C=C(/C(OC(=O)C)(C)C)\C)C(=C(O)C(=O)C5)C)C)C(O)C2O)C1)C(=O)OC
MOL008097	0.6955	0.3045	0.8215	Bruceae Fructus	yadanzioside L	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)/C=C(/C(O)(C)C)\C)C(=C(OC3OC(C(O)C(O)C3O)CO)C(=O)C5)C)C)C(O)C2O)C1)C(=O)OC
MOL008098	0.7353	0.2647	0.8276	Bruceae Fructus	yadanzioside L_qt	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)/C=C(/C(O)(C)C)\C)C(=C(O)C(=O)C5)C)C)C(O)C2O)C1)C(=O)OC
MOL008099	0.6508	0.3492	0.8133	Bruceae Fructus	yadanzioside M	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)c3ccccc3)C(C(=O)C(=C5)OC3OC(C(O)C(O)C3O)CO)C)C)C(O)C2O)C1)C(=O)OC
MOL008100	0.6714	0.3286	0.8220	Bruceae Fructus	yadanzioside M_qt	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)c3ccccc3)C(C(=O)C(=C5)O)C)C)C(O)C2O)C1)C(=O)OC
MOL008101	0.6346	0.3654	0.7992	Bruceae Fructus	yadanzioside N	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)/C=C(/C(C)C)\C)C(C=C(OC3OC(C(O)C(O)C3O)CO)C5=O)C)C)C(O)C2O)C1)C(=O)OC
MOL008102	0.6338	0.3662	0.7445	Bruceae Fructus	yadanzioside N_qt	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)/C=C(/C(C)C)\C)C(C=C(O)C5=O)C)C)C(O)C2O)C1)C(=O)OC
MOL008103	0.5921	0.4079	0.7784	Bruceae Fructus	yadanzioside O	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)/C=C(/C(OC(=O)C)(C)C)\C)C(C(=O)C(=C5)OC3OC(C(O)C(O)C3O)CO)C)C)C(O)C2O)C1)C(=O)OC

MOL008104	0.5715	0.4285	0.7152	Bruceae Fructus	yadanzioside O_qt	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)/C=C(/C(OC(=O)C)(C)C)\C)C(C(=O)C(=C5)O)C)C)C(O)C2O)C1)C(=O)OC
MOL008105	0.6230	0.3770	0.7994	Bruceae Fructus	yadanzioside P	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)/C=C(/C(C)C)\C)C(=C(OC3OC(C(O)C(O)C3O)CO)C(=O)C5)C)C(O)C2O)C1)C(=O)OC
MOL008106	0.7982	0.2018	0.8513	Bruceae Fructus	bruceine A	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)CC(C)C)C(=C(O)C(=O)C5)C)C(O)C2O)C1)C(=O)OC
MOL008107	0.7145	0.2855	0.8192	Bruceae Fructus	yadanziolide C	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)/C=C(/C(O)(C)C)\C)C(C(=O)C(=C5)OC3OC(C(O)C(O)C3O)CO)C)C)C(O)C2O)C1)C(=O)OC
MOL008108	0.7388	0.2612	0.8244	Bruceae Fructus	yadanziolide C_qt	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)/C=C(/C(O)(C)C)\C)C(C(=O)C(=C5)O)C)C)C(O)C2O)C1)C(=O)OC
MOL008109	0.8980	0.1020	0.7623	Bruceae Fructus	yadanziolide D	Not Available	FALSE	O1C2(C3(O)C4(C(C(CC4OC(=O)C3O)(C3OC(=O)C=C3C)C)C(O)C2O)C1)C
MOL008110	0.7485	0.2515	0.8037	Bruceae Fructus	bruceoside B	Not Available	FALSE	C123C4C(OC3)(C(C(C1C1(C(CC2OC(=O)C4OC(=O)C=C(C)C)C(=C(C(=O)C1)OC1OC(C(C(C1O)O)O)CO)C)C)O)O)C(=O)OC
MOL008111	0.7994	0.2006	0.8575	Bruceae Fructus	bruceoside B_qt	Not Available	FALSE	C123C4C(OC3)(C(C(C1C1(C(CC2OC(=O)C4OC(=O)C=C(C)C)C(=C(C(=O)C1)O)C)C)O)O)C(=O)OC
MOL008112	0.7353	0.2647	0.8276	Bruceae Fructus	bruceine C	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3OC(=O)/C=C(\C(O)(C)C)/C)C(=C(O)C(=O)C5)C)C)C(O)C2O)C1)C(=O)OC
MOL008113	0.9458	0.0542	0.8393	Bruceae Fructus	bruceine E	Not Available	FALSE	O1C2(C3(O)C4(C(C5(C(CC4OC(=O)C3O)C(=CC(O)C5O)C)C)C(O)C2O)C1)C
MOL008114	0.9329	0.0671	0.8397	Bruceae Fructus	bruceine F	Not Available	FALSE	O1C2(C3(O)C4(C(C5(C(CC4OC(=O)C3O)C(=CC(O)C5O)C)C)C(O)C2O)C1)CO
MOL008115	0.9291	0.0709	0.8141	Bruceae Fructus	bruceine G	Not Available	FALSE	O1C2(C3C4(C(C5(C(C(O)C4OC(=O)C3O)C(=CC(=O)C5)C)C)C(O)C2O)C1)C
MOL008116	0.9335	0.0665	0.8394	Bruceae Fructus	bruceine H	Not Available	FALSE	O1C2(C3(O)C4(C(C5(C(CC4OC(=O)C3O)C(=CC(=O)C5O)C)C)C(O)C2O)C1)CO
MOL008117	0.8705	0.1295	0.7578	Bruceae Fructus	bruceine I	Not Available	FALSE	O1C2(C3C4(C(C5(C(CC4OC(=O)C3)C(=C(O)C(=O)C5)C)C)C(O)C2O)C1)C(=O)OCC
MOL008118	0.5546	0.4454	0.6482	Coicis Semen	Coixenolide	Not Available	FALSE	O(C(C(OC(=O)CCCCCCC/C=C\CCCCCC)C)C)C(=O)CCCCCCCCC/C=C/CCCCCC
MOL008120	0.9288	0.0712	0.9719	Morindae Officinalis Radix	(S)-4-Nonanolide	441574	FALSE	C1(OC(=O)CC1)CCCCC
MOL008120	0.9288	0.0712	0.9719	Siphonostegiae Herba	(S)-4-Nonanolide	441574	FALSE	C1(OC(=O)CC1)CCCCC
MOL008120	0.9288	0.0712	0.9719	Coicis Semen	(S)-4-Nonanolide	441574	FALSE	C1(OC(=O)CC1)CCCCC
MOL008121	0.4349	0.5651	0.6376	Akebiae Frucyus	2-Monoolein	5319879	FALSE	C(CO)(OC(=O)CCCCCCC/C=C\CCCCCCCC)CO
MOL008121	0.4349	0.5651	0.6376	Coicis Semen	2-Monoolein	5319879	FALSE	C(CO)(OC(=O)CCCCCCC/C=C\CCCCCCCC)CO

MOL008126	0.9242	0.0758	0.9296	Coicis Semen	2-ethyl-3-hydroxyhexyl butyrate	Not Available	FALSE	C(=O)(CCC)OCC(C(CCC)O)CC
MOL008127	0.8733	0.1267	0.9626	Siphonostegiae Herba	Ermanin	5352001	FALSE	o1c(c(OC)c(=O)c2c1cc(O)cc2O)c1ccc(OC)cc1
MOL008128	0.8944	0.1056	0.8381	Siphonostegiae Herba	ZINC02042359	1715160	FALSE	CC(=O)CCCC(CCCC(C)C)C
MOL008128	0.8944	0.1056	0.8381	Ephedra Herba	ZINC02042359	1715160	FALSE	CC(=O)CCCC(CCCC(C)C)C
MOL008129	0.9543	0.0457	0.9542	Siphonostegiae Herba	(1S,2S,5S)-2-isopropyl-5-methyl-1-cyclohexanol	1715097	FALSE	OC1C(CCC(C1)C)C(C)C
MOL008130	0.9583	0.0417	0.9014	Siphonostegiae Herba	ascaridole	12308625	FALSE	O1OC2(CCC1(C(C)C)C=C2)C
MOL008130	0.9583	0.0417	0.9014	Zanthoxyli Pericarpium	ascaridole	12308625	FALSE	O1OC2(CCC1(C(C)C)C=C2)C
MOL008131	0.8815	0.1185	0.9022	Siphonostegiae Herba	(2R)-3-(phenoxy)propane-1,2-diol	855016	FALSE	C(C(CO)O)Oc1ccccc1
MOL008132	0.9499	0.0501	0.8831	Siphonostegiae Herba	Isocantleyine	126750	FALSE	OC1C(c2c(C1)c(cnc2)C(=O)OC)C
MOL008133	0.6789	0.3211	0.6950	Siphonostegiae Herba	macranthoin F	Not Available	FALSE	O(C1C(OC(=O)/C=C\c2cc(O)c(O)cc2)C(O)CC(O)(C1)C(=O)OC)C(=O)/C=C\c1cc(O)c(O)cc1
MOL008134	0.8989	0.1011	0.9285	Siphonostegiae Herba	amylcyclopropane	75640	FALSE	C1(CC1)CCCCC
MOL008135	0.8390	0.1610	0.7279	Siphonostegiae Herba	3,4-di-O-caffeoylquinic acid	Not Available	FALSE	C1(CC(C(C(C1)OC(=O)/C=C\c1cc(c(cc1)O)O)O)OC(=O)/C=C\c1cc(c(cc1)O)O)(C(=O)O)O
MOL008136	0.8025	0.1975	0.6277	Siphonostegiae Herba	3-hydroxy-16-methyl heptadecanoic acid	Not Available	FALSE	C(=O)(CC(CCCCCCCCCCCCCC(C)C)O)O
MOL008137	0.9649	0.0351	0.8897	Siphonostegiae Herba	3-methyl-bycyclo[2.2.2.]octanone	Not Available	FALSE	C12C(=O)CC(CC1C)CC2
MOL008138	0.9348	0.0652	0.9517	Siphonostegiae Herba	ZINC02011663	445789	FALSE	OC(CCCCC)CC
MOL008138	0.9348	0.0652	0.9517	Schizonepetae Herba	ZINC02011663	445789	FALSE	OC(CCCCC)CC
MOL008138	0.9348	0.0652	0.9517	Menthae Herba	ZINC02011663	445789	FALSE	OC(CCCCC)CC
MOL008138	0.9348	0.0652	0.9517	Allii Fistulost Bulbus	ZINC02011663	445789	FALSE	OC(CCCCC)CC
MOL008138	0.9348	0.0652	0.9517	Panacis Quinquefolii Radix	ZINC02011663	445789	FALSE	OC(CCCCC)CC
MOL008139	0.9608	0.0392	0.9413	Siphonostegiae Herba	Synox TBC	7381	FALSE	c1(c(cc(cc1)C(C)(C)C)O)O

MOL008141	0.1505	0.8495	0.6648	Ricini Semen	7beta,12-Dimethoxy-8,11,13-abietatrien-11-ol	21159045	FALSE	C1C(C2C(CC1)(c1c(C(C2)OC)cc(c(c1O)OC)C(C)C)C)(C)C
MOL008142	0.9376	0.0624	0.8826	Ricini Semen	Ricinin	10666	TRUE	O(c1c(c(=O)n(cc1)C)C#N)C
MOL008142	0.9376	0.0624	0.8826	Codonopsis Radix	Ricinin	10666	TRUE	O(c1c(c(=O)n(cc1)C)C#N)C
MOL008143	0.8226	0.1774	0.6731	Ricini Semen	Nouracid CS 80	643684	FALSE	C(CCCCC(C/C=C\CCCCCCCC(=O)O)O)C
MOL008143	0.8226	0.1774	0.6731	Ganoderma	Nouracid CS 80	643684	FALSE	C(CCCCC(C/C=C\CCCCCCCC(=O)O)O)C
MOL008144	0.8325	0.1675	0.8396	Ricini Semen	rosthorin A	Not Available	FALSE	O1C2(O)C34C(C5(C(C2O)C(CCC5)(C)C)C1)C(O)CC(C3O)C(=C)C4=O
MOL008145	0.6725	0.3275	0.6350	Ricini Semen	Costaclavine	821486	FALSE	c1c2c3c(cc1)C1C(Cc3c[nH]2)N(CC(C1)C)C
MOL008146	0.8040	0.1960	0.6155	Ricini Semen	Riddelline	Not Available	FALSE	C/C=C\1/C(=O)OC2CCN3C2C(=CC3)COC(=O)C(C(=C)C1)(O)CO
MOL008147	0.5573	0.4427	0.7691	Ricini Semen	Sebiferic acid	Not Available	FALSE	C12C(CCC3C1(CCC3C(=C)C)C)(C1(C(CC2)C(C(CC1)C(=C)C)(CCC(=O)O)C)C)C
MOL008148	0.9165	0.0835	0.8274	Ricini Semen	Suberogorgin	Not Available	FALSE	C1CC2C(CC(=O)C32C1(C=C(C3C)C(=O)O)C)C
MOL008150	0.8895	0.1105	0.8859	Platycladi Semen	Methyl undecenate	8138	FALSE	C(CCC(=O)OC)CCCCCC=C
MOL008152	0.9398	0.0602	0.9578	Ephedra Herba	Methyl heptoate	7826	FALSE	C(=O)(CCCCCC)OC
MOL008152	0.9398	0.0602	0.9578	Hoveniae Dulcis Semen	Methyl heptoate	7826	FALSE	C(=O)(CCCCCC)OC
MOL008152	0.9398	0.0602	0.9578	Platycladi Semen	Methyl heptoate	7826	FALSE	C(=O)(CCCCCC)OC
MOL008154	0.9248	0.0752	0.9219	Platycladi Semen	Nona-2,6-dienal	643731	FALSE	C(C/C=C/C=O)/C=C\CC
MOL008155	0.8698	0.1302	0.8126	Microctis Folium	isorhamnetin3-O-D-glucopyranoside	Not Available	FALSE	c1(cc(c2c(c1)OC(C(C2=O)OC1CC(C(C(C1O)O)O)O)CO)c1ccc(c(c1)OC)O)O)O
MOL008156	0.9213	0.0787	0.9047	Microctis Folium	isorhamnetin3-O-D-glucopyranoside_qt	Not Available	FALSE	c1(cc(c2c(c1)OC(C(C2=O)O)c1ccc(c(c1)OC)O)O)O
MOL008157	0.8527	0.1473	0.7937	Microctis Folium	isoviolanthin	Not Available	FALSE	c1c(c(c2c(c1C1C(C(C(C(O1)CO)O)O)O)OC(CC2=O)c1ccc(cc1)O)O)C1OC(C(C(C1O)O)O)C
MOL008158	0.8811	0.1189	0.8240	Microctis Folium	kaempferol-3-O-β-D-glucopyranoside	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1CC(C(C(C1O)O)O)O)CO)c1ccc(cc1)O)O)O

MOL008160	0.5750	0.4250	0.6203	Microctis Folium	Tritetracontane	522398	FALSE	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
MOL008161	0.8729	0.1271	0.7977	Microctis Folium	violanthin	Not Available	FALSE	c1(cc(=O)c2c(c(c(c(c2o1)C1OC(C(C(C1O)O)O)C)O)C1OC(C(C(C1O)O)O)CO)O)c1ccc(cc1)O
MOL008163	0.9079	0.0921	0.9178	Dichroae Radix	(2E,4Z)-hepta-2,4-dienal	11788274	FALSE	O=C/C=C/C=C\CC
MOL008164	0.9337	0.0663	0.9590	Dichroae Radix	(2R)-2-methylpentanal	6994104	FALSE	O=CC(CCC)C
MOL008165	0.9210	0.0790	0.9282	Campsis Flos	2-Decanone	12741	FALSE	C(CCCCC)CCC(=O)C
MOL008165	0.9210	0.0790	0.9282	Dichroae Radix	2-Decanone	12741	FALSE	C(CCCCC)CCC(=O)C
MOL008166	0.9250	0.0750	0.9644	Ephedra Herba	(E)-Pent-2-en-1-ol	5364920	FALSE	OC/C=C/CC
MOL008166	0.9250	0.0750	0.9644	Dichroae Radix	(E)-Pent-2-en-1-ol	5364920	FALSE	OC/C=C/CC
MOL008167	0.8363	0.1637	0.8008	Dichroae Radix	3,9-Dodecadiyne	143841	FALSE	C(CCC#CCC)CC#CCC
MOL008168	0.9212	0.0788	0.9400	Dichroae Radix	3-hexanone,2,4-dimethyl-	25021574	FALSE	C(=O)(C(CC)C)C(C)C
MOL008169	0.9537	0.0463	0.7528	Dichroae Radix	(1R)-(-)-thuj-3-ene	12444325	FALSE	C1=C(C2C(C1)(C(C)C)C2)C
MOL008170	0.9428	0.0572	0.9284	Dichroae Radix	3-methyl-3,4-divinyl-1-cyclohexene	Not Available	FALSE	C1(C(CCC=C1)C=C)(C)C=C
MOL008171	0.9295	0.0705	0.9403	Dichroae Radix	CIS-3-heptenyl acetate	21159742	FALSE	C(/C=C\CCC)COC(=O)C
MOL008174	0.9203	0.0797	0.9308	Dichroae Radix	(E)-hept-4-en-2-one	5363123	FALSE	O=C(C/C=C/CC)C
MOL008175	0.9308	0.0692	0.9571	Dichroae Radix	Ethyl 3-butenoate	74172	FALSE	O(CC)C(=O)CC=C
MOL008176	0.8713	0.1287	0.8472	Dichroae Radix	2-[(1S,3Z,7Z)-4,8-dimethyl-1-cyclodeca-3,7-dienyl]propan-2-ol	6432240	FALSE	OC(C1CC/C(=C\CC/C(=C\C1)/C)/C)(C)C

MOL008177	0.8398	0.1602	0.7993	Dichroae Radix	4,8-dimethoxy-1-methyl-3-(3-methyl-2-oxobut-3-enyl)quinolin-2-one	11243539	FALSE	O(c1c2c(n(c(=O)c1CC(=O)C(=C)C)C)c(OC)ccc2)C
MOL008178	0.8828	0.1172	0.8564	Dichroae Radix	3-(2-keto-3-methyl-but-3-enyl)-4,8-dimethoxy-carbostyril	11426211	FALSE	O(c1c2c([nH]c(=O)c1CC(=O)C(=C)C)c(OC)ccc2)C
MOL008180	0.8773	0.1227	0.6970	Dichroae Radix	3-[3-[(2R,3S)-3-hydroxy-2-piperidyl]-2-oxo-propyl]quinazolin-4-one	9851692	FALSE	OC1C(NCCC1)CC(=O)Cn1c(=O)c2c(nc1)cccc2
MOL008181	0.9312	0.0688	0.7843	Dichroae Radix	1,1-diethylpropyl benzene	20136	FALSE	C(c1ccccc1)(CC)(CC)CC
MOL008183	0.8925	0.1075	0.8490	Dichroae Radix	Evolitrin	196980	FALSE	o1c2nc3c(c(OC)c2cc1)ccc(OC)c3
MOL008184	0.7637	0.2363	0.6351	Dichroae Radix	(2R)-1-(4,8-dimethoxyfuro[2,3-b]quinolin-7-yl)oxy-3-methylbutane-2,3-diol	673465	FALSE	O(CC(O)C(O)(C)C)c1c(OC)c2nc3occc3c(OC)c2cc1
MOL008185	0.8966	0.1034	0.9339	Dichroae Radix	2-Propylfuran	77907	FALSE	c1(CCC)ccco1
MOL008185	0.8966	0.1034	0.9339	Campsis Flos	2-Propylfuran	77907	FALSE	c1(CCC)ccco1
MOL008185	0.8966	0.1034	0.9339	Momordicae Fructus	2-Propylfuran	77907	FALSE	c1(CCC)ccco1
MOL008186	0.9158	0.0842	0.8859	Dichroae Radix	Isobutyryl chloride	62325	FALSE	CC(C)C(=O)Cl
MOL008187	0.8168	0.1832	0.6555	Dichroae Radix	isofebrifugine	Not Available	FALSE	O1C2C(NCCC2)CC1(O)Cn1c(=O)c2c(nc1)cccc2
MOL008188	0.6813	0.3187	0.8446	Dipsaci Radix	Japonine	442915	FALSE	O(c1c(n(c2c(c1=O)cc(OC)cc2)C)c1ccccc1)C
MOL008188	0.6813	0.3187	0.8446	Dichroae Radix	Japonine	442915	FALSE	O(c1c(n(c2c(c1=O)cc(OC)cc2)C)c1ccccc1)C
MOL008189	0.9093	0.0907	0.6747	Dichroae Radix	Kokusagine	Not Available	FALSE	O1c2c3nc4occc4c(OC)c3ccc2OC1
MOL008190	0.9085	0.0915	0.7796	Dichroae Radix	megastigma-3,7(E),9-triene	Not Available	FALSE	C1=CC(C(C(C1)(C)C)/C=C/C=C)C
MOL008192	0.9011	0.0989	0.6413	Dichroae Radix	NEOPENTANE	10041	FALSE	C(C)(C)(C)C

MOL008193	0.7797	0.2203	0.7933	Dichroae Radix	4,8-dimethoxy-1-methyl-3-(3-methyl-2-oxobutyl)quinolin-2-one	11278088	FALSE	O(c1c(CC(=O)C(C)C)c(=O)n(c2c1cccc2OC)C)C
MOL008194	0.8189	0.1811	0.7337	Dichroae Radix	(3R,4S)-3,4-dihydroxy-2,2,6-trimethyl-3,4-dihydropyrano[5,6-c]quinolin-5-one	21573064	FALSE	O1C(C(C(c2c(=O)n(c3c(c12)cccc3)C)O)O)(C)C
MOL008195	0.7255	0.2745	0.7905	Dichroae Radix	Orixinone	5320309	FALSE	O1c2c3nc(OC)c(CC(=O)C(C)C)c(OC)c3ccc2OC1
MOL008197	0.6512	0.3488	0.7833	Dichroae Radix	Pteleprenine	167633	FALSE	O1c2c3n(c(=O)c(c(OC)c3ccc2OC1)CC=C(C)C)C
MOL008198	0.9035	0.0965	0.8950	Dichroae Radix	Vinyl methacrylate	77921	FALSE	O(C(=O)C(=C)C)C=C
MOL008199	0.8168	0.1832	0.6555	Dichroae Radix	α-Dichroine	Not Available	FALSE	O1C2C(NCCC2)CC1(O)Cn1c(=O)c2c(nc1)cccc2
MOL008200	0.9480	0.0520	0.9161	Dichroae Radix	1-Methyl-5,6-divinyl-1-cyclohexene	Not Available	FALSE	C1(C(C(=CCC1)C)C=C)C=C
MOL008201	0.8612	0.1388	0.7739	Dichroae Radix	2,4,6-trimethyl-1-nonene	Not Available	FALSE	C(CC(CC(=C)C)C)(CCC)C
MOL008202	0.3950	0.6050	0.7476	Impatientis Semen	3-[(E)-2-[(1R,4aS,5R,6R,8aR)-6-hydroxy-5,8a-dimethyl-2-methylene-5-methylol-decalin-1-yl]vinyl]-5H-furan-2-one	5708351	FALSE	C12C(C(/C=C/C3=CCOC3=O)C(=C)CC2)(CCC(C1(CO)C)O)C

MOL008202	0.3950	0.6050	0.7476	Andrographis Herba	3-[(E)-2-[(1R,4aS,5R,6R,8aR)-6-hydroxy-5,8a-dimethyl-2-methylene-5-methylol-decalin-1-yl]vinyl]-5H-furan-2-one	5708351	FALSE	C12C(C(/C=C/C3=CCOC3=O)C(=C)CC2)(CCC(C1(CO)C)O)C
MOL008203	0.5347	0.4653	0.6987	Andrographis Herba	14-deoxy-11-oxo-andrographolide	Not Available	FALSE	C1C2C(CCC(C2(C)CO)O)(C(C(=C)C1)C(=O)CC1=CCOC1=O)C
MOL008204	0.6657	0.3343	0.8107	Andrographis Herba	Mono-O-methylwightin	5319878	FALSE	c1(cc(=O)c2c(cc(c(c2o1)OC)OC)O)c1c(c(ccc1)OC)OC
MOL008205	0.7056	0.2944	0.8453	Andrographis Herba	5-hydroxy-7,8-dimethoxy flavanone	Not Available	FALSE	O1C(CC(=O)c2c1c(OC)ccc2)c1cc(OC)c(O)cc1
MOL008206	0.7929	0.2071	0.9723	Moslae Herba	Moslosooflavone	188316	FALSE	o1c2c(c(O)cc(OC)c2OC)c(=O)cc1c1ccccc1
MOL008206	0.7929	0.2071	0.9723	Andrographis Herba	Moslosooflavone	188316	FALSE	o1c2c(c(O)cc(OC)c2OC)c(=O)cc1c1ccccc1
MOL008206	0.7929	0.2071	0.9723	Scutellariae Barbatae Herba	Moslosooflavone	188316	FALSE	o1c2c(c(O)cc(OC)c2OC)c(=O)cc1c1ccccc1
MOL008207	0.9107	0.0893	0.8914	Andrographis Herba	2-[(4R,4aS)-4,7-dimethyl-2,3,4,4a,5,6-hexahydronaphthalen-1-yl]acrylic acid	11424773	FALSE	C1C(=CC2=C(CCC(C2C1)C)C(=C)C(=O)O)C
MOL008208	0.5696	0.4304	0.6183	Andrographis Herba	TETRACONTANE	20149	FALSE	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
MOL008208	0.5696	0.4304	0.6183	Ranunculi Ternati Radix	TETRACONTANE	20149	FALSE	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
MOL008209	0.7786	0.2214	0.7908	Andrographis Herba	Deoxycamptothecine	Not Available	FALSE	c12c(cccc1)nc1c(c2)Cn2c1cc1c(c2=O)COC(=O)C1CC
MOL008211	0.9258	0.0742	0.7366	Andrographis Herba	Deoxypeganin	442894	FALSE	c1cccc2c1CN1C(=N2)CCC1
MOL008212	0.1789	0.8211	0.6786	Andrographis Herba	(-)-Neoarctin B	3083466	FALSE	C1(C(Cc2cc(c(c(c2)OC)O)OC)C(=O)OC1)Cc1ccc(c(c1)OC)c1c(cc(cc1)CC1COC(=O)C1Cc1cc(c(c(c1)OC)O)OC)OC
MOL008214	0.4667	0.5333	0.7605	Andrographis Herba	Paniculatin	Not Available	FALSE	CC(C(=O)C(OC(=O)CC(C)C)C1(CCC2C1OC(=O)CC2)OC)C

MOL008215	0.9158	0.0842	0.7961	Andrographis Herba	Paniculide B	Not Available	FALSE	C12C(CC3C(=C(C(=O)O3)CCC=C(C)C)C1O)(O2)C
MOL008216	0.8987	0.1013	0.7986	Andrographis Herba	Paniculide C	Not Available	FALSE	C12C(CC3C(=C(C(=O)O3)CCC=C(C)C)C1=O)(O2)CO
MOL008217	0.3721	0.6279	0.7404	Andrographis Herba	Paniculogenin	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2O)C2C(CC1)(C1C(C2)OC2(C1C)C(CC(C)CO2)O)C)C)O
MOL008219	0.2702	0.7298	0.7387	Andrographis Herba	3-[2-[(1R,4aS,5R,8aS)-5,8a-dimethyl-2-methylene-5-methylol-decalin-1-yl]ethyl]-5H-furan-2-one	11666871	FALSE	OCC1(C2C(C(C(=C)CC2)CCC2=CCOC2=O)(CCC1)C)C
MOL008220	0.4777	0.5223	0.7309	Andrographis Herba	andrographidine A	Not Available	FALSE	C1(C(C(C(CC1CO)Oc1c2c(c(c(c1)OC)OC)OC(CC2=O)c1ccccc1)O)O)O
MOL008221	0.8504	0.1496	0.7916	Andrographis Herba	andrographidine B	Not Available	FALSE	c1cc(c(c(c1)OC1OC(C(C(C1O)O)O)CO)O)c1oc2c(c(=O)c1)c(cc(c2OC)OC)O
MOL008222	0.8628	0.1372	0.8644	Andrographis Herba	andrographidine B_qt	13963776	FALSE	c1cc(c(c(c1)O)O)c1oc2c(c(=O)c1)c(cc(c2OC)OC)O
MOL008223	0.6484	0.3516	0.7604	Andrographis Herba	andrographidine C	Not Available	FALSE	c1cc(ccc1)c1oc2c(c(=O)c1)c(cc(c2OC)OC)OC1OC(C(C(C1O)O)O)CO
MOL008224	0.6330	0.3670	0.6323	Andrographis Herba	andrographidine D	Not Available	FALSE	c1(c(c(ccc1)c1oc2c(c(=O)c1)c(cc(c2OC)OC)OC1OC(C(C(C1O)O)O)CO)OC)OC
MOL008226	0.3638	0.6362	0.7185	Andrographis Herba	14-deoxyandrographolide	Not Available	FALSE	C1(C2C(C(C(=C)CC2)CCC2=CCOC2=O)(CCC1O)C)(CO)C
MOL008227	0.6279	0.3721	0.6992	Andrographis Herba	andrographidine E	Not Available	FALSE	c1c(c(ccc1)c1oc2c(c(=O)c1)c(cc(c2OC)OC)OC1OC(C(C(C1O)O)O)CO)OC
MOL008228	0.7436	0.2564	0.8529	Andrographis Herba	Andrographin	5318506	FALSE	c1c(c(ccc1)c1oc2c(c(=O)c1)c(cc(c2OC)OC)O)OC
MOL008229	0.7324	0.2676	0.6747	Andrographis Herba	Andrographin F	5318512	FALSE	O1C(C(C(C(C1CO)O)O)O)Oc1c2c(=O)cc(oc2c(c(c1)OC)OC)c1c(c(c(cc1)O)OC)OC
MOL008230	0.6895	0.3105	0.7755	Andrographis Herba	andrographidine F_qt	13963777	FALSE	Oc1c2c(=O)cc(oc2c(c(c1)OC)OC)c1c(c(c(cc1)O)OC)OC
MOL008231	0.4754	0.5246	0.6264	Andrographis Herba	andropanoside	Not Available	FALSE	C1(C(C(C(OC1CO)OCC1(C2C(CCC1O)(C(C(=C)CC2)C/C=C\1/C(COC1=O)O)C)C)O)O)O

MOL008232	0.4913	0.5087	0.6921	Andrographis Herba	(3Z,4S)-3-[2-[(1R,4aS,5R,6R,8aS)-6-hydroxy-5,8a-dimethyl-2-methylene-5-methylol-decalin-1-yl]ethylidene]-4-hydroxy-tetrahydrofuran-2-one	7067324	FALSE	OC1C(C2C(C(C(=C)CC2)C/C=C\2/C(O)COC2=O)(CC1)C)(CO)C
MOL008234	0.4516	0.5484	0.7251	Andrographis Herba	andrographolide-19-β-D-glucoside_qt	Not Available	FALSE	C1C(CC2C(C1)(C(C(=C)CC2(CO)C)C/C=C\1/C(O)COC1=O)C)O
MOL008238	0.2702	0.7298	0.7387	Andrographis Herba	3-[2-[(1S,4aR,5S,8aR)-5,8a-dimethyl-2-methylene-5-methylol-decalin-1-yl]ethyl]-5H-furan-2-one	23238929	FALSE	C1(C2(C(C(CCC2)(C)CO)CCC1=C)C)CCC1=CCOC1=O
MOL008239	0.7789	0.2211	0.8697	Andrographis Herba	Quercetin tetramethyl(3',4',5,7) ether	97142	FALSE	o1c2c(c(=O)c(O)c1c1cc(OC)c(OC)cc1)c(OC)cc(OC)c2
MOL008240	0.6679	0.3321	0.7315	Hydnocarpi Anthelminticae Semen	(E)-3-[4-[(1R,2R)-2-hydroxy-2-(4-hydroxy-3-methoxy-phenyl)-1-methylol-ethoxy]-3-methoxy-phenyl]acrolein	21582571	FALSE	c1(cc(ccc1OC(C(c1ccc(c(c1)OC)O)O)CO)/C=C/C=O)OC
MOL008241	0.8613	0.1387	0.8259	Hydnocarpi Anthelminticae Semen	1,2-Bis(4-hydroxy-3-methoxyphenyl)-1,3-propanediol	12468617	FALSE	OC(C(c1cc(OC)c(O)cc1)CO)c1cc(OC)c(O)cc1

MOL008242	0.5705	0.4295	0.6618	Hydnocarpi Anthelminticae Semen	mulberrofuran K	Not Available	FALSE	O1C2(Oc3c(C4C2C(CC(=C4)C)c2c1cc(O)cc2)c(O)cc(c3)c1oc2c(c1)ccc(O)c2)c1c(O)cc(O)cc1
MOL008243	0.7288	0.2712	0.6808	Hydnocarpi Anthelminticae Semen	mulberroside C	Not Available	FALSE	O1C(C(O)Cc2c1cc1oc(cc1c2)c1cc(OC2OCC(O)C(O)C2O)cc(O)c1)(C)C
MOL008245	0.8752	0.1248	0.7946	Angelicae Sinensis Radix	DODECENE	8183	FALSE	C=CCCCCCCCCCC
MOL008245	0.8752	0.1248	0.7946	Farfarae Flos	DODECENE	8183	FALSE	C=CCCCCCCCCCC
MOL008245	0.8752	0.1248	0.7946	Lysimachiae Foenigraeci Herba	DODECENE	8183	FALSE	C=CCCCCCCCCCC
MOL008245	0.8752	0.1248	0.7946	Fritiliariae Irrhosae Bulbus	DODECENE	8183	FALSE	C=CCCCCCCCCCC
MOL008250	0.9132	0.0868	0.8506	Angelicae Sinensis Radix	ESEN	6811	FALSE	C1(=O)c2c(C(=O)O1)cccc2
MOL008251	0.9497	0.0503	0.8699	Angelicae Sinensis Radix	sedanolide	12315451	FALSE	O1C(C2CCCC=C2C1=O)CCCC
MOL008252	0.9526	0.0474	0.8878	Angelicae Sinensis Radix	senkyunolide	54753664	FALSE	O1C(C2=C(C1=O)C=CCC2)CCCC
MOL008254	0.2190	0.7810	0.7258	Angelicae Sinensis Radix	Isotetandrine	Not Available	FALSE	O1c2c3C(N(CCc3cc(OC)c2OC)C)Cc2cc(Oc3ccc(CC4N(CCc5c4cc1c(OC)c5)C)cc3)c(OC)cc2
MOL008254	0.2190	0.7810	0.7258	Mahoniae Caulis	Isotetandrine	Not Available	FALSE	O1c2c3C(N(CCc3cc(OC)c2OC)C)Cc2cc(Oc3ccc(CC4N(CCc5c4cc1c(OC)c5)C)cc3)c(OC)cc2
MOL008254	0.2190	0.7810	0.7258	Mahoniae Folum	Isotetandrine	Not Available	FALSE	O1c2c3C(N(CCc3cc(OC)c2OC)C)Cc2cc(Oc3ccc(CC4N(CCc5c4cc1c(OC)c5)C)cc3)c(OC)cc2
MOL008254	0.2190	0.7810	0.7258	Mahoniae Eadix	Isotetandrine	Not Available	FALSE	O1c2c3C(N(CCc3cc(OC)c2OC)C)Cc2cc(Oc3ccc(CC4N(CCc5c4cc1c(OC)c5)C)cc3)c(OC)cc2
MOL008259	0.4749	0.5251	0.6514	Angelicae Sinensis Radix	2,6-di(phenyl)thiopyran-4-thione	11832833	FALSE	c1(cc(=S)cc(s1)c1ccccc1)c1ccccc1
MOL008260	0.9220	0.0780	0.9428	Angelicae Sinensis Radix	o-Xylenol	10687	FALSE	c1(c(c(ccc1)C)C)O
MOL008261	0.9005	0.0995	0.8389	Angelicae Sinensis Radix	2,4,6-trimethyl-Octane	59734807	FALSE	CC(CC(CC(CC)C)C)C
MOL008262	0.9541	0.0459	0.8585	Angelicae Sinensis Radix	Mesitaldehyde	10254	FALSE	C(=O)c1c(cc(cc1C)C)C
MOL008263	0.9454	0.0546	0.9253	Angelicae Sinensis Radix	Isoxylaldehyde	22015	FALSE	O=Cc1c(ccc(c1)C)C
MOL008265	0.9551	0.0449	0.8865	Angelicae Sinensis Radix	2-valerylbenzoic acid	5315165	FALSE	C(=O)(c1c(cccc1)C(=O)CCCC)O
MOL008266	0.8834	0.1166	0.8852	Angelicae Sinensis Radix	(Z)-2-Hexenyl hexanoate	5352973	FALSE	CCC/C=C/COC(=O)CCCCC
MOL008267	0.8095	0.1905	0.6185	Angelicae Sinensis Radix	2-Methylhexadecanoic acid	Not Available	FALSE	C(=O)(C(CCCCCCCCCCCCCCC)C)O
MOL008268	0.9506	0.0494	0.9462	Angelicae Sinensis Radix	cis-Isoeugenol	1549041	FALSE	O(c1cc(ccc1O)/C=C\C)C

MOL008270	0.8797	0.1203	0.8430	Angelicae Sinensis Radix	2-methyldodecan-5-one	5319599	FALSE	CC(CCC(=O)CCCCCCC)C
MOL008271	0.9055	0.0945	0.8579	Rose Rugosae Flos	3,7-dimethyl-nonane	42626759	FALSE	C(CC(CC)C)CC(CC)C
MOL008271	0.9055	0.0945	0.8579	Angelicae Sinensis Radix	3,7-dimethyl-nonane	42626759	FALSE	C(CC(CC)C)CC(CC)C
MOL008272	0.9624	0.0376	0.9399	Angelicae Sinensis Radix	1,1,5-trimethyl-2-formylcyclohexa-2,5-diene-4-one	Not Available	FALSE	C1(=CC(=O)C(=CC1(C)C)C)C=O
MOL008273	0.9210	0.0790	0.9369	Angelicae Sinensis Radix	4-Methyl-6-hepten-3-one	25018179	FALSE	CCC(=O)C(CC=C)C
MOL008274	0.9381	0.0619	0.9713	Angelicae Sinensis Radix	6-Ethylresorcinol	17927	FALSE	Oc1cc(O)c(cc1)CC
MOL008275	0.9072	0.0928	0.8411	Angelicae Sinensis Radix	5-Indolol	16054	FALSE	Oc1cc2c([nH]cc2)cc1
MOL008276	0.9124	0.0876	0.9062	Angelicae Sinensis Radix	Undecanol-6	32045	FALSE	CCCCCC(CCCCC)O
MOL008277	0.8765	0.1235	0.7660	Angelicae Sinensis Radix	7,10-PENTADECADIYNOIC ACID	30942	FALSE	C(=O)(CCCCCC#CCC#CCCCC)O
MOL008278	0.3101	0.6899	0.6133	Angelicae Sinensis Radix	4-chloro-N-[1-methyl-5-[[1-methyl-5-[[1-methyl-5-(2-morpholinoethylcarbamoyl)pyrrol-3-yl]carbamoyl]pyrrol-3-yl]carbamoyl]pyrrol-3-yl]-5-[2-(2-pyridyl)ethylamino]isothiazole-3-carboxamide	488866	FALSE	Clc1c(nsc1NCCc1ncccc1)C(=O)Nc1cc(n(c1)C)C(=O)Nc1cc(n(c1)C)C(=O)Nc1cc(n(c1)C)C(=O)NCCN1CCOCC1
MOL008279	0.9067	0.0933	0.9075	Angelicae Sinensis Radix	Amyl ketone	13561	FALSE	O=C(CCCCC)CCCCC
MOL008279	0.9067	0.0933	0.9075	Achyranthis Bidentatae Radix	Amyl ketone	13561	FALSE	O=C(CCCCC)CCCCC

MOL008280	0.9333	0.0667	0.9263	Angelicae Sinensis Radix	Isoamylbenzene	16294	FALSE	C(CCc1ccccc1)(C)C
MOL008281	0.9316	0.0684	0.9596	Angelicae Sinensis Radix	(Z)-2-[[(Z)-2-methylbut-2-enoyl]oxymethyl]but-2-enoic acid	6440421	FALSE	C(=O)(/C(=C\C)/COC(=O)/C(=C\C)/C)O
MOL008282	0.8706	0.1294	0.9601	Angelicae Sinensis Radix	Tropone	10881	FALSE	O=c1cccccc1
MOL008284	0.8994	0.1006	0.9677	Ginkgo Folium	BUA	264	FALSE	OC(=O)CCC
MOL008284	0.8994	0.1006	0.9677	Hippophae Fructus	BUA	264	FALSE	OC(=O)CCC
MOL008284	0.8994	0.1006	0.9677	Allii Fistulost Bulbus	BUA	264	FALSE	OC(=O)CCC
MOL008284	0.8994	0.1006	0.9677	Angelicae Sinensis Radix	BUA	264	FALSE	OC(=O)CCC
MOL008284	0.8994	0.1006	0.9677	Cistanches Herba	BUA	264	FALSE	OC(=O)CCC
MOL008284	0.8994	0.1006	0.9677	Momordicae Fructus	BUA	264	FALSE	OC(=O)CCC
MOL008284	0.8994	0.1006	0.9677	Ginkgo Semen	BUA	264	FALSE	OC(=O)CCC
MOL008284	0.8994	0.1006	0.9677	Codonopsis Radix	BUA	264	FALSE	OC(=O)CCC
MOL008284	0.8994	0.1006	0.9677	Euphorbiae Helioscopiae Herba	BUA	264	FALSE	OC(=O)CCC
MOL008285	0.9525	0.0475	0.8916	Gossampiniflos	(3S)-3-butyl-3H-isobenzofuran-1-one	11116832	FALSE	O1C(CCCC)c2c(C1=O)cccc2
MOL008285	0.9525	0.0475	0.8916	Angelicae Sinensis Radix	(3S)-3-butyl-3H-isobenzofuran-1-one	11116832	FALSE	O1C(CCCC)c2c(C1=O)cccc2
MOL008286	0.9516	0.0484	0.8722	Angelicae Sinensis Radix	()-Camphoric acid	101807	FALSE	C(=O)(C1(CCC(C(=O)O)C1(C)C)C)O
MOL008287	0.9596	0.0404	0.9083	Angelicae Sinensis Radix	(3E)-3-butylidene-7-hydroxy-2-benzofuran-1-one	5852943	FALSE	C1(=O)O/C(=C/CCC)/c2cccc(c12)O
MOL008288	0.5892	0.4108	0.7617	Angelicae Sinensis Radix	Coniferyl ferulate	6441913	FALSE	O(c1cc(ccc1O)/C=C/COC(=O)/C=C/c1cc(OC)c(O)cc1)C
MOL008288	0.5892	0.4108	0.7617	Notopterygii Rhizoma Et Radix	Coniferyl ferulate	6441913	FALSE	O(c1cc(ccc1O)/C=C/COC(=O)/C=C/c1cc(OC)c(O)cc1)C
MOL008291	0.9616	0.0384	0.9330	Angelicae Sinensis Radix	2,4-Xylylaldehyde	61814	FALSE	O=Cc1c(cc(cc1)C)C
MOL008292	0.9295	0.0705	0.9517	Angelicae Sinensis Radix	m-Ethylphenol	12101	FALSE	Oc1cc(CC)ccc1

MOL008293	0.9546	0.0454	0.9396	Angelicae Sinensis Radix	1,5,5,6-tetramethyl-1,3-Cyclohexadiene	Not Available	FALSE	C1(=CC=CC(C1C)(C)C)C
MOL008295	0.5551	0.4449	0.7383	Achyranthis Asperae Herba	(threo)-3-hydroxy-1-(4-hydroxy-3-methoxyphenyl)_qt	Not Available	FALSE	c1(c(c(cc(c1)/C=C/CO)OC)OC(C)C(c1cc(c(cc1)O)OC)O)OC
MOL008296	0.9146	0.0854	0.6551	Achyranthis Asperae Herba	1,4-Dimethylnaphthalene	11304	FALSE	c1(ccc(c2ccccc12)C)C
MOL008296	0.9146	0.0854	0.6551	Gossampiniflos	1,4-Dimethylnaphthalene	11304	FALSE	c1(ccc(c2ccccc12)C)C
MOL008297	0.8870	0.1130	0.9687	Achyranthis Asperae Herba	Methakrylsaeure	4093	FALSE	C(=O)(C(=C)C)O
MOL008298	0.9242	0.0758	0.8904	Achyranthis Asperae Herba	Tremetone	78673	FALSE	O1C(Cc2c1ccc(c2)C(=O)C)C(=C)C
MOL008299	0.9515	0.0485	0.9093	Achyranthis Asperae Herba	3-(2,3-dihydroxy-isopentyl)-4-hydroxy-acetophenone	Not Available	FALSE	c1(ccc(c(c1)CC(C(C)(O)C)O)O)C(=O)C
MOL008300	0.6474	0.3526	0.6071	Achyranthis Asperae Herba	36,47-dihydroxyhenpentacontan-4-one	Not Available	FALSE	CCCC(=O)CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(CCCCCCCCCCC(CCCC)O)O
MOL008302	0.7134	0.2866	0.7714	Achyranthis Asperae Herba	Isoparvifuran	617473	FALSE	o1c2c(c(c1C)c1ccccc1)cc(O)c(OC)c2
MOL008303	0.8727	0.1273	0.7494	Achyranthis Asperae Herba	5H-benzocycloheptен-1-ol , 6, 7, 8, 9-	Not Available	FALSE	c12c(C(CCCC1(C)C)C)c(cc(c2)C)O
MOL008304	0.9509	0.0491	0.8353	Achyranthis Asperae Herba	7, 8-dihydroxy-4,5-dimethyl-3,4-dihydronaphthalen-1(2H)-one	Not Available	FALSE	C1(=O)CCC(c2c(cc(c(c12)O)O)C)C

MOL008305	0.6540	0.3460	0.7773	Achyranthis Asperae Herba	Ardisiacrispin A	Not Available	FALSE	C1C2C3(CCC1(C)C=O)C(CC1(C2(CCC2C1(CCC1C(C(CCC21C)OC1C(C(C(CO1)OC1C(C(C(C(O1)CO)O)O)O)Oc1c(cccc1C)C)C)OC1C(C(C(C(C1)CO)O)O)O)(C)C)C)OC3)C)O
MOL008306	0.5429	0.4571	0.7197	Achyranthis Asperae Herba	Ardisiacrispin A_qt	Not Available	FALSE	C1C2C3(CCC1(C)C=O)C(CC1(C2(CCC2C1(CCC1C(C(CCC21C)OC1C(C(C(CO1)OC1C(C(C(C(O1)CO)O)O)O)Oc1c(cccc1C)C)C)O)(C)C)C)OC3)C)O
MOL008307	0.9186	0.0814	0.6958	Achyranthis Asperae Herba	1,7-Dimethylnaphthalene	11326	FALSE	c1(cccc2ccc(cc12)C)C
MOL008307	0.9186	0.0814	0.6958	Gossampiniflos	1,7-Dimethylnaphthalene	11326	FALSE	c1(cccc2ccc(cc12)C)C
MOL008308	0.8712	0.1288	0.7932	Achyranthis Asperae Herba	73088-51-4	6450454	FALSE	C12C/C=C(/C(CCC(=C)C1CC2(C)C)O)\C
MOL008309	0.9564	0.0436	0.9164	Achyranthis Asperae Herba	2,5-Dimethoxyacetophenone	70991	FALSE	C(=O)(C)c1c(ccc(c1)OC)OC
MOL008310	0.9619	0.0381	0.8188	Achyranthis Asperae Herba	Euparone	104654	FALSE	o1c2c(cc(c(O)c2)C(=O)C)cc1C(=O)C
MOL008312	0.5494	0.4506	0.6156	Achyranthis Asperae Herba	Eupatorin A_qt	Not Available	FALSE	c1(c(c(cc(c1)/C=C/CO)OC)OC(COC(=O)C)C(c1cc(c(cc1)O)OC)O)OC
MOL008313	0.9196	0.0804	0.8568	Achyranthis Asperae Herba	Gymnastone	Not Available	FALSE	c1(c(cc2c(c1)cc(o2)C(CO)(O)CO)C(=O)C)O
MOL008314	0.9245	0.0755	0.7114	Achyranthis Asperae Herba	ETHYLNAPHTHALENE	14315	FALSE	c1(cccc2ccccc12)CC
MOL008315	0.9003	0.0997	0.9732	Achyranthis Asperae Herba	Stilon	7768	FALSE	N1C(=O)CCCCC1
MOL008315	0.9003	0.0997	0.9732	Sojae Semen Nigrum	Stilon	7768	FALSE	N1C(=O)CCCCC1
MOL008317	0.3817	0.6183	0.6043	Ginkgo Folium	Hydroginkgol	68146	FALSE	Oc1cc(CCCCCCCCCCCCCCCC)ccc1
MOL008317	0.3817	0.6183	0.6043	Achyranthis Asperae Herba	Hydroginkgol	68146	FALSE	Oc1cc(CCCCCCCCCCCCCCCC)ccc1
MOL008318	0.7595	0.2405	0.8219	Achyranthis Asperae Herba	ardisiacrispin B	Not Available	FALSE	O1C23C(C4(C(C5(C(CC4)C(C(OC4OCC(OC6OC(C(O)C(O)C6OC6OC(C(O)C(O)C6O)C)CO)C(O)C4OC4OC(C(O)C(O)C4O)CO)CC5)(C)C)C)CC3)C)(CC(O)C3(C2CC(CC3)(C)C=O)C1)C
MOL008318	0.7595	0.2405	0.8219	Ardisiae Japonicae Herba	ardisiacrispin B	Not Available	FALSE	O1C23C(C4(C(C5(C(CC4)C(C(OC4OCC(OC6OC(C(O)C(O)C6OC6OC(C(O)C(O)C6O)C)CO)C(O)C4OC4OC(C(O)C(O)C4O)CO)CC5)(C)C)C)CC3)C)(CC(O)C3(C2CC(CC3)(C)C=O)C1)C
MOL008319	0.8836	0.1164	0.6061	Achyranthis Asperae Herba	α-Santalol	Not Available	FALSE	OC/C(=C\CCC1(C2(C3C2CC1C3)C)C)/C
MOL008319	0.8836	0.1164	0.6061	Chebulae Fructus	α-Santalol	Not Available	FALSE	OC/C(=C\CCC1(C2(C3C2CC1C3)C)C)/C

MOL008320	0.5469	0.4531	0.6933	Achyranthis Asperae Herba	Ecdysteron	3032482	FALSE	C12(C3=CC(=O)C4C(C3CCC1(C(CC2)C(C(CCC(C)(C)O)O)(C)O)C)(CC(C(C4)O)O)C)O
MOL008321	0.9375	0.0625	0.8281	Achyranthis Asperae Herba	12,13-dihydroxyeuparin	Not Available	FALSE	c1(c(cc2c(c1)cc(o2)C(O)(CO)C)O)C(=O)C
MOL008322	0.9232	0.0768	0.6803	Achyranthis Asperae Herba	5-methyl-7-phenyl-6H-1,4-diazepine-2,3-dicarbonitrile	300512	FALSE	N1=C(CC(=NC(=C1C#N)C#N)C)c1ccccc1
MOL008323	0.9321	0.0679	0.7397	Achyranthis Asperae Herba	4,7-Dimethylindan	23151	FALSE	C1CCc2c(ccc(c12)C)C
MOL008324	0.9234	0.0766	0.9190	Malvae Fructus	2,6-Dimethyl-3,5,7-octatriene-2-ol, ,E,E-	5363695	FALSE	CC(/C=C/C=C(/C=C)\C)(O)C
MOL008325	0.8810	0.1190	0.9131	Malvae Fructus	1-methyl-6,7-dioxabicyclo[3.2.1]octane	Not Available	FALSE	C12(CCCC(OO1)C2)C
MOL008326	0.4833	0.5167	0.6253	Malvae Fructus	14,17-Octadecadienoic acid, methyl ester	5365751	FALSE	C(=O)(CCCCCCCCCCCC/C=C/CC=C)OC
MOL008327	0.8730	0.1270	0.9713	Malvae Fructus	N-Nitroso-3-pyrroline	25371	FALSE	N1(CC=CC1)N=O
MOL008328	0.8364	0.1636	0.6460	Malvae Fructus	2-(prop-2-enoytoxy)tetradecane	Not Available	FALSE	CC(CCCCCCCCCCCC)O/C=C/C(=O)O
MOL008329	0.9570	0.0430	0.9744	Malvae Fructus	()-Dihydrocarveol	89755	FALSE	C1(C(CCC(C1)C(=C)C)C)O
MOL008329	0.9570	0.0430	0.9744	Capsici Fructus	()-Dihydrocarveol	89755	FALSE	C1(C(CCC(C1)C(=C)C)C)O
MOL008330	0.9037	0.0963	0.9160	Malvae Fructus	3,5-octadien-2-ol	Not Available	FALSE	CC(/C=C/C=C/CC)O
MOL008330	0.9037	0.0963	0.9160	Cucurbitae Moschatae Semen	3,5-octadien-2-ol	Not Available	FALSE	CC(/C=C/C=C/CC)O
MOL008331	0.7326	0.2674	0.7415	Malvae Fructus	3-(prop-2-enoyloxy)dodecane	Not Available	FALSE	CCC(CCCCCCCCC)OC(=O)C=C

MOL008333	0.6629	0.3371	0.6338	Malvae Fructus	7-methyl-Z-tetradecen-1-ol acetate	Not Available	FALSE	C(=C\CCCCC(CCCCCCC)C)\OC(=O)C
MOL008335	0.7756	0.2244	0.7190	Malvae Fructus	Z,Z-2,5-Pentadecadien-1-ol	5364952	FALSE	C(/C=C\C/C=C\CCCCCCCCC)O
MOL008337	0.9342	0.0658	0.9263	Malvae Fructus	cyclopropane octanoic acid	57346156	FALSE	C1(CC1)CCCCCCCC(=O)O
MOL008338	0.8632	0.1368	0.8849	Malvae Fructus	N-(2-hydroxyethyl) capramide	111739	FALSE	CCCCCCCCCC(=O)NCCO
MOL008339	0.8862	0.1138	0.9677	Malvae Fructus	4,4-dimethyloxolan-2-one	26312	FALSE	C1(CC(=O)OC1)(C)C
MOL008340	0.9281	0.0719	0.9329	Malvae Fructus	Ethyl 6-acetoxyhexanoate	113640	FALSE	C(CCCCOC(=O)C)C(=O)OCC
MOL008341	0.9023	0.0977	0.9279	Malvae Fructus	N-(2-hydroxyethyl) octanamide	559169	FALSE	C(=O)(CCCCCCC)NCCO
MOL008342	0.8904	0.1096	0.9717	Malvae Fructus	trans-1,2-Cyclopentanediol	225711	FALSE	C1(C(CCC1)O)O
MOL008343	0.9279	0.0721	0.9326	Malvae Fructus	2-Nonenal	5354833	FALSE	C(=O)/C=C\CCCCCC
MOL008344	0.9324	0.0676	0.9460	Malvae Fructus	(Z)-2-octen-2-ol	59918853	FALSE	C/C(=C/CCCCC)/O
MOL008345	0.9658	0.0342	0.8949	Malvae Fructus	1,1-dichloro-2-hexyl-cyclopropane	12936734	FALSE	C1(C(C1)CCCCCC)(Cl)Cl
MOL008346	0.9379	0.0621	0.9473	Malvae Fructus	amoxyethylene	21459	FALSE	C(CCCC)OC=C
MOL008347	0.8190	0.1810	0.8182	Allii Sativi Bulbus	1,2,4,6-Tetrathiepane	520423	FALSE	S1CSCSSC1
MOL008348	0.8573	0.1427	0.8454	Allii Sativi Bulbus	Dithiolane	79045	FALSE	S1SCCC1
MOL008349	0.8631	0.1369	0.8263	Allii Sativi Bulbus	3-Chlorothiophene	87017	FALSE	c1(ccsc1)Cl
MOL008350	0.8863	0.1137	0.9024	Allii Sativi Bulbus	3-Ethenyl-1,2-dithia-cyclohex-5-ene	Not Available	FALSE	S1SC=CCC1C=C

MOL008351	0.8988	0.1012	0.8905	Allii Sativi Bulbus	3-Ethylthiophene	74530	FALSE	s1cc(CC)cc1
MOL008352	0.8893	0.1107	0.8572	Allii Sativi Bulbus	3-(isoamylthio) prop-1-ene	534495	FALSE	C(CC(C)C)SCC=C
MOL008353	0.8855	0.1145	0.9659	Allii Sativi Bulbus	6-Methyl-1-thio-2,4-cyciohexadiene	Not Available	FALSE	S1C=CC=CC1C
MOL008354	0.8678	0.1322	0.8140	Allii Sativi Bulbus	allicin	51380898	FALSE	S(=O)(SCC=C)CC=C
MOL008354	0.8678	0.1322	0.8140	Allii Fistulost Bulbus	allicin	51380898	FALSE	S(=O)(SCC=C)CC=C
MOL008355	0.9065	0.0935	0.9686	Allii Sativi Bulbus	Allylthiol	13367	FALSE	C(=C)CS
MOL008356	0.9094	0.0906	0.9646	Allii Sativi Bulbus	Benzaldoxime	5324611	FALSE	C(=N\O)/c1ccccc1
MOL008357	0.8350	0.1650	0.7895	Allii Sativi Bulbus	Thioform	9264	FALSE	C1SCSCS1
MOL008358	0.8635	0.1365	0.8760	Allii Sativi Bulbus	Oil garlic	11617	TRUE	S(CC=C)CC=C
MOL008358	0.8635	0.1365	0.8760	Allii Fistulost Bulbus	Oil garlic	11617	TRUE	S(CC=C)CC=C
MOL008358	0.8635	0.1365	0.8760	Capsici Fructus	Oil garlic	11617	TRUE	S(CC=C)CC=C
MOL008360	0.8566	0.1434	0.8480	Allii Sativi Bulbus	Dithiolane	20970	FALSE	S1CCSC1
MOL008361	0.9092	0.0908	0.9637	Allii Sativi Bulbus	3-METHYL-2-THIABUTANE	15246	FALSE	C(SC)(C)C
MOL008362	0.8118	0.1882	0.6480	Allii Sativi Bulbus	Methyl allyl tetrasulfide	525329	FALSE	S(SSC)SCC=C
MOL008363	0.8507	0.1493	0.7367	Allii Sativi Bulbus	Methylallyl trisulfide	61926	FALSE	S(CC=C)SSC
MOL008364	0.9083	0.0917	0.9533	Allii Sativi Bulbus	Dimethylthiourea	2723631	FALSE	S=C(NC)NC
MOL008365	0.8767	0.1233	0.7124	Allii Sativi Bulbus	Propyl n-butyl disulfide	522458	FALSE	S(SCCC)CCCC
MOL008366	0.7915	0.2085	0.7844	Allii Sativi Bulbus	protoerubosideB	Not Available	FALSE	O1C2C(C3C(C4C(C5(C(C(O)C4)(C(OC4OC(C(OC6OC(C(O)C(OC7OC(C(O)C(O)C7O)CO)C6OC6OC(C(O)C(O)C6O)CO)CO)C(O)C4O)CO)CCC5)C)C)CC3)C2)C(C1(O)CCC(COC1OC(C(O)C(O)C1O)CO)C)C
MOL008367	0.3534	0.6466	0.6387	Allii Sativi Bulbus	protoerubosideB_qt	Not Available	FALSE	O1C2C(C3C(C4C(C5(C(C(O)C4)(C(O)CCC5)C)C)CC3)C2)C(C1(O)CCC(CO)C)C
MOL008368	0.9003	0.0997	0.9595	Allii Sativi Bulbus	2,2-Dimethoxyethylamine	89728	FALSE	C(CN)(OC)OC
MOL008369	0.9003	0.0997	0.9677	Allii Sativi Bulbus	3-Butenoic acid	32743	FALSE	OC(=O)CC=C

MOL008370	0.9243	0.0757	0.8618	Allii Sativi Bulbus	2,5-Dimethylthiophene	12514	FALSE	c1(sc(cc1)C)C
MOL008371	0.8649	0.1351	0.8714	Allii Sativi Bulbus	2-Ethenyl-1,3-dithia-cyclohex-5-ene	Not Available	FALSE	S1C(SC=CC1)C=C
MOL008372	0.9101	0.0899	0.8660	Allii Sativi Bulbus	2-ethyl-1,3-dithiane	521915	FALSE	C1CCSC(S1)CC
MOL008373	0.9153	0.0847	0.9070	Allii Sativi Bulbus	2-ISOPROPYL-1,3-DIOXOLANE	13201	FALSE	O1C(OCC1)C(C)C
MOL008374	0.8824	0.1176	0.8612	Allii Sativi Bulbus	3,4-Dimethylthiophene	79089	FALSE	Cc1cscc1C
MOL008375	0.9033	0.0967	0.7930	Codonopsis Radix	(1R)-2,3,4,9-tetrahydro-1H-$b-carboline-1-carboxylic acid	6920097	FALSE	c12c([nH]c3c1cccc3)C(NCC2)C(=O)O
MOL008376	0.8508	0.1492	0.6496	Codonopsis Radix	13-Methyl pentadecanoic acid	12113497	FALSE	C(CCCCCCCCCCC(=O)O)C(C)CC
MOL008377	0.9080	0.0920	0.8237	Nelumbinis Plumula	Galuteolin	5317471	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(oc(cc2=O)c2cc(O)c(O)cc2)cc(O)c1)CO
MOL008377	0.9080	0.0920	0.8237	Codonopsis Radix	Galuteolin	5317471	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(oc(cc2=O)c2cc(O)c(O)cc2)cc(O)c1)CO
MOL008378	0.9175	0.0825	0.8681	Codonopsis Radix	o-(o-Methoxyphenoxy)phenol	572803	FALSE	O(c1c(OC)cccc1)c1c(O)cccc1
MOL008378	0.9175	0.0825	0.8681	Hemerocallis Radix	o-(o-Methoxyphenoxy)phenol	572803	FALSE	O(c1c(OC)cccc1)c1c(O)cccc1
MOL008379	0.7802	0.2198	0.6835	Codonopsis Radix	tangshenoside I	Not Available	FALSE	O1C(OC(CC(=O)OC/C=C/c2cc(OC)c(OC3OC(C(O)C(O)C3O)CO)c(OC)c2)(CC(=O)O)C)C(O)C(O)C(O)C1CO
MOL008380	0.9376	0.0624	0.8356	Codonopsis Radix	tangshenoside I_qt	Not Available	FALSE	OC(CC(=O)OC/C=C\c1cc(OC)c(O)c(OC)c1)(CC(=O)O)C
MOL008381	0.5210	0.4790	0.6392	Codonopsis Radix	tangshenoside III	Not Available	FALSE	c1(c(c(c(c(c1)/C=C/CO)C/C=C\c1cc(c(c(c1)OC)OC1C(O)C(O)C(O)C(O1)CO)OC)OC)OC1C(O)C(O)C(O)C(O1)CO)OC

MOL008382	0.4346	0.5654	0.6527	Codonopsis Radix	tangshenoside III_qt	Not Available	FALSE	c1(c(c(c(c(c1)/C=C\CO)C/C=C\c1cc(c(c(c1)OC)O)OC)OC)O)OC
MOL008383	0.5598	0.4402	0.7245	Codonopsis Radix	tangshenoside IV	Not Available	FALSE	C(=O)(CC(CC(=O)OC/C=C/c1c(c(c(c(c1)OC)OC1OC(C(C(C1O)O)O)CO)OC)C/C=C/c1cc(c(c(c1)OC)OC1OC(C(C(C1O)O)O)CO)OC)(OC1OC(C(C(C1O)O)O)CO)C)O
MOL008385	0.9393	0.0607	0.9023	Zanthoxyli Pericarpium	T-BUTYLBENZENE	7366	FALSE	C(c1ccccc1)(C)(C)C
MOL008385	0.9393	0.0607	0.9023	Codonopsis Radix	T-BUTYLBENZENE	7366	FALSE	C(c1ccccc1)(C)(C)C
MOL008385	0.9393	0.0607	0.9023	Chrysanthemi Flos	T-BUTYLBENZENE	7366	FALSE	C(c1ccccc1)(C)(C)C
MOL008386	0.9240	0.0760	0.9289	Codonopsis Radix	2,6-NONADIENOL	5320191	FALSE	CC/C=C/CC/C=C/CO
MOL008387	0.8555	0.1445	0.6877	Codonopsis Radix	3-METHYLCARBAZOLE	20746	FALSE	c1(ccc2c(c1)c1c([nH]2)cccc1)C
MOL008388	0.8953	0.1047	0.8674	Codonopsis Radix	L-Sulforaphane	9577379	FALSE	CS(=O)CCCCN=C=S
MOL008389	0.9172	0.0828	0.7801	Codonopsis Radix	4-Phenylbicyclo[2,2,2]octan-1-ol	327096	FALSE	c1ccc(cc1)C12CCC(CC1)(O)CC2
MOL008389	0.9172	0.0828	0.7801	Cistanches Herba	4-Phenylbicyclo[2,2,2]octan-1-ol	327096	FALSE	c1ccc(cc1)C12CCC(CC1)(O)CC2
MOL008391	0.2081	0.7919	0.6542	Codonopsis Radix	5alpha-Stigmastan-3,6-dione	Not Available	FALSE	C1C(=O)CC2C(C1)(C1C(CC2=O)C2C(CC1)(C(CC2)C(C)CCC(C(C)C)CC)C)C
MOL008393	0.4355	0.5645	0.7803	Codonopsis Radix	7-(beta-Xylosyl)cephalomannine_qt	Not Available	FALSE	C1(C(=O)C2(C(C(C3(C(C1=C(C(C3)OC(=C)C(C(c1ccccc1)NC(=O)/C(=C/C)/C)O)C)(C)C)O)OC(=O)c1ccccc1)C1(C(CC2O)OC1)OC(=O)C)C)OC(=O)C
MOL008394	0.9431	0.0569	0.9385	Codonopsis Radix	Butylcyclohexane	15506	FALSE	C1CC(CCC1)CCCC
MOL008395	0.9557	0.0443	0.7848	Codonopsis Radix	Codonopsine	442631	FALSE	c1c(ccc(c1OC)OC)C1C(C(C(N1C)C)O)O
MOL008396	0.7807	0.2193	0.7324	Codonopsis Radix	Coelogin	Not Available	FALSE	c1(cc2c3c(c1)CCc1c3c(CO2)c(c(c1OC)OC)O)O
MOL008397	0.2148	0.7852	0.7044	Panacis Quinquefolii Radix	Daturilin	Not Available	FALSE	C1=CC(=O)C2(C(=CCC3C2CCC2(C3CCC2C2C3CC(OC2)(C(=C)C(=O)O3)C)C)C1)C

MOL008397	0.2148	0.7852	0.7044	Codonopsis Radix	Daturilin	Not Available	FALSE	C1=CC(=O)C2(C(=CCC3C2CCC2(C3CCC2C2C3CC(OC2)(C(=C)C(=O)O3)C)C)C1)C
MOL008398	0.9144	0.0856	0.8112	Codonopsis Radix	Ethyl-p-digallate	5317260	FALSE	c1(cc(c(c(c1)O)OC(=O)c1cc(c(c(c1)O)O)O)O)C(=O)OCC
MOL008399	0.3019	0.6981	0.7047	Asteris Radix Et Rhizoma	fritillaziebinol	Not Available	FALSE	C1CC(C2C(C1)(C1C3(CC2)CC(CC1)C(C3)(CCl)O)C)(C)C
MOL008399	0.3019	0.6981	0.7047	Codonopsis Radix	fritillaziebinol	Not Available	FALSE	C1CC(C2C(C1)(C1C3(CC2)CC(CC1)C(C3)(CCl)O)C)(C)C
MOL008400	0.8339	0.1661	0.9166	Puerariae Flos	glycitein	5317750	FALSE	c1(c(cc2c(c1)occ(c2=O)c1ccc(cc1)O)OC)O
MOL008400	0.8339	0.1661	0.9166	Codonopsis Radix	glycitein	5317750	FALSE	c1(c(cc2c(c1)occ(c2=O)c1ccc(cc1)O)OC)O
MOL008400	0.8339	0.1661	0.9166	Sojae Semen Praeparatum	glycitein	5317750	FALSE	c1(c(cc2c(c1)occ(c2=O)c1ccc(cc1)O)OC)O
MOL008400	0.8339	0.1661	0.9166	Lycii Fructus	glycitein	5317750	FALSE	c1(c(cc2c(c1)occ(c2=O)c1ccc(cc1)O)OC)O
MOL008402	0.9368	0.0632	0.8980	Codonopsis Radix	BHG	181215	FALSE	O1C(C(O)C(O)C(O)C1OCCCCCC)CO
MOL008403	0.9126	0.0874	0.8112	Codonopsis Radix	Hexyl-beta-D-glucopyranosyl-(1-2)-beta-D-glucopyranoside	14655096	FALSE	O(CCCCCC)C1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL008404	0.9080	0.0920	0.9653	Codonopsis Radix	(2S)-2-ammonio-4-[(R)-methylsulfinyl]butyrate	11862103	FALSE	CS(=O)CCC(N)C(=O)O
MOL008404	0.9080	0.0920	0.9653	Ginkgo Semen	(2S)-2-ammonio-4-[(R)-methylsulfinyl]butyrate	11862103	FALSE	CS(=O)CCC(N)C(=O)O
MOL008406	0.3649	0.6351	0.8205	Codonopsis Radix	Spinoside A	Not Available	FALSE	C1(=CC2C(=CCC3C2(CCC2(C3(CC(C2C(C(=O)/C=C/C(C)(C)O)(O)C)OC2C(C(C(CO2)OC(=C)O)O)OC(=O)C)C)C)C(C1=O)(C)C)O

MOL008407	0.1969	0.8031	0.6164	Codonopsis Radix	(8S,9S,10R,13R,14S,17R)-17-[(E,2R,5S)-5-ethyl-6-methylhept-3-en-2-yl]-10,13-dimethyl-1,2,4,7,8,9,11,12,14,15,16,17-dodecahydrocyclopenta[a]phenanthren-3-one	14807783	FALSE	C12(C(C3C(C4(C(=CC3)CC(=O)CC4)C)CC2)CCC1C(/C=C/C(C(C)C)CC)C)C
MOL008409	0.9311	0.0689	0.8305	Codonopsis Radix	Tangshenoside II	14135593	FALSE	c1(c(c(cc(c1)C(C=C)O)OC)OC1OC(C(C(C1O)O)O)CO)OC
MOL008410	0.9416	0.0584	0.9623	Codonopsis Radix	Tangshenoside II_qt	Not Available	FALSE	c1(c(c(cc(c1)C(C=C)O)OC)O)OC
MOL008412	0.1920	0.8080	0.6460	Codonopsis Radix	alpha-Stigmasta-7,22-dien-3-one	Not Available	FALSE	C1C(=O)CC2C(C1)(C1C(=CC2)C2C(CC1)(C(CC2)C(C)/C=C/C(C(C)C)CC)C)C
MOL008413	0.8960	0.1040	0.9675	Codonopsis Radix	Codopiloic acid	178371	FALSE	O1CC(=NC=C1)C(=O)O
MOL008415	0.2061	0.7939	0.6369	Codonopsis Radix	delta7-Stigmastenone-3	Not Available	FALSE	C1C(=O)CC2C(C1)(C1C(=CC2)C2C(CC1)(C(CC2)C(C)CCC(C(C)C)CC)C)C
MOL008418	0.8823	0.1177	0.7499	Catechu	(-)-angelicoidenol-2-O-β-D-glucopyranoside	Not Available	FALSE	C1(OC(C(C(C1O)O)O)CO)OC1CC(C(CC)O)C(C1(C)C)(C)C
MOL008419	0.9232	0.0768	0.8407	Catechu	(-)-angelicoidenol-2-O-β-D-glucopyranoside_qt	Not Available	FALSE	OC1CC(C(CC)O)C(C1(C)C)(C)C

MOL008420	0.9290	0.0710	0.8143	Catechu	5-Hydroxy-2-[2-(4-hydroxyphenyl)acetyl]-3-methoxy-benzoic acid	Not Available	FALSE	c1c(cc(c(c1OC)C(=O)Cc1ccc(cc1)O)C(=O)O)O
MOL008421	0.8769	0.1231	0.8892	Catechu	Cis-dihydro quercetin	59044266	FALSE	CC1C(=O)c2c(cc(cc2OC1c1cc(c(cc1)O)O)O)O
MOL008422	0.9260	0.0740	0.8495	Catechu	Afzelechin	442154	FALSE	c12c(OC(C(C1)O)c1ccc(cc1)O)cc(cc2O)O
MOL008423	0.9402	0.0598	0.8922	Catechu	berchemiaside A	Not Available	FALSE	c1ccc2c(c1O)C(=O)CCC2OC1OC(C(C(C1O)O)O)CO
MOL008424	0.9467	0.0533	0.8405	Catechu	berchemiaside A_qt	44576009	FALSE	c1ccc2c(c1O)C(=O)CCC2O
MOL008425	0.7694	0.2306	0.7437	Catechu	berchemiaside B	Not Available	FALSE	c1cc(c2c(c1O)C(=O)CCC2OC1OC(C(C(C1O)O)O)COC(=O)/C=C/c1ccc(cc1)O)O
MOL008426	0.8570	0.1430	0.9004	Catechu	(R)-2,6-dihydroxy-2-(4-hydroxybenzyl)-4-methoxybenzofuran-3(2H)-one	Not Available	FALSE	c1(cc(c2c(c1)OC(C2=O)(Cc1ccc(cc1)O)O)OC)O
MOL008427	0.8397	0.1603	0.8812	Catechu	maesopsino-O-glucoside80	Not Available	FALSE	Cc1cc(cc2c1C(=O)C(O2)(Cc1ccc(cc1)O)O)O
MOL008428	0.9432	0.0568	0.7813	Catechu	3,4,8,10-tetrahydroxy-5H-chromeno[3,2-c]isochromen-7-one	11461162	FALSE	c1(cc(c2c(c1)oc1c(c2=O)OCc2c1ccc(c2O)O)O)O
MOL008429	0.8965	0.1035	0.8229	Catechu	(R)-5-((R)-1-(3,4-dihydroxyphenyl)-3-oxobutyl)dihydrofuran-2(3H)-one	Not Available	FALSE	C(C(C1OC(=O)CC1)c1ccc(c(c1)O)O)C(=O)C

MOL008430	0.8965	0.1035	0.7879	Catechu	5,7-dihydroxy-2-(4-hydroxyphenyl)-3-methyl-chromone	15661821	FALSE	c1(cc(c2c(c1)oc(c(c2=O)C)c1ccc(cc1)O)O)O
MOL008431	0.9290	0.0710	0.8530	Catechu	(2R,3S)-2-(3,4-dihydroxyphenyl)chroman-3,7,8-triol	11033582	FALSE	c1(ccc2c(c1O)OC(C(C2)O)c1cc(c(cc1)O)O)O
MOL008432	0.9139	0.0861	0.8057	Catechu	Fisetinidol	442397	FALSE	c1(ccc2c(c1)OC(C(C2)O)c1cc(c(cc1)O)O)O
MOL008433	0.6655	0.3345	0.7866	Rubi Fructus	(1R,2R,4aS,6aS,6aR,6bR,8aR,12aR,14bS)-1,11-dihydroxy-1,2,6a,6b,9,9,12a-heptamethyl-10-oxo-3,4,5,6,6a,7,8,8a,13,14b-decahydro-2H-picene-4a-carboxylic acid	12045007	FALSE	C12(C(C3(C(CC1)C(C(=O)C(=C3)O)(C)C)C)CC=C1C2(CCC2(C1C(C(CC2)C)(O)C)C(=O)O)C)C
MOL008434	0.8756	0.1244	0.8200	Rubi Fructus	gamma-curcumene	12304273	FALSE	C(C1=CC=C(CC1)C)(CCC=C(C)C)C
MOL008435	0.9217	0.0783	0.8270	Rubi Fructus	H-2-indenone,2,4,5,6,7,7a-hexahydro-3-(1-methylethyl)-7a-methyl	Not Available	FALSE	O=C1CC2(C(=C1C(C)C)CCCC2)C
MOL008436	0.8574	0.1426	0.8126	Ginkgo Folium	Kaempferol-7-rhamnoside	25079965	FALSE	CC1C(C(C(C(O1)Oc1cc(c2c(c1)oc(c1ccc(cc1)O)c(c2=O)O)O)O)O)O
MOL008436	0.8574	0.1426	0.8126	Rubi Fructus	Kaempferol-7-rhamnoside	25079965	FALSE	CC1C(C(C(C(O1)Oc1cc(c2c(c1)oc(c1ccc(cc1)O)c(c2=O)O)O)O)O)O

MOL008437	0.9246	0.0754	0.9150	Rubi Fructus	2-[(2S,5S)-5-ethenyl-5-methyloxolan-2-yl]propan-2-ol	6432254	FALSE	O1C(CCC1(C)C=C)C(O)(C)C
MOL008437	0.9246	0.0754	0.9150	Mume Fructus	2-[(2S,5S)-5-ethenyl-5-methyloxolan-2-yl]propan-2-ol	6432254	FALSE	O1C(CCC1(C)C=C)C(O)(C)C
MOL008437	0.9246	0.0754	0.9150	Eriobotryae Folium	2-[(2S,5S)-5-ethenyl-5-methyloxolan-2-yl]propan-2-ol	6432254	FALSE	O1C(CCC1(C)C=C)C(O)(C)C
MOL008438	0.6680	0.3320	0.7469	Rubi Fructus	[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl] (1R,2R,4aS,6aR,6aS,6bR,8aR,9R,10R,11R,12aR,14bS)-1,10,11-trihydroxy-9-(hydroxymethyl)-1,2,6a,6b,9,12a-hexamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylate	16118969	FALSE	C12=CCC3C4(C(C(C(C(C4)O)O)(CO)C)CCC3(C1(CCC1(C2C(C(CC1)C)(O)C)C(=O)OC1C(C(C(C(O1)CO)O)O)O)C)C)C
MOL008439	0.7394	0.2606	0.7373	Rubi Fructus	Niga-ichigoside F1 aglycone	490367	FALSE	C12=CCC3C4(C(C(C(C(C4)O)O)(CO)C)CCC3(C1(CCC1(C2C(C(CC1)C)(O)C)C(=O)O)C)C)C

MOL008440	0.8799	0.1201	0.7782	Rubi Fructus	1-[2,4-dihydroxy-6-[(2S,3S,4R,5S,6S)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]-3-(4-hydroxyphenyl)propan-1-one	7059603	FALSE	c1(c(OC2OC(C(C(C2O)O)O)CO)cc(cc1O)O)C(=O)CCc1ccc(cc1)O
MOL008441	0.7632	0.2368	0.7856	Rubi Fructus	Procyanidin B-23,3'-di-O-gallate	Not Available	FALSE	c1c(c2c(cc1O)OC(C(C2c1c(cc(c2c1OC(C(C2)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)c1cc(c(cc1)O)O)O
MOL008442	0.7022	0.2978	0.7572	Rubi Fructus	Procyanidin B-23,3'-di-O-gallate_qt	12967793	FALSE	c1c(c2c(cc1O)OC(C(C2c1c(cc(c2c1OC(C(C2)O)c1cc(c(cc1)O)O)O)O)O)c1cc(c(cc1)O)O)O
MOL008443	0.8878	0.1122	0.9563	Rubi Fructus	2,5-Dimethylfuran	12266	FALSE	c1(oc(cc1)C)C
MOL008444	0.9619	0.0381	0.8976	Rubi Fructus	1-(2,6-dichloro-3-fluorophenyl) ethanone	2733982	FALSE	c1(c(c(ccc1Cl)F)Cl)C(=O)C
MOL008445	0.9291	0.0709	0.9660	Rubi Fructus	(3R)-3-methylpentan-2-one	6999802	FALSE	C(C(=O)C)(CC)C
MOL008446	0.9281	0.0719	0.9610	Rubi Fructus	2,6-Cresotaldehyde	585174	FALSE	C(=O)c1c(O)cccc1C

MOL008447	0.7405	0.2595	0.7570	Rubi Fructus	(1S,4aR,6aR,6aS,6bR,8aR,10R,11R,12aR,14bS)-1,10,11-trihydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	15385516	FALSE	C12=CCC3C4(C(C(C(C(C4)O)O)(C)C)CCC3(C1(CCC1(C2C(C(CC1)(C)C)O)C(=O)O)C)C)C
MOL008449	0.9411	0.0589	0.9622	Rubi Fructus	cis-p-2-menthen- 1-ol	6427100	FALSE	OC1CCC(C(C)(C)C)C=C1
MOL008451	0.9458	0.0542	0.9235	Euonymi Alati Ramulus	Methyl atratate	78435	FALSE	c1(c(c(c(cc1C)O)C)O)C(=O)OC
MOL008452	0.9483	0.0517	0.8883	Euonymi Alati Ramulus	methyl 2,4-dimethoxy-6-methylbenzoate	601782	FALSE	c1(c(c(cc(c1)OC)C)C(=O)OC)OC
MOL008453	0.8100	0.1900	0.7288	Euonymi Alati Ramulus	USNIC ACID	Not Available	FALSE	C12(c3c(OC1=CC(=O)C(C2=O)C(=O)C)c(c(c(c3O)C)O)C(=O)C)C
MOL008454	0.3795	0.6205	0.8237	Uncariae Ramulus Cumuncis	27-nor-olean-3-hydroxy-28→13 oate	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2C3(CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O3)C)C)(C)C)O
MOL008456	0.3691	0.6309	0.6685	Uncariae Ramulus Cumuncis	(3E,4R)-4-(1,3-benzodioxol-5-ylmethyl)-3-[(3,4,5-trimethoxyphenyl)methylidene]oxolan-2-one	11165431	FALSE	c1(c(cc(cc1OC)/C=C\1/C(=O)OCC1Cc1ccc2c(c1)OCO2)OC)OC
MOL008457	0.6582	0.3418	0.9278	Uncariae Ramulus Cumuncis	Tetrahydroalstonine	Not Available	FALSE	c12C3N(CC4C(C3)C(=COC4C)C(=O)OC)CCc1c1c([nH]2)cccc1
MOL008457	0.6582	0.3418	0.9278	Cornus Officinalis Sieb. Et Zucc.	Tetrahydroalstonine	Not Available	FALSE	c12C3N(CC4C(C3)C(=COC4C)C(=O)OC)CCc1c1c([nH]2)cccc1
MOL008458	0.7983	0.2017	0.8048	Uncariae Ramulus Cumuncis	Angustidine	Not Available	FALSE	c1(=O)n2c(cc3cc(ncc13)C)c1c(CC2)c2ccccc2[nH]1

MOL008460	0.6476	0.3524	0.7898	Uncariae Ramulus Cumuncis	geissoschizinc acid	Not Available	FALSE	c1ccc2c(c1)c1c(C3N(CC1)C/C(=C\C)/C(C3)/C(=C\OC)/C(=O)O)[nH]2
MOL008462	0.7568	0.2432	0.8489	Uncariae Ramulus Cumuncis	Strictosamide _qt	Not Available	FALSE	c1ccc2c(c1)c1c(C3CC4C(=COC(C4C=C)O)C(=O)N3CC1)[nH]2
MOL008465	0.2304	0.7696	0.8234	Uncariae Ramulus Cumuncis	(E)-16,17-Didehydro-17-methoxy-17,18-seco-3-beta-yohimban-16-carboxylic acid methyl ester	3037884	FALSE	C12c3c(c4c([nH]3)cccc4)CCN1CC(C(C2)/C(=C\OC)/C(=O)OC)CC
MOL008466	0.1711	0.8289	0.7637	Uncariae Ramulus Cumuncis	Dihydrocoryn antheine	Not Available	FALSE	c1ccc2c(c1)c1c(C3(CC(C(CN3CC1)CC)/C(=C\OC)/C(=O)OC)C)[nH]2
MOL008468	0.2227	0.7773	0.8514	Uncariae Ramulus Cumuncis	methyl (E)-2-[(2S,3Z,12bS)-3-ethylidene-2,4,6,7,12,12b-hexahydro-1H-indolo[3,2-h]quinolizin-2-yl]-3-methoxyprop-2-enoate	10021817	FALSE	c1ccc2c(c1)c1c(C3N(CC1)C/C(=C\C)/C(C3)/C(=C\OC)/C(=O)OC)[nH]2
MOL008472	0.2188	0.7812	0.6909	Uncariae Ramulus Cumuncis	hirsutasideA	Not Available	FALSE	c1ccc2c(c1)c1c(C(NC(C1)C(=O)OCC)CC1C(=COC(C1C=C)C)C(=O)OC)[nH]2
MOL008476	0.2065	0.7935	0.7736	Uncariae Ramulus Cumuncis	hirsutasideB	Not Available	FALSE	c1ccc2c(c1)c1c(c(nc(c1)C(=O)OCC)CC1C(=CCC(C1C=C)C)C(=O)OC)[nH]2
MOL008478	0.2147	0.7853	0.8411	Uncariae Ramulus Cumuncis	methyl (E)-2-[(2S,3R,12bS)-3-vinyl-1,2,3,4,6,7,12,12b-octahydroindolo[3,2-h]quinolizin-2-yl]-3-methoxy-prop-2-enoate	3037997	FALSE	c1ccc2c(c1)c1c(C3CC(C(CN3CC1)C=C)/C(=C\OC)/C(=O)OC)[nH]2

MOL008479	0.9140	0.0860	0.8280	Ginseng Folium	5,7-dihydroxy-2-(4-hydroxyphenyl)-3-[(2R,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	5318755	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL008479	0.9140	0.0860	0.8280	Pyrrosiae Folium	5,7-dihydroxy-2-(4-hydroxyphenyl)-3-[(2R,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	5318755	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL008479	0.9140	0.0860	0.8280	Uncariae Ramulus Cumuncis	5,7-dihydroxy-2-(4-hydroxyphenyl)-3-[(2R,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	5318755	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1

MOL008479	0.9140	0.0860	0.8280	Anisi Stellati Fructus	5,7-dihydroxy-2-(4-hydroxyphenyl)-3-[(2R,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	5318755	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL008482	0.3735	0.6265	0.7802	Uncariae Ramulus Cumuncis	(2S,12bR)-methyl 2-((E)-1-oxobut-2-en-2-yl)-1,2,6,7,12,12b-hexahydroindolo[2,3-a]quinolizine-3-carboxylate	Not Available	FALSE	c1ccc2c(c1)c1c(C3CC(C(=CN3CC1)C(=O)OC)/C(=C\C)/C=O)[nH]2
MOL008485	0.3618	0.6382	0.6960	Uncariae Ramulus Cumuncis	hirsutasideC	Not Available	FALSE	c1ccc2c(c1)c1c([nH]2)c(ncc1CCC1C(=COC(C1C=C)C)C(=O)O)CC1C(=COC(C1C=C)C)C(=O)OC
MOL008487	0.6186	0.3814	0.7634	Uncariae Ramulus Cumuncis	hirsutine	Not Available	FALSE	C1CC=C2C(C1)(C1N(C2)CCc2c1cc(c(c2)O)OC)C(=O)C
MOL008488	0.5641	0.4359	0.9169	Uncariae Ramulus Cumuncis	yohimbine	8969	FALSE	c12C3N(CC4C(C3)C(C(CC4)O)C(=O)OC)CCc1c1c([nH]2)cccc1
MOL008488	0.5641	0.4359	0.9169	Capsellae Herba	yohimbine	8969	FALSE	c12C3N(CC4C(C3)C(C(CC4)O)C(=O)OC)CCc1c1c([nH]2)cccc1
MOL008489	0.2147	0.7853	0.8411	Uncariae Ramulus Cumuncis	delta(sup 18)-Hirsutine	3037151	FALSE	c1ccc2c(c1)c1c(C3N(CC1)CC(C(C3)/C(=C\OC)/C(=O)OC)C=C)[nH]2
MOL008490	0.6442	0.3558	0.7813	Uncariae Ramulus Cumuncis	isocorynanthe ic acid	Not Available	FALSE	c1ccc2c(c1)c1c(C3N(CC1)CC(C(C3)/C(=C\OC)/C(=O)O)C=C)[nH]2
MOL008491	0.7806	0.2194	0.7046	Uncariae Ramulus Cumuncis	ncariasideA	Not Available	FALSE	C1C(C(C(C(OC1CO)OC1CCC2(C(C1(C)C)CCC1(C2CC(=O)C2=C1CCC1(C2C(C(CC1)C)C)C(=O)OC1OC(C(C(C1O)O)O)CO)C)C)O)O)O
MOL008492	0.6530	0.3470	0.7438	Uncariae Ramulus Cumuncis	ncariasideA_qt	Not Available	FALSE	OC1CCC2(C(C1(C)C)CCC1(C2CC(=O)C2=C1CCC1(C2C(C(CC1)C)C)C(=O)O)C)C

MOL008493	0.9180	0.0820	0.9079	Choerospondiatis Fructus	2-hydroxy-1,2,3-propane tricarboxylic acid-2-ethyl ester	21154104	FALSE	C(C(CC(=O)O)(C(=O)OCC)O)C(=O)O
MOL008494	0.8946	0.1054	0.7514	Radix Euphorbiae Pekinensis	3,3'-Di-O-methylellagic acid	Not Available	FALSE	O=c1oc2c(OC)c(O)cc3c2c2c(oc3=O)c(OC)c(O)cc12
MOL008494	0.8946	0.1054	0.7514	Polygoni Orientalis Fructus	3,3'-Di-O-methylellagic acid	Not Available	FALSE	O=c1oc2c(OC)c(O)cc3c2c2c(oc3=O)c(OC)c(O)cc12
MOL008494	0.8946	0.1054	0.7514	Choerospondiatis Fructus	3,3'-Di-O-methylellagic acid	Not Available	FALSE	O=c1oc2c(OC)c(O)cc3c2c2c(oc3=O)c(OC)c(O)cc12
MOL008495	0.8947	0.1053	0.7872	Choerospondiatis Fructus	kaempferol-5-O-arabinoside	44633238	FALSE	c1(c(O)c(=O)c2c(cc(O)cc2o1)OC1C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL008496	0.9287	0.0713	0.7985	Choerospondiatis Fructus	5,7-dihydroxy-3-[(2R,3S,4S,5S,6R)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-2-(3,4,5-trihydroxyphenyl)chromone	9890615	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)C)c1cc(O)c(O)c(O)c1
MOL008497	0.2429	0.7571	0.6058	Choerospondiatis Fructus	stigmastan-7-one	Not Available	FALSE	O=C1C2C3C(C(CC3)C(CCC(C(C)C)CC)C)(CCC2C2(C(C1)CCCC2)C)C
MOL008498	0.7574	0.2426	0.9071	Choerospondiatis Fructus	ursolicacid	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3C)C)C(=O)O)C)(CC2)C)(CC1)C)(C)C
MOL008499	0.2056	0.7944	0.7254	Trigonellae Semen	(25R)-Spirost-5-en-3β-ol acetate	Not Available	FALSE	C(=O)(C)OC1CCC2(C(=CCC3C4CC5OC6(C(C5C4(C)CCC23)C)OCC(CC6)C)C1)C
MOL008500	0.9329	0.0671	0.9619	Trigonellae Semen	1-PENTANOL, 2-METHYL	637757	FALSE	C(C(CCC)C)O
MOL008501	0.6884	0.3116	0.8669	Trigonellae Semen	Gitonin	Not Available	FALSE	C1(C(CC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)OC1OC(C(C(C1O)O)OC1OC(C(C(C1O)O)O)CO)CO)O
MOL008502	0.3332	0.6668	0.6949	Trigonellae Semen	C08899	Not Available	FALSE	C1(C(CC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)O)O

MOL008504	0.8907	0.1093	0.7794	Trigonellae Semen	5,7,3'-Trihydroxy-5'-methylisoflavone	Not Available	FALSE	c1c(c(=O)c2c(cc(cc2o1)O)O)c1cc(cc(c1)C)O
MOL008505	0.5871	0.4129	0.7796	Trigonellae Semen	Schisandrol	Not Available	FALSE	c1(c(c2c(cc1O)CC(C(Cc1c2c(c(c(c1)O)OC)OC)C)(O)C)OC)OC
MOL008506	0.2799	0.7201	0.7501	Trigonellae Semen	Tigogenone	Not Available	FALSE	C1C(=O)CC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C
MOL008507	0.5160	0.4840	0.7145	Trigonellae Semen	Tricornine	Not Available	FALSE	CC(=O)OCC12CCC(C34C1C(C(C1(C5C3CC(C5OC)C(C1)OC)O)(C4N(C2)CC)O)OC)OC
MOL008508	0.8394	0.1606	0.8207	Trigonellae Semen	5,7-dihydroxy-2-(4-hydroxyphenyl)-6-methyl-8-((2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)-4H-chromen-4-one	Not Available	FALSE	c1(cc(=O)c2c(O)c(c(O)c(c2o1)C1C(O)C(O)C(O)C(O1)CO)C)c1ccc(O)cc1
MOL008509	0.5563	0.4437	0.7212	Trigonellae Semen	Vitexin-2-O-p-coumarate	Not Available	FALSE	O1C(C(OC(=O)/C=C\c2ccc(O)cc2)C(O)C(O)C1CO)c1c2oc(cc(=O)c2c(O)cc1O)c1ccc(O)cc1
MOL008510	0.8801	0.1199	0.7921	Trigonellae Semen	Vitexin-7-glucoside	Not Available	FALSE	c1(cc(c2c(c1C1OC(C(C(C1O)O)O)CO)oc(cc2=O)c1ccc(cc1)O)O)OC1OC(C(C(C1O)O)O)CO
MOL008511	0.8571	0.1429	0.8397	Trigonellae Semen	Vitexin-7-glucoside_qt	Not Available	FALSE	c1(cc(c2c(c1C1OC(C(C(C1O)O)O)CO)oc(cc2=O)c1ccc(cc1)O)O)O
MOL008512	0.6254	0.3746	0.6977	Trigonellae Semen	Vitisin C	16145527	FALSE	c1cc(ccc1C1C(c2c(O1)cc(cc2C1c2c(OC1c1ccc(cc1)O)ccc(c2)/C=C/c1cc(cc2c1C(C(O2)c1ccc(cc1)O)c1cc(cc(c1)O)O)O)O)c1cc(cc(c1)O)O)O
MOL008513	0.8774	0.1226	0.7699	Trigonellae Semen	apigenin-6-xyloside-8-glucoside	Not Available	FALSE	c1(cc(=O)c2c(O)c(c(O)c(c2o1)OC1C(O)C(O)C(O)C(O1)CO)OC1C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL008515	0.9319	0.0681	0.8587	Trigonellae Semen	gentianine	Not Available	FALSE	O1C(=O)c2c(C(C1)C=C)ccnc2
MOL008518	0.3332	0.6668	0.6949	Trigonellae Semen	lilagenin	Not Available	FALSE	C1(C(CC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)CCC(CO2)C)C)C)O)O
MOL008519	0.3012	0.6988	0.7449	Trigonellae Semen	neotigogenin	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(O)CC5)C)CC3)C2)C)C(C21OCC(CC2)C)C

MOL008520	0.9207	0.0793	0.7995	Trigonellae Semen	9,11-Dimethyl-11-ethyl-10,12-dihydroxy-dodecanoicacid	Not Available	FALSE	C(=O)(CCCCCCCC(C(C(CO)(CC)C)O)C)O
MOL008522	0.3012	0.6988	0.7449	Trigonellae Semen	sarsasapogeni	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(O)CC5)C)CC3)C2)C)C(C21OCC(CC2)C)C
MOL008523	0.3332	0.6668	0.6949	Trigonellae Semen	sitogenin	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(O)C(O)C5)C)CC3)C2)C)C(C21OCC(CC2)C)C
MOL008525	0.3077	0.6923	0.7078	Trigonellae Semen	Yuccagenin	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(=CC4)CC(O)C(O)C5)C)CC3)C2)C)C(C21OCC(CC2)C)C
MOL008526	0.8593	0.1407	0.7876	Trigonellae Semen	Carpesia lactone	Not Available	FALSE	C12C(CCC(C3C1C(=CC3=O)C)C)C(C(=O)O2)C
MOL008527	0.9563	0.0437	0.8701	Cichorii Radix	(Z)-4,5-Dihydro-6,7-trans-dihydroxy-3-butylidene phthalide	Not Available	FALSE	C1C(C(C2=C(C1)/C(=C\CCC)/OC2=O)O)O
MOL008528	0.7411	0.2589	0.8363	Cichorii Radix	Chikusetsu saponin Ib	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1OC(C(C(C1O)O)O)CO)C)C)(C)C)OC1OC(C(C(C1O)O)OC1OCC(C(C1O)O)O)C(=O)O
MOL008529	0.7553	0.2447	0.9079	Cichorii Radix	(4aS,6aR,6aS,6bR,8aS,10R,12aR,14bS)-10-hydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	11869662	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O
MOL008530	0.9325	0.0675	0.8769	Cichorii Radix	Cichoriin	442101	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2oc(=O)ccc2cc1O)CO
MOL008531	0.6473	0.3527	0.6290	Cichorii Radix	Cicutol	5315864	FALSE	C(CCC#CC#C/C=C/C=C/C=C/CCCC)O
MOL008532	0.8691	0.1309	0.8586	Cichorii Radix	Deoxylapachol	97448	FALSE	c1cccc2c1C(=O)C=C(C2=O)CC=C(C)C
MOL008533	0.9082	0.0918	0.7325	Cichorii Radix	D-DCTA	5470299	FALSE	C(C(OC(=O)/C=C/c1cc(c(cc1)O)O)C(=O)O)(OC(=O)/C=C/c1cc(c(cc1)O)O)C(=O)O

MOL008534	0.9184	0.0816	0.9549	Cichorii Radix	Izalpinin	5318691	FALSE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccccc1)O)OC
MOL008534	0.9184	0.0816	0.9549	Alpiniae Oxyphyliae Fructus	Izalpinin	5318691	FALSE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccccc1)O)OC
MOL008535	0.8786	0.1214	0.8007	Cichorii Radix	Lactucin	Not Available	FALSE	O1C2C(C(O)CC(=C3C2C(=CC3=O)CO)C)C(=C)C1=O
MOL008537	0.3218	0.6782	0.6046	Cichorii Radix	Lactucopicrin	Not Available	FALSE	C1=C(C2C(=C(C)CC(C3C2OC(=O)C3=C)OC(=O)Cc2ccc(cc2)O)C1=O)CO
MOL008538	0.8810	0.1190	0.8857	Cichorii Radix	Lageracetal	22210	FALSE	C(CC(OCCCC)OCCCC)C
MOL008539	0.7633	0.2367	0.6362	Cichorii Radix	(2R)-3-[3-(5-allyl-2-hydroxyphenyl)-4-hydroxyphenyl]propane-1,2-diol	11066525	FALSE	c1cc(cc(c2cc(ccc2O)CC=C)c1O)CC(CO)O
MOL008540	0.9007	0.0993	0.9223	Cichorii Radix	Mono-p-coumaroyl glyceride	Not Available	FALSE	c1c(ccc(c1)O)CCC(=O)OCC(O)CO
MOL008541	0.6573	0.3427	0.8379	Cichorii Radix	Purpurea glycoside B	Not Available	FALSE	OC12C3C(C4(C(CC3)CC(OC3OC(C(OC5OC(C(O)C(O)C5)C)C(OC5OC(C(O)C(OC6OC(C(O)C(O)C6O)CO)C5)C)C3)C)CC4)C)CCC1(C(C(O)C2)C1=CC(=O)OC1)C
MOL008542	0.5216	0.4784	0.7670	Cichorii Radix	Gitoxigenin	348482	FALSE	OC12C3C(C4(C(CC3)CC(O)CC4)C)CCC1(C(C(O)C2)C1=CC(=O)OC1)C
MOL008543	0.6337	0.3663	0.8464	Cichorii Radix	Desace	28620	FALSE	OC12C3C(C4(C(CC3)CC(OC3OC(C(OC5OC(C(OC6OC(C(OC7OC(C(O)C(O)C(O)C7O)CO)C(O)C6)C)C(O)C5)C)C(O)C3)C)CC4)C)CC(O)C1(C(CC2)C1=CC(=O)OC1)C
MOL008544	0.5441	0.4559	0.7268	Cichorii Radix	DOG	15478	FALSE	OC12C3C(C4(C(CC3)CC(O)CC4)C)CC(O)C1(C(CC2)C1=CC(=O)OC1)C
MOL008545	0.6304	0.3696	0.8255	Cichorii Radix	Purpureaglykosid A	Not Available	FALSE	OC12C3C(C4(C(CC3)CC(OC3OC(C(OC5OC(C(O)C(O)C5)C)C(OC5OC(C(O)C(OC6OC(C(O)C(O)C6O)CO)C5)C)C3)C)CC4)C)CCC1(C(CC2)C1=CC(=O)OC1)C
MOL008546	0.8722	0.1278	0.8173	Cichorii Radix	cichorioside B	Not Available	FALSE	C1(=C2C(C3C(C(C1)O)C(C(=O)O3)C)C(=CC2=O)COC1C(C(C(C(O1)CO)O)O)O)C
MOL008547	0.8990	0.1010	0.7839	Cichorii Radix	cichorioside B_qt	9970764	FALSE	C1(=C2C(C3C(C(C1)O)C(C(=O)O3)C)C(=CC2=O)CO)C
MOL008552	0.9323	0.0677	0.8757	Cichorii Radix	7-hydroxy-6-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-2-one	5420916	FALSE	c12c(cc(c(c1)OC1OC(C(C(C1O)O)O)CO)O)oc(=O)cc2

MOL008553	0.9143	0.0857	0.8188	Cichorii Radix	inulin	14656614	FALSE	C1(C(OC(C1O)CO)(COC1(OC(C(C1O)O)CO)COC1(OC(C(C1O)O)CO)CO)O)O
MOL008555	0.9429	0.0571	0.9769	Cichorii Radix	Methyl 4-hydroxyphenylacetate	518900	FALSE	c1(ccc(cc1)O)CC(=O)OC
MOL008556	0.9296	0.0704	0.9045	Cichorii Radix	monocaffeyltartaric acid	Not Available	FALSE	c1(cc(c(cc1)O)O)/C=C/C(=O)C(C(=O)O)(C(C(=O)O)O)O
MOL008558	0.4023	0.5977	0.7041	Cichorii Radix	ψ-taraxasterol	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CC=C(C1C)C)C)C)C)(C)C)O
MOL008559	0.4696	0.5304	0.6771	Tribulifructus	(2aR,2'R,4R,6aR,6bS,8aS,8bR,11aS,12aR,12bR)-4-((S)-2-(2,6-dimethylphenyl)propoxy)-5',5',6a,8a-tetramethyl-8-methylenedocosahydro-1H-spiro[pentaleno[2,1-a]phenanthrene-10,2'-pyran]	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C2C(C(=C)C1)(C1C(C2)CC2(C1)CCC(CO2)(C)C)C)C)OCC(C)c1c(cccc1C)C
MOL008560	0.2877	0.7123	0.7641	Tribulifructus	(2aS,2'R,5'R,6aS,6bS,8aS,8bR,9S,11aR,12aR,12bR)-5',6a,8a,9-tetramethylicosahydro-1H-spiro[pentaleno[2,1-a]phenanthrene-10,2'-pyran]-8(2H)-one	Not Available	FALSE	C1CCC2C(C1)(C1C(CC2)C2C(C(=O)C1)(C1C(C2)CC2(C1C)CCC(CO2)C)C)C

MOL008561	0.7013	0.2987	0.7821	Tribulifructus	(2S,2'S,3R,3'R,4R,4'R,5R,5'R)-2,2'-(((2R,3R,4R,5R,6R)-2-(((2S,3R,4R,5R,6R)-2,4-dihydroxy-6-(((2aS,4R,6aS,6bS,8aS,8bS,9S,10R,11aR,12aR,12bR)-10-methoxy-6a,8a,9-trimethyl-10-((R)-3-(((2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyra	Not Available	FALSE	C1(C(C(C(OC1)OC1C(C(OC(C1OC1C(C(C(CO1)O)O)O)OC1C(C(C(OC1O)OC1CCC2(C(C1)CCC1C2CCC2(C1CC1C2C(C(O1)(CCC(OC1C(C(C(C(O1)CO)O)O)O)C)OC)C)C)C)OC1C(C(C(C(O1)C)O)O)O)O)CO)O)O)O)O
MOL008563	0.2127	0.7873	0.6657	Tribulifructus	(3R,8S,9S,10R,13R,14R,17S)-17-((2S,5R)-5-ethyl-6-methylheptan-2-yl)-3-hydroxy-10,13-dimethyl-3,4,8,9,10,11,12,13,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-7(2H)-one	Not Available	FALSE	C1C(CC2=CC(=O)C3C(C2(C1)C)CCC1(C3CCC1C(C)CCC(CC)C(C)C)C)O

MOL008564	0.6110	0.3890	0.7699	Tribulifructus	3β-hydroxy-5α-pregn-16(17)en-20-one-3-O-β-D-xylopyranosyl(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl(1→4)-[α-L-rhamnopyranosyl(1→2)]-β-D-galactopyranoside	Not Available	FALSE	C1(C(C(C(OC1)OC(C(CCO)O)C(C(O)OC1C(C(C(OC1O)OC1CC2C(CC1)(C1C(CC2)C2C(CC1)(C(CC2)C(=O)C)C)C)OC1C(C(C(C(O1)C)O)O)O)O)OC1C(C(C(CO1)O)O)O)O)O)O
MOL008565	0.2497	0.7503	0.7753	Tribulifructus	3β-hydroxy-5α-pregn-16(17)en-20-one-3-O-β-D-xylopyranosyl(1→2)-[β-D-xylopyranosyl-(1→3)]-β-D-glucopyranosyl(1→4)-[α-L-rhamnopyranosyl(1→2)]-β-D-galactopyranoside_qt	Not Available	FALSE	C1CC2C(CC1)(C1C(CC2)C2C(CC1)(C(CC2)C(=O)C)C)C
MOL008566	0.5904	0.4096	0.7384	Tribulifructus	4-ketopinores	Not Available	FALSE	c1(ccc(cc1OC)C1C2C(C(=O)O1)C(OC2)c1cc(c(cc1)O)OC)O

MOL008567	0.2261	0.7739	0.6042	Tribulifructus	(3R,7R,8S,9S,10S,13R,14S,17R)-17-((2R,5S)-5-ethyl-6-methylheptan-2-yl)-3,10-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-7-ol	Not Available	FALSE	C1C(CC2=CC(C3C(C2(C1)C)CCC1C3CCC1C(CCC(C)C)CC)C)O)C
MOL008568	0.9021	0.0979	0.8075	Tribulifructus	(Z)-3-(3,4-dihydroxyphenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	16119508	FALSE	c1(c(ccc(c1)/C=C\C(=O)NCCc1ccc(cc1)O)O)O
MOL008570	0.8797	0.1203	0.7496	Tribulifructus	Yajeine	5280953	FALSE	c12c3c([nH]c1c(ncc2)C)cc(cc3)OC
MOL008571	0.2973	0.7027	0.7595	Tribulifructus	(2'R,5'R,6aS,6bS,8aR,8bS,11aR,12aR,12bR)-5',6a,8a-trimethyl-1,3',4',5',6,6a,6b,6',7,8a,8b,9,11a,12,12a,12b-hexadecahydrospiro[naphtho[2',1':4,5]indeno[2,1-b]furan-10,2'-pyran]-4,8(2H,5H)-dione	Not Available	FALSE	C1C(=O)C=C2C(C1)(C1C(CC2)C2C(C(=O)C1)(C1C(C2)OC2(C1)OCC(CC2)C)C)C

MOL008572	0.7110	0.2890	0.8282	Tribulifructus	(2aS,2'R,4R,5'R,6aS,6bS,8aS,8bS,9S,11aR,12aR,12bR)-4-(((2R,3R,4S,5S,6R)-5-(((2R,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-(((2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)tetrahydro-2H-pyran-2-yl)oxy)-3-hydroxy-6-(h	Not Available	FALSE	C1(C(C(C(OC1CO)OC1C(C(C(OC1CO)OC1CC2C(CC1)(C1C(CC2)C2C(C(=O)C1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)O)OC1C(C(C(CO1)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)O)O)O

MOL008573	0.2742	0.7258	0.7380	Tribulifructus	(2aS,2'R,4R,5'R,6aS,6bS,8aS,8bS,9S,11aR,12aR,12bR)-4-(((2R,3R,4S,5S,6R)-5-(((2R,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-(((2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)tetrahydro-2H-pyran-2-yl)oxy)-3-hydroxy-6-(h	Not Available	FALSE	C1CC2C(CC1)(C1C(CC2)C2C(C(=O)C1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C
MOL008574	0.2153	0.7847	0.6992	Tribulifructus	(2aS,2'R,4R,6aS,6bS,8aR,8bS,9S,11aR,12aR,12bR)-4-ethoxy-2a,8a,9-trimethylicosahydrospiro[naphtho[2',1':4,5]indeno[2,1-b]furan-10,2'-pyran]-8(2H)-one	Not Available	FALSE	C1C(CC2(C(C1)C1C(CC2)C2C(C(=O)C1)(C1C(C2)OC2(C1C)CCCCO2)C)C)OCC
MOL008576	0.3332	0.6668	0.6949	Tribulifructus	Gitogenin	Not Available	FALSE	C1(C(CC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)CCC(CO2)C)C)C)O)O
MOL008577	0.2023	0.7977	0.6987	Tribulifructus	zymostrol	92746	FALSE	C12C3=C(C4(C(CC3)CC(CC4)O)C)CCC1(C(CC2)C(CCC=C(C)C)C)C

MOL008578	0.3431	0.6569	0.7584	Tribulifructus	(2S,2aS,2'R,4S,5'R,6aR,6bS,8aS,8bS,9S,11aR,12aS,12bR)-5',6a,8a,9-tetramethyldocosahydrospiro[naphtho[2',1':4,5]indeno[2,1-b]furan-10,2'-pyran]-2,4-diol	Not Available	FALSE	C1C2(C(CC(C1)O)C(CC1C2CCC2(C1CC1C2C(C2(O1)OCC(CC2)C)C)C)O)C
MOL008579	0.6529	0.3471	0.8695	Tribulifructus	(2aS,2'R,4R,5'S,6R,6aR,6bS,8aS,8bS,9S,11aR,12aR,12bR)-4-(((2R,3R,4S,5R,6R)-3,4-dihydroxy-6-(hydroxymethyl)-5-(((2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)tetrahydro-2H-pyran-2-yl)oxy)-5',6,8a,9-tetramethylicosahydro	Not Available	FALSE	C1(C(C(C(OC1CO)OC1C(C(C(OC1CO)OC1CC(C2C(C1)CCC1C2CC(=O)C2(C1CC1C2C(C2(O1)CCC(CO2)C)C)C)C)O)O)O)O)O
MOL008580	0.2912	0.7088	0.6585	Tribulifructus	spirostanol	Not Available	FALSE	C1CCC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C
MOL008581	0.3012	0.6988	0.7449	Tribulifructus	tigogenin	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)O
MOL008582	0.3326	0.6674	0.6585	Tribulifructus	trillin	Not Available	FALSE	C1(OC(C(C(C1O)O)O)CO)OC1CC2=CCC3C4C(C5C(OC6(C5C)CCC(CO6)C)C4)(CCC3C2(CC1)C)C
MOL008582	0.3326	0.6674	0.6585	Broussonetiae Fructus	trillin	Not Available	FALSE	C1(OC(C(C(C1O)O)O)CO)OC1CC2=CCC3C4C(C5C(OC6(C5C)CCC(CO6)C)C4)(CCC3C2(CC1)C)C

MOL008583	0.2378	0.7622	0.7459	Tribulifructus	beta-Sitosterol	Not Available	FALSE	C1CCC2C(C1C)C1C(CC2)C2C(C(=O)C1)(C1C(C2)OC2(C1C)CCC(CO2)C)C
MOL008584	0.2701	0.7299	0.6857	Tribulifructus	beta-Sitosterol-beta-D-glucopyranoside_qt	Not Available	FALSE	C12C3(C(CC1OC1(C2C)CCC(CO1)C)C1C(CC3)C2(C(=CC1)CCCC2)C)C
MOL008585	0.7150	0.2850	0.7769	Tribulifructus	(2S,2'S,3R,3'R,4R,4'R,5R,5'R)-2,2'-(((2S,3R,4R,5R,6R)-2-(((2R,3R,5R,6R)-6-(((2aS,6aR,6bS,8aS,8bS,9S,10R,11aR,12aR,12bS)-10-(3-(((2S,3R,4R,5S,6R)-6-ethyl-3,4,5-trihydroxytetrahydro-2H-pyran-2-yl)oxy)-3-methylbutyl)-2a,6a,8a,9,10-pentamethyloctadecahyd	Not Available	FALSE	C1(C(C(C(OC1)OC1C(C(OC(C1OC1C(C(C(CO1)O)O)O)OC1CC(C(OC1CO)OC1CCC2(C(C1)(CCC1C2CCC2(C1CC1C2C(C(O1)(CCC(OC1C(C(C(C(O1)CC)O)O)O)(C)C)C)C)C)C)OC1C(C(C(C(O1)C)O)O)O)CO)O)O)O)O

MOL008586	0.3457	0.6543	0.6530	Tribulifructus	(2S,2'S,3R,3'R,4R,4'R,5R,5'R)-2,2'-(((2S,3R,4R,5R,6R)-2-(((2R,3R,5R,6R)-6-(((2aS,6aR,6bS,8aS,8bS,9S,10R,11aR,12aR,12bS)-10-(3-(((2S,3R,4R,5S,6R)-6-ethyl-3,4,5-trihydroxytetrahydro-2H-pyran-2-yl)oxy)-3-methylbutyl)-2a,6a,8a,9,10-pentamethylooctadecahyd	Not Available	FALSE	C1CCC2(C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC(C1C)(CCC(C)C)C)C)C)C
MOL008587	0.8618	0.1382	0.8836	Tribulifructus	terrestric acid	Not Available	FALSE	C1(=NC(=O)NC(N1)C(=O)O)N
MOL008588	0.8789	0.1211	0.8243	Tribulifructus	terrestriamide	Not Available	FALSE	C1(C(CCC(C1)/C=C\C(=O)NCC(=O)C1CCC(CC1)O)O)O
MOL008589	0.3076	0.6924	0.6646	Tribulifructus	furostanol	Not Available	FALSE	C1CCC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC(C1C)CCC(CC)C)C)C
MOL008590	0.4032	0.5968	0.6875	Tribulifructus	(2aR,2'S,4R,4'R,5'S,6aS,6bS,8aS,8bR,9S,11aR,12aR,12bR)-4,4'-dihydroxy-5',6a,8a,9-tetramethylicosahydro-1H-spiro[pentaleno[2,1-a]phenanthrene-10,2'-pyran]-8(2H)-one	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C2C(C(=O)C1)(C1C(C2)CC2(C1C)CC(C(CO2)C)O)C)C)O

MOL008591	0.3383	0.6617	0.6951	Tribulifructus	(2aR,2'R,4R,5'R,6aS,6bS,8aS,8bR,9S,11aS,12aR,12bR)-4-hydroxy-5',6a,8a,9-tetramethylicosahydrospiro[naphtho[2',1':4,5]indeno[2,1-b]furan-10,2'-pyran]-8(2H)-one	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C2C(C(=O)C1)(C1C(C2)OC2(C1C)CCC(CO2)C)C)C)O
MOL008592	0.7754	0.2246	0.8001	Tribulifructus	Automatically Name	Not Available	FALSE	C1(C(C(C(OC1CO)OC1C(C(C(OC1CO)OC1C(CC2(C(C1)CCC1C2CCC2(C1CC1C2C(=C(O1)CCC(COC1C(C(C(C(O1)CO)O)O)O)C)C)C)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)O)O
MOL008593	0.2739	0.7261	0.7551	Tribulifructus	(2aR,5S,6aS,6bS,8aS,8bS,11aS,12aR,12bR)-10-isopentyl-6a,8a,9-trimethyl-2,2a,3,4,5,6,6a,6b,7,8,8a,8b,11a,12,12a,12b-hexadecahydro-1H-naphtho[2',1':4,5]indeno[2,1-b]furan-5-ol	Not Available	FALSE	C1(CCC2C(C1)(C1C(CC2)C2C(CC1)(C1C(C2)OC(=C1C)CCC(C)C)C)C)O
MOL008594	0.6689	0.3311	0.6618	Impatientis Semen	methyl (Z)-hexadec-7-enoate	14029831	FALSE	C(=O)(CCCCC/C=C\CCCCCCCC)OC
MOL008594	0.6689	0.3311	0.6618	Perillae Fructus	methyl (Z)-hexadec-7-enoate	14029831	FALSE	C(=O)(CCCCC/C=C\CCCCCCCC)OC
MOL008596	0.7979	0.2021	0.7371	Impatientis Semen	balsaminone A	Not Available	FALSE	o1c2c(c3c1C(=O)c1c(C3=O)cccc1)c(OC)c(O)c1c2cccc1
MOL008597	0.7310	0.2690	0.7372	Impatientis Semen	balsaminone B	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(c3oc4c(c3c1OC)C(=O)c1c(C4=O)cccc1)cccc2)CO

MOL008602	0.6667	0.3333	0.6398	Impatientis Semen	methyl (E)-hexadec-2-enoate	5362679	FALSE	C(=O)(/C=C/CCCCCCCCCCCCC)OC
MOL008603	0.2846	0.7154	0.6282	Impatientis Semen	(1R,2S,2'S,4aR,4bR,6aR,7R,8S,10aR,10bR,12aS)-7-(hydroxymethyl)-2'-[(2S)-1-hydroxypropan-2-yl]-4a,4b,7,10a-tetramethylspiro[3,4,5,6,6a,8,9,10,10b,11,12,12a-dodecahydro-1H-chrysene-2,5'-oxane]-1,8-diol	21729342	FALSE	O1C(CCC2(C(C3C(C4(C(C5(C(C(C(CC5)O)(CO)C)CC4)C)CC3)C)(CC2)C)O)C1)C(CO)C
MOL008604	0.7609	0.2391	0.8273	Impatientis Semen	hosenkosides A	Not Available	FALSE	O1C(CCC2(C(C3C(C4(C(C5(C(C(C(CC5)OC5OC(C(C(C5OC5OC(C(C(C5O)O)O)CO)O)O)CO)(COC5OC(C(C(C5O)O)O)CO)C)CC4)C)CC3)C)(CC2)C)O)C1)C(CO)C
MOL008605	0.2846	0.7154	0.6282	Impatientis Semen	hosenkosides D_qt	Not Available	FALSE	O1C(CCC2(C(C3C(C4(C(C5(C(C(C(CC5)O)(CO)C)CC4)C)CC3)C)(CC2)C)O)C1)C(CO)C
MOL008606	0.7652	0.2348	0.8184	Impatientis Semen	hosenkosides B	Not Available	FALSE	O1C(CCC2(C(C3C(C4(C(C5(C(C(C(CC5)OC5OC(C(C(C5OC5OC(C(C(C5O)O)O)CO)O)O)CO)(CO)C)C4)C)CC3)C)(CC2)C)O)C1)C(COC1OC(C(C(C1O)O)O)CO)C
MOL008607	0.2846	0.7154	0.6282	Impatientis Semen	hosenkosides E_qt	Not Available	FALSE	O1C(CCC2(C(C3C(C4(C(C5(C(C(C(CC5)O)(CO)C)CC4)C)CC3)C)(CC2)C)O)C1)C(CO)C
MOL008608	0.7655	0.2345	0.8182	Impatientis Semen	hosenkosides C	Not Available	FALSE	O1C(C(C(C(C1CO)O)O)O)OC1C(C(C(OC1OC1C(C2C(C3C(C4(C(C(C(CC4)(CO)CC/C=C(\CO)/C)O)CC3)C)(CC2)C)(CC1)C)(COC1OC(C(C(C1O)O)O)CO)C)CO)O)O
MOL008610	0.7633	0.2367	0.8127	Impatientis Semen	hosenkosides D	Not Available	FALSE	O1C(CCC2(C(C3C(C4(C(C5(C(C(C(CC5)OC5OC(C(C(C5O)O)O)CO)(COC5OC(C(C(C5O)O)O)CO)C)C4)C)CC3)C)(CC2)C)O)C1)C(CO)C
MOL008611	0.7330	0.2670	0.8592	Impatientis Semen	hosenkosides E	Not Available	FALSE	O1C(CCC2(C(C3C(C4(C(C5(C(C(C(CC5)OC5OC(C(C(C5OC5OC(C(C(C5O)O)O)CO)O)O)CO)(CO)C)C4)C)CC3)C)(CC2)C)O)C1)C(CO)C

MOL008612	0.7682	0.2318	0.6219	Impatientis Semen	(2E,4E,6E,8E)-octadeca-2,4,6,8-tetraenoic acid	11778225	FALSE	C(=O)(/C=C/C=C/C=C/C=C/CCCCCCCCC)O
MOL008613	0.9011	0.0989	0.8878	Impatientis Semen	2,2-Dimethyloctane	85150	FALSE	C(CCCCCC)(C)(C)C
MOL008615	0.9271	0.0729	0.9412	Impatientis Semen	Methyl 9-oxononanoate	74732	FALSE	C(=O)(CCCCCCCC=O)OC
MOL008615	0.9271	0.0729	0.9412	Perillae Fructus	Methyl 9-oxononanoate	74732	FALSE	C(=O)(CCCCCCCC=O)OC
MOL008615	0.9271	0.0729	0.9412	Sterculiae Lychnophorae Semen	Methyl 9-oxononanoate	74732	FALSE	C(=O)(CCCCCCCC=O)OC
MOL008616	0.2355	0.7645	0.7137	Rosae Laevigatae Fructus	(+)-2-N-Methylfangchinoline	Not Available	FALSE	c1c2c3c(c(c1OC)O)Oc1c(cc4CCN(C(Cc5ccc(Oc6c(ccc(CC3[N+](CC2)(C)C)c6)OC)cc5)c4c1)C)OC
MOL008617	0.7394	0.2606	0.7373	Rosae Laevigatae Fructus	19a-hydroxyasiatic acid	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1(C)O)C)C(=O)O)C)C)(C)CO)O)O
MOL008619	0.7290	0.2710	0.7293	Rosae Laevigatae Fructus	1α,2α,3β,19α-tetrahydroxyurs-12-en-28-oic acid	Not Available	FALSE	C1(C(C(C2C(C1O)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(=O)O)CCC(C1(O)C)C)C)C)(C)C)O)O
MOL008620	0.7087	0.2913	0.7847	Rosae Laevigatae Fructus	Euscaphic acid 3,4-monoacetonide	Not Available	FALSE	C12C(C(C3C(C1)(C1C(CC3)(C3(C(=CC1)C1C(CC3)(CCC(C1(C)O)C)C(=O)O)C)C)(C)C)OC(O2)(C)C
MOL008621	0.3061	0.6939	0.7473	Rosae Laevigatae Fructus	Methyl 2alpha-hydroxyursolate	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1C)C)C(=O)OC)C)C)(C)C)O)O
MOL008622	0.1513	0.8487	0.7302	Rosae Laevigatae Fructus	Methyl trametenolate	Not Available	FALSE	C1C(C(C2C(C1)(C1=C(CC2)C2(C(CC1)(C(CC2)C(CCC=C(C)C)C(=O)OC)C)C)(C)C)O
MOL008623	0.7451	0.2549	0.7902	Rosae Laevigatae Fructus	2α,3α-dihydroxyolean-12-en-28-oic acid	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O)O
MOL008625	0.2813	0.7187	0.7634	Quisqualis Indica	Methyl 3beta-hydroxyurs-12-en-28-oate	636516	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(C(CC2)C)C)C(=O)OC

MOL008625	0.2813	0.7187	0.7634	Rosae Laevigatae Fructus	Methyl 3beta-hydroxyurs-12-en-28-oate	636516	FALSE	C12(C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCC(C1(C)C)O)C)C)C(CC2)C)C)C(=O)OC
MOL008626	0.7473	0.2527	0.7092	Quisqualis Indica	pedunculagin	Not Available	FALSE	O1C2C3OC(=O)c4c(c5c(C(=O)OCC3OC(O)C2OC(=O)c2c(c3c(C1=O)cc(O)c(O)c3O)c(O)c(O)c(O)c2)cc(O)c(O)c5O)c(O)c(O)c(O)c4
MOL008626	0.7473	0.2527	0.7092	Rosae Laevigatae Fructus	pedunculagin	Not Available	FALSE	O1C2C3OC(=O)c4c(c5c(C(=O)OCC3OC(O)C2OC(=O)c2c(c3c(C1=O)cc(O)c(O)c3O)c(O)c(O)c(O)c2)cc(O)c(O)c5O)c(O)c(O)c(O)c4
MOL008626	0.7473	0.2527	0.7092	Rose Rugosae Flos	pedunculagin	Not Available	FALSE	O1C2C3OC(=O)c4c(c5c(C(=O)OCC3OC(O)C2OC(=O)c2c(c3c(C1=O)cc(O)c(O)c3O)c(O)c(O)c(O)c2)cc(O)c(O)c5O)c(O)c(O)c(O)c4
MOL008627	0.6885	0.3115	0.7662	Rosae Laevigatae Fructus	2α,3β-dihydroxylup-20(29)-en-28-oic acid	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(=O)O)CCC1C(=C)C)C)C)(C)C)O)O
MOL008628	0.4142	0.5858	0.7796	Rosae Laevigatae Fructus	4'-Methyl-N-methylcoclaurine	Not Available	FALSE	c1(ccc2c(c1)CCN(C2Cc1ccc(cc1)OC)C)OC
MOL008629	0.9310	0.0690	0.8205	Rosae Laevigatae Fructus	6-Methylindole	137928	FALSE	c1c(cc2c(c1)cc[nH]2)C
MOL008630	0.7408	0.2592	0.7912	Corydalis Bungeanae Herba	11-epicorynoline	Not Available	FALSE	c12c(cc3c(c1)CC(C1(C3CCc3c1ccc1c3OCO1)C)O)OCO2
MOL008631	0.8344	0.1656	0.7318	Corydalis Bungeanae Herba	12-hydroxycorynoline	Not Available	FALSE	O1COc2c1c1CN(C3C(C(C(c4c3cc3OCOc3c4)O)O)(c1cc2)C)C
MOL008632	0.7655	0.2345	0.7188	Corydalis Bungeanae Herba	bungeanine	Not Available	FALSE	C1Oc2c(O1)c1c(cc2)C2(C(=NC1)c1c(CC2C(=O)OC)cc2c(c1)OCO2)C
MOL008633	0.7272	0.2728	0.8030	Corydalis Bungeanae Herba	(S)-Cheilanthifoline	Not Available	FALSE	O1c2c3CN4C(Cc3ccc2OC1)c1c(CC4)cc(OC)c(O)c1
MOL008635	0.5641	0.4359	0.9169	Corydalis Bungeanae Herba	coryincine	3058605	FALSE	OC1C(C2C(CN3C(C2)c2[nH]c4c(c2CC3)cccc4)CC1)C(=O)OC
MOL008636	0.7737	0.2263	0.7864	Corydalis Bungeanae Herba	corynoline	Not Available	FALSE	O1COc2c1c1CN(C3C(C(Cc4c3cc3OCOc3c4)O)(c1cc2)C)C
MOL008637	0.8652	0.1348	0.7718	Corydalis Bungeanae Herba	d-isocorynoline	Not Available	FALSE	OC1C2(C(NCc3c2ccc2OCOc32)c2c(C1)cc1OCOc1c2)C
MOL008638	0.7737	0.2263	0.7864	Corydalis Bungeanae Herba	13-epicorynoline	Not Available	FALSE	c12ccc3c(c1OCO2)CN(C1C3(C(Cc2c1cc1c(c2)OCO1)O)C)C
MOL008639	0.7737	0.2263	0.7864	Corydalis Bungeanae Herba	epicorynoline	Not Available	FALSE	OC1C2(C(N(Cc3c2ccc2OCOc32)C)c2c(C1)cc1OCOc1c2)C
MOL008640	0.7986	0.2014	0.7630	Corydalis Bungeanae Herba	isocorynoline	Not Available	FALSE	O1c2c(OC1)c1c(cc2)C2(C(N(C1)C)c1c(CO2)cc2c(c1)OCO2)C

MOL008641	0.8600	0.1400	0.7245	Corydalis Bungeanae Herba	Norsanguinarine	Not Available	FALSE	O1c2c3c(c4c(nc3)c3c(cc4)cc4OCOc4c3)ccc2OC1
MOL008642	0.8226	0.1774	0.8166	Corydalis Bungeanae Herba	noryuziphine	Not Available	FALSE	c1(cc2c(cc1)CCNC2Cc1ccc(cc1)O)OC
MOL008643	0.7980	0.2020	0.6731	Corydalis Bungeanae Herba	spallidamine	Not Available	FALSE	c1cc2c(c3N(C(c4c5c(ccc4c13)OCO5)CC(=O)O)C)cc1OCOc1c2
MOL008644	0.7911	0.2089	0.7867	Corydalis Bungeanae Herba	tetrahydrocorysamine	Not Available	FALSE	O1COc2c1c1CN3CCc4c(C3C(c1cc2)C)cc1c(c4)OCO1
MOL008645	0.5866	0.4134	0.7762	Corydalis Bungeanae Herba	yuziphine	Not Available	FALSE	c1cc(cc2c1CCN(C2Cc1ccc(cc1)O)C)OC
MOL008646	0.5820	0.4180	0.6653	Corydalis Bungeanae Herba	6-acetonyldihydrosanguinarine	Not Available	FALSE	O1c2c3C(N(c4c(c3ccc2OC1)ccc1c4cc2OCOc2c1)C)CC(=O)C
MOL008647	0.8309	0.1691	0.7609	Jujubae Fructus	Moupinamide	5280537	FALSE	O(c1cc(/C=C/C(=O)NCCc2ccc(O)cc2)ccc1O)C
MOL008647	0.8309	0.1691	0.7609	Corydalis Bungeanae Herba	Moupinamide	5280537	FALSE	O(c1cc(/C=C/C(=O)NCCc2ccc(O)cc2)ccc1O)C
MOL008648	0.7537	0.2463	0.7249	Corydalis Bungeanae Herba	acetylcorynoline	Not Available	FALSE	O1COc2c1c1c(cc2)C2(C(NC1)c1c(CC2OC(=O)C)cc2c(c1)OCO2)C
MOL008650	0.9395	0.0605	0.9399	Apocyniveneti Folium	o-Methylanisole	33637	FALSE	c1(c(cccc1)C)OC
MOL008651	0.9286	0.0714	0.9612	Apocyniveneti Folium	Pyroterebaldehyde	21457	FALSE	C(=O)CC=C(C)C
MOL008652	0.8986	0.1014	0.9731	Momordicae Fructus	(2R)-2-methyloxolan-3-one	7060522	FALSE	C1(=O)C(OCC1)C
MOL008652	0.8986	0.1014	0.9731	Apocyniveneti Folium	(2R)-2-methyloxolan-3-one	7060522	FALSE	C1(=O)C(OCC1)C
MOL008653	0.8889	0.1111	0.9406	Hippophae Fructus	Acetylfuran	14505	FALSE	c1(C(=O)C)ccco1
MOL008653	0.8889	0.1111	0.9406	Achyranthis Bidentatae Radix	Acetylfuran	14505	FALSE	c1(C(=O)C)ccco1
MOL008653	0.8889	0.1111	0.9406	Momordicae Fructus	Acetylfuran	14505	FALSE	c1(C(=O)C)ccco1
MOL008653	0.8889	0.1111	0.9406	Ardisiae Japonicae Herba	Acetylfuran	14505	FALSE	c1(C(=O)C)ccco1
MOL008653	0.8889	0.1111	0.9406	Perillae Fructus	Acetylfuran	14505	FALSE	c1(C(=O)C)ccco1
MOL008653	0.8889	0.1111	0.9406	Apocyniveneti Folium	Acetylfuran	14505	FALSE	c1(C(=O)C)ccco1
MOL008653	0.8889	0.1111	0.9406	Campsis Flos	Acetylfuran	14505	FALSE	c1(C(=O)C)ccco1
MOL008655	0.9177	0.0823	0.9438	Apocyniveneti Folium	3,3-Dimethylpent-1-ene	18852	FALSE	C(CC)(C=C)(C)C
MOL008656	0.9138	0.0862	0.9689	Cinnamomi Ramulus	(1R,3R,4S)-3,4-dimethylcyclohexan-1-ol	6994302	FALSE	C1(C(CCC(C1)O)C)C

MOL008656	0.9138	0.0862	0.9689	Ginkgo Folium	(1R,3R,4S)-3,4-dimethylcyclohexan-1-ol	6994302	FALSE	C1(C(CCC(C1)O)C)C
MOL008656	0.9138	0.0862	0.9689	Apocyniveneti Folium	(1R,3R,4S)-3,4-dimethylcyclohexan-1-ol	6994302	FALSE	C1(C(CCC(C1)O)C)C
MOL008657	0.9198	0.0802	0.9213	Capsici Fructus	isoamylcyclopentane	517741	FALSE	C1(CCCC1)CCC(C)C
MOL008658	0.9353	0.0647	0.9664	Litchi Semen	ZINC02041097	637497	FALSE	C(C(C)O)CO
MOL008658	0.9353	0.0647	0.9664	Citri Sarcodactylis Fructus	ZINC02041097	637497	FALSE	C(C(C)O)CO
MOL008658	0.9353	0.0647	0.9664	Capsici Fructus	ZINC02041097	637497	FALSE	C(C(C)O)CO
MOL008658	0.9353	0.0647	0.9664	Sesami Nigrum Semen	ZINC02041097	637497	FALSE	C(C(C)O)CO
MOL008658	0.9353	0.0647	0.9664	Hordei Fructus Germinatus	ZINC02041097	637497	FALSE	C(C(C)O)CO
MOL008659	0.8782	0.1218	0.9669	Capsici Fructus	1-Ethynylcyclopentanol	87074	FALSE	C1(CCCC1)(C#C)O
MOL008660	0.8941	0.1059	0.9598	Capsici Fructus	METHYLCYCLOHEXENE	11574	FALSE	C1(=CCCCC1)C
MOL008661	0.9250	0.0750	0.9428	Viticis Negundo Folium	Vinyl amyl ketone	61346	FALSE	C(=O)(CCCCC)C=C
MOL008661	0.9250	0.0750	0.9428	Polygonati Odorati Rhizoma	Vinyl amyl ketone	61346	FALSE	C(=O)(CCCCC)C=C
MOL008661	0.9250	0.0750	0.9428	Schizonepetae Spica	Vinyl amyl ketone	61346	FALSE	C(=O)(CCCCC)C=C
MOL008661	0.9250	0.0750	0.9428	Meliae Azedarach Fructus	Vinyl amyl ketone	61346	FALSE	C(=O)(CCCCC)C=C
MOL008661	0.9250	0.0750	0.9428	Capsici Fructus	Vinyl amyl ketone	61346	FALSE	C(=O)(CCCCC)C=C
MOL008662	0.7892	0.2108	0.6675	Capsici Fructus	2,2,3,6-tetramethyl-alpha-propyl-cyclohexane	Not Available	FALSE	C1(C(C(CCC1C)C)(C)C)CCC(O)CCC
MOL008663	0.9163	0.0837	0.9708	Capsici Fructus	biacetyl	650	FALSE	C(=O)(C(=O)C)C
MOL008663	0.9163	0.0837	0.9708	Panacis Japonici Rhizoma	biacetyl	650	FALSE	C(=O)(C(=O)C)C
MOL008663	0.9163	0.0837	0.9708	Sesami Nigrum Semen	biacetyl	650	FALSE	C(=O)(C(=O)C)C

MOL008664	0.9275	0.0725	0.9654	Capsici Fructus	2,3-Pentadione	11747	FALSE	C(=O)(C(=O)C)CC
MOL008666	0.9032	0.0968	0.9380	Capsici Fructus	Allyl glycol	8116	FALSE	O(CC=C)CCO
MOL008667	0.9113	0.0887	0.8896	Capsici Fructus	2-butyloctanoic acid	Not Available	FALSE	C(CCCCCC)(CCCC)C(=O)O
MOL008668	0.9141	0.0859	0.9572	Cinnamomi Ramulus	2-ethoxypropanol	Not Available	FALSE	C(C(C)OCC)O
MOL008668	0.9141	0.0859	0.9572	Capsici Fructus	2-ethoxypropanol	Not Available	FALSE	C(C(C)OCC)O
MOL008669	0.9298	0.0702	0.9624	Momordicae Fructus	(S)-2-Ethylhexanoic acid	135309	FALSE	C(CCCC)(C(=O)O)CC
MOL008669	0.9298	0.0702	0.9624	Capsici Fructus	(S)-2-Ethylhexanoic acid	135309	FALSE	C(CCCC)(C(=O)O)CC
MOL008670	0.8515	0.1485	0.8614	Capsici Fructus	Baran	12542	FALSE	C(=O)(CF)N
MOL008671	0.9519	0.0481	0.8990	Achyranthis Bidentatae Radix	PRZ	32594	FALSE	c1(c(nccn1)OC)CC(C)C
MOL008671	0.9519	0.0481	0.8990	Capsici Fructus	PRZ	32594	FALSE	c1(c(nccn1)OC)CC(C)C
MOL008672	0.9113	0.0887	0.9666	Capsici Fructus	ZINC00901303	6971249	FALSE	C(CC)(C=O)C
MOL008672	0.9113	0.0887	0.9666	Sesami Nigrum Semen	ZINC00901303	6971249	FALSE	C(CC)(C=O)C
MOL008673	0.9097	0.0903	0.9041	Capsici Fructus	2-Nonyl acetate	13240755	FALSE	CCCCCCCC(OC(=O)C)C
MOL008674	0.9252	0.0748	0.9337	Capsici Fructus	2-Octynal	74610	FALSE	C(CCCC)C#CC=O
MOL008674	0.9252	0.0748	0.9337	Ginkgo Folium	2-Octynal	74610	FALSE	C(CCCC)C#CC=O
MOL008675	0.9180	0.0820	0.9251	Rose Rugosae Flos	3-HEPTEN-2-ONE	5364578	FALSE	C(=C\CCC)/C(=O)C
MOL008675	0.9180	0.0820	0.9251	Capsici Fructus	3-HEPTEN-2-ONE	5364578	FALSE	C(=C\CCC)/C(=O)C
MOL008676	0.9324	0.0676	0.9745	Capsici Fructus	3-Methyl-1,5-pentanediol	20524	FALSE	C(CCO)(CCO)C
MOL008677	0.9092	0.0908	0.9704	Capsici Fructus	3-methyl-4-oxo-pentanoic acid	12576879	FALSE	C(CC(=O)O)(C(=O)C)C
MOL008678	0.9300	0.0700	0.9690	Capsici Fructus	Pentanol-3	11428	FALSE	C(CC)(CC)O
MOL008678	0.9300	0.0700	0.9690	Menthae Herba	Pentanol-3	11428	FALSE	C(CC)(CC)O
MOL008679	0.9335	0.0665	0.9607	Capsici Fructus	Isohexanol	12296	FALSE	C(CCC(C)C)O
MOL008679	0.9335	0.0665	0.9607	Mori Fructus	Isohexanol	12296	FALSE	C(CCC(C)C)O

MOL008680	0.8569	0.1431	0.6680	Foeniculi Fructus	acetaldehyde	177	FALSE	C(=O)C
MOL008680	0.8569	0.1431	0.6680	Peucedanidecursivi Radix	acetaldehyde	177	FALSE	C(=O)C
MOL008680	0.8569	0.1431	0.6680	Peucedani Radix	acetaldehyde	177	FALSE	C(=O)C
MOL008680	0.8569	0.1431	0.6680	Capsici Fructus	acetaldehyde	177	FALSE	C(=O)C
MOL008680	0.8569	0.1431	0.6680	Achyranthis Bidentatae Radix	acetaldehyde	177	FALSE	C(=O)C
MOL008681	0.9615	0.0385	0.9262	Capsici Fructus	(1S)-2,6,6-trimethylcyclohex-2-ene-1-carbaldehyde	11073610	FALSE	C1(C(=CCCC1(C)C)C)C=O
MOL008682	0.7031	0.2969	0.8530	Capsici Fructus	alpha-Solamarine	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC2C1C(C1(O2)NCC(CC1)C)C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)OC1OC(C(C(C1O)O)O)CO)O)CO
MOL008683	0.3243	0.6757	0.7531	Capsici Fructus	alpha-Solamarine_qt	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC2C1C(C1(O2)NCC(CC1)C)C)C)O
MOL008684	0.9057	0.0943	0.8023	Capsici Fructus	bis(1,1-dimethylethyl)-diazene	Not Available	FALSE	C(/N=N/C(C)(C)C)(C)(C)C
MOL008686	0.7401	0.2599	0.8138	Capsici Fructus	(4-hydroxy-3-methoxyphenyl)methyl (E)-8-methylnon-6-enoate	9839519	FALSE	c1(c(ccc(c1)COC(=O)CCCC/C=C/C(C)C)O)OC
MOL008687	0.3321	0.6679	0.6164	Capsici Fructus	capsicastrine	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC(C1C(C1NCC(CC1)C)C)O)C)OC1OC(C(C(C1O)O)O)CO
MOL008688	0.2378	0.7622	0.6943	Capsici Fructus	capsicastrine_qt	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC(C1C(C1NCC(CC1)C)C)O)C)O
MOL008689	0.8712	0.1288	0.8184	Capsici Fructus	Capsidiol	161937	FALSE	C1C(C(C2(C(=CCC(C2)C(=C)C)C1O)C)C)O
MOL008691	0.3636	0.6364	0.6148	Ginkgo Semen	alpha-Carotene/beta,epsilon-Carotene	6419725	FALSE	C1(C(CCC=C1C)(C)C)/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C
MOL008691	0.3636	0.6364	0.6148	Capsici Fructus	alpha-Carotene/beta,epsilon-Carotene	6419725	FALSE	C1(C(CCC=C1C)(C)C)/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C
MOL008692	0.8308	0.1692	0.7203	Capsici Fructus	carotol	Not Available	FALSE	OC12C(CCC1C(C)C)(CC=C(CC2)C)C
MOL008694	0.9116	0.0884	0.9723	Capsici Fructus	Cyclohexylmethanol	7507	FALSE	C1(CCCCC1)CO
MOL008695	0.1225	0.8775	0.6292	Euryales Semen	δ-tocopherol	12444418	FALSE	c12c(CCC(O1)(CCCC(CCCC(CCCC(C)C)C)C)C)cc(cc2C)O

MOL008695	0.1225	0.8775	0.6292	Canavaliae Semen	δ-tocopherol	12444418	FALSE	c12c(CCC(O1)(CCCC(CCCC(CCCC(C)C)C)C)C)cc(cc2C)O
MOL008695	0.1225	0.8775	0.6292	Capsici Fructus	δ-tocopherol	12444418	FALSE	c12c(CCC(O1)(CCCC(CCCC(CCCC(C)C)C)C)C)cc(cc2C)O
MOL008696	0.4534	0.5466	0.6720	Capsici Fructus	decumbesterone A	Not Available	FALSE	C1(CC2C(CC1O)(C1C(=CC2=O)C2(C(CC1)(C(CC2)C(O)(C(CC(C(=C)C)C(C)O)O)C)C)O)C)O
MOL008698	0.8058	0.1942	0.7509	Capsici Fructus	Dihydrocapsaicin	107982	FALSE	c1(cc(c(cc1)O)OC)CNC(=O)CCCCCCC(C)C
MOL008699	0.8608	0.1392	0.6634	Sesami Nigrum Semen	MSM	1068	FALSE	S(C)C
MOL008699	0.8608	0.1392	0.6634	Hippophae Fructus	MSM	1068	FALSE	S(C)C
MOL008699	0.8608	0.1392	0.6634	Cistanches Herba	MSM	1068	FALSE	S(C)C
MOL008699	0.8608	0.1392	0.6634	Capsici Fructus	MSM	1068	FALSE	S(C)C
MOL008701	0.9292	0.0708	0.9614	Capsici Fructus	L-Glycerose	439723	FALSE	C(=O)C(O)CO
MOL008702	0.8590	0.1410	0.6633	Ephedra Herba	eth	6324	FALSE	CC
MOL008702	0.8590	0.1410	0.6633	Capsici Fructus	eth	6324	FALSE	CC
MOL008703	0.8574	0.1426	0.6619	Capsici Fructus	SCC	6343	FALSE	C(C)S
MOL008704	0.9369	0.0631	0.9663	Capsici Fructus	Ethyl (R)-3-hydroxybutanoate	440030	FALSE	C(=O)(CC(C)O)OCC
MOL008705	0.9352	0.0648	0.9615	Capsici Fructus	Butyric ether	7762	FALSE	C(=O)(CCC)OCC
MOL008705	0.9352	0.0648	0.9615	Hemerocallis Radix	Butyric ether	7762	FALSE	C(=O)(CCC)OCC
MOL008706	0.9411	0.0589	0.9603	Capsici Fructus	Ethyl cyclohexylpropionate	61466	FALSE	C1(CCC(=O)OCC)CCCCC1
MOL008707	0.9010	0.0990	0.9008	Sesami Nigrum Semen	Ethylisobutyrate	7342	FALSE	C(=O)(OCC)C(C)C
MOL008707	0.9010	0.0990	0.9008	Capsici Fructus	Ethylisobutyrate	7342	FALSE	C(=O)(OCC)C(C)C
MOL008708	0.9172	0.0828	0.9172	Capsici Fructus	1-ethoxyoctane	94664	FALSE	O(CCCCCCCC)CC
MOL008709	0.9411	0.0589	0.9593	Capsici Fructus	Ethyl valerate	10882	FALSE	C(=O)(CCCC)OCC
MOL008709	0.9411	0.0589	0.9593	Sesami Nigrum Semen	Ethyl valerate	10882	FALSE	C(=O)(CCCC)OCC
MOL008710	0.9240	0.0760	0.9656	Capsici Fructus	EGDEE	12375	FALSE	C(COCC)OCC
MOL008711	0.8549	0.1451	0.6667	Capsici Fructus	ETO	6354	FALSE	C1CO1
MOL008712	0.9115	0.0885	0.9445	Capsici Fructus	Wine oil	7797	FALSE	C(=O)(CCCCCC)OCC
MOL008713	0.9361	0.0639	0.9540	Meliae Azedarach Fructus	Ethyl hexoate	31265	FALSE	C(=O)(CCCCC)OCC
MOL008713	0.9361	0.0639	0.9540	Capsici Fructus	Ethyl hexoate	31265	FALSE	C(=O)(CCCCC)OCC
MOL008713	0.9361	0.0639	0.9540	Hippophae Fructus	Ethyl hexoate	31265	FALSE	C(=O)(CCCCC)OCC
MOL008714	0.9090	0.0910	0.9030	Capsici Fructus	Hexyl methacrylate	8872	FALSE	O(C(=O)C(=C)C)CCCCCC
MOL008715	0.6607	0.3393	0.6525	Capsici Fructus	icarside E5	Not Available	FALSE	C1(C(C(C(OC1CO)Oc1c(cc(cc1C(Cc1ccc(c(c1)OC)O)CO)/C=C/CO)OC)O)O)O
MOL008716	0.8084	0.1916	0.7056	Capsici Fructus	icarside E5_qt	Not Available	FALSE	Oc1c(cc(cc1C(Cc1ccc(c(c1)OC)O)CO)/C=C/CO)O

MOL008717	0.9208	0.0792	0.8633	Capsici Fructus	NOS	6021	FALSE	n1(c2c(nc1)c(=O)[nH]cn2)C1OC(C(C1O)O)CO
MOL008719	0.8918	0.1082	0.6670	Capsici Fructus	IPA	3776	FALSE	C(C)(C)O
MOL008719	0.8918	0.1082	0.6670	Capsellae Herba	IPA	3776	FALSE	C(C)(C)O
MOL008721	0.8882	0.1118	0.8826	Capsici Fructus	Isobutenal	6562	FALSE	C(=C)(C=O)C
MOL008722	0.9064	0.0936	0.9636	Zanthoxyli Pericarpium	Butenone	6570	FALSE	C(=O)(C=C)C
MOL008722	0.9064	0.0936	0.9636	Capsici Fructus	Butenone	6570	FALSE	C(=O)(C=C)C
MOL008724	0.9400	0.0600	0.9740	Capsici Fructus	SPD	1102	FALSE	C(NCCCN)CCCN
MOL008725	0.8962	0.1038	0.8187	Capsici Fructus	DMF	6228	FALSE	N(C=O)(C)C
MOL008726	0.9170	0.0830	0.9675	Capsici Fructus	Neopentanol	6404	FALSE	C(CO)(C)(C)C
MOL008727	0.9342	0.0658	0.9792	Capsici Fructus	EHBN	41223	FALSE	N(CCCCO)(CC)N=O
MOL008728	0.8595	0.1405	0.7871	Capsici Fructus	NONIVAMIDE	2998	FALSE	O=C(NCc1cc(OC)c(O)cc1)CCCCCCCC
MOL008729	0.8612	0.1388	0.7908	Capsici Fructus	Nordihydrocapsacin	168836	FALSE	c1(c(ccc(c1)CNC(=O)CCCCCC(C)C)O)OC
MOL008730	0.8452	0.1548	0.7012	Capsici Fructus	Actinex	71398	FALSE	c1(ccc(cc1O)CC(C(Cc1ccc(c(c1)O)O)C)C)O
MOL008732	0.9287	0.0713	0.9561	Rose Rugosae Flos	LNK	8003	FALSE	C(CC)CC
MOL008732	0.9287	0.0713	0.9561	Capsici Fructus	LNK	8003	FALSE	C(CC)CC
MOL008733	0.9069	0.0931	0.9081	Capsici Fructus	Hexyl valerate	70694	FALSE	C(=O)(OCCCCCC)CCCC
MOL008734	0.9248	0.0752	0.9525	Capsici Fructus	PENTENE	8004	FALSE	C=CCCC
MOL008735	0.7174	0.2826	0.8572	Capsici Fructus	solanine	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC2C1C(C1N2CC(CC1)C)C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)OC1OC(C(C(C1O)O)O)CO)O)CO
MOL008736	0.3950	0.6050	0.6667	Capsici Fructus	solanine_qt	Not Available	FALSE	OC1CCC2(C(=CCC3C2CCC2(C3CC3C2C(C2N3CC(CC2)C)C)C)C1)C
MOL008737	0.7031	0.2969	0.8530	Capsici Fructus	solasonine	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC2C1C(C1(O2)NCC(CC1)C)C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)OC1OC(C(C(C1O)O)O)CO)O)CO
MOL008738	0.3243	0.6757	0.7531	Capsici Fructus	solasonine_qt	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC2C1C(C1(O2)NCC(CC1)C)C)C)O
MOL008738	0.3243	0.6757	0.7531	Lilii Bulbus	solasonine_qt	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC2C1C(C1(O2)NCC(CC1)C)C)C)O
MOL008739	0.8513	0.1487	0.7482	Capsici Fructus	Solavetivone	442399	FALSE	C1(=O)CC(C2(C(=C1)C)CC(CC2)C(=C)C)C
MOL008739	0.8513	0.1487	0.7482	Lycii Fructus	Solavetivone	442399	FALSE	C1(=O)CC(C2(C(=C1)C)CC(CC2)C(=C)C)C
MOL008740	0.6969	0.3031	0.6084	Capsici Fructus	tetradecyl oxirane	53470714	FALSE	C1(CO1)CCCCCCCCCCCCCC
MOL008741	0.9214	0.0786	0.9563	Capsici Fructus	3-Methylpent-2-ene	642661	FALSE	C/C=C(/CC)\C
MOL008742	0.7634	0.2366	0.6620	Capsici Fructus	(2R)-2-tridecyloxirane	11107067	FALSE	O1C(C1)CCCCCCCCCCCC
MOL008743	0.8554	0.1446	0.7924	Capsici Fructus	1-Tridecyne	117754	FALSE	C(CCCCCC#C)CCCCC

MOL008744	0.8839	0.1161	0.9667	Capsici Fructus	(3R)-2,2,3-trimethyloxirane	6999849	FALSE	C1(C(O1)C)(C)C
MOL008745	0.9464	0.0536	0.9001	Capsici Fructus	3-methoxy-4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybenzoic acid	14132337	FALSE	C1(C(C(C(OC1CO)Oc1c(cc(cc1)C(=O)O)OC)O)O)O
MOL008746	0.8785	0.1215	0.6733	Aauropi Folium	1-oxaspiro-[2,5]octane,5,5-dimethyl-4-(3-methyl-1,3-butadienyl	Not Available	FALSE	O1CC21C(C(CCC2)(C)C)/C=C/C(=C)C
MOL008747	0.4722	0.5278	0.7941	Aauropi Folium	RETINAL	638015	FALSE	C1(=C(CCCC1(C)C)C)/C=C/C(=C/C=C/C(=C/C=O)/C)/C
MOL008748	0.9520	0.0480	0.8988	Aauropi Folium	[(1R,2R)-2-methyl-2-(4-methylpent-3-enyl)cyclopropyl]methanol	10920919	FALSE	C1(C(C1)(CCC=C(C)C)C)CO
MOL008749	0.9220	0.0780	0.9001	Aauropi Folium	2-Methyl-4-(2,6,6-trimethylcyclohex-1-enyl)but-2-en-1-ol	5369482	FALSE	C(/C(=C/CC1=C(CCCC1(C)C)C)/C)O
MOL008753	0.7423	0.2577	0.7468	Verbenae Herb	2α,3β,23-trihydroxyurs-12-en-28-oic acid	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3C)C)C(=O)O)C)(CC2)C)(CC1O)C)(CO)C
MOL008754	0.9116	0.0884	0.7223	Verbenae Herb	cadinene	Not Available	FALSE	C1CC(C2C(C1C)C=CC(C2)C)C
MOL008755	0.8551	0.1449	0.8873	Verbenae Herb	diosmetin7-neohesperidoside	69964214	FALSE	c12c(c(=O)cc(o1)c1cc(c(cc1)OC)O)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL008756	0.9066	0.0934	0.8395	Verbenae Herb	hastatoside	Not Available	FALSE	O(C1OC=C(C2(O)C1C(CC2=O)C)C(=O)OC)C1OC(C(O)C(O)C1O)CO
MOL008757	0.9296	0.0704	0.8157	Verbenae Herb	hastatoside_qt	Not Available	FALSE	OC1OC=C(C2(O)C1C(CC2=O)C)C(=O)OC
MOL008758	0.9310	0.0690	0.8168	Verbenae Herb	3,4-Dihydroverbenalin	Not Available	FALSE	C12C(OCC(C1C(=O)CC2C)CC(=O)O)OC1C(C(C(C(O1)CO)O)O)O

MOL008759	0.9509	0.0491	0.8293	Verbenae Herb	3,4-Dihydroverbenalin_qt	Not Available	FALSE	C12C(OCC(C1C(=O)CC2C)CC(=O)O)O
MOL008760	0.7574	0.2426	0.9071	Verbenae Herb	3-Hydroxy-12-ursen-28-oic acid	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C)C(C)C4C3=CCC21)C)O
MOL008763	0.7613	0.2387	0.8412	Verbenae Herb	3α,24-dihydroxyolean-12-en-28-oicacid	53393622	FALSE	C12CC(C)(C)CCC1(CCC1(C)C2=CCC2C3(C)CCC(O)C(C)(CO)C3CCC12C)C(=O)O
MOL008764	0.8817	0.1183	0.7200	Gossampiniflos	(+)-8-Hydroxycalamenone	442519	FALSE	c12c(C(CCC1C)C(C)C)cc(cc2O)C
MOL008766	0.8738	0.1262	0.6848	Gossampiniflos	BHT-OH	146102	FALSE	C(C1=CC(C=C(C1=O)C(C)(C)C)(C)O)(C)(C)C
MOL008766	0.8738	0.1262	0.6848	Linderae Radix	BHT-OH	146102	FALSE	C(C1=CC(C=C(C1=O)C(C)(C)C)(C)O)(C)(C)C
MOL008767	0.9079	0.0921	0.7331	Ephedra Herba	2,6-Dimethylnaphthalene	11387	FALSE	c1c(ccc2cc(ccc12)C)C
MOL008767	0.9079	0.0921	0.7331	Gossampiniflos	2,6-Dimethylnaphthalene	11387	FALSE	c1c(ccc2cc(ccc12)C)C
MOL008768	0.9201	0.0799	0.7181	Gossampiniflos	2-ISOPROPYLNAPHTHALENE	16238	FALSE	c12c(ccc(c1)C(C)C)cccc2
MOL008769	0.9080	0.0920	0.8284	Gossampiniflos	1,2-benzothiazole	9225	FALSE	c12c(snc1)cccc2
MOL008770	0.9470	0.0530	0.8114	Gossampiniflos	()-Camphorquinone	641916	FALSE	C12(C(C(C(=O)C1=O)CC2)(C)C)C
MOL008771	0.9090	0.0910	0.9032	Gossampiniflos	Wine ether	31251	FALSE	C(=O)(CCCCCCCC)OCC
MOL008771	0.9090	0.0910	0.9032	Ranunculi Ternati Radix	Wine ether	31251	FALSE	C(=O)(CCCCCCCC)OCC
MOL008772	0.2571	0.7429	0.8185	Gossampiniflos	104086-74-0	3050416	FALSE	C1CC(C2C(C1)(C1C(CC2)(C(CC(=CC1)C=O)O)C=O)C)(C)C
MOL008774	0.9013	0.0987	0.6797	Gossampiniflos	2,3,5-Trimethylnaphthalene	16732	FALSE	c12c(cc(c(c2)C)C)cccc1C
MOL008775	0.8745	0.1255	0.7081	Gossampiniflos	(1S,4S,5S)-1-isopropyl-4,8-dimethyl-7-spiro[4.5]dec-8-enone	12480741	FALSE	C1(CCC(C21CC(=O)C(=CC2)C)C(C)C)C

MOL008776	0.8976	0.1024	0.8970	Gossampiniflos	aromadendrin-4'-methylether	Not Available	FALSE	c1(cc(c2c(c1)OC(C(C2=O)O)c1ccc(cc1)OC)O)O
MOL008777	0.9241	0.0759	0.9317	Gossampiniflos	Butylbenzene	7705	FALSE	c1(ccccc1)CCCC
MOL008777	0.9241	0.0759	0.9317	Thalluslaminariae	Butylbenzene	7705	FALSE	c1(ccccc1)CCCC
MOL008778	0.9082	0.0918	0.9068	Gossampiniflos	1-DECYNE	12997	FALSE	C(CCCC#C)CCCC
MOL008778	0.9082	0.0918	0.9068	Sterculiae Lychnophorae Semen	1-DECYNE	12997	FALSE	C(CCCC#C)CCCC
MOL008779	0.7767	0.2233	0.6892	Gossampiniflos	isocalamendiol	Not Available	FALSE	C1CC(C2C(C1CC(C)C)(CC(=C)CC2)O)(C)O
MOL008780	0.9156	0.0844	0.8604	Gossampiniflos	Isocoumarin	68108	FALSE	c1(=O)c2c(cco1)cccc2
MOL008780	0.9156	0.0844	0.8604	Citri Sarcodactylis Fructus	Isocoumarin	68108	FALSE	c1(=O)c2c(cco1)cccc2
MOL008781	0.2170	0.7830	0.6622	Thalictri Glandulosissimi Et	2'-northaliphylline	Not Available	FALSE	C1N(C2c3c(C1)cc(c(c3Oc1cc3c(cc1OC)C(NCC3)Cc1ccc(cc1)Oc1c(ccc(C2)c1)OC)O)OC)C
MOL008782	0.2210	0.7790	0.6989	Thalictri Glandulosissimi Et	2-northalmine	Not Available	FALSE	O1c2c3c(C(N(CC3)C)Cc3ccc(Oc4cc(CC5NCCc6c5cc1c(OC)c6)ccc4OC)cc3)cc(OC)c2O
MOL008783	0.2117	0.7883	0.7226	Thalictri Glandulosissimi Et	Thalmidine	Not Available	FALSE	O1c2c3C(N(CCc3cc(OC)c2OC)C)Cc2cc(Oc3ccc(CC4N(CCc5c4cc(OC)c1c5)C)cc3)c(OC)cc2
MOL008784	0.2137	0.7863	0.7245	Thalictri Glandulosissimi Et	O-methylthalmine	Not Available	FALSE	N1(CCc2c3C1Cc1ccc(cc1)Oc1cc(ccc1OC)CC1c4c(cc(c(Oc2c(c(c3)OC)OC)c4)OC)CCN1C)C
MOL008785	0.1758	0.8242	0.8658	Thalictri Glandulosissimi Et	Adiantifoline	167937	FALSE	O(c1c2c3C(N(CC2)C)Cc2c(c3c(OC)c1OC)cc(OC)c(Oc1c(CC3N(CCc4c3cc(OC)c(OC)c4)C)cc(OC)c(OC)c1)c2)C
MOL008786	0.6410	0.3590	0.8109	Thalictri Glandulosissimi Et	baicalidine	Not Available	FALSE	c1(cc2c(cc1OC)CC1c3c2c(c2c(c3CCN1C)OCO2)OC)OC
MOL008787	0.1596	0.8404	0.8546	Thalictri Glandulosissimi Et	5-O-demethylthalistyline	181902	FALSE	c12c(OCO1)c(c1c(c2)C(N(CC1)C)Cc1ccc(cc1)Oc1cc(ccc1OC)CC1c2c(CC[N+]1(C)C)c(c(c(c2)OC)OC)O)OC
MOL008789	0.2258	0.7742	0.7314	Thalictri Glandulosissimi Et	Hernandezine	Not Available	FALSE	O1c2c3C(N(CCc3c(OC)c(OC)c2OC)C)Cc2cc(Oc3ccc(CC4N(CCc5c4cc1c(OC)c5)C)cc3)c(OC)cc2
MOL008790	0.7703	0.2297	0.6273	Thalictri Glandulosissimi Et	Isolinoleic acid	5312483	FALSE	OC(=O)CCCC/C=C\C/C=C\CCCCCCCC
MOL008791	0.2072	0.7928	0.7337	Thalictri Glandulosissimi Et	isothalidezine	Not Available	FALSE	C1N(C2c3c(C1)c(c(c(c3Oc1c(cc3CCN(C(Cc4ccc(Oc5c(ccc(C2)c5)OC)cc4)c3c1)C)OC)OC)OC)O)C
MOL008792	0.6723	0.3277	0.8439	Thalictri Glandulosissimi Et	11-Hydroxynoracronycine	5378702	FALSE	c1(cccc2c1n(c1c(c2=O)c(cc2c1C=CC(O2)(C)C)O)C)O
MOL008794	0.0963	0.9037	0.9249	Thalictri Glandulosissimi Et	neothalibrine-2'-alpha-N-oxide	Not Available	FALSE	C1[N+](C(c2c(C1)cc(c(c2)OC)OC)Cc1ccc(cc1)Oc1cc(ccc1OC)CC1c2c(CCN1C)cc(c(c2)O)OC)(C)[O-]
MOL008795	0.2005	0.7995	0.7289	Thalictri Glandulosissimi Et	northalidasine	Not Available	FALSE	c1cc2ccc1Oc1cc(CC3c4c(Oc5c6CCN(C(C2)c6cc(c5OC)OC)C)c(c(cc4CCN3)OC)OC)ccc1OC

MOL008796	0.2213	0.7787	0.7085	Thalictri Glandulosissimi Et	5-hydroxythalmine	Not Available	FALSE	c1c2ccc(c1)CC1c3c(CCN1C)c(c(c(c3)OC)O)Oc1c(c(c3c(c1)C(N(CC3)C)Cc1cc(O2)c(cc1)OC)O)OC
MOL008797	0.6102	0.3898	0.7497	Thalictri Glandulosissimi Et	(R)-Reticuline	440586	FALSE	O(c1cc2c(C(N(CC2)C)Cc2cc(O)c(OC)cc2)cc1O)C
MOL008798	0.5003	0.4997	0.6188	Thalictri Glandulosissimi Et	tembetarine	167718	FALSE	O(c1cc2c(C([N+](CC2)(C)C)Cc2cc(O)c(OC)cc2)cc1O)C
MOL008799	0.6784	0.3216	0.7877	Thalictri Glandulosissimi Et	STOCK1N-08335	6352241	FALSE	c1(c(cc2c(c1)c1c3C(C2)NCCc3c(c(c1OC)OC)O)OC)OC
MOL008800	0.5838	0.4162	0.6976	Thalictri Glandulosissimi Et	thalbaicalidine	10384584	FALSE	O(c1c2c3C(N(CCc3c(O)c1OC)C)Cc1c2cc(OC)c(OC)c1)C
MOL008802	0.9107	0.0893	0.7651	Thalictri Glandulosissimi Et	4-methoxy-7-methyl-8,9-dihydro-[1,3]dioxolo[4,5-f]isoquinolin-6-one	14355975	FALSE	C1(=O)N(CCc2c3c(c(cc12)OC)OCO3)C
MOL008803	0.2099	0.7901	0.7013	Thalictri Glandulosissimi Et	thalfoetidine	Not Available	FALSE	O1c2c3c(C(N(CC3)C)Cc3ccc(Oc4cc(CC5N(CCc6c5cc1c(OC)c6OC)C)ccc4O)cc3)cc(OC)c2OC
MOL008804	0.1153	0.8847	0.8446	Thalictri Glandulosissimi Et	thalibulamine	13892261	FALSE	c1(c(cc(cc1)CC1N(CCc2cc(c(cc12)OC)OC)C)Oc1cc2c(c3c4c(CCN(C4C2)C)c(c(c3OC)OC)OC)cc1OC)O
MOL008805	0.7056	0.2944	0.7944	Thalictri Glandulosissimi Et	7-oxobaicaline	Not Available	FALSE	n1ccc2c3c(c4c(C(=O)c13)cc(c(c4)OC)OC)c(c1OCOc21)OC
MOL008806	0.1768	0.8232	0.8698	Thalictri Glandulosissimi Et	TBL	21470	TRUE	O(c1c2c3C(N(CCc3cc1OC)C)Cc1c2cc(OC)c(Oc2c(CC3N(CCc4c3cc(OC)c(OC)c4)C)cc(OC)c(OC)c2)c1)C
MOL008807	0.2314	0.7686	0.6761	Thalictri Glandulosissimi Et	NSC-93674	Not Available	FALSE	O1c2c3C(N(CCc3cc(OC)c2O)C)Cc2ccc(Oc3cc(CC4N(CCc5c4cc1c(OC)c5)C)ccc3O)cc2
MOL008808	0.3801	0.6199	0.6844	Thalictri Glandulosissimi Et	thalicsimidine	Not Available	FALSE	O(c1c2c3C(N(CC2)C)Cc2c(c3c(OC)c1OC)cc(OC)c(OC)c2)C
MOL008809	0.2099	0.7901	0.6990	Thalictri Glandulosissimi Et	58092-24-3	Not Available	FALSE	O1c2c3c(C(N(CC3)C)Cc3ccc(Oc4cc(CC5N(CCc6c5cc1c(OC)c6)C)ccc4O)cc3)cc(OC)c2OC
MOL008810	0.2151	0.7849	0.7275	Thalictri Glandulosissimi Et	Thalidasin	Not Available	FALSE	O1c2c3C(N(CCc3cc(OC)c2OC)C)Cc2cc(Oc3ccc(CC4N(CCc5c4cc(OC)c(OC)c15)C)cc3)c(OC)cc2
MOL008811	0.7906	0.2094	0.7255	Thalictri Glandulosissimi Et	thalidastine	Not Available	FALSE	c12c(OCO1)cc1c(c2)C(C[n+]2c1cc1c(c2)c(c(cc1)O)OC)O
MOL008812	0.1171	0.8829	0.8424	Thalictri Glandulosissimi Et	thalidezine	10101101	FALSE	C1(N(CCc2cc(c(cc12)OC)O)C)Cc1ccc(cc1)Oc1c2c(c3c4c(CCN(C4C2)C)c(c(c3OC)OC)OC)cc(c1OC)OC
MOL008813	0.1846	0.8154	0.8680	Thalictri Glandulosissimi Et	Thalifaberine	159246	FALSE	O(c1c2c3C(N(CC2)C)Cc2c(c3c(OC)c1OC)cc(OC)c(OC)c2Oc1ccc(CC2N(CCc3c2cc(OC)c(OC)c3)C)cc1)C
MOL008814	0.1130	0.8870	0.8517	Thalictri Glandulosissimi Et	thalifaramine	10100789	FALSE	C1(N(CCc2cc(c(cc12)O)OC)C)Cc1ccc(cc1)Oc1c2c(c3c4c(CCN(C4C2)C)cc(c3OC)OC)cc(c1OC)OC

MOL008815	0.5090	0.4910	0.8195	Thalictri Glandulosissimi Et	N,O,O-trimethylsparsiflorine	Not Available	FALSE	c1c(ccc2c1c1c3C(C2)N(C=Cc3cc(c1OC)OC)C)OC
MOL008817	0.1466	0.8534	0.7929	Thalictri Glandulosissimi Et	thalifaricine	10484580	FALSE	N1(CCc2c3c(c4c(CC13)c(c(c(c4)OC)O)Oc1ccc(cc1)CC1N(CCc3cc(c(cc13)O)OC)C)c(c(c2OC)OC)OC)C
MOL008818	0.1182	0.8818	0.8566	Thalictri Glandulosissimi Et	thalifaroline	13892259	FALSE	N1(CCc2c3c(c4c(CC13)c(c(c(c4)OC)OC)Oc1ccc(cc1)CC1N(CCc3cc(c(cc13)OC)OC)C)c(c(c2O)OC)OC)C
MOL008819	0.1338	0.8662	0.8705	Thalictri Glandulosissimi Et	thalifaronine	10055201	FALSE	N1(CCc2c3c(c4c(CC13)c(c(c(c4)OC)OC)Oc1ccc(cc1)CC1N(CCc3cc(c(cc13)OC)OC)C)c(c(c2)OC)OC)C
MOL008820	0.2084	0.7916	0.7352	Thalictri Glandulosissimi Et	Thalisopine	Not Available	FALSE	O1c2c3C(N(CCc3c(O)c(OC)c2OC)C)Cc2ccc(Oc3cc(CC4N(CCc5c4cc1c(OC)c5)C)ccc3OC)cc2
MOL008821	0.1565	0.8435	0.8596	Thalictri Glandulosissimi Et	thalilutine	21763780	FALSE	N1(CCc2c(c(c(c3c2C1CC1c3cc(c(c1)OC1c(cc(c(c1)OC)OC)CC1N(CCc2c1cc(c(c2)OC)OC)C)OC)OC)OC)OC
MOL008823	0.1866	0.8134	0.8525	Thalictri Glandulosissimi Et	thalmelatidine	56842063	FALSE	O(c1c2c3C(N(CC2)C)CC2(c3c(OC)c1OC)cc(OC)c(Oc1c(CC3N(CCc4c3cc(OC)c3OCOc43)C)cc(OC)c(OC)c1)c2)C
MOL008825	0.1799	0.8201	0.8601	Thalictri Glandulosissimi Et	N-demethylthalistyline	Not Available	FALSE	O1c2cc3C(N(CCc3c(OC)c2OC1)C)Cc1ccc(Oc2cc(CC3N(CCc4c3cc(OC)c(OC)c4OC)C)ccc2OC)cc1
MOL008826	0.1736	0.8264	0.6940	Thalictri Glandulosissimi Et	105437-18-1	Not Available	FALSE	O1c2cc3C(N(CCc3c(O)c2OC)C)Cc2cc(Oc3ccc(CC4=NCCc5c1c(OC)c(OC)cc45)cc3)c(OC)cc2
MOL008827	0.2121	0.7879	0.6889	Thalictri Glandulosissimi Et	STOCK1N-06254	Not Available	FALSE	O1c2c3c(C(N(CC3)C)Cc3ccc(Oc4cc(CC5N(CCc6c5cc1c(OC)c6)C)ccc4OC)cc3)cc(OC)c2O
MOL008828	0.1281	0.8719	0.8656	Thalictri Glandulosissimi Et	thalmineline	Not Available	FALSE	C1(N(CCc2c(c(cc12)OC)OC)O)CC1c(cc(c(c1)OC)OC)Oc1cc2c(c3c4c(CCN(C4C2)C)c(c(c3OC)OC)OC)cc1OC
MOL008829	0.2263	0.7737	0.7322	Thalictri Glandulosissimi Et	thalrugosamine	Not Available	FALSE	O1c2c3C(N(CCc3c(OC)c(OC)c2OC)C)Cc2ccc(Oc3cc(CC4N(CCc5c4cc1c(OC)c5)C)ccc3OC)cc2
MOL008830	0.2141	0.7859	0.6990	Thalictri Glandulosissimi Et	Thalrugosidine	Not Available	FALSE	O1c2c3C(N(CCc3cc(OC)c2O)C)Cc2cc(Oc3ccc(CC4N(CCc5c4cc(OC)c(OC)c15)C)cc3)c(OC)cc2
MOL008831	0.1590	0.8410	0.6919	Thalictri Glandulosissimi Et	73609-02-6	Not Available	FALSE	c12ccc(cc1)Oc1cc(ccc1OC)CC1c3c(CCN1C=O)cc(c(c3Oc1c3CCN(C(C2)c3cc(c1OC)OC)C)OC)OC
MOL008833	0.4949	0.5051	0.6129	Thalictri Glandulosissimi Et	xanthoplanine	14262868	FALSE	O(c1c2c3C([N+](CCc3cc1OC)(C)C)Cc1c2cc(OC)c(O)c1)C
MOL008836	0.5759	0.4241	0.6306	Bovis Calculus	N-(3alpha,12alpha-dihydroxy-5beta-cholan-24-oyl)glycine	3035026	FALSE	OC1C2(C(C3C(C4(C(CC3)CC(O)CC4)C)C1)CCC2C(CCC(=O)NCC(=O)O)C)C

MOL008837	0.6960	0.3040	0.6808	Bovis Calculus	(2S)-2-[(2S,3S)-4-[3-[(1R)-1-(3,4-dihydroxybenzyl)-2-hydroxy-2-keto-ethoxy]-3-keto-propyl]-2-(3,4-dihydroxyphenyl)-7-hydroxy-2,3-dihydrobenzofuran-3-carbonyl]oxy-3-(3,4-dihydroxyphenyl)propionic acid	5319055	FALSE	c1(c(cc(cc1)C1Oc2c(C1C(=O)OC(Cc1cc(c(cc1)O)O)C(=O)O)c(ccc2O)CCC(=O)OC(Cc1ccc(c(c1)O)O)C(=O)O)O)O
MOL008838	0.2755	0.7245	0.6658	Bovis Calculus	methyl (4R)-4-[(3R,5S,7S,8R,9S,10S,12S,13R,14S,17R)-3,7,12-trihydroxy-10,13-dimethyl-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl]pentanoate	10477353	FALSE	OC1C2(C(C3C(C4(C(CC3O)CC(O)CC4)C)C1)CCC2C(CCC(=O)OC)C)C
MOL008839	0.2209	0.7791	0.6041	Bovis Calculus	Methyl desoxycholate	Not Available	FALSE	OC1C2(C(C3C(C4(C(CC3)CC(O)CC4)C)C1)CCC2C(CCC(=O)OC)C)C
MOL008842	0.5403	0.4597	0.7892	Bovis Calculus	chenodeoxycholic acid	10133	FALSE	OC1C2C3C(C(CC3)C(CCC(=O)O)C)(CCC2C2(C(C1)CC(O)CC2)C)C
MOL008843	0.9255	0.0745	0.7430	Bovis Calculus	Cherianoine	5315819	FALSE	COc1c(O)c(c2c(c1)ccn(c2=O)C)OC

MOL008844	0.2155	0.7845	0.7002	Bovis Calculus	methyl (4R)-4-[(3R,5S,7R,8R,9S,10S,13R,14S,17R)-3,7-dihydroxy-10,13-dimethyl-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl]pentanoate	11069533	FALSE	OC1C2C3C(C(CC3)C(CCC(=O)OC)C)(CCC2C2(C(C1)CC(O)CC2)C)C
MOL008845	0.5299	0.4701	0.6085	Bovis Calculus	Deoxycholic Acid	Not Available	FALSE	OC1C2(C(C3C(C4(C(CC3)CC(O)CC4)C)C1)CCC2C(CCC(=O)O)C)C
MOL008846	0.3257	0.6743	0.9600	Bovis Calculus	ZINC01280365	1403454	FALSE	C1C(=O)C=C2C(C1)(C1C(CC2)C2C(CC1)(C(CC2)C(=O)CO)C)C
MOL008847	0.1987	0.8013	0.8985	Lasiosphaera Seu Calvatia	Isoergotamine	Not Available	FALSE	c12c3CC4C(=CC(CN4C)C(=O)NC4(C(=O)N5C(O4)(C4CCCN4C(=O)C5Cc4ccccc4)O)C)c1cccc2[nH]c3
MOL008847	0.1987	0.8013	0.8985	Corayceps	Isoergotamine	Not Available	FALSE	c12c3CC4C(=CC(CN4C)C(=O)NC4(C(=O)N5C(O4)(C4CCCN4C(=O)C5Cc4ccccc4)O)C)c1cccc2[nH]c3
MOL008847	0.1987	0.8013	0.8985	Bovis Calculus	Isoergotamine	Not Available	FALSE	c12c3CC4C(=CC(CN4C)C(=O)NC4(C(=O)N5C(O4)(C4CCCN4C(=O)C5Cc4ccccc4)O)C)c1cccc2[nH]c3
MOL008848	0.6511	0.3489	0.7149	Bovis Calculus	GCH	10140	FALSE	OC1C2(C(C3C(C4(C(CC3O)CC(O)CC4)C)C1)CCC2C(CCC(=O)NCC(=O)O)C)C
MOL008848	0.6511	0.3489	0.7149	Sojae Semen Nigrum	GCH	10140	FALSE	OC1C2(C(C3C(C4(C(CC3O)CC(O)CC4)C)C1)CCC2C(CCC(=O)NCC(=O)O)C)C
MOL008849	0.4510	0.5490	0.6146	Cistanches Herba	(+)-pinoresinol-O-β-D-glucopyranoside	Not Available	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(OC2OC(C(O)C(O)C2O)CO)cc1
MOL008850	0.9290	0.0710	0.9539	Cistanches Herba	m-Anisidine	10824	FALSE	O(c1cc(N)ccc1)C
MOL008851	0.9362	0.0638	0.9186	NA	(4R,5S)-4,5-diethyl-1,2-dimethylcyclohexene	22216712	FALSE	C1(=C(CC(C(C1)CC)CC)C)C

MOL008852	0.5825	0.4175	0.7447	Cistanches Herba	(1R,4aR,4bR,10aS)-7-isopropyl-1,4a-dimethyl-2,3,4,4b,5,6,10,10a-octahydrophenanthrene-1-carboxylic acid	7067292	FALSE	C(=O)(C1(C)C2C(C3CCC(=CC3=CC2)C(C)C)(CCC1)C)O
MOL008853	0.9560	0.0440	0.9186	Cistanches Herba	(1S,4S,7R)-7-bicyclo[2.2.2]oct-2-enol	21675470	FALSE	C1C2C=CC(C1O)CC2
MOL008854	0.2777	0.7223	0.6107	NA	bis[(2R)-2-ethylhexyl] benzene-1,2-dicarboxylate	7057919	FALSE	c1(ccccc1C(=O)OCC(CC)CCCC)C(=O)OCC(CC)CCCC
MOL008855	0.9241	0.0759	0.7468	Cistanches Herba	Cistanin	Not Available	FALSE	O1Cc2c3c(ccoc13)cc2
MOL008856	0.6129	0.3871	0.7180	Cistanches Herba	Cistanoside A	Not Available	FALSE	C1(C(C(C(C(O1)OCCc1cc(c(cc1)OC)O)O)OC1OC(C(C(C1O)O)O)C)OC(=O)/C=C/c1cc(c(cc1)O)O)COC1OC(C(C(C1O)O)O)CO
MOL008857	0.6679	0.3321	0.6943	Cistanches Herba	Cistanoside A_qt	Not Available	FALSE	C1(C(C(C(C(O1)OCCc1cc(c(cc1)OC)O)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)CO
MOL008858	0.6620	0.3380	0.7018	Cistanches Herba	.beta.-D-Glucopyranoside, 2-(4-hydroxy-3-methoxyphenyl)ethyl 3-O-(6-deoxy-.alpha.-L-mannopyranosyl)-4-O-[(2E)-3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]-	5315929	FALSE	C1(C(C(C(C(O1)OCCc1ccc(c(c1)OC)O)O)OC1OC(C(C(C1O)O)O)C)OC(=O)/C=C/c1cc(c(cc1)O)O)CO
MOL008859	0.8888	0.1112	0.7564	Cistanches Herba	Cistanoside E	Not Available	FALSE	C1(C(C(C(C(O1)OCCc1ccc(c(c1)OC)O)O)OC1CC(C(C(C1O)O)O)O)O)CO
MOL008860	0.9345	0.0655	0.8526	Cistanches Herba	Cistanoside E_qt	Not Available	FALSE	C1(C(C(C(C(O1)OCCc1ccc(c(c1)OC)O)O)O)O)CO

MOL008861	0.8841	0.1159	0.7485	Cistanches Herba	Cistanoside F	Not Available	FALSE	C1(C(C(C(C(O1)O)O)OC1OC(C(C(C1O)O)O)C)OC(=O)CCc1ccc(c(c1)O)O)CO
MOL008862	0.8911	0.1089	0.7492	Cistanches Herba	Cistanoside H	Not Available	FALSE	C1(C(C(C(C(O1)OCCc1cc(c(cc1)O)O)OC(=O)C)OC1CC(C(C(C1O)O)O)O)O)CO
MOL008863	0.9541	0.0459	0.9537	Cistanches Herba	1-Methyl-4-isoallyl-cyclohexane	Not Available	FALSE	C1(CCC(CC1)/C=C/C)C
MOL008864	0.9408	0.0592	0.8488	Cistanches Herba	[(7S,8R)-7-hydroxy-5,6,7,8-tetrahydro-3H-pyrrolizin-1-yl]methyl (2R)-2-hydroxy-2-(1-hydroxyethyl)-3-methylbutanoate	6546284	FALSE	C12C(CCN1CC=C2COC(=O)C(C(C)O)(O)C(C)C)O
MOL008865	0.5718	0.4282	0.7544	Cistanches Herba	Epimedin A	11972345	FALSE	c1(ccc2c(c1CC=C(C)C)oc(c(c2=O)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO)c1ccc(cc1)OC)OC1OC(C(C(C1O)O)O)CO
MOL008867	0.9318	0.0682	0.8690	Cistanches Herba	Leonuride(ajugol)	Not Available	FALSE	C1(CC(C2C1C=COC2OC1C(C(C(C(O1)CO)O)O)O)(O)C)O
MOL008868	0.9456	0.0544	0.8249	Cistanches Herba	Leonuride(ajugol)_qt	Not Available	FALSE	C1(CC(C2C1C=COC2O)(O)C)O
MOL008869	0.9293	0.0707	0.9553	Cistanches Herba	methyl 2-dimethylaminoacetate	81569	FALSE	CN(CC(=O)OC)C

MOL008870	0.6614	0.3386	0.6984	Cistanches Herba	[(2R,3R,4S,5R,6R)-5-acetyloxy-6-[2-(3,4-dihydroxyphenyl)ethoxy]-2-(hydroxymethyl)-4-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-3-yl] (E)-3-(3,4-dihydroxyphenyl)prop-2-enoate	21629996	FALSE	c1(c(ccc(c1)/C=C/C(=O)OC1C(C(C(OC1CO)OCCc1cc(c(cc1)O)O)OC(=O)C)OC1OC(C(C(C1O)O)O)C)O)O
MOL008871	0.1219	0.8781	0.7546	Cistanches Herba	Marckine	72341	FALSE	C1c2c(C3N(C1)CC(C(C3)CC1NCCc3c1[nH]c1c3cc(cc1)O)CC)cc(c(c2)OC)OC
MOL008872	0.5576	0.4424	0.7065	Cistanches Herba	cistanoside B	Not Available	FALSE	O(C1C(OC(=O)/C=C\c2cc(OC)c(O)cc2)C(OC(OCCc2cc(OC)c(O)cc2)C1O)COC1OC(C(O)C(O)C1O)CO)C1OC(C(O)C(O)C1O)C
MOL008873	0.5425	0.4575	0.6605	Cistanches Herba	cistanoside B_qt	Not Available	FALSE	O(C1C(OC(=O)/C=C/c2cc(OC)c(O)cc2)C(OC(OCCc2cc(OC)c(O)cc2)C1O)CO)C1OC(C(O)C(O)C1O)C
MOL008874	0.8570	0.1430	0.8288	Cistanches Herba	Ethyl disulfide	8077	FALSE	S(SCC)CC
MOL008875	0.7264	0.2736	0.7281	Cistanches Herba	echinacoside	Not Available	FALSE	O(C1C(OC(=O)/C=C\c2cc(O)c(O)cc2)C(OC(OCCc2cc(O)c(O)cc2)C1O)COC1OC(C(O)C(O)C1O)CO)C1OC(C(O)C(O)C1O)C
MOL008876	0.7807	0.2193	0.7349	Cistanches Herba	echinacoside_qt	Not Available	FALSE	O(C1C(OC(=O)/C=C/c2cc(O)c(O)cc2)C(OC(OCCc2cc(O)c(O)cc2)C1O)CO)C1OC(C(O)C(O)C1O)C
MOL008877	0.9197	0.0803	0.9261	Cistanches Herba	2,3-Dimethylheptane	24884356	FALSE	CC(C(CCCC)C)C
MOL008878	0.9076	0.0924	0.7888	Cistanches Herba	n-Decyl glucoside	62142	FALSE	O(CCCCCCCCCC)C1C(C(C(C(O1)CO)O)O)O
MOL008879	0.9155	0.0845	0.9599	Typhonii Rhizoma	SBU	7843	FALSE	CCCC
MOL008879	0.9155	0.0845	0.9599	Ginkgo Folium	SBU	7843	FALSE	CCCC
MOL008879	0.9155	0.0845	0.9599	Cistanches Herba	SBU	7843	FALSE	CCCC
MOL008879	0.9155	0.0845	0.9599	Ginkgo Semen	SBU	7843	FALSE	CCCC

MOL008880	0.8633	0.1367	0.7507	Cistanches Herba	2,6-diisobutyl-4-methylphenol	5315473	FALSE	c1(cc(cc(c1O)CC(C)C)C)CC(C)C
MOL008881	0.9478	0.0522	0.9384	Cistanches Herba	3,4,5,5-Tetramethyl-2-cyclopenten-1-one	Not Available	FALSE	C1(=O)C=C(C(C1(C)C)C)C
MOL008882	0.9574	0.0426	0.8588	Cistanches Herba	3,4-Dioxymethulene-5methoxy-1-(1-oxopropyl) benzene	Not Available	FALSE	c1c(c2c(cc1C(=O)CC)COO2)OC
MOL008883	0.8834	0.1166	0.8485	Salviae Chinensis Herba	Dehydrovomifoliol	688492	FALSE	C1(C(=CC(=O)CC1(C)C)C)(/C=C/C(=O)C)O
MOL008884	0.7805	0.2195	0.6952	Salviae Chinensis Herba	lithospermic acid	Not Available	FALSE	c12C(C(Oc1c(ccc2/C=C/C(=O)OC(Cc1cc(c(cc1)O)O)C(=O)O)O)c1cc(c(cc1)O)O)C(=O)O
MOL008885	0.6979	0.3021	0.6748	Salviae Chinensis Herba	(2R)-2-[(2R,3R)-4-[(E)-3-[(1R)-1-(3,4-dihydroxybenzyl)-2-hydroxy-2-keto-ethoxy]-3-keto-prop-1-enyl]-2-(3,4-dihydroxyphenyl)-7-hydroxy-2,3-dihydrobenzofuran-3-carbonyl]oxy-3-(3,4-dihydroxyphenyl)propionic acid	11629084	FALSE	C1(C(Oc2c1c(/C=C/C(=O)OC(C(=O)O)Cc1cc(c(cc1)O)O)ccc2O)c1cc(c(cc1)O)O)C(=O)OC(C(=O)O)Cc1cc(c(cc1)O)O
MOL008886	0.9509	0.0491	0.9700	Crataegi Folium	2-Methoxyphenethylamine	74896	FALSE	c1(c(cccc1)OC)CCN

MOL008887	0.9396	0.0604	0.9437	Crataegi Folium	(1S)-1-phenylethanamine	75818	FALSE	c1(ccccc1)C(C)N
MOL008888	0.8646	0.1354	0.8226	Crataegi Folium	Vitexin-2-O-rhamnoside	Not Available	FALSE	c12c(C3C(OC4C(C(C(C(O4)C)O)O)O)C(C(C(O3)CO)O)O)c(cc(c1c(=O)cc(o2)c1ccc(cc1)O)O)O
MOL008889	0.8571	0.1429	0.8397	Crataegi Folium	5,7-dihydroxy-2-(4-hydroxyphenyl)-8-[(2R,3R,4R,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]chromone	9910645	FALSE	c12c(C3C(O)C(C(C(O3)CO)O)O)c(cc(c1c(=O)cc(o2)c1ccc(cc1)O)O)O
MOL008889	0.8571	0.1429	0.8397	Viticis Cannabifoliae Fructus	5,7-dihydroxy-2-(4-hydroxyphenyl)-8-[(2R,3R,4R,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]chromone	9910645	FALSE	c12c(C3C(O)C(C(C(O3)CO)O)O)c(cc(c1c(=O)cc(o2)c1ccc(cc1)O)O)O
MOL008890	0.9273	0.0727	0.9650	Crataegi Folium	DIETHYLAMINE	8021	FALSE	N(CC)CC
MOL008891	0.8594	0.1406	0.6694	Crataegi Folium	NEH	6341	FALSE	C(C)N
MOL008892	0.9136	0.0864	0.9658	Crataegi Folium	Valamine	6558	FALSE	C(CN)(C)C
MOL008893	0.5072	0.4928	0.7626	Pseudolaricis Cortex	pseudolarifuroic	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=CCC3(C(C1=CC2)(CCC3C(Cc1occ(c1)C(=O)O)C)C)C)(C)C
MOL008894	0.3986	0.6014	0.7449	Pseudolaricis Cortex	pseudolarolide A	Not Available	FALSE	O1C2C(C3(C(C4C5(C6(C5)C(CC4)C(C(=O)CC6)(C)C)CC3)(C2)C)C)C(CC21OC(=O)C(C2)C)C
MOL008895	0.9325	0.0675	0.8437	Pseudolaricis Cortex	pseudolaroside C	15139313	FALSE	c1(ccc(cc1)C(=O)OC)OC1OC(C(C(C1O)O)O)O)CO

MOL008896	0.9296	0.0704	0.7948	Pseudolaricis Cortex	(2R,3R,4S,5R,6S)-3-isopropyl-2-methylol-6-(phenoxy)-5-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]oxy-tetrahydropyran-3,4,5-triol	179289	FALSE	O1C(C(O)(C(O)C(OC2OC(C(O)C(O)C2O)CO)(O)C1Oc1ccccc1)C(C)C)CO
MOL008897	0.9271	0.0729	0.8283	Pseudolaricis Cortex	Coleoside B_qt	Not Available	FALSE	O1C(C(O)(C(O)C(O)(O)C1Oc1ccccc1)C(C)C)CO
MOL008898	0.9341	0.0659	0.9685	Pseudolaricis Cortex	methyl (3S,4S,5R)-3,4,5-trihydroxycyclohexene-1-carboxylate	10867095	FALSE	C(=O)(C1=CC(O)C(O)C(O)C1)OC
MOL008899	0.6206	0.3794	0.6578	Pseudolaricis Cortex	Pseudolaric acid A	Not Available	FALSE	O1C(C2C3(OC(=O)C)C(CC2)(CC=C(CC3)C)C1=O)(C)/C=C/C=C(\C)/C(=O)O
MOL008900	0.6523	0.3477	0.6275	Pseudolaricis Cortex	Pseudolaric acid B	Not Available	FALSE	O1C(C2C3(OC(=O)C)C(CC2)(CC=C(CC3)C(=O)OC)C1=O)(C)/C=C/C=C(\C)/C(=O)O
MOL008901	0.7067	0.2933	0.6701	Pseudolaricis Cortex	Pseudolaric acid C	Not Available	FALSE	O1C(C2C3(O)C(CC2)(CC=C(CC3)C(=O)OC)C1=O)(C)/C=C/C=C(/C)\C(=O)O
MOL008903	0.9341	0.0659	0.8962	Vaccariae Semen	1-[(2S,3S,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]pyrimidine-2,4-dione	6604651	FALSE	c1(=O)[nH]c(=O)ccn1C1OC(C(C1O)O)CO
MOL008904	0.8713	0.1287	0.7697	Vaccariae Semen	9H-xanthene-2-carboxylic acid	12439784	FALSE	C1c2cc(ccc2Oc2ccccc12)C(=O)O
MOL008905	0.8852	0.1148	0.7691	Vaccariae Semen	beta-Vicianosyl-3-quercetin	Not Available	FALSE	C1C(C(C(C(O1)OCC1C(C(C(C(O1)Oc1c(c2ccc(c(c2)O)O)oc2c(c1=O)c(cc(c2)O)O)O)O)O)O)O)O
MOL008906	0.7261	0.2739	0.6042	Ginkgo Folium	Hydroginkgolinic acid	5318118	FALSE	c1(cccc(c1C(=O)O)CCCCCCCCCCCCCC)O

MOL008906	0.7261	0.2739	0.6042	Mume Fructus	Hydroginkgolinic acid	5318118	FALSE	c1(cccc(c1C(=O)O)CCCCCCCCCCCCCC)O
MOL008906	0.7261	0.2739	0.6042	Vaccariae Semen	Hydroginkgolinic acid	5318118	FALSE	c1(cccc(c1C(=O)O)CCCCCCCCCCCCCC)O
MOL008907	0.5143	0.4857	0.6570	Vaccariae Semen	segetalin A	Not Available	FALSE	O=C1N2C(CCC2)C(=O)NC(C(C)C)C(=O)NC(Cc2c3c([nH]c2)cccc3)C(=O)NC(C(=O)NCC(=O)NC1C(C)C)C
MOL008909	0.5146	0.4854	0.7662	Vaccariae Semen	(3R,6R,9R,12S,15R,21S)-3,9-bis(benzyl)-15-isobutyl-6-methyl-12-methylol-1,4,7,10,13,16,19-heptazabicyclo[19.3.0]tetracosane-2,5,8,11,14,17,20-heptone	21458012	FALSE	N12CCCC1C(=O)NCC(=O)NC(C(=O)NC(C(=O)NC(C(=O)NC(C(=O)NC(C2=O)Cc1ccccc1)C)Cc1ccccc1)CO)CC(C)C
MOL008910	0.8792	0.1208	0.7900	Vaccariae Semen	vaccarin	Not Available	FALSE	O1C(C(OC2OCC(O)C(O)C2O)C(O)C(O)C1CO)c1c(O)c2c(oc(cc2=O)c2ccc(OC3OC(C(O)C(O)C3O)CO)cc2)cc1O
MOL008911	0.8621	0.1379	0.8440	Vaccariae Semen	vaccarin_qt	51340236	FALSE	Oc1c(c(O)cc2oc(cc(=O)c12)c1ccc(O)cc1)C1OC(C(O)C(O)C1O)CO
MOL008913	0.1714	0.8286	0.8000	Vaccariae Semen	Meldenin	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(C(C2OC(=O)C)O)C2=CCC(C2(CC1)C)c1cocc1)C)(C)C
MOL008915	0.7932	0.2068	0.8318	Chrysanthemi Indici Flos	acacetin-7-O-β-D-galactopyranoside	Not Available	FALSE	c1(cc(=O)c2c(c(c(cc2o1)O)C1C(C(C(C(O1)CO)O)O)O)O)c1ccc(cc1)OC
MOL008916	0.4745	0.5255	0.7044	Chrysanthemi Indici Flos	angeloylajadin	Not Available	FALSE	C12C(=C(C(C3C1OC(=O)C3=C)OC(=O)/C(=C\C)/C)C)CC1C2(O1)C
MOL008917	0.5387	0.4613	0.6690	Chrysanthemi Indici Flos	angeloylcumambrin B	Not Available	FALSE	C12=C(C(C3C(C1C1(C(C2)O1)C)OC(=O)C3=C)OC(=O)/C(=C(\C)/O)/C)C
MOL008918	0.6313	0.3687	0.7365	Chrysanthemi Indici Flos	Arteglasin A	Not Available	FALSE	O1C2(C3C(=C(CC(OC(=O)C)C4C3OC(=O)C4=C)C)CC12)C
MOL008920	0.9317	0.0683	0.7743	Chrysanthemi Indici Flos	[(1S,3S)-2,2-dimethyl-3-(2-methylprop-1-enyl)cyclopropyl]methanol	6993677	FALSE	C(O)C1C(C1C=C(C)C)(C)C

MOL008921	0.9554	0.0446	0.8050	Chrysanthemi Flos	(1R,5S)-4,7,7-trimethylbicyclo[3.1.1]hept-3-en-6-one	11789373	FALSE	C12C(=CCC(C1=O)C2(C)C)C
MOL008921	0.9554	0.0446	0.8050	Chrysanthemi Indici Flos	(1R,5S)-4,7,7-trimethylbicyclo[3.1.1]hept-3-en-6-one	11789373	FALSE	C12C(=CCC(C1=O)C2(C)C)C
MOL008922	0.8914	0.1086	0.8394	Chrysanthemi Indici Flos	chrysanthetriol	Not Available	FALSE	OC(C1CC(O)C(=C)CCC(O)C(=C)CC1)(C)C
MOL008923	0.8583	0.1417	0.7980	Chrysanthemi Indici Flos	3-Methylanthralin	10288	FALSE	c1ccc2c(c1O)c(c1c(c2)cc(cc1O)C)O
MOL008924	0.6381	0.3619	0.7076	Chrysanthemi Indici Flos	Azuleno(4,5-b)furan-2(3H)-one, 4-(acetyloxy)-3a,4,5,6,6a,7,9a,9b-octahydro-6-hydroxy-6,9-dimethyl-3-methylene-, (3aR-(3aalpha,4alpha,6alpha,6aalpha,9aalpha,9bbeta))-	174867	FALSE	O1C2C3C(C(O)(CC(OC(=O)C)C2C(=C)C1=O)C)CC=C3C
MOL008925	0.8966	0.1034	0.8003	Chrysanthemi Indici Flos	(3aR,4S,6R,6aR,9aR,9bR)-4,6-dihydroxy-6,9-dimethyl-3-methylene-4,5,6a,7,9a,9b-hexahydro-3aH-azuleno[5,4-d]furan-2-one	9992975	FALSE	O1C2C3C(C(O)(CC(O)C2C(=C)C1=O)C)CC=C3C
MOL008928	0.4289	0.5711	0.7500	Chrysanthemi Indici Flos	handelin chrysanthelide	Not Available	FALSE	O1C2C(C3(C4(C5C(C3)(C(O)(CCC3C5OC(=O)C3=C)C)C=C4)C)C1=O)CC(OC(=O)C)C(O)(C1C2C(=CC1)C)C
MOL008929	0.9213	0.0787	0.8832	Chrysanthemi Indici Flos	indicumenone	46173956	FALSE	OC(C1CC(=O)C(=CC1)C)(C/C=C/C(O)(C)C)C

MOL008931	0.2692	0.7308	0.6384	Schisandrae Chinensis Fructus	Gomisin T	Not Available	FALSE	c12CC(C(Cc3c(c1c(c(c(c2)OC)OC)OC)c(c(c(c3)O)OC)OC)C)C
MOL008932	0.4532	0.5468	0.7915	Schisandrae Chinensis Fructus	(-)-Gomisin L1	Not Available	FALSE	c12CC(C(Cc3c(c1c(c1c(c2)OCO1)OC)c(c(c(c3)OC)OC)O)C)C
MOL008933	0.7803	0.2197	0.7040	Schisandrae Chinensis Fructus	beta-Sesquiphellandrene	Not Available	FALSE	C(=C(C)C)CC(C)C(C1C=CC(=C)CC1)C
MOL008934	0.4512	0.5488	0.7262	Schisandrae Chinensis Fructus	(-)-Gomisin L2	Not Available	FALSE	c12CC(C(Cc3c(c1c(c1c(c2)OCO1)OC)c(c(c(c3)O)OC)OC)C)C
MOL008935	0.9221	0.0779	0.8668	Schisandrae Chinensis Fructus	thymoquinol 2-glucoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1CO)Oc1cc(c(cc1C(C)C)O)C
MOL008936	0.9663	0.0337	0.9400	Schisandrae Chinensis Fructus	Thymoquinol	95779	FALSE	Oc1cc(c(cc1C(C)C)O)C
MOL008937	0.9181	0.0819	0.8682	Schisandrae Chinensis Fructus	thymoquinol 5-glucoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1CO)Oc1cc(c(cc1C)O)C(C)C
MOL008938	0.9198	0.0802	0.8113	Schisandrae Chinensis Fructus	zingerone glucoside	Not Available	FALSE	c1cc(c(cc1CCC(=O)C)OC)OC1OC(C(O)C(O)C1O)CO
MOL008939	0.8302	0.1698	0.7293	Schisandrae Chinensis Fructus	(9aS)-2,5,9,9-tetramethyl-3,4,6,7,8,9a-hexahydrobenzo[7]annulene	24798710	FALSE	C1CC(=CC2C1=C(CCCC2(C)C)C)C
MOL008940	0.8558	0.1442	0.6232	Schisandrae Chinensis Fructus	γ-Cadinene	12358781	FALSE	C1C=C(CC2C1C(=C)CCC2C(C)C)C
MOL008941	0.9059	0.0941	0.8448	Asari Radix Et Rhizoma	(E)-9-Isopropyl-6-methyl-5,9-decadiene-2-one	5318635	FALSE	CC(=O)CC/C=C(/CCC(=C)C(C)C)\C
MOL008941	0.9059	0.0941	0.8448	Aucklandiae Radix	(E)-9-Isopropyl-6-methyl-5,9-decadiene-2-one	5318635	FALSE	CC(=O)CC/C=C(/CCC(=C)C(C)C)\C
MOL008941	0.9059	0.0941	0.8448	Schisandrae Chinensis Fructus	(E)-9-Isopropyl-6-methyl-5,9-decadiene-2-one	5318635	FALSE	CC(=O)CC/C=C(/CCC(=C)C(C)C)\C

MOL008942	0.8698	0.1302	0.7281	Schisandrae Chinensis Fructus	1,1alpha,4,5,6,7,7alpha,7beta-Octahydro-1,1,7,7alpha-tetramethyl-2H-cyclopropa(alpha)-naphthalen-2-one	12305213	FALSE	C1(CCCC2=CC(=O)C3C(C12C)C3(C)C)C
MOL008943	0.8729	0.1271	0.8741	Schisandrae Chinensis Fructus	1,2,3,3alpha,8,8alpha-Hexahydro-2,2,8-trimethyl-5,6-azulenedimethanol	Not Available	FALSE	C12C(CC(C1)(C)C)C(C=C(C(=C2)CO)CO)C
MOL008944	0.8431	0.1569	0.6870	Schisandrae Chinensis Fructus	1-(1,5-Dimethyl-4-hexenyl)-4-methyl benzene	Not Available	FALSE	C1(CCC(CC1)C(C)CCC=C(C)C)C
MOL008945	0.9444	0.0556	0.9369	Oroxyli Semen	Benzoylacetone	7166	FALSE	c1cccc(c1)C(=O)CC(=O)C
MOL008945	0.9444	0.0556	0.9369	Schisandrae Chinensis Fructus	Benzoylacetone	7166	FALSE	c1cccc(c1)C(=O)CC(=O)C
MOL008946	0.2572	0.7428	0.7120	Schisandrae Chinensis Fructus	Schisanhenol	Not Available	FALSE	c12CC(C(Cc3c(c1c(c(c(c2)OC)OC)OC)c(c(c(c3)OC)OC)O)C)C
MOL008947	0.2133	0.7867	0.6007	Schisandrae Chinensis Fructus	2,4-Dimethyl-6(3-methyl-isobuten-5-isopropyl)-phenyl-3,5 hexanedione	Not Available	FALSE	c1(cc(cc(c1)C/C(=C(/C(=O)C(C)C)\C)/O)C(=C(C)C)C)C(C)C
MOL008948	0.9162	0.0838	0.9431	Schisandrae Chinensis Fructus	3-carbomethoxy-3-hydroxy-glutaric acid	12566215	FALSE	C(=O)(OC)C(CC(=O)O)(CC(=O)O)O
MOL008949	0.8161	0.1839	0.7462	Schisandrae Chinensis Fructus	3-Methyl betuletol	Not Available	FALSE	C1(=C(C(c2c(C1)oc(c(c2=O)OC)c1ccc(cc1)OC)O)OC)O
MOL008950	0.7369	0.2631	0.6810	Schisandrae Chinensis Fructus	3-Phenyldecane	Not Available	FALSE	c1(ccccc1)C(CC)CCCCCCC

MOL008951	0.9279	0.0721	0.8994	Schisandrae Chinensis Fructus	3alpha-Tigloyloxytropane	Not Available	FALSE	C1(OC(=O)/C(=C/C)/C)CC2CCC(N2C)C1
MOL008952	0.8438	0.1562	0.6497	Schisandrae Chinensis Fructus	4,7-dimethyl-7-(4-methylpent-3-enyl)bicyclo[2.2.1]heptan-3-ol	Not Available	FALSE	C12CC(C(CC1)(C2(CCC=C(C)C)C)C)O
MOL008954	0.4567	0.5433	0.7905	Schisandrae Chinensis Fructus	SMR000445689	Not Available	FALSE	c12CC(C(Cc3c(c1c(c1c(c2)OCO1)O)c(c(c(c3)OC)OC)OC)C)C
MOL008956	0.1295	0.8705	0.6050	Schisandrae Chinensis Fructus	Angeloylgomisin O	Not Available	FALSE	c12c(c(c3c(c1)CC(C(C(c1c3c(OC)c(c(c1)OC)OC)OC(=O)/C(=C/C)/C)C)C)OC)OCO2
MOL008957	0.1726	0.8274	0.6157	Schisandrae Chinensis Fructus	Schizandrer B	Not Available	FALSE	c12c(c(c3c(c1)CC(C(C(c1c3c(OC)c(c(c1)OC)OC)OC(=O)/C(=C/C)/C)(C)O)C)OC)OCO2
MOL008958	0.0967	0.9033	0.6261	Schisandrae Chinensis Fructus	Angeloylgomisin Q	Not Available	FALSE	c1(c(c(c2c(c1)CC(C(C(c1c2c(OC)c(c(c1)OC)OC)OC(=O)/C(=C/C)/C)(C)O)C)OC)OC)OC
MOL008959	0.1282	0.8718	0.6046	Schisandrae Chinensis Fructus	Angeloylisogomisin O	Not Available	FALSE	c1(c(c(c2c(c1)CC(C(C(c1c2c(OC)c2c(c1)OCO2)OC(=O)/C(=C/C)/C)C)C)OC)OC)OC
MOL008960	0.1106	0.8894	0.7260	Schisandrae Chinensis Fructus	Benzoylgomisin H	Not Available	FALSE	c1(c(c(c2c(c1)CC(C(Cc1c2c(c(c(c1)OC)OC)OC)(C)O)C)Oc1ccccc1)OC)OC
MOL008961	0.1399	0.8601	0.6755	Schisandrae Chinensis Fructus	Benzoylgomisin O	Not Available	FALSE	c1(c(c(c2c(c1)CC(C(C(c1c2c(OC)c2c(c1)OCO2)Oc1ccccc1)C)C)OC)OC)OC
MOL008962	0.1429	0.8571	0.6965	Schisandrae Chinensis Fructus	Benzoylgomisin P	Not Available	FALSE	c12c(c(c3c(c1)CC(C(C(c1c3c(c(c(c1)OC)OC)OC)Oc1ccccc1)(C)O)C)OC)OCO2
MOL008963	0.1054	0.8946	0.7124	Schisandrae Chinensis Fructus	Benzoylgomisin Q	Not Available	FALSE	c1(c(c(c2c(c1)CC(C(C(c1c2c(c(c(c1)OC)OC)OC)Oc1ccccc1)(C)O)C)OC)OC)OC
MOL008965	0.7568	0.2432	0.6182	Schisandrae Chinensis Fructus	Clupanodonic acid	5315978	FALSE	C(C/C=C/C/C=C/CC/C=C/CCC(=O)O)/C=C/CC
MOL008967	0.8516	0.1484	0.7341	Schisandrae Chinensis Fructus	Epiguaipyridine	13857098	FALSE	n1c2c(ccc1C)C(CCC(C2)C(=C)C)C
MOL008968	0.4523	0.5477	0.7301	Schisandrae Chinensis Fructus	Gomisin-A	Not Available	FALSE	c12CC(C(Cc3c(c1c(c(c(c2)OC)OC)OC)c(c1c(c3)OCO1)OC)C)(C)O
MOL008969	0.3632	0.6368	0.6483	Schisandrae Chinensis Fructus	Gomisin B	Not Available	FALSE	c12C(C(C(Cc3c(c1c(c1c(c2)OCO1)OC)c(c1c(c3)OCO1)OC)C)(C)O)OC(=O)C=C(C)C
MOL008970	0.1429	0.8571	0.6965	Schisandrae Chinensis Fructus	Gomisin C	Not Available	FALSE	c12C(C(C(Cc3c(c1c(c(c(c2)OC)OC)OC)c(c1c(c3)OCO1)OC)C)(C)O)Oc1ccccc1
MOL008971	0.5093	0.4907	0.6694	Schisandrae Chinensis Fructus	Gomisin D	Not Available	FALSE	c12C3C(C(Cc4c(c1c(c(c(c2)OC)OC)OC)c(c1c(c4)OCO1)OCC(C(C(=O)O3)(O)C)C)C)(C)O
MOL008972	0.3963	0.6037	0.6480	Schisandrae Chinensis Fructus	Gomisin E	Not Available	FALSE	c12C3C(C(Cc4c(c1c(c(c(c2)OC)OC)OC)c(c1c(c4)OCO1)OCC(C(C(=O)O3)(O)C)C)C)C

MOL008973	0.1508	0.8492	0.6402	Schisandrae Chinensis Fructus	Gomisin F	Not Available	FALSE	c12C(C(C(Cc3c(c1c(c1c(c2)OCO1)OC)c(c(c(c3)OC)OC)OC)C)(O)C)OC(=O)C=C(C)C
MOL008974	0.1407	0.8593	0.6963	Schisandrae Chinensis Fructus	Gomisin G	Not Available	FALSE	c12C(C(C(Cc3c(c1c(c1c(c2)OCO1)OC)c(c(c(c3)OC)OC)OC)C)(O)C)Oc1ccccc1
MOL008975	0.4003	0.5997	0.7239	Schisandrae Chinensis Fructus	Gomisin H	Not Available	FALSE	c12CC(C(Cc3c(c1c(c(c(c2)OC)OC)OC)c(c(c(c3)OC)OC)O)C)(O)C
MOL008976	0.4548	0.5452	0.7422	Schisandrae Chinensis Fructus	Gomisin J	Not Available	FALSE	c12CC(C(Cc3c(c1c(c(c(c2)O)OC)OC)c(c(c(c3)O)OC)OC)C)C
MOL008977	0.4673	0.5327	0.7198	Schisandrae Chinensis Fructus	AIDS446185	Not Available	FALSE	c12C(C(C(Cc3c(c1c(c(c(c2)OC)OC)OC)c(c1c(c3)OCO1)OC)C)C)O
MOL008978	0.6701	0.3299	0.7395	Schisandrae Chinensis Fructus	Gomisin R	Not Available	FALSE	OC1C(C(Cc2c(c3c1cc1OCOc1c3OC)c(OC)c1OCOc1c2)C)C
MOL008980	0.8520	0.1480	0.7072	Schisandrae Chinensis Fructus	Gomphrenin I	Not Available	FALSE	N1(C/C=C\2/CC(NC(=C2)C(=O)O)C(=O)O)c2cc(c(cc2CC1C(=O)O)O)OC1OC(C(C(C1O)O)O)CO
MOL008981	0.9345	0.0655	0.6426	Schisandrae Chinensis Fructus	Gomphrenin I_qt	Not Available	FALSE	c1(c(cc2c(c1)CC(N2C/C=C\1/CC(NC(=C1)C(=O)O)C(=O)O)C(=O)O)O)O
MOL008982	0.7358	0.2642	0.7772	Schisandrae Chinensis Fructus	Hexahydroxytaxadiene	Not Available	FALSE	C1(=C2C(C(CC1O)(C(C1C(C(C2O)O)(CCC(C1=C)O)C)O)O)(C)C)C
MOL008983	0.8748	0.1252	0.8094	Schisandrae Chinensis Fructus	5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-6-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	5318663	FALSE	c1cc(cc(c1O)OC)c1oc2c(c(=O)c1)c(c(c(c2)O)OC1C(C(C(C(O1)CO)O)O)O)O
MOL008984	0.9418	0.0582	0.9522	Schisandrae Chinensis Fructus	(1R)-1-phenylpropan-1-ol	640199	FALSE	c1cccc(c1)C(CC)O
MOL008985	0.8594	0.1406	0.7285	Schisandrae Chinensis Fructus	Psilostachyin A	Not Available	FALSE	O1C2(C(O)(C3OC(=O)C(=C)C3CCC2C)C)CCC1=O
MOL008986	0.8941	0.1059	0.7850	Schisandrae Chinensis Fructus	Rugosal	Not Available	FALSE	C12(C3(C(C=C(C(C1)OO3)C=O)O)C(CC2)C(C)C)C
MOL008986	0.8941	0.1059	0.7850	Rose Rugosae Flos	Rugosal	Not Available	FALSE	C12(C3(C(C=C(C(C1)OO3)C=O)O)C(CC2)C(C)C)C
MOL008987	0.1614	0.8386	0.6473	Schisandrae Chinensis Fructus	Schisanhenol acetate	Not Available	FALSE	c1(c(c2c(cc1OC)CC(C(Cc1c2c(c(c(c1)OC)OC)OC)C)C)OC(=O)C)OC
MOL008988	0.9244	0.0756	0.8399	Schisandrae Chinensis Fructus	Schizonepetoside A	Not Available	FALSE	C1(CCC(C(=O)C1)/C(=C/OC1C(C(C(C(O1)CO)O)O)O)/C)C

MOL008989	0.9525	0.0475	0.9780	Schizonepetae Herba	schizonepetoside A_qt	Not Available	FALSE	C1(CCC(C(=O)C1)/C(=C/O)/C)C
MOL008989	0.9525	0.0475	0.9780	Schisandrae Chinensis Fructus	schizonepetoside A_qt	Not Available	FALSE	C1(CCC(C(=O)C1)/C(=C/O)/C)C
MOL008990	0.9326	0.0674	0.9095	Ligustici Rhizoma Et Radix	2-[(1R)-4-methyl-1-cyclohex-3-enyl]propan-2-yl acetate	11469649	FALSE	C1(C(OC(=O)C)(C)C)CCC(=CC1)C
MOL008990	0.9326	0.0674	0.9095	Asari Radix Et Rhizoma	2-[(1R)-4-methyl-1-cyclohex-3-enyl]propan-2-yl acetate	11469649	FALSE	C1(C(OC(=O)C)(C)C)CCC(=CC1)C
MOL008990	0.9326	0.0674	0.9095	Schisandrae Chinensis Fructus	2-[(1R)-4-methyl-1-cyclohex-3-enyl]propan-2-yl acetate	11469649	FALSE	C1(C(OC(=O)C)(C)C)CCC(=CC1)C
MOL008991	0.9640	0.0360	0.8048	Schisandrae Chinensis Fructus	Thujyalcohol	12304610	FALSE	C1(C2CC2(CC1O)C(C)C)C
MOL008992	0.5499	0.4501	0.7795	Schisandrae Chinensis Fructus	Wuweizisu C	Not Available	FALSE	c1c2c(c(c3c1OCO3)OC)c1c(cc3c(c1OC)OCO3)CC(C(C2)C)C
MOL008993	0.8571	0.1429	0.8142	Schisandrae Chinensis Fructus	Wyerone	643733	FALSE	c1cc(oc1/C=C/C(=O)OC)C(=O)C#C/C=C\CC
MOL008994	0.8912	0.1088	0.7006	Schisandrae Chinensis Fructus	alpha-Cuparenol	5316200	FALSE	c1c(ccc(c1)C1(C(C(CC1)O)(C)C)C)C
MOL008995	0.9410	0.0590	0.9530	Boschniakia Rossica Herba	2,3,4-Trihydroxy-benzenepropanoic acid	5322049	FALSE	c1c(c(c(c(c1)CCC(=O)O)O)O)O
MOL008996	0.9615	0.0385	0.8765	Boschniakia Rossica Herba	Boschniakine	442507	FALSE	c12c(c(cnc1)C=O)CCC2C
MOL008997	0.9485	0.0515	0.9087	Boschniakia Rossica Herba	Boschnialactone	442420	FALSE	C12C(CC(=O)OC1)CCC2C
MOL009000	0.9241	0.0759	0.8406	Corayceps	(2R,3S,5S)-5-(6-aminopurin-9-yl)-2-(hydroxymethyl)oxolan-3-ol	12800099	FALSE	O1C(n2c3ncnc(N)c3nc2)CC(O)C1CO

MOL009001	0.9282	0.0718	0.7694	Corayceps	(2R,3R,4S)-2-(6-aminopurin-9-yl)-4-(hydroxymethyl)oxolan-3-ol	15480629	FALSE	n1cnc2c(c1N)ncn2C1C(C(CO1)CO)O
MOL009002	0.3634	0.6366	0.7441	Corayceps	Cordylagenin	Not Available	FALSE	C1C(CC2C(C1O)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)O
MOL009003	0.7082	0.2918	0.6882	Eucommiae Cortex	(2S,3R,4S,5S,6R)-2-[4-[(1R,3aR,4S,6aS)-6a-hydroxy-4-[3-methoxy-4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]-3,3a,4,6-tetrahydro-1H-furo[4,3-c]furan-1-yl]-2-methoxyphenoxy]-6-(hydroxymethyl)oxane-3,4,5-triol	21633110	FALSE	O(C1OC(C(C(C1O)O)O)CO)c1c(cc(C2C3(C(C(OC3)c3cc(c(cc3)OC3OC(C(C(C3O)O)O)CO)OC)CO2)O)cc1)OC

MOL009004	0.5977	0.4023	0.6704	Eucommiae Cortex	(2S,3R,4S,5S,6R)-2-[4-[(1S,3aS,4R,6aR)-3a-hydroxy-4-(4-hydroxy-3-methoxyphenyl)-3,4,6,6a-tetrahydro-1H-furo[4,3-c]furan-1-yl]-2-methoxyphenoxy]-6-(hydroxymethyl)oxane-3,4,5-triol	21591950	FALSE	C12C(COC1c1cc(c(cc1)OC1OC(C(C(C1O)O)O)O)CO)OC)(C(OC2)c1cc(c(cc1)O)OC)O
MOL009005	0.9444	0.0556	0.9545	Prinsepiae Nux	(+-)-Threo-guaiacylglycerol	51382654	FALSE	c1c(c(cc(c1)C(C(CO)O)O)OC)O
MOL009005	0.9444	0.0556	0.9545	Eucommiae Cortex	(+-)-Threo-guaiacylglycerol	51382654	FALSE	c1c(c(cc(c1)C(C(CO)O)O)OC)O
MOL009006	0.8710	0.1290	0.7795	Eucommiae Cortex	(4aS,8aR)-3-isopropylidene-8a-methyl-5-methylene-2-decalinone	13986100	FALSE	C1CC(=C)C2C(C1)(CC(=O)C(=C(C)C)C2)C
MOL009007	0.4834	0.5166	0.6242	Eucommiae Cortex	Eucommin A	442836	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(OC2OC(C(O)C(O)C2O)CO)c(OC)c1
MOL009008	0.5840	0.4160	0.6755	Eucommiae Cortex	(+)-Medioresinol di-O-beta-D-glucopyranoside	Not Available	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(OC3OC(C(O)C(O)C3O)CO)cc2)C1)c1cc(OC)c(OC2OC(C(O)C(O)C2O)CO)c(OC)c1
MOL009009	0.4757	0.5243	0.7025	Eucommiae Cortex	(+)-medioresinol	Not Available	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(O)c(OC)c1
MOL009009	0.4757	0.5243	0.7025	Lobeliae Chinensis Herba	(+)-medioresinol	Not Available	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(O)c(OC)c1
MOL009010	0.5866	0.4134	0.6647	Eucommiae Cortex	(+)-Pinoresinol-di-O-β-D-glucoside	Not Available	FALSE	C1(OCC2C1COC2c1ccc(c(c1)OC)OC1C(C(C(C(CO)O1)O)O)O)c1cc(c(cc1)OC1OC(C(C(C1O)O)O)CO)OC

MOL009011	0.4510	0.5490	0.6146	Eucommiae Cortex	(+)-Pinoresinol-.beta.-D-glucoside	486614	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(OC2OC(C(O)C(O)C2O)CO)cc1
MOL009011	0.4510	0.5490	0.6146	Daturae Flos	(+)-Pinoresinol-.beta.-D-glucoside	486614	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(OC2OC(C(O)C(O)C2O)CO)cc1
MOL009011	0.4510	0.5490	0.6146	Drynariae Rhizoma	(+)-Pinoresinol-.beta.-D-glucoside	486614	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)cc2)C1)c1cc(OC)c(OC2OC(C(O)C(O)C2O)CO)cc1
MOL009012	0.7040	0.2960	0.7121	Eucommiae Cortex	(2S,3R,4S,5S,6R)-2-[4-[[(3S,4R,5S)-3-hydroxy-5-(4-hydroxy-3-methoxyphenyl)-4-(hydroxymethyl)oxolan-3-yl]methyl]-2-methoxyphenoxy]-6-(hydroxymethyl)oxane-3,4,5-triol	14033815	FALSE	C1(OC(C(C(C1O)O)O)CO)Oc1c(cc(cc1)CC1(C(C(OC1)c1cc(c(cc1)O)OC)CO)O)OC

MOL009013	0.6855	0.3145	0.7168	Eucommiae Cortex	(2S,3R,4S,5S,6R)-2-[4-[(2S,3R,4S)-4-hydroxy-3-(hydroxymethyl)-4-[[3-methoxy-4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]methyl]oxolan-2-yl]-2-methoxyphenoxy]-6-(hydroxymethyl)oxane-3,4,5-triol	21633108	FALSE	C1(OC(C(C(C1O)O)O)CO)Oc1c(cc(cc1)CC1(C(C(OC1)c1cc(c(cc1)OC1C(C(C(C(O1)CO)O)O)O)OC)CO)O)OC
MOL009014	0.6262	0.3738	0.6883	Eucommiae Cortex	(2S,3R,4S,5S,6R)-2-[4-[(2S,3R,4S)-4-hydroxy-4-[(4-hydroxy-3-methoxyphenyl)methyl]-3-(hydroxymethyl)oxolan-2-yl]-2-methoxyphenoxy]-6-(hydroxymethyl)oxane-3,4,5-triol	14033813	FALSE	C1(OC(C(C(C1O)O)O)CO)Oc1ccc(cc1OC)C1OCC(C1CO)(O)Cc1cc(c(cc1)O)OC
MOL009015	0.5410	0.4590	0.7570	Eucommiae Cortex	(-)-Tabernemontanine	Not Available	FALSE	O(C(=O)C1C2C(CN(C1Cc1c([nH]c3c1cccc3)C(=O)C2)C)CC)C
MOL009017	0.9379	0.0621	0.9557	Eucommiae Cortex	3-Furyl-2-ethylacrolein	6435826	FALSE	o1c(/C=C(\CC)/C=O)ccc1
MOL009017	0.9379	0.0621	0.9557	Eucommiae Folium	3-Furyl-2-ethylacrolein	6435826	FALSE	o1c(/C=C(\CC)/C=O)ccc1

MOL009018	0.9521	0.0479	0.9523	Eucommiae Folium	MHP	91	FALSE	Oc1cc(CCC(=O)O)ccc1
MOL009018	0.9521	0.0479	0.9523	Eucommiae Cortex	MHP	91	FALSE	Oc1cc(CCC(=O)O)ccc1
MOL009019	0.9064	0.0936	0.9576	Eucommiae Cortex	(2R,3R)-3-hydroxyproline	10725382	FALSE	C1CNC(C1O)C(=O)O
MOL009020	0.8933	0.1067	0.8177	Eucommiae Cortex	[(1S,4aR,5S,7S,7aS)-5-hydroxy-7-methyl-1-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4a,5,6,7a-tetrahydro-1H-cyclopenta[c]pyran-7-yl] ethanoate	14355414	FALSE	C12C(C(OC=C1)OC1OC(C(C(C1O)O)O)CO)C(CC2O)(C)OC(=O)C
MOL009021	0.9531	0.0469	0.8132	Eucommiae Cortex	Ajugoside_qt	Not Available	FALSE	C12C(C(OC=C1)O)C(CC2O)(C)OC(=O)C
MOL009023	0.9512	0.0488	0.8524	Eucommiae Cortex	Aucubin_qt	Not Available	FALSE	OC1C2C(C=CO1)C(C=C2CO)O
MOL009024	0.3431	0.6569	0.7584	Eucommiae Cortex	Chlorogenin	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2O)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)O
MOL009025	0.6168	0.3832	0.6581	Eucommiae Cortex	3-[4-(1H-indol-3-yl)-3H-thiazol-2-ylidene]indole	5293082	FALSE	s1/c(=C/2\c3c(N=C2)cccc3)/[nH]c(c2c3c([nH]c2)cccc3)c1
MOL009027	0.2436	0.7564	0.7507	Fritillariae Pallidiflorae Bulbus	Cyclopamine	442972	FALSE	C1C(CC2=CCC3C(C2(C1)C)CC1=C(C2(CCC31)OC1C(C2C)NCC(C1)C)C)O
MOL009027	0.2436	0.7564	0.7507	Fritiliariae Irrhosae Bulbus	Cyclopamine	442972	FALSE	C1C(CC2=CCC3C(C2(C1)C)CC1=C(C2(CCC31)OC1C(C2C)NCC(C1)C)C)O
MOL009027	0.2436	0.7564	0.7507	Eucommiae Cortex	Cyclopamine	442972	FALSE	C1C(CC2=CCC3C(C2(C1)C)CC1=C(C2(CCC31)OC1C(C2C)NCC(C1)C)C)O
MOL009028	0.6274	0.3726	0.6629	Eucommiae Cortex	Dehydrodiconiferyl alcohol 4,gamma'-di-O-beta-D-glucopyanoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc(C2Oc3c(C2CO)cc(cc3OC)/C=C/COC2OC(C(O)C(O)C2O)CO)ccc1OC)CO

MOL009029	0.5001	0.4999	0.7644	Eucommiae Cortex	Dehydrodiconiferyl alcohol 4,gamma'-di-O-beta-D-glucopyanoside_qt	Not Available	FALSE	O1C(C(c2c1c(OC)cc(c2)/C=C/CO)CO)c1cc(O)c(OC)cc1
MOL009030	0.4684	0.5316	0.7464	Eucommiae Cortex	Dehydrodieugenol	165225	FALSE	c1c(cc(c(c1OC)O)c1cc(cc(c1O)OC)CC=C)CC=C
MOL009031	0.2431	0.7569	0.8342	Eucommiae Cortex	Cinchonan-9-al, 6'-methoxy-, (9R)-	94175	FALSE	OC(C1N2CC(C(C1)CC2)C=C)c1c2c(ncc1)ccc(OC)c2
MOL009032	0.8109	0.1891	0.7862	Drynariae Rhizoma	Threo-dihydroxydehydrodiconiferyl alcohol	26208563	FALSE	O1C(C(c2c1c(OC)cc(c2)C(O)C(O)CO)CO)c1cc(OC)c(O)cc1
MOL009032	0.8109	0.1891	0.7862	Eucommiae Cortex	Threo-dihydroxydehydrodiconiferyl alcohol	26208563	FALSE	O1C(C(c2c1c(OC)cc(c2)C(O)C(O)CO)CO)c1cc(OC)c(O)cc1
MOL009033	0.9052	0.0948	0.9593	Eucommiae Cortex	(2R,3S)-2-amino-3-hydroxy-succinic acid	6603868	FALSE	OC(=O)C(C(C(=O)O)N)O
MOL009034	0.9294	0.0706	0.8722	Eucommiae Folium	Eucommiol	154373	FALSE	C1(C(CC(=C1CO)CO)O)CCO
MOL009034	0.9294	0.0706	0.8722	Eucommiae Cortex	Eucommiol	154373	FALSE	C1(C(CC(=C1CO)CO)O)CCO
MOL009035	0.9364	0.0636	0.8842	Eucommiae Cortex	Eucommioside-II	6325167	FALSE	C1(C(CC(=C1CO)CO)OC1OC(C(C(C1O)O)O)CO)CCO
MOL009036	0.9258	0.0742	0.8866	Eucommiae Cortex	Eucommiosid[illegible]	6325166	FALSE	C1(C(CC(=C1CO)CO)O)CCOC1OC(C(C(C1O)O)O)CO
MOL009037	0.9326	0.0674	0.8877	Eucommiae Cortex	Genioisidic acid	Not Available	FALSE	C1=C(C2C(C(O1)OC1OC(C(C(C1O)O)O)CO)C(=CC2)CO)C(=O)O
MOL009038	0.9068	0.0932	0.7293	Eucommiae Cortex	GBGB	3082301	FALSE	C1=C(C2C(C(O1)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)C(=CC2)CO)C(=O)OC
MOL009039	0.9435	0.0565	0.8991	Eucommiae Cortex	ZINC00394284	6950715	TRUE	O(CC(O)CO)c1c(OC)cccc1
MOL009040	0.7751	0.2249	0.7386	Figwort Root	harpagoside	5281542	FALSE	C12(C(C(OC=C1)OC1OC(C(C(C1O)O)O)CO)C(CC2O)(OC(=O)/C=C/c1ccccc1)C)O
MOL009040	0.7751	0.2249	0.7386	Eucommiae Cortex	harpagoside	5281542	FALSE	C12(C(C(OC=C1)OC1OC(C(C(C1O)O)O)CO)C(CC2O)(OC(=O)/C=C/c1ccccc1)C)O
MOL009041	0.7834	0.2166	0.7509	Eucommiae Cortex	Harpagoside_qt	25026347	FALSE	C12(C(C(OC=C1)O)C(CC2O)(OC(=O)/C=C/c1ccccc1)C)O
MOL009042	0.8714	0.1286	0.8264	Eucommiae Cortex	Helenalin	23205	FALSE	C1=CC2C(C1=O)(C(C1C(OC(=O)C1=C)CC2C)O)C
MOL009042	0.8714	0.1286	0.8264	Centipedae Herba	Helenalin	23205	FALSE	C1=CC2C(C1=O)(C(C1C(OC(=O)C1=C)CC2C)O)C

MOL009043	0.8846	0.1154	0.7905	Eucommiae Cortex	SPBio_000310	Not Available	FALSE	C1C2C(C(=O)CCC3C(C1)(O3)C)CC2(C)C
MOL009044	0.4629	0.5371	0.6897	Eucommiae Cortex	Melafolone	Not Available	FALSE	c1cccc(c1)/C=C/C(=O)c1c(OC)c(c(c(c1O)OC)O)OC(=O)C(CC)C
MOL009045	0.9017	0.0983	0.9185	Eucommiae Cortex	Methyl 2-chloroacrylate	6659	FALSE	C=C(C(=O)OC)Cl
MOL009046	0.9012	0.0988	0.8749	Eucommiae Cortex	Chlorogenic acid methyl ester	6476139	FALSE	C1C(C(C(CC1(O)C(=O)OC)OC(=O)/C=C/c1cc(c(cc1)O)O)O)O
MOL009046	0.9012	0.0988	0.8749	Eriobotryae Folium	Chlorogenic acid methyl ester	6476139	FALSE	C1C(C(C(CC1(O)C(=O)OC)OC(=O)/C=C/c1cc(c(cc1)O)O)O)O
MOL009047	0.2663	0.7337	0.6910	Eucommiae Cortex	(+)-Eudesmin	73117	FALSE	C12C(C(OC1)c1ccc(c(c1)OC)OC)COC2c1cc(c(cc1)OC)OC
MOL009048	0.9214	0.0786	0.9116	Eucommiae Cortex	cis-pinosylvin	9548840	FALSE	c1c(cc(cc1O)/C=C\c1ccccc1)O
MOL009049	0.9363	0.0637	0.9631	Eucommiae Cortex	(4S,5S)-4-hydroxy-5-pentyloxolan-2-one	10464767	FALSE	C1(C(CC(=O)O1)O)CCCCC
MOL009050	0.9078	0.0922	0.7628	Eucommiae Cortex	Ulmoside	Not Available	FALSE	C12C(C(OC=C1)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)C(CC2O)CO
MOL009051	0.9501	0.0499	0.8546	Eucommiae Cortex	Ulmoside_qt	Not Available	FALSE	C12C(C(OC=C1)O)C(CC2O)CO
MOL009052	0.9177	0.0823	0.9554	Eucommiae Cortex	(2S)-2-ammonio-6-ureidohexanoate	6991977	FALSE	C(=O)(C(CCCCNC(=O)N)N)O
MOL009053	0.5280	0.4720	0.7065	Eucommiae Cortex	4-[(2S,3R)-5-[(E)-3-hydroxyprop-1-enyl]-7-methoxy-3-methylol-2,3-dihydrobenzofuran-2-yl]-2-methoxy-phenol	11824478	FALSE	O1C(C(c2c1c(OC)cc(c2)/C=C/CO)CO)c1cc(OC)c(O)cc1

MOL009053	0.5280	0.4720	0.7065	Aurantii Fructus Immaturus	4-[(2S,3R)-5-[(E)-3-hydroxyprop-1-enyl]-7-methoxy-3-methylol-2,3-dihydrobenzofuran-2-yl]-2-methoxy-phenol	11824478	FALSE	O1C(C(c2c1c(OC)cc(c2)/C=C/CO)CO)c1cc(OC)c(O)cc1
MOL009056	0.6463	0.3537	0.7348	Eucommiae Cortex	liriodendrin	Not Available	FALSE	O1C(C2C(C(OC2)c2c(OC3OC(C(O)C(O)C3O)CO)cc(OC)c(OC3OC(C(O)C(O)C3O)CO)c2OC)C1)c1c(OC2OC(C(O)C(O)C2O)CO)cc(OC)c(OC2OC(C(O)C(O)C2O)CO)c1OC
MOL009057	0.6786	0.3214	0.6088	Eucommiae Cortex	liriodendrin_qt	Not Available	FALSE	O1C(C2C(C(OC2)c2c(O)cc(OC)c(O)c2OC)C1)c1c(O)cc(OC)c(O)c1OC
MOL009058	0.8890	0.1110	0.8057	Eucommiae Cortex	quercetin-3-sophoroside	Not Available	FALSE	O(C1C(O)C(O)C(OC1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1)CO)C1OC(C(O)C(O)C1O)CO
MOL009059	0.9418	0.0582	0.9706	Eucommiae Cortex	trans-4-Hydroxycyclohexane-1-carboxylic acid	151138	FALSE	C1(C(=O)O)CCC(CC1)O
MOL009060	0.8979	0.1021	0.8011	Drynariae Rhizoma	(+)-catechin-5-O-β-D-glucopyranoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2CC(O)C(Oc2cc(O)c1)c1cc(O)c(O)cc1)CO
MOL009062	0.8967	0.1033	0.8168	Drynariae Rhizoma	Aureusidin-6-glucoside	5321164	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2O/C(=C\c3cc(O)c(O)cc3)/C(=O)c2c(O)c1)CO
MOL009063	0.2990	0.7010	0.7075	Drynariae Rhizoma	Cyclolaudenol acetate	Not Available	FALSE	O(C1C(C2C3(C4(C3)C(C3(C(CC4)(C(CC3)C(CCC(C)C(=C)C)C)C)C)CC2)CC1)(C)C)C(=O)C
MOL009064	0.8726	0.1274	0.8202	Drynariae Rhizoma	Epiafzelechin 5-O-beta-D-glucopyranoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2CC(O)C(Oc2cc(O)c1)c1ccc(O)cc1)CO

MOL009065	0.8953	0.1047	0.8097	Drynariae Rhizoma	(2R,3R,4R,5S,6R)-2-[(2R,3R)-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-chroman-3-yl]oxy-6-(hydroxymethyl)tetrahydropyran-3,4,5-triol	14104303	FALSE	O1C(OC2C(Oc3c(C2)c(O)cc(O)c3)c2cc(O)c(O)cc2)C(O)C(O)C(O)C1CO
MOL009066	0.9099	0.0901	0.8379	Chrysanthemi Flos	Eriodictyol 7-glucuronide	124258	FALSE	O1C(Oc2cc3OC(CC(=O)c3c(O)c2)c2cc(O)c(O)cc2)C(O)C(O)C(O)C1C(=O)O
MOL009066	0.9099	0.0901	0.8379	Drynariae Rhizoma	Eriodictyol 7-glucuronide	124258	FALSE	O1C(Oc2cc3OC(CC(=O)c3c(O)c2)c2cc(O)c(O)cc2)C(O)C(O)C(O)C1C(=O)O
MOL009067	0.3566	0.6434	0.6462	Drynariae Rhizoma	Isoglaucanone	Not Available	FALSE	C1CC(C2C(C1)(C1C(CC2)(C2(C(CC1)C1(C(CC2)CC(=O)C1)C)C)C)C)(C)C
MOL009068	0.8877	0.1123	0.7783	Drynariae Rhizoma	Kaempferol 7-alpha-L-arabinoside	Not Available	FALSE	O1C(Oc2cc3oc(c(O)c(=O)c3c(O)c2)c2ccc(O)cc2)C(O)C(O)C(O)C1
MOL009069	0.8788	0.1212	0.7786	Drynariae Rhizoma	Lucenin-2	442615	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c(C2OC(C(O)C(O)C2O)CO)c(O)c2c1oc(cc2=O)c1cc(O)c(O)cc1
MOL009070	0.9168	0.0832	0.8296	Polygoni Cuspidati Rhizoma Et Radix	Luteolin 7-O-glucuronide	5280601	FALSE	O1C(Oc2cc3oc(cc(=O)c3c(O)c2)c2cc(O)c(O)cc2)C(O)C(O)C(O)C1C(=O)O
MOL009070	0.9168	0.0832	0.8296	Schizonepetae Herba	Luteolin 7-O-glucuronide	5280601	FALSE	O1C(Oc2cc3oc(cc(=O)c3c(O)c2)c2cc(O)c(O)cc2)C(O)C(O)C(O)C1C(=O)O
MOL009070	0.9168	0.0832	0.8296	Drynariae Rhizoma	Luteolin 7-O-glucuronide	5280601	FALSE	O1C(Oc2cc3oc(cc(=O)c3c(O)c2)c2cc(O)c(O)cc2)C(O)C(O)C(O)C1C(=O)O
MOL009071	0.8751	0.1249	0.8088	Drynariae Rhizoma	Luteolin 7-glucoside-4'-neohesperidoside	Not Available	FALSE	O(C1C(O)C(O)C(OC1Oc1c(O)cc(cc1)c1oc2cc(OC3OC(C(O)C(O)C3O)CO)cc(O)c2c(=O)c1)CO)C1OC(C(O)C(O)C1O)C
MOL009072	0.8746	0.1254	0.8452	Lunulatae Herba	Prunin	92794	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1ccc(O)cc1)CO
MOL009072	0.8746	0.1254	0.8452	Drynariae Rhizoma	Prunin	92794	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1ccc(O)cc1)CO
MOL009072	0.8746	0.1254	0.8452	Menthae Herba	Prunin	92794	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1ccc(O)cc1)CO
MOL009073	0.7022	0.2978	0.7572	Drynariae Rhizoma	Procyanidin D	13269089	FALSE	O1C(C(O)C(c2c3OC(C(O)Cc3c(O)cc2O)c2cc(O)c(O)cc2)c2c1cc(O)cc2O)c1cc(O)c(O)cc1

MOL009074	0.6144	0.3856	0.7663	Drynariae Rhizoma	Chitranone	633072	FALSE	Oc1c(C2=C(C(=O)c3c(C2=O)c(O)ccc3)C)ccc2c1C(=O)C=C(C2=O)C
MOL009075	0.2944	0.7056	0.7176	Drynariae Rhizoma	cycloartenone	Not Available	FALSE	O=C1C(C2C3(C4(C3)C(C3(C(CC4)(C(CC3)C(CCC=C(C)C)C)C)C)CC2)CC1)(C)C
MOL009076	0.3725	0.6275	0.6835	Drynariae Rhizoma	cyclolaudenol	Not Available	FALSE	OC1C(C2C3(C4(C3)C(C3(C(CC4)(C(CC3)C(CCC(C)C(=C)C)C)C)C)CC2)CC1)(C)C
MOL009077	0.8828	0.1172	0.6887	Drynariae Rhizoma	davallioside A	Not Available	FALSE	O(C1C(Oc2c(C1)c(O)cc(O)c2C1NC(=O)CC1)c1cc(O)c(O)cc1)C1OC(C(O)C(O)C1O)CO
MOL009078	0.8287	0.1713	0.7294	Drynariae Rhizoma	davallioside A_qt	Not Available	FALSE	OC1C(Oc2c(C1)c(O)cc(O)c2C1NC(=O)CC1)c1cc(O)c(O)cc1
MOL009079	0.8828	0.1172	0.6887	Drynariae Rhizoma	davallioside B	Not Available	FALSE	N1C(=O)CCC1c1c2c(CC(C(O2)c2cc(c(cc2)O)O)OC2C(O)C(O)C(O)C(O2)CO)c(cc1O)O
MOL009080	0.8287	0.1713	0.7294	Drynariae Rhizoma	davallioside B_qt	Not Available	FALSE	N1C(=O)CCC1c1c2c(CC(C(O2)c2cc(c(cc2)O)O)O)c(cc1O)O
MOL009081	0.8981	0.1019	0.8052	Drynariae Rhizoma	eriodictyol-7-O-glucoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(O)cc1)CO
MOL009082	0.4001	0.5999	0.6642	Drynariae Rhizoma	Fernene	441679	FALSE	C12(C(C3C(=CC2)C2(C(CC3)C(CCC2)(C)C)C)(CCC2(C1CCC2C(C)C)C)C)C
MOL009083	0.3437	0.6563	0.6549	Drynariae Rhizoma	ferna-7-9(11)-diene	13857712	FALSE	C1(CCC2C1(C)CCC1(C2(C)CC=C2C1=CCC1C2(CCCC1(C)C)C)C)C(C)C
MOL009084	0.9279	0.0721	0.7349	Drynariae Rhizoma	(4-hydroxyphenyl)-(2,4,6-trihydroxyphenyl)methanone	11311158	FALSE	Oc1c(C(=O)c2ccc(O)cc2)c(O)cc(O)c1
MOL009087	0.8956	0.1044	0.8402	Drynariae Rhizoma	marioside_qt	Not Available	FALSE	OC1C2(C(C(C1)CC(=O)OC)CC=C(CC2)C(=O)OC)C
MOL009088	0.8816	0.1184	0.8851	Drynariae Rhizoma	Neoeriocitrin	114627	FALSE	O(C1C(O)C(O)C(OC1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(O)cc1)CO)C1OC(C(O)C(O)C1O)C
MOL009089	0.6985	0.3015	0.7534	Drynariae Rhizoma	procyanidin B-5	Not Available	FALSE	O(C1(Oc2c(C(O)C1O)c(O)cc(O)c2)c1cc(O)c(O)cc1)C1C(Oc2c(C1)c(O)cc(O)c2)c1cc(O)c(O)cc1
MOL009092	0.8001	0.1999	0.7043	Chebulae Fructus	Pentagalloylglucose	65238	FALSE	O1C(C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C1OC(=O)c1cc(O)c(O)c(O)c1)COC(=O)c1cc(O)c(O)c(O)c1
MOL009092	0.8001	0.1999	0.7043	Phyllanthi Fructus	Pentagalloylglucose	65238	FALSE	O1C(C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C1OC(=O)c1cc(O)c(O)c(O)c1)COC(=O)c1cc(O)c(O)c(O)c1
MOL009092	0.8001	0.1999	0.7043	Cortex Moutan	Pentagalloylglucose	65238	FALSE	O1C(C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C1OC(=O)c1cc(O)c(O)c(O)c1)COC(=O)c1cc(O)c(O)c(O)c1
MOL009092	0.8001	0.1999	0.7043	Paeoniae Radix Alba	Pentagalloylglucose	65238	FALSE	O1C(C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C1OC(=O)c1cc(O)c(O)c(O)c1)COC(=O)c1cc(O)c(O)c(O)c1

MOL009092	0.8001	0.1999	0.7043	Juglandis Semen	Pentagalloylglucose	65238	FALSE	O1C(C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C1OC(=O)c1cc(O)c(O)c(O)c1)COC(=O)c1cc(O)c(O)c(O)c1
MOL009092	0.8001	0.1999	0.7043	Radix Paeoniae Rubra	Pentagalloylglucose	65238	FALSE	O1C(C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C1OC(=O)c1cc(O)c(O)c(O)c1)COC(=O)c1cc(O)c(O)c(O)c1
MOL009093	0.8605	0.1395	0.6915	Juglandis Semen	1,2,3,6-Tetragalloylglucose	73178	FALSE	O(C1C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C(O)C(O1)COC(=O)c1cc(O)c(O)c(O)c1)C(=O)c1cc(O)c(O)c(O)c1
MOL009094	0.3592	0.6408	0.6321	Juglandis Semen	9,10,12,13-dimethylene octadecanoate	Not Available	FALSE	CCCCCC1C(C1)CC1C(C1)CCCCCCCC(=O)OC
MOL009095	0.4002	0.5998	0.6549	Broussonetiae Fructus	9,10-methylene octadecanoate	71366172	FALSE	CCCCCCCCC1C(CCCCCCCC(=O)OC)C1
MOL009095	0.4002	0.5998	0.6549	Juglandis Semen	9,10-methylene octadecanoate	71366172	FALSE	CCCCCCCCC1C(CCCCCCCC(=O)OC)C1
MOL009096	0.9281	0.0719	0.8741	Juglandis Semen	Methyl 9-cyclopropylnonanoate	543433	FALSE	C1CC1CCCCCCCCC(=O)OC
MOL009098	0.8210	0.1790	0.7520	Juglandis Semen	casuariin	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC(C(OC(=O)c1c2c(c(c(c1)O)O)O)C1C2C(c3c(c(c(c(c4c(C(=O)C1)cc(c(c4O)O)O)c3C(=O)O2)O)O)O)O)O)O)O
MOL009099	0.8057	0.1943	0.7601	Juglandis Semen	casuarinin	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC(C(OC(=O)c1c2c(c(c(c1)O)O)O)C1C2C(O)c3c(c(c(c(c3O)O)O)c3c(cc(c(c3O)O)O)C(=O)O1)C(=O)O2)OC(=O)c1cc(c(c(c1)O)O)O)O)O
MOL009101	0.7415	0.2585	0.7360	Juglandis Semen	euprostin A	Not Available	FALSE	Oc1c(cc2c(c1O)c1c(cc(c(c1O)O)O)C(=O)OCC1C(OC2=O)C(C(C(O1)OC(=O)c1cc(c(c(c1Oc1cc2c3c(c1O)oc(=O)c1c3c(oc2=O)cc(c1O)O)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O
MOL009102	0.8637	0.1363	0.6846	Juglandis Semen	gemin D	Not Available	FALSE	c1(c(cc(cc1O)C(=O)OC(C(O)C=O)C1C(O)COC(=O)c2c(c3c(C(=O)O1)cc(c(c3O)O)O)c(c(c(c2)O)O)O)O)O

MOL009103	0.8606	0.1394	0.6913	Juglandis Semen	[(2R,3S,4S,5R,6S)-4-hydroxy-5,6-bis[(3,4,5-trihydroxybenzoyl)oxy]-2-[(3,4,5-trihydroxybenzoyl)oxymethyl]oxan-3-yl] 3,4,5-trihydroxybenzoate	11297287	FALSE	O(C1C(OC(=O)c2cc(O)c(O)c(O)c2)C(O)C(OC(=O)c2cc(O)c(O)c(O)c2)C(O1)COC(=O)c1cc(O)c(O)c(O)c1)C(=O)c1cc(O)c(O)c(O)c1
MOL009104	0.7502	0.2498	0.6429	Juglandis Semen	glansreginin A	Not Available	FALSE	C(C(C(C)C/C=C/C=C(/C(=O)OCC1C(C(C(C(O1)OC1(CC(=O)Nc2c1cccc2)C(=O)O)O)O)O)\C)O)C(=O)O
MOL009105	0.8606	0.1394	0.7256	Juglandis Semen	glansreginin B	Not Available	FALSE	O1C(C(C(C(C1OC1(OC(C(C1O)O)CO)CO)O)O)O)COC(=O)/C(=C/C=C/CC(C)C(CC(=O)O)O)/C
MOL009106	0.5871	0.4129	0.7232	Juglandis Semen	glansrin A	Not Available	FALSE	c1c(c(c(c(c1C(=O)O)Oc1c(cc2c(c1O)c1c(cc(c(c1O)O)O)C(=O)OCC1C(OC2=O)C2C(C(O1)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1c(c3c(C(=O)O2)cc(c(c3O)O)O)c(c(c(c1)O)O)O)O)O)O)O
MOL009107	0.4938	0.5062	0.7292	Juglandis Semen	glansrin B	Not Available	FALSE	Oc1c(cc2c(c1O)c1c(cc(c3c1Oc1c(O3)c(c(c(c1)O)O)O)O)C(=O)OCC1C(OC2=O)C2C(C(O1)O)OC(=O)c1c(c3c(C(=O)O2)cc(c(c3O)O)O)c(c(c(c1)O)O)O)O
MOL009108	0.7574	0.2426	0.7274	Juglandis Semen	glansrin C	Not Available	FALSE	c1(c(cc2c(c1O)Oc1c(OC2=O)c2c(cc1O)C(=O)OCC(C(OC(=O)c1c2c(c(c(c1)O)O)O)O)C1C2C(c3c(c(c(c(c4c(C(=O)C1)cc(c(c4O)O)O)c3C(=O)O2)O)O)O)O)O)O
MOL009109	0.4358	0.5642	0.7267	Juglandis Semen	glansrin D	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC1C(C(C(C(O1)OC(=O)c1c(c(c(c(c1)O)O)O)O)Oc1c(c(c3c(c1)C(=O)OCC1C(OC(=O)c4c3c(c(c(c4)O)O)O)O)C3C(C(O1)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1c(c4c(C(=O)O3)cc(c(c4O)O)O)c(c(c(c1)O)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)OC(=O)c1c2c(c(c(c1)O)O)O)O)O
MOL009110	0.4387	0.5613	0.7217	Juglandis Semen	heterophylliin D	Not Available	FALSE	Oc1c(cc2c(c1O)c1c(cc(c(c1O)O)O)C(=O)OCC1C(OC2=O)C2C(C(O1)OC(=O)c1c(c(c(c(c1)O)O)O)O)c1c(c(c3c(c1)C(=O)OCC1C(OC(=O)c4c3c(c(c(c4)O)O)O)O)C3C(C(O1)OC(=O)c1cc(O)c(O)c(O)c1)OC(=O)c1c(c4c(C(=O)O3)cc(c(c4O)O)O)c(c(c(c1)O)O)O)O)OC(=O)c1c(c3c(c(c(cc3C(=O)O2)O)O)O)c(c(c(c1)O)O)O)O
MOL009111	0.8827	0.1173	0.6833	Juglandis Semen	hippomanin A	Not Available	FALSE	C1(c2c(cc(c1O)O)C(=O)OCC1C(OC(=O)c3c2c(c(c(c3)O)O)O)O)C(C(C(O1)O)OC(=O)c1cc(c(c(c1)O)O)O)O
MOL009112	0.8879	0.1121	0.6894	Juglandis Semen	isostrictinin	Not Available	FALSE	C1(C2C(C(OC1CO)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1c(c3c(cc(c(c3O)O)O)C(=O)O2)c(c(c(c1)O)O)O)O

MOL009114	0.8629	0.1371	0.7170	Juglandis Semen	1,2-di-O-galloyl-4,6-HHDP-bata-D-glucose	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC1C(C(C(C(O1)OC(=O)c1c(c(c(c(c1)O)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O)OC(=O)c1c2c(c(c(c1)O)O)O)O)O
MOL009115	0.9438	0.0562	0.7989	Juglandis Semen	juglone	3806	FALSE	Oc1c2c(ccc1)C(=O)C=CC2=O
MOL009116	0.3853	0.6147	0.6462	Juglandis Semen	Methyl sterculate	115261	FALSE	C(CCCCCC1=C(CCCCCCCCC)C1)CC(=O)OC
MOL009117	0.4002	0.5998	0.6549	Juglandis Semen	methyl 8-[(1R,2S)-2-octylcyclopropyl]octanoate	11381345	FALSE	C(CCCCCCC1C(CCCCCCCCC(=O)OC)C1)C
MOL009117	0.4002	0.5998	0.6549	Broussonetiae Fructus	methyl 8-[(1R,2S)-2-octylcyclopropyl]octanoate	11381345	FALSE	C(CCCCCCC1C(CCCCCCCCC(=O)OC)C1)C
MOL009118	0.9626	0.0374	0.8431	Juglandis Semen	Methyl tri-O-methylgallate	15956	FALSE	c1c(cc(c(c1OC)OC)OC)C(=O)OC
MOL009119	0.5916	0.4084	0.7232	Juglandis Semen	platycaryanin A	Not Available	FALSE	Oc1c(cc2c(c1O)c1c(cc(c(c1O)Oc1c(c(c(cc1C(=O)O)O)O)O)O)C(=O)OCC1C(OC2=O)C2C(C(O1)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1c(c3c(C(=O)O2)cc(c(c3O)O)O)c(c(c(c1)O)O)O)O
MOL009120	0.7816	0.2184	0.7570	Juglandis Semen	pterocarinin A	Not Available	FALSE	c1(cc2c(c(c1O)O)c1c3c(c(c(c1O)O)O)C(C(OC3=O)C(OC2=O)C1C(COC(=O)c2cc(c3c(C(=O)O1)cc(c(c3O)O)O)c(c(c2O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)C(=O)C(C(C(CO)O)O)O)O
MOL009121	0.5988	0.4012	0.7224	Juglandis Semen	rugosin C	Not Available	FALSE	c12c(c(c(cc1C(=O)OC1C3C(C(OC1COC(=O)c1c2c(c(c(c1)Oc1c(c(c(cc1C(=O)O)O)O)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1c(c2c(C(=O)O3)cc(c(c2O)O)O)c(c(c(c1)O)O)O)O)O)O
MOL009122	0.4326	0.5674	0.7403	Juglandis Semen	rugosin F	Not Available	FALSE	Oc1c(cc2c(c1O)c1c(cc(c(c1O)O)O)C(=O)OCC1C(OC2=O)C(C(C(O1)OC(=O)c1c(c(c(c(c1)O)O)O)O)c1c(c(c2c(c1)C(=O)OCC1C(OC(=O)c3c2c(c(c(c3)O)O)O)C2C(C(O1)OC(=O)c1cc(O)c(O)c(O)c1)OC(=O)c1c(c3c(C(=O)O2)cc(c(c3O)O)O)c(c(c(c1)O)O)O)O)O)OC(=O)c1cc(O)c(O)c(O)c1)OC(=O)c1cc(O)c(O)c(O)c1)O
MOL009123	0.7658	0.2342	0.7394	Juglandis Semen	stenophyllanin A	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC(C(OC(=O)c1c2c(c(c(c1)O)O)O)C1C2C(c3c(c(c(c(c3O)O)O)c3c(cc(c(c3O)O)O)C(=O)O1)C(=O)O2)c1c(cc(c2c1OC(C(C2)O)c1cc(c(c1)O)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O
MOL009124	0.8418	0.1582	0.7151	Juglandis Semen	tellimagrandin I	Not Available	FALSE	c1(c(c(cc(c1)C(=O)OC(C=O)C(C1OC(=O)c2c(c3c(cc(c3O)O)O)C(=O)OCC1O)c(c(c(c2)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O)O

MOL009125	0.3920	0.6080	0.6565	Juglandis Semen	11,12-methylene octadecanoate	14345321	FALSE	C1(CCCCCC)C(C1)CCCCCCCCCC(=O)OC
MOL009127	0.4301	0.5699	0.7182	Juglandis Semen	1-desgalloylrugosin F	Not Available	FALSE	Oc1c(cc2c(c1O)c1c(cc(c(c1O)O)O)C(=O)OCC1C(OC2=O)C(C(C(O1)OC(=O)c1c(c(c(c(c1)O)O)O)c1c(c(c2c(c1)C(=O)OCC1C(OC(=O)c3c2c(c(c(c3)O)O)O)C2C(CO1)OC(=O)c1c(c3c(C(=O)O2)cc(c(c3O)O)O)c(c(c(c1)O)O)O)O)O)OC(=O)c1cc(O)c(O)c(O)c1)OC(=O)c1cc(O)c(O)c(O)c1)O
MOL009128	0.8920	0.1080	0.7228	Juglandis Semen	2,3-HHDP-D-glucopyranose	Not Available	FALSE	C1(C2C(C(OC1CO)O)OC(=O)c1c(c3c(cc(c(c3O)O)O)C(=O)O2)c(c(c(c1)O)O)O)O
MOL009129	0.7700	0.2300	0.6693	Juglandis Semen	6,7-methylene octadecanoate	Not Available	FALSE	C(=O)(CCCCC1C(CCCCCCCCCCC)C1)O
MOL009130	0.4096	0.5904	0.6545	Juglandis Semen	8,9-methylene octadecanoate	Not Available	FALSE	CCCCCCCCCC1CC1CCCCCCC(=O)OC
MOL009132	0.9353	0.0647	0.9713	Chebulae Fructus	3-Dehydroshikimate	439774	FALSE	C1(=CC(=O)C(C(C1)O)O)C(=O)O
MOL009133	0.8748	0.1252	0.6694	Maydis Seigma	Tannic acid (Corilagin)	452707	FALSE	O1C(C(O)C(OC(=O)c2cc(O)c(O)c(O)c2)C(O)C1OC(=O)c1cc(O)c(O)c(O)c1)COC(=O)c1cc(O)c(O)c(O)c(O)c1
MOL009133	0.8748	0.1252	0.6694	Farfarae Flos	Tannic acid (Corilagin)	452707	FALSE	O1C(C(O)C(OC(=O)c2cc(O)c(O)c(O)c2)C(O)C1OC(=O)c1cc(O)c(O)c(O)c1)COC(=O)c1cc(O)c(O)c(O)c(O)c1
MOL009133	0.8748	0.1252	0.6694	Chebulae Fructus	Tannic acid (Corilagin)	452707	FALSE	O1C(C(O)C(OC(=O)c2cc(O)c(O)c(O)c2)C(O)C1OC(=O)c1cc(O)c(O)c(O)c1)COC(=O)c1cc(O)c(O)c(O)c(O)c1
MOL009134	0.9348	0.0652	0.9421	Chebulae Fructus	D-Altro-3-heptulose	192877	FALSE	OC(C(O)C(=O)C(O)CO)C(O)CO
MOL009135	0.7911	0.2089	0.7084	Chebulae Fructus	ellipticine	3213	TRUE	c12c(c(c3c(c2C)cncc3)C)[nH]c2c1cccc2
MOL009136	0.7719	0.2281	0.7986	Chebulae Fructus	Peraksine	Not Available	FALSE	C1CCC2C(C1)[NH]C1C2CC2N3C1CC1C(C3C)COC(C21)O
MOL009137	0.2431	0.7569	0.8342	Chebulae Fructus	(R)-(6-methoxy-4-quinolyl)-[(2R,4R,5S)-5-vinylquinuclidin-2-yl]methanol	5748152	FALSE	OC(C1N2CC(C(C1)CC2)C=C)c1c2c(ncc1)ccc(OC)c2
MOL009138	0.9347	0.0653	0.7794	Chebulae Fructus	Teresautalic acid	Not Available	FALSE	OC(=O)C1(C2(C3C2CC1C3)C)C

MOL009139	0.9174	0.0826	0.8813	Chebulae Fructus	(2Z)-2-[(E)-3-cyano-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyprop-2-enylidene]butanedioic acid	5322040	FALSE	C1(C(C(C(C(O1)O/C(=C/C=C(\C(=O)O)/CC(=O)O)/C#N)O)O)O)CO
MOL009140	0.9328	0.0672	0.9490	Chebulae Fructus	Triglochinin_qt	Not Available	FALSE	O/C(=C/C=C(\C(=O)O)/CC(=O)O)/C#N
MOL009141	0.7218	0.2782	0.7370	Chebulae Fructus	(1S,4aR,6aR,6aS,6bR,8aR,9R,10R,11R,12aR,14bS)-1,10,11-trihydroxy-2,2,6a,6b,9,12a-hexamethyl-9-methylol-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	12444386	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3O)(C)C)C(=O)O)C)(CC2)C)(CC1O)C)(CO)C
MOL009142	0.9104	0.0896	0.8742	Chebulae Fructus	beta-Glucogallin	Not Available	FALSE	O1C(OC(=O)c2cc(O)c(O)c(O)c2)C(O)C(O)C(O)C1OC
MOL009143	0.7024	0.2976	0.7332	Chebulae Fructus	chebulagic acid	Not Available	FALSE	C12C3C(OC(=O)C(C4c5c(OC(=O)C4O)c(c(cc5C(=O)O2)O)O)O)CC(=O)O)C(OC1OC(=O)c1cc(c(c(c1)O)O)O)COC(=O)c1c(c2c(C(=O)O3)cc(c(c2O)O)O)c(c(c(c1O)O)O)O
MOL009144	0.8720	0.1280	0.7603	Phyllanthi Fructus	chebulinic acid	Not Available	FALSE	C12C(C(OC(=O)C(C3c4c(OC(=O)C3O)c(c(cc4C(=O)O2)O)O)O)CC(=O)O)C(OC1OC(=O)c1cc(c(c(c1)O)O)O)COC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O
MOL009144	0.8720	0.1280	0.7603	Chebulae Fructus	chebulinic acid	Not Available	FALSE	C12C(C(OC(=O)C(C3c4c(OC(=O)C3O)c(c(cc4C(=O)O2)O)O)O)CC(=O)O)C(OC1OC(=O)c1cc(c(c(c1)O)O)O)COC(=O)c1cc(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O
MOL009145	0.5247	0.4753	0.7003	Chebulae Fructus	chebupentol	Not Available	FALSE	C1(C(CC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(CO)CCC(C)(C)C(C4C3=CCC21)O)C)O)O

MOL009146	0.4314	0.5686	0.7167	Chebulae Fructus	punicalagin	Not Available	FALSE	C12C(OC(=O)c3c(c4c(C(=O)O2)cc(c(c4O)O)O)c(c(c(c3)O)O)O)C(OC2C1OC(=O)c1c(c3c4c5c6c(c(c7c(C(=O)OC2)cc(c(c7O)O)O)c(c(c6oc4=O)O)O)c(=O)oc5c(c3O)O)c(c(c(c1)O)O)O)O
MOL009146	0.4314	0.5686	0.7167	Granati Pericarpium	punicalagin	Not Available	FALSE	C12C(OC(=O)c3c(c4c(C(=O)O2)cc(c(c4O)O)O)c(c(c(c3)O)O)O)C(OC2C1OC(=O)c1c(c3c4c5c6c(c(c7c(C(=O)OC2)cc(c(c7O)O)O)c(c(c6oc4=O)O)O)c(=O)oc5c(c3O)O)c(c(c(c1)O)O)O)O
MOL009146	0.4314	0.5686	0.7167	Quisqualis Indica	punicalagin	Not Available	FALSE	C12C(OC(=O)c3c(c4c(C(=O)O2)cc(c(c4O)O)O)c(c(c(c3)O)O)O)C(OC2C1OC(=O)c1c(c3c4c5c6c(c(c7c(C(=O)OC2)cc(c(c7O)O)O)c(c(c6oc4=O)O)O)c(=O)oc5c(c3O)O)c(c(c(c1)O)O)O)O
MOL009148	0.3736	0.6264	0.8525	Chebulae Fructus	Catharanthamine	Not Available	FALSE	C1(C2(C3C4(C(C1(O)C(=O)OC)N(c1c4cc(c(c1)OC)C1(C4C5CN(CCc6c1[nH]c1c6cccc1)CC(C5)(O4)CC)C(=O)OC)C)CCN3CC=C2)CC)OC(=O)C
MOL009149	0.7142	0.2858	0.7972	Chebulae Fructus	Cheilanthifoline	Not Available	FALSE	c12c(CCN3Cc4c(CC13)ccc1OCOc41)cc(c(c2)OC)O
MOL009149	0.7142	0.2858	0.7972	Menispermi Rhizoma	Cheilanthifoline	Not Available	FALSE	c12c(CCN3Cc4c(CC13)ccc1OCOc41)cc(c(c2)OC)O
MOL009150	0.8802	0.1198	0.9058	Allii Tuberosi Semen	2-METHYLTHIOPHENE	11126	FALSE	s1c(ccc1)C
MOL009151	0.8168	0.1832	0.6410	Allii Tuberosi Semen	4-Methyltridecane	Not Available	FALSE	C(CCCCCCCCC)(CCC)C
MOL009153	0.9434	0.0566	0.8890	Allii Tuberosi Semen	Tuberosine B	Not Available	FALSE	c1ccc2c(c1)C(CCN2)(O)C(=O)O
MOL009154	0.3819	0.6181	0.7996	Allii Tuberosi Semen	Tuberostemoenone	Not Available	FALSE	C123C(=O)CCCCN1C(CC2=C1C(C3CC)OC(=O)C1C)C1OC(=O)C(C1)C
MOL009155	0.3743	0.6257	0.6911	Nelumbinis Plumula	14-Methyl-24-methylene-dihydromangiferodiol	Not Available	FALSE	OC1C(C2C3(C4(C3)C(C3(C(CC4)(C(CC3)C(CCC(=C)C(CO)C)C)C)CC2)CC1)(C)C
MOL009156	0.4142	0.5858	0.7796	Nelumbinis Plumula	4'-methyl-N-methylcoclaurine	Not Available	FALSE	O(c1cc2c(C(N(CC2)C)Cc2ccc(OC)cc2)cc1)C
MOL009157	0.4099	0.5901	0.7748	Nelumbinis Plumula	NSC90384	259803	FALSE	OC12C3C(C4(C(CC3)CC(O)CC4)C)C(O)CC1(C(CC2)c1ccc(=O)oc1)C
MOL009158	0.8628	0.1372	0.7428	Nelumbinis Plumula	Isolimocitrol-3-beta-D-glucoside	5318586	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)c(OC)c(O)c2OC)c1cc(O)c(OC)cc1)CO

MOL009159	0.8867	0.1133	0.8030	Nelumbinis Plumula	3,5,7-trihydroxy-2-(3-hydroxy-4-methoxy-phenyl)-6,8-dimethoxy-chromone	15290461	FALSE	Oc1c(oc2c(c1=O)c(O)c(OC)c(O)c2OC)c1cc(O)c(OC)cc1
MOL009160	0.8497	0.1503	0.9263	Nelumbinis Plumula	Loureirin A	5319081	FALSE	O(c1c(CCC(=O)c2ccc(O)cc2)ccc(OC)c1)C
MOL009161	0.9328	0.0672	0.8601	Nelumbinis Plumula	(1R)-6-methoxy-1,2-dimethyl-3,4-dihydro-1H-isoquinolin-7-ol	40091	FALSE	O(c1cc2c(C(N(CC2)C)C)cc1O)C
MOL009162	0.9525	0.0475	0.8475	Nelumbinis Plumula	N-Methylheliamine	27694	FALSE	O(c1cc2CCN(Cc2cc1OC)C)C
MOL009163	0.8708	0.1292	0.7843	Nelumbinis Plumula	Nelumboside	11968794	FALSE	O(C1C(O)C(O)C(OC1C(=O)O)Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1)C1OC(C(O)C(O)C1O)CO
MOL009163	0.8708	0.1292	0.7843	Folium Nelumbinis	Nelumboside	11968794	FALSE	O(C1C(O)C(O)C(OC1C(=O)O)Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1)C1OC(C(O)C(O)C1O)CO
MOL009164	0.3150	0.6850	0.7492	Nelumbinis Plumula	Nudicauline	Not Available	FALSE	C123C4C(CN(C1C(C4OC)(C1(C4C2CC(C4OC(=O)C)C(C1)OC)O)O)CC)(CCC3OC)COC(=O)c1c(N2C(=O)CC(C2=O)C)cccc1
MOL009165	0.8896	0.1104	0.9638	Nelumbinis Plumula	1-sulfinylpropane	441491	FALSE	CCC=S=O
MOL009166	0.8426	0.1574	0.8166	Nelumbinis Plumula	anonaine	Not Available	FALSE	O1c2c3c4C(NCCc4cc2OC1)Cc1c3cccc1
MOL009166	0.8426	0.1574	0.8166	Folium Nelumbinis	anonaine	Not Available	FALSE	O1c2c3c4C(NCCc4cc2OC1)Cc1c3cccc1
MOL009167	0.2916	0.7084	0.8158	Nelumbinis Plumula	(1R)-6,7-dimethoxy-1-(4-methoxybenzyl)-2-methyl-3,4-dihydro-1H-isoquinoline	821338	FALSE	O(c1cc2C(N(CCc2cc1OC)C)Cc1ccc(OC)cc1)C
MOL009168	0.1191	0.8809	0.8732	Nelumbinis Plumula	isoliensinine	5274591	FALSE	O(c1cc2C(N(CCc2cc1OC)C)Cc1ccc(OC)cc1)c1cc(CC2N(CCc3c2cc(O)c(OC)c3)C)ccc1O
MOL009169	0.0823	0.9177	0.9288	Nelumbinis Plumula	Liensinine	160644	FALSE	O(c1cc2C(N(CCc2cc1OC)C)Cc1ccc(O)cc1)c1cc(CC2N(CCc3c2cc(OC)c(OC)c3)C)ccc1O
MOL009170	0.5293	0.4707	0.6305	Nelumbinis Plumula	lotusine	5274587	FALSE	O(c1cc2C([N+](CCc2cc1O)(C)C)Cc1ccc(O)cc1)C

MOL009171	0.1180	0.8820	0.9138	Nelumbinis Plumula	Neferin	159654	FALSE	O(c1cc2C(N(CCc2cc1OC)C)Cc1ccc(OC)cc1)c1cc(CC2N(CCc3c2cc(OC)c(OC)c3)C)ccc1O
MOL009172	0.5069	0.4931	0.7542	Nelumbinis Plumula	Pronuciferin	Not Available	FALSE	O(c1c2C3(CC4N(CCc(c24)cc1OC)C)C=CC(=O)C=C3)C
MOL009173	0.6797	0.3203	0.7797	Nelumbinis Plumula	1,4-Di(p-tolyl)-trans-2-buten-1,4-dione	883995	FALSE	O=C(c1ccc(cc1)C)/C=C/C(=O)c1ccc(cc1)C
MOL009176	0.6669	0.3331	0.6508	Ephedrae Radix Et Rhizoma	ephedrannin A	Not Available	FALSE	c1(cc(c2c(c1)OC1(C(C2c2c3c(c(cc2O1)O)c(=O)c(c(o3)c1ccc(cc1)O)O)O)c1ccc(cc1)O)O)O
MOL009177	0.6109	0.3891	0.6118	Ephedrae Radix Et Rhizoma	ephedrannin B	Not Available	FALSE	c1(cc(c2c(c1)OC1(CC2c2c3c(c(cc2O1)O)c(=O)c(c(o3)c1ccc(cc1)O)O)c1ccc(cc1)O)O)O
MOL009178	0.6588	0.3412	0.6951	Ephedrae Radix Et Rhizoma	mahuannin A	Not Available	FALSE	O1C2(Oc3c(C(C2O)c2c1cc(O)c1c2OC(C(O)C1)c1ccc(O)cc1)c(O)cc(O)c3)c1ccc(O)cc1
MOL009179	0.6588	0.3412	0.6951	Ephedrae Radix Et Rhizoma	mahuannin B	Not Available	FALSE	c1(cc(c2c(c1)OC1(C(C2c2c3c(c(cc2O1)O)CC(C(O3)c1ccc(cc1)O)O)O)c1ccc(cc1)O)O)O
MOL009180	0.5795	0.4205	0.6580	Ephedrae Radix Et Rhizoma	Mahuannin D	Not Available	FALSE	O1C2(Oc3c(C(C2)c2c1cc(O)c1c2OC(C(O)C1)c1ccc(O)cc1)c(O)cc(O)c3)c1ccc(O)cc1
MOL009181	0.5795	0.4205	0.6580	Ephedrae Radix Et Rhizoma	mahuannin E	Not Available	FALSE	c1(cc(c2c(c1)OC1(CC2c2c3c(c(cc2O1)O)CC(C(O3)c1ccc(cc1)O)O)c1ccc(cc1)O)O)O
MOL009182	0.6542	0.3458	0.6526	Ephedrae Radix Et Rhizoma	mahuannin F	Not Available	FALSE	c12c(c(cc(c1)O)O)C1C(C(=O)O2)(c2ccc(cc2)O)Oc2c1c1c(c(c2)O)CC(C(O1)c1ccc(cc1)O)O
MOL009183	0.8895	0.1105	0.7264	Ephedrae Radix Et Rhizoma	(E,9S,12R,13R)-9,12,13-trihydroxyoctadec-10-enoic acid	11099581	FALSE	OC(CCCCC)C(O)/C=C/C(O)CCCCCCCC(=O)O
MOL009184	0.6542	0.3458	0.6526	Ephedrae Radix Et Rhizoma	mahuannin G	Not Available	FALSE	c1(ccc(cc1)C12C(=O)Oc3c(C1c1c(cc(c4c1OC(C(C4)O)c1ccc(cc1)O)O)O2)c(cc(c3)O)O)O
MOL009185	0.6637	0.3363	0.6853	Ephedrae Radix Et Rhizoma	mahuannin H	Not Available	FALSE	C1(C2(C(c3c(O1)cc(cc3O)O)c1c(cc(c3c1OC(C(C3)O)c1ccc(cc1)O)O)O2)c1ccc(cc1)O)O
MOL009186	0.6637	0.3363	0.6853	Ephedrae Radix Et Rhizoma	mahuannin I	Not Available	FALSE	C1(C2(C(c3c(O1)cc(cc3O)O)c1c(cc(c3c1OC(C(C3)O)c1ccc(cc1)O)O)O2)c1ccc(cc1)O)O
MOL009187	0.6732	0.3268	0.6500	Ephedrae Radix Et Rhizoma	mahuannin J	Not Available	FALSE	C1(C2(C(c3c(O1)cc(cc3O)O)c1c(cc(c3c1oc(c(c3=O)O)c1ccc(cc1)O)O)O2)c1ccc(cc1)O)O
MOL009188	0.6732	0.3268	0.6500	Ephedrae Radix Et Rhizoma	mahuannin K	Not Available	FALSE	C1(C2(C(c3c(O1)cc(cc3O)O)c1c(cc(c3c1oc(c(c3=O)O)c1ccc(cc1)O)O)O2)c1ccc(cc1)O)O
MOL009189	0.9570	0.0430	0.9684	Ephedrae Radix Et Rhizoma	Tybraine	64782	FALSE	c1cccc(c1)C(C(C)N(C)C)O
MOL009189	0.9570	0.0430	0.9684	Ephedra Herba	Tybraine	64782	FALSE	c1cccc(c1)C(C(C)N(C)C)O
MOL009190	0.9518	0.0482	0.9786	Ephedra Herba	Usaf cs-6	10297	TRUE	c1cccc(c1)C(C(C)N)O
MOL009190	0.9518	0.0482	0.9786	Ephedrae Radix Et Rhizoma	Usaf cs-6	10297	TRUE	c1cccc(c1)C(C(C)N)O

MOL009191	0.9518	0.0482	0.9786	Ephedrae Radix Et Rhizoma	Cathine	441457	FALSE	c1cccc(c1)C(C(C)N)O
MOL009192	0.9570	0.0430	0.9684	Ephedrae Radix Et Rhizoma	(1R,2R)-2-dimethylamino-1-phenylpropan-1-ol	5706040	FALSE	OC(C(N(C)C)C)c1ccccc1
MOL009194	0.9570	0.0430	0.9684	Ephedra Herba	()-N-Methylpseudoephedrine	7059596	FALSE	OC(C(N(C)C)C)c1ccccc1
MOL009194	0.9570	0.0430	0.9684	Ephedrae Radix Et Rhizoma	()-N-Methylpseudoephedrine	7059596	FALSE	OC(C(N(C)C)C)c1ccccc1
MOL009195	0.9631	0.0369	0.9156	Ephedrae Radix Et Rhizoma	(4S,5R)Ephedroxane	12153184	FALSE	c1(ccccc1)C1OC(=O)N(C1C)C
MOL009198	0.3461	0.6539	0.8600	Myristicae Semen	(+)-Anwulignan	10404245	FALSE	c1(c(ccc(c1)CC(C(C)Cc1ccc2c(c1)OCO2)C)O)OC
MOL009198	0.3461	0.6539	0.8600	Schisandrae Sphenantherae Fructus	(+)-Anwulignan	10404245	FALSE	c1(c(ccc(c1)CC(C(C)Cc1ccc2c(c1)OCO2)C)O)OC
MOL009199	0.3587	0.6413	0.6248	Schisandrae Sphenantherae Fructus	Interiotherin B	Not Available	FALSE	OC1(C(Cc2c(c3c(C1OC(=O)/C(=C/C)/C)cc1OCOc1c3OC)c(OC)c1OCOc1c2)C)C
MOL009200	0.5463	0.4537	0.7003	Schisandrae Sphenantherae Fructus	changnanic acid	Not Available	FALSE	C12(C(CCC3C1(C2)CCC1(C3(CCC1C(C)CC/C=C(/C)\C(=O)O)C)C)C(=C)C)CCC(=O)O
MOL009201	0.1332	0.8668	0.6011	Schisandrae Sphenantherae Fructus	heteroclitin A	Not Available	FALSE	c12c(c3c(C(C(C(C1)C)C)OC(=O)C(C)CC)cc1c(c3OC)OCO1)c(c(c(c2)OC)OC)OC
MOL009202	0.1282	0.8718	0.6046	Schisandrae Sphenantherae Fructus	heteroclitin B	Not Available	FALSE	c12c(c3c(C(C(C(C1)C)C)OC(=O)/C(=C/C)/C)cc1c(c3OC)OCO1)c(c(c(c2)OC)OC)OC
MOL009203	0.1282	0.8718	0.6046	Schisandrae Sphenantherae Fructus	heteroclitin C	Not Available	FALSE	c12c(c3c(C(C(C(C1)C)C)OC(=O)/C(=C\C)/C)cc1c(c3OC)OCO1)c(c(c(c2)OC)OC)OC
MOL009204	0.2193	0.7807	0.6822	Schisandrae Sphenantherae Fructus	heteroclitin D	Not Available	FALSE	C12=CC(=C(C(=O)C31c1c(C(C(C(C2)C)C)OC(=O)/C(=C/C)/C)cc2c(c1OC3)OCO2)OC)OC
MOL009205	0.3556	0.6444	0.6776	Schisandrae Sphenantherae Fructus	heteroclitin E	Not Available	FALSE	C12=CC(=C(C(=O)C31c1c(C(C(C(C2O)C)C)OC(=O)/C(=C/C)/C)cc2c(c1OC3)OCO2)OC)OC
MOL009207	0.6617	0.3383	0.8075	Schisandrae Sphenantherae Fructus	heteroclitin G	Not Available	FALSE	c12c(cc3c(c1OC)C14C(C3O)(C(CC1=CC(=C(C4=O)C)OC)C)C)OCO2
MOL009208	0.2181	0.7819	0.6649	Schisandrae Sphenantherae Fructus	interiotherin A	Not Available	FALSE	O(C1C(C(Cc2c(c3c1cc1OCOc1c3OC)c(OC)c1OCOc1c2)C)C)C(=O)c1ccccc1
MOL009209	0.2752	0.7248	0.7362	Schisandrae Sphenantherae Fructus	Kadsulactone A	Not Available	FALSE	OC1C2C3(C4(C(C5(C(CC4)(C(CC5)C(C4OC(=O)C(=CC4)C)C)C)C)C1)C3)C=CC(=O)OC2(C)C
MOL009210	0.2632	0.7368	0.7093	Schisandrae Sphenantherae Fructus	Kadsulignan C	Not Available	FALSE	c12cc3c4c(c1OCO2)OCC14C(=O)C(=C(C=C1C(C(C(C3OC(=O)c1ccccc1)C)(O)C)OC(=O)C)OC)OC
MOL009211	0.2592	0.7408	0.7516	Schisandrae Sphenantherae Fructus	kadsulactone	Not Available	FALSE	C1C(=O)C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C(CC2)C(C1OC(=O)C(=CC1)C)C)C)C)C3)(C)C

MOL009212	0.3588	0.6412	0.7208	Schisandrae Sphenantherae Fructus	kadsulignan A	Not Available	FALSE	c12C34C(=CC(=O)C(=C4OC)OC)CC(C(C(c1cc(c(c2OC)OC)OC)O3)C)C
MOL009213	0.3242	0.6758	0.6555	Schisandrae Sphenantherae Fructus	kadsulignan B	Not Available	FALSE	c12C34C(=CC(=O)C(=C4OC)OC)C(C(C(C(c1cc(c(c2OC)OC)OC)O3)C)C)OC(=O)C
MOL009214	0.3027	0.6973	0.6912	Kadsurae Coccineae Radix Et Caulis	Kadsuranin	Not Available	FALSE	O1c2cc3CC(C(Cc4c(c3c(OC)c2OC1)c(OC)c(OC)c(OC)c4)C)C
MOL009214	0.3027	0.6973	0.6912	Schisandrae Sphenantherae Fructus	Kadsuranin	Not Available	FALSE	O1c2cc3CC(C(Cc4c(c3c(OC)c2OC1)c(OC)c(OC)c(OC)c4)C)C
MOL009215	0.2974	0.7026	0.6501	Schisandrae Sphenantherae Fructus	Kadsurin	Not Available	FALSE	O(C1C(C(Cc2c(c3c1cc1OCOc1c3OC)c(OC)c(OC)c(OC)c2)C)C)C(=O)C
MOL009217	0.5152	0.4848	0.7293	Schisandrae Sphenantherae Fructus	neokadsuranic acid A	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=CC3C(C1CC2)(CCC(C3=C)C(CC/C=C(/C)\C(=O)O)C)C)(C)C
MOL009218	0.5207	0.4793	0.7136	Schisandrae Sphenantherae Fructus	neokadsuranic acid B	Not Available	FALSE	C1C(=O)C(C2C(C1)(C)C1=C(CC2)C2(C(C1)C(=C)C(CC2)C(C)CC/C=C(/C)\C(=O)O)C)(C)C
MOL009219	0.5091	0.4909	0.6728	Schisandrae Sphenantherae Fructus	neokadsuranic acid C	Not Available	FALSE	C1C(=O)C(C2C(C1)(C)C1=C(CC2)C2(C(C1)C(C(CC2)C(C)CC/C=C(/C)\C(=O)O)O)C)(C)C
MOL009220	0.4902	0.5098	0.7167	Schisandrae Sphenantherae Fructus	neokadsurani n	Not Available	FALSE	O1c2cc3C4C(C(C(c5c(c3c(OC)c2OC1)c(OC)c(OC)c(OC)c5)O4)C)C
MOL009221	0.1654	0.8346	0.7394	Schisandrae Sphenantherae Fructus	Kadsulignan D	Not Available	FALSE	c12cc3c4c(c1OCO2)OCC14C(=O)C(=C(C=C1C(C(C(C3OC(=O)/C(=C/C)/C)C)(O)C)OC(=O)/C(=C/C)/C)OC)OC
MOL009222	0.1499	0.8501	0.7082	Schisandrae Sphenantherae Fructus	schisanlacton e A	Not Available	FALSE	C1(=O)C=CC2=CC3=C(CCC2C(O1)(C)C)C1(C(CC3)(C(CC1)C(C)C1CC=C(C(=O)O1)C)C)C
MOL009223	0.2231	0.7769	0.7415	Schisandrae Sphenantherae Fructus	schisanlacton e B	Not Available	FALSE	O1C(C2C3(C4(C(C5(C(CC4)(C(CC5)C(C4OC(=O)C(=CC4)C)C)C)C)CC2)C3)C=CC1=O)(C)C
MOL009224	0.5276	0.4724	0.7028	Schisandrae Sphenantherae Fructus	schisanlacton e E	Not Available	FALSE	C1(=O)C(=CCC(O1)C(C1C2(C(CC1)(C)C1C3(CC2)C(C(CC1)C(=C)C)(C3)CCC(=O)O)C)C)C
MOL009225	0.2592	0.7408	0.7516	Schisandrae Sphenantherae Fructus	schisanlacton e F	Not Available	FALSE	C1C(=O)C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C(CC2)C(C)C1OC(=O)C(=CC1)C)C)C)C3)(C)C
MOL009226	0.0635	0.9365	0.8044	Schisandrae Sphenantherae Fructus	schisantherin J	Not Available	FALSE	c12c(c3c(cc1OCO2)C(C(C(C(c1c3c(c(c(c1)OC)OC)OC)OC(=O)c1ccccc1)(C)O)C)OC(=O)C(C)CC)OC
MOL009227	0.3748	0.6252	0.6250	Schisandrae Sphenantherae Fructus	schisantherin L	Not Available	FALSE	c12c(cc3c(c1OC)c1c(C(C(C(C3O)C)C)OC(=O)/C(=C/C)/C)cc3c(c1OC)OCO3)OCO2
MOL009228	0.1358	0.8642	0.7026	Schisandrae Sphenantherae Fructus	schisantherin M	Not Available	FALSE	c12c(cc3c(c1OC)c1c(C(C(C(C3OC(=O)/C(=C\C)/C)C)C)OC(=O)/C(=C/C)/C)cc3c(c1OC)OCO3)OCO2
MOL009229	0.6593	0.3407	0.7576	Schisandrae Sphenantherae Fructus	schizandronic acid	Not Available	FALSE	C1C(=O)C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C(CC2)C(CC/C=C(/C)\C(=O)O)C)C)C)C3)(C)C
MOL009230	0.1916	0.8084	0.6684	Schisandrae Sphenantherae Fructus	taiwanschirin D	Not Available	FALSE	c12c3C(C(C(C/C(=C/C(=O)OC)/C1(C(=O)C(=O)OC)COc2c1c(c3)OOC1)C)C)OC(=O)CCCCC
MOL009231	0.2965	0.7035	0.7269	Schisandrae Sphenantherae Fructus	Kadsulignan E	Not Available	FALSE	c12cc3c4c(c1OCO2)OCC14C(=C(C(=O)C=C1C(C(C(C3OC(=O)c1ccccc1)C)(O)C)OC(=O)C)OC)OC
MOL009232	0.3669	0.6331	0.6750	Schisandrae Sphenantherae Fructus	Kadsulignan F	Not Available	FALSE	c12cc3c4c(c1OCO2)OCC14C(=C(C(=O)C=C1C(C(C(C3OC(=O)C)C)(O)C)OC(=O)/C(=C/C)/C)OC)OC

MOL009233	0.1606	0.8394	0.7556	Schisandrae Sphenantherae Fructus	Kadsulignan G	Not Available	FALSE	c12cc3c4c(c1OCO2)OCC14C(=C(C(=O)C=C1C(C(C(C3OC(=O)/C(=C/C)/C)C)(O)C)OC(=O)/C(=C/C)/C)OC)OC
MOL009234	0.1464	0.8536	0.7564	Schisandrae Sphenantherae Fructus	angusifolin A	Not Available	FALSE	c12c(c3c(cc1OCO2)C(C(C(Cc1c3c(c2c(c1)OCO2)OC)(C)OC(=O)c1ccccc1)C)OC(=O)c1ccccc1)OC
MOL009235	0.2276	0.7724	0.6782	Schisandrae Sphenantherae Fructus	angusifolin B	Not Available	FALSE	c12c(c3c(cc1OCO2)C(C(C(Cc1c3c(c2c(c1)OCO2)OC)(C)OC(=O)c1ccccc1)C)OC(=O)C)OC
MOL009236	0.2903	0.7097	0.6765	Schisandrae Sphenantherae Fructus	angusifolin C	Not Available	FALSE	c12c(c3c(cc1OCO2)C(C(C(Cc1c3c(c2c(c1)OCO2)OC)(C)OC(=O)c1ccccc1)C)O)OC
MOL009237	0.2220	0.7780	0.8300	Myristicae Semen	2,3-dihydro-7-methoxy-2-(3-methoxy-4,5-methylenedioxyphenyl)-3-methyl-5-(E)-propenyl-benzofuran	52326145	FALSE	O1C(C(c2c1c(cc(c2)/C=C/C)OC)C)c1cc(c2c(c1)OCO2)OC
MOL009238	0.9339	0.0661	0.9085	Eriobotryae Folium	Methoxyeugenol	226486	FALSE	c1(c(cc(cc1OC)CC=C)OC)O
MOL009238	0.9339	0.0661	0.9085	Myristicae Semen	Methoxyeugenol	226486	FALSE	c1(c(cc(cc1OC)CC=C)OC)O
MOL009239	0.5049	0.4951	0.7924	Myristicae Semen	4-[(1R,2S)-2-(4-allyl-2,6-dimethoxyphenoxy)-1-hydroxypropyl]-2-methoxyphenol	21636106	FALSE	c1(c(ccc(c1)C(C(C)Oc1c(cc(cc1OC)CC=C)OC)O)O)OC
MOL009240	0.4262	0.5738	0.8643	Myristicae Semen	4-[(2R,3R,4S,5S)-5-(1,3-benzodioxol-5-yl)-3,4-dimethyl-2-tetrahydrofuranyl]-2-methoxyphenol	10450045	FALSE	C1(C(OC(C1C)c1ccc(c(c1)OC)O)c1cc2c(cc1)OCO2)C

MOL009241	0.2940	0.7060	0.7578	Myristicae Semen	2,6-dimethoxy-4-[(2S,3S)-7-methoxy-3-methyl-5-[(E)-prop-1-enyl]-2,3-dihydrobenzofuran-2-yl]phenol	11703153	FALSE	c1c(c2c(cc1/C=C/C)C(C(O2)c1cc(c(c(c1)OC)O)OC)C)OC
MOL009242	0.4262	0.5738	0.8643	Myristicae Semen	4-[(2R,3S,4S,5S)-5-(1,3-benzodioxol-5-yl)-3,4-dimethyl-2-tetrahydrofuranyl]-2-methoxyphenol	10088741	FALSE	C1(C(C(OC1c1ccc(c(c1)OC)O)c1cc2c(cc1)OCO2)C)C
MOL009243	0.4423	0.5577	0.6621	Myristicae Semen	Isoguaiacin	Not Available	FALSE	c1(c(cc2c(c1)CC(C(C2c1ccc(c(c1)OC)O)C)C)O)OC
MOL009244	0.5394	0.4606	0.8440	Myristicae Semen	Machilin D	13939327	FALSE	c1cc(cc(c1O)OC)C(C(Oc1c(cc(cc1)/C=C/C)OC)C)O
MOL009245	0.4869	0.5131	0.8142	Myristicae Semen	Myristargenol A	26195072	FALSE	c1(c(cc(cc1)C(C(C(Cc1ccc2c(c1)OCO2)C)C)O)OC)O
MOL009246	0.6871	0.3129	0.8063	Myristicae Semen	Myristargenol B	26195071	FALSE	c1(c(cc(cc1)CC(C(C(c1cc(c(cc1)O)OC)O)C)C)OC)O
MOL009247	0.6564	0.3436	0.7293	Myristicae Semen	Phenol, 4,4'-((2R,3R,4S,5S)-tetrahydro-3,4-dimethyl-2,5-furandiyl)bis(2-methoxy-, rel-	156517	FALSE	C1(C(OC(C1C)c1ccc(c(c1)OC)O)c1cc(c(cc1)O)OC)C
MOL009248	0.2988	0.7012	0.8525	Myristicae Semen	Licarin A	5281836	FALSE	c1(cc(c2c(c1)C(C(O2)c1cc(c(cc1)O)OC)C)OC)/C=C/C
MOL009250	0.8192	0.1808	0.6602	Myristicae Semen	OKO	3039	FALSE	COP(=O)(OC)OC=C(Cl)Cl

MOL009251	0.3461	0.6539	0.8600	Myristicae Semen	4-[(2R,3S)-4-(1,3-benzodioxol-5-yl)-2,3-dimethylbutyl]-2-methoxyphenol	10381847	FALSE	c1c(cc2c(c1)OCO2)CC(C(Cc1cc(c(cc1)O)OC)C)C
MOL009252	0.9580	0.0420	0.7912	Myristicae Semen	(1R,4S,5S)-1-isopropyl-4-methyl-4-bicyclo[3.1.0]hexanol	11228920	FALSE	C1C(C2C(C1)(C2)C(C)C)(C)O
MOL009252	0.9580	0.0420	0.7912	Citri Sarcodactylis Fructus	(1R,4S,5S)-1-isopropyl-4-methyl-4-bicyclo[3.1.0]hexanol	11228920	FALSE	C1C(C2C(C1)(C2)C(C)C)(C)O
MOL009253	0.6411	0.3589	0.6495	Myristicae Semen	4-[(2S,3S,4R,5R)-5-(4-hydroxy-3-methoxyphenyl)-3,4-dimethyloxolan-2-yl]-2,6-dimethoxyphenol	13870579	FALSE	c1c(c(c(cc1C1OC(C(C1C)C)c1ccc(c(c1)OC)O)OC)O)OC
MOL009254	0.3840	0.6160	0.8486	Myristicae Semen	galbacin	11175182	FALSE	c1c2c(ccc1C1OC(C(C1C)C)c1ccc3c(c1)OCO3)OCO2
MOL009255	0.2693	0.7307	0.8993	Myristicae Semen	5-[(2S,3S)-7-methoxy-3-methyl-5-[(E)-prop-1-enyl]-2,3-dihydrobenzofuran-2-yl]-1,3-benzodioxole	10860310	FALSE	O1C(C(c2c1c(OC)cc(c2)/C=C/C)C)c1cc2OCOc2cc1
MOL009256	0.4450	0.5550	0.7023	Myristicae Semen	MALABARICONE B	163001	FALSE	c1(cccc(c1C(=O)CCCCCCCCc1ccc(cc1)O)O)O
MOL009257	0.4653	0.5347	0.6731	Myristicae Semen	MALABARICONE C	100313	FALSE	c1(cccc(c1C(=O)CCCCCCCCc1cc(c(cc1)O)O)O)O
MOL009259	0.2469	0.7531	0.6068	Myristicae Semen	Kudos	40463	FALSE	c1(cccc1OC1ccccc1)COC(=O)C1C(C1C=C(C)C)(C)C

MOL009260	0.9664	0.0336	0.9487	Myristicae Semen	IPMC	4944	TRUE	c1(ccccc1OC(=O)NC)OC(C)C
MOL009261	0.6991	0.3009	0.7038	Myristicae Semen	Propranolol, L-	91536	TRUE	c1c(c2c(cc1)cccc2)OCC(O)CNC(C)C
MOL009262	0.9757	0.0243	0.9667	Myristicae Semen	S-Atenolol	175540	FALSE	O=C(N)Cc1ccc(OCC(O)CNC(C)C)cc1
MOL009263	0.6564	0.3436	0.7293	Myristicae Semen	saucernetindiol	40580526	FALSE	c1c(c(ccc1C1OC(C(C1C)C)c1ccc(c(c1)OC)O)O)OC
MOL009264	0.6564	0.3436	0.7293	Myristicae Semen	tetrahydrofuroguaiacin B	13870572	FALSE	c1c(c(ccc1C1OC(C(C1C)C)c1ccc(c(c1)OC)O)O)OC
MOL009265	0.4497	0.5503	0.7000	Myristicae Semen	threo-austrobailignan-5	Not Available	FALSE	c1(c(cc2c(c1)C=C(C(C2c1ccc(c(c1)OC)O)C)C)O)OC
MOL009266	0.9620	0.0380	0.8042	Myristicae Semen	trans-carane-cis 4-ol	Not Available	FALSE	C12CC(C(CC1C2(C)C)O)C
MOL009267	0.6564	0.3436	0.7293	Myristicae Semen	4-[(2R,3S,4S,5S)-5-(4-hydroxy-3-methoxyphenyl)-3,4-dimethyloxolan-2-yl]-2-methoxyphenol	10736226	FALSE	c1c(c(ccc1C1OC(C(C1C)C)c1ccc(c(c1)OC)O)O)OC
MOL009268	0.9564	0.0436	0.9425	Myristicae Semen	2',4'-Dimethoxypropiophenone	70020	FALSE	C(=O)(CC)c1c(cc(cc1)OC)OC
MOL009269	0.9085	0.0915	0.8281	Granati Pericarpium	luteolin 7-O-glycoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2oc(cc(=O)c2c(O)c1)c1cc(O)c(O)cc1)CO
MOL009270	0.9369	0.0631	0.8180	Granati Pericarpium	officinalisin	Not Available	FALSE	C1(C(COC2(C1(CO)C2O)OCCCC)O)O
MOL009271	0.9573	0.0427	0.9256	Granati Pericarpium	09762_FLUKA	6602484	FALSE	O=C1CC2N(C(CCC2)C1)C
MOL009272	0.7465	0.2535	0.7058	Quisqualis Indica	Punicalin	Not Available	FALSE	c12c3c4c5c(c6c(C(=O)OCC7C(OC(=O)c8c(c1c(c(c3oc5=O)O)O)c(c(c(c8)O)O)O)C(C(C(O7)O)O)O)cc(c(c6O)O)O)c(c(c4oc2=O)O)O
MOL009272	0.7465	0.2535	0.7058	Granati Pericarpium	Punicalin	Not Available	FALSE	c12c3c4c5c(c6c(C(=O)OCC7C(OC(=O)c8c(c1c(c(c3oc5=O)O)O)c(c(c(c8)O)O)O)C(C(C(O7)O)O)O)cc(c(c6O)O)O)c(c(c4oc2=O)O)O
MOL009273	0.9461	0.0539	0.9434	Granati Pericarpium	1-Methyl-3-isopropoxy cyclohexane	Not Available	FALSE	C1CCC(CC1C)OC(C)C
MOL009274	0.3019	0.6981	0.7047	Granati Pericarpium	Fritillaziebinol	Not Available	FALSE	ClCC1(O)C2CC3(C(C4(C(CC3)C(CCC4)(C)C)C)CC2)C1

MOL009275	0.8057	0.1943	0.7601	Granati Pericarpium	casuarinin	Not Available	FALSE	c1(c(cc2c(c1O)c1c3c(c(c(c1O)O)O)C(O)C(OC3=O)C(OC2=O)C1OC(=O)c2cc(c(c(c2c2c(C(=O)OCC1OC(=O)c1cc(c(c(c1)O)O)O)cc(c(c2O)O)O)O)O)O)O)O
MOL009276	0.6219	0.3781	0.7447	Granati Pericarpium	granatin B	Not Available	FALSE	c1(cc(c(c(c1)O)O)O)C(=O)OC1C2C3C(C(O1)COC(=O)c1c(c(c(c(c1)O)O)O)c1c(c(c(cc1C(=O)O3)O)O)O)OC(=O)c1c3C4C(C(O)(O)C(=O)C=C4C(=O)O2)(Oc3c(c(c1)O)O)O
MOL009277	0.6169	0.3831	0.6128	Astragali Cpmplanatisemen	formononetin-7-O-beta-D-glucoside	Not Available	FALSE	c1(ccc2c(c1)occ(c2=O)c1ccc(cc1)OC)OC1C(O)C(O)C(O)C(O1)CO
MOL009278	0.9325	0.0675	0.9087	Ginkgo Folium	Laricitrin	5282154	FALSE	o1c(c2cc(OC)c(O)c(O)c2)c(O)c(=O)c2c1cc(O)cc2O
MOL009278	0.9325	0.0675	0.9087	Ardisiae Japonicae Herba	Laricitrin	5282154	FALSE	o1c(c2cc(OC)c(O)c(O)c2)c(O)c(=O)c2c1cc(O)cc2O
MOL009278	0.9325	0.0675	0.9087	Astragali Cpmplanatisemen	Laricitrin	5282154	FALSE	o1c(c2cc(OC)c(O)c(O)c2)c(O)c(=O)c2c1cc(O)cc2O
MOL009279	0.9107	0.0893	0.8017	Astragali Cpmplanatisemen	laricitrin-3-O-bata-glucopyranoside	Not Available	FALSE	c1c(cc(c2c1oc(c(c2=O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(c(c1)OC)O)O)O)O
MOL009280	0.9067	0.0933	0.7966	Astragali Cpmplanatisemen	4H-1-Benzopyran-4-one, 2-(3-(beta-D-glucopyranosyloxy)-4-hydroxy-5-methoxyphenyl)-3,5,7-trihydroxy-	5487255	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc(cc(OC)c1O)c1oc2c(c(=O)c1O)c(O)cc(O)c2)CO
MOL009280	0.9067	0.0933	0.7966	Ardisiae Japonicae Herba	4H-1-Benzopyran-4-one, 2-(3-(beta-D-glucopyranosyloxy)-4-hydroxy-5-methoxyphenyl)-3,5,7-trihydroxy-	5487255	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc(cc(OC)c1O)c1oc2c(c(=O)c1O)c(O)cc(O)c2)CO

MOL009281	0.8020	0.1980	0.7398	Astragali Cpmplanatisemen	4H-1-Benzopyran-4-one, 3-((6-O-acetyl-beta-D-glucopyranosyl)oxy)-5-hydroxy-2-(4-hydroxyphenyl)-7-methoxy-	5487254	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(OC)c2)c1ccc(O)cc1)COC(=O)C
MOL009282	0.8975	0.1025	0.8169	Equiseti Hiemalis Herba	Quercetin-3-O-.beta.-D-glucopyranoside	15959354	FALSE	O(C1CC(C(O)C(O)C1O)CO)c1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1
MOL009282	0.8975	0.1025	0.8169	Astragali Cpmplanatisemen	Quercetin-3-O-.beta.-D-glucopyranoside	15959354	FALSE	O(C1CC(C(O)C(O)C1O)CO)c1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1
MOL009284	0.8652	0.1348	0.8161	Astragali Cpmplanatisemen	rhamnocitrin-3-O-beta-glucoside	Not Available	FALSE	c1c(cc(c2c1oc(c(c2=O)OC1C(C(C(C(O1)CO)O)O)O)O)c1ccc(cc1)O)O)OC
MOL009289	0.7297	0.2703	0.6712	Astragali Cpmplanatisemen	Calycosin-7-O-beta-D-glucopyranoside	Not Available	FALSE	c1cc(cc2c1c(=O)c(co2)c1cc(c(cc1)OC)O)OC1OC(C(C(C1O)O)O)CO
MOL009290	0.7297	0.2703	0.6712	Astragali Cpmplanatisemen	calycosin-7-O-beta-D-glucoside	Not Available	FALSE	c1(ccc2c(c1)occ(c2=O)c1ccc(c(c1)O)OC)OC1C(O)C(O)C(O)C(O1)CO
MOL009291	0.9263	0.0737	0.8212	Astragali Cpmplanatisemen	cannabiscitrin	Not Available	FALSE	c1c(cc(c2c1oc(cc2=O)c1cc(c(c(c1)O)O)OC1OC(C(C(C1O)O)O)CO)O)O
MOL009292	0.9385	0.0615	0.9002	Ginkgo Folium	MYF	5281701	FALSE	c1c(cc(c2c1oc(cc2=O)c1cc(c(c(c1)O)O)O)O)O)O
MOL009292	0.9385	0.0615	0.9002	Astragali Cpmplanatisemen	MYF	5281701	FALSE	c1c(cc(c2c1oc(cc2=O)c1cc(c(c(c1)O)O)O)O)O)O
MOL009293	0.8650	0.1350	0.8281	Astragali Cpmplanatisemen	complanatuside	Not Available	FALSE	c1c(cc(c2c1oc(c(c2=O)OC1C(C(C(C(O1)CO)O)O)O)O)c1ccc(cc1)OC1C(C(C(C(O1)CO)O)O)O)O)OC
MOL009294	0.9247	0.0753	0.9435	Saussureae Involucratae Herba	LOF	444718	FALSE	OC(Cc1ccccc1)C(=O)O
MOL009295	0.7958	0.2042	0.7413	Saussureae Involucratae Herba	Flazin	5377686	FALSE	o1c(c2nc(cc3c2[nH]c2c3cccc2)C(=O)O)ccc1CO
MOL009295	0.7958	0.2042	0.7413	Momordicae Fructus	Flazin	5377686	FALSE	o1c(c2nc(cc3c2[nH]c2c3cccc2)C(=O)O)ccc1CO
MOL009297	0.8883	0.1117	0.8903	Saussureae Involucratae Herba	jaceosidin	5379096	FALSE	o1c2c(c(O)c(OC)c(O)c2)c(=O)cc1c1cc(OC)c(O)cc1

MOL009298	0.8246	0.1754	0.8107	Saussureae Involucratae Herba	Oroselol	160600	FALSE	o1c(C(O)(C)C)cc2c1ccc1c2oc(=O)cc1
MOL009298	0.8246	0.1754	0.8107	Nardostachyos Radix Et Rhizoma	Oroselol	160600	FALSE	o1c(C(O)(C)C)cc2c1ccc1c2oc(=O)cc1
MOL009299	0.9190	0.0810	0.8272	Saussureae Involucratae Herba	scopolin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(OC)cc2c(oc(=O)cc2)c1)CO
MOL009300	0.8645	0.1355	0.7802	Saussureae Involucratae Herba	Azuleno(4,5-b)furan-2(3H)-one, decahydro-4-hydroxy-3-methyl-6,9-bis(methylene)-, (3R-(3alpha,3abeta,4alpha,6abeta,9abeta,9balpha))-	147111	FALSE	O1C2C3C(CCC3=C)C(=C)CC(O)C2C(C1=O)C
MOL009301	0.9316	0.0684	0.9577	Saussureae Involucratae Herba	Xylitol	Not Available	FALSE	C(C(C(C(CCO)O)O)O)CO
MOL009302	0.9132	0.0868	0.9658	Cuscutae Semen	ZINC02034518	6999790	FALSE	OC(C)C=C
MOL009303	0.7451	0.2549	0.7246	Cuscutae Semen	Cuscutoside B	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)CO1)c1cc2OCOc2cc1C1OCC2C1COC2c1cc2OCOc2cc1
MOL009304	0.9091	0.0909	0.6745	Cuscutae Semen	InChI=1/C12H16N2O/c1-13-6-9-5-10(8-13)11-3-2-4-12(15)14(11)7-9/h2-4,9-10H,5-8H2,1H	Not Available	FALSE	O=c1n2CC3CC(CN(C3)C)c2ccc1
MOL009305	0.8995	0.1005	0.7288	Sojae Semen Nigrum	Vincubine	13220	FALSE	O=C1CC(NC(C1)(C)C)(C)C
MOL009305	0.8995	0.1005	0.7288	Mume Fructus	Vincubine	13220	FALSE	O=C1CC(NC(C1)(C)C)(C)C
MOL009306	0.8818	0.1182	0.9667	Mume Fructus	tert-Butylurea	14233	FALSE	O=C(NC(C)(C)C)N
MOL009307	0.8473	0.1527	0.8023	Mume Fructus	Naringenin-4'-glucoside-7-neohesperidoside	Not Available	FALSE	C1(C(C(C(OC1CO)Oc1cc(c2c(c1)OC(CC2=O)c1ccc(cc1)OC1OC(C(C(C1O)O)O)CO)O)OC1OC(C(C(C1O)O)O)C)O)O
MOL009308	0.9133	0.0867	0.8176	Mume Fructus	Thujin	5359430	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1)C

MOL009308	0.9133	0.0867	0.8176	Eriobotryae Folium	Thujin	5359430	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1)C
MOL009309	0.8619	0.1381	0.8024	Mume Fructus	2-(3,4-dihydroxyphenyl)-5-hydroxy-7-methoxy-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxychromen-4-one	5491382	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(OC)c2)c1cc(O)c(O)cc1)C
MOL009310	0.8182	0.1818	0.8119	Mume Fructus	Rhamnocitrin 3-rhamnoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(OC)c2)c1ccc(O)cc1)C
MOL009312	0.8390	0.1610	0.7279	Dipsaci Radix	(E,E)-3,5-Di-O-caffeoylquinic acid	Not Available	FALSE	O(C1CC(O)(CC(OC(=O)/C=C/c2cc(O)c(O)cc2)C1O)C(=O)O)C(=O)/C=C/c1cc(O)c(O)cc1
MOL009313	0.9233	0.0767	0.8785	Dipsaci Radix	Mesitol	10698	FALSE	c1(c(cc(cc1C)C)C)O
MOL009314	0.9499	0.0501	0.8831	Dipsaci Radix	Cantleyine	442515	FALSE	OC1C(c2c(C1)c(cnc2)C(=O)OC)C
MOL009315	0.8871	0.1129	0.8338	Dipsaci Radix	Cantleyoside	Not Available	FALSE	ClCC(OC(Cl)CCl)Cl
MOL009316	0.6785	0.3215	0.7724	Dipsaci Radix	Cauloside A	Not Available	FALSE	C1(C(C(C(OC1)OC1C(C2C(CC1)C1C(CC2)(C)C2C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)(CO)C)O)O)O
MOL009317	0.6584	0.3416	0.7807	Dipsaci Radix	Cauloside A_qt	Not Available	FALSE	OC1C(C2C(CC1)C1C(CC2)(C)C2C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)(CO)C
MOL009318	0.7028	0.2972	0.8314	Dipsaci Radix	Dipsacobioside	Not Available	FALSE	C1(CCC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C)(C)CC4C3=CCC21C)OC1C(OC2C(O)C(O)C(O)C(O2)C)C(O)C(O)CO1
MOL009319	0.7590	0.2410	0.8022	Dipsaci Radix	Dipsaeussaponin B	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C)C1OCC(OC2OC(C(O)C(O)C2O)CO)C(OC2OC(C(O)C(O)C2O)CO)C1OC1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)C)C
MOL009321	0.7143	0.2857	0.7750	Dipsaci Radix	Macranthoidin B	Not Available	FALSE	C1(CCC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C(=O)OC5C(O)C(O)C(O)C(O5)COC5C(O)C(O)C(O)C(O5)CO)CCC(C)(C)CC4C3=CCC21C)OC1C(OC2C(O)C(OC3C(O)C(O)C(OC4C(O)C(O)C(O)C(O4)CO)C(O3)CO)C(O)C(O2)C)C(O)C(O)CO1
MOL009324	0.2664	0.7336	0.6453	Papaveris Pericarpium	Cryptogenin	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC(=O)C1C(C(=O)CCC(CO)C)C)C)O
MOL009325	0.8883	0.1117	0.7199	Papaveris Pericarpium	Sanleng acid	Not Available	FALSE	C(CCCCCC(C(/C=C/C(CCCCC(=O)O)O)O)O)CC

MOL009326	0.8920	0.1080	0.9008	Papaveris Pericarpium	Thellungianin F	Not Available	FALSE	c1(ccc(cc1)OC(=O)C(CC)C)/C=C/C
MOL009327	0.3953	0.6047	0.8802	Papaveris Pericarpium	Noskapin	31411	FALSE	c12c(c(c3c(c1)CCN(C3C1c3c(C(=O)O1)c(c(cc3)OC)OC)C)OC)OCO2
MOL009328	0.4442	0.5558	0.7137	Papaveris Pericarpium	5-[[(1S)-6,7-dimethoxy-2-methyl-3,4-dihydro-1H-isoquinolin-1-yl]methyl]-2-methoxyphenol	821396	FALSE	O(c1cc2C(N(CCc2cc1OC)C)Cc1cc(O)c(OC)cc1)C
MOL009330	0.3953	0.6047	0.8802	Papaveris Pericarpium	Noscapine	275196	TRUE	c12C(C3c4c(C(=O)O3)c(c(cc4)OC)OC)N(CCc2cc2c(c1OC)OCO2)C
MOL009331	0.5214	0.4786	0.7477	Papaveris Pericarpium	Palaudine	167736	FALSE	O(c1cc2c(nccc2cc1OC)Cc1cc(O)c(OC)cc1)C
MOL009332	0.8268	0.1732	0.7902	Papaveris Pericarpium	Dihydrosecurinine	Not Available	FALSE	C1(=O)CC2=CCC3CC2(O1)C1N3CCCC1
MOL009333	0.6102	0.3898	0.7497	Linderae Radix	(S)-Reticuline	439653	FALSE	O(c1cc2c(C(N(CC2)C)Cc2cc(O)c(OC)cc2)cc1O)C
MOL009333	0.6102	0.3898	0.7497	Papaveris Pericarpium	(S)-Reticuline	439653	FALSE	O(c1cc2c(C(N(CC2)C)Cc2cc(O)c(OC)cc2)cc1O)C
MOL009334	0.5776	0.4224	0.7324	Papaveris Pericarpium	salutaridine	24856366	FALSE	O(C1=CC2C(=CC1=O)C(N(CC2)C)Cc1cc(O)c(OC)cc1)C
MOL009335	0.4897	0.5103	0.8503	Papaveris Pericarpium	Erythroculine	12308908	FALSE	c1(c(cc2c(c1)CCN1C32C(=CCC(C3)OC)CC1)C(=O)OC)OC
MOL009336	0.6300	0.3700	0.6793	Papaveris Pericarpium	Narcotoline	70897566	FALSE	c12cc3c(c(O)c1OCO2)C(N(CC3)C)C1c2ccc(c(c2C(=O)O1)OC)OC
MOL009337	0.8532	0.1468	0.6805	Papaveris Pericarpium	Nardol	12313130	FALSE	C12C(CC(CCC1=C)C(C)C)C(CC2)(O)C
MOL009338	0.9215	0.0785	0.8469	Papaveris Pericarpium	Norswertianin	5281658	FALSE	c1(ccc2c(c1O)c(=O)c1c(o2)cc(cc1O)O)O
MOL009339	0.7353	0.2647	0.7472	Papaveris Pericarpium	Papaverrubine B	Not Available	FALSE	COc1c(OC)cc2c(c1)CCNC1C2OC(c2c1ccc1c2OCO1)OC
MOL009340	0.3146	0.6854	0.7461	Alpiniae Oxyphyliae Fructus	(2E)-2-[2-[(1S,4aS,8aS)-5,5,8a-trimethyl-2-methylene-1-decalinyl]ethylidene]butanedial	11077520	FALSE	C1(=C)CCC2C(C1C/C=C(/C=O)\CC=O)(CCCC2(C)C)C
MOL009341	0.8828	0.1172	0.8648	Zanthoxyli Pericarpium	6,8-Nonadien-2-one, 8-methyl-5-(1-methylethyl)-, (S-(E))-	6451337	FALSE	CC(=O)CCC(C(C)C)/C=C/C(=C)C

MOL009341	0.8828	0.1172	0.8648	Alpiniae Oxyphyliae Fructus	6,8-Nonadien-2-one, 8-methyl-5-(1-methylethyl)-, (S-(E))-	6451337	FALSE	CC(=O)CCC(C(C)C)/C=C/C(=C)C
MOL009342	0.8651	0.1349	0.7681	Alpiniae Oxyphyliae Fructus	isocyperol	Not Available	FALSE	OC1C(=C)C2C(CCC(C2)C(=C)C)(CC1)C
MOL009343	0.8385	0.1615	0.6988	Alpiniae Oxyphyliae Fructus	(1R,4aR,7R,8aR)-7-isopropenyl-1,4a-dimethyl-1-decalinol	15560330	FALSE	C1CCC2(C(C1(O)C)CC(CC2)C(=C)C)C
MOL009344	0.4626	0.5374	0.7944	Alpiniae Oxyphyliae Fructus	neonootkatol	Not Available	FALSE	c1(c(ccc(c1)CC(O)CCCCCc1ccccc1)O)OC
MOL009345	0.8246	0.1754	0.7601	Alpiniae Oxyphyliae Fructus	nootkatol	Not Available	FALSE	OC1CC(C2(CC(CCC2=C1)C(=C)C)C)C
MOL009346	0.5283	0.4717	0.6953	Alpiniae Oxyphyliae Fructus	oxyphyllacinol	Not Available	FALSE	OC(CCCCc1ccccc1)CCc1cc(OC)c(O)cc1
MOL009347	0.8928	0.1072	0.8197	Alpiniae Oxyphyliae Fructus	(4S,5S,6R)-5,6-dihydroxy-4-isopropyl-6-methyl-2,3,4,5,7,8-hexahydronaphthalen-1-one	10082923	FALSE	C1CC(=O)C2=C(C1C(C)C)C(C(CC2)(O)C)O
MOL009348	0.8928	0.1072	0.8197	Alpiniae Oxyphyliae Fructus	Oxyphyllenodiol B	5279294	FALSE	C1CC(=O)C2=C(C1C(C)C)C(C(CC2)(O)C)O
MOL009349	0.9582	0.0418	0.8825	Alpiniae Oxyphyliae Fructus	(4aR,7R,8R)-7,8-dihydroxy-4a,8-dimethyl-4,5,6,7-tetrahydro-3H-naphthalen-2-one	10262534	FALSE	C1(CCC2(C(=CC(=O)CC2)C1(C)O)C)O
MOL009350	0.9582	0.0418	0.8825	Alpiniae Oxyphyliae Fructus	Oxyphyllenone B	44310512	FALSE	C1(CCC2(C(=CC(=O)CC2)C1(C)O)C)O
MOL009351	0.8593	0.1407	0.7930	Alpiniae Oxyphyliae Fructus	Oxyphyllol A	637451	FALSE	OC1(C2=CC(CCC2(CCC1)C)C(=C)C)C

MOL009352	0.8403	0.1597	0.8199	Alpiniae Oxyphyliae Fructus	(4R,4aS,6S,8R)-8-hydroxy-6-isopropenyl-4,4a-dimethyl-3,4,5,6,7,8-hexahydronaphthalen-2-one	11128252	FALSE	C1(=O)C=C2C(C(C1)C)(CC(CC2O)C(=C)C)C
MOL009353	0.8356	0.1644	0.7612	Alpiniae Oxyphyliae Fructus	(1S,4R,4aS,6R,8aS)-6-isopropenyl-4,4a-dimethyldecalin-1,8a-diol	10857540	FALSE	C1C(C2(C(C(C1)C)(CC(CC2)C(=C)C)C)O)O
MOL009354	0.7648	0.2352	0.6126	Alpiniae Oxyphyliae Fructus	selin-11-en-4 α-ol	Not Available	FALSE	C1CC(C2(C(C1)(CCC(C2)C(=C)C)C)C)(C)O
MOL009356	0.8904	0.1096	0.9595	Alpiniae Oxyphyliae Fructus	Tectochrysin	5281954	FALSE	c1ccccc1c1cc(=O)c2c(o1)cc(cc2O)OC
MOL009357	0.4817	0.5183	0.7699	Alpiniae Oxyphyliae Fructus	yakuchinone a	133145	FALSE	O=C(CCCCc1ccccc1)CCc1cc(OC)c(O)cc1
MOL009358	0.4412	0.5588	0.7389	Alpiniae Oxyphyliae Fructus	yakuchinone b	6440365	FALSE	O=C(CCCCc1ccccc1)/C=C/c1cc(OC)c(O)cc1
MOL009359	0.9590	0.0410	0.7628	Alpiniae Oxyphyliae Fructus	γ-pinene	12314302	FALSE	C12C(C(C=CC1C)C2)(C)C
MOL009360	0.2756	0.7244	0.6727	Stemonae Radix	12-Oxoarundoin	Not Available	FALSE	C1C(C(C2C(C1)(C1=CC(=O)C3(C(C1CC2)(CCC1(C3CCC1C(C)C)C)C)C)(C)C)OC
MOL009361	0.2107	0.7893	0.6570	Stemonae Radix	13,15-Dideoxyaconitine	Not Available	FALSE	C1C(C2(C3C4(C1OC)C(N(C2)CC)C(C3OC)C1(C2C4CC(C2OC(=O)c2ccccc2)C(C1)OC)OC(=O)C)COC)O
MOL009362	0.9207	0.0793	0.8582	Stemonae Radix	4'-methylpinosylvin	Not Available	FALSE	c1cccc(c1)/C=C\c1cc(c(c(c1)O)C)O
MOL009363	0.1822	0.8178	0.6650	Stemonae Radix	tuberostemonine C	Not Available	FALSE	C12C(C(C3C4C1CC(N4CCCC3)C1OC(=O)C(C1)C)CC)OC(=O)C2C
MOL009364	0.1822	0.8178	0.6650	Stemonae Radix	tuberostemonine	Not Available	FALSE	C12CCCCN3C1C(C1C(C2CC)OC(=O)C1C)CC3C1OC(=O)C(C1)C
MOL009365	0.1568	0.8432	0.6816	Stemonae Radix	tuberostemonine H	Not Available	FALSE	C12(C(C3C4C(C1C(C(=O)O2)C)CC(N4CCCC3)C1OC(=O)C(C1)C)CC)C
MOL009366	0.1568	0.8432	0.6816	Stemonae Radix	tuberostemonine J	Not Available	FALSE	C12(C(C3C4C(C1C(C(=O)O2)C)CC(N4CCCC3)C1OC(=O)C(C1)C)CC)C
MOL009367	0.1568	0.8432	0.6816	Stemonae Radix	tuberostemonine K	Not Available	FALSE	C12(C(C3C4C(C1C(C(=O)O2)C)CC(N4CCCC3)C1OC(=O)C(C1)C)CC)C

MOL009368	0.1568	0.8432	0.6816	Stemonae Radix	tuberostemonine N	Not Available	FALSE	C12(C(C3C4C(C1C(C(=O)O2)C)CC(N4CCCC3)C1OC(=O)C(C1)C)CC)C
MOL009369	0.3261	0.6739	0.7643	Stemonae Radix	tuberostemoninol	Not Available	FALSE	N12CCCCC3(C1=C(C1C(C3CC)OC(=O)C1C)CC2C1OC(=O)C(C1)C)O
MOL009371	0.9173	0.0827	0.7281	Stemonae Radix	tuberostemospironine	Not Available	FALSE	O1C2(C(C(C1=O)C)O)C1N(CCCC2)C(=O)CC1
MOL009372	0.2419	0.7581	0.6957	Stemonae Radix	Tubocurarine	Not Available	FALSE	C1c2c3C([N+](C1)(C)C)Cc1cc(c(cc1)O)Oc1c(cc4CCN(C(Cc5ccc(Oc3c(c(c2)OC)O)cc5)c4c1)C)OC
MOL009374	0.7991	0.2009	0.7987	Stemonae Radix	7-methoxy-3-methyl-2,5-dihydroxy-9,10-dihydrophenanthrene	60205844	FALSE	C1c2c(c3c(C1)cc(cc3O)OC)cc(c(c2)O)C
MOL009376	0.5667	0.4333	0.7418	Stemonae Radix	bisdehydrostemonine	Not Available	FALSE	c12cccn1CCCC1C2C(/C(=C/2\C(=C(C(=O)O2)C)OC)/O1)C
MOL009377	0.2241	0.7759	0.7564	Stemonae Radix	bisdehydrotuberostemonine	Not Available	FALSE	C1(OC(=O)C(C1)C)c1cc2c3n1CCCCC3C(C1C2C(C(=O)O1)C)CC
MOL009379	0.5430	0.4570	0.6880	Stemonae Radix	2-oxostenine	Not Available	FALSE	C12C3C(C4C(C1CC)OC(=O)C4C)CC(=O)N3CCCC2
MOL009380	0.2373	0.7627	0.6357	Stemonae Radix	bisdehydrostemoninine	Not Available	FALSE	O1C2C(C(C31OC(=O)C(=C3)C)CC)c1n(CCC2)c(C2OC(=O)C(C2)C)cc1
MOL009383	0.2241	0.7759	0.7564	Stemonae Radix	bisdehydrotuberostemonine B	Not Available	FALSE	c12c3n(c(c1)C1OC(=O)C(C1)C)CCCCC3C(C1C2C(C(=O)O1)C)CC
MOL009384	0.2241	0.7759	0.7564	Stemonae Radix	bisdehydrotuberostemonine C	Not Available	FALSE	c12c3n(c(c1)C1OC(=O)C(C1)C)CCCCC3C(C1C2C(C(=O)O1)C)CC
MOL009387	0.2241	0.7759	0.7564	Stemonae Radix	didehydrotuberostemonine	Not Available	FALSE	O1C2C(C3c4n(c(cc4C2C(C1=O)C)C1OC(=O)C(C1)C)CCCC3)CC
MOL009389	0.2241	0.7759	0.7564	Stemonae Radix	epi-bisdehydrotuberostemonine J	Not Available	FALSE	C12C(C3c4c(C1C(C(=O)O2)C)cc(n4CCCC3)C1OC(=O)C(C1)C)CC
MOL009390	0.2373	0.7627	0.6357	Stemonae Radix	isobisdehydrostemoninine	Not Available	FALSE	C12(OC3C(C1CC)c1n(c(cc1)C1OC(=O)C(C1)C)CCC3)C=C(C(=O)O2)C
MOL009391	0.2241	0.7759	0.7564	Stemonae Radix	isodidehydrotuberostemonine	Not Available	FALSE	C12C(C3c4c(C1C(C(=O)O2)C)cc(n4CCCC3)C1OC(=O)C(C1)C)CC
MOL009392	0.2906	0.7094	0.6966	Stemonae Radix	isomaistemonine	Not Available	FALSE	C1C(N2C3(C1)C(=C(C(=O)C13OC(=O)C(=C1OC)C)C)CCCC2)C1OC(=O)C(C1)C
MOL009394	0.5409	0.4591	0.7414	Stemonae Radix	stemonamine	Not Available	FALSE	O1C2(C34N(CCC3)CCCCC4=C(C2=O)C)C(=C(C1=O)C)OC

MOL009396	0.1822	0.8178	0.6650	Stemonae Radix	isotuberostemonine	Not Available	FALSE	N12CCCCC3C1C(C1C(C3CC)OC(=O)C1C)CC2C1OC(=O)C(C1)C
MOL009398	0.3601	0.6399	0.7084	Stemonae Radix	lupan-3-one	11015452	FALSE	C12(C(C3C(CC2)(CCC3C(C)C)C)CCC2C1(CCC1C2(CCC(=O)C1(C)C)C)C)C
MOL009399	0.2906	0.7094	0.6966	Stemonae Radix	Maistemonine	Not Available	FALSE	O1C2(C34N(C(CC3)C3OC(=O)C(C3)C)CCCCC4=C(C2=O)C)C(=C(C1=O)C)OC
MOL009400	0.2719	0.7281	0.6734	Stemonae Radix	n-oxytuberostemonine	Not Available	FALSE	C12(C3C(C(C4C1N(C(C2)C1OC(=O)C(C1)C)CCCC4)CC)OC(=O)C3C)O
MOL009403	0.4512	0.5488	0.6414	Stemonae Radix	neostenine	Not Available	FALSE	C12C(C3C4C(C1C(C(=O)O2)C)CCN4CCCC3)CC
MOL009404	0.1822	0.8178	0.6650	Stemonae Radix	neotuberostemonine	Not Available	FALSE	O1C2C(C3C4N(C(C3)C3OC(=O)C(C3)C)CCCCC4C2CC)C(C1=O)C
MOL009405	0.4544	0.5456	0.7438	Stemonae Radix	neotuberostemoninol	Not Available	FALSE	C12(C3(C(=O)N(C(C1)C1OC(=O)C(C1)C)CCCC3)C(C1C2C(C(=O)O1)C)CC)O
MOL009406	0.3378	0.6622	0.7790	Stemonae Radix	neotuberostemonol	Not Available	FALSE	C12(C3C(C(C4=C1N(C(C2)C1OC(=O)C(C1)C)CCCC4)CC)OC(=O)C3C)O
MOL009407	0.3375	0.6625	0.7371	Stemonae Radix	oxotuberostemonine	Not Available	FALSE	O1C2C3C(C(O)C(C4=C3N(C2C2OC(=O)C(C2)C)CCCC4)CC)C(C1=O)C
MOL009408	0.3257	0.6743	0.7672	Stemonae Radix	oxotuberostemonine Ⅱ	Not Available	FALSE	C12=C3N(CCCC1)C(CC13C(C(C2CC)O)C(C(=O)O1)C)C1OC(=O)C(C1)C
MOL009411	0.2906	0.7094	0.6966	Stemonae Radix	protostemotinine	Not Available	FALSE	C12(OC(=O)C(=C1OC)C)C13N(C(C4OC(=O)C(C4)C)CC3)CCCCC1=C(C2=O)C
MOL009413	0.7178	0.2822	0.6810	Stemonae Radix	sessilifoliamide B	12116760	FALSE	C1(C(C2CCCCN3C2CCC3=O)CC)OC(=O)C(C1)C
MOL009414	0.6803	0.3197	0.7091	Stemonae Radix	sessilifoliamide C	12116761	FALSE	C1(C(C2CCCCN3C2CCC3=O)CC)OC(=O)C(=C1)C
MOL009415	0.7336	0.2664	0.6641	Stemonae Radix	sessilifoliamide D	12116762	FALSE	C(=O)(C(C1CCCCN2C1CCC2=O)CC)CC(C(=O)OC)C
MOL009420	0.4544	0.5456	0.7438	Stemonae Radix	sessilifoliamide I	Not Available	FALSE	C12(C3(C(=O)N(C(C1)C1OC(=O)C(C1)C)CCCC3)C(C1C2C(C(=O)O1)C)CC)O
MOL009421	0.4042	0.5958	0.7560	Stemonae Radix	sessilifoline A	Not Available	FALSE	C12C34C(C(C5C2C(C(=O)O5)C)CC)CCCC(N3C(C1)C1OC(=O)C(C1)C)O4
MOL009422	0.4574	0.5426	0.6785	Stemonae Radix	sessilifoline B	Not Available	FALSE	C12(C3C(C4C(C1CC)OC(=O)C4)CCN3CCCC2)C
MOL009423	0.3089	0.6911	0.7791	Stemonae Radix	sessilistemonamine A	Not Available	FALSE	C1(=O)OC2C(C1(C)O)C13C(C2CC)CCCCN1C(CC3)C1OC(=O)C(C1)C
MOL009424	0.3089	0.6911	0.7791	Stemonae Radix	sessilistemonamine B	Not Available	FALSE	C1(=O)OC2C(C1(C)O)C13C(C2CC)CCCCN1C(CC3)C1OC(=O)C(C1)C
MOL009425	0.3089	0.6911	0.7791	Stemonae Radix	sessilistemonamine C	Not Available	FALSE	C1(=O)OC2C(C1(C)O)C13C(C2CC)CCCCN1C(CC3)C1OC(=O)C(C1)C
MOL009426	0.1873	0.8127	0.7607	Stemonae Radix	sessilistemonamine D	Not Available	FALSE	C1(CC(C(=O)O1)C)C1CCC23N1CCCCC3C(C1OC(=O)C2(C1)C)CC
MOL009427	0.9241	0.0759	0.7196	Stemonae Radix	stemoamide	Not Available	FALSE	C1(=O)OC2C(C1C)C1N(C(=O)CC1)CCC2

MOL009429	0.3705	0.6295	0.6789	Stemonae Radix	stemofoline	Not Available	FALSE	O1C23O/C(=C\4/OC(=O)C(=C4OC)C)/C(C3C3N4C(C2CC4)(C1C3)CCCC)C
MOL009430	0.5007	0.4993	0.7521	Stemonae Radix	stemonamide	Not Available	FALSE	C1(=O)N2C3(CC1)C(=C(C(=O)C13CC(=O)C(=C1OC)C)C)CCCC2
MOL009432	0.2489	0.7511	0.6201	Stemonae Radix	stemoninine A	Not Available	FALSE	C1(C(=O)OC2(C1)OC1C(C2CC)c2n(c(cc2)C2OC(=O)C(C2)C)CCC1)C
MOL009433	0.2489	0.7511	0.6201	Stemonae Radix	stemoninine B	Not Available	FALSE	C1(C(=O)OC2(C1)OC1C(C2CC)c2n(c(cc2)C2OC(=O)C(C2)C)CCC1)C
MOL009434	0.6735	0.3265	0.6188	Stemonae Radix	stemoninoamide	Not Available	FALSE	C1(=O)C(=CC2(O1)OC1C(C2CC)C2N(C(=O)CC2)CCC1)C
MOL009437	0.4512	0.5488	0.6414	Stemonae Radix	16625-37-9	Not Available	FALSE	C12C(C3C4C(C1C(C(=O)O2)C)CCN4CCCC3)CC
MOL009438	0.9496	0.0504	0.9600	Stemonae Radix	WLN: QVR D1	7470	FALSE	Cc1ccc(cc1)C(=O)O
MOL009439	0.9296	0.0704	0.8617	Stemonae Radix	2-methyl-5-(2-phenylethyl)resorcinol	10376477	FALSE	c1cccc(c1)CCc1cc(c(c(c1)O)C)O
MOL009440	0.9013	0.0987	0.7785	Stemonae Radix	stilbostemin D	15222503	FALSE	c1(c(c(cc(c1)CCc1c(cccc1)OC)O)C)O
MOL009442	0.6735	0.3265	0.6188	Stemonae Radix	tuberostemoamide	Not Available	FALSE	C1CCC2C(C3N1C(=O)CC3)C(C1(O2)C=C(C(=O)O1)C)CC
MOL009443	0.3819	0.6181	0.7996	Stemonae Radix	tuberostemoenone	Not Available	FALSE	C1(CC(C(=O)O1)C)C1CC2=C3C(C(=O)OC3C(C32N1CCCCC3=O)CC)C
MOL009444	0.1822	0.8178	0.6650	Stemonae Radix	tuberostemonine A	Not Available	FALSE	C12C(C(C3C4C1CC(N4CCCC3)C1OC(=O)C(C1)C)CC)OC(=O)C2C
MOL009445	0.1822	0.8178	0.6650	Stemonae Radix	tuberostemonine B	Not Available	FALSE	C12C(C(C3C4C1CC(N4CCCC3)C1OC(=O)C(C1)C)CC)OC(=O)C2C
MOL009446	0.9135	0.0865	0.9010	Lilii Bulbus	1-O-feruloylglycerol	Not Available	FALSE	c1(c(ccc(c1)/C=C\C(=O)OCC(O)CO)O)OC
MOL009447	0.8841	0.1159	0.9066	Lilii Bulbus	regaloside D_qt	Not Available	FALSE	O(CC(O)CO)C(=O)/C=C/c1ccc(cc1)O
MOL009448	0.7532	0.2468	0.7920	Lilii Bulbus	26-O-beta-D-Glucopyranosyl-3beta,26-dihydroxy-cholestan-16,22-dioxo-3-O-alpha-L-rhamnopyranosyl-(1-2)-beta-D-glucopyranoside	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C2C(CC1)(C(C(=O)C2)C(C(=O)CCC(C)COC1OC(C(C(C1O)O)O)CO)C)C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO

MOL009449	0.2620	0.7380	0.6378	Lilii Bulbus	26-O-beta-D-Glucopyranosyl-3beta,26-dihydroxy-cholesten-16,22-dioxo-3-O-alpha-L-rhamnopyranosyl-(1-2)-beta-D-glucopyranoside_qt	Not Available	FALSE	OC1CCC2(C(C1)CCC1C2CCC2(C1CC(=O)C2C(C(=O)CCC(C)CO)C)C)C
MOL009450	0.8932	0.1068	0.8265	Lilii Bulbus	2-aminobenzoate-3,7-dimethyl-1,6-octadien-3-ol	Not Available	FALSE	O(C(CCC=C(C)C)(C)C=C)C(=O)c1c(N)cccc1
MOL009451	0.9483	0.0517	0.7603	Zanthoxyli Pericarpium	.alpha.-Carene	6430755	FALSE	C12C=C(CCC1C2(C)C)C
MOL009451	0.9483	0.0517	0.7603	Rhododendri Daurici Folium	.alpha.-Carene	6430755	FALSE	C12C=C(CCC1C2(C)C)C
MOL009451	0.9483	0.0517	0.7603	Lilii Bulbus	.alpha.-Carene	6430755	FALSE	C12C=C(CCC1C2(C)C)C
MOL009452	0.9303	0.0697	0.9058	Lilii Bulbus	(2S)-2-methyl-3-phenylpropanal	1715215	FALSE	CC(Cc1ccccc1)C=O
MOL009453	0.5921	0.4079	0.6773	Lilii Bulbus	3,6'-O-diferuloylsucrose	Not Available	FALSE	c1c(c(cc(c1)/C=C\C(=O)OC1C(OC(C1O)CO)(OC1CC(C(C(C1O)O)O)OC(=O)/C=C/c1ccc(c(c1)OC)O)CO)OC)O
MOL009454	0.7782	0.2218	0.8243	Lilii Bulbus	3-O-beta-D-Glucopyranosyl betulinic acid-28-O-beta-D-glucopyranosyl-(1-6)-beta-D-glucopyranoside	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC1C(=C)C)C(=O)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)C)C)(C)C)OC1OC(C(C(C1O)O)O)CO

MOL009455	0.6899	0.3101	0.8784	Lilii Bulbus	3-O-beta-D-Glucopyranosyl betulinic acid-28-O-beta-D-glucopyranosyl-(1-6)-beta-D-glucopyranoside_qt	Not Available	FALSE	OC1CCC2(C(C1(C)C)CCC1(C2CC=C2C1(CCC1(C(=O)O)C2C(C(=C)C)CC1)C)C)C
MOL009456	0.9619	0.0381	0.7507	Lilii Bulbus	β-thujene	Not Available	FALSE	C12(C=CC(C1C2)C)C(C)C
MOL009456	0.9619	0.0381	0.7507	Menthae Herba	β-thujene	Not Available	FALSE	C12(C=CC(C1C2)C)C(C)C
MOL009457	0.6377	0.3623	0.6714	Lilii Bulbus	colchicoside	92763	FALSE	O(c1c(OC2OC(C(C(C2O)O)O)CO)cc2c(c1OC)c1c(C(CC2)NC(=O)C)cc(=O)c(cc1)OC)C
MOL009458	0.4043	0.5957	0.8523	Lilii Bulbus	3-Demethylcolchicine	299664	FALSE	O(C)c1ccc2c3c(c(OC)c(O)cc3CCC(NC(=O)C)c2cc1=O)OC
MOL009459	0.9119	0.0881	0.8862	Lilii Bulbus	bicyclo[6. 1. 0]non-1-ene	Not Available	FALSE	C12=CCCCCCC1C2
MOL009460	0.8968	0.1032	0.9485	Lilii Bulbus	(1S,2R)-1-ethyl-2-methylcyclopropane	640655	FALSE	C1(C(C1)C)CC
MOL009461	0.9320	0.0680	0.9420	Lilii Bulbus	Geraniol formate	5354882	FALSE	O=COC/C=C(/C)\CCC=C(C)C
MOL009462	0.6729	0.3271	0.8638	Lilii Bulbus	ophipogonin D	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC2C1C(C1(O2)OCC(CC1)C)C)C)OC1C(C(C(C(O1)CO)O)OC1C(C(C(CO1)O)O)O)OC1C(C(C(C(O1)C)O)O)O
MOL009463	0.9212	0.0788	0.9283	Lilii Bulbus	lilioside C	15559912	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)CC(CO)O
MOL009464	0.7362	0.2638	0.8048	Lilii Bulbus	26-O-β-D-glucopyranosyl-3β,26-dihydroxy-5-cholesten-16,22-dioxo-3-O-α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranoside	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC(=O)C1C(C(=O)CCC(C)COC1OC(C(C(C1O)O)O)C)C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO

MOL009465	0.2664	0.7336	0.6453	Lilii Bulbus	26-O-β-D-glucopyranosyl-3β,26-dihydroxy-5-cholesten-16,22-dioxo-3-O-α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranoside_qt	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC(=O)C1C(C(=O)CCC(C)CO)C)C)O
MOL009466	0.7074	0.2926	0.8283	Lilii Bulbus	27-O-(3-hydroxy-3-methylglutaroyl)-isonarthogenin-3-O-α-L-rhamnopyranosyl-(1→2)-O-[β-D-glucopyranosyl-(1→4)]-β-D-glucopyranosid	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3CC3C1C(C1(O3)CCC(COC(=O)CC(CC(=O)O)(O)C)CO1)C)C)CC(CC2)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)OC1C(C(C(C(O1)CO)O)O)O)CO)C
MOL009467	0.5800	0.4200	0.7289	Lilii Bulbus	27-O-(3-hydroxy-3-methylglutaroyl)-isonarthogenin-3-O-α-L-rhamnopyranosyl-(1→2)-O-[β-D-glucopyranosyl-(1→4)]-β-D-glucopyranosid_qt	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3CC3C1C(C1(O3)CCC(COC(=O)CC(O)(CC(=O)O)C)CO1)C)C)CC(CC2)O)C
MOL009468	0.6642	0.3358	0.8230	Lilii Bulbus	β1-solamargine	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3CC3C1C(C1(O3)CCC(C)CN1)C)C)CC(CC2)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO)C

MOL009469	0.7007	0.2993	0.8535	Lilii Bulbus	solasodine-3-O-α-L-rhamnopyranosyl-(1→2)-O-[β-D-glucopyranosyl-(1→4)]-β-D-glucopyranoside	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3CC3C1C(C1(O3)CCC(C)CN1)C)C)CC(CC2)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)OC1C(C(C(C(O1)CO)O)O)O)CO)C
MOL009470	0.7321	0.2679	0.7964	Lilii Bulbus	26-O-β-D-glucopyranosyl-3β,26-dihydroxy-cholestan-16,22-dioxo-3-O-α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranoside	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C2C(CC1)(C(C(=O)C2)C(C(=O)CCC(C)COC1OC(C(C(C1O)O)O)C)C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO
MOL009471	0.2620	0.7380	0.6378	Lilii Bulbus	26-O-β-D-glucopyranosyl-3β,26-dihydroxy-cholestan-16,22-dioxo-3-O-α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranoside_qt	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C2C(CC1)(C(C(=O)C2)C(C(=O)CCC(C)CO)C)C)C)O
MOL009472	0.7699	0.2301	0.8454	Lilii Bulbus	26-O-β-D-glucopyranosyl-nuatigenin-3-O-α-L-rhamnopyranosyl(1→2)-β-D-glucopyranoside	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3CC3C1C(C1(O3)CCC(O1)(C)COC1C(C(C(C(O1)CO)O)O)O)C)C)CC(CC2)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO)C

MOL009473	0.3265	0.6735	0.7360	Lilii Bulbus	26-O-β-D-glucopyranosyl-nuatigenin-3-O-α-L-rhamnopyranosyl(1→2)-β-D-glucopyranoside_qt	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3CC3C1C(C1(O3)CCC(O1)(C)CO)C)C)CC(CC2)O)C
MOL009474	0.7423	0.2577	0.8185	Lilii Bulbus	26-O-β-D-glucopyranosylnuatigenin-3-O-α-L-rhamnopyranosyl(1→2)-o-[β-D-glucopyranosyl(1→4)]-β-D-glucopyranoside	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3CC3C1C(C1(O3)CCC(O1)(C)COC1C(C(C(C(O1)CO)O)O)O)C)C)CC(CC2)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)OC1C(C(C(C(O1)CO)O)O)O)CO)C
MOL009475	0.4810	0.5190	0.7841	Lilii Bulbus	26-O-β-D-glucopyranosylnuatigenin-3-O-α-L-rhamnopyranosyl(1→2)-o-[β-D-glucopyranosyl(1→4)]-β-D-glucopyranoside_qt	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3CC3C1C(C1(O3)CCC(O1)(C)COC1OC(CO)C(O)C(O)C1O)C)C)CC(CC2)O)C
MOL009476	0.6793	0.3207	0.8511	Lilii Bulbus	brownioside	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3CC3C1C(C1(O3)CCC(COC(=O)CC(CC(=O)O)(O)C)CO1)C)C)CC(CC2)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO)C
MOL009477	0.5800	0.4200	0.7289	Lilii Bulbus	brownioside_qt	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3CC3C1C(C1(O3)CCC(COC(=O)CC(O)(CC(=O)O)C)CO1)C)C)CC(CC2)O)C
MOL009478	0.6980	0.3020	0.8580	Lilii Bulbus	deacylbrownioside	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3CC3C1C(C1(O3)CCC(CO)CO1)C)C)CC(CC2)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO)C
MOL009479	0.3404	0.6596	0.7770	Lilii Bulbus	deacylbrownioside_qt	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3CC3C1C(C1(O3)CCC(CO)CO1)C)C)CC(CC2)O)C
MOL009480	0.9414	0.0586	0.8231	Lilii Bulbus	regaloside A	Not Available	FALSE	O1C(C(O)C(O)C(O)C1OCC(O)COC(=O)/C=C/c1ccc(O)cc1)CO

MOL009481	0.8904	0.1096	0.7384	Lilii Bulbus	regaloside B	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)C(COC(=O)C)COC(=O)/C=C\c1ccc(cc1)O
MOL009482	0.8094	0.1906	0.8680	Lilii Bulbus	regaloside B_qt	Not Available	FALSE	OC(COC(=O)C)COC(=O)/C=C/c1ccc(cc1)O
MOL009483	0.9394	0.0606	0.8349	Lilii Bulbus	regaloside D	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)C(CO)COC(=O)/C=C\c1ccc(cc1)O
MOL009484	0.8996	0.1004	0.7539	Lilii Bulbus	regaloside E	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)C(COC(=O)C)COC(=O)/C=C\c1cc(c(cc1)O)O
MOL009485	0.8736	0.1264	0.8828	Lilii Bulbus	regaloside E_qt	Not Available	FALSE	OC(COC(=O)C)COC(=O)/C=C/c1cc(c(cc1)O)O
MOL009486	0.9244	0.0756	0.7852	Lilii Bulbus	regaloside F	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)CC(COC(=O)/C=C/c1cc(c(cc1)O)OC)O
MOL009487	0.9135	0.0865	0.9010	Lilii Bulbus	regaloside F_qt	Not Available	FALSE	OCC(COC(=O)/C=C/c1cc(c(cc1)O)OC)O
MOL009489	0.9598	0.0402	0.9671	Lilii Bulbus	trans-4-(Isopropyl)-1-methylcyclohex-2-en-1-ol	122484	FALSE	C1(C=CC(CC1)C(C)C)(O)C
MOL009489	0.9598	0.0402	0.9671	Aucklandiae Radix	trans-4-(Isopropyl)-1-methylcyclohex-2-en-1-ol	122484	FALSE	C1(C=CC(CC1)C(C)C)(O)C
MOL009490	0.9301	0.0699	0.9481	Lilii Bulbus	Hex-3-enyl acetate	5352557	FALSE	C(C/C=C/CC)OC(=O)C
MOL009491	0.9382	0.0618	0.8868	Morindae Officinalis Radix	1,2-diethyl-3-methylcyclohexylamine	Not Available	FALSE	NC1(C(C(CCC1)C)CC)CC
MOL009492	0.7846	0.2154	0.7959	Morindae Officinalis Radix	1,2-dihydroxy-3-methyl-9,10-anthraquinone	429241	FALSE	c1(c(c(cc2C(=O)c3ccccc3C(=O)c12)C)O)O
MOL009493	0.8367	0.1633	0.8252	Morindae Officinalis Radix	1,3-Dihydroxy-2-methoxyanthraquinone	146101	FALSE	c1(c(c(cc2C(=O)c3ccccc3C(=O)c12)O)OC)O
MOL009494	0.8038	0.1962	0.8281	Morindae Officinalis Radix	1,4-dihydroxy-2-methoxy-7-methylanthracenequinone	12416403	FALSE	c1(c(cc(c2C(=O)c3ccc(cc3C(=O)c12)C)O)OC)O

MOL009495	0.6249	0.3751	0.7788	Morindae Officinalis Radix	2-hydroxy-1,5-dimethoxy-6-(methoxymethyl)-9,10-anthraquinone	16203753	FALSE	c12c(C(=O)c3c(C1=O)c(c(cc3)COC)OC)c(c(cc2)O)OC
MOL009496	0.8437	0.1563	0.8071	Morindae Officinalis Radix	1,5,7-trihydroxy-6-methoxy-2-methoxymethylanthracenequinone	Not Available	FALSE	c1(c(ccc2C(=O)c3c(c(c(cc3C(=O)c12)O)OC)O)COC)O
MOL009497	0.9490	0.0510	0.8848	Morindae Officinalis Radix	1,5-diethyl-2,3-dimethylcyclohexylamine	Not Available	FALSE	NC1(C(C(CC(C1)CC)C)C)CC
MOL009498	0.8303	0.1697	0.7769	Morindae Officinalis Radix	1,6-Dihydroxy-2,4-dimethoxyanthraquinone	126726	FALSE	c1(c(cc(c2C(=O)c3cc(ccc3C(=O)c12)O)OC)OC)O
MOL009499	0.8242	0.1758	0.7823	Morindae Officinalis Radix	1,6-Dihydroxy-2-methoxyanthraquinone	132521	FALSE	c1(c(ccc2C(=O)c3cc(ccc3C(=O)c12)O)OC)O
MOL009500	0.7285	0.2715	0.7994	Morindae Officinalis Radix	1,6-dihydroxy-5-methoxy-2-(methoxymethyl)-9,10-anthraquinone	11674044	FALSE	c1(c(ccc2C(=O)c3c(c(ccc3C(=O)c12)O)OC)COC)O
MOL009501	0.7661	0.2339	0.7761	Morindae Officinalis Radix	1-hydroxy-2,3-dimethyl-9,10-anthraquinone	1382	FALSE	c1(c(c(cc2C(=O)c3ccccc3C(=O)c12)C)C)O
MOL009502	0.8347	0.1653	0.8178	Morindae Officinalis Radix	1-hydroxy-3-methylol-9,10-anthraquinone	171106	FALSE	c1(cc(cc2C(=O)c3ccccc3C(=O)c12)CO)O
MOL009503	0.8081	0.1919	0.8162	Morindae Officinalis Radix	1-hydroxy-3-methoxy-9,10-anthraquinone	13412786	FALSE	c1(cc(cc2C(=O)c3ccccc3C(=O)c12)OC)O

MOL009504	0.8358	0.1642	0.8101	Morindae Officinalis Radix	1-hydroxy-6-hydroxymethylanthracenequinone	44595036	FALSE	c1(cccc2C(=O)c3cc(ccc3C(=O)c12)CO)O
MOL009505	0.8397	0.1603	0.7227	Morindae Officinalis Radix	1-hydroxy-7-hydroxymethylanthracenequinone	Not Available	FALSE	c1(cccc2C(=O)c3ccc(cc3C(=O)c12)CO)O
MOL009506	0.8273	0.1727	0.7877	Peucedani Radix	Hydroxyanthraquinone	8512	FALSE	c12c(C(=O)c3c(C1=O)cccc3)cccc2O
MOL009506	0.8273	0.1727	0.7877	Morindae Officinalis Radix	Hydroxyanthraquinone	8512	FALSE	c12c(C(=O)c3c(C1=O)cccc3)cccc2O
MOL009507	0.9410	0.0590	0.8233	Morindae Officinalis Radix	1-isobutyl-2,5-dimethylcyclohexylamine	Not Available	FALSE	NC1(C(CCC(C1)C)C)CC(C)C
MOL009508	0.9193	0.0807	0.8592	Morindae Officinalis Radix	1-methyl-3-propylcyclooctane	Not Available	FALSE	C1(CC(CCCCC1)CCC)C
MOL009509	0.5764	0.4236	0.6762	Ginkgo Folium	2-phenyldodecane	Not Available	FALSE	c1(ccccc1)C(CCCCCCCCCC)C
MOL009509	0.5764	0.4236	0.6762	Morindae Officinalis Radix	2-phenyldodecane	Not Available	FALSE	c1(ccccc1)C(CCCCCCCCCC)C
MOL009509	0.5764	0.4236	0.6762	Panacis Quinquefolii Radix	2-phenyldodecane	Not Available	FALSE	c1(ccccc1)C(CCCCCCCCCC)C
MOL009510	0.8364	0.1636	0.7110	Morindae Officinalis Radix	1F-Fructofuranosylnystose	3085157	FALSE	O1C(OCC2(OC(C(O)C2O)CO)OC2OC(C(O)C(O)C2O)CO)(C(O)C(O)C1CO)COC1(OC(C(O)C1O)CO)COC1(OC(C(O)C1O)CO)CO
MOL009511	0.9112	0.0888	0.9244	Morindae Officinalis Radix	2,5,5-trimethylhex-1-ene	545898	FALSE	C=C(CCC(C)(C)C)C
MOL009512	0.7506	0.2494	0.8088	Morindae Officinalis Radix	methyl 9,10-dioxoanthracene-2-carboxylate	3146261	FALSE	c1c(ccc2C(=O)c3ccccc3C(=O)c12)C(=O)OC

MOL009513	0.6330	0.3670	0.8274	Morindae Officinalis Radix	2-hydroxy-1,8-dimethoxy-7-methoxymethylanthraceneq uinone	Not Available	FALSE	c1(c(ccc2C(=O)c3ccc(c(c3C(=O)c12)OC)COC)O)OC
MOL009514	0.7081	0.2919	0.8377	Morindae Officinalis Radix	1-methoxy-2-hydroxyanthraquinone	80309	FALSE	c1(c(ccc2C(=O)c3ccccc3C(=O)c12)O)OC
MOL009515	0.8692	0.1308	0.7964	Morindae Officinalis Radix	2-hydroxy-3-hydroxymethylanthracenequinone	44445519	FALSE	c1c(c(cc2C(=O)c3ccccc3C(=O)c12)CO)O
MOL009516	0.8418	0.1582	0.7772	Morindae Officinalis Radix	2-Hydroxyanthraquinone	11796	FALSE	c1ccc2c(c1)C(=O)c1c(C2=O)ccc(c1)O
MOL009517	0.8584	0.1416	0.8245	Morindae Officinalis Radix	1,3,6-trihydroxy-2-methoxy-9,10-anthraquinone	11659239	FALSE	c1(c(c(cc2C(=O)c3cc(ccc3C(=O)c12)O)O)OC)O
MOL009518	0.8674	0.1326	0.7207	Morindae Officinalis Radix	2-methyl-p-methylphenyl-2-heptene	Not Available	FALSE	C/C=C/CCCCc1c(cc(cc1)C)C
MOL009519	0.8915	0.1085	0.8522	Morindae Officinalis Radix	(2R,3S)-(+)-3',5-Dihydroxy-4',7-dimethoxydihydroflavonol	5316762	FALSE	c1c(cc(c2c1OC(C(C2=O)O)c1ccc(c(c1)O)OC)O)OC
MOL009520	0.8813	0.1187	0.7136	Morindae Officinalis Radix	3,8-dimethylundecane	Not Available	FALSE	CCC(CCCCC(CCC)C)C
MOL009520	0.8813	0.1187	0.7136	Rose Rugosae Flos	3,8-dimethylundecane	Not Available	FALSE	CCC(CCCCC(CCC)C)C
MOL009520	0.8813	0.1187	0.7136	Eriobotryae Folium	3,8-dimethylundecane	Not Available	FALSE	CCC(CCCCC(CCC)C)C

MOL009521	0.7071	0.2929	0.8562	Morindae Officinalis Radix	3-hydroxy-1,2-dimethoxyanthracenequinone	57509304	FALSE	c1(c(c(cc2C(=O)c3ccccc3C(=O)c12)O)OC)OC
MOL009523	0.9024	0.0976	0.9243	Morindae Officinalis Radix	3-Ethynylphenol	139144	FALSE	C#Cc1cc(ccc1)O
MOL009526	0.3085	0.6915	0.7794	Morindae Officinalis Radix	3beta,5-alkenyl-spirostol	Not Available	FALSE	C1C2C(C3C(C1)(C1C(C3)CC3(C1C)OCC(CC3)C)C)CC=C1C2(CCC(C1)O)C
MOL009527	0.7469	0.2531	0.8471	Morindae Officinalis Radix	4-hydroxymethyl-1,3-dimethoxyanthracenequinone	Not Available	FALSE	c1(cc(c(c2C(=O)c3ccccc3C(=O)c12)CO)OC)OC
MOL009528	0.9039	0.0961	0.9572	Morindae Officinalis Radix	(4R,5S)-5-hydroxyhexan-4-olide	10887941	FALSE	C1(=O)CCC(C(C)O)O1
MOL009529	0.0835	0.9165	0.6387	Morindae Officinalis Radix	5alpha-Hydroxy-2alpha-(alpha-methylbutyryl)-oxy-7beta,9alpha,10beta-triacetoxy-4(20),11-taxadiene	Not Available	FALSE	C1(C(C2(C(C(C3C(C1=C(CC3)C)(C)C)OC(=O)C(CC)C)C(=C)C(CC2OC(=O)C)O)C)OC(=O)C)OC(=O)C
MOL009530	0.9291	0.0709	0.8760	Morindae Officinalis Radix	6-alpha-hydroxyadoxoside	Not Available	FALSE	C1(C=C(C2C1C=COC2OC1C(O)C(O)C(O)C(O)C(O1)CO)O)O
MOL009531	0.9332	0.0668	0.8536	Morindae Officinalis Radix	6-alpha-hydroxyadoxoside_qt	Not Available	FALSE	C1(C=C(C2C1C=COC2O)O)O
MOL009532	0.8875	0.1125	0.7961	Morindae Officinalis Radix	6beta,7beta-epoxy-8-epi-splendoside	11166049	FALSE	C12C(C(C3C1C(=COC3OC1C(O)C(O)C(O)C(O)C(O1)CO)C(=O)OC)(O)CO)O2
MOL009533	0.9198	0.0802	0.7989	Morindae Officinalis Radix	6beta,7beta-epoxy-8-epi-splendoside_qt	Not Available	FALSE	C12C(C(C3C1C(=COC3O)C(=O)OC)(O)CO)O2

MOL009535	0.8679	0.1321	0.7315	Morindae Officinalis Radix	Nystose	166775	FALSE	O(C1(OC(C(O)C1O)CO)COC1(OC(C(O)C1O)CO)CO)CC1(OC(C(O)C1O)CO)OC1OC(C(O)C(O)C1O)CO
MOL009536	0.6541	0.3459	0.8473	Morindae Officinalis Radix	alizarin-1-methyl ether	Not Available	FALSE	O=C1c2ccccc2C(=O)c2c1c(c(O)cc2)OCC
MOL009537	0.6638	0.3362	0.7339	Morindae Officinalis Radix	americanin A	Not Available	FALSE	O1C(C(Oc2c1ccc(c2)/C=C/C=O)CO)c1cc(O)c(O)cc1
MOL009538	0.7175	0.2825	0.7320	Morindae Officinalis Radix	4-[3-Hydroxymethyl-6-(3-hydroxy-propenyl)-2,3-dihydro-benzo[1,4]dioxin-2-yl]-benzene-1,2-diol	637304	FALSE	O1C(C(Oc2c1ccc(c2)/C=C/CO)CO)c1cc(O)c(O)cc1
MOL009539	0.7401	0.2599	0.7626	Morindae Officinalis Radix	2-Anthraquinonecarboxaldehyde	344310	FALSE	c1c(ccc2C(=O)c3ccccc3C(=O)c12)C=O
MOL009540	0.9210	0.0790	0.8818	Morindae Officinalis Radix	asperuloside acid	Not Available	FALSE	C12C(C(OC=C1C(=O)O)OC1C(O)C(O)C(O)C(O1)CO)C(=CC2O)CO
MOL009542	0.9029	0.0971	0.8749	Morindae Officinalis Radix	Majantol	175948	FALSE	c1(CC(CO)(C)C)cc(ccc1)C
MOL009543	0.9060	0.0940	0.8306	Morindae Officinalis Radix	ZINC03107553	7035404	FALSE	c12ccccc1C(C2)O
MOL009544	0.8578	0.1422	0.6933	Lycii Fructus	Hypogaeic acid	5318393	FALSE	C(=O)(CCCCC/C=C\CCCCCCCC)O
MOL009544	0.8578	0.1422	0.6933	Morindae Officinalis Radix	Hypogaeic acid	5318393	FALSE	C(=O)(CCCCC/C=C\CCCCCCCC)O
MOL009545	0.8503	0.1497	0.6891	Morindae Officinalis Radix	citrifolinin A-1	Not Available	FALSE	O1C=C(C2C(C1OC1C(C(C(C(O1)CO)O)O)O)C(C1C2O1)COC(C1(C2C(C3C1C(OC=C3C(=O)OC)OC1C(C(C(C(O1)CO)O)O)O)O2)O)O)C(=O)OC
MOL009546	0.9077	0.0923	0.8355	Morindae Officinalis Radix	deacetyl asperuloside	Not Available	FALSE	C1(C(O)C(C(C(O1)CO)O)O)OC1OC=C2C3C1C(=CC3OC2=O)CO
MOL009547	0.9210	0.0790	0.8818	Morindae Officinalis Radix	desacetyl asperulosidic acid	12315349	FALSE	O(C1OC=C(C2C1C(=CC2O)CO)C(=O)O)C1OC(C(O)C(O)C1O)CO
MOL009548	0.9468	0.0532	0.8480	Morindae Officinalis Radix	desacetyl asperulosidic acid_qt	Not Available	FALSE	OC1OC=C(C2C1C(=CC2O)CO)C(=O)O
MOL009549	0.9253	0.0747	0.9643	Morindae Officinalis Radix	Ether	3283	FALSE	O(CC)CC
MOL009550	0.8653	0.1347	0.7033	Morindae Officinalis Radix	heptasaccharide	Not Available	FALSE	C1(C(C(C(OC1COC1OCC(C(C1O)O)O)OC1C(C(OC1COC1C(C(C(CO1)O)O)O)OC1C(C(C(OC1COC1C(C(C(CO1)O)O)O)OC1C(C(C(OC1CO)O)O)O)O)O)O)O)O)O

MOL009551	0.3492	0.6508	0.6840	Morindae Officinalis Radix	isoprincepin	Not Available	FALSE	C1(Oc2c(OC1CO)ccc(c2)C1OCC2C1COC2c1cc(c(cc1)O)O)c1ccc(c(c1)O)O
MOL009552	0.9181	0.0819	0.9191	Morindae Officinalis Radix	m-Tolualdehyde	12105	FALSE	C(=O)c1cc(ccc1)C
MOL009553	0.9230	0.0770	0.8828	Morindae Officinalis Radix	Monotropein	73466	FALSE	O(C1OC=C(C2C1C(O)(C=C2)CO)C(=O)O)C1OC(C(O)C(O)C1O)CO
MOL009554	0.9363	0.0637	0.8775	Morindae Officinalis Radix	monotropein_qt	Not Available	FALSE	OC1OC=C(C2C1C(O)(C=C2)CO)C(=O)O
MOL009555	0.9433	0.0567	0.8319	Morindae Officinalis Radix	morindacin	44583980	FALSE	C1(=O)C(C2C(O1)C=C(C2CO)CO)CO
MOL009556	0.9586	0.0414	0.8839	Morindae Officinalis Radix	(4aR,7aS)-7-methylol-4,4a,5,7a-tetrahydro-3H-cyclopenta[c]pyran-1-one	10397184	FALSE	C1(=O)C2C(CCO1)CC=C2CO
MOL009557	0.8349	0.1651	0.7403	Morindae Officinalis Radix	morinipticoside	Not Available	FALSE	C1(C(O)C(O)C(O)C(O1)CO)OC1C2C(C(=CO1)C(=O)OC)C1C(C32C=C(C(=O)O3)C(=O)c2ccc(cc2)O)O
MOL009558	0.8499	0.1501	0.7262	Morindae Officinalis Radix	2-hydroxyethyl 5-hydroxy-2-(2-hydroxybenzoyl)-4-(hydroxymethyl)benzoate	24763413	FALSE	c1(cc(c(cc1C(=O)OCCO)O)CO)C(=O)c1ccccc1O
MOL009559	0.8884	0.1116	0.7656	Morindae Officinalis Radix	morintrifolins B	Not Available	FALSE	c1(c(c(c(cc1C(=O)OCCO)O)C)O)C(=O)c1ccc(c(c1O)OC)O

MOL009560	0.9214	0.0786	0.8413	Morindae Officinalis Radix	methyl (1S,4aS,6R,7R,7aS)-6-hydroxy-7-(hydroxymethyl)-1-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-1,4a,5,6,7,7a-hexahydrocyclopenta[d]pyran-4-carboxylate	10453987	FALSE	C12C(C(OC=C1C(=O)OC)OC1OC(C(C(C1O)O)O)CO)C(C(C2)O)CO
MOL009561	0.9369	0.0631	0.8180	Morindae Officinalis Radix	officinalisin	Not Available	FALSE	O1C2(OCCCC)C(C2O)(C(O)C(O)C1)CO
MOL009562	0.7695	0.2305	0.7226	Morindae Officinalis Radix	Ohioensin-A	Not Available	FALSE	C1(=O)CC2C3c4c1c(cc(c4c1c(C3Oc3c2cccc3)cc(cc1)O)O)O
MOL009563	0.9169	0.0831	0.9698	Morindae Officinalis Radix	NPG	31344	FALSE	OCC(CO)(C)C
MOL009564	0.7552	0.2448	0.7883	Morindae Officinalis Radix	rotungenic acid	Not Available	FALSE	C1(CCC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C)C(C)(C4C3=CCC21O)C)O
MOL009565	0.7301	0.2699	0.8572	Paederiae Scandentis Herba	Rubiadin-1-methyl ether	96191	FALSE	c12c(C(=O)c3c(C1=O)cccc3)cc(c(c2OC)C)O
MOL009565	0.7301	0.2699	0.8572	Morindae Officinalis Radix	Rubiadin-1-methyl ether	96191	FALSE	c12c(C(=O)c3c(C1=O)cccc3)cc(c(c2OC)C)O
MOL009567	0.9168	0.0832	0.8390	Fritiliariae Irrhosae Bulbus	1-O-feruloyl glycerol	Not Available	FALSE	c1cc(cc(c1O)OC)/C=C/C(=C)OCC(CO)O
MOL009568	0.9174	0.0826	0.9065	Fritiliariae Irrhosae Bulbus	Methylbenzylideneacetone	5370646	FALSE	O=C(/C(=C/c1ccccc1)/C)C
MOL009569	0.9431	0.0569	0.7564	Fritiliariae Irrhosae Bulbus	4,7-DIMETHYLBENZOFURAN	33109	FALSE	o1ccc2c1c(ccc2C)C
MOL009570	0.4831	0.5169	0.6504	Fritiliariae Irrhosae Bulbus	Methyl stearolate	534587	FALSE	C(#CCCCCCCCC)CCCCCCCC(=O)OC
MOL009572	0.4462	0.5538	0.7175	Fritiliariae Irrhosae Bulbus	Chuanbeinone	Not Available	FALSE	N12CC3C4C(C5C(C6(CCC(CC6C(=O)C5)O)C)C4)CCC3C(C2CCC(C1)C)C
MOL009573	0.3278	0.6722	0.6644	Fritillariae Pallidiflorae Bulbus	cycloposine	25078000	FALSE	O1C2(CCC3C4C(C5(C(=CC4)CC(OC4OC(C(O)C(O)C4O)CO)CC5)C)CC3=C2C)C(C2NCC(CC12)C)C
MOL009573	0.3278	0.6722	0.6644	Fritiliariae Irrhosae Bulbus	cycloposine	25078000	FALSE	O1C2(CCC3C4C(C5(C(=CC4)CC(OC4OC(C(O)C(O)C4O)CO)CC5)C)CC3=C2C)C(C2NCC(CC12)C)C

MOL009574	0.9233	0.0767	0.9106	Fritiliariae Irrhosae Bulbus	4-amino-1-[(2R,3R,4S,5S)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]pyrimidin-2-one	6603781	FALSE	C1(n2c(=O)nc(cc2)N)OC(C(C1O)O)CO
MOL009575	0.5548	0.4452	0.6321	Fritillariaeussuriensis Bulbus	delavine	Not Available	FALSE	O1C23C4N(CC5(C(C4(C4C6C2(OC1)CC(OC)C(C4)C6OC)C(OC)CC5)C3O)COC)CC
MOL009575	0.5548	0.4452	0.6321	Fritiliariae Irrhosae Bulbus	delavine	Not Available	FALSE	O1C23C4N(CC5(C(C4(C4C6C2(OC1)CC(OC)C(C4)C6OC)C(OC)CC5)C3O)COC)CC
MOL009576	0.4762	0.5238	0.6550	Fritiliariae Irrhosae Bulbus	ebeiedinone	Not Available	FALSE	C1CCC2(C(C1)C(=O)CC1C3CCC4C(C)C5CCC(C)C[NH+]5CC4C3CC21)C
MOL009576	0.4762	0.5238	0.6550	Fritillariaeussuriensis Bulbus	ebeiedinone	Not Available	FALSE	C1CCC2(C(C1)C(=O)CC1C3CCC4C(C)C5CCC(C)C[NH+]5CC4C3CC21)C
MOL009577	0.8425	0.1575	0.7582	Fritiliariae Irrhosae Bulbus	Aklavinon	159776	FALSE	OC1(C(c2c(C(O)C1)c(O)c1c(c2)C(=O)c2c(C1=O)c(O)ccc2)C(=O)OC)CC
MOL009578	0.9478	0.0522	0.8298	Fritiliariae Irrhosae Bulbus	(Z)-3-(3,4,5-trimethoxyphenyl)acrylic acid	1715138	FALSE	C(=O)(/C=C\c1cc(c(c(c1)OC)OC)OC)O
MOL009579	0.3106	0.6894	0.7897	Fritiliariae Irrhosae Bulbus	ent-(16S)-atisan-13,17-oxide	Not Available	FALSE	O1C2C3CC4C(CC3C1)(C2)CCC1C4(CCCC1(C)C)C
MOL009580	0.3084	0.6916	0.7811	Fritiliariae Irrhosae Bulbus	ent-17-norkauran-16-one	Not Available	FALSE	O=C1C2CC3(C(C4(C(CC3)C(CCC4)(C)C)C)CC2)C1
MOL009581	0.2577	0.7423	0.7698	Fritiliariae Irrhosae Bulbus	ent-kaur-15-en-17-ol	Not Available	FALSE	OCC1=CC23C(C4(C(C(CCC4)(C)C)CC2)C)CCC1C3
MOL009582	0.5462	0.4538	0.7618	Fritillariaeussuriensis Bulbus	Sipeimine	Not Available	FALSE	C12C(C3C(C2)C2C(CC3)C(C3N(C2)CC(CC3)C)(C)O)CC(=O)C2C1(CCC(C2)O)C
MOL009582	0.5462	0.4538	0.7618	Fritillariae Pallidiflorae Bulbus	Sipeimine	Not Available	FALSE	C12C(C3C(C2)C2C(CC3)C(C3N(C2)CC(CC3)C)(C)O)CC(=O)C2C1(CCC(C2)O)C
MOL009582	0.5462	0.4538	0.7618	Fritiliariae Irrhosae Bulbus	Sipeimine	Not Available	FALSE	C12C(C3C(C2)C2C(CC3)C(C3N(C2)CC(CC3)C)(C)O)CC(=O)C2C1(CCC(C2)O)C
MOL009583	0.6031	0.3969	0.7282	Fritillariae Pallidiflorae Bulbus	STOCK1N-49993	Not Available	FALSE	C12C(C3C(C2)C2C(CC3)C(C3N(C2)CC(CC3)C)(C)O)CC(=O)C2C1(CCC(C2)OC1C(O)C(O)C(O)C(O1)CO)C
MOL009583	0.6031	0.3969	0.7282	Fritiliariae Irrhosae Bulbus	STOCK1N-49993	Not Available	FALSE	C12C(C3C(C2)C2C(CC3)C(C3N(C2)CC(CC3)C)(C)O)CC(=O)C2C1(CCC(C2)OC1C(O)C(O)C(O)C(O1)CO)C
MOL009583	0.6031	0.3969	0.7282	Fritillariaeussuriensis Bulbus	STOCK1N-49993	Not Available	FALSE	C12C(C3C(C2)C2C(CC3)C(C3N(C2)CC(CC3)C)(C)O)CC(=O)C2C1(CCC(C2)OC1C(O)C(O)C(O)C(O1)CO)C

MOL009584	0.5462	0.4538	0.7618	Fritiliariae Irrhosae Bulbus	imperialine-3 β-D-glucoside_qt	Not Available	FALSE	C12C(C3C(C2)C2C(CC3)C(C3N(C2)CC(CC3)C)(C)O)CC(=O)C2C1(CCC(C2)O)C
MOL009584	0.5462	0.4538	0.7618	Fritillariaeussuriensis Bulbus	imperialine-3 β-D-glucoside_qt	Not Available	FALSE	C12C(C3C(C2)C2C(CC3)C(C3N(C2)CC(CC3)C)(C)O)CC(=O)C2C1(CCC(C2)O)C
MOL009584	0.5462	0.4538	0.7618	Fritillariae Pallidiflorae Bulbus	imperialine-3 β-D-glucoside_qt	Not Available	FALSE	C12C(C3C(C2)C2C(CC3)C(C3N(C2)CC(CC3)C)(C)O)CC(=O)C2C1(CCC(C2)O)C
MOL009585	0.6153	0.3847	0.7345	Fritiliariae Irrhosae Bulbus	Imperialine-β-N-oxide	Not Available	FALSE	C12C(C3C(C2)C2C(CC3)C(C3[N+](C2)(CC(CC3)C)O)(C)O)CC(=O)C2C1(CCC(C2)O)C
MOL009585	0.6153	0.3847	0.7345	Fritillariae Pallidiflorae Bulbus	Imperialine-β-N-oxide	Not Available	FALSE	C12C(C3C(C2)C2C(CC3)C(C3[N+](C2)(CC(CC3)C)O)(C)O)CC(=O)C2C1(CCC(C2)O)C
MOL009586	0.5559	0.4441	0.7268	Fritiliariae Irrhosae Bulbus	isoverticine	Not Available	FALSE	C1(CCC2(C(C1)C(CC1C3CCC4C(C)(C5CCC(C)CN5CC4C3CC21)O)O)C)O
MOL009587	0.6146	0.3854	0.7152	Fritiliariae Irrhosae Bulbus	isoverticine-beta-N-oxide	Not Available	FALSE	C1(CCC2(C(C1)C(CC1C3CCC4C(C)(C5CCC(C)C[N+]5(CC4C3CC21)O)O)O)C)O
MOL009588	0.5641	0.4359	0.6851	Fritiliariae Irrhosae Bulbus	Korseveriline	Not Available	FALSE	C1C(CC2C(C1)(C1CC3C(C1CC2O)(CCC1C3CN2C(C1C)CCC(C2)C)O)C)O
MOL009589	0.4673	0.5327	0.7443	Fritiliariae Irrhosae Bulbus	Korseverinine	Not Available	FALSE	C1C(CC2C(C1)(C1=C(CC2O)C2C(C1)C1C(CC2)C(C2N(C1)CC(CC2)C)C)C)O
MOL009590	0.2458	0.7542	0.7169	Fritiliariae Irrhosae Bulbus	Korsevinine	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2=O)C2C(CC1)(C(CC2)C(C)C1=NC2C(CC1O2)C)C)C)O
MOL009591	0.5659	0.4341	0.7471	Fritiliariae Irrhosae Bulbus	Korsine	Not Available	FALSE	OC1C2C3C(C(C4N(C3)CC(CC4O)C)C)CCC2C2=C1C1(C(CC2)CC(O)CC1)C
MOL009593	0.5462	0.4538	0.7618	Fritillariaeussuriensis Bulbus	verticinone	Not Available	FALSE	C12C(C3C(C2)C2C(CC3)C(C3N(C2)CC(CC3)C)(C)O)CC(=O)C2C1(CCC(C2)O)C
MOL009593	0.5462	0.4538	0.7618	Fritillariae Pallidiflorae Bulbus	verticinone	Not Available	FALSE	C12C(C3C(C2)C2C(CC3)C(C3N(C2)CC(CC3)C)(C)O)CC(=O)C2C1(CCC(C2)O)C
MOL009593	0.5462	0.4538	0.7618	Fritiliariae Irrhosae Bulbus	verticinone	Not Available	FALSE	C12C(C3C(C2)C2C(CC3)C(C3N(C2)CC(CC3)C)(C)O)CC(=O)C2C1(CCC(C2)O)C
MOL009594	0.8911	0.1089	0.8439	Fritiliariae Irrhosae Bulbus	Nemerol	4058	TRUE	O(C(=O)C1(CCN(CC1)C)c1ccccc1)CC
MOL009595	0.9171	0.0829	0.7869	Fritiliariae Irrhosae Bulbus	2-(chloromethyl)-7-methyl-[1,3,4]thiadiazolo[2,3-b]pyrimidin-5-one	385795	FALSE	ClCc1sc2n(n1)c(=O)cc(n2)C
MOL009596	0.4462	0.5538	0.7175	Fritiliariae Irrhosae Bulbus	sinpemine A	Not Available	FALSE	O=C1C2C(C3C(C4C(C5C(CC4)C(C4N(C5)CC(CC4)C)C)C3)C1)(CCC(O)C2)C
MOL009596	0.4462	0.5538	0.7175	Fritillariae Pallidiflorae Bulbus	sinpemine A	Not Available	FALSE	O=C1C2C(C3C(C4C(C5C(CC4)C(C4N(C5)CC(CC4)C)C)C3)C1)(CCC(O)C2)C

MOL009597	0.7388	0.2612	0.8567	Fritiliariae Irrhosae Bulbus	solanidine 3-O-α-L-rhamnopyranosyl-(1-2)-[β-D-glucopyranosyl-(1-4)]-β-D-glucopyranoside	Not Available	FALSE	O(C1CC2=CCC3C4C(C5C(N6C(C5C)CCC(C6)C)C4)(CCC3C2(CC1)C)C)C1OC(C(O)C(O)C1OC1OC(C(OC2OC(C(O)C(O)C2O)CO)C(O)C1O)C)CO
MOL009598	0.1187	0.8813	0.7663	Fritiliariae Irrhosae Bulbus	solanine	2335	FALSE	O(CC[N+](Cc1ccccc1)(C)C)CCOc1ccc(C(CC(C)(C)C)(C)C)cc1
MOL009599	0.4462	0.5538	0.7175	Fritiliariae Irrhosae Bulbus	songbeinone	Not Available	FALSE	C1(CCC2(C(C1)C(=O)CC1C3CCC4C(C)C5CCC(C)CN5CC4C3CC21)C)O
MOL009600	0.2894	0.7106	0.7791	Fritiliariae Irrhosae Bulbus	songbeisine	Not Available	FALSE	C1(=O)C2C3(C(CCC2C2CCC4(C(=C12)C)OC1C(NCC(C1)C)C4C)CC(CC3)O)C
MOL009603	0.5604	0.4396	0.6222	Lycii Fructus	13,17,21-trimethyltritriacontane	Not Available	FALSE	CCCCCCCCCCCCCC(CCCC(CCCC(CCCCCCCCCCCCC)C)C)C
MOL009605	0.9431	0.0569	0.8853	Lycii Fructus	1,2,3,4,5-Pentamethylcyclopentadiene	77667	FALSE	CC1C(=C(C)C(=C1C)C)C
MOL009606	0.8481	0.1519	0.8286	Lycii Fructus	(4aS,7R)-7-isopropenyl-1,4a-dimethyl-5,6,7,8-tetrahydronaphthalen-2-one	10976879	FALSE	C1(C(=C)C)CCC2(C)C(=C(C(=O)C=C2)C)C1
MOL009607	0.9388	0.0612	0.7621	Lycii Fructus	(1R,4aR,5S,8aS)-1,5-dimethyldecalin	21717998	FALSE	C1(CCCC2C(CCCC12)C)C
MOL009608	0.9098	0.0902	0.7983	Lycii Fructus	WLN: E6E	12368	FALSE	BrCCCCCCBr
MOL009609	0.8402	0.1598	0.7055	Lycii Fructus	1,6-dimethyl-1-isopropyl-1,2,3,4,4a,7-hexahydronaphthalene	Not Available	FALSE	C1(CCCC2C=C(CC=C12)C)(C(C)C)C
MOL009610	0.9333	0.0667	0.7655	Lycii Fructus	(1S,4aS,6S,8aR)-1,6-dimethyldecalin	21718000	FALSE	C1(CCCC2CC(CCC12)C)C

MOL009612	0.2269	0.7731	0.6687	Lycii Fructus	(24R)-4alpha-Methyl-24-ethylcholesta-7,25-dien-3beta-ylacetate	Not Available	FALSE	C1C(C(C2C(C1)(C1C(=CC2)C2(C(CC1)(C(CC2)C(CCC(C(=C)C)CC)C)C)C)C)C)OC(=O)C
MOL009615	0.3595	0.6405	0.6920	Lycii Fructus	24-Methylenecycloartan-3beta,21-diol	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C2(CCC2(C1(CCC2C(CO)CCC(=C)C(C)C)C)C)C3)O
MOL009616	0.4364	0.5636	0.6147	Lycii Fructus	24-Methylenecycloartanol ferulate	Not Available	FALSE	C(=C\c1cc(c(cc1)O)OC)/C(=O)OC1CCC23C(C1(C)C)CCC1C2(CCC2(C1(CCC2C(C)CCC(=C)C(C)C)C)C)C3
MOL009620	0.2694	0.7306	0.6107	Lycii Fructus	24-methyl-31-norlanost-9(11)-enol	Not Available	FALSE	OC1C(C2C(C3=CCC4(C(C3CC2)(CCC4C(CCC(C(C)C)C)C)C)C)(CC1)C)C
MOL009621	0.2510	0.7490	0.6702	Lycii Fructus	24-methylenelanost-8-enol	Not Available	FALSE	C1C2=C(C3(C(C1)(C(CC3)C(CCC(=C)C(C)C)C)C)C)CCC1C2(CCC(C1(C)C)O)C
MOL009622	0.2167	0.7833	0.6060	Lycii Fructus	Fucosterol	5281328	FALSE	OC1CC2=CCC3C4C(C(CC4)C(CC/C(=C\C)/C(C)C)C)(CCC3C2(CC1)C)C
MOL009622	0.2167	0.7833	0.6060	Thalluslaminariae	Fucosterol	5281328	FALSE	OC1CC2=CCC3C4C(C(CC4)C(CC/C(=C\C)/C(C)C)C)(CCC3C2(CC1)C)C
MOL009624	0.9396	0.0604	0.7999	Lycii Fructus	(2S,3S,4aR,8aR)-2,3-dimethyldecalin	21718043	FALSE	C1C(C(CC2CCCCC12)C)C
MOL009628	0.9598	0.0402	0.8669	Lycii Fructus	(2-fluoro-2-methoxycyclopropyl)benzene	Not Available	FALSE	c1(ccccc1)C1C(C1)(OC)F
MOL009629	0.9052	0.0948	0.8520	Lycii Fructus	2-methyl-5-ethyloctane	Not Available	FALSE	CC(CCC(CCC)CC)C
MOL009630	0.8988	0.1012	0.8712	Lycii Fructus	2-o-(beta-d-glucopyranosyl)-ascorbic acid	54693473	FALSE	OC1=C(C(=O)OC1C(O)CO)OC1C(O)C(O)C(O)C(O1)CO
MOL009631	0.3834	0.6166	0.6818	Lycii Fructus	31-Norcyclolaudenol	Not Available	FALSE	CC(CCCC(C)C(=C)C)C1C2(C(CC1)(C1C3(CC2)C2(C(CC1)C(C(CC2)O)C)C3)C)C

MOL009632	0.3604	0.6396	0.7107	Lycii Fructus	31-norcycloartanol	Not Available	FALSE	OC1C(C2C3(C4(C3)C(C3(C(CC4)(C(CC3)C(CCCC(C)C)C)C)C)CC2)CC1)C
MOL009633	0.2316	0.7684	0.6763	Lycii Fructus	31-norlanost-9(11)-enol	Not Available	FALSE	OC1C(C2C(C3=CCC4(C(C3CC2)(CCC4C(CCCC(C)C)C)C)C)(CC1)C)C
MOL009634	0.2016	0.7984	0.6998	Lycii Fructus	31-norlanosterol	Not Available	FALSE	C1(CCC2(C(C1C)CCC1=C2CCC2(C1(CCC2C(CCC=C(C)C)C)C)C)C)O
MOL009636	0.8968	0.1032	0.8396	Lycii Fructus	4-((2Z,5E)-5-methylhepta-2,5-dien-2-yl)cyclohex-1-ene	Not Available	FALSE	C/C(=C/C/C(=C/C)/C)/C1CC=CCC1
MOL009637	0.7377	0.2623	0.7966	Lycii Fructus	4-[(Z,1R)-3-(4-methoxyphenyl)-1-vinylprop-2-enyl]phenol	23626544	FALSE	c1c(ccc(c1)/C=C\C(c1ccc(cc1)O)C=C)OC
MOL009638	0.8959	0.1041	0.9798	Lycii Fructus	1-(2-hydrazino-4-methyl-5-pyrimidinyl)ethanone	341594	FALSE	c1(nc(c(cn1)C(=O)C)C)NN
MOL009639	0.2183	0.7817	0.6621	Lycii Fructus	Lophenol	160482	FALSE	C1(CCC2(C(C1C)CC=C1C3CCC(C(CCCC(C)C)C)C3(C)CCC21)C)O
MOL009640	0.2337	0.7663	0.6457	Lycii Fructus	4alpha,14alpha,24-trimethylcholesta-8,24-dienol	Not Available	FALSE	C1(CCC2(C(C1C)CCC1=C2CCC2(C1(CCC2C(CCC(=C(C)C)C)C)C)C)C)O
MOL009641	0.2103	0.7897	0.6135	Lycii Fructus	4alpha,24-dimethylcholesta-7,24-dienol	Not Available	FALSE	C1(CCC2(C(C1C)CC=C1C3CCC(C(CCC(=C(C)C)C)C)C3(C)CCC21)C)O
MOL009642	0.2128	0.7872	0.6471	Lycii Fructus	4alpha-methyl-24-ethylcholesta-7,24-dienol	Not Available	FALSE	C1(CCC2(C(C1C)CC=C1C3CCC(C(CCC(=C(C)C)CC)C)C3(C)CCC21)C)O
MOL009643	0.8717	0.1283	0.7067	Lycii Fructus	5-Butylnonane	300476	FALSE	CCCCC(CCCC)CCCC

MOL009644	0.2296	0.7704	0.6530	Lycii Fructus	6-Fluoroindole-7-Dehydrocholesterol	Not Available	FALSE	OC1CC2=C(C=C3C4C(C(CC4)C(CCCC(C)C)C)(CCC3C2(CC1)C)C)F
MOL009645	0.8920	0.1080	0.8170	Lycii Fructus	7-O-Methylluteolin-6-C-beta-glucoside	Not Available	FALSE	C1(C(C(C(C(O1)Oc1c(c2c(cc1OC)OC(CC2=O)c1cc(c(cc1)O)O)O)O)O)O)CO
MOL009646	0.9351	0.0649	0.8962	Lycii Fructus	7-O-Methylluteolin-6-C-beta-glucoside_qt	Not Available	FALSE	Oc1c(c2c(cc1OC)OC(CC2=O)c1cc(c(cc1)O)O)O
MOL009649	0.5095	0.4905	0.6530	Lycii Fructus	Anhydrorhodovibrin	5368308	FALSE	O(C(C/C=C/C(=C/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C=C(/CCC=C(C)C)\C)\C)\C)/C)/C)/C)(C)C)C
MOL009650	0.8739	0.1261	0.9139	Lycii Fructus	Atropine	637577	FALSE	C12CC(CC(N1C)CC2)OC(=O)C(c1ccccc1)CO
MOL009651	0.2725	0.7275	0.6015	Lycii Fructus	Cryptoxanthin monoepoxide	Not Available	FALSE	C1C(CC2(C(C1(C)C)(O2)/C=C/C(=C\C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CCCC1(C)C)C)\C)\C)/C)/C)C)O
MOL009652	0.3106	0.6894	0.7040	Lycii Fructus	Cycloartanol acetate	Not Available	FALSE	C1(C(C2C3(CC1)C1(C(CC2)C2(C(CC1)(C)C(CC2)C(CCCC(C)C)C)C)C3)(C)C)OC(=O)C
MOL009653	0.3701	0.6299	0.6919	Lobeliae Chinensis Herba	Cycloeucalenol	Not Available	FALSE	OC1C(C2C3(C4(C3)C(C3(C(CC4)(C(CC3)C(CCC(=C)C(C)C)C)C)C)CC2)CC1)C
MOL009653	0.3701	0.6299	0.6919	Mori Cortex	Cycloeucalenol	Not Available	FALSE	OC1C(C2C3(C4(C3)C(C3(C(CC4)(C(CC3)C(CCC(=C)C(C)C)C)C)C)CC2)CC1)C
MOL009653	0.3701	0.6299	0.6919	Perillae Fructus	Cycloeucalenol	Not Available	FALSE	OC1C(C2C3(C4(C3)C(C3(C(CC4)(C(CC3)C(CCC(=C)C(C)C)C)C)C)CC2)CC1)C
MOL009653	0.3701	0.6299	0.6919	Lycii Fructus	Cycloeucalenol	Not Available	FALSE	OC1C(C2C3(C4(C3)C(C3(C(CC4)(C(CC3)C(CCC(=C)C(C)C)C)C)C)CC2)CC1)C
MOL009654	0.7861	0.2139	0.8090	Lycii Fructus	Cyclofoetoside B	Not Available	FALSE	C1(C(OCC(C1O)O)OC1C(C2C3(CC1)C1(C(CC2)C2(C(CC1)(C(C(C2)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)C)C(CCC(C(C)(O)C)O)C)C)C3)(C)CO)O
MOL009655	0.4757	0.5243	0.6627	Lycii Fructus	Cyclofoetoside B_qt	Not Available	FALSE	OC1C(C)(CO)C2C3(C4(C3)C(CC2)C2(C(C)(CC4)C(C(O)C2)C(CCC(C(O)(C)C)O)C)C)CC1
MOL009656	0.4373	0.5627	0.6190	Lycii Fructus	(E,E)-1-ethyl octadeca-3,13-dienoate	Not Available	FALSE	C(=O)(C/C=C/CCCCCCCC/C=C/CCCC)OCC
MOL009657	0.9613	0.0387	0.9576	Lycii Fructus	Ethyl p-toluate	66743	FALSE	c1(C(=O)OCC)ccc(cc1)C
MOL009658	0.9126	0.0874	0.9760	Bamusaeconcretiosilicea	DGL	23327	FALSE	OC(=O)C(N)CCC(=O)O
MOL009658	0.9126	0.0874	0.9760	Lycii Fructus	DGL	23327	FALSE	OC(=O)C(N)CCC(=O)O
MOL009659	0.2991	0.7009	0.7372	Lycii Fructus	Hypaconitine	Not Available	FALSE	C1CC2(C3C4(C1OC)C1C5C(C(C3OC)C4N(C)C2)C(C(C(C5OC(=O)c2ccccc2)(C1)O)OC)O)OC(=O)C)COC

MOL009660	0.9124	0.0876	0.8323	Lycii Fructus	methyl (1R,4aS,7R,7aS)-4a,7-dihydroxy-7-methyl-1-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-1,5,6,7a-tetrahydrocyclopenta[d]pyran-4-carboxylate	11968619	FALSE	C1=C(C2(C(C(O1)OC1C(C(C(C(O1)CO)O)O)O)C(CC2)(O)C)O)C(=O)OC
MOL009661	0.9475	0.0525	0.8121	Lycii Fructus	Ipolamiide_qt	Not Available	FALSE	C1=C(C2(C(C(O1)O)C(CC2)(O)C)O)C(=O)OC
MOL009662	0.6405	0.3595	0.7815	Lycii Fructus	Lantadene A	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(CC(C1)(C)C)OC(=O)/C(=C/C)/C)C(=O)O)C)C)(C)C
MOL009663	0.8898	0.1102	0.8050	Lycii Fructus	Maaliol	Not Available	FALSE	OC1(C2C3C(C3(C)C)CCC2(C(=O)CC1)C)C
MOL009664	0.8331	0.1669	0.6789	Lycii Fructus	Physalin A	Not Available	FALSE	C1=CCC2=CC(C3C(C2(C1=O)C)CCC1(C24C(C(=O)C3(O4)O)C3(C(=C)C(=O)OC(C2(OC1=O)C)C3)C)O)O
MOL009665	0.8704	0.1296	0.8241	Lycii Fructus	Physcion-8-O-beta-D-gentiobioside	5320543	FALSE	c1(cc(c2c(c1)C(=O)c1c(C2=O)c(cc(c1)OC)O)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)C
MOL009667	0.8573	0.1427	0.6940	Ardisiae Japonicae Herba	11Z-hexadecenoic acid	5312414	FALSE	C(=O)(CCCCCCCCC/C=C\CCCC)O
MOL009667	0.8573	0.1427	0.6940	Lycii Fructus	11Z-hexadecenoic acid	5312414	FALSE	C(=O)(CCCCCCCCC/C=C\CCCC)O
MOL009668	0.7779	0.2221	0.8106	Lycii Fructus	Zederone	Not Available	FALSE	C1CC2(C(C(=O)c3c(C/C(=C/1)/C)occ3C)O2)C
MOL009669	0.8492	0.1508	0.8806	Lycii Fructus	aminoethyl thiosulfite	Not Available	FALSE	S(=S)(OCCN)O
MOL009670	0.8826	0.1174	0.9419	Lycii Fructus	2-Pyridylamine	10439	FALSE	c1(ccccn1)N
MOL009673	0.9407	0.0593	0.7180	Lycii Fructus	cis,trans-1,6-dimethyl-spiro-[4,5]-decane	Not Available	FALSE	C1(CCCC21C(CCCC2)C)C
MOL009675	0.9610	0.0390	0.9611	Lycii Fructus	Ethyl anisate	60979	FALSE	O(C(=O)c1ccc(OC)cc1)CC
MOL009676	0.9068	0.0932	0.9690	Lycii Fructus	DGN	6992096	FALSE	OC(=O)C(N)CCC(=O)N

MOL009677	0.2225	0.7775	0.7095	Lycii Fructus	lanost-8-en-3beta-ol	440560	FALSE	OC1C(C2C(C3=C(C4(C(C(CC4)C(CCCC(C)C)C)(CC3)C)C)CC2)(CC1)C)(C)C
MOL009678	0.2225	0.7775	0.7095	Lycii Fructus	lanost-8-enol	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1=C2CCC2(C1(C)CCC2C(CCCC(C)C)C)C)C)O
MOL009679	0.2113	0.7887	0.6437	Lycii Fructus	lathosterol	65728	FALSE	C12C3=CCC4C(C3CCC1(C(CC2)C(CCCC(C)C)C)C)(CCC(C4)O)C
MOL009681	0.2382	0.7618	0.6489	Lycii Fructus	Obtusifoliol	65252	FALSE	OC1C(C2C(C3=C(C4(C(C(CC4)C(CCC(=C)C(C)C)C)(CC3)C)C)CC2)(CC1)C)C
MOL009681	0.2382	0.7618	0.6489	Calyx Seu Fructus Physalis	Obtusifoliol	65252	FALSE	OC1C(C2C(C3=C(C4(C(C(CC4)C(CCC(=C)C(C)C)C)(CC3)C)C)CC2)(CC1)C)C
MOL009681	0.2382	0.7618	0.6489	Perillae Fructus	Obtusifoliol	65252	FALSE	OC1C(C2C(C3=C(C4(C(C(CC4)C(CCC(=C)C(C)C)C)(CC3)C)C)CC2)(CC1)C)C
MOL009685	0.9407	0.0593	0.7180	Lycii Fructus	trans,trans-1,6-dimethyl-spiro-[4,5]-decane	Not Available	FALSE	C1(CCCC21C(CCCC2)C)C
MOL009686	0.7346	0.2654	0.6841	Sojae Semen Nigrum	SBB008790	144130	FALSE	C(CCC#CCCCC)CCCCCCCO
MOL009687	0.8731	0.1269	0.7817	Sojae Semen Nigrum	11-Phenoxyundecanoic acid	81597	FALSE	c1(ccccc1)OCCCCCCCCCCC(=O)O
MOL009690	0.9463	0.0537	0.9182	Sojae Semen Nigrum	(1,2-DIMETHYLPROPYL)BENZENE	12482226	FALSE	c1(C(C(C)C)C)ccccc1
MOL009691	0.9001	0.0999	0.8637	Sojae Semen Nigrum	1,3-dimethylbutylbenzene	49836662	FALSE	c1(ccccc1)C(CC(C)C)C
MOL009692	0.8926	0.1074	0.8693	Sojae Semen Nigrum	(1Z,5Z)-cyclodeca-1,5-diene	5792121	FALSE	C\1=C\CC/C=C\CCCC1
MOL009693	0.9234	0.0766	0.8250	Sojae Semen Nigrum	Cyclopentenylpyrrolidine	81570	FALSE	N1(CCCC1)C1=CCCC1
MOL009694	0.9435	0.0565	0.8919	Sojae Semen Nigrum	2-Benzyl-2-isopropenylmalononitrile	561221	FALSE	C(=C)(C)C(C#N)(C#N)Cc1ccccc1
MOL009696	0.8984	0.1016	0.9335	Sojae Semen Nigrum	2,4-Dimethylpyrrole	39539	FALSE	c1(cc([nH]c1)C)C
MOL009697	0.9486	0.0514	0.8798	Sojae Semen Nigrum	2,5-Dimethyl-1-propylpyrrole	527547	FALSE	n1(c(ccc1C)C)CCC
MOL009698	0.8899	0.1101	0.9516	Sojae Semen Nigrum	Imidazole, 2-acetoxy-	558451	FALSE	c1([nH]ccn1)OC(=O)C

MOL009699	0.9599	0.0401	0.8364	Sojae Semen Nigrum	2-ethyl-1,2,3-propanetriylbutanoate	Not Available	FALSE	C1(=O)C2(C(C)C(C)(C2)CO1)CC
MOL009701	0.9217	0.0783	0.8941	Sojae Semen Nigrum	3,6,6-trimethylundecyl-2,5,10-trione	Not Available	FALSE	C(=O)(C(CC(=O)C(CCCC(=O)C)(C)C)C)C
MOL009702	0.9421	0.0579	0.9311	Sojae Semen Nigrum	3-Ethoxy-4-methoxyphenol	580771	FALSE	c1(c(ccc(c1)O)OC)OCC
MOL009703	0.9232	0.0768	0.8964	Sojae Semen Nigrum	HXD	5312804	FALSE	C(=O)(CC(CCCCCCCCC)O)O
MOL009704	0.8260	0.1740	0.8626	Sojae Semen Nigrum	3-Methylthiophene-2-carbonitrile	521617	FALSE	c1(c(ccs1)C)C#N
MOL009705	0.9032	0.0968	0.8129	Sojae Semen Nigrum	Skatol	6736	FALSE	[nH]1cc(c2ccccc12)C
MOL009706	0.8772	0.1228	0.8993	Sojae Semen Nigrum	Pramoxine	4886	TRUE	N1(CCOCC1)CCCOc1ccc(cc1)OCCCC
MOL009707	0.8795	0.1205	0.8038	Sojae Semen Nigrum	4-Dodecene	5364443	FALSE	C(CCCC)CC/C=C/CCC
MOL009708	0.9310	0.0690	0.9712	Sojae Semen Nigrum	Pentoxone	7884	FALSE	C(C(OC)(C)C)C(=O)C
MOL009709	0.7677	0.2323	0.8793	Sojae Semen Nigrum	5-methoxy-n-4-phenylbutylcyclohexa-1-4-dienamine	Not Available	FALSE	N(CCCCc1ccccc1)C1=CCC=C(C1)OC
MOL009710	0.9261	0.0739	0.7994	Sojae Semen Nigrum	(S)-bupropion	667684	FALSE	Clc1cc(C(=O)C(NC(C)(C)C)C)ccc1
MOL009711	0.2944	0.7056	0.7176	Sojae Semen Nigrum	Cycloartenone	Not Available	FALSE	C1(=O)C(C2C3(CC1)C1(C(CC2)C2(C(CC1)(C)C(CC2)C(CCC=C(C)C)C)C)C3)(C)C
MOL009712	0.5324	0.4676	0.7338	Sojae Semen Nigrum	Genkdaphin	5317554	FALSE	c12c(ccc(c1)C1OCC3C1C(=O)OC3c1ccc3c(c1)OCO3)OCO2
MOL009713	0.7360	0.2640	0.8468	Sojae Semen Nigrum	Soyasaponin	Not Available	FALSE	C1(CC(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(CC(C1)(C)C)O)C)C)C)(CO)C)OC1OC(C(C(C1OC1OC(C(C(C1OC1OC(C(CC1O)O)C)O)O)O)CO)O)O)C(=O)O
MOL009714	0.4190	0.5810	0.7700	Sojae Semen Nigrum	Soyasaponin_qt	Not Available	FALSE	C1(CC(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(CC(C1)(C)C)O)C)C)C)C)(CO)C)O
MOL009715	0.8956	0.1044	0.8261	Sojae Semen Nigrum	N,N'-bis(3-aminopropyl)heptane-1,7-diamine	492218	FALSE	NCCCNCCCCCCCNCCCN
MOL009716	0.8562	0.1438	0.6227	Sojae Semen Nigrum	Cadina-9,11(12)-diene	Not Available	FALSE	C1C(CC2C(C1)C(=CCC2C(=C)C)C)C
MOL009717	0.7657	0.2343	0.6440	Sojae Semen Nigrum	Pinolenic acid	5312493	FALSE	OC(=O)CCC/C=C/CC/C=C/C/C=C/CCCCC

MOL009718	0.9511	0.0489	0.8251	Sojae Semen Nigrum	Phenylcyclopropane	70112	FALSE	C1(c2ccccc2)CC1
MOL009719	0.8921	0.1079	0.9540	Sojae Semen Nigrum	(2S)-2,3-dihydroxypropanoic acid	6326776	FALSE	OCC(C(=O)O)O
MOL009720	0.7746	0.2254	0.7030	Cyathulae Radix	daidzin	107971	FALSE	c12c(c(=O)c(co2)c2ccc(cc2)O)ccc(c1)OC1OC(C(C(C1O)O)O)CO
MOL009720	0.7746	0.2254	0.7030	Radix Puerariae	daidzin	107971	FALSE	c12c(c(=O)c(co2)c2ccc(cc2)O)ccc(c1)OC1OC(C(C(C1O)O)O)CO
MOL009720	0.7746	0.2254	0.7030	Sojae Semen Nigrum	daidzin	107971	FALSE	c12c(c(=O)c(co2)c2ccc(cc2)O)ccc(c1)OC1OC(C(C(C1O)O)O)CO
MOL009720	0.7746	0.2254	0.7030	Sojae Semen Praeparatum	daidzin	107971	FALSE	c12c(c(=O)c(co2)c2ccc(cc2)O)ccc(c1)OC1OC(C(C(C1O)O)O)CO
MOL009722	0.8826	0.1174	0.8386	Sojae Semen Nigrum	L-Folinic acid	149436	FALSE	O=c1nc([nH]c2NCC(N(c12)C=O)CNc1ccc(cc1)C(=O)NC(CCC(=O)O)C(=O)O)N
MOL009723	0.9352	0.0648	0.9630	Sojae Semen Nigrum	HPN	136449	FALSE	C(CC(=O)N)CCCC
MOL009724	0.9008	0.0992	0.8390	Sojae Semen Nigrum	Heptylbenzene	14115	FALSE	c1(CCCCCCC)ccccc1
MOL009725	0.7079	0.2921	0.6208	Sojae Semen Nigrum	Palmitonitrile	69424	FALSE	C(CCCCCCCC)CCCCCCC#N
MOL009725	0.7079	0.2921	0.6208	Sesami Nigrum Semen	Palmitonitrile	69424	FALSE	C(CCCCCCCC)CCCCCCC#N
MOL009726	0.8769	0.1231	0.8954	Sojae Semen Nigrum	indole	Not Available	FALSE	N1=C2C(C=C1)C=CC=C2
MOL009727	0.8939	0.1061	0.9654	Lasiosphaera Seu Calvatia	LEVA	11579	FALSE	C(=O)(CCC(=O)O)C
MOL009727	0.8939	0.1061	0.9654	Ranunculi Ternati Radix	LEVA	11579	FALSE	C(=O)(CCC(=O)O)C
MOL009727	0.8939	0.1061	0.9654	Amygdalus Communis Vas	LEVA	11579	FALSE	C(=O)(CCC(=O)O)C
MOL009727	0.8939	0.1061	0.9654	Sojae Semen Nigrum	LEVA	11579	FALSE	C(=O)(CCC(=O)O)C
MOL009728	0.8584	0.1416	0.7384	Sojae Semen Nigrum	malonyl-genistin	Not Available	FALSE	C(=O)(CC(=O)OCC1C(C(C(C(O1)Oc1cc2c(c(=O)c(co2)c2ccc(cc2)O)c(c1)O)O)O)O)O
MOL009731	0.4699	0.5301	0.6100	Sojae Semen Nigrum	Methyl cis-11-octadecenoate	5364505	FALSE	C(CCCC/C=C\CCCCCC)CCCCC(=O)OC
MOL009733	0.4823	0.5177	0.6881	Sojae Semen Nigrum	methyl 12-oxooctadec-9-enoate	6386109	FALSE	C(=O)(CCCCCCC/C=C/CC(=O)CCCCCC)OC
MOL009735	0.6027	0.3973	0.6827	Sojae Semen Nigrum	N-(p-Hydroxyphenethyl) actinidine	442550	FALSE	c1(c[n+](cc2c1CCC2C)CCc1ccc(cc1)O)C
MOL009737	0.8926	0.1074	0.8774	Sojae Semen Nigrum	sialic acid	25322860	FALSE	O1C(C(NC(=O)C)C(O)CC1(O)C(=O)O)C(O)C(O)C(O)CO

MOL009738	0.4800	0.5200	0.7116	Abri Herba	(3R,4S,4aR,6aR,6aS,6bR,8aR,9S,10S,12aR,14bS)-2,2,4a,6a,6b,9,12a-heptamethyl-9-methylol-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-3,4,10-triol	12442849	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(CO)C)C)C1C(CC3)(C(C(C(C1)(C)C)O)O)C)C)C
MOL009738	0.4800	0.5200	0.7116	Sojae Semen Nigrum	(3R,4S,4aR,6aR,6aS,6bR,8aR,9S,10S,12aR,14bS)-2,2,4a,6a,6b,9,12a-heptamethyl-9-methylol-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-3,4,10-triol	12442849	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)O)(CO)C)C)C1C(CC3)(C(C(C(C1)(C)C)O)O)C)C)C
MOL009739	0.4192	0.5808	0.7722	Sojae Semen Nigrum	Soyasapogenol B	12442852	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CC(C(C1)(C)C)O)C)C)C)(CO)C)O
MOL009740	0.3914	0.6086	0.7497	Sojae Semen Nigrum	Sapogenol C	3083637	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C=CC(C1)(C)C)C)C)C)(CO)C)O
MOL009741	0.2978	0.7022	0.7363	Sojae Semen Nigrum	Soyasapogenol D	Not Available	FALSE	C1C(C(C2C(C1)(C1C(C(C2)OC2C(C(=C3C(C2)(CCC(C3)(C)C)C)CC1)C)C)(C)CO)O
MOL009742	0.3835	0.6165	0.8196	Sojae Semen Nigrum	Soyasapogenol E	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CC(=O)C(C1)(C)C)C)C)C)(CO)C)O
MOL009743	0.7656	0.2344	0.7860	Sojae Semen Nigrum	Soyasaponin A1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(C(C(C1)(C)C)O)OC1OCC(C(C1O)OC1OC(C(C(C1O)O)O)CO)O)C)C)C)(CO)C)OC1OC(C(C(C1OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO)O)O)C(=O)O

MOL009744	0.7656	0.2344	0.7860	Sojae Semen Nigrum	Soyasaponin A2	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(C(C(C1)(C)C)O)OC1OCC(C(C1O)OC1OC(C(C(C1O)O)O)CO)O)C)C)C)(CO)C)OC1OC(C(C(C1OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)O)CO)O)O)C(=O)O
MOL009745	0.4800	0.5200	0.7116	Sojae Semen Nigrum	Soyasaponin A3_qt	Not Available	FALSE	OC1CCC2(C(C1(CO)C)CCC1(C2CC=C2C1(CCC1(C2CC(C(C1O)O)(C)C)C)C)C)C
MOL009746	0.7800	0.2200	0.8309	Sojae Semen Nigrum	Soyasaponin A3	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(C(C(C1)(C)C)O)O)C)C)C)(CO)C)OC1OC(C(C(C1OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)O)CO)O)O)C(=O)O
MOL009747	0.7761	0.2239	0.8069	Sojae Semen Nigrum	Soyasaponin A5	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(C(C(C1)(C)C)O)OC1OCC(C(C1O)OC1OCC(C(C1O)O)O)O)C)C)C)(CO)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)C(=O)O
MOL009748	0.7697	0.2303	0.8113	Sojae Semen Nigrum	Soyasaponin A6	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(C(C(C1)(C)C)O)OC1OCC(C(C1O)OC1OCC(C(C1O)O)O)O)C)C)C)(CO)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)C(=O)O
MOL009749	0.9198	0.0802	0.7319	Sojae Semen Nigrum	Squamatic acid	5321482	FALSE	c1c(c(c(c(c1C)C(=O)Oc1cc(c(c(c1C)O)C(=O)O)C)O)C(=O)O)OC
MOL009750	0.8675	0.1325	0.7954	Sojae Semen Nigrum	URC	1175	FALSE	c12c(c(=O)[nH]c(=O)[nH]2)[nH]c(=O)[nH]1
MOL009750	0.8675	0.1325	0.7954	Abri Herba	URC	1175	FALSE	c12c(c(=O)[nH]c(=O)[nH]2)[nH]c(=O)[nH]1
MOL009752	0.8602	0.1398	0.9118	Polygonati Rhizoma	2',7-dihydroxy-3',4'-dimethoxyisoflavane	Not Available	FALSE	C1(=Cc2ccc(cc2OC1)O)c1cc(c(cc1O)OC)OC
MOL009753	0.8836	0.1164	0.9518	Polygonati Rhizoma	4-methylolfurfural	5318289	FALSE	o1c(cc(CO)c1)C=O
MOL009754	0.8906	0.1094	0.8441	Polygonati Rhizoma	Oroxin A	5320313	FALSE	c1(c(c2c(cc1OC1OC(C(C(C1O)O)O)CO)oc(cc2=O)c1ccccc1)O)O
MOL009754	0.8906	0.1094	0.8441	Oroxyli Semen	Oroxin A	5320313	FALSE	c1(c(c2c(cc1OC1OC(C(C(C1O)O)O)CO)oc(cc2=O)c1ccccc1)O)O
MOL009755	0.8520	0.1480	0.7301	Polygonati Rhizoma	2-Acridinecarboxylic acid	3041556	FALSE	c1c(ccc2nc3ccccc3cc12)C(=O)O
MOL009756	0.5932	0.4068	0.6751	Polygonati Rhizoma	liriodendrin	Not Available	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(OC3OC(C(O)C(O)C3O)CO)c(OC)c2)C1)c1cc(OC)c(OC2OC(C(O)C(O)C2O)CO)c(OC)c1
MOL009757	0.9358	0.0642	0.9195	Polygonati Rhizoma	n-butyl-β-D-fructopyranoside	13059907	FALSE	C1C(C(C(C(O1)(OCCCC)CO)O)O)O

MOL009758	0.7708	0.2292	0.6351	Polygonati Rhizoma	2-Propen-1-one, 1-(2,4-dihydroxyphenyl)-3-(4-(beta-D-glucopyranosyloxy)phenyl)-, (2E)-	5318591	FALSE	C(=O)(/C=C/c1ccc(cc1)OC1C(O)C(O)C(O)C(O1)CO)c1c(cc(cc1)O)O
MOL009759	0.7325	0.2675	0.7959	Polygonati Rhizoma	sibiricoside A	Not Available	FALSE	C12(C(CC3C1C(C(O3)(CCC(C)OC1OC(C(C(C1O)O)O)CO)OC)C)C1C(CC2)C2(C(=CC1)CC(CC2)OC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)CO)O)OC1C(C(C(CO1)O)O)O)OC1OC(C(C(C1O)O)O)CO)O)O)C)C
MOL009760	0.2749	0.7251	0.7394	Polygonati Rhizoma	sibiricoside A_qt	Not Available	FALSE	C12(C(CC3C1C(C(O3)(CCC(C)O)OC)C)C1C(CC2)C2(C(=CC1)CC(CC2)O)C)C
MOL009761	0.7488	0.2512	0.8301	Polygonati Rhizoma	sibiricoside B	Not Available	FALSE	C12(C(CC3C1C(C)C1(O3)OCC(CC1O)C)(C1C(CC2)C2(C(=CC1)CC(CC2)OC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)CO)O)OC1C(C(C(CO1)O)O)O)OC1OC(C(C(C1O)O)O)CO)O)O)C)O)C
MOL009762	0.4156	0.5844	0.7385	Polygonati Rhizoma	sibiricoside B_qt	Not Available	FALSE	C12(C(CC3C1C(C)C1(O3)OCC(CC1O)C)(C1C(CC2)C2(C(=CC1)CC(CC2)O)C)O)C
MOL009764	0.8811	0.1189	0.7809	Polygonati Rhizoma	vitexin xyloside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1c1c2oc(cc(=O)c2c(O)cc1O)c1ccc(O)cc1)COC1OC(O)C(O)C(O)C1O
MOL009766	0.3100	0.6900	0.7270	Polygonati Rhizoma	zhonghualiaoine 1	Not Available	FALSE	C1C2C(C3C(C1)(C(C(=O)C3)C(CC1C(C(C)C)C1C)C)C)CC1C3(C2(C(CC(C3)O)O)C)O1
MOL009767	0.9507	0.0493	0.9664	Dioscoreaebulbiferae	3-[(3R)-3-methyl-1-piperidyl]propylamine	6999015	FALSE	N1(CC(CCC1)C)CCCN
MOL009768	0.8579	0.1421	0.7905	Dioscoreaebulbiferae	2,4,5,6-tetrahydroxyphenanthrene	Not Available	FALSE	c12c3c(ccc1ccc(c2O)O)cc(cc3O)O
MOL009769	0.8972	0.1028	0.8324	Dioscoreaebulbiferae	9,10-dihydrophenanthrene-2,3,5,7-tetrol	22753774	FALSE	c12c3c(CCc1cc(c(c2)O)O)cc(cc3O)O
MOL009770	0.9404	0.0596	0.8631	Dioscoreaebulbiferae	2-(4-methoxyphenyl)ethyl-O-β-D-glucopyranoside	Not Available	FALSE	c1(ccc(cc1)CCOC1OC(C(C(C1O)O)O)CO)OC

MOL009771	0.9542	0.0458	0.9764	Dioscoreaebulbiferae	p-Methoxyphenethyl alcohol	69705	FALSE	c1(ccc(cc1)CCO)OC
MOL009772	0.7235	0.2765	0.8258	Dioscoreaebulbiferae	3,5,3'-trimethoxyquercetin	Not Available	FALSE	c1(c(c(=O)c2c(o1)cc(cc2OC)O)OC)c1cc(c(c(c1)OC)O)OC
MOL009773	0.8458	0.1542	0.8219	Dioscoreaebulbiferae	7-hydroxy-2-(4-hydroxyphenyl)-3,5-dimethoxy-chromone	10470863	FALSE	o1c2c(c(=O)c(OC)c1c1ccc(O)cc1)c(OC)cc(O)c2
MOL009774	0.8816	0.1184	0.8935	Dioscoreaebulbiferae	3,7-Di-O-methylquercetin	5280417	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC)OC)c1cc(c(cc1)O)O
MOL009775	0.9275	0.0725	0.8710	Dioscoreaebulbiferae	3-phenyl-2-propenol-O-β-D-glucopyranoside	Not Available	FALSE	c1ccc(cc1)/C=C/COC1OC(C(C(C1O)O)O)CO
MOL009776	0.9236	0.0764	0.9162	Dioscoreaebulbiferae	Styrylcarbinol	5280511	FALSE	c1ccc(cc1)/C=C\CO
MOL009777	0.4407	0.5593	0.6463	Dioscoreaebulbiferae	8-epidiosbulbin E acetate	Not Available	FALSE	C12CC(C3C(C1)C1(C(CC3OC(=O)C)C(=O)OC(C1)c1cocc1)C)C(=O)O2
MOL009778	0.9389	0.0611	0.8981	Smilacis Glabrae Rhixoma	n-butyl-α-D-fructoufranoside	13386214	FALSE	O1C(OCCCC)(C(O)C(O)C1CO)CO
MOL009778	0.9389	0.0611	0.8981	Semiaquilegiae Radix	n-butyl-α-D-fructoufranoside	13386214	FALSE	O1C(OCCCC)(C(O)C(O)C1CO)CO
MOL009778	0.9389	0.0611	0.8981	Dioscoreaebulbiferae	n-butyl-α-D-fructoufranoside	13386214	FALSE	O1C(OCCCC)(C(O)C(O)C1CO)CO
MOL009779	0.9462	0.0538	0.9703	Dioscoreaebulbiferae	ZINC02517032	107428	FALSE	OC(C(O)CO)C(O)C(=O)CO
MOL009780	0.9095	0.0905	0.7570	Dioscoreaebulbiferae	Demethylbatatasin IV	442699	FALSE	Oc1c(CCc2cc(O)cc(O)c2)cccc1
MOL009781	0.9466	0.0534	0.7955	Dioscoreaebulbiferae	dihydrodioscorine	Not Available	FALSE	C1C2(C3CCC1N(C3)C)CC(CC(=O)O2)C
MOL009782	0.9392	0.0608	0.9178	Dioscoreaebulbiferae	Dihydroresveratrol	185914	FALSE	Oc1cc(CCc2ccc(O)cc2)cc(O)c1
MOL009782	0.9392	0.0608	0.9178	Rhododendri Daurici Folium	Dihydroresveratrol	185914	FALSE	Oc1cc(CCc2ccc(O)cc2)cc(O)c1

MOL009782	0.9392	0.0608	0.9178	Smilacis Glabrae Rhixoma	Dihydroresveratrol	185914	FALSE	Oc1cc(CCc2ccc(O)cc2)cc(O)c1
MOL009784	0.8807	0.1193	0.7526	Dioscoreaebulbiferae	diosbuibin J	44130234	FALSE	C1(CC(C2(C(C1)C1(C(CC2=O)C(=O)OC(C1)c1coccc1)C)O)C(=O)O)O
MOL009785	0.6295	0.3705	0.6344	Dioscoreaebulbiferae	diosbuilbin K	46845277	FALSE	C1(CC(C2C(C1)C1(C(CC2=O)C(=O)OC(C1)c1coccc1)C)C(=O)OC)O
MOL009786	0.8497	0.1503	0.6933	Dioscoreaebulbiferae	diosbuilbin L	Not Available	FALSE	C1(CC(C2C(C1)C1(C(CC2=O)C(=O)OC(C1)c1coccc1)C)C(=O)O)O
MOL009787	0.7396	0.2604	0.7004	Dioscoreaebulbiferae	diosbuilbin M	Not Available	FALSE	C12CC(C3(C(C1)C1(C(CC3=O)C(=O)OC(C1)c1coccc1)C)O)C(=O)O2
MOL009788	0.5968	0.4032	0.7141	Dioscoreaebulbiferae	diosbulbin A	Not Available	FALSE	O1C23C(C4C(C(OC3=O)C2)C(CC(O)C4)C(=O)OC)(CC1c1ccoc1)C
MOL009789	0.8547	0.1453	0.7378	Dioscoreaebulbiferae	diosbulbin C	Not Available	FALSE	O1C23C(C4C(C(OC3=O)C2)C(CC(O)C4)C(=O)O)(CC1c1ccoc1)C
MOL009790	0.6391	0.3609	0.7242	Dioscoreaebulbiferae	diosbulbin D	Not Available	FALSE	O1C2CC3C4(C(CC(=O)C3C(C2)C1=O)C(=O)OC(C4)c1ccoc1)C
MOL009791	0.7121	0.2879	0.7471	Dioscoreaebulbiferae	diosbulbin E	Not Available	FALSE	O1C2CC3C4(C(CC(O)C3C(C2)C1=O)C(=O)OC(C4)c1ccoc1)C
MOL009792	0.6295	0.3705	0.6344	Dioscoreaebulbiferae	Diosbulbin F	181851	FALSE	O1C(CC2(C3C(C(CC(O)C3)C(=O)OC)C(=O)CC2C1=O)C)c1ccoc1
MOL009793	0.6571	0.3429	0.7268	Dioscoreaebulbiferae	diosbulbin G	Not Available	FALSE	O1C2C3C(C4(C(C2)C(=O)OC(C4)c2ccoc2)C)CC(O)CC3C1=O
MOL009795	0.8274	0.1726	0.7784	Dioscoreaebulbiferae	diosbulbinoside D	Not Available	FALSE	O1C(=O)C2C3=C(CC4C(C3CC1C2)(CC(OC4=O)c1cocc1)COC1C(O)C(O)C(O)C(O1)CO)OC1C(O)C(O)C(O)C(O1)CO
MOL009796	0.7599	0.2401	0.6961	Dioscoreaebulbiferae	diosbulbinoside D_qt	Not Available	FALSE	O1C(=O)C2C3=C(CC4C(C3CC1C2)(CC(OC4=O)c1cocc1)CO)O
MOL009797	0.7964	0.2036	0.7521	Dioscoreaebulbiferae	diosbulbinoside F	Not Available	FALSE	C1(=O)C2C(CC(O1)c1cocc1)(C1C(=C(C2)OC2C(O)C(O)C(O)C(O2)CO)C(CC(C1)O)C(=O)OC)COC1C(O)C(O)C(O)C(O1)CO
MOL009798	0.7484	0.2516	0.6163	Dioscoreaebulbiferae	diosbulbinoside F_qt	Not Available	FALSE	C1(=O)C2C(CC(O1)c1cocc1)(C1C(=C(C2)O)C(CC(C1)O)C(=O)OC)CO
MOL009799	0.9140	0.0860	0.8280	Dioscoreaebulbiferae	kaempferol-3-O-β-D-galactopyranoside	12358430	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)CO
MOL009800	0.2664	0.7336	0.6453	Dioscoreaebulbiferae	kryptogenin	Not Available	FALSE	O=C1C(C2(C(C3C(C4(C(=CC3)CC(O)CC4)C)CC2)C1)C)C(C)C(=O)CCC(CO)C
MOL009801	0.9280	0.0720	0.7859	Dioscoreaebulbiferae	myricetin-3-O-beta-D-galactopyranoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)c(O)c1)CO

MOL009803	0.6391	0.3609	0.7242	Dioscoreaebulbiferae	neodiosbulbin	Not Available	FALSE	C12CC(C3C(C1)C1(C(CC3=O)C(=O)OC(C1)c1cocc1)C)C(=O)O2
MOL009804	0.6499	0.3501	0.8433	Dioscoreaebulbiferae	prosapogenin A of dioscin	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CC2C1C(C1(O2)OCC(CC1)C)C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO
MOL009805	0.6771	0.3229	0.8609	Dioscoreaebulbiferae	taccaoside	Not Available	FALSE	O(C1C(C(C(C(O1)C)O)O)O)C1C(C(OC(OC2CC3=CCC4C(C3(CC2)C)CCC2(C4CC3C2C(C2(CCC(CO2)C)O3)C)C)C1OC1OC(C(C(C1O)O)O)C)CO)O
MOL009807	0.6261	0.3739	0.6610	Macacae Calcalus Gasteris	CHD	221493	FALSE	OC1C2(C(C3C(C4(C(CC3O)CC(O)CC4)C)C1)CCC2C(CCC(=O)O)C)C
MOL009808	0.9111	0.0889	0.9179	Sesami Nigrum Semen	2,3,5-trimethyl-Hexane	59954463	FALSE	C(CC(C)C)(C(C)C)C
MOL009809	0.9082	0.0918	0.8608	Sesami Nigrum Semen	2,3-dimethyl-Nonane	Not Available	FALSE	CC(C(CCCCCC)C)C
MOL009810	0.8848	0.1152	0.8805	Sesami Nigrum Semen	2,4-DIMETHYL-1-HEPTaNE	Not Available	FALSE	C(C(CCC)C)C(=C)C
MOL009811	0.9392	0.0608	0.9052	Sesami Nigrum Semen	3-Ethyl-2,6-dimethylpyrazine	26334	FALSE	c1(c(nc(cn1)C)C)CC
MOL009812	0.8964	0.1036	0.8510	Sesami Nigrum Semen	2,5-dimethyl-Nonane	Not Available	FALSE	CC(CCC(CCCC)C)C
MOL009813	0.9254	0.0746	0.9672	Ephedra Herba	(2R)-2-methylbutan-1-ol	637572	FALSE	OCC(CC)C
MOL009813	0.9254	0.0746	0.9672	Sesami Nigrum Semen	(2R)-2-methylbutan-1-ol	637572	FALSE	OCC(CC)C
MOL009814	0.8811	0.1189	0.9314	Sesami Nigrum Semen	2-Methylpyrrole	12489	FALSE	c1(ccc[nH]1)C
MOL009815	0.8640	0.1360	0.7095	Sesami Nigrum Semen	3-ethyl-methyl-Decane	Not Available	FALSE	C(CC(CCCCCCC)CC)C
MOL009816	0.9246	0.0754	0.9709	Sesami Nigrum Semen	HBS	447765	FALSE	OC(C(=O)C)C
MOL009817	0.8129	0.1871	0.6416	Sesami Nigrum Semen	3-methyl-Tridecane	25113498	FALSE	C(CCC(CC)C)CCCCCCC
MOL009818	0.9151	0.0849	0.8565	Sesami Nigrum Semen	4,5-dimethylnonane	Not Available	FALSE	CCCC(C(CCCC)C)C
MOL009819	0.8347	0.1653	0.6415	Sesami Nigrum Semen	4,6-dimethyl-Dodecan	Not Available	FALSE	C(CC(CCC)C)(CCCCCC)C

MOL009820	0.8755	0.1245	0.7122	Sesami Nigrum Semen	4,7-Dimethylundecane	Not Available	FALSE	CCCC(CCC(CCCC)C)C
MOL009821	0.8736	0.1264	0.7116	Sesami Nigrum Semen	4,8-dimethyl-Undecane	Not Available	FALSE	CCCC(CCCC(CCC)C)C
MOL009822	0.8886	0.1114	0.7876	Sesami Nigrum Semen	4-ethyl-Decane	Not Available	FALSE	CCCC(CCCCCC)CC
MOL009824	0.9060	0.0940	0.8896	Sesami Nigrum Semen	4-methyl-Nonane	70702301	FALSE	C(C(CCC)C)CCCC
MOL009825	0.9155	0.0845	0.9114	Sesami Nigrum Semen	4-methyloctane	53770446	FALSE	C(CCCC)(CCC)C
MOL009826	0.8738	0.1262	0.7070	Sesami Nigrum Semen	5,7-dimethylundecane	Not Available	FALSE	CCCCC(CC(CCCC)C)C
MOL009827	0.8720	0.1280	0.7061	Sesami Nigrum Semen	6-methyl-Dodecane	42626542	FALSE	CCCCCC(CCCCCC)C
MOL009829	0.9334	0.0666	0.9443	Sesami Nigrum Semen	Amyl propionate	12217	FALSE	C(=O)(OCCCCC)CC
MOL009830	0.8278	0.1722	0.8814	Sesami Nigrum Semen	EHD	Not Available	TRUE	C1CCC2(C1)[C@H]1[C@H]2[C@H]2CC[C@H]([C@@H]2O)COC(=O)C1(O)CC
MOL009831	0.9096	0.0904	0.9708	Farfarae Flos	Diethylacetic acid	6915	FALSE	OC(=O)C(CC)CC
MOL009831	0.9096	0.0904	0.9708	Sesami Nigrum Semen	Diethylacetic acid	6915	FALSE	OC(=O)C(CC)CC
MOL009832	0.9205	0.0795	0.9756	Sesami Nigrum Semen	(2R,4S)-4-hydroxypipecolinic acid	40507948	FALSE	C1CNC(CC1O)C(=O)O
MOL009833	0.7548	0.2452	0.6811	Sesami Nigrum Semen	Tetradecyl cyanide	87568	FALSE	N#CCCCCCCCCCCCCC
MOL009834	0.4556	0.5444	0.6119	Sesami Nigrum Semen	sesamolin	101746	FALSE	c1c2c(cc(c1)C1C3C(CO1)C(OC3)Oc1cc3c(cc1)OCO3)OCO2
MOL009835	0.4592	0.5408	0.6636	Sesami Nigrum Semen	Sesamolinol	443019	FALSE	C12C(C(OC1)Oc1cc(c(cc1)O)OC)COC2c1ccc2c(c1)OCO2
MOL009836	0.8919	0.1081	0.7932	Sesami Nigrum Semen	Sesamoside	Not Available	FALSE	C1(OC=C(C2(C1C1(C(C2O)O1)C)O)C(=O)OC)OC1OC(C(C(C1O)O)O)CO
MOL009837	0.9256	0.0744	0.8041	Sesami Nigrum Semen	Sesamoside_qt	Not Available	FALSE	C1(OC=C(C2(C1C1(C(C2O)O1)C)O)C(=O)OC)O
MOL009838	0.8281	0.1719	0.7597	Sesami Nigrum Semen	Myristonitrile	64678	FALSE	N#CCCCCCCCCCCCCC
MOL009840	0.6882	0.3118	0.6759	Sesami Nigrum Semen	Citrusin B_qt	Not Available	FALSE	c1(c(ccc(c1)C(C(CO)Oc1c(OC)cc(cc1OC)/C=C\CO)O)O)OC
MOL009842	0.6266	0.3734	0.7066	Sesami Nigrum Semen	cytochrome C	Not Available	FALSE	S(C(C1=C(C2=N/C/1=C\c1[nH]c(/C=C/3\N=C(/C=c/4\[nH]/c(=C\2)/c(c4C)C(SCC(N)C(=O)NC)C)C(=C3CCC(=O)O)C)c(c1C)CCC(=O)O)C)CC(N)C(=O)NC
MOL009843	0.9186	0.0814	0.9362	Sesami Nigrum Semen	Propionic ether	7749	FALSE	C(=O)(OCC)CC

MOL009844	0.9381	0.0619	0.9703	Paederiae Scandentis Herba	I-Amyl acetate	31276	FALSE	C(CCOC(=O)C)(C)C
MOL009844	0.9381	0.0619	0.9703	Mume Flos	I-Amyl acetate	31276	FALSE	C(CCOC(=O)C)(C)C
MOL009844	0.9381	0.0619	0.9703	Sesami Nigrum Semen	I-Amyl acetate	31276	FALSE	C(CCOC(=O)C)(C)C
MOL009845	0.8778	0.1222	0.8466	Sesami Nigrum Semen	Methyl decenoate	543920	FALSE	C(CCC(=O)OC)CCCCCCC=C
MOL009846	0.8899	0.1101	0.8072	Sesami Nigrum Semen	Pedaliin	5320439	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(O)c2c(oc(cc2=O)c2cc(O)c(O)cc2)cc1OC)CO
MOL009847	0.9255	0.0745	0.8851	Sesami Nigrum Semen	Pedalitin	31161	FALSE	Oc1c(O)c2c(oc(cc2=O)c2cc(O)c(O)cc2)cc1OC
MOL009848	0.8977	0.1023	0.8279	Sesami Nigrum Semen	planteose	Not Available	FALSE	O1C(OC2OC(C(O)C(O)C2O)CO)(C(O)C(O)C1COC1OC(C(O)C(O)C1O)CO)CO
MOL009849	0.4331	0.5669	0.7622	Magnoliae Flos	ZINC05223929	11869417	FALSE	O1C(C2C(C(OC2)c2cc3OCOc3cc2)C1)c1cc2OCOc2cc1
MOL009849	0.4331	0.5669	0.7622	Sesami Nigrum Semen	ZINC05223929	11869417	FALSE	O1C(C2C(C(OC2)c2cc3OCOc3cc2)C1)c1cc2OCOc2cc1
MOL009849	0.4331	0.5669	0.7622	Asari Radix Et Rhizoma	ZINC05223929	11869417	FALSE	O1C(C2C(C(OC2)c2cc3OCOc3cc2)C1)c1cc2OCOc2cc1
MOL009850	0.8577	0.1423	0.7583	Sesami Nigrum Semen	sesamose	Not Available	FALSE	O1C(OC2OC(C(O)C(O)C2O)CO)(C(O)C(O)C1COC1OC(C(O)C(O)C1O)COC1OC(C(O)C(O)C1O)CO)CO
MOL009851	0.9182	0.0818	0.9018	Sesami Nigrum Semen	27400-71-1	6436632	FALSE	C(C)(C)/C=C/C=C(/C)\C=C
MOL009852	0.9550	0.0450	0.8746	Sesami Nigrum Semen	Prehnitol	10263	FALSE	c1(c(c(c(cc1)C)C)C)C
MOL009855	0.2107	0.7893	0.6152	Gynostemmae Pentaphylli Herba	(24S)-Ethylcholesta-5,22,25-trans-3beta-ol	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CCC1C(C)/C=C/C(C(=C)C)CC)C)O
MOL009856	0.9186	0.0814	0.9153	Gynostemmae Pentaphylli Herba	2,4-dimethyl-4-octanol	Not Available	FALSE	CC(CC(CCCC)(O)C)C
MOL009857	0.9053	0.0947	0.9080	Gynostemmae Pentaphylli Herba	(4E,6E)-octa-4,6-dien-3-one	11230835	FALSE	C/C=C/C=C/C(=O)CC
MOL009858	0.9052	0.0948	0.9375	Gynostemmae Pentaphylli Herba	2-dimethylaminopentanoic acid	30030436	FALSE	C(=O)(C(CCC)N(C)C)O
MOL009859	0.9325	0.0675	0.9483	Gynostemmae Pentaphylli Herba	2-Ethylhexenal	5354264	FALSE	C(=O)/C(=C/CCC)/CC
MOL009860	0.2171	0.7829	0.7185	Gynostemmae Pentaphylli Herba	2α-hydroxypanaxadiol	Not Available	FALSE	C1(C2C(CC(C1O)O)(C1C(CC2)(C2(C(C(C1)O)C(C1(CCCC(O1)(C)C)C)CC2)C)C)(C)C

MOL009861	0.9333	0.0667	0.9730	Gynostemmae Pentaphylli Herba	3,4-Difluoroanisole	568250	FALSE	c1(c(ccc(c1)OC)F)F
MOL009862	0.9321	0.0679	0.9386	Gynostemmae Pentaphylli Herba	ZINC01680040	6994068	FALSE	C=CC(CCCCCC)O
MOL009863	0.6916	0.3084	0.8340	Gynostemmae Pentaphylli Herba	3-o-beta-d-glucopyranosyl2alpha,3beta,12beta,20(S)-3hydroxy-dammarane24-ene20-o-beta-d-glucopyranoside	Not Available	FALSE	C1C2C(C3(C(C1O)C(CC3)C(OC1C(C(C(C(O1)CO)O)O)O)(C)CCC=C(C)C)C)(CCC1C2(CC(C(C1(C)C)OC1C(C(C(C(O1)CO)O)O)O)O)C)C
MOL009864	0.2356	0.7644	0.6800	Gynostemmae Pentaphylli Herba	3-o-beta-d-glucopyranosyl2alpha,3beta,12beta,20(S)-3hydroxy-dammarane24-ene20-o-beta-d-glucopyranoside_qt	Not Available	FALSE	C1C2C(C3(C(C1O)C(CC3)C(O)(C)CCC=C(C)C)C)(CCC1C2(CC(C(C1(C)C)O)O)C)C
MOL009865	0.8856	0.1144	0.9474	Gynostemmae Pentaphylli Herba	4-amino-5-ethoxyimidazole	Not Available	FALSE	c1[nH]c(c(n1)OCC)N
MOL009866	0.8999	0.1001	0.9718	Gynostemmae Pentaphylli Herba	p-Mercaptophenol	240147	FALSE	c1(ccc(cc1)S)O
MOL009867	0.2263	0.7737	0.6713	Gynostemmae Pentaphylli Herba	4α,14α-dimethyl-5α-ergosta-7,9(11),24(28)-trien-3β-ol	Not Available	FALSE	C1C(C(C2C(C1)(C1=CCC3(C(C1=CC2)(CCC3C(CCC(=C)C(C)C)C)C)C)C)C)O
MOL009868	0.9506	0.0494	0.9685	Gynostemmae Pentaphylli Herba	5-[2-butylethyl]-2-pyrrolone	Not Available	FALSE	N1=C(C=CC1=O)CCCCCC
MOL009869	0.8784	0.1216	0.9553	Gynostemmae Pentaphylli Herba	5-Methylfurfuryl alcohol	520911	FALSE	c1(oc(cc1)C)CO

MOL009870	0.7228	0.2772	0.8012	Gynostemmae Pentaphylli Herba	6'-malonylgypenoside V	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)COC(=O)CC(=O)O)CO)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(C(O)C(O)C1O)COC1OC(C(O)C(O)C1O)C)(CCC=C(C)C)C)C
MOL009871	0.2305	0.7695	0.7376	Gynostemmae Pentaphylli Herba	6'-malonylgypenoside V_qt	Not Available	FALSE	OC1C2C(C3(C)C(C4(C(CC3)C(C)(C(O)CC4)C)C)C1)(CCC2C(O)(CCC=C(C)C)C)C
MOL009872	0.9008	0.0992	0.9114	Gynostemmae Pentaphylli Herba	6-O-malonyl-beta-methyl-D-glucopyranoside	5319243	FALSE	C1(C(C(C(OC1COC(=O)CC(=O)O)OC)O)O)O
MOL009873	0.8218	0.1782	0.7120	Gynostemmae Pentaphylli Herba	7-(6-O-Malony-beta-D-glucopyransyloxy)-3-(4-hydroxphenyl)-4H-1-benzopyran-4-one	Not Available	FALSE	C(=O)(CC(=O)OCC1C(C(C(C(O1)Oc1ccc2c(c1)OCC(C2=O)c1ccc(cc1)O)O)O)O)O
MOL009874	0.8047	0.1953	0.7313	Gynostemmae Pentaphylli Herba	Malonylawobanin	Not Available	FALSE	c1(cc(c2c(c1)[o+]c(c(c2)OC1C(C(C(C(O1)COC(=O)/C=C\c1ccc(cc1)O)O)O)O)c1cc(c(c(c1)O)O)O)OC1C(C(C(C(O1)COC(=O)CC(=O)O)O)O)O)O
MOL009875	0.9502	0.0498	0.9660	Gynostemmae Pentaphylli Herba	ZINC00407077	6951558	FALSE	c1(c(nccn1)C(CC)C)OC
MOL009876	0.8925	0.1075	0.8747	Gynostemmae Pentaphylli Herba	Decylaldehyde DMA	24513	FALSE	O(C(OC)CCCCCCCCC)C
MOL009877	0.2228	0.7772	0.7144	Gynostemmae Pentaphylli Herba	cucurbita-5,24-dienol	Not Available	FALSE	C1C2(C(C3(C(C1)(C(CC3)C(CCC=C(C)C)C)C)C)CC=C1C2CCC(C1(C)C)O)C
MOL009879	0.9273	0.0727	0.9514	Gynostemmae Pentaphylli Herba	cyclopentyl 2-methoxyacetate	550010	FALSE	C(=O)(COC)OC1CCCC1

MOL009880	0.7496	0.2504	0.8413	Gynostemmae Pentaphylli Herba	(2S,3R,4S,5S,6R)-2-[(2S)-2-[(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-6-[(2R,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]oxy-3,12-dihydroxy-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,	24721561	FALSE	C12C(C3(C(C(C2)O)C(CC3)C(OC2OC(C(C(C2O)O)O)CO)(CCC=C(C)C)C)C)(CC(C2C1(CCC(C2(C)C)O)C)OC1C(OC2OC(C(C(C2O)O)O)O)CO)C(C(C(O1)CO)O)O)C
MOL009881	0.3423	0.6577	0.7298	Gynostemmae Pentaphylli Herba	gynosaponin TN-1	Not Available	FALSE	C1C2C(C3(C(C1O)C(CC3)C(C)(CCC=C(C)C)OC1C(C(C(O1)CO)O)O)C)(CCC1C2(CC(C(C1(C)C)O)O)C)C
MOL009882	0.2356	0.7644	0.6800	Gynostemmae Pentaphylli Herba	gynosaponin TN-1_qt	Not Available	FALSE	C1C2C(C3(C(C1O)C(CC3)C(C)(CCC=C(C)C)O)C)(CCC1C2(CC(C(C1(C)C)O)O)C)C
MOL009883	0.7256	0.2744	0.8470	Gynostemmae Pentaphylli Herba	gynsenoside Rd	Not Available	FALSE	C1C2C(C3(C(C1O)C(CC3)C(OC1C(C(C(O1)CO)O)O)O)(C)CCC=C(C)C)(CCC1C2(CCC(C1(C)C)OC1C(C(C(O1)CO)O)O)OC1OC(C(C(C1O)O)O)C)C
MOL009884	0.2305	0.7695	0.7376	Gynostemmae Pentaphylli Herba	gynsenoside Rd_qt	Not Available	FALSE	C1C2C(C3(C(C1O)C(CC3)C(O)(C)CCC=C(C)C)C)(CCC1C2(CCC(C1(C)C)O)C)C
MOL009885	0.7270	0.2730	0.8354	Gynostemmae Pentaphylli Herba	Gypenoside LII	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(COC1OC(C(C(C1O)O)O)CO)O)C)C)C=O)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)C)O)O
MOL009886	0.2531	0.7469	0.6733	Gynostemmae Pentaphylli Herba	Gypenoside LII_qt	Not Available	FALSE	OCC(C1C2C(C3(CCC4C(C(O)CCC4(C3CC2O)C=O)(C)C)C)(CC1)C)(CCC=C(C)C)O
MOL009887	0.7154	0.2846	0.8074	Gynostemmae Pentaphylli Herba	Gypenoside XXXVII	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)O)COC1OCC(C(C1O)O)O)C)C)C=O)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)O)CO

MOL009888	0.2069	0.7931	0.7569	Gynostemmae Pentaphylli Herba	Gypenoside XXXVI_qt	Not Available	FALSE	OC(C1C2C(C3(CCC4C(C(CCC4(C3CC2)C=O)O)(C)C)C)(CC1)C)(CCC=C(C)C)C
MOL009889	0.7547	0.2453	0.7945	Gynostemmae Pentaphylli Herba	Gypenoside I	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)COC3OC(C(O)C(O)C3O)C)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(C(O)C(O)C1O)COC1OC(C(O)C(O)C1O)CO)(CCC=C(C)C)C)C
MOL009890	0.7438	0.2562	0.7917	Gynostemmae Pentaphylli Herba	Gypenoside II	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)C)C)C)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)COC1OC(C(C(C1O)O)O)C
MOL009891	0.7282	0.2718	0.8093	Gynostemmae Pentaphylli Herba	Gypenoside IV	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)C)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009892	0.7118	0.2882	0.8238	Gynostemmae Pentaphylli Herba	Gypenoside IX	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)C)C)(C)C)OC1OC(C(C(C1O)O)O)C)O
MOL009893	0.6958	0.3042	0.8643	Gynostemmae Pentaphylli Herba	Gypenoside L	Not Available	FALSE	C1C(C(C2C(C1)C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)O)C)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009894	0.2461	0.7539	0.6761	Gynostemmae Pentaphylli Herba	Gypenoside L_qt	Not Available	FALSE	OC1CCC2C(C1(C)C)CCC1(C2CC(C2C1(C)CCC2C(O)(C)CCC=C(C)C)O)C
MOL009895	0.6836	0.3164	0.8646	Gynostemmae Pentaphylli Herba	Gypenoside LI	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO)O
MOL009896	0.2356	0.7644	0.6800	Gynostemmae Pentaphylli Herba	Gypenoside LI_qt	Not Available	FALSE	OC1C(O)CC2(C)C(C1(C)C)CCC1(C2CC(C2C1(C)CCC2C(O)(C)CCC=C(C)C)O)C
MOL009897	0.7270	0.2730	0.8354	Gynostemmae Pentaphylli Herba	Gypenoside III	Not Available	FALSE	C1CC(C(C2CCC3(C4(CCC(C4C(CC3C12C=O)O)C(COC1OC(C(C(C1O)O)O)CO)(CCC=C(C)C)O)C)C)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)C)O)O
MOL009898	0.2531	0.7469	0.6733	Gynostemmae Pentaphylli Herba	Gypenoside III_qt	Not Available	FALSE	C1CC(C(C2CCC3(C4(CCC(C4C(CC3C12C=O)O)C(CO)(CCC=C(C)C)O)C)C)(C)C)O
MOL009899	0.6583	0.3417	0.8624	Gynostemmae Pentaphylli Herba	Gypenoside LIII	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C=O)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)CO)O)O
MOL009900	0.2257	0.7743	0.7237	Gynostemmae Pentaphylli Herba	Gypenoside XL_qt	Not Available	FALSE	OC1CCC2(C(C1(C)C)CCC1(C2CC(C2C1(CCC2C(CCC=C(C)C)(O)C)C)O)C)C=O
MOL009901	0.6695	0.3305	0.8626	Gynostemmae Pentaphylli Herba	Gypenoside LIV	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)O)C)C)CO)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)CO)O)O
MOL009902	0.2500	0.7500	0.7073	Gynostemmae Pentaphylli Herba	Gypenoside LXV_qt	Not Available	FALSE	OC1CCC2(C(C1(C)C)CCC1(C2CC(C2C1(CCC2C(CCC=C(C)C)(C)O)C)O)C)CO

MOL009903	0.6887	0.3113	0.8179	Gynostemmae Pentaphylli Herba	Gypenoside LIX	Not Available	FALSE	C1C(C(C2C(C1)C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CC/C=C(/CO)\C)(C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)C)(C)C)O
MOL009904	0.2619	0.7381	0.6233	Gynostemmae Pentaphylli Herba	Gypenoside LXI_qt	Not Available	FALSE	C1C(C(C2C(C1)C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CC/C=C(/CO)\C)(C)O)C)C)(C)C)O
MOL009905	0.7109	0.2891	0.8239	Gynostemmae Pentaphylli Herba	Gypenoside LV	Not Available	FALSE	C1C(C(C2C(C1)C1C(CC2)(C2(C(CC1)C(CC2)C(CC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)CO)(C)C)OC1OC(C(C(C1O)O)O)CO
MOL009906	0.2401	0.7599	0.7551	Gynostemmae Pentaphylli Herba	Gypenoside LV_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(C(C)(O)CCC=C(C)C)CC2)C)C)CO)(C)C)O
MOL009907	0.7387	0.2613	0.8114	Gynostemmae Pentaphylli Herba	Gypenoside LVI	Not Available	FALSE	C1C(C(C2C(C1)C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009908	0.7242	0.2758	0.8263	Gynostemmae Pentaphylli Herba	Gypenoside LVII	Not Available	FALSE	C1C(C(C2C(C1)C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)C)(C)C)OC1OC(C(C(C1O)O)O)CO
MOL009909	0.7213	0.2787	0.8051	Gynostemmae Pentaphylli Herba	Gypenoside LVIII	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CC/C=C(/CC)\C)(C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)C)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)CO)O)O
MOL009910	0.2370	0.7630	0.7176	Gynostemmae Pentaphylli Herba	Gypenoside LVIII_qt	Not Available	FALSE	OC1CCC2(C)C(C1(C)C)CCC1(C2CC(C2C1(CCC2C(O)(CC/C=C(/CC)\C)C)C)O)C
MOL009911	0.6833	0.3167	0.8491	Gynostemmae Pentaphylli Herba	Gypenoside LX	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)C)(C)C)O)O
MOL009912	0.2356	0.7644	0.6800	Gynostemmae Pentaphylli Herba	Gypenoside LX_qt	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(C(O)C1)C(C(C)(O)CCC=C(C)C)CC2)C)C)C)(C)C)O)O
MOL009913	0.7486	0.2514	0.8033	Gynostemmae Pentaphylli Herba	Gypenoside LXI	Not Available	FALSE	C1C(C(C2C(C1)C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CC/C=C(/CO)\C)(C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009914	0.7410	0.2590	0.8114	Gynostemmae Pentaphylli Herba	Gypenoside LXII	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)CO)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009915	0.7317	0.2683	0.8088	Gynostemmae Pentaphylli Herba	Gypenoside LXIII	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)CO)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009916	0.7312	0.2688	0.8277	Gynostemmae Pentaphylli Herba	Gypenoside LXIV	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)CO)(C)C)OC1OC(C(C(C1O)O)O)CO

MOL009917	0.6879	0.3121	0.8510	Gynostemmae Pentaphylli Herba	Gypenoside LXV	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)C)CO)(C)C)O
MOL009918	0.6368	0.3632	0.7987	Gynostemmae Pentaphylli Herba	Gypenoside LXVI	Not Available	FALSE	C1C(C(C2C(C1)C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)C)C)C)(C)C)O
MOL009919	0.7445	0.2555	0.8111	Gynostemmae Pentaphylli Herba	Gypenoside LXVIII	Not Available	FALSE	C1(C(C(C2C(C1)C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO)O
MOL009920	0.2673	0.7327	0.6316	Gynostemmae Pentaphylli Herba	Gypenoside LXVIII_qt	Not Available	FALSE	OC1C(CC2C(C1(C)C)CCC1(C2CC(C2C1(CCC2C(O)(CCC=C(C)C)C)C)O)C)O
MOL009921	0.7384	0.2616	0.8060	Gynostemmae Pentaphylli Herba	Gypenoside LXX	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CC/C=C(/CO)\C)(C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)C)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009922	0.2382	0.7618	0.6965	Gynostemmae Pentaphylli Herba	Gypenoside XX_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(O)C1)C(C(C)(O)CC/C=C(/CO)\C)CC2)C)C)C)(C)C)O
MOL009923	0.6210	0.3790	0.7763	Gynostemmae Pentaphylli Herba	Gypenoside LXXI	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC(C(=C)C)O)(C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)C)C)(C)C)O
MOL009924	0.2351	0.7649	0.7161	Gynostemmae Pentaphylli Herba	Gypenoside LXXI_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(C(C)(O)CCC(C(=C)C)O)CC2)C)C)C)(C)C)O
MOL009925	0.7486	0.2514	0.8265	Gynostemmae Pentaphylli Herba	Gypenoside LXXII	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)CO)C)C)O)(C)C)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)C
MOL009926	0.7066	0.2934	0.8321	Gynostemmae Pentaphylli Herba	Gypenoside LXXIII	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)C)C)C)(C)C)OC1OC(C(C(C1O)O)O)CO)O
MOL009927	0.2207	0.7793	0.7083	Gynostemmae Pentaphylli Herba	Gypenoside LXXIII_qt	Not Available	FALSE	C1(CC2(C3CCC4C(CCC4C(CCC=C(C)C)(O)C)(C)C3(CCC2C(C)(C1O)C)C)C)O
MOL009928	0.6753	0.3247	0.7448	Gynostemmae Pentaphylli Herba	Gypenoside LXXIV	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)CO)C)C)O)(C)C)OC1OC(C(C(C1O)O)O)CO
MOL009929	0.5977	0.4023	0.7200	Gynostemmae Pentaphylli Herba	Gypenoside LXXIX	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)CO)C)C)CO)(C)C)OC1OC(C(C(C1O)O)O)CO
MOL009930	0.6885	0.3115	0.8411	Gynostemmae Pentaphylli Herba	Gypenoside LXXV	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)C)C)C)(C)C)O
MOL009931	0.3584	0.6416	0.7283	Gynostemmae Pentaphylli Herba	Gypenoside LXXVI	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)CO)C)C)C)O)(C)C)O

MOL009932	0.6525	0.3475	0.8114	Gynostemmae Pentaphylli Herba	Gypenoside LXXVII	Not Available	FALSE	C1C(C(C2C(C1)C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)C)(C)C)O
MOL009933	0.7613	0.2387	0.8084	Gynostemmae Pentaphylli Herba	Gypenoside VI	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)CO)C)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)C)O)O)CO
MOL009934	0.7256	0.2744	0.8470	Gynostemmae Pentaphylli Herba	Gypenoside VII	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)CO)C)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009935	0.6583	0.3417	0.8624	Gynostemmae Pentaphylli Herba	Gypenoside VIII	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OCC(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CC4)(C)C)C=O)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL009936	0.2257	0.7743	0.7237	Gynostemmae Pentaphylli Herba	Gypenoside VIII_qt	Not Available	FALSE	OC1C2C(CCC2C(O)(CCC=C(C)C)C)(C2(C(C3(C=O)C(CC2)C(C(O)CC3)(C)C)C1)C)C
MOL009937	0.7319	0.2681	0.8231	Gynostemmae Pentaphylli Herba	Gypenoside XI	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)CO)C)C)(C)C)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)C
MOL009938	0.5928	0.4072	0.7475	Gynostemmae Pentaphylli Herba	Gypenoside XII	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)CO)C)C)(C)C)OC1OC(C(C(C1O)O)O)CO
MOL009939	0.6384	0.3616	0.8211	Gynostemmae Pentaphylli Herba	Gypenoside XIII	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)C)(C)C)O
MOL009940	0.6330	0.3670	0.8178	Gynostemmae Pentaphylli Herba	Gypenoside XIV	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)C)C(C1CCC2(C3(CCC4C(C(CCC4(C3CC(C12)O)C)O)(C)C)C)C)(CCC=C(C)C)C
MOL009941	0.6330	0.3670	0.8178	Gynostemmae Pentaphylli Herba	Gypenoside XIX	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)C)C)C)(C)C)O
MOL009942	0.7478	0.2522	0.8063	Gynostemmae Pentaphylli Herba	Gypenoside XIX2	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CC/C=C(/CO)\C)(C)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)C)C)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009943	0.6812	0.3188	0.8683	Gynostemmae Pentaphylli Herba	Gypenoside XL	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)O)C)C=O)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009944	0.6808	0.3192	0.8562	Gynostemmae Pentaphylli Herba	Gypenoside XLI	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)(C)O)C)CO)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009945	0.2401	0.7599	0.7551	Gynostemmae Pentaphylli Herba	Gypenoside XLI_qt	Not Available	FALSE	OC1CCC2(CO)C(C1(C)C)CCC1(C2CCC2C1(CCC2C(O)(CCC=C(C)C)C)C)C

MOL009946	0.7524	0.2476	0.8041	Gynostemmae Pentaphylli Herba	Gypenoside XLII	Not Available	FALSE	C1C(C(C2C(C1)C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009947	0.7439	0.2561	0.8060	Gynostemmae Pentaphylli Herba	Gypenoside XLVII	Not Available	FALSE	C1C(C(C2C(C1)C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)C)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009948	0.7490	0.2510	0.8185	Gynostemmae Pentaphylli Herba	Gypenoside XLIV	Not Available	FALSE	C1C(C(C2C(C1)C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)C)(C)C)OC1OC(C(C(C1O)O)O)CO
MOL009949	0.7201	0.2799	0.8125	Gynostemmae Pentaphylli Herba	Gypenoside XLIX	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)COC1OC(C(C(C1O)O)O)CO)C)C)C=O)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)C)OC1OC(C(C(C1O)O)O)CO)O
MOL009950	0.7341	0.2659	0.8194	Gynostemmae Pentaphylli Herba	Gypenoside XLV	Not Available	FALSE	C1C(C(C2C(C1)C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)C)C)(C)C)OC1OC(C(C(C1O)O)O)C)O
MOL009951	0.7369	0.2631	0.8387	Gynostemmae Pentaphylli Herba	Gypenoside XLVI	Not Available	FALSE	C1C(C(C2C(C1)C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)CO)C)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009952	0.7473	0.2527	0.8101	Gynostemmae Pentaphylli Herba	Gypenoside XLVIII	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)(O)COC1OC(C(C(C1O)O)O)CO)C)C)C=O)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)C)OC1CC(C(C(C1O)O)O)CO)O
MOL009953	0.2084	0.7916	0.6943	Gynostemmae Pentaphylli Herba	Gypenoside XLVIII_qt	Not Available	FALSE	OC1CCC2(C(C1(C)C)CCC1(C2CCC2C1(CCC2C(CCC=C(C)C)(O)CO)C)C)C=O
MOL009954	0.7126	0.2874	0.8096	Gynostemmae Pentaphylli Herba	Gypenoside XV	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1OC1OCC(C(C1O)O)O)O)O)O)CO)C)C)(C)C)OC1OC(C(C(C1O)O)O)C)OC1OCC(C(C1O)O)O
MOL009955	0.7305	0.2695	0.8091	Gynostemmae Pentaphylli Herba	Gypenoside XVI	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)C)C)C)(C)C)OC1OC(C(C(C1OC1OCC(C(C1O)O)O)O)O)CO
MOL009956	0.7426	0.2574	0.8234	Gynostemmae Pentaphylli Herba	Gypenoside XVII	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)C)C)(C)C)OC1OC(C(C(C1O)O)O)CO
MOL009957	0.7501	0.2499	0.8477	Gynostemmae Pentaphylli Herba	Gypenoside XVIII	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)(O)C1OC(C(C(C1O)O)O)CO)C)C)CO)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)O)CO)O)O)CO
MOL009958	0.2535	0.7465	0.7539	Gynostemmae Pentaphylli Herba	Gypenoside XVIII_qt	Not Available	FALSE	OC1CCC2(C(C1(C)C)CCC1(C2CCC2C1(CCC2C(CCC=C(C)C)O)C)C)CO

MOL009959	0.7496	0.2504	0.7906	Gynostemmae Pentaphylli Herba	Gypenoside XX	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CC/C=C(/CO)\C)(C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)COC1OC(C(C(C1O)O)O)C)O)C
MOL009960	0.6735	0.3265	0.8184	Gynostemmae Pentaphylli Herba	Gypenoside XXI	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CC/C=C(/CO)\C)(C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)C)(C)C)O
MOL009961	0.7323	0.2677	0.8099	Gynostemmae Pentaphylli Herba	Gypenoside XXII	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)C)CO)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009962	0.2535	0.7465	0.7539	Gynostemmae Pentaphylli Herba	Gypenoside XXX_qt	Not Available	FALSE	C1C(O)C(C)(C2CCC3(C(C2(CO)C1)CCC1C3(C)CCC1C(CCC=C(C)C)O)C)C
MOL009963	0.7367	0.2633	0.8478	Gynostemmae Pentaphylli Herba	Gypenoside XXIV	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)(C1OC(C(C(C1O)O)O)CO)O)C)C)C=O)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)O)CO)O)O)CO
MOL009964	0.2157	0.7843	0.7532	Gynostemmae Pentaphylli Herba	Gypenoside XXIX_qt	Not Available	FALSE	OC1CCC2(C(C1(C)C)CCC1(C2CCC2C1(CCC2C(CCC=C(C)C)O)C)C)C=O
MOL009965	0.6314	0.3686	0.8477	Gynostemmae Pentaphylli Herba	Gypenoside XXIX	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)O)C)C)C=O)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)CO)O)O
MOL009966	0.7084	0.2916	0.8353	Gynostemmae Pentaphylli Herba	Gypenoside XXV	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)(COC1OC(C(C(C1O)O)O)CO)O)C)C)C=O)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)CO)O)O
MOL009967	0.2084	0.7916	0.6943	Gynostemmae Pentaphylli Herba	Gypenoside XXV_qt	Not Available	FALSE	C1C(O)C(C)(C)C2C(C3C(C4(C(CC3)C(CC4)C(CCC=C(C)C)(CO)O)C)(C)CC2)(C=O)C1
MOL009968	0.6880	0.3120	0.8411	Gynostemmae Pentaphylli Herba	Gypenoside XXVI	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)OC1OC(C(C(C1O)O)O)CO)C)C)C=O)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)CO)O)O
MOL009969	0.2157	0.7843	0.7532	Gynostemmae Pentaphylli Herba	Gypenoside XXXV_qt	Not Available	FALSE	C12C3(C=O)C(C(C)(C(O)CC3)C)CCC1(C1(C(CC2)C(C(O)CCC=C(C)C)CC1)C)C
MOL009970	0.6810	0.3190	0.8340	Gynostemmae Pentaphylli Herba	Gypenoside XXVII	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)O)C)C)CO)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)O)CO)O)O)CO
MOL009971	0.2668	0.7332	0.6959	Gynostemmae Pentaphylli Herba	Gypenoside XXVII_qt	Not Available	FALSE	OC1CCC2(C(C1)CCC1(C2CCC2C1(CCC2C(CCC=C(C)C)O)C)C)CO
MOL009972	0.6683	0.3317	0.8412	Gynostemmae Pentaphylli Herba	Gypenoside XXVIII	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)O)C)C)C=O)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)O)CO)O)O)CO
MOL009973	0.2493	0.7507	0.7158	Gynostemmae Pentaphylli Herba	Gypenoside XXVIII_qt	Not Available	FALSE	OC1CCC2(C(C1)CCC1(C2CCC2C1(CCC2C(CCC=C(C)C)O)C)C)C=O

MOL009974	0.6247	0.3753	0.7159	Gynostemmae Pentaphylli Herba	Gypenoside XXX	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)OC1OC(C(C(C1O)O)O)CO)C)C)CO)(C)C)OC1OC(C(C(C1O)O)O)CO
MOL009975	0.6905	0.3095	0.8670	Gynostemmae Pentaphylli Herba	Gypenoside XXXI	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)O)C)C)CO)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009976	0.7017	0.2983	0.7107	Gynostemmae Pentaphylli Herba	Gypenoside XXXII	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)(OC1OC(C(C(C1O)O)O)CO)O)C)C)CO)(C)C)OC1OC(C(C(C1O)O)O)CO
MOL009977	0.2815	0.7185	0.7170	Gynostemmae Pentaphylli Herba	Gypenoside XXXII_qt	Not Available	FALSE	C12C3(CO)C(C(C)(C)C(O)CC3)CCC1(C1(C)C(CC2)C(CC1)C(CCC=C(C)C)(O)O)C
MOL009978	0.6734	0.3266	0.8687	Gynostemmae Pentaphylli Herba	Gypenoside XXXIII	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)O)C)C)C=O)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009979	0.7274	0.2726	0.8077	Gynostemmae Pentaphylli Herba	Gypenoside XXXIV	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)C)C)C)C=O)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009980	0.7004	0.2996	0.8651	Gynostemmae Pentaphylli Herba	Gypenoside XXXIX	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)CO)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009981	0.2500	0.7500	0.7073	Gynostemmae Pentaphylli Herba	Gypenoside XXXIX_qt	Not Available	FALSE	OC1CCC2(C(C1(C)C)CCC1(C2CC(O)C2C1(CCC2C(O)(CCC=C(C)C)C)C)C)CO
MOL009982	0.7163	0.2837	0.8091	Gynostemmae Pentaphylli Herba	Gypenoside XXXV	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)C)C=O)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009983	0.7312	0.2688	0.8083	Gynostemmae Pentaphylli Herba	Gypenoside XXXVI	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)C)C)C)C=O)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009984	0.6808	0.3192	0.8562	Gynostemmae Pentaphylli Herba	Gypenoside XXXVIII	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)(C)O)C)C)CO)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009985	0.6749	0.3251	0.8138	Gynostemmae Pentaphylli Herba	Gypentonoside A	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(=O)C1)C(CC2)C(CC(=O)C=C(C)C)(C)O)C)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)OC1OC(C(C(C1O)O)O)C)O)COC1OC(C(C(C1O)O)O)C
MOL009986	0.2058	0.7942	0.7235	Gynostemmae Pentaphylli Herba	Gypentonoside A_qt	Not Available	FALSE	OC1CCC2(C(C1(C)C)CCC1(C2CC(=O)C2C1(CCC2C(CC(=O)C=C(C)C)(C)O)C)C)C

MOL009987	0.7488	0.2512	0.8174	Gynostemmae Pentaphylli Herba	Gypinoside III	Not Available	FALSE	C1(C(C2C(CC1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO)C)C)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009988	0.7337	0.2663	0.8111	Gynostemmae Pentaphylli Herba	Gypinoside LXVII	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O)C)C)CO)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO)O
MOL009989	0.2422	0.7578	0.6868	Gynostemmae Pentaphylli Herba	Gypinoside LXVII_qt	Not Available	FALSE	OC1C(CC2(C(C1(C)C)CCC1(C2CCC2C1(CCC2C(O)(CCC=C(C)C)C)C)C)CO)O
MOL009990	0.7403	0.2597	0.8037	Gynostemmae Pentaphylli Herba	Gypinoside VII	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)O)COC1OC(C(C(C1O)O)O)C)C)C)(C)C)OC1OC(C(C(C1O)O)O)O)COC1OC(C(C(C1O)O)O)O)C
MOL009991	0.7442	0.2558	0.8106	Gynostemmae Pentaphylli Herba	Gypnoside V	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)O)COC1OC(C(C(C1O)O)O)C)C)C)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO
MOL009992	0.7411	0.2589	0.8610	Gynostemmae Pentaphylli Herba	Gypsogenin	92825	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)C)(C)C=O)O
MOL009993	0.9070	0.0930	0.8932	Gynostemmae Pentaphylli Herba	(2R,3R,4R,5R)-2,3,5,6-tetrahydroxy-4-[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhexanal	3037558	FALSE	C1(OC(C(C(C=O)O)O)C(CO)O)OC(C(C(C1O)O)O)CO
MOL009994	0.9523	0.0477	0.8965	Gynostemmae Pentaphylli Herba	N,N-Dimethylconiine	Not Available	FALSE	CCCC1[N+](CCCC1)(C)C
MOL009995	0.8267	0.1733	0.7926	Gynostemmae Pentaphylli Herba	ombuoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(OC)c2)c1cc(OC)c(O)cc1)COC1OC(C(O)C(O)C1O)C
MOL009996	0.7353	0.2647	0.7681	Gynostemmae Pentaphylli Herba	Onjisaponin F	Not Available	FALSE	O1CC(C(C1OC1C(C(OC(C1OC1OCC(C(C1O)OC1OCC(C(C1O)O)O)O)C)OC1C(OC(C(C1O)OC(=O)/C=C/c1cc(c(c(c1)OC)OC)OC)C)OC(=O)C12CCC3(C4(CCC5C(C(CC5(C4CC=C3C1CC(CC2)(C)C)C)O)OC1CC(C(C(C1O)O)O)CO)(C(=O)O)C)C)CO)O)O)(CO)O
MOL009997	0.9410	0.0590	0.8730	Gynostemmae Pentaphylli Herba	1-isochromanone	78429	FALSE	C1(=O)OCCc2ccccc12

MOL009998	0.8790	0.1210	0.9490	Gynostemmae Pentaphylli Herba	Toddaculin	5321960	FALSE	c12c(ccc(=O)o1)c(c(c(c2)OC)CC=C(C)C)OC
MOL009999	0.1720	0.8280	0.6975	Farfarae Flos	12-Methoxy-6,8,11,13-abietatraen-11-ol	14827287	FALSE	c1(c2c(cc(c1OC)C(C)C)C=CC1C2(CCCC1(C)C)C)O
MOL010000	0.8506	0.1494	0.7330	Farfarae Flos	21964-48-7	30874	FALSE	C=CCCCCCCCCCC=C
MOL010003	0.3518	0.6482	0.7123	Farfarae Flos	7beta-angeloyloxyoplopa-3(14)Z,8(10)-dien-2-one	Not Available	FALSE	C1(CC(C2C(C1=C)CC(=O)/C/2=C/C)C(C)C)OC(=O)C=C(C)C
MOL010004	0.3177	0.6823	0.8046	Farfarae Flos	7beta-(4-methylsenecioyloxy)oplopa-3(14)E,8(10)-dien-2-one	Not Available	FALSE	C1(CC(C2C(C1=C)CC(=O)/C/2=C/C)C(C)C)OC(=O)/C(=C\C)/C
MOL010008	0.8982	0.1018	0.8913	Farfarae Flos	(1R,4S,6R)-1-methyl-4-(6-methylhepta-1,5-dien-2-yl)-7-oxabicyclo[4.1.0]heptan-2-one	10704868	FALSE	C(CC=C(C)C)C(=C)C1CC2C(C(=O)C1)(C)O2
MOL010010	0.4008	0.5992	0.6106	Farfarae Flos	14(R)-hydroxy-7beta-isovaleroyloxyoplop-8(10)-en-2-one	Not Available	FALSE	C1(CC(C2C(C1=C)CC(=O)C2C(O)C)C(C)C)OC(=O)CC(C)C
MOL010018	0.9193	0.0807	0.9442	Farfarae Flos	pedatisectine E	Not Available	FALSE	C(C(C(CO)O)O)(O)c1cnc(cn1)C
MOL010019	0.4023	0.5977	0.7041	Farfarae Flos	Phi-Taraxasterol	12305110	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(CC2)(CC=C(C1C)C)C)C)C)(C)C)O
MOL010020	0.9029	0.0971	0.9037	Farfarae Flos	(3R)-undec-1-en-3-ol	11171230	FALSE	C=CC(CCCCCCCC)O
MOL010021	0.9184	0.0816	0.9826	Farfarae Flos	R-methyl 2-pyrrolidin-2-yl-acetate	11571818	FALSE	C1CCNC1CC(=O)OC
MOL010026	0.9425	0.0575	0.8003	Farfarae Flos	Tussilagine	185071	FALSE	OC1(C(C2N(C1)CCC2)C(=O)OC)C
MOL010029	0.8873	0.1127	0.7847	Farfarae Flos	tutin	Not Available	FALSE	C1(C2C3(C(C(C1OC2=O)O)(C1(C2C3O2)OC1)C)O)C(=C)C

MOL010030	0.8795	0.1205	0.7103	Farfarae Flos	2,6-dimethyl-undecane	Not Available	FALSE	C(CCCC(C)C)(CCCCC)C
MOL010031	0.9191	0.0809	0.9553	Farfarae Flos	EGBE	8133	FALSE	O(CCCC)CCO
MOL010032	0.9194	0.0806	0.9094	Farfarae Flos	3-(2-propenyl)-cyclooctene	Not Available	FALSE	C1=CC(CCCCC1)CC=C
MOL010033	0.8390	0.1610	0.7279	Farfarae Flos	3,5-o-dicaffeoylquinic acid	Not Available	FALSE	C1(C(C(CC(C1)(C(=O)O)O)OC(=O)/C=C\c1cc(c(cc1)O)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O
MOL010034	0.8690	0.1310	0.8134	Farfarae Flos	3,7,11-Trimethyl-dodeca-2,4,6,10-tetraenal	5365928	FALSE	C(=O)/C=C(/C=C/C=C(/CCC=C(C)C)\C)\C
MOL010035	0.8638	0.1362	0.8314	Farfarae Flos	NSC21907	228781	FALSE	O1CC(COC1CCCCCCCC)(C)C
MOL010036	0.7634	0.2366	0.7752	Farfarae Flos	6,6-dimethyl-2-methylene-7-(3-oxobutylidene)oxepan-3-ylmethyl acetic acid ester	Not Available	FALSE	O1/C(=C\CC(=O)C)/C(CCC(C1=C)COC(=O)C)(C)C
MOL010037	0.8398	0.1602	0.7980	Farfarae Flos	6-isopropenyl-4,8a-dimethyl-1,2,3,5,6,7,8,8a-octahydro-naphthalen-2-ol	Not Available	FALSE	OC1CC2(C(=C(C1)C)CC(CC2)C(=C)C)C
MOL010038	0.3094	0.6906	0.6263	Farfarae Flos	alpha-Carotene-5,6-epoxide	Not Available	FALSE	C1CCC2(C(C1(C)C)(/C=C/C(=C\C=C/C(=C/C=C/C=C(/C=C\C=C(/C=C/C1C(=CCCC1(C)C)C)\C)\C)/C)/C)O2)C
MOL010039	0.3996	0.6004	0.7624	Farfarae Flos	arnidiol	Not Available	FALSE	OC1C2(C(C3C(C4(C(C5(C(CC4)C(C(O)CC5)(C)C)C)CC3)C)(C1)C)C(C(=C)CC2)C)C
MOL010039	0.3996	0.6004	0.7624	Centipedae Herba	arnidiol	Not Available	FALSE	OC1C2(C(C3C(C4(C(C5(C(CC4)C(C(O)CC5)(C)C)C)CC3)C)(C1)C)C(C(=C)CC2)C)C
MOL010040	0.3925	0.6075	0.7529	Farfarae Flos	bauer-7-ene-3beta-16alpha-diol	Not Available	FALSE	C1C2(C(C3=CCC4C(C3C1)(CCC(C4(C)C)O)C)(CC(C1(C2C(C(CC1)C)C)C)O)C)C

MOL010041	0.3966	0.6034	0.6969	Farfarae Flos	D:C-Friedours-7-en-3beta-ol (8CI)	111220	FALSE	C1C(C(C2C(C1)(C1C(=CC2)C2(C(CC1)(C1C(CC2)(CCC(C1C)C)C)C)C)C)(C)C)O
MOL010042	0.9176	0.0824	0.9478	Farfarae Flos	WLN: ZVR	2331	FALSE	NC(=O)c1ccccc1
MOL010043	0.8679	0.1321	0.7021	Farfarae Flos	bicyclo[10.1.0]tridec-1-ene	Not Available	FALSE	C12C/C/1=C/CCCCCCCCC2
MOL010044	0.8308	0.1692	0.7203	Anisi Stellati Fructus	C09628	442347	FALSE	OC12C(CCC1C(C)C)(CC=C(CC2)C)C
MOL010044	0.8308	0.1692	0.7203	Farfarae Flos	C09628	442347	FALSE	OC12C(CCC1C(C)C)(CC=C(CC2)C)C
MOL010045	0.8892	0.1108	0.7623	Farfarae Flos	cis-lanceol	Not Available	FALSE	OC/C(=C/1\C2C(C(CC1)C)CCC(=C2)C)/C
MOL010046	0.8667	0.1333	0.8009	Farfarae Flos	Cycloundecene(Z)	5362796	FALSE	C\1=C\CCCCCCCCC1
MOL010047	0.8871	0.1129	0.8249	Farfarae Flos	dextrin	Not Available	FALSE	O1C(C(OC2OC(C(O)C(O)C2O)CO)C(O)C(O)C1OC1C(O)C(O)C(OC1CO)O)CO
MOL010048	0.5999	0.4001	0.6180	Farfarae Flos	octadecan-2E,13Z-dien-1-ol	5283306	FALSE	C(=C\CCCCCCCCC/C=C\CCCC)/CO
MOL010049	0.4114	0.5886	0.7226	Farfarae Flos	faradiol	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)C)(CCC1(C2CC(=CC1)C)C)C
MOL010050	0.7023	0.2977	0.6696	Farfarae Flos	farcarineiol	Not Available	FALSE	C(CCCCCC)/C=C/C(O)C#CC#CC(C=C)O
MOL010051	0.7643	0.2357	0.6720	Farfarae Flos	farfugin A	Not Available	FALSE	c12c(cc3c(c1C(CCC2)C)occ3C)C
MOL010053	0.8892	0.1108	0.8660	Farfarae Flos	(E)-10-methylundec-1-en-1-ol	Not Available	FALSE	C(=C\CCCCCCCC(C)C)/O
MOL010054	0.9040	0.0960	0.8110	Farfarae Flos	kaempferol-3-arabinoside	Not Available	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O)CO1)c1ccc(cc1)O
MOL010055	0.8777	0.1223	0.7272	Farfarae Flos	Femara	3902	FALSE	N#Cc1ccc(cc1)C(n1cncn1)c1ccc(cc1)C#N
MOL010056	0.6789	0.3211	0.6950	Farfarae Flos	methyl 3,4-o-dicaffeoylquinate	Not Available	FALSE	C1(C(C(CC(C1)(C(=O)OC)O)OC(=O)/C=C\c1cc(c(cc1)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O)O
MOL010057	0.6880	0.3120	0.6986	Farfarae Flos	methyl 3,5-o-dicaffeoylquinate	Not Available	FALSE	C1(C(C(CC(C1)(C(=O)OC)O)OC(=O)/C=C\c1cc(c(cc1)O)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O
MOL010058	0.9012	0.0988	0.8749	Farfarae Flos	methyl 3-o-caffeoylquinate	Not Available	FALSE	C1(C(C(CC(C1)(C(=O)OC)O)OC(=O)/C=C\c1cc(c(cc1)O)O)O)O
MOL010059	0.5403	0.4597	0.6728	Farfarae Flos	methyl 4,5-o-dicaffeoylquinate	Not Available	FALSE	C1(C(CCC(C1)(C(=O)OC)O)OC(=O)/C=C/c1cc(c(cc1)O)O)OC(=O)/C=C/c1cc(c(cc1)O)O
MOL010061	0.8993	0.1007	0.8891	Momordicae Fructus	10-Undecenal	8187	FALSE	C(CCCCC=O)CCCC=C
MOL010061	0.8993	0.1007	0.8891	Lysimachiae Foenigraeci Herba	10-Undecenal	8187	FALSE	C(CCCCC=O)CCCC=C

MOL010062	0.7436	0.2564	0.8145	Momordicae Fructus	11-dehydroxymogroside III	17752184	FALSE	C12C(C3C(=CC2)C(C(CC3)OC2OC(C(C(C2O)O)O)CO)(C)C)(CCC2(C1(CCC2C(CCC(OC1OC(COC2OC(C(C(C2O)O)O)CO)C(C(C1O)O)O)C(C)(C)O)C)C)C
MOL010063	0.2754	0.7246	0.6518	Momordicae Fructus	11-dehydroxymogroside III_qt	Not Available	FALSE	C12C(C3C(=CC2)C(C(CC3)O)(C)C)(CCC2(C1(CCC2C(CCC(O)C(C)(O)C)C)C)C
MOL010064	0.7425	0.2575	0.8064	Momordicae Fructus	11-deoxymogroside III	Not Available	FALSE	C12C(C3(C(=CC2)C(C(CC3)OC2OC(C(C(C2O)O)O)CO)(C)C)C)(CCC2(C1(CCC2C(CCC(OC1OC(COC2OC(C(C(C2O)O)O)CO)C(C(C1O)O)O)C(C)(C)O)C)C)C
MOL010065	0.2674	0.7326	0.6558	Momordicae Fructus	11-deoxymogroside III_qt	Not Available	FALSE	C12C(C3(C(=CC2)C(C(CC3)O)(C)C)C)(CCC2(C1(CCC2C(CCC(O)C(C)(O)C)C)C)C
MOL010066	0.7890	0.2110	0.7770	Momordicae Fructus	11-oxomogroside V	44423070	FALSE	OC1C2(C(C3(C(C(CC3)C(CCC(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)COC3OC(C(O)C(O)C3O)CO)C(O)(C)C)C)(C1)C)CC=C1C2CCC(OC2OC(C(O)C(O)C2O)COC2OC(C(O)C(O)C2O)CO)C1(C)C)C
MOL010067	0.2801	0.7199	0.6514	Momordicae Fructus	mogrol	14525327	FALSE	OC1CC2(C(C3C1(C1C(=CC3)C(C(O)CC1)(C)C)C)(CCC2C(CCC(O)C(O)(C)C)C)C)C
MOL010068	0.4884	0.5116	0.7940	Momordicae Fructus	(3S,8S,9R,10R,13R,14S,17R)-3-hydroxy-17-[(2R,5R)-6-hydroxy-6-methyl-5-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyheptan-2-yl]-4,4,9,13,14-pentamethyl-1,2,3,7,8,10,12,15,16,17-decahydrocyclopenta[a]phenanthren-11-one	11093434	FALSE	C12C(C3C(=CC2)C(C)(C)C(CC3)O)(C(=O)CC2(C1(CCC2C(CCC(OC1C(C(C(C(O1)CO)O)O)O)C(C)(C)O)C)C)C)C
MOL010069	0.2456	0.7544	0.6693	Momordicae Fructus	NSC710352	399493	FALSE	C12C(C3C(=CC2)C(C)(C)C(CC3)O)(C(=O)CC2(C1(CCC2C(CCC(O)C(O)(C)C)C)C)C)C

MOL010070	0.7021	0.2979	0.8387	Momordicae Fructus	11-oxomogroside Ⅱ A1	Not Available	FALSE	C1C(C(C2=CCC3C(C2(C1)C)(C(=O)CC1(C3(CCC1C(CCC(C(C)(C)O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)CO)O)O)O)C)C)C)(C)C)O
MOL010071	0.2418	0.7582	0.6869	Momordicae Fructus	12-oxomogroside IE1_qt	Not Available	FALSE	C1C(C(C2=CCC3C(C2(C1)C)(C(=O)CC1(C3(CCC1C(CCC(C(C)(C)O)O)C)C)C)C)(C)C)O
MOL010072	0.7033	0.2967	0.8335	Momordicae Fructus	11-oxomogroside Ⅱ E	Not Available	FALSE	C1C(C(C2=CCC3C(C2(C1)C)(C(=O)CC1(C3(CCC1C(C)CCC(C(C)(C)O)OC1OC(C(O)C(O)C1O)CO)C)C)(C)C)OC1OC(C(O)C(O)C1O)CO
MOL010073	0.2418	0.7582	0.6869	Momordicae Fructus	11-oxomogroside Ⅱ E_qt	Not Available	FALSE	C1C(C(C2=CCC3C(C2(C1)C)(C(=O)CC1(C3(CCC1C(C)CCC(C(C)(C)O)O)C)C)C)(C)C)O
MOL010074	0.7401	0.2599	0.8121	Momordicae Fructus	11-oxoymogroside Ⅲ	17752183	FALSE	C12C(C3C(=CC2)C(C(CC3)OC2OC(C(C(C2O)O)O)CO)(C)C)(C(=O)CC2(C1(CCC2C(CCC(OC1OC(COC2OC(C(C(C2O)O)O)CO)C(C(C1O)O)O)C(C)(C)O)C)C)C
MOL010075	0.7611	0.2389	0.7911	Momordicae Fructus	11-oxomogroside ⅣA	Not Available	FALSE	C1C(C(C2=CCC3C(C2(C1)C)(C(=O)CC1(C3(CCC1C(CCC(C(C)(C)O)OC1OC(COC2OC(C(C(C2O)O)O)CO)C(C(C1O)O)O)C)C)C)(C)C)OC1OC(COC2OC(C(C(C2O)O)O)CO)C(C(C1O)O)O
MOL010076	0.2418	0.7582	0.6869	Momordicae Fructus	11-oxomogroside ⅣA_qt	Not Available	FALSE	C1C(C(C2=CCC3C(C2(C1)C)(C(=O)CC1(C3(CCC1C(CCC(C(C)(C)O)O)O)C)C)C)(C)C)O
MOL010077	0.4476	0.5524	0.7867	Momordicae Fructus	11-oxomogroside IA1	Not Available	FALSE	C1C(C(C2=CCC3C(C2(C1)C)(C(=O)CC1(C3(CCC1C(CCC(C(C)(C)O)OC1OC(C(O)C(O)C1O)CO)C)C)C)(C)C)O
MOL010078	0.3572	0.6428	0.7140	Momordicae Fructus	12-oxomogroside IE1	Not Available	FALSE	C1C(C(C2=CCC3C(C2(C1)C)(C(=O)CC1(C3(CCC1C(CCC(C(C)(C)O)O)C)C)C)(C)C)OC1OC(C(O)C(O)C1O)CO
MOL010079	0.6320	0.3680	0.6413	Momordicae Fructus	(14R)-14-methylhexadec-8-yn-1-ol	10944926	FALSE	OCCCCCCCC#CCCCCC(CC)C
MOL010080	0.8219	0.1781	0.8862	Momordicae Fructus	BUTYL ISOBUTYL PHTHALATE	28813	FALSE	O(CC(C)C)C(=O)c1c(C(=O)OCCCC)cccc1
MOL010080	0.8219	0.1781	0.8862	Allii Fistulost Bulbus	BUTYL ISOBUTYL PHTHALATE	28813	FALSE	O(CC(C)C)C(=O)c1c(C(=O)OCCCC)cccc1
MOL010082	0.8785	0.1215	0.9318	Momordicae Fructus	WLN: T5NJ A1 BVH	14504	FALSE	c1(n(ccc1)C)C=O
MOL010083	0.9199	0.0801	0.7768	Momordicae Fructus	Zoba ERN	7005	FALSE	Oc1c2c(ccc1)cccc2

MOL010084	0.5284	0.4716	0.8131	Momordicae Fructus	20-hydroxy-11-oxomogroside I A1	Not Available	FALSE	C1C(C(C2=CCC3C(C2(C1)C)(C(=O)CC1(C3(CCC1C(C)(CCC(C(C)(C)O)OC1OC(C(O)C(O)C1O)CO)O)C)C)C)(C)C)O
MOL010085	0.2666	0.7334	0.6828	Momordicae Fructus	20-hydroxy-11-oxomogroside I A1_qt	Not Available	FALSE	C1C(C(C2=CCC3C(C2(C1)C)(C(=O)CC1(C3(CCC1C(C)(CCC(C(C)(C)O)O)O)C)C)C)(C)C)O
MOL010086	0.9429	0.0571	0.9400	Momordicae Fructus	[(2R,4R)-4-acetyloxypentan-2-yl] acetate	12641386	FALSE	O(C(CC(OC(=O)C)C)C)C(=O)C
MOL010087	0.7202	0.2798	0.6138	Momordicae Fructus	2-hexadecanol	25021739	FALSE	OC(CCCCCCCCCCCCCC)C
MOL010088	0.8751	0.1249	0.9643	Momordicae Fructus	2-Methyl-1,3-cyclopentadione	13005	FALSE	C1(C(=O)CCC1=O)C
MOL010089	0.9045	0.0955	0.9697	Momordicae Fructus	2-Methylenecycloheptanone	543153	FALSE	O=C1CCCCCC1=C
MOL010090	0.9313	0.0687	0.9384	Citri Fructus	557951_ALDRICH	11286536	FALSE	C(CCCCC)CC(C)O
MOL010090	0.9313	0.0687	0.9384	Caryophylliflos	557951_ALDRICH	11286536	FALSE	C(CCCCC)CC(C)O
MOL010090	0.9313	0.0687	0.9384	Momordicae Fructus	557951_ALDRICH	11286536	FALSE	C(CCCCC)CC(C)O
MOL010091	0.8700	0.1300	0.8182	Momordicae Fructus	(2R)-tridecan-2-ol	10420345	FALSE	OC(CCCCCCCCCCC)C
MOL010091	0.8700	0.1300	0.8182	Rose Rugosae Flos	(2R)-tridecan-2-ol	10420345	FALSE	OC(CCCCCCCCCCC)C
MOL010092	0.9429	0.0571	0.9400	Momordicae Fructus	3-(acetyloxy)-1-methylbutyl acetate	40429805	FALSE	C(CC(OC(=O)C)C)(OC(=O)C)C
MOL010093	0.9142	0.0858	0.9407	Momordicae Fructus	trans-1,2-Diacetylethylene	5363639	FALSE	CC(=O)/C=C/C(=O)C
MOL010094	0.8987	0.1013	0.8886	Momordicae Fructus	3-Octyne	84849	FALSE	C(C#CCC)CCC
MOL010095	0.9267	0.0733	0.7398	Momordicae Fructus	3-PHENYLPYRIDINE	13886	FALSE	c1(c2cccnc2)ccccc1
MOL010096	0.8826	0.1174	0.8725	Momordicae Fructus	4-Cyclopentene-1,3-dione	70258	FALSE	C1(=O)CC(=O)C=C1

MOL010097	0.4562	0.5438	0.7376	Momordicae Fructus	5alpha,6alpha-expoxymogroside I E1	Not Available	FALSE	C12C(C3(C4(C(C2)O4)C(C(CC3)OC2OC(C(C(C2O)O)O)CO)(C)C)C)(C(CC2(C1(CCC2C(CCC(O)C(C)(C)O)C)C)C)O)C
MOL010098	0.3248	0.6752	0.6802	Momordicae Fructus	5alpha,6alpha-expoxymogroside I E1_qt	Not Available	FALSE	C12C(C3(C4(C(C2)O4)C(C(CC3)O)(C)C)C)(C(CC2(C1(CCC2C(CCC(O)C(C)(O)C)C)C)C)O)C
MOL010099	0.9435	0.0565	0.8446	Momordicae Fructus	Myristicin aldehyde	22016	FALSE	c12c(c(cc(c1)C=O)OC)OCO2
MOL010100	0.7292	0.2708	0.8337	Momordicae Fructus	7-oxomogroside Ⅱ E	Not Available	FALSE	C1C(C(C2=CC(=O)C3C(C2(C1)C)(C(CC1(C3(CCC1C(C)CCC(C(C)(C)O)OC1OC(C(O)C(O)C1O)CO)C)O)C)(C)C)OC1OC(C(O)C(O)C1O)CO
MOL010101	0.2739	0.7261	0.6790	Momordicae Fructus	7-oxomogroside Ⅱ E_qt	Not Available	FALSE	C1C(C(C2=CC(=O)C3C(C2(C1)C)(C(CC1(C3(CCC1C(C)CCC(C(C)(C)O)O)C)C)O)C)(C)C)O
MOL010102	0.7789	0.2211	0.7819	Momordicae Fructus	7-oxomogroside Ⅴ	Not Available	FALSE	OC1C2(C(C3(C(C(CC3)C(CCC(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)COC3OC(C(O)C(O)C3O)CO)C(O)(C)C)C)(C1)C)C)C(=O)C=C1C2CCC(OC2OC(C(O)C(O)C2O)COC2OC(C(O)C(O)C2O)CO)C1(C)C
MOL010103	0.2653	0.7347	0.6743	Momordicae Fructus	7-oxomogroside Ⅴ_qt	Not Available	FALSE	OC1C2(C(C3(C(C(CC3)C(CCC(O)C(O)(C)C)C)(C1)C)C)C(=O)C=C1C2CCC(O)C1(C)C)C
MOL010104	0.9240	0.0760	0.9228	Momordicae Fructus	Caproleic acid	61743	FALSE	OC(=O)CCCCCCCC=C
MOL010106	0.7446	0.2554	0.8458	Momordicae Fructus	Sapindoside B	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(CO)C)OC1OCC(C(C1OC1OC(C(C(C1O)OC1OCC(C(C1O)O)O)O)C)O)O
MOL010106	0.7446	0.2554	0.8458	Caulis Akebiae	Sapindoside B	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(CO)C)OC1OCC(C(C1OC1OC(C(C(C1O)OC1OCC(C(C1O)O)O)O)C)O)O
MOL010107	0.7613	0.2387	0.8412	Momordicae Fructus	Sapindoside B_qt	Not Available	FALSE	C1CC2(C(C(C1O)(CO)C)CCC1(C2CC=C2C1(CCC1(C2CC(C)(CC1)C)C(=O)O)C)C)C
MOL010107	0.7613	0.2387	0.8412	Caulis Akebiae	Sapindoside B_qt	Not Available	FALSE	C1CC2(C(C(C1O)(CO)C)CCC1(C2CC=C2C1(CCC1(C2CC(C)(CC1)C)C(=O)O)C)C)C
MOL010108	0.7711	0.2289	0.8199	Momordicae Fructus	siraitic acid C	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(CO)C)OC1OCC(C(C1OC1OC(C(C(C1O)OC1OCC(C(C1O)O)OC1OC(C(C(C1O)O)O)CO)O)C)O)O
MOL010109	0.7206	0.2794	0.7771	Momordicae Fructus	siraitic acid D	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(CO)C)OC1OCC(C(C1OC1OC(C(C(C1O)OC1OCC(C(C1O)O)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)COC1OC(C(C(C1O)O)O)C)O)C)O)O

MOL010110	0.4897	0.5103	0.7569	Momordicae Fructus	siraitic acid E	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1OCC(C(C1OC1OC(C(C(C1O)OC1OCC(C(C1O)O)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)COC1OC(C(C(C1O)O)O)C)O)C)O)O)C)C)(CO)C)OC1OCC(C(C1OC1OC(C(C(C1O)OC1OCC(C(C1O)O)O)O)C)O)O
MOL010111	0.7613	0.2387	0.8412	Momordicae Fructus	siraitic acid E_qt	40469782	FALSE	C1C2C(C3(C(=C1)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)(CCC1C2(CCC(C1(C)CO)O)C)C
MOL010112	0.7869	0.2131	0.7379	Momordicae Fructus	TRIDECYL ACETATE	14071	FALSE	CC(=O)OCCCCCCCCCCCCC
MOL010113	0.8921	0.1079	0.9688	Momordicae Fructus	WLN: T5OV CHJ E1	11559	FALSE	C1(=CCC(=O)O1)C
MOL010114	0.8807	0.1193	0.8663	Momordicae Fructus	BA (VAN)	7657	FALSE	c1(COCc2ccccc2)ccccc1
MOL010115	0.9231	0.0769	0.8238	Momordicae Fructus	Damasione	5374527	FALSE	C1(=C(CCCC1(C)C)C)C(=O)/C=C/C
MOL010115	0.9231	0.0769	0.8238	Eucommiae Folium	Damasione	5374527	FALSE	C1(=C(CCCC1(C)C)C)C(=O)/C=C/C
MOL010115	0.9231	0.0769	0.8238	Eriobotryae Folium	Damasione	5374527	FALSE	C1(=C(CCCC1(C)C)C)C(=O)/C=C/C
MOL010116	0.9414	0.0586	0.9604	Momordicae Fructus	BUTYL CROTONATE	5366039	FALSE	O(CCCC)C(=O)/C=C/C
MOL010117	0.9377	0.0623	0.9584	Momordicae Fructus	Butyl tiglate	5352450	FALSE	C(=O)(OCCCC)/C(=C/C)/C
MOL010118	0.9435	0.0565	0.9697	Momordicae Fructus	butyl 3-hydroxybutanoate	14360282	FALSE	O(CCCC)C(=O)CC(O)C
MOL010119	0.9415	0.0585	0.9593	Momordicae Fructus	Butyl butyrate	7983	FALSE	CCCCOC(=O)CCC
MOL010120	0.8406	0.1594	0.7115	Momordicae Fructus	(1S,4R,4aR,8aR)-1-isopropyl-4,7-dimethyl-2,3,4,5,6,8a-hexahydro-1H-naphthalen-4a-ol	11770062	FALSE	OC12C(C(CCC1C)C(C)C)C=C(CC2)C
MOL010120	0.8406	0.1594	0.7115	Thalluslaminariae	(1S,4R,4aR,8aR)-1-isopropyl-4,7-dimethyl-2,3,4,5,6,8a-hexahydro-1H-naphthalen-4a-ol	11770062	FALSE	OC12C(C(CCC1C)C(C)C)C=C(CC2)C

MOL010120	0.8406	0.1594	0.7115	Tamaricis Cacumen	(1S,4R,4aR,8aR)-1-isopropyl-4,7-dimethyl-2,3,4,5,6,8a-hexahydro-1H-naphthalen-4a-ol	11770062	FALSE	OC12C(C(CCC1C)C(C)C)C=C(CC2)C
MOL010121	0.9298	0.0702	0.8839	Momordicae Fructus	(3S,8aS)-3-methyl-2,3,6,7,8,8a-hexahydropyrrolo[2,1-f]pyrazine-1,4-dione	13879951	FALSE	N1C(C(=O)N2C(C1=O)CCC2)C
MOL010122	0.9431	0.0569	0.8141	Momordicae Fructus	ZINC04023242	7074740	FALSE	C1(NC(=O)C2N(C1=O)CCC2)CC(C)C
MOL010123	0.9361	0.0639	0.9629	Caryophylliflos	ZINC00394787	6950754	FALSE	C(OC(=O)C)(CC)C
MOL010123	0.9361	0.0639	0.9629	Momordicae Fructus	ZINC00394787	6950754	FALSE	C(OC(=O)C)(CC)C
MOL010124	0.9254	0.0746	0.9174	Momordicae Fructus	3-decenoic acid	5282725	FALSE	C(=O)(C/C=C/CCCCCC)O
MOL010125	0.4469	0.5531	0.7423	Momordicae Fructus	esgoside	Not Available	FALSE	O1C23C4(C(C5(C(CC4=O)C(OC(=O)CC5OC(=O)C)(C)C)C)CCC2(C(OC(=O)C13)c1ccoc1)C)C
MOL010126	0.8358	0.1642	0.8080	Momordicae Fructus	grosvenorine	Not Available	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)OC1C(OC2C(O)C(O)C(O)C(O2)C)C(O)C(O)C(O1)CO)OC1C(O)C(O)C(O)C(O1)C)c1ccc(cc1)O
MOL010127	0.9400	0.0600	0.9589	Mume Flos	Hexyl acetate	8908	FALSE	CCCCCCOC(=O)C
MOL010127	0.9400	0.0600	0.9589	Rose Rugosae Flos	Hexyl acetate	8908	FALSE	CCCCCCOC(=O)C
MOL010127	0.9400	0.0600	0.9589	Momordicae Fructus	Hexyl acetate	8908	FALSE	CCCCCCOC(=O)C
MOL010127	0.9400	0.0600	0.9589	Ardisiae Japonicae Herba	Hexyl acetate	8908	FALSE	CCCCCCOC(=O)C
MOL010128	0.8977	0.1023	0.8916	Momordicae Fructus	Heptyl iobutyrate	61304	FALSE	C(=O)(C(C)C)OCCCCCCC
MOL010129	0.8574	0.1426	0.8126	Momordicae Fructus	kaempferol 7-o-alpha-l-rhamnopyranoside	Not Available	FALSE	C1(C(C(C(C(O1)Oc1cc(c2c(c1)oc(c(c2=O)O)c1ccc(cc1)O)O)O)O)O)C
MOL010130	0.8757	0.1243	0.9664	Momordicae Fructus	Corylon	6660	FALSE	C1(=C(CCC1=O)C)O
MOL010131	0.4046	0.5954	0.6838	Momordicae Fructus	mogroester	Not Available	FALSE	C1(CCC23C(C1(C)C)CC=C1C4(C)CCC(C(CCC=C(C)C)COC(=O)c5ccccc5)C4(C)CCC21C3)OC(=O)c1ccccc1

MOL010132	0.7198	0.2802	0.8303	Momordicae Fructus	mogroside Ⅱ A1	Not Available	FALSE	C1C(C(C2=CCC3C(C2C1)(C(CC1(C3(CCC1C(CCC(OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)CO)O)O)O)C(C)(C)O)C)C)O)C)(C)C)O
MOL010133	0.2801	0.7199	0.6514	Momordicae Fructus	mogroside Ⅱ A1_qt	Not Available	FALSE	C1C(C(C2=CCC3C(C2C1)(C(CC1(C3(CCC1C(CCC(O)C(C)(C)O)C)C)O)C)(C)C)O
MOL010134	0.7392	0.2608	0.8156	Momordicae Fructus	mogroside Ⅱ B	Not Available	FALSE	C1C(C(C2=CCC3C(C2(C1)C)(C(CC1(C3(CCC1C(C)CCC(C(C)(C)OC1OC(C(O)C(O)C1O)CO)O)C)C)O)C)(C)C)OC1OC(C(O)C(O)C1O)CO
MOL010135	0.2793	0.7207	0.6677	Momordicae Fructus	mogroside Ⅱ B_qt	Not Available	FALSE	C1C(C(C2=CCC3C(C2(C1)C)(C(CC1(C3(CCC1C(C)CCC(C(C)(C)O)O)C)C)O)C)(C)C)O
MOL010136	0.7189	0.2811	0.8263	Momordicae Fructus	mogroside Ⅱ E	Not Available	FALSE	C1C(C(C2=CCC3C(C2(C1)C)(C(CC1(C3(CCC1C(C)CCC(C(C)(C)O)OC1OC(C(O)C(O)C1O)CO)C)C)O)C)(C)C)OC1OC(C(O)C(O)C1O)CO
MOL010137	0.2793	0.7207	0.6677	Momordicae Fructus	mogroside Ⅱ E_qt	Not Available	FALSE	C1C(C(C2=CCC3C(C2(C1)C)(C(CC1(C3(CCC1C(C)CCC(C(C)(C)O)O)C)C)O)C)(C)C)O
MOL010138	0.7881	0.2119	0.7724	Momordicae Fructus	mogroside Ⅵ	56843594	FALSE	OC1C2(C(C3(C(C(CC3)C(CCC(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)COC3OC(C(O)C(O)C3O)CO)C(O)(C)C)C)(C1)C)C)CC=C1C2CCC(OC2OC(C(O)C(O)C2OC2OC(C(O)C(O)C2O)CO)COC2OC(C(O)C(O)C2O)CO)C1(C)C)C
MOL010139	0.7587	0.2413	0.8125	Momordicae Fructus	(2R,3R,4S,5S,6R)-2-[[(3S,8S,9R,10R,11R,13R,14S,17R)-11-hydroxy-17-[(2R,5R)-6-hydroxy-6-methyl-5-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]oxan-2-yl]oxyheptan-2-yl]-4,4,9,13,14-pentamethyl	24720988	FALSE	C12C(C3C(=CC2)C(C(CC3)OC2OC(C(C(C2O)O)O)CO)(C)C)(C(CC2(C1(CCC2C(CCC(OC1OC(COC2OC(C(C(C2O)O)O)CO)C(C(C1O)O)O)C(C)(C)O)C)C)C)O)C

MOL010140	0.7458	0.2542	0.8098	Momordicae Fructus	mogroside ⅢA2	Not Available	FALSE	C1C(C(C2=CCC3C(C2(C1)C)(C(CC1(C3(CCC1C(CCC(C(C)(C)O)OC1OC(C(C(C1O)O)O)CO)C)C)C)O)C)(C)C)OC1OC(COC2OC(C(C(C2O)O)O)CO)C(C(C1O)O)O
MOL010141	0.2793	0.7207	0.6677	Momordicae Fructus	mogroside ⅣE_qt	Not Available	FALSE	C1C(C(C2=CCC3C(C2(C1)C)(C(CC1(C3(CCC1C(CCC(C)(C)O)O)C)C)C)O)C)(C)C)O
MOL010142	0.7695	0.2305	0.7953	Momordicae Fructus	mogroside Ⅳ	Not Available	FALSE	OC1C2(C(C3(C(C(CC3)C(CCC(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)C(O)(C)C)C)(C1)C)CC=C1C2CCC(OC2OC(C(O)C(O)C2O)COC2OC(C(O)C(O)C2O)CO)C1(C)C)C
MOL010143	0.2801	0.7199	0.6514	Momordicae Fructus	mogroside Ⅳ_qt	Not Available	FALSE	OC1CC2(C(C3C1(C1C(=CC3)C(C(O)CC1)(C)C)C)(CCC2C(CCC(O)C(O)(C)C)C)C)C
MOL010144	0.7719	0.2281	0.7899	Momordicae Fructus	mogroside ⅣA	Not Available	FALSE	C1C(C(C2=CCC3C(C2(C1)C)(C(CC1(C3(CCC1C(CCC(C(C)(C)O)OC1OC(COC2OC(C(C(C2O)O)O)O)CO)C(C(C1O)O)O)C)C)O)C)(C)C)OC1OC(COC2OC(C(C(C2O)O)O)CO)C(C(C1O)O)O
MOL010145	0.7679	0.2321	0.7920	Momordicae Fructus	mogroside ⅣE	Not Available	FALSE	C1C(C(C2=CCC3C(C2(C1)C)(C(CC1(C3(CCC1C(CCC(C(C)(C)O)OC1C(C(O)C(C(O1)CO)O)OC1OC(C(C(C1O)O)O)CO)C)C)O)C)(C)C)OC1OC(COC2OC(C(C(C2O)O)O)CO)C(C(C1O)O)O
MOL010146	0.7779	0.2221	0.7776	Momordicae Fructus	mogroside V	Not Available	FALSE	OC1C2(C(C3(C(C(CC3)C(CCC(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)COC3OC(C(O)C(O)C3O)CO)C(O)(C)C)C)(C1)C)CC=C1C2CCC(OC2OC(C(O)C(O)C2O)COC2OC(C(O)C(O)C2O)CO)C1(C)C)C
MOL010147	0.4685	0.5315	0.7707	Momordicae Fructus	mogroside ⅠA1	Not Available	FALSE	C1C(C(C2=CCC3C(C2(C1)C)(C(CC1(C3(CCC1C(CCC(C(C)(C)O)OC1OC(C(O)C(O)C(O)C1O)CO)C)C)C)O)C)(C)C)O
MOL010148	0.3783	0.6217	0.7070	Momordicae Fructus	mogroside ⅠE1	Not Available	FALSE	C1C(C(C2=CCC3C(C2(C1)C)(C(CC1(C3(CCC1C(CCC(C(C)(C)O)O)C)C)C)O)C)(C)C)OC1OC(C(O)C(O)C1O)CO
MOL010149	0.7450	0.2550	0.6720	Momordicae Fructus	Myristyl acetate	12531	FALSE	O(CCCCCCCCCCCCCC)C(=O)C
MOL010149	0.7450	0.2550	0.6720	Rose Rugosae Flos	Myristyl acetate	12531	FALSE	O(CCCCCCCCCCCCCC)C(=O)C
MOL010150	0.5704	0.4296	0.6213	Momordicae Fructus	1-Heptatriacotanol	537071	FALSE	OCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
MOL010151	0.7909	0.2091	0.7775	Momordicae Fructus	neomogroside	Not Available	FALSE	OCC1OC(C(C(C1O)O)O)OC1C(OC2C(C3=CCC4C(C3CC2)(C(O)CC2(C4(CCC2C(CCC(C(O)(C)C)OC2OC(C(O)C(O)C2COC2C(C(C(C(CO)O2)O)O)O)O)OC2C(C(C(C(O2)CO)O)O)O)C)C)C)(C)C)OC(C(C1O)O)COC1C(C(C(C(O1)CO)O)O)O
MOL010152	0.7566	0.2434	0.7971	Momordicae Fructus	siamenoide I	Not Available	FALSE	C1(C(C(C(OC1CO)OC1C(C2=CCC3C(C2CC1)(C(CC1(C3(CCC1C(CCC(OC1C(C(C(C(O1)COC1C(C(C(C(O1)CO)O)O)O)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)C(C)(C)O)C)C)O)C)(C)C)O)O)O

MOL010153	0.2801	0.7199	0.6514	Momordicae Fructus	siamenoide I_qt	Not Available	FALSE	OC1C(C2=CCC3C(C2CC1)(C(CC1(C3(CCC1C(CCC(O)C(C)(C)O)C)C)C)O)C)(C)C
MOL010154	0.6428	0.3572	0.7487	Lunulatae Herba	5,7-dimethoxyphenanthrene-2,6-diol	10445823	FALSE	c1(ccc2c(c1)ccc1c2c(c(c(c1)OC)O)OC)O
MOL010155	0.9082	0.0918	0.8226	Lunulatae Herba	(5S,6R,7R,8S)-5,6,7,8-tetrahydroxy-2-[2-(2-hydroxyphenyl)ethyl]-5,6,7,8-tetrahydrochromen-4-one	21768736	FALSE	C1(C(C(c2c(C1O)oc(cc2=O)CCc1c(cccc1)O)O)O)O
MOL010156	0.7570	0.2430	0.8732	Lunulatae Herba	beta-peltoboykinolic acid	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C(=O)O)CCC4(C)CCC(C)(C)CC4C3=CCC21)C)O
MOL010157	0.8770	0.1230	0.7251	Lunulatae Herba	chrysograyanone	Not Available	FALSE	C1(C(=CC(=O)C1(c1c(c(=O)c2c(o1)cc(cc2O)OC)OC)O)OC)(C(=O)OC)O
MOL010158	0.8099	0.1901	0.6450	Lunulatae Herba	2-(5-hydroxy-4-keto-3,7-dimethoxy-chromen-2-yl)-3,5-dimethoxy-p-benzoquinone	10045780	FALSE	C1(=O)C(=C(C(=O)C(=C1)OC)OC)c1c(c(=O)c2c(o1)cc(cc2O)OC)OC
MOL010159	0.6749	0.3251	0.6356	Lunulatae Herba	2-[4,5-dimethoxy-2-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]-5-hydroxy-3,6,7-trimethoxychromen-4-one	10008104	FALSE	c1(c(c(=O)c2c(o1)cc(c(c2O)OC)OC)OC)c1c(cc(c(c1)OC)OC)OC1C(O)C(O)C(O)C(O1)CO

MOL010160	0.7542	0.2458	0.6253	Lunulatae Herba	5-hydroxy-2-(2-hydroxy-4,5-dimethoxy-phenyl)-3,6,7-trimethoxy-chromone	13871363	FALSE	c1(c(c(=O)c2c(o1)cc(c(c2O)OC)OC)OC)c1c(cc(c(c1)OC)OC)O
MOL010161	0.6822	0.3178	0.7535	Lunulatae Herba	1,5,6-trimethoxyphenanthrene-2,7-diol	11983285	FALSE	c1(c(ccc2c3c(c(c(cc3ccc12)O)OC)OC)O)OC
MOL010162	0.5865	0.4135	0.8993	Lunulatae Herba	NCI60_035895	Not Available	FALSE	C1CC(C2C(C1)(C1C3(CC2)C(C2=C(C(=O)OC2=C1)CO)O3)C)(C)C
MOL010163	0.6918	0.3082	0.8449	Lunulatae Herba	fischeriana B	Not Available	FALSE	C1(C(C(C(C(O1)OCC1=C2C(=CC3C4(C2O4)CCC2C3(CCCC2(C)C)C)OC1=O)O)O)O)CO
MOL010164	0.5865	0.4135	0.8993	Lunulatae Herba	fischeriana B_qt	Not Available	FALSE	OCC1=C2C(=CC3C4(C2O4)CCC2C3(CCCC2(C)C)C)OC1=O
MOL010165	0.4262	0.5738	0.8740	Lunulatae Herba	Jolkinolide A	Not Available	FALSE	O1C23C(C4(C(C(CCC4)(C)C)CC3)C)C=C3OC(=O)C(=C3C12)C
MOL010166	0.5470	0.4530	0.8586	Lunulatae Herba	Jolkinolide B	Not Available	FALSE	O1C23C(C4(C(CC3)C(CCC4)(C)C)C)C3OC43OC(=O)C(=C4C12)C
MOL010167	0.9043	0.0957	0.8155	Lunulatae Herba	kaempferol 3-o-beta-d-glucuronic acid	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1OC(C(C(C1O)O)O)C(=O)O)c1ccc(cc1)O)O)O
MOL010168	0.8822	0.1178	0.8398	Lunulatae Herba	5,7-dihydroxy-2-(4-hydroxyphenyl)-3-[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-chromone	15558501	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)C

MOL010168	0.8822	0.1178	0.8398	Eriobotryae Folium	5,7-dihydroxy-2-(4-hydroxyphenyl)-3-[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-chromone	15558501	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)C
MOL010169	0.7048	0.2952	0.6598	Lunulatae Herba	maoyancaosu	Not Available	FALSE	O1C(C(O)c2cc(O)c(O)cc2)COc2c1cc1c(oc(=O)cc1)c2
MOL010170	0.8683	0.1317	0.7577	Lunulatae Herba	quercetin-3-o-(2'-galloyl)-beta-d-galacopyranoside	Not Available	FALSE	O1C(C(O)C(O)C(OC(=O)c2cc(O)c(O)c(O)c2)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1)CO
MOL010171	0.9072	0.0928	0.8001	Lunulatae Herba	quercetin-3-o-beta-d-glucuronide	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1OC(C(C(C1O)O)O)C(=O)O)c1ccc(c(c1)O)O)O)O
MOL010172	0.9133	0.0867	0.8176	Lunulatae Herba	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-[(2R,3S,4R,5S,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-chromone	5320852	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1)C
MOL010173	0.7288	0.2712	0.8071	Lunulatae Herba	Saponin	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)C2(C(=CC1)C1C(C(C2)O)(C(C(C(C1)(C)C)OC(=O)/C(=C\C)/C)OC(=O)C)CO)C)(C)C=O)OC1OC(C(C(C1OC1OCC(C(C1OC1OCC(C(C1O)O)O)O)O)O)OC1(C(C(C(C(O1)CO)O)O)O)C)O)C(=O)O
MOL010174	0.3500	0.6500	0.7723	Lunulatae Herba	Saponin_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)C2(C(=CC1)C1C(C(C2)O)(C(C(C(C1)(C)C)OC(=O)/C(=C\C)/C)OC(=O)C)CO)C)(C)C=O)O

MOL010175	0.7482	0.2518	0.7320	Humulus Scandens (Lour.) Merr.	Tannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1
MOL010175	0.7482	0.2518	0.7320	Broussonetiae Fructus	Tannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1
MOL010175	0.7482	0.2518	0.7320	Sterculiae Lychnophorae Semen	Tannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1
MOL010175	0.7482	0.2518	0.7320	Menispermi Rhizoma	Tannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1
MOL010175	0.7482	0.2518	0.7320	Trollius Chinensis	Tannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1
MOL010175	0.7482	0.2518	0.7320	Sapindi Mukorossiperic Arpium	Tannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1
MOL010175	0.7482	0.2518	0.7320	Citrus Aurantium	Tannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1
MOL010175	0.7482	0.2518	0.7320	Herba Pyrolae	Tannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1

MOL010175	0.7482	0.2518	0.7320	Ilicis Purpureae Folium	Tannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1
MOL010175	0.7482	0.2518	0.7320	Gleditsiae Fructus Abnormalis	Tannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1
MOL010175	0.7482	0.2518	0.7320	Gleditsiae Spina	Tannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1
MOL010175	0.7482	0.2518	0.7320	Cortex Hibisci	Tannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1
MOL010175	0.7482	0.2518	0.7320	Radix Salviae	Tannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1
MOL010175	0.7482	0.2518	0.7320	Hordei Fructus Germinatus	Tannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1
MOL010175	0.7482	0.2518	0.7320	Radix Aconiti Kusnezoffii	Tannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1
MOL010175	0.7482	0.2518	0.7320	Smilacis Glabrae Rhixoma	Tannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1

MOL010175	0.7482	0.2518	0.7320	Mori Fructus	Tannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1
MOL010175	0.7482	0.2518	0.7320	Dioscoreaebulbiferae	Tannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1
MOL010175	0.7482	0.2518	0.7320	Areca Catechu L.	Tannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1
MOL010175	0.7482	0.2518	0.7320	Lunulatae Herba	Tannin	Not Available	FALSE	O1C(C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C(OC(=O)c2cc(OC(=O)c3cc(O)c(O)c(O)c3)c(O)c(O)c2)C1OC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1)COC(=O)c1cc(OC(=O)c2cc(O)c(O)c(O)c2)c(O)c(O)c1
MOL010176	0.4819	0.5181	0.7659	Fritillariaeussuriensis Bulbus	cordiline	Not Available	FALSE	C1C(CC2C(C1)(C1=C(CC2)C2CCC3C(C2C1O)CN1C(C3C)CCC(C1)C)C)O
MOL010177	0.4653	0.5347	0.7403	Fritillariaeussuriensis Bulbus	ebeiedine	Not Available	FALSE	OC1C2C(C3C(C4C(C3)C3=C(CC4)C(C4N(C3)CC(CC4)C)C)C1)(CCC(O)C2)C
MOL010178	0.4845	0.5155	0.6473	Fritillariaeussuriensis Bulbus	heilonine	Not Available	FALSE	N12CC(CCC1C(c1c(C2)c2c(cc1)C1C(C3(C(C(C1)O)CC(CC3)O)C)C2)C)C
MOL010180	0.5126	0.4874	0.8181	Fritillariaeussuriensis Bulbus	pingbeidinoside	Not Available	FALSE	OC1C(C2(C(C3C(C4(C(=CC3)CC(O)CC4)C)CC2)C1)C)C(O)(C(O)C1OC(OC2CCCNC2)(C(O)C(O)(C1O)C)C)C
MOL010181	0.7566	0.2434	0.7010	Fritillariaeussuriensis Bulbus	pingbeimine C	Not Available	FALSE	C1C(CC2C(C1)(C1C(C(C2=O)O)C2(C(C1)C1C(C(C2)O)C(C2N(C1)CC(CC2)C)(O)C)O)C)O
MOL010182	0.2794	0.7206	0.6900	Fritillariaeussuriensis Bulbus	pingbeininoside	Not Available	FALSE	OC1C(C2(C(C3C(C4(C(=CC3)CC(OC3OC(C(O)C(O)C3O)CO)CC4)C)CC2)C1)C)C(C1N(CC(O)(CC1)C)C)C
MOL010183	0.1758	0.8242	0.6211	Fritillariaeussuriensis Bulbus	pingbeininoside_qt	Not Available	FALSE	OC1C(C2(C(C3C(CC2)C2(CCC(O)CC2=CC3)C)C1)C)C(C1N(CC(O)(CC1)C)C)C
MOL010184	0.1758	0.8242	0.6211	Fritillariaeussuriensis Bulbus	Pingbeinine	131457	FALSE	OC1C(C2(C(C3C(C4(C(=CC3)CC(O)CC4)C)CC2)C1)C)C(C1N(CC(O)(CC1)C)C)C
MOL010185	0.7043	0.2957	0.8640	Fritillariaeussuriensis Bulbus	pingbeisaponin	Not Available	FALSE	O(C1C(OC2C(O)C(O)C(O)C(O2)C)C(O)C(O)C(O1)CO)C1CCC2(C(=CCC3C4CC5OC6(C(C5C4(C)CCC23)C)OCC(C(C6)O)C)C1)C
MOL010186	0.3518	0.6482	0.7816	Fritillariaeussuriensis Bulbus	pingbeisaponin_qt	Not Available	FALSE	OC1CCC2(C(=CCC3C4CC5OC6(C(C5C4(C)CCC23)C)OCC(C(C6)O)C)C1)C
MOL010187	0.7073	0.2927	0.6832	Fritillariaeussuriensis Bulbus	Pingpeimine A	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2O)C2(C(C1)C1C(C(C2)O)C(C2N(C1)CC(CC2)C)(O)C)O)C)O

MOL010188	0.7823	0.2177	0.6781	Fritillariaeussuriensis Bulbus	Pingpeimine B	Not Available	FALSE	C1(CC2C(CC1)(C1C(CC2O)C2(C(C1)(C1C(C(C2)O)C(C2N(C1)CC(CC2)C)(O)C)O)O)C)O
MOL010189	0.8524	0.1476	0.7357	Fritillariaeussuriensis Bulbus	Pinguisone	442388	FALSE	c12CC3(C(C(c1cco2)C)(C(=O)CC3C)C)C
MOL010191	0.6031	0.3969	0.7282	Fritillariae Pallidiflorae Bulbus	sipeimine-3β-D-glucoside	Not Available	FALSE	C12C(C3C(C2)C2C(CC3)C(C3N(C2)CC(CC3)C)(C)O)CC(=O)C2C1(CCC(C2)OC1C(O)C(O)C(O)C(O1)CO)C
MOL010191	0.6031	0.3969	0.7282	Fritillariaeussuriensis Bulbus	sipeimine-3β-D-glucoside	Not Available	FALSE	C12C(C3C(C2)C2C(CC3)C(C3N(C2)CC(CC3)C)(C)O)CC(=O)C2C1(CCC(C2)OC1C(O)C(O)C(O)C(O1)CO)C
MOL010192	0.5462	0.4538	0.7618	Fritillariae Pallidiflorae Bulbus	sipeimine-3β-D-glucoside_qt	Not Available	FALSE	C12C(C3C(C2)C2C(CC3)C(C3N(C2)CC(CC3)C)(C)O)CC(=O)C2C1(CCC(C2)O)C
MOL010192	0.5462	0.4538	0.7618	Fritillariaeussuriensis Bulbus	sipeimine-3β-D-glucoside_qt	Not Available	FALSE	C12C(C3C(C2)C2C(CC3)C(C3N(C2)CC(CC3)C)(C)O)CC(=O)C2C1(CCC(C2)O)C
MOL010193	0.6693	0.3307	0.6412	Fritillariaeussuriensis Bulbus	ussuriendine	Not Available	FALSE	OC12N3C(C(c4c1c1CC5C6(C(C(O)CC5c1cc4)CC(O)CC6)C)C)CCC(C2)C3
MOL010194	0.6410	0.3590	0.6693	Fritillariaeussuriensis Bulbus	ussuriendinone	Not Available	FALSE	OC12N3C(C(c4c1c1CC5C6(C(CC(O)CC6)C(=O)CC5c1cc4)C)C)CCC(C2)C3
MOL010195	0.5334	0.4666	0.6325	Fritillariaeussuriensis Bulbus	ussurienine	Not Available	FALSE	O(C12N3C(C(c4c1c1CC5C6(C(C(O)CC5c1cc4)CC(O)CC6)C)C)CCC(C2)C3)C
MOL010197	0.5462	0.4538	0.7618	Fritillariaeussuriensis Bulbus	verticinone	Not Available	FALSE	OC1(C2C(C3C(C4C(C3)C3(C(C(=O)C4)CC(O)CC3)C)CC2)CN2C1CCC(C2)C)C
MOL010198	0.9280	0.0720	0.9566	Sterculiae Lychnophorae Semen	(2S)-2-methylenanthic acid	6999930	FALSE	C(CCCCC)(C(=O)O)C
MOL010199	0.9221	0.0779	0.9627	Sterculiae Lychnophorae Semen	2-methyl-hexanoic acid	6999858	FALSE	C(C(=O)O)(CCCC)C
MOL010200	0.9346	0.0654	0.9639	Sterculiae Lychnophorae Semen	ARB	439764	FALSE	C1(C(C(OCC1O)O)O)O
MOL010200	0.9346	0.0654	0.9639	Bamusaeconcretiosilicea	ARB	439764	FALSE	C1(C(C(OCC1O)O)O)O
MOL010201	0.9435	0.0565	0.9547	Sterculiae Lychnophorae Semen	dimethyl 3-methyl-heptanedioate	Not Available	FALSE	C(=O)(CCCC(CC(=O)OC)C)OC
MOL010202	0.9196	0.0804	0.9499	Sterculiae Lychnophorae Semen	galactosacetic acid	Not Available	FALSE	C(C(O)C(O)C(O)C(O)CO)CC(=O)O
MOL010204	0.9313	0.0687	0.9299	Sterculiae Lychnophorae Semen	METHYL 8-NONYNOATE	23433	FALSE	C(CCCC#C)CCC(=O)OC
MOL010205	0.4897	0.5103	0.6560	Sterculiae Lychnophorae Semen	Flexricin P-1	5354133	FALSE	C(=O)(CCCCCCC/C=C\CC(O)CCCCCC)OC
MOL010207	0.9359	0.0641	0.9619	Sterculiae Lychnophorae Semen	methyl 4-methyl-hexanoate	Not Available	FALSE	C(CCC(=O)OC)(CC)C

MOL010208	0.9126	0.0874	0.9044	Sterculiae Lychnophorae Semen	methyl 8-methyl-decanoate	Not Available	FALSE	C(=O)(CCCCCCC(CC)C)OC
MOL010209	0.8910	0.1090	0.8887	Sterculiae Lychnophorae Semen	METHYL UNDECANOATE	15607	FALSE	C(CCC(=O)OC)CCCCCCC
MOL010210	0.8995	0.1005	0.9119	Sterculiae Lychnophorae Semen	trans-1-methyl-2-(2'-propenyl)cyclopropane	Not Available	FALSE	CC1C(/C=C/C)C1
MOL010211	0.2653	0.7347	0.6815	Hippophae Fructus	14,15-dimethyl-alpha-sitosterol	Not Available	FALSE	OC1C(C2C(C3C(=CC2)C2(C(C(CC2C)C(CC/C(=C/C)/C(C)C)C)(CC3)C)C)(CC1)C)C
MOL010212	0.2506	0.7494	0.6611	Hippophae Fructus	14-methyl-alpha-sitosterol	Not Available	FALSE	OC1C(C2C(C3C(=CC2)C2(C(C(CC2)C(CC/C(=C/C)/C(C)C)C)(CC3)C)C)(CC1)C)C
MOL010214	0.9309	0.0691	0.9799	Hippophae Fructus	(2S,4S)-2,4-dimethyl-1,3-dioxane	23617239	FALSE	O1C(CCOC1C)C
MOL010215	0.9133	0.0867	0.9105	Hippophae Fructus	2,6-DIMETHYL HEPTANE	14069	FALSE	C(CC(C)C)CC(C)C
MOL010216	0.8839	0.1161	0.9690	Hippophae Fructus	WLN: L6V BUTJ	13594	FALSE	O=C1CCCC=C1
MOL010218	0.8845	0.1155	0.9613	Hippophae Fructus	MBD	340	FALSE	Cc1cccc(O)c1O
MOL010219	0.8973	0.1027	0.9370	Hippophae Fructus	3-Pyridol	7971	FALSE	Oc1cccnc1
MOL010220	0.9187	0.0813	0.9216	Hippophae Fructus	4-Methylheptane	11512	FALSE	C(CCC)(CCC)C
MOL010223	0.9596	0.0404	0.9665	Hippophae Fructus	Dmbc formate	61464	FALSE	O(C(Cc1ccccc1)(C)C)C=O
MOL010224	0.9285	0.0715	0.8894	Hippophae Fructus	3-O-Ethylascorbic acid	150736	FALSE	O1C(C(O)CO)C(=C(O)C1=O)OCC
MOL010224	0.9285	0.0715	0.8894	Sapindi Mukorossiperic Arpium	3-O-Ethylascorbic acid	150736	FALSE	O1C(C(O)CO)C(=C(O)C1=O)OCC
MOL010225	0.9368	0.0632	0.9422	Hippophae Fructus	Methyl benzyl ether	10869	FALSE	O(Cc1ccccc1)C
MOL010226	0.9378	0.0622	0.9633	Hippophae Fructus	Butyl isovalerate	7981	FALSE	O(CCCC)C(=O)CC(C)C
MOL010230	0.2709	0.7291	0.6439	Hippophae Fructus	ST5330591	2723613	FALSE	O(C1CC2=CCC3C4C(C(CC4)C(CCCC(C)C)C)(CCC3C2(CC1)C)C)C(=O)c1ccccc1

MOL010231	0.8848	0.1152	0.8867	Hippophae Fructus	cis-3-Hexenyl hexoate	5352543	FALSE	O(C(=O)CCCCC)CC/C=C\CC
MOL010232	0.5107	0.4893	0.6239	Hippophae Fructus	cislycopene	56841918	FALSE	C(CC=C(C)C)/C(=C/C=C\C(=C\C=C/C(=C/C=C\C=C(\C=C/C=C(/C=C\C=C(\CCC=C(C)C)/C)\C)/C)/C)\C)/C
MOL010233	0.9313	0.0687	0.9689	Hippophae Fructus	Bis-DHA	440667	FALSE	O1C(C(O)CO)C(=O)C(=O)C1=O
MOL010234	0.5100	0.4900	0.6437	Lycii Fructus	delta-Carotene	5281230	FALSE	C1(C(C(=CCC1)C)/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C=C(/CCC=C(C)C)\C)\C)\C)/C)/C)(C)C
MOL010234	0.5100	0.4900	0.6437	Capsici Fructus	delta-Carotene	5281230	FALSE	C1(C(C(=CCC1)C)/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C=C(/CCC=C(C)C)\C)\C)\C)/C)/C)(C)C
MOL010234	0.5100	0.4900	0.6437	Hippophae Fructus	delta-Carotene	5281230	FALSE	C1(C(C(=CCC1)C)/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C=C(/CCC=C(C)C)\C)\C)\C)/C)/C)(C)C
MOL010235	0.7693	0.2307	0.8144	Hippophae Fructus	(25R)-2alpha,15beta-dihydroxy-5alpha-spirostan-3beta-yl beta-D-glucopyranosyl-(1->3)-beta-D-galactopyranosyl-(1->2)-[beta-D-xylopyranosyl-(1->3)]-beta-D-glucopyranosyl-(1->4)-beta-D-galactopyranoside	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(OC4OC(C(OC6OC(C(O)C(OC7OCC(O)C(O)C7O)C6OC6OC(C(O)C(OC7OC(C(O)C(O)C7O)CO)C6O)CO)CO)C(O)C4O)CO)C(O)C5)C)CC3)C2O)C)C(C21OCC(CC2)C)C
MOL010236	0.3637	0.6363	0.7112	Hippophae Fructus	Digitogenin	Not Available	FALSE	O1C2C(C3(C(C4C(C5(C(CC4)CC(O)C(O)C5)C)CC3)C2O)C)C(C21OCC(CC2)C)C
MOL010237	0.9543	0.0457	0.9542	Hippophae Fructus	(1R,2R,5S)-2-Isopropyl-5-methylcyclohexanol	6566020	FALSE	OC1C(CCC(C1)C)C(C)C
MOL010242	0.9091	0.0909	0.8683	Hippophae Fructus	(2R,4R)-2-phenylchroman-4-ol	6923719	FALSE	O1C(CC(O)c2c1cccc2)c1ccccc1
MOL010243	0.8226	0.1774	0.8178	Hippophae Fructus	flavane-3,4-diol	Not Available	FALSE	O1C(C(O)C(O)c2c1cccc2)c1ccccc1

MOL010244	0.8797	0.1203	0.9002	Hippophae Fructus	(2S)-Flavanone	439652	FALSE	O1C(CC(=O)c2c1cccc2)c1ccccc1
MOL010245	0.8597	0.1403	0.8515	Mahoniae Eadix	flavone	10680	TRUE	o1c(c2ccccc2)cc(=O)c2c1cccc2
MOL010245	0.8597	0.1403	0.8515	Gleditsiae Spina	flavone	10680	TRUE	o1c(c2ccccc2)cc(=O)c2c1cccc2
MOL010245	0.8597	0.1403	0.8515	Ginkgo Semen	flavone	10680	TRUE	o1c(c2ccccc2)cc(=O)c2c1cccc2
MOL010245	0.8597	0.1403	0.8515	Mahoniae Caulis	flavone	10680	TRUE	o1c(c2ccccc2)cc(=O)c2c1cccc2
MOL010245	0.8597	0.1403	0.8515	Mahoniae Folum	flavone	10680	TRUE	o1c(c2ccccc2)cc(=O)c2c1cccc2
MOL010245	0.8597	0.1403	0.8515	Hippophae Fructus	flavone	10680	TRUE	o1c(c2ccccc2)cc(=O)c2c1cccc2
MOL010246	0.8841	0.1159	0.8880	Hippophae Fructus	Flavonol	11349	FALSE	o1c(c2ccccc2)c(O)c(=O)c2c1cccc2
MOL010248	0.5002	0.4998	0.6468	Hippophae Fructus	gamma-carotene	Not Available	FALSE	C1(CCCC(=C1/C=C\C(=C\C=C\C(=C\C=C\C=C(\C=C\C=C(\C=C\C=C(\CCC=C(C)C)/C)/C)/C)\C)\C)C)(C)C
MOL010249	0.9332	0.0668	0.9664	Hippophae Fructus	gluconalgun	12702415	FALSE	O(C(CO)C)C(=O)c1ccccc1
MOL010250	0.4327	0.5673	0.6011	Hippophae Fructus	hemin	Not Available	FALSE	OC(=O)CCc1c/2=C/c3[nH]c(c(c3CCC(=O)O)C)/C=C/3\N=C(C(=C3C=C)C)/C=C/3\N=C(/C=c(\[nH]2)/c1C)C(=C3C=C)C
MOL010252	0.5891	0.4109	0.6043	Hippophae Fructus	Heptadecanal	71552	FALSE	C(CCCCCCCCCC)CCCCCC=O
MOL010253	0.9079	0.0921	0.9178	Hippophae Fructus	(Z,E)-2,4-heptadienal	6428554	FALSE	O=C/C=C\C=C\CC
MOL010254	0.8515	0.1485	0.7424	Hippophae Fructus	hippophaenin A	Not Available	FALSE	O1C(C2OC(=O)c3c(c4c(C(=O)OC2C(=O)O)cc(O)c(O)c4O)c(O)c(O)c(O)c3)C(OC(=O)c2cc(O)c(O)c(O)c2)COC(=O)c2c(c3c(C1=O)cc(O)c(O)c3O)c(O)c(O)c(O)c2
MOL010255	0.9110	0.0890	0.9119	Hippophae Fructus	Isobutyl caproate	7775	FALSE	O(CC(C)C)C(=O)CCCCC
MOL010256	0.8644	0.1356	0.8638	Hippophae Fructus	Isobutyl octanoate	79582	FALSE	O(CC(C)C)C(=O)CCCCCCC
MOL010257	0.9498	0.0502	0.9723	Hippophae Fructus	Isoamyl benzoate	7193	FALSE	O(CCC(C)C)C(=O)c1ccccc1
MOL010258	0.9177	0.0823	0.9330	Hippophae Fructus	Isoamyl caproate	16617	FALSE	O(CCC(C)C)C(=O)CCCCC
MOL010259	0.9310	0.0690	0.9592	Ephedra Herba	Apple oil	12613	FALSE	O(CCC(C)C)C(=O)CC(C)C
MOL010259	0.9310	0.0690	0.9592	Ligustici Rhizoma Et Radix	Apple oil	12613	FALSE	O(CCC(C)C)C(=O)CC(C)C
MOL010259	0.9310	0.0690	0.9592	Rhododendri Daurici Folium	Apple oil	12613	FALSE	O(CCC(C)C)C(=O)CC(C)C
MOL010259	0.9310	0.0690	0.9592	Hippophae Fructus	Apple oil	12613	FALSE	O(CCC(C)C)C(=O)CC(C)C
MOL010260	0.8862	0.1138	0.8691	Hippophae Fructus	Isoamyl octylate	16255	FALSE	O(CCC(C)C)C(=O)CCCCCCC
MOL010261	0.8764	0.1236	0.8492	Hippophae Fructus	isorhamnetin-3-O-β-rutinoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(OC)c(O)cc1)COC1OC(C(O)C(O)C1O)C
MOL010262	0.8977	0.1023	0.8170	Hippophae Fructus	isorhamnetin-3-O-galactoside	Not Available	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1OC(C(C(C1O)O)O)CO)c1cc(c(cc1)O)OC

MOL010264	0.1988	0.8012	0.6290	Hippophae Fructus	Lichesterol	5281329	FALSE	OC1CC2=CCC3=C(CCC4(C3CCC4C(C)/C=C/C(C(C)C)C)C)C2(CC1)C
MOL010265	0.9356	0.0644	0.9480	Zanthoxyli Pericarpium	cis-linalol pyranoxide	6428574	FALSE	O1C(C(O)CCC1(C)C=C)(C)C
MOL010265	0.9356	0.0644	0.9480	Hippophae Fructus	cis-linalol pyranoxide	6428574	FALSE	O1C(C(O)CCC1(C)C=C)(C)C
MOL010266	0.9246	0.0754	0.9150	Hippophae Fructus	linalool oxide B (cis-THF)	6428573	FALSE	O1C(CCC1(C)C=C)C(O)(C)C
MOL010266	0.9246	0.0754	0.9150	Ginkgo Folium	linalool oxide B (cis-THF)	6428573	FALSE	O1C(CCC1(C)C=C)C(O)(C)C
MOL010267	0.5107	0.4893	0.6239	Citri Grandis Exocarpium	LYC	446925	FALSE	C(CC=C(C)C)/C(=C/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C=C(/CCC=C(C)C)\C)\C)\C)/C)/C)/C
MOL010267	0.5107	0.4893	0.6239	Hippophae Fructus	LYC	446925	FALSE	C(CC=C(C)C)/C(=C/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C=C(/CCC=C(C)C)\C)\C)\C)/C)/C)/C
MOL010267	0.5107	0.4893	0.6239	Rose Rugosae Flos	LYC	446925	FALSE	C(CC=C(C)C)/C(=C/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C=C(/CCC=C(C)C)\C)\C)\C)/C)/C)/C
MOL010268	0.9486	0.0514	0.9198	Hippophae Fructus	D 3 (ester)	20392	FALSE	O(C(=O)c1c(cccc1)C(=O)O)C
MOL010270	0.9110	0.0890	0.9150	Hippophae Fructus	Amyl hexoate	10886	FALSE	C(=O)(OCCCCC)CCCCC
MOL010271	0.6164	0.3836	0.7377	Hippophae Fructus	propelargonidin	Not Available	FALSE	O(C1(C(C(c2c(cc(cc2O1)O)O)O)O)c1ccc(cc1)O)C1C(Oc2c(C1)c(cc(c2)O)O)c1cc(c(cc1)O)O
MOL010272	0.9372	0.0628	0.9557	Hippophae Fructus	PROPYL ISOVALERATE	11176	FALSE	C(C(=O)OCCC)C(C)C
MOL010273	0.4249	0.5751	0.8130	Hippophae Fructus	Quassin	Not Available	FALSE	O1C2C3(C(C4(C(C2)C(C=C(OC)C4=O)C)C)C(=O)C(=C(C3CC1=O)C)OC)C
MOL010274	0.2039	0.7961	0.6125	Hippophae Fructus	stigmastadienone	45109823	FALSE	C12(C(C3C(C4(C(=CC=CC4=O)CC3)C)CC2)CCC1C(CCC(C(C)C)CC)C)C
MOL010276	0.4650	0.5350	0.7771	Hippophae Fructus	(2E,4E,6E,8Z)-3,7-dimethyl-9-(2,6,6-trimethyl-1-cyclohexenyl) nona-2,4,6,8-tetraen-1-ol	11173703	FALSE	OC/C=C(/C=C/C=C(/C=C\C1=C(CCCC1(C)C)C)\C)\C
MOL010281	0.1161	0.8839	0.6286	Hippophae Fructus	vitamin E-delta	Not Available	FALSE	c1c(cc2c(c1C)OC(C(C2)CCCC(C)CCCC(C)CCCC(C)C)C)O
MOL010284	0.9421	0.0579	0.9705	Mori Fructus	(2S,3R,4S,5R)-hexane-2,3,4,5-tetrol	15140200	FALSE	CC(O)C(O)C(O)C(O)C
MOL010285	0.9080	0.0920	0.8951	Mori Fructus	1-Ethyl-2-propylcyclohexane	Not Available	FALSE	C1(C(CCCC1)CCC)CC

MOL010286	0.9413	0.0587	0.8732	Mori Fructus	IEA	10685	FALSE	c12c([nH]cc1CCO)cccc2
MOL010287	0.8947	0.1053	0.9420	Mori Fructus	WLN: T6NJ BG CQ	81136	FALSE	c1(c(nccc1)Cl)O
MOL010288	0.8975	0.1025	0.9523	Mori Fructus	3,5-Dimethylcyclopentene	59039511	FALSE	C1(CC(C=C1)C)C
MOL010289	0.9165	0.0835	0.7773	Mori Fructus	3-Allylbenzothiazoliumbromide	3347407	FALSE	c12c(sc[n+]1CC=C)cccc2
MOL010290	0.8071	0.1929	0.9512	Mori Fructus	3-Aminoacrylonitrile	5362818	FALSE	N/C=C/C#N
MOL010291	0.9225	0.0775	0.7960	Mori Fructus	3-benzofuranylmethanol	3666346	FALSE	o1cc(c2c1cccc2)CO
MOL010292	0.9235	0.0765	0.9209	Mori Fructus	3-Hydroxybenzylhydrazine	1663	FALSE	c1(cc(ccc1)O)CNN
MOL010293	0.9304	0.0696	0.9617	Mori Fructus	Methionol	10448	FALSE	C(CSC)CO
MOL010294	0.9224	0.0776	0.8874	Mori Fructus	4-(3-hydroxypropyl)phenol	82452	FALSE	C(CCc1ccc(cc1)O)O
MOL010295	0.9481	0.0519	0.9547	Mori Fructus	q-Lure	19137	FALSE	CC(=O)CCc1ccc(cc1)OC(=O)C
MOL010296	0.9060	0.0940	0.7719	Mori Fructus	4-(2,6,6-Trimethyl-1-cyclohexenl-yl)-3-buten-2-ol	Not Available	FALSE	CC(/C=C/C1C(=C(C(CC1)(C)C)C=O)C)O
MOL010297	0.9152	0.0848	0.8879	Rose Rugosae Flos	4-Ethyloctane	54176650	FALSE	C(CCCC)(CCC)CC
MOL010297	0.9152	0.0848	0.8879	Mori Fructus	4-Ethyloctane	54176650	FALSE	C(CCCC)(CCC)CC
MOL010298	0.9248	0.0752	0.9435	Mori Fructus	(2R)-4-methoxy-2,5-dimethylfuran-3-one	11815467	FALSE	C1(=C(OC(C1=O)C)C)OC
MOL010299	0.8574	0.1426	0.9629	Mori Fructus	Metacyl	12283	FALSE	c1(cc(=O)[nH]c(=O)[nH]1)C
MOL010303	0.9079	0.0921	0.8978	Mori Fructus	(2E,4E)-5-chloro-4-methylhepta-2,4-diene	13673764	FALSE	C/C=C/C(=C(\CC)/Cl)/C

MOL010304	0.8756	0.1244	0.8803	Mori Fructus	Hydroxymethyl 2-hydroxy-2-methylpropionate	547682	FALSE	O(C(=O)C(O)(C)C)CCO
MOL010305	0.9409	0.0591	0.9192	Mori Fructus	2-ethoxy-6-(methoxymethyl)phenol	586449	FALSE	O(Cc1c(c(ccc1)OCC)O)C
MOL010306	0.9310	0.0690	0.9433	Mori Fructus	Butyl acrylate	8846	FALSE	C(=O)(C=C)OCCCC
MOL010307	0.8739	0.1261	0.9637	Mori Fructus	Methylmethoxyamine	14232	FALSE	N(C)OC
MOL010308	0.9539	0.0461	0.9440	Mori Fructus	p-Menthane, trans	7459	FALSE	C1(C(C)C)CCC(CC1)C
MOL010309	0.8581	0.1419	0.9652	Bolbostemae Paniculati Bulbus	Cyt	597	FALSE	n1c(cc[nH]c1=O)N
MOL010310	0.5356	0.4644	0.8327	Bolbostemae Paniculati Bulbus	7β,18,20,26-Tetrahydroxy-20(s)-24E-dammaragonene-3-O-α-L-(3'-acetyl)-arabinopyranose-(l-2)-β-D-glucopyranoside	Not Available	FALSE	CC1(C2C(C3CCC4C(C3(C(C2)C)CO)(C)CCC4C(CC/C=C(/CO)\C)(O)C)(CCC1OC1OC(CO)C(C(C1OC1OCC(C(C1O)O)OC(=O)C)O)O)C)C
MOL010311	0.2392	0.7608	0.7190	Bolbostemae Paniculati Bulbus	7β,18,20,26-Tetrahydroxy-20(s)-24E-dammaragonene-3-O-α-L-(4'-acetyl)-arabinopyranose-(l-2)-β-D-glucopyranoside_qt	Not Available	FALSE	CC1(C2C(C3CCC4C(C3(C(C2)C)CO)(CCC4C(CC/C=C(/CO)\C)(O)C)C)(CCC1O)C)C
MOL010312	0.9574	0.0426	0.8975	Bolbostemae Paniculati Bulbus	methyl 4-[2-formyl-5-(methoxymethyl)pyrrol-1-yl]butanoate	10911621	FALSE	c1c(n(c(c1)C=O)CCCC(=O)OC)COC

MOL010313	0.8899	0.1101	0.7710	Bolbostemae Paniculati Bulbus	4-(2-formyl-5-carbooxymethyl-pyrrole-1-yl)-3-phenyl-methyl propanoate	Not Available	FALSE	c1c(n(c(c1)C=O)C(C(=O)OC)Cc1ccccc1)COC
MOL010316	0.2004	0.7996	0.6487	Bolbostemae Paniculati Bulbus	Δ7,16,25,26-stigmastatrienol	Not Available	FALSE	OC1CC2C(CC1)(C1C(=CC2)C2C(CC1)(C(=CC2)C(CCC(C(=C)C)CC)C)C)C
MOL010318	0.2075	0.7925	0.6293	Bolbostemae Paniculati Bulbus	Δ7,22,25-triene-3-ol	Not Available	FALSE	OC1CC2C(CC1)(C1C(=CC2)C2C(CC1)(C(CC2)C(/C=C/C(C(=C)C)CC)C)C)C
MOL010321	0.5627	0.4373	0.8263	Bolbostemae Paniculati Bulbus	7β,18,20,26-Tetrahydroxy-20(s)-24E-dammaragonene-3-O-α-L-(4'-acetyl)-arabinopyranose-(l-2)-β-D-glucopyranoside	Not Available	FALSE	CC1(C2C(C3CCC4C(C3(C(C2)C)CO)(C)CCC4C(CC/C=C(/CO)\C)(O)C)(CCC1OC1OC(COC(=O)C)C(C(C1OC1OCC(C(C1O)O)O)O)O)C)C
MOL010323	0.6220	0.3780	0.7866	Bolbostemae Paniculati Bulbus	7β,18,20,26-Tetrahydroxy-20(s)-24E-dammaragonene-3-O-α-L-arabinopyranose-(l-2)-β-D-(6'-acetyl)-glucopyranoside	Not Available	FALSE	CC1(C2C(C3CCC4C(C3(C(C2)C)C)(C)CCC4C(CC/C=C(/CO)\C)(O)C)(CCC1OC1OC(CO)C(C(C1OC1OCC(C(C1O)O)O)O)O)C)C
MOL010324	0.2220	0.7780	0.7352	Bolbostemae Paniculati Bulbus	7β,20,26-trihydroxy-20(s)-24E-dammaragonene-3-O-α-L-arabinopyranose-(l-2)-β-D-(6'-acetyl)-glucopyranoside_qt	Not Available	FALSE	CC1(C2C(C3CCC4C(C3(C(C2)C)C)(C)CCC4C(CC/C=C(\C)/CO)(C)O)(CCC1O)C)C

MOL010325	0.5054	0.4946	0.7996	Bolbostemae Paniculati Bulbus	7β,20,26-trihydroxy-20(s)-24E-dammaragonene-3-O-α-L-arabinopyranose-(l-2)-β-D-(6'-acetyl)-glucopyranoside	Not Available	FALSE	CC1(C2C(C3CCC4C(C3(C(C2)C)C)(C)CCC4C(CC/C=C(/CO)\C)(O)C)(CCC1OC1OC(CO)C(C(C1OC1OCC(C(C1O)OC(=O)C)O)O)O)C)C
MOL010326	0.4452	0.5548	0.7936	Bolbostemae Paniculati Bulbus	7β,20,26-trihydroxy-20(s)-24E-dammaragonene-3-O-α-L-(3'-acetyl)-arabinopyranose-(l-2)-β-D-glucopyranoside	Not Available	FALSE	CC1(C2C(C3CCC4C(C3(C(C2)C)C)(C)CCC4C(CC/C=C(/CO)\C)(O)C)(CCC1OC1OC(CO)C(C(C1OC1OCC(C(C1O)O)OC(=O)C)O)O)C)C
MOL010327	0.5598	0.4402	0.8455	Bolbostemae Paniculati Bulbus	7β,20,26-trihydroxy-20(s)-24E-dammaragonene-3-O-α-L-(4'-acetyl)-arabinopyranose-(l-2)-β-D-glucopyranoside	Not Available	FALSE	CC1(C2C(C3CCC4C(C3(C(C2)C)C=O)(C)CCC4C(CC/C=C(/CO)\C)(O)C)(CCC1OC1OC(CO)C(C(C1OC1OCC(C(C1O)OC(=O)C)O)O)O)C)C
MOL010328	0.2165	0.7835	0.7415	Bolbostemae Paniculati Bulbus	7β,20,26-trihydroxy-20(s)-24E-dammaragonene-3-O-α-L-(4'-acetyl)-arabinopyranose-(l-2)-β-D-glucopyranoside_qt	Not Available	FALSE	CC1(C2C(C3CCC4C(C3(C(C2)C)C=O)(C)CCC4C(CC/C=C(/CO)\C)(O)C)(CCC1O)C)C

MOL010329	0.5336	0.4664	0.8377	Bolbostemae Paniculati Bulbus	7β,20,26-trihydroxy-8-formyl-20(s)-24E-dammaragonene-3-O-α-L-(3'-acetyl)-arabinopyranose-(l-2)-β-D-glucopyranoside	Not Available	FALSE	CC1(C2C(C3CCC4C(C3(C(C2)C)C=O)(C)CCC4C(CC/C=C(/CO)\C)(O)C)(CCC1OC1OC(CO)C(C(C1OC1OCC(C(C1O)O)OC(=O)C)O)O)C)C
MOL010330	0.3635	0.6365	0.7307	Bolbostemae Paniculati Bulbus	7β,20,26-trihydroxy-8-formyl-20(s)-24E-dammaragonene-3-O-α-L-(4'-acetyl)-arabinopyranose-(l-2)-β-D-glucopyranoside	Not Available	FALSE	C(C1OC2OC3C(CC4(C5CC=C6C7CC(CCC7(CCC6(C5(CCC4C3(C)CO)C)C)C(=O)OC3OCC(C(C3OC3OC(C(C(C3O)OC3OCC(C(C3O)O)O)OC(=O)CC(CC(=O)OC3COC(OC2C(C1O)O)C(C3O)O)(C)O)C)O)O)(C)C)C)O)OC(=O)CCCCCCCCCCCCCCC
MOL010334	0.7300	0.2700	0.8558	Bolbostemae Paniculati Bulbus	tubeimoside IV	Not Available	FALSE	O(C1C(OC2C(O)C(O)C(O)CO2)C(O)C(O)C(O1)CO)C1CCC2(C(C1(C)C)CC(C1(CO)C3(C)CCC(C(CC/C=C(\CO)/C)(C)O)C3CCC21)O)C
MOL010335	0.4646	0.5354	0.7853	Bolbostemae Paniculati Bulbus	tubeimosideV	Not Available	FALSE	C(C1(C2C3(C4CC=C5C6CC(CCC6(CCC5(C4(CC2)C)C)C(=O)OC2OCC(C(C2OC2OC(C(C(C2O)OC2OCC(C(C2O)O)O)OC(=O)CC(CC(=O)OCC2OC(OC4C(OC1C(C3)O)OC(CO)C(C4O)O)C(C(C2O)O)O)(C)O)C)O)O)(C)C)C)O
MOL010336	0.9027	0.0973	0.9693	Bamusaeconcretiosilicea	D-Asparaginsaeure	83887	FALSE	OC(=O)C(N)CC(=O)O
MOL010337	0.6646	0.3354	0.7145	Bamusaeconcretiosilicea	Hypocrellin	Not Available	FALSE	OC1(C(c2c3c4c(C1)c(OC)c(O)c1c4c(c4c3c(c(O)c2OC)C(=O)C=C4OC)C(=CC1=O)OC)C(=O)C)C
MOL010338	0.5847	0.4153	0.6509	Bamusaeconcretiosilicea	1H-Cyclohepta(ghi)perylene-5,12-dione, 3-acetyl-6,11-dihydroxy-4,8,9,13-tetramethoxy-2-methyl-	Not Available	FALSE	O(C1=C2c3c4c(c5c6c3c(cc(OC)c6c(OC)cc5O)C(=O)C1=O)c(O)c(OC)c(c4=C(C2)C)C(=O)C)C

MOL010339	0.5943	0.4057	0.6941	Bamusaeconcretiosilicea	hypocrellin C	Not Available	FALSE	O(C1=C2c3c4c(c5c6c3c(C(=O)C1O)cc(OC)c6=C(OC)CC5=O)c(O)c(OC)c(c4=C(C2)C)C(=O)C)C
MOL010340	0.6187	0.3813	0.7088	Bamusaeconcretiosilicea	shiraiachrome A	Not Available	FALSE	OC1(C(c2c3C4=C1C=C(OC)C(=O)C4c1c4c3c(c(O)c(=O)c2OC)cc(OC)c4c(OC)cc1O)C(=O)C)C
MOL010341	0.6393	0.3607	0.6772	Bamusaeconcretiosilicea	shiraiachrome B	Not Available	FALSE	c1(O)c2C(=O)C(=C3c4c2c(c(c1)OC)c1c2c4C(=C(C(=O)c2c(cc1OC)O)OC)CC(C3C(=O)C)(O)C)OC
MOL010342	0.5888	0.4112	0.6951	Bamusaeconcretiosilicea	shiraiachrome C	Not Available	FALSE	c1(O)c2C(=O)C(=C3c4c2c(c(c1)OC)c1c2c4C(=C(C(=O)c2c(cc1OC)O)OC)CC(=C3C(=O)C)C)OC
MOL010344	0.4960	0.5040	0.7485	Sapindi Mukorossi Semen	Mukuroziside Ⅱa	Not Available	FALSE	O(C1C(OC2OC(C(O)C(O)C2O)C)C(OC(C1O)CO)OCC(CCC/C(=C/CC/C(=C/OC1OC(C(O)C(OC2OC(C(O)C(O)C2O)C)C1OC1OC(C(O)C(O)C1O)C)CO)/C)/C)C)C1OC(C(O)C(O)C1O)C
MOL010344	0.4960	0.5040	0.7485	Sapindi Mukorossiperic Arpium	Mukuroziside Ⅱa	Not Available	FALSE	O(C1C(OC2OC(C(O)C(O)C2O)C)C(OC(C1O)CO)OCC(CCC/C(=C/CC/C(=C/OC1OC(C(O)C(OC2OC(C(O)C(O)C2O)C)C1OC1OC(C(O)C(O)C1O)C)CO)/C)/C)C)C1OC(C(O)C(O)C1O)C
MOL010345	0.9017	0.0983	0.8554	Sapindi Mukorossiperic Arpium	mukuroziside Ia_qt	Not Available	FALSE	OCC(CCC/C(=C/CC/C(=C/O)/C)/C)C
MOL010345	0.9017	0.0983	0.8554	Sapindi Mukorossi Semen	mukuroziside Ia_qt	Not Available	FALSE	OCC(CCC/C(=C/CC/C(=C/O)/C)/C)C

MOL010346	0.4974	0.5026	0.7521	Sapindi Mukorossiperic Arpium	(2S,3R,4R,5R,6R)-2-[[(2R,3R,4S,5R,6R)-5-hydroxy-2-[(2Z,6E,10E)-11-[[(2R,3R,4S,5R,6R)-5-hydroxy-6-(hydroxymethyl)-3,4-bis[[(2S,3R,4R,5R,6R)-3,4,5-trihydroxy-6-methyl-2-tetrahydropyranyl]oxy]-2-tetrahydropyranyl]oxy]-2,6,10-trimethylundeca-2,6,10-trienoxy]-	21550518	FALSE	O(C1C(OC2OC(C(O)C(O)C2O)C)C(OC(C1O)CO)OC/C(=C\CC/C(=C/CC/C(=C/OC1OC(C(O)C(OC2OC(C(O)C(O)C2O)C)C1OC1OC(C(O)C(O)C1O)C)CO)/C)/C)/C)C1OC(C(O)C(O)C1O)C

MOL010346	0.4974	0.5026	0.7521	Sapindi Mukorossi Semen	(2S,3R,4R,5R,6R)-2-[[(2R,3R,4S,5R,6R)-5-hydroxy-2-[(2Z,6E,10E)-11-[[(2R,3R,4S,5R,6R)-5-hydroxy-6-(hydroxymethyl)-3,4-bis[[(2S,3R,4R,5R,6R)-3,4,5-trihydroxy-6-methyl-2-tetrahydropyranyl]oxy]-2-tetrahydropyranyl]oxy]-2,6,10-trimethylundeca-2,6,10-trienoxy]-	21550518	FALSE	O(C1C(OC2OC(C(O)C(O)C2O)C)C(OC(C1O)CO)OC/C(=C\CC/C(=C/CC/C(=C/OC1OC(C(O)C(OC2OC(C(O)C(O)C2O)C)C1OC1OC(C(O)C(O)C1O)C)CO)/C)/C)/C)C1OC(C(O)C(O)C1O)C
MOL010347	0.9085	0.0915	0.8628	Sapindi Mukorossi Semen	Mukuroziside I_qt	Not Available	FALSE	OC/C(=C\CC/C(=C/CC/C(=C/O)/C)/C)/C
MOL010347	0.9085	0.0915	0.8628	Sapindi Mukorossiperic Arpium	Mukuroziside I_qt	Not Available	FALSE	OC/C(=C\CC/C(=C/CC/C(=C/O)/C)/C)/C
MOL010348	0.5214	0.4786	0.7332	Sapindi Mukorossi Semen	mukuroziside Ia	Not Available	FALSE	O(C1C(OC2OC(C(O)C(O)C2O)C)C(OC(C1O)CO)O/C=C(/CC/C=C(/CCCC(COC1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)C)CO)C)\C)\C)C1OC(C(O)C(O)C1O)C
MOL010348	0.5214	0.4786	0.7332	Sapindi Mukorossiperic Arpium	mukuroziside Ia	Not Available	FALSE	O(C1C(OC2OC(C(O)C(O)C2O)C)C(OC(C1O)CO)O/C=C(/CC/C=C(/CCCC(COC1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)C)CO)C)\C)\C)C1OC(C(O)C(O)C1O)C
MOL010349	0.9017	0.0983	0.8554	Sapindi Mukorossiperic Arpium	Mukuroziside Ⅰa_qt	Not Available	FALSE	O/C=C(/CC/C=C(/CCCC(CO)C)\C)\C

MOL010350	0.5258	0.4742	0.7369	Sapindi Mukorossi Semen	(2S,3R,4R,5R,6R)-2-[[(2R,3R,4S,5R,6R)-2-[(1E,5E,9Z)-11-[[(2R,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[[(2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-methyl-2-tetrahydropyranyl]oxy]-2-tetrahydropyranyl]oxy]-2,6,10-trimethylundeca-1,5,9-trienoxy]-5-hydroxy-6-(	21550516	FALSE	O(C1C(OC2OC(C(O)C(O)C2O)C)C(OC(C1O)CO)O/C=C(/CC/C=C(/CC/C=C(\COC1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)C)CO)/C)\C)\C)C1OC(C(O)C(O)C1O)C

MOL010350	0.5258	0.4742	0.7369	Sapindi Mukorossiperic Arpium	(2S,3R,4R,5R,6R)-2-[[(2R,3R,4S,5R,6R)-2-[(1E,5E,9Z)-11-[[(2R,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[[(2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-methyl-2-tetrahydropyranyl]oxy]-2-tetrahydropyranyl]oxy]-2,6,10-trimethylundeca-1,5,9-trienoxy]-5-hydroxy-6-(	21550516	FALSE	O(C1C(OC2OC(C(O)C(O)C2O)C)C(OC(C1O)CO)O/C=C(/CC/C=C(/CC/C=C(\COC1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)C)CO)/C)\C)\C)C1OC(C(O)C(O)C1O)C
MOL010351	0.6885	0.3115	0.8370	Sapindi Mukorossiperic Arpium	Mukurozi-saponin E1	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1OC1OC(C(O)C(OC2OCC(OC(=O)C)C(O)C2O)C1O)C
MOL010352	0.7613	0.2387	0.8412	Sapindi Mukorossi Semen	mukurozisaponin X_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C
MOL010352	0.7613	0.2387	0.8412	Sapindi Mukorossiperic Arpium	mukurozisaponin X_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C
MOL010353	0.6592	0.3408	0.8227	Sapindi Mukorossi Semen	mukurozisaponin G	Not Available	FALSE	C1C(C(C(C(O1)OC1C(C(OC(C1O)C)OC1C(OCC(C1O)O)OC1C(C2C(CC1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)CO)O)O)OC(=O)C)OC(=O)C
MOL010353	0.6592	0.3408	0.8227	Sapindi Mukorossiperic Arpium	mukurozisaponin G	Not Available	FALSE	C1C(C(C(C(O1)OC1C(C(OC(C1O)C)OC1C(OCC(C1O)O)OC1C(C2C(CC1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)CO)O)O)OC(=O)C)OC(=O)C
MOL010354	0.7863	0.2137	0.8130	Sapindi Mukorossiperic Arpium	mukurozisaponin X	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)C)(CC2)C)(CC1)C)(CO)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)C)C

MOL010354	0.7863	0.2137	0.8130	Sapindi Mukorossi Semen	mukurozisaponin X	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)C)(CC2)C)(CC1)C)(CO)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)C)C
MOL010355	0.7708	0.2292	0.7944	Sapindi Mukorossiperic Arpium	mukurozisaponin Y1	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1OC1OC(C(O)C(OC2OCC(O)C(O)C2O)C1O)C
MOL010355	0.7708	0.2292	0.7944	Sapindi Mukorossi Semen	mukurozisaponin Y1	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1OC1OC(C(O)C(OC2OCC(O)C(O)C2O)C1O)C
MOL010356	0.7708	0.2292	0.7944	Sapindi Mukorossiperic Arpium	mukurozisaponin Y2	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1OC1OC(C(O)C(OC2OCC(O)C(O)C2O)C1O)C
MOL010356	0.7708	0.2292	0.7944	Sapindi Mukorossi Semen	mukurozisaponin Y2	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1OC1OC(C(O)C(OC2OCC(O)C(O)C2O)C1O)C
MOL010357	0.5022	0.4978	0.6855	Sapindi Mukorossiperic Arpium	Pyishiauoside Ⅰb	Not Available	FALSE	C1(C(C(OC(C1O)(C)OC1C(C(C(OC1OC/C=C(/CC/C=C(/CC/C=C(\C)/CO)\C)\C)CO)O)OC1OC(C(C(C1O)O)O)C)C)O)O
MOL010358	0.8893	0.1107	0.8362	Sapindi Mukorossiperic Arpium	Pyishiauoside Ⅰb_qt	Not Available	FALSE	OC/C=C(/CC/C=C(/CC/C=C(\C)/CO)\C)\C

MOL010359	0.6960	0.3040	0.8276	Sapindi Mukorossi Semen	(4aS,6aR,6aS,6bR,8aR,9R,10S,12aR,14bS)-10-[[(2R,3R,4S,5S,6S)-4,5-dihydroxy-6-methyl-3-[[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-2-tetrahydropyranyl]oxy]-2-tetrahydropyranyl]oxy]-9-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,	24721244	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)C)O)O)(CO)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C

MOL010359	0.6960	0.3040	0.8276	Sapindi Mukorossiperic Arpium	(4aS,6aR,6aS,6bR,8aR,9R,10S,12aR,14bS)-10-[[(2R,3R,4S,5S,6S)-4,5-dihydroxy-6-methyl-3-[[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-2-tetrahydropyranyl]oxy]-2-tetrahydropyranyl]oxy]-9-(hydroxymethyl)-2,2,6a,6b,9,12a-hexamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,	24721244	FALSE	C12(C3(C(=CCC1C1(C(CC2)C(C(CC1)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)C)O)O)(CO)C)C)C1C(CC3)(CCC(C1)(C)C)C(=O)O)C)C
MOL010360	0.7711	0.2289	0.8199	Sapindi Mukorossi Semen	Sapindoside C	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1OC1OC(C(O)C(OC2OCC(OC3OC(C(O)C(O)C3O)CO)C(O)C2O)C1O)C
MOL010360	0.7711	0.2289	0.8199	Sapindi Mukorossiperic Arpium	Sapindoside C	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1OC1OC(C(O)C(OC2OCC(OC3OC(C(O)C(O)C3O)CO)C(O)C2O)C1O)C
MOL010361	0.7613	0.2387	0.8412	Sapindi Mukorossiperic Arpium	sapindoside E_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C
MOL010361	0.7613	0.2387	0.8412	Sapindi Mukorossi Semen	sapindoside E_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C
MOL010362	0.7206	0.2794	0.7771	Sapindi Mukorossiperic Arpium	Sapindoside D	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1OC1OC(C(O)C(OC2OCC(OC3OC(C(O)C(O)C3OC3OC3OC(C(O)C(O)C3O)CO)COC3OC(C(O)C(O)C3O)C)C(O)C2O)C1O)C

MOL010362	0.7206	0.2794	0.7771	Sapindi Mukorossi Semen	Sapindoside D	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1OC1OC(C(O)C(OC2OCC(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)COC3OC(C(O)C(O)C3O)C)C(O)C2O)C1O)C
MOL010363	0.4897	0.5103	0.7569	Sapindi Mukorossiperic Arpium	sapindoside E	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OCC(O)C(O)C3OC3OC(C(O)C(OC4OCC(OC5OC(C(O)C(O)C5OC5OC(C(O)C(O)C(O)C5O)CO)COC5OC(C(O)C(O)C5O)C)C(O)C4O)C3O)C)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1OC1OC(C(O)C(OC2OCC(O)C(O)C2O)C1O)C
MOL010363	0.4897	0.5103	0.7569	Sapindi Mukorossi Semen	sapindoside E	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OCC(O)C(O)C3OC3OC(C(O)C(OC4OCC(OC5OC(C(O)C(O)C5OC5OC(C(O)C(O)C(O)C5O)CO)COC5OC(C(O)C(O)C5O)C)C(O)C4O)C3O)C)C)(CC2)C)(CC1)C)(CO)C)C1OCC(O)C(O)C1OC1OC(C(O)C(OC2OCC(O)C(O)C2O)C1O)C
MOL010364	0.4279	0.5721	0.7774	Sapindi Mukorossiperic Arpium	Sapogenin ST-1	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(O)CC(C3)(C)C)CO)C)(CC2)C)(CC1)C)(C)C
MOL010367	0.3229	0.6771	0.7725	Fritillariae Pallidiflorae Bulbus	Yibeissine	Not Available	FALSE	C1C(CC2C(C1)(C)C1C(CC2=O)C2CCC3(C(=C2C1O)C)C(C1C(CC(CN1)C)O3)C)O
MOL010368	0.1509	0.8491	0.7044	Fritillariae Pallidiflorae Bulbus	Yinyanghuo A	Not Available	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1cc(c2c(c1)C=CC(O2)(C)C)CC(O)C(=C)C)O)O
MOL010371	0.5579	0.4421	0.7560	Fritillariae Pallidiflorae Bulbus	Siraitic acid A	Not Available	FALSE	C1C(C(C23C(C1)C1(C(CC2)C2(C(CC1=O)(C(CC2)C(C)CC/C=C(/C(=O)O)\C)C)C)CO3)C)O
MOL010372	0.2144	0.7856	0.6484	Fritillariae Pallidiflorae Bulbus	valivine	Not Available	FALSE	C1(CCC2(C(=CCC3C4C(CC(C(C)C5N(CCCCC5)C)(C4(C)CCC23)O)O)C1)C)O
MOL010373	0.4955	0.5045	0.6261	Fritillariae Pallidiflorae Bulbus	yibeinoside A	Not Available	FALSE	O(C1CC2(C3C(C4C(C5C(CC4)C(C4N(C5)CC(CC4)C)C)C3)CC(=O)C2CC1)C)C1OC(C(O)C(O)C1O)CO
MOL010374	0.4412	0.5588	0.7262	Fritillariae Pallidiflorae Bulbus	yibeinoside A_qt	Not Available	FALSE	OC1CC2(C3C(C4C(C5C(CC4)C(C4N(C5)CC(CC4)C)C)C3)CC(=O)C2CC1)C
MOL010375	0.5121	0.4879	0.6820	Fritillariae Pallidiflorae Bulbus	Yibeinoside B	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2=O)C2C(C1)C1C(CC2)C(C2N(C1)CC(CC2)C)C)C)OC1OC(C(C(C1O)O)O)CO
MOL010376	0.4462	0.5538	0.7175	Fritillariae Pallidiflorae Bulbus	Yibeinoside B_qt	Not Available	FALSE	OC1CCC2(C(C1)C(=O)CC1C2CC2C1CCC1C2CN2C(C1C)CCC(C2)C)C
MOL010377	0.6437	0.3563	0.8282	Fritillariae Pallidiflorae Bulbus	Yibeinoside C	Not Available	FALSE	C1(C(C(C(C(O1)OC1C(OC(C(C1O)O)O)OC1CCC2(C(C1)C(=O)CC1C2CCC2(C1CCC2C(C)C1NCC(CC1)C)C)C)CO)O)O)O)CO
MOL010378	0.2311	0.7689	0.6699	Fritillariae Pallidiflorae Bulbus	Yibeinoside C_qt	Not Available	FALSE	OC1CCC2(C(C1)C(=O)CC1C2CCC2(C1CCC2C(C)C1NCC(CC1)C)C)C
MOL010379	0.5108	0.4892	0.6846	Polygonati Odorati Rhizoma	7'-n-butanol-N-trans-feruloyloctopamine	Not Available	FALSE	C(=C\c1cc(c(cc1)O)OC)\C(=O)NCC(c1ccc(cc1)O)OCCCC

MOL010381	0.9011	0.0989	0.9639	Polygonati Odorati Rhizoma	Azetidinecarboxylic acid	11862171	FALSE	C1CNC1C(=O)O
MOL010382	0.5355	0.4645	0.7778	Polygonati Odorati Rhizoma	Convallasaponin A	Not Available	FALSE	C1C(CC2(C(C1O)(C1C(CC2)C2C(CC1)(C1C(C2)OC2(C1C)OCC(CC2)C)C)C)O)OC1OCC(C(C1O)O)O
MOL010383	0.4015	0.5985	0.7272	Polygonati Odorati Rhizoma	Convallasaponin A_qt	Not Available	FALSE	OC1CC(O)C2(C(O)(C1)CCC1C2CCC2(C1CC1C2C(C2(OCC(C)CC2)O1)C)C)C
MOL010384	0.7000	0.3000	0.8287	Polygonati Odorati Rhizoma	3-o-beta-d-glucopyranosyl-(1-2)-[beta-d-xylopyranosyl-(1-3)]-beta-d-glucopyranosyl-(1-4)-galactopyranosyl-25(S)-spirost-5(6)-en-3beta-ol	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3CC3C1C(C1(O3)OCC(CC1)C)C)CC(CC2)OC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)CO)O)OC1C(C(C(CO1)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)O)O)C
MOL010385	0.2872	0.7128	0.7586	Polygonati Odorati Rhizoma	3-o-beta-d-glucopyranosyl-(1-2)-[beta-d-xylopyranosyl-(1-3)]-beta-d-glucopyranosyl-(1-4)-galactopyranosyl-25(S)-spirost-5(6)-en-3beta-ol_qt	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3CC3C1C(C1(O3)OCC(CC1)C)C)C)CC(CC2)O)C

MOL010386	0.7340	0.2660	0.8311	Polygonati Odorati Rhizoma	3-o-beta-d-glucopyranosyl-(1-2)-[beta-d-xylopyranosyl-(1-3)]-beta-d-glucopyranosyl-(1-4)-galactopyranosyl-25(S)-spirost-5(6)-en-3beta,14alpho-diol	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3(CC3C1C(C1(O3)OCC(CC1)C)C)O)C)CC(CC2)OC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)CO)O)OC1C(C(C(CO1)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)O)O)C
MOL010387	0.3575	0.6425	0.7312	Polygonati Odorati Rhizoma	3-o-beta-d-glucopyranosyl-(1-2)-[beta-d-xylopyranosyl-(1-3)]-beta-d-glucopyranosyl-(1-4)-galactopyranosyl-25(S)-spirost-5(6)-en-3beta,14alpho-diol_qt	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3(CC3C1C(C1(O3)OCC(CC1)C)C)O)C)CC(CC2)O)C
MOL010388	0.7340	0.2660	0.8311	Polygonati Odorati Rhizoma	25(R)spirost-5-en-3beta-ol-3-o-beta-d-glucopyranosyl-(1-2)-[beta-d-xylylpyranylosyl-(1-3)]-beta-d-glucopyranosyl-(1-4)-beta-d-galactopyranose	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3(CC3C1C(C1(O3)OCC(CC1)C)C)O)C)CC(CC2)OC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)CO)O)OC1C(C(C(CO1)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)O)O)C

MOL010389	0.3575	0.6425	0.7312	Polygonati Odorati Rhizoma	25(R)spirost-5-en-3beta-ol-3-o-beta-d-glucopyranosyl-(1-2)-[beta-d-xylylpyranylosyl-(1-3)]-beta-d-glucopyranosyl-(1-4)-beta-d-galactopyranose_qt	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3(CC3C1C(C1(O3)OCC(CC1)C)C)O)C)CC(CC2)O)C
MOL010390	0.3575	0.6425	0.7312	Polygonati Odorati Rhizoma	25(S and R)-spirost-5-en-3beta,14alpho-diol	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3(CC3C1C(C1(O3)OCC(CC1)C)C)O)C)CC(CC2)O)C
MOL010391	0.7000	0.3000	0.8287	Polygonati Odorati Rhizoma	25(R,S)spirost-5-en-3beta-ol-3-o-beta-d-glucopyranosyl-(1-2)-[beta-d-xylylpyranylosyl-(1-3)]-beta-d-glucopyranosyl-(1-4)-beta-d-galactopyranose	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3CC3C1C(C1(O3)OCC(CC1)C)C)CC(CC2)OC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)CO)O)OC1C(C(C(CO1)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)O)O)C

MOL010392	0.7476	0.2524	0.8244	Polygonati Odorati Rhizoma	25(R,S)spirost-5-ene-3beta,14alpha-diol-3-o-beta-d-glucopyranosyl-(1-2)-[beta-d-glucopyranosyl-(1-3)]-beta-d-glucopyranosyl-(1-4)-beta-d-galactopyranose	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3(CC3C1C(C1(O3)OCC(CC1)C)C)O)C)CC(CC2)OC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)CO)O)OC1C(C(C(C(O1)CO)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)O)O)C
MOL010393	0.7226	0.2774	0.8253	Polygonati Odorati Rhizoma	25(R,S)spirost-5-ene-3beta,14alpha-diol-3-o-beta-d-glucopyranosyl-(1-2)-[beta-d-xylylpyranylosyl-(1-3)]-beta-d-glucopyranosyl-(1-4)-beta-d-galactopyranose	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3CC3C1C(C1(O3)OCC(CC1)C)C)C)CC(CC2)OC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)CO)O)OC1C(C(C(C(O1)CO)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)O)C
MOL010394	0.2872	0.7128	0.7586	Polygonati Odorati Rhizoma	STOCK1N-66370	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3CC3C1C(C1(O3)OCC(CC1)C)C)C)CC(CC2)O)C
MOL010395	0.7286	0.2714	0.7769	Polygonati Odorati Rhizoma	4',5,7-trihydroxy-6-methyl-8-methoxy-homoisoflavanone	46886730	FALSE	O1CC(C(=O)c2c1c(c(c(c2O)C)O)OC)Cc1ccc(cc1)O
MOL010396	0.7506	0.2494	0.6739	Polygonati Odorati Rhizoma	4',5,7-trihydroxy-6,8-dimethyl-homoisoflavanone	46886731	FALSE	O1CC(C(=O)c2c1c(c(c(c2O)C)O)C)Cc1ccc(cc1)O

MOL010397	0.7340	0.2660	0.8311	Polygonati Odorati Rhizoma	(3beta,14alpha)-3-o-beta-d-glucopyranosyl-(1-2)-[beta-d-xylopyranosyl-(1-3)]-beta-d-glucopyranosyl(1-4)-beta-d-galacopyranosyl-14-hydroxy-(25S)-spirost-5-ene	Not Available	FALSE	C1C2C(C3(C(C1)(C1C(C3)OC3(C1C)OCC(CC3)C)C)O)CC=C1C2(CCC(C1)OC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)CO)O)OC1C(C(C(CO1)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)O)O)C
MOL010398	0.3575	0.6425	0.7312	Polygonati Odorati Rhizoma	polygosides A_qt	Not Available	FALSE	C1C2C(C3(C(C1)(C1C(C3)OC3(C1C)OCC(CC3)C)C)O)CC=C1C2(CCC(C1)O)C
MOL010399	0.7000	0.3000	0.8287	Polygonati Odorati Rhizoma	(3beta,14alpha)-3-o-beta-d-glucopyranosyl-(1-2)-[beta-d-xylopyranosyl-(1-3)]-beta-d-glucopyranosyl-(1-4)-beta-d-galacopyranosyl-yamogenin	Not Available	FALSE	C1C2C(C3C(C1)(C1C(C3)OC3(C1C)OCC(CC3)C)C)CC=C1C2(CCC(C1)OC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)CO)O)OC1C(C(C(CO1)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)O)O)C
MOL010400	0.6861	0.3139	0.8086	Polygonati Odorati Rhizoma	(22S)-sipirost-5-ene-1beta,3beta,16beta,22-tetrol-1-o-alpha-l-rhamnopyranosyl-16-o-beta-d-glucopyranoside	Not Available	FALSE	C1C2C(C3C(C1)(C(C(C3)OC1C(C(C(C(O1)CO)O)O)O)C(C(CCC(C)C)O)C)C)CC=C1C2(C(CC(C1)O)OC1OC(C(C(C1O)O)O)C)C

MOL010401	0.2960	0.7040	0.6411	Polygonati Odorati Rhizoma	(22S)-sipirost-5-ene-1beta,3beta,16beta,22-tetrol-1-o-alpha-l-rhamnopyranosyl-16-o-beta-d-glucopyranoside_qt	Not Available	FALSE	C1C2C(C3C(C1)(C(C(C3)O)C(C(CCC(C)C)O)C)C)CC=C1C2(C(CC(C1)O)O)C
MOL010402	0.7754	0.2246	0.7874	Polygonati Odorati Rhizoma	polyfuroside	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3CC3C1C(C(O3)(O)CCC(COC1C(C(C(C(O1)CO)O)O)O)C)C)C)CC(CC2)OC1OC(C(C(C1O)O)OC1OC(C(C(C1OC1C(C(C(C(O1)CO)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)O)CO)CO)C
MOL010403	0.3408	0.6592	0.7742	Polygonati Odorati Rhizoma	polyfuroside_qt	Not Available	FALSE	C12(C(=CCC3C1CCC1(C3CC3C1C(C(O3)(O)CCC(CO)C)C)C)CC(CC2)O)C
MOL010404	0.7392	0.2608	0.8423	Polygonati Odorati Rhizoma	polygosides A	Not Available	FALSE	C1C2C(C3(C(C1)(C1C(C3)OC3(C1C)OCC(CC3)C)C)O)CC=C1C2(CCC(C1)OC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O)O)C
MOL010405	0.7392	0.2608	0.8423	Polygonati Odorati Rhizoma	polygosides B	Not Available	FALSE	C1C2C(C3(C(C1)(C1C(C3)OC3(C1C)OCC(CC3)C)C)O)CC=C1C2(CCC(C1)OC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O)O)C
MOL010406	0.3575	0.6425	0.7312	Polygonati Odorati Rhizoma	polygosides B_qt	Not Available	FALSE	C1C2C(C3(C(C1)(C1C(C3)OC3(C1C)OCC(CC3)C)C)O)CC=C1C2(CCC(C1)O)C
MOL010407	0.7485	0.2515	0.7812	Polygonati Odorati Rhizoma	polygosides E	Not Available	FALSE	C1C2C(C3=CC=C(C3(C1)C)C(C(=O)CCC(COC1OC(C(C(C1O)O)O)CO)C)C)CC=C1C2(CCC(C1)OC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(CO1)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)O)C
MOL010408	0.2214	0.7786	0.6108	Polygonati Odorati Rhizoma	polygosides E_qt	Not Available	FALSE	C1C2C(C3=CC=C(C3(C1)C)C(C(=O)CCC(CO)C)C)CC=C1C2(CCC(C1)O)C
MOL010409	0.7487	0.2513	0.7911	Polygonati Odorati Rhizoma	polygosides D	Not Available	FALSE	C1C2C(C3=CC=C(C3(C1)C)C(C(=O)CCC(COC1OC(C(C(C1O)O)O)CO)C)C)CC=C1C2(CCC(C1)OC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O)O)C
MOL010410	0.9227	0.0773	0.9290	Polygonati Odorati Rhizoma	2-Methylnonan-3-one	79518	FALSE	CC(C(=O)CCCCCC)C
MOL010411	0.8844	0.1156	0.6970	Polygonati Odorati Rhizoma	4',5,7-trihydroxy-6-methyl-homoisoflavanone	Not Available	FALSE	c12c(C(=O)C(CO1)Cc1ccc(cc1)O)c(c(c(c2)O)C)O

MOL010412	0.6602	0.3398	0.8254	Polygonati Odorati Rhizoma	4'-methoxy-5,7-dihydroxy-6,8-dimethyl-homoisflavanone	Not Available	FALSE	c12c(C(=O)C(CO1)Cc1ccc(cc1)OC)c(c(c(c2C)O)C)O
MOL010413	0.9265	0.0735	0.9593	Polygonati Odorati Rhizoma	4-methyl-2-hexanone	38989048	FALSE	C(CC(=O)C)(CC)C
MOL010416	0.8561	0.1439	0.6611	Broussonetiae Fructus	methyl pentadecanoic acid	54465023	FALSE	C(CCCCCCCCCCC)CC(C(=O)O)C
MOL010417	0.7705	0.2295	0.6313	Broussonetiae Fructus	8,11-OCTADECADIENOIC ACID	5312487	FALSE	OC(=O)CCCCCC/C=C/C/C=C/CCCCCC
MOL010419	0.1225	0.8775	0.6292	Broussonetiae Fructus	8-methyltocol	92094	FALSE	O1C(CCCC(CCCC(CCCC(C)C)C)C)(CCc2c1c(cc(O)c2)C)C
MOL010421	0.7089	0.2911	0.7639	Broussonetiae Fructus	isoterihanine	6482370	FALSE	C1CC2(C3[NH+](CC4CC(C(CC4C13)O)OC)C)CC1OCOC1C2
MOL010422	0.4640	0.5360	0.6854	Broussonetiae Fructus	Methyl malvalate	283632	FALSE	C1(=C(C1)CCCCCCCC)CCCCCCC(=O)OC
MOL010423	0.9398	0.0602	0.9540	Broussonetiae Fructus	Methyl 8-oxooctanoate	535040	FALSE	C(=O)(CCCCCCC=O)OC
MOL010424	0.7703	0.2297	0.6316	Momordicae Semen	(10E,13E)-octadeca-10,13-dienoic acid	22457197	FALSE	C(=O)(CCCCCCCC/C=C/C/C=C/CCCC)O
MOL010424	0.7703	0.2297	0.6316	Broussonetiae Fructus	(10E,13E)-octadeca-10,13-dienoic acid	22457197	FALSE	C(=O)(CCCCCCCC/C=C/C/C=C/CCCC)O
MOL010425	0.8379	0.1621	0.6992	Broussonetiae Fructus	oxyavicine	Not Available	FALSE	c12c(cc3c(c1)OCO3)c1c(cc2)c2c(c(=O)n1C)cc1c(c2)OCO1
MOL010426	0.4723	0.5277	0.6089	Broussonetiae Fructus	Methyl petroselate	5362717	FALSE	C(=O)(CCCC/C=C\CCCCCCCCCC)OC
MOL010427	0.7146	0.2854	0.6655	Asteris Radix Et Rhizoma	16beta,17-dihydroxy-(-)-kauran-19-ate-beta-D-glucose ester	Not Available	FALSE	C1CC(C2C(C1)(C1C3(CC2)CC(CC1)C(C3)(O)CO)C)(C(=O)OC1C(O)C(O)C(O)C(O1)CO)C

MOL010428	0.7614	0.2386	0.8339	Asteris Radix Et Rhizoma	16beta,17-dihydroxy-(-)-kauran-19-ate-beta-D-glucose ester_qt	Not Available	FALSE	C1CC(C2C(C1)(C1C3(CC2)CC(CC1)C(C3)(O)CO)C)(C(=O)O)C
MOL010429	0.3907	0.6093	0.6974	Asteris Radix Et Rhizoma	18,19-dihydroxy-5alpha,10beta-neo-cleroda-diene-butenylhydroxyoate	15408737	FALSE	C1C=C(C2(C(C1)C(C(CC2)C)(CCC1=CCOC1=O)C)CO)CO
MOL010430	0.8705	0.1295	0.8773	Asteris Radix Et Rhizoma	(4-allyl-2,6-dimethoxy-phenyl) 3-methylbutanoate	23727651	FALSE	c1c(c(c(cc1CC=C)OC)OC(=O)CC(C)C)OC
MOL010431	0.8923	0.1077	0.9164	Asteris Radix Et Rhizoma	4-allyl-2-meth-oxyphenyl 2-methylbutanoate	Not Available	FALSE	c1c(c(ccc1CC=C)OC(=O)C(CC)C)OC
MOL010432	0.9342	0.0658	0.8982	Asteris Radix Et Rhizoma	3-(1-carbomethoxy ethenoxy)-4-hydroxy-benzoic acid	23727652	FALSE	c1(ccc(c(c1)OC(=C)C(=O)OC)O)C(=O)O
MOL010433	0.8851	0.1149	0.8731	Asteris Radix Et Rhizoma	5-(1-carboxyethenoxy)-2-hydroxybenzoic acid	23727686	FALSE	c1(cc(ccc1O)OC(=C)C(=O)O)C(=O)O
MOL010434	0.8016	0.1984	0.7264	Asteris Radix Et Rhizoma	5,6-dihydroxy-2,7,3',4'-tetramethoxyflavonol	14376225	FALSE	c1(c(c(c2c(c1)oc(c(c2=O)OC)c1cc(c(cc1)OC)OC)O)O)OC

MOL010435	0.8141	0.1859	0.7979	Asteris Radix Et Rhizoma	5,6-dihydroxy-3,7-dimethoxy-2-(4-methoxyphenyl)chromone	10043097	FALSE	c1(c(c(c2c(c1)oc(c(c2=O)OC)c1ccc(cc1)OC)O)O)OC
MOL010436	0.9331	0.0669	0.8194	Asteris Radix Et Rhizoma	(-)-angelicoidenol-2-beta-d-glucopyranoside	Not Available	FALSE	C1C(C2CC(C1(C)C2(C)C)OC1C(C(C(C(O1)CO)O)O)O)O
MOL010437	0.9636	0.0364	0.8239	Asteris Radix Et Rhizoma	64911-68-8	182459	FALSE	C1C(C2CC(C1(C)C2(C)C)O)O
MOL010438	0.9057	0.0943	0.7123	Asteris Radix Et Rhizoma	(-)-angelicoidenol-2-o-beta-apiofuranosyl-(1-6)-beta-d-glucopyranoside	Not Available	FALSE	C1C(C2CC(C1(C)C2(C)C)OC1C(C(C(C(O1)COC1C(C(CO1)(CO)O)O)O)O)O)O
MOL010439	0.9636	0.0364	0.8239	Asteris Radix Et Rhizoma	(-)-angelicoidenol-2-o-beta-apiofuranosyl-(1-6)-beta-d-glucopyranoside_qt	42150278	FALSE	C1C(C2CC(C1(C)C2(C)C)O)O
MOL010440	0.6814	0.3186	0.7747	Asteris Radix Et Rhizoma	aster saponin A	Not Available	FALSE	O1CC(C(C1OC1C(C(OC(C1O)OC1C(C(COC1OC(=O)C12C(CC3(C4(C(C5(C(C(C(C(C5)O)OC5OC(C(C(C5O)O)O)COC5OCC(C(C5O)O)O)(C)C)CC4)C)CC=C3C2CC(CC1)(C)C)C)C)O)O)O)C)OC1OCC(C(C1O)OC1OCC(C(C1O)O)O)O)O)(O)CO

MOL010441	0.7417	0.2583	0.7566	Asteris Radix Et Rhizoma	(4aR,5R,6aR,6aS,6bR,8aR,10R,11S,12aR,14bS)-5,10,11-trihydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	20055767	FALSE	OC(=O)C12C(CC3(C4(C(C5(C(C(C(C(C5)O)O)(C)C)CC4)C)CC=C3C2CC(CC1)(C)C)C)C)O
MOL010442	0.6660	0.3340	0.7707	Asteris Radix Et Rhizoma	aster saponin B	Not Available	FALSE	O1CC(C(C1OC1C(C(OC(C1O)OC1C(C(COC1OC(=O)C12C(CC3(C4(C(C5(C(C(C(CC5)OC5OC(C(C(C5O)O)O)COC5OCC(C(C5O)O)O)(C)C)CC4)C)CC=C3C2CC(CC1)(C)C)C)C)O)O)O)C)OC1OCC(C(C1O)OC1OCC(C(C1O)O)O)O)(O)CO
MOL010443	0.6737	0.3263	0.7720	Asteris Radix Et Rhizoma	aster saponin C	Not Available	FALSE	O1CC(C(C1OC1C(C(OC(C1O)OC1C(C(COC1OC(=O)C12C(CC3(C4(C(C5(C(C(C(C(C5)O)OC5OC(C(C(C5O)O)O)COC5OCC(C(C5O)O)O)(C)C)CC4)C)CC=C3C2CC(CC1)(C)C)C)C)O)O)OC1OC(C(C(C1O)O)O)C)OC1OCC(C(C1O)OC1OCC(C(C1O)O)O)O)O)(O)CO
MOL010444	0.6591	0.3409	0.7664	Asteris Radix Et Rhizoma	aster saponin D	Not Available	FALSE	O1CC(C(C1OC1C(C(OC(C1O)OC1C(C(COC1OC(=O)C12C(CC3(C4(C(C5(C(C(C(CC5)OC5OC(C(C(C5O)O)O)COC5OCC(C(C5O)O)O)(C)C)CC4)C)CC=C3C2CC(CC1)(C)C)C)C)O)O)OC1OC(C(C(C1O)O)O)C)C)OC1OCC(C(C1O)OC1OCC(C(C1O)O)O)O)O)(O)CO
MOL010445	0.7124	0.2876	0.7820	Asteris Radix Et Rhizoma	aster saponin E	Not Available	FALSE	O1CC(C(C1OC(=O)C12C(CC3(C4(C(C5(C(C(C(C5)O)OC5OC(C(C(C5O)O)O)COC5OCC(C(C5O)O)O)(C)C)CC4)C)CC=C3C2CC(CC1)(C)C)C)C)O)OC1OC(C(C(C1O)O)OC1OCC(C(C1O)OC1OCC(C(C1O)O)O)O)O)C)O)O
MOL010446	0.6987	0.3013	0.7773	Asteris Radix Et Rhizoma	aster saponin F	Not Available	FALSE	O1CC(C(C1OC(=O)C12C(CC3(C4(C(C5(C(C(CC5)OC5OC(C(C(C5O)O)O)COC5OCC(C(C5O)O)O)(C)C)CC4)C)CC=C3C2CC(CC1)(C)C)C)C)O)OC1OC(C(C(C1O)O)OC1OCC(C(C1O)OC1OCC(C(C1O)O)O)O)O)C)O)O
MOL010447	0.7590	0.2410	0.8007	Asteris Radix Et Rhizoma	aster saponin G	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(C(O)C4)(CCC(C3)(C)C)C(=O)OC3OCC(O)C(OC4OCC(O)C(O)C4O)C3OC3OC(C(O)C(O)C3O)C)C)(CC2)C)(CC1O)C)(C)C)C1OC(C(O)C(O)C1O)COC1OCC(O)C(O)C1O

MOL010448	0.7417	0.2583	0.7566	Asteris Radix Et Rhizoma	aster saponin G_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(C(O)C4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C
MOL010449	0.7722	0.2278	0.7912	Asteris Radix Et Rhizoma	asterbatanoside J	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1C(C(C(C(O1)C)O)O)OC1C(C(C(C(O1)C)O)OC1C(C(C(CO1)O)O)O)O)C)C)(C)C(=O)O)OC1C(C(C(C(O1)COC1C(C(C(C(O1)C(O)O)O)O)O)O)O)O
MOL010450	0.7229	0.2771	0.7402	Asteris Radix Et Rhizoma	asterbatanoside K_qt	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C(=O)O)O)O
MOL010451	0.7481	0.2519	0.7785	Asteris Radix Et Rhizoma	asterbatanoside K	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1C(C(C(C(O1)C)O)O)OC1C(C(C(C(O1)C)OC1C(C(C(CO1)O)O)O)OC1C(C(C(CO1)O)O)O)O)C)C)(C)C(=O)O)OC1C(C(C(C(O1)COC1C(C(C(C(O1)CO)O)O)O)O)O)O)O
MOL010453	0.7963	0.2037	0.6001	Asteris Radix Et Rhizoma	astin A	Not Available	FALSE	N12CC(C(C1C(=O)NC(C(=O)NC(C(=O)NC(CC(=O)NC(C2=O)C(O)C)c1ccccc1)CO)CC)Cl)Cl
MOL010458	0.8710	0.1290	0.8270	Asteris Radix Et Rhizoma	celereoin	Not Available	FALSE	O1C(C(O)(C)C)Cc2c1cc1oc(=O)ccc1c2O
MOL010459	0.9314	0.0686	0.9451	Asteris Radix Et Rhizoma	(e)-3,6-dihydroxymethyl-4,5-dihydroxy-2-en-octanoic acid	Not Available	FALSE	C(C(C(C(/C(=C/C(=O)O)/CO)O)O)CC)O
MOL010461	0.4429	0.5571	0.7028	Asteris Radix Et Rhizoma	epifriedelanol	12309540	FALSE	OC1C(C2(C(C3(C(C4(C(C5C(CC4)(CCC(C5)(C)C)C)(CC3)C)C)CC2)C)CC1)C)C
MOL010464	0.2988	0.7012	0.6734	Asteris Radix Et Rhizoma	(3S)-3-methyl-5-[(1S,4aS,8aS)-5,5,8a-trimethyl-2-methylidenedecahydronaphthalen-1-yl]pent-1-en-3-ol	10891602	FALSE	C1CC(C2C(C1)(C(C(=C)CC2)CCC(C=C)(O)C)C)(C)C
MOL010467	0.8929	0.1071	0.8279	Asteris Radix Et Rhizoma	Lachnophyllol acetate	5318914	FALSE	CCCC#CC#C/C=C/COC(=O)C
MOL010468	0.7679	0.2321	0.8515	Asteris Radix Et Rhizoma	Lacinilene-C-7-methyl ether	108125	FALSE	COc1c(C)cc2c(c1)C(C(=O)C=C2C(C)C)(O)C
MOL010469	0.8881	0.1119	0.7705	Asteris Radix Et Rhizoma	Oxyayanin B	442621	FALSE	O1c2c(c(=O)c(OC)c1c1cc(O)c(OC)cc1)c(O)c(O)c(OC)c2
MOL010470	0.6411	0.3589	0.7766	Asteris Radix Et Rhizoma	rabdosinatol	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CC(C13C2CCC(C(=C)C1O)C3O)O)C

MOL010471	0.9158	0.0842	0.8335	Asteris Radix Et Rhizoma	shanzhiside methyl ester	Not Available	FALSE	C1(C2C(C(=CO1)C(=O)OC)C(CC2(C)O)O)OC1C(O)C(O)C(O)C(O1)CO
MOL010472	0.9469	0.0531	0.8078	Asteris Radix Et Rhizoma	shanzhiside methyl ester_qt	Not Available	FALSE	C1(C2C(C(=CO1)C(=O)OC)C(CC2(C)O)O)O
MOL010473	0.2223	0.7777	0.6905	Asteris Radix Et Rhizoma	shionone	12315507	FALSE	O=C1C(C2(C(C3(C(C4(C(CC3)(CC(CC4)(CCC=C(C)C)C)C)C)CC2)C)CC1)C)C
MOL010474	0.8654	0.1346	0.6950	Asteris Radix Et Rhizoma	(2R,3S,4S,5R,6R)-2-[[(2R,3R,4R)-3,4-dihydroxy-4-methylol-tetrahydrofuran-2-yl]oxymethyl]-6-[[(1R,2R,4S)-3,3-dimethylnorbornan-2-yl]methoxy]tetrahydropyran-3,4,5-triol	21626476	FALSE	O1CC(C(C1OCC1OC(C(C(C1O)O)O)O)OCC1C(C2CCC1C2)(C)C)O)(O)CO
MOL010475	0.9447	0.0553	0.7969	Asteris Radix Et Rhizoma	shionoside A_qt	12302318	FALSE	OCC1C(C2CCC1C2)(C)C
MOL010476	0.8888	0.1112	0.7873	Asteris Radix Et Rhizoma	shionoside B	46881259	FALSE	O1C2(C(O)(C(C1)(CC(=O)C2)C)/C=C/C(OC1OC(C(O)C(O)C1O)CO)C)C
MOL010477	0.9058	0.0942	0.7854	Asteris Radix Et Rhizoma	shionoside B_qt	Not Available	FALSE	O1C2(C(O)(C(C1)(CC(=O)C2)C)/C=C/C(O)C)C
MOL010479	0.9447	0.0553	0.7969	Asteris Radix Et Rhizoma	shionoside C_qt	12302323	FALSE	OCC1C(C2CC1CC2)(C)C
MOL010481	0.9407	0.0593	0.7464	Arecae Semen	WLN: GR DSWR DG	6625	FALSE	S(=O)(=O)(c1ccc(cc1)Cl)c1ccc(cc1)Cl
MOL010482	0.4493	0.5507	0.8305	Arecae Semen	WLN: 6OVR BVO6	6786	FALSE	C(=O)(c1c(C(=O)OCCCCCC)cccc1)OCCCCCC
MOL010483	0.9305	0.0695	0.9069	Arecae Semen	dehydeoacetic acid	1712264	FALSE	O1C(=O)C(C(=O)C=C1C)C(=O)C
MOL010486	0.8932	0.1068	0.9435	Arecae Semen	Ethyl furoate	11980	FALSE	o1c(ccc1)C(=O)OCC
MOL010487	0.9155	0.0845	0.9676	Arecae Semen	Guvacoline	160492	FALSE	O(C(=O)C1=CCCNC1)C
MOL010488	0.8208	0.1792	0.6372	Arecae Semen	10Z-heptadecenoic acid	5312435	FALSE	C(=O)(CCCCCCCC/C=C\CCCCCC)O

MOL010489	0.9461	0.0539	0.8873	Ephedra Herba	Resivit	440833	FALSE	O1c2c(C(O)C(O)C1c1cc(O)c(O)cc1)c(O)cc(O)c2
MOL010489	0.9461	0.0539	0.8873	Arecae Semen	Resivit	440833	FALSE	O1c2c(C(O)C(O)C1c1cc(O)c(O)cc1)c(O)cc(O)c2
MOL010489	0.9461	0.0539	0.8873	Cyperi Rhizoma	Resivit	440833	FALSE	O1c2c(C(O)C(O)C1c1cc(O)c(O)cc1)c(O)cc(O)c2
MOL010489	0.9461	0.0539	0.8873	Peanut Skin	Resivit	440833	FALSE	O1c2c(C(O)C(O)C1c1cc(O)c(O)cc1)c(O)cc(O)c2
MOL010491	0.7560	0.2440	0.7510	Litchi Semen	procyanidin A1	Not Available	FALSE	C12(C(C(c3c(O1)cc(c1c3OC(C(C1)O)c1cc(c(cc1)O)O)O)c1c(O2)cc(cc1O)O)O)c1cc(c(cc1)O)O
MOL010491	0.7560	0.2440	0.7510	Arecae Semen	procyanidin A1	Not Available	FALSE	C12(C(C(c3c(O1)cc(c1c3OC(C(C1)O)c1cc(c(cc1)O)O)O)c1c(O2)cc(cc1O)O)O)c1cc(c(cc1)O)O
MOL010492	0.9500	0.0500	0.9414	Arecae Semen	Arekolin	2230	FALSE	C1(=CCCN(C1)C)C(=O)OC
MOL010493	0.7238	0.2762	0.7911	Linderae Radix	Flindersiachromone	441964	FALSE	c1(cc(=O)c2ccccc2o1)CCc1ccccc1
MOL010494	0.6567	0.3433	0.8127	Linderae Radix	DPMC	125296	FALSE	c1(cc(=O)c2c(ccc(c2o1)O)O)CCc1ccc(cc1)OC
MOL010495	0.5765	0.4235	0.8415	Linderae Radix	6,7-dimethoxy-2-(2-phenylethyl)chromone	5316872	FALSE	c1(cc(=O)c2cc(c(cc2o1)OC)OC)CCc1ccccc1
MOL010496	0.4772	0.5228	0.8424	Linderae Radix	DMPEC	195226	FALSE	c1(cc(=O)c2cc(c(cc2o1)OC)OC)CCc1ccc(cc1)OC
MOL010497	0.7870	0.2130	0.8202	Linderae Radix	6-hydroxy-2-(2-phenylethyl)chromone	5318315	FALSE	c1(cc(=O)c2cc(ccc2o1)O)CCc1ccccc1
MOL010498	0.7057	0.2943	0.8162	Linderae Radix	6-Hmpec	130350	FALSE	c1(cc(=O)c2cc(ccc2o1)O)CCc1ccc(cc1)OC
MOL010499	0.6771	0.3229	0.8391	Linderae Radix	6-methoxy-2-(2-phenylethyl)chromone	5319482	FALSE	c1(cc(=O)c2cc(ccc2o1)OC)CCc1ccccc1
MOL010500	0.5592	0.4408	0.8232	Linderae Radix	6-methoxy-2-[2-(3-methoxyphenyl)ethyl]chromone	5319468	FALSE	c1(cc(=O)c2cc(ccc2o1)OC)CCc1cc(ccc1)OC
MOL010501	0.7762	0.2238	0.7479	Linderae Radix	7,9-ditert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione	545303	FALSE	O1C(=O)CCC21C=C(C(=O)C(=C2)C(C)(C)C)C(C)(C)C
MOL010502	0.8954	0.1046	0.7607	Linderae Radix	agarotetrol	70677591	FALSE	o1c2C(O)C(O)C(O)C(O)c2c(=O)cc1CCc1ccccc1
MOL010503	0.8742	0.1258	0.8066	Linderae Radix	baimuxinal	Not Available	FALSE	OC(C1CC2(CC1)C(CCC=C2C=O)C)(C)C
MOL010504	0.9257	0.0743	0.8186	Linderae Radix	baimuxinic acid	Not Available	FALSE	OC(C1CC2(CC1)C(CCC=C2C(=O)O)C)(C)C

MOL010505	0.8337	0.1663	0.7036	Linderae Radix	2H-3,9a-Methano-1-benzoxepin-9-methanol, octahydro-2,2,5a-trimethyl-, (3R-(3alpha,5aalpha,9alpha,9aalpha))-	Not Available	FALSE	C1CCC(C23C1(CCC(C2)C(O3)(C)C)C)CO
MOL010505	0.8337	0.1663	0.7036	Smilacis Glabrae Rhixoma	2H-3,9a-Methano-1-benzoxepin-9-methanol, octahydro-2,2,5a-trimethyl-, (3R-(3alpha,5aalpha,9alpha,9aalpha))-	Not Available	FALSE	C1CCC(C23C1(CCC(C2)C(O3)(C)C)C)CO
MOL010506	0.9265	0.0735	0.9491	Linderae Radix	BUCB	8177	FALSE	C(COCCO)OCCCC
MOL010508	0.8535	0.1465	0.7886	Linderae Radix	Dihydrokaranone	177072	FALSE	O=C1C(=C(C)C)CC2(C(CCCC2=C1)C)C
MOL010509	0.8486	0.1514	0.8322	Linderae Radix	gmelofuran	Not Available	FALSE	o1c2c3C(C(C(C)C)CC(=O)c3c1)CC(C2=O)C
MOL010510	0.8954	0.1046	0.7607	Linderae Radix	isoagarotetrol	Not Available	FALSE	o1c2C(O)C(O)C(O)C(O)c2c(=O)cc1CCc1ccccc1
MOL010512	0.8288	0.1712	0.7288	Linderae Radix	2-[(2R,8R,8aS)-8,8a-dimethyl-2,3,4,6,7,8-hexahydro-1H-naphthalen-2-yl]propan-2-ol	9859337	FALSE	C1C(CCC2=CCCC(C12C)C)C(O)(C)C
MOL010513	0.8816	0.1184	0.8798	Linderae Radix	(3R)-7-hydroxy-3-isopropenyl-tetralin-5-carbaldehyde	14681764	FALSE	c1(cc(cc2CCC(Cc12)C(=C)C)O)C=O

MOL010515	0.9345	0.0655	0.8719	Linderae Radix	Phenylpropynoic acid	69475	FALSE	c1(C#CC(=O)O)ccccc1
MOL010516	0.8597	0.1403	0.7172	Linderae Radix	sinenofuranal	Not Available	FALSE	O1C23C(C(CCC(C2)C1(C)C)C)CCC3C=O
MOL010517	0.9122	0.0878	0.7055	Linderae Radix	sinenofuranol	Not Available	FALSE	C12CCC(C31OC(C(CC2C)C3)(C)C)CO
MOL010518	0.8893	0.1107	0.7625	Linderae Radix	3,4-dihydroxydihydroagarofuran	Not Available	FALSE	C1CC(C(C23C1(CCC(C(O2)(C)C)C3)C)(O)C)O
MOL010519	0.9041	0.0959	0.8946	Linderae Radix	64130-69-4	6440940	FALSE	C12=C(CCC2C(CCC1/C=C(/C(=O)O)\C)C)C
MOL010520	0.8606	0.1394	0.8907	Linderae Radix	Velleral	Not Available	FALSE	C1C(CC2C=C(C(C=C(C12)C)C=O)C=O)(C)C
MOL010521	0.8709	0.1291	0.8054	Linderae Radix	guaia-1(10),11-dien-15-al	Not Available	FALSE	O=CC1=C2C(C(CC2)C)CC(CC1)C(=C)C
MOL010522	0.9068	0.0932	0.6753	Linderae Radix	3,5-Di-t-butylphenol	70825	FALSE	C(c1cc(C(C)(C)C)cc(c1)O)(C)(C)C
MOL010523	0.8531	0.1469	0.6073	Linderae Radix	4,5,9,10-Dehydro-isolongifolene	Not Available	FALSE	C123C(=CC=CC3(C)C)C(C(C1)C=C2)(C)C
MOL010524	0.8377	0.1623	0.6908	Linderae Radix	4-hydroxydihydroagarofuran	Not Available	FALSE	C1CCC(C23C1(CCC(C(O2)(C)C)C3)C)(O)C
MOL010525	0.9103	0.0897	0.9241	Canavaliae Semen	Canavalmine	125776	FALSE	C(CNCCCCN)CNCCCCN
MOL010526	0.9033	0.0967	0.9617	Canavaliae Semen	Guanidinooxypropylamine	126170	FALSE	NCCCONC(=N)N
MOL010527	0.7721	0.2279	0.6194	Citrus Aurantium	9,10-Octadecadienoic acid	107568	FALSE	C(=O)(CCCCCCCC=C=CCCCCCCC)O
MOL010528	0.8564	0.1436	0.7051	Citrus Aurantium	humulene epoxide	Not Available	FALSE	O1C2(C1CC(C)(C)/C=C/C/C(=C\CC2)/C)C
MOL010529	0.9588	0.0412	0.9673	Citrus Aurantium	cis-jasmone	1549018	FALSE	C1(=C(CCC1=O)C)C/C=C\CC
MOL010530	0.8928	0.1072	0.9067	Citrus Aurantium	2,7-dimethylocta-2,6-diene	519299	FALSE	C(=CCCC=C(C)C)(C)C
MOL010531	0.8977	0.1023	0.7138	Nardostachyos Radix Et Rhizoma	1,1,3-trimethylindene	588777	FALSE	c12c(C(=CC1(C)C)C)cccc2
MOL010532	0.9550	0.0450	0.8591	Nardostachyos Radix Et Rhizoma	Actinidine	68231	FALSE	n1cc2c(c(c1)C)CCC2C
MOL010534	0.8799	0.1201	0.8129	Nardostachyos Radix Et Rhizoma	debilone	Not Available	FALSE	OC1CC2C(C2(C)C)C2(C1=CC(=O)CC2C)C
MOL010535	0.8445	0.1555	0.6397	Nardostachyos Radix Et Rhizoma	1,2,9,10-tetradehydroaristolane	Not Available	FALSE	C12C(C1CC=C1C2(C(CC=C1)C)C)(C)C

MOL010536	0.7954	0.2046	0.7567	Aucklandiae Radix	(3aS,6aR,9aR,9bR)-3,6,9-trimethylene-3a,4,5,6a,7,8,9a,9b-octahydroazuleno[5,4-d]furan-2-one	11673075	FALSE	O1C2C(C(=C)C1=O)CCC(=C)C1CCC(=C)C21
MOL010536	0.7954	0.2046	0.7567	Nardostachyos Radix Et Rhizoma	(3aS,6aR,9aR,9bR)-3,6,9-trimethylene-3a,4,5,6a,7,8,9a,9b-octahydroazuleno[5,4-d]furan-2-one	11673075	FALSE	O1C2C(C(=C)C1=O)CCC(=C)C1CCC(=C)C21
MOL010537	0.9089	0.0911	0.7454	Nardostachyos Radix Et Rhizoma	(1S,4R)-1,4-dimethyltetralin	12453628	FALSE	c12c(C(CCC1C)C)cccc2
MOL010538	0.3675	0.6325	0.7654	Nardostachyos Radix Et Rhizoma	[(9S)-8,8-dimethyl-2-oxo-9,10-dihydropyrano[6,5-h]chromen-9-yl] (E)-2-methylbut-2-enoate	668078	FALSE	O1C(C(OC(=O)/C(=C/C)/C)Cc2c1ccc1c2oc(=O)cc1)(C)C
MOL010539	0.8532	0.1468	0.6805	Nardostachyos Radix Et Rhizoma	nardol	Not Available	FALSE	OC1(C2C(CC1)C(=C)CCC(C2)C(C)C)C
MOL010540	0.8614	0.1386	0.7949	Nardostachyos Radix Et Rhizoma	Nardosinone	Not Available	FALSE	O1OC(C2C3(C(CCC=C3C(=O)CC12)C)C)(C)C
MOL010543	0.7934	0.2066	0.8315	Nardostachyos Radix Et Rhizoma	acaciin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(OC)cc1)COC1OC(C(O)C(O)C1O)C
MOL010545	0.9481	0.0519	0.9374	Cinnamomi Ramulus	2-Methoxycinnamic Acid	734154	FALSE	C(=O)(/C=C/c1c(cccc1)OC)O
MOL010546	0.8409	0.1591	0.7128	Cinnamomi Ramulus	ST069309	Not Available	FALSE	c12c3c4c(cc1CCCN2CCC3)cc(c(=O)o4)C(=O)O
MOL010547	0.9462	0.0538	0.9282	Cinnamomi Ramulus	2-Phenylpropenal	10312	FALSE	C(=O)C(=C)c1ccccc1

MOL010548	0.9475	0.0525	0.9498	Cinnamomi Ramulus	beta-Methoxystyrene	5368493	FALSE	c1(ccccc1)/C=C/OC
MOL010549	0.8941	0.1059	0.9594	Cinnamomi Ramulus	m-Formylphenol	101	FALSE	c1(cc(ccc1)O)C=O
MOL010550	0.8763	0.1237	0.8523	Cinnamomi Ramulus	4-Methyl-2-(1,5-dimethyl-4-hexenyl)-3-cyclohexen-1-ol	Not Available	FALSE	C1(C(C=C(CC1)C)C(CCC=C(C)C)C)O
MOL010551	0.9578	0.0422	0.8766	Ephedra Herba	DMEP	8344	FALSE	c1(c(cccc1)C(=O)OCCOC)C(=O)OCCOC
MOL010551	0.9578	0.0422	0.8766	Cinnamomi Ramulus	DMEP	8344	FALSE	c1(c(cccc1)C(=O)OCCOC)C(=O)OCCOC
MOL010552	0.9506	0.0494	0.7955	Cinnamomi Ramulus	2-Methyl-N-phenylmaleimide	689222	FALSE	N1(c2ccccc2)C(=O)C(=CC1=O)C
MOL010552	0.9506	0.0494	0.7955	Anisi Stellati Fructus	2-Methyl-N-phenylmaleimide	689222	FALSE	N1(c2ccccc2)C(=O)C(=CC1=O)C
MOL010553	0.8942	0.1058	0.8107	Cinnamomi Ramulus	β-Bisabolene	13677920	FALSE	c1(ccccc1)C(=C)CCC=C(C)C
MOL010554	0.8945	0.1055	0.8224	Cinnamomi Ramulus	694-87-1	69667	FALSE	c12c(CC1)cccc2
MOL010554	0.8945	0.1055	0.8224	Eucommiae Folium	694-87-1	69667	FALSE	c12c(CC1)cccc2
MOL010555	0.8237	0.1763	0.8332	Cinnamomi Ramulus	1,2-Dibenzoylethane	136322	FALSE	c1(C(=O)CCC(=O)c2ccccc2)ccccc1
MOL010556	0.8945	0.1055	0.9101	Cinnamomi Ramulus	WLN: BVO2R	7194	FALSE	C(=O)(c1ccccc1)OCCc1ccccc1
MOL010557	0.9479	0.0521	0.9514	Cinnamomi Ramulus	WLN: 2OVR	7165	FALSE	C(=O)(c1ccccc1)OCC
MOL010557	0.9479	0.0521	0.9514	Caryophylliflos	WLN: 2OVR	7165	FALSE	C(=O)(c1ccccc1)OCC
MOL010557	0.9479	0.0521	0.9514	Allii Fistulost Bulbus	WLN: 2OVR	7165	FALSE	C(=O)(c1ccccc1)OCC
MOL010558	0.9481	0.0519	0.9374	Cinnamomi Ramulus	Substance H 36	1622530	FALSE	C(=O)(/C=C\c1c(cccc1)OC)O
MOL010559	0.9471	0.0529	0.9324	Cinnamomi Ramulus	2-Coumarinate	5280841	FALSE	C(=O)(/C=C\c1c(cccc1)O)O
MOL010560	0.9440	0.0560	0.9650	Cinnamomi Ramulus	WLN: VHO2R	7711	FALSE	c1(CCOC=O)ccccc1
MOL010561	0.9594	0.0406	0.9122	Cinnamomi Ramulus	2-Methoxyphenylacetone	78887	FALSE	c1(c(cccc1)OC)CC(=O)C
MOL010562	0.9337	0.0663	0.9533	Cinnamomi Ramulus	Hydro Cinnamicacid	Not Available	FALSE	C(=O)(/C=C/C1C=CC=CC1)O
MOL010563	0.9315	0.0685	0.9122	Cinnamomi Ramulus	Methyl (Z)-cinnamate	6428458	FALSE	C(=O)(/C=C\c1ccccc1)OC
MOL010564	0.9022	0.0978	0.9619	Sargassum	NK	6998	FALSE	c1(c(cccc1)O)C=O

MOL010564	0.9022	0.0978	0.9619	Cinnamomi Ramulus	NK	6998	FALSE	c1(c(cccc1)O)C=O
MOL010564	0.9022	0.0978	0.9619	Solidaginis Herba	NK	6998	FALSE	c1(c(cccc1)O)C=O
MOL010565	0.8822	0.1178	0.8487	Kadsurae Coccineae Radix Et Caulis	Carmine	14749	FALSE	c12c(C(=O)c3c(C1=O)c(c(c(c3)O)C(=O)O)C)c(c(c(c2O)C1OC(C(C(C1O)O)O)CO)O)O
MOL010566	0.4687	0.5313	0.6240	Kadsurae Coccineae Radix Et Caulis	kadsuric acid	Not Available	FALSE	C(=O)(CCC1(C(C(=C)C)CCC2C3(C)CCC(C(CC/C=C(\C(=O)O)/C)C)C3(C)CC=C12)C)O
MOL010567	0.5118	0.4882	0.7534	Kadsurae Coccineae Radix Et Caulis	acetoxyl oxokadsurane	Not Available	FALSE	O1CC23c4c(C(OC(=O)C)C(C(CC2=CC(=C(OC)C3=O)OC)C)C)cc2OCOc2c14
MOL010568	0.9278	0.0722	0.9460	Kadsurae Coccineae Radix Et Caulis	2-Methylheptan-3-one	25611	FALSE	C(=O)(C(C)C)CCCC
MOL010569	0.4902	0.5098	0.7167	Kadsurae Coccineae Radix Et Caulis	neokadsuranin	Not Available	FALSE	O1C2C(C(C1c1c(c3c2cc2OCOc2c3OC)c(OC)c(OC)c(OC)c1)C)C
MOL010570	0.4788	0.5212	0.6282	Kadsurae Coccineae Radix Et Caulis	seco-coccinic acid E	24896697	FALSE	OC(CCC(C1C2(C(C3=CCC(C(C3CC2)(CCC(=O)O)C)C(=C)C)(CC1)C)C)C)C(=C)C
MOL010571	0.4093	0.5907	0.6840	Kadsurae Coccineae Radix Et Caulis	acetylbinankadsurin A	Not Available	FALSE	O1COc2c1c(c1c(c2)C(C(C(Cc2c1c(c(c2)OC)OC)O)C)C)OC(=O)C)OC
MOL010573	0.1680	0.8320	0.6901	Kadsurae Coccineae Radix Et Caulis	benzoyl oxokadsurane	Not Available	FALSE	O1CC23c4c(C(OC(=O)c5ccccc5)C(C(CC2=CC(=C(OC)C3=O)OC)C)C)cc2OCOc2c14
MOL010574	0.8940	0.1060	0.8096	Sargassum	OBT	13625	FALSE	s1c(=O)[nH]c2c1cccc2
MOL010575	0.9361	0.0639	0.8475	Sargassum	2,3-dihydro-1H-quinolin-4-one	117158	FALSE	N1CCC(=O)c2ccccc12
MOL010576	0.9182	0.0818	0.8644	Sargassum	4-hydroxy-3H-2-benzofuran-1-one	12662077	FALSE	c12c(C(=O)OC1)cccc2O
MOL010577	0.8683	0.1317	0.6011	Sargassum	ZINC04026398	Not Available	FALSE	OC1(C2C(C3C(C2)(C(CC3)C)CC1)(C)C)C
MOL010579	0.8766	0.1234	0.8060	Sargassum	alginic acid	Not Available	FALSE	O(C1C(O)C(O)C(OC1C(=O)O)OC)C1OC(C(OC)C(O)C1O)C(=O)O
MOL010580	0.7223	0.2777	0.8517	Sargassum	Diglycol dibenzoate	8437	FALSE	C(COCCOC(=O)c1ccccc1)OC(=O)c1ccccc1
MOL010585	0.2752	0.7248	0.6315	Radix Euphorbiae Pekinensis	Daucosterol_qt	Not Available	FALSE	OC1CC2=CCC3C(C2(CC1)C)(CCC1(C3CCC1C(CCC(C(C)C)CC)C)C)C
MOL010586	0.8926	0.1074	0.9120	Radix Euphorbiae Pekinensis	Formononetin	46881075	FALSE	c1(ccc2c(c1)OCC(C2=O)c1ccc(cc1)OC)O
MOL010587	0.6262	0.3738	0.6789	Radix Euphorbiae Pekinensis	trifohrhizin 6'-monoacetate	Not Available	FALSE	c12c(cc3c(c1)C1C(C3)c3c(OC1)cc(cc3)CC1OC(C(C(C1O)O)O)COC(=O)C)OCO2
MOL010588	0.5013	0.4987	0.7652	Radix Euphorbiae Pekinensis	d-Pinoresinol	12309637	FALSE	c1cc(cc(c1O)OC)C1OCC2C1COC2c1cc(c(cc1)O)OC

MOL010589	0.1019	0.8981	0.6441	Radix Euphorbiae Pekinensis	Isokurarinone	Not Available	FALSE	c12c(c(c(cc1O)O)CC(CC=C(C)C)C(=C)C)C(=O)CC(O2)c1ccc(cc1OC)O
MOL010591	0.9185	0.0815	0.8635	Paederiae Scandentis Herba	(7S)-7-methyl-6,7-dihydro-5H-cyclopenta[b]pyrazine	6931359	FALSE	c12c(nccn2)CCC1C
MOL010592	0.9109	0.0891	0.8233	Paederiae Scandentis Herba	Asperulosidic acid	11968867	FALSE	O(C1OC=C(C2C1C(=CC2O)COC(=O)C)C(=O)O)C1OC(C(O)C(O)C1O)CO
MOL010593	0.9442	0.0558	0.8175	Paederiae Scandentis Herba	asperulosidic acid_qt	Not Available	FALSE	OC1OC=C(C2C1C(=CC2O)COC(=O)C)C(=O)O
MOL010594	0.5042	0.4958	0.7479	Paederiae Scandentis Herba	(2S,3S)-2-(4-hydroxy-3-methoxy-phenyl)-5-methoxy-3-methylol-2,3-dihydropyrano[5,6-h][1,4]benzodioxin-9-one	11982428	FALSE	O1C(C(Oc2c1c1oc(=O)ccc1cc2OC)CO)c1cc(OC)c(O)cc1
MOL010595	0.8922	0.1078	0.8936	Paederiae Scandentis Herba	Octatrienal	5283331	FALSE	C(=O)/C=C/C=C/C=C/C
MOL010596	0.9215	0.0785	0.9668	Paederiae Scandentis Herba	2-methylbut-2-en-1-ol	6433417	FALSE	C(/C(=C/C)/C)O
MOL010598	0.9256	0.0744	0.9404	Paederiae Scandentis Herba	Hexylbenzoate	23235	FALSE	c1(C(=O)OCCCCCC)ccccc1
MOL010599	0.8084	0.1916	0.7865	Paederiae Scandentis Herba	Isobutyl decanoate	121738	FALSE	C(C(=O)OCC(C)C)CCCCCCCC
MOL010600	0.8612	0.1388	0.8103	Paederiae Scandentis Herba	linalyl isobutyrate	36690114	FALSE	C(OC(=O)C(C)C)(CCC=C(C)C)(C=C)C
MOL010601	0.7472	0.2528	0.7763	Paederiae Scandentis Herba	2α-hydroxyursolic acid	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3C)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C
MOL010602	0.8932	0.1068	0.8948	Paederiae Scandentis Herba	methyl propyl carbonate	10129937	FALSE	C(=O)(OCCC)OC
MOL010603	0.8554	0.1446	0.6220	Paederiae Scandentis Herba	Paederoside	Not Available	FALSE	S(C(=O)OCC1=CC2OC(=O)C3=COC(OC4OC(C(O)C(O)C4O)CO)C1C23)C
MOL010604	0.8972	0.1028	0.7124	Paederiae Scandentis Herba	paederoside_qt	Not Available	FALSE	S(C(=O)OCC1=CC2OC(=O)C3=COC(O)C1C23)C
MOL010605	0.8423	0.1577	0.6802	Paederiae Scandentis Herba	paederosidic acid methyl ester	Not Available	FALSE	S(C(=O)OCC1=CC(O)C2C1C(OC1OC(C(O)C(O)C1O)CO)OC=C2C(=O)OC)C

MOL010606	0.9134	0.0866	0.6391	Paederiae Scandentis Herba	paederosidic acid methyl ester_qt	Not Available	FALSE	S(C(=O)OCC1=CC(O)C2C1C(O)OC=C2C(=O)OC)C
MOL010607	0.8759	0.1241	0.9555	Paederiae Scandentis Herba	3,4-dimethylcyclopent-2-en-1-one	637895	FALSE	C1(=O)C=C(C(C1)C)C
MOL010609	0.9584	0.0416	0.8650	Paederiae Scandentis Herba	S(-)-Secobarbital	30019	FALSE	C1(C(=O)NC(=O)NC1=O)(C(CCC)C)CC=C
MOL010610	0.9308	0.0692	0.9549	Eriobotryae Folium	2-Hexenol	5318042	FALSE	C(/C=C/CCC)O
MOL010610	0.9308	0.0692	0.9549	Thalluslaminariae	2-Hexenol	5318042	FALSE	C(/C=C/CCC)O
MOL010610	0.9308	0.0692	0.9549	Ephedra Herba	2-Hexenol	5318042	FALSE	C(/C=C/CCC)O
MOL010610	0.9308	0.0692	0.9549	Campsis Flos	2-Hexenol	5318042	FALSE	C(/C=C/CCC)O
MOL010610	0.9308	0.0692	0.9549	Amygdalus Communis Vas	2-Hexenol	5318042	FALSE	C(/C=C/CCC)O
MOL010611	0.7222	0.2778	0.7563	Thalluslaminariae	4-(3,5-dihydroxyphenoxy)-9-[6-(3,5-dihydroxyphenoxy)-2,4,7,9-tetrahydroxyoxanthren-1-yl]oxanthrene-1,3,6,8-tetrol	137388	FALSE	O1c2c(Oc3c1c(c(cc3O)O)Oc1cc(cc(c1)O)O)c(c(cc2O)O)c1c2c(Oc3c(O2)c(cc(c3Oc2cc(cc(c2)O)O)O)O)c(cc1O)O
MOL010612	0.7641	0.2359	0.7580	Thalluslaminariae	9-(3,5-dihydroxyphenoxy)-2-[9-(3,5-dihydroxyphenoxy)-1,3,6,8-tetrahydroxyoxanthren-2-yl]oxanthrene-1,3,6,8-tetrol	3008867	FALSE	O1c2c(Oc3c1c(cc(c3Oc1cc(cc(c1)O)O)O)O)c(c(c(c2)O)c1c(c2c(Oc3c(O2)c(c(cc3O)O)Oc2cc(cc(c2)O)O)cc1O)O)O
MOL010613	0.9080	0.0920	0.9328	Thalluslaminariae	Felosan	64950	FALSE	c1c(cccn1)C(=O)NC
MOL010614	0.9029	0.0971	0.9201	Thalluslaminariae	gamma-Glu-ala-gly	5489007	FALSE	C(=O)(CNC(=O)C(NC(=O)CCC(C(=O)O)N)C)O
MOL010616	0.8302	0.1698	0.7582	Thalluslaminariae	eckol	145937	FALSE	O1c2c(Oc3c1c(cc(c3)O)O)c(cc(c2Oc1cc(cc(c1)O)O)O)O
MOL010618	0.9211	0.0789	0.9199	Thalluslaminariae	(E)-5-Decenol	5283292	FALSE	C(CCC/C=C/CCCC)O
MOL010619	0.9147	0.0853	0.8966	Thalluslaminariae	laminine	440121	FALSE	C(CCCC(C(=O)O)N)[N+](C)(C)C

MOL010620	0.7743	0.2257	0.7174	Thalluslaminariae	Phlorofucofuroeckol A	130976	FALSE	O1c2c(Oc3c1c(cc1c3c3c(o1)c(c(cc3O)O)Oc1cc(cc(c1)O)O)O)c(cc(c2Oc1cc(cc(c1)O)O)O)O
MOL010621	0.9044	0.0956	0.9086	Thalluslaminariae	2,4-octadienal	5283329	FALSE	C(=O)/C=C/C=C/CCC
MOL010622	0.7700	0.2300	0.6369	Thalluslaminariae	Stearidonic acid	5312508	FALSE	C(=O)(CCCC/C=C\C/C=C\C/C=C\C/C=C\CC)O
MOL010623	0.4352	0.5648	0.7176	Thalluslaminariae	FRIEDELIN	Not Available	FALSE	C1C(=O)C(C2(C(C1)C1(C(CC2)(C2(C(CC1)(C1C(CC2)(CCC(C1)(C)C)C)C)C)C)C)C)C
MOL010624	0.9248	0.0752	0.9219	Thalluslaminariae	2,6-nonadienal	636687	FALSE	C(=O)/C=C/CC/C=C/CC
MOL010624	0.9248	0.0752	0.9219	Campsis Flos	2,6-nonadienal	636687	FALSE	C(=O)/C=C/CC/C=C/CC
MOL010625	0.2212	0.7788	0.6482	Thalluslaminariae	24-Methylenecholesterol	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1)C)CCC1(C3CCC1C(CCC(=C)CC(C)C)C)C)O
MOL010626	0.6704	0.3296	0.7634	Thalluslaminariae	89079-38-9	16132364	FALSE	c1(cc(cc(c1)O)Oc1c(cc(c2c1Oc1c(O2)c(c(cc1O)O)c1c2Oc3c(Oc2c(cc1O)O)c(c(cc3O)Oc1c(cc(cc1O)O)O)Oc1cc(cc(c1)O)O)O)O)O
MOL010627	0.5932	0.4068	0.6751	Meliae Cortex	(+)-Syringaresinol-di-O-β-D-glucosid	Not Available	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(OC3OC(C(O)C(O)C3O)CO)c(OC)c2)C1)c1cc(OC)c(OC2OC(C(O)C(O)C2O)CO)c(OC)c1
MOL010628	0.5284	0.4716	0.6200	Meliae Cortex	(+)-Syringaresinol-di-O-β-D-glucosid _qt	12309695	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(O)c(OC)c2)C1)c1cc(OC)c(O)c(OC)c1
MOL010629	0.7596	0.2404	0.6767	Meliae Cortex	4,8-dimethoxy-1-vinyl-beta-carboline	5318875	FALSE	c1cc2c(c(c1)OC)[nH]c1c2c(cnc1C=C)OC
MOL010630	0.9467	0.0533	0.8405	Meliae Cortex	isosclerone	13369486	FALSE	C1(=O)CCC(c2cccc(c12)O)O
MOL010631	0.2377	0.7623	0.7976	Meliae Cortex	kulactone	Not Available	FALSE	O1C2C(C3(C(C4=CCC5C(C4CC3)(CCC(=O)C5(C)C)C)(C2)C)C)C(C1=O)CCC=C(C)C
MOL010632	0.1992	0.8008	0.7729	Meliae Cortex	kulinone	Not Available	FALSE	OC1C(C2(C(C3=CCC4C(C3CC2)(CCC(=O)C4(C)C)C)(C1)C)C)C(CCC=C(C)C)C
MOL010633	0.2687	0.7313	0.8004	Meliae Cortex	kulolactone	Not Available	FALSE	O1C2C(C3(C(C4=CCC5C(C4CC3)(CCC(O)C5(C)C)C)(C2)C)C)C(C1=O)CCC=C(C)C
MOL010634	0.9136	0.0864	0.9606	Meliae Cortex	D-Gulonic acid	152304	FALSE	OC(C(O)C(O)C(=O)O)C(O)CO
MOL010635	0.5642	0.4358	0.7186	Meliae Cortex	meliacarpinin C	Not Available	FALSE	O1C2C(C3C4(C5C2OCC5(C(OC(=O)/C(=C/C)/C)CC4OC(=O)C)C)COC3(OC)C(=O)OC)(C2(O)C1(C1CC2OC2OC=CC12O)C)C
MOL010636	0.2689	0.7311	0.6602	Meliae Cortex	melianotriol	Not Available	FALSE	O1C(O)C(C2C3(C(C4=CCC5C(C4CC3)(CCC(O)C5(C)C)C)(CC2)C)C)CC1C(O)C(O)(C)C

MOL010637	0.9325	0.0675	0.9658	Meliae Cortex	Dimethyl malonate	7943	FALSE	O(C(=O)CC(=O)OC)C
MOL010638	0.1047	0.8953	0.7625	Meliae Cortex	nimbolin A	Not Available	FALSE	O1C2C3C(C4C(C2OC(=O)/C=C/c2ccccc2)(C2=CCC(C2(CC4)C)c2ccoc2)C)(C(OC(=O)C)CC(OC(=O)C)C3(C1)C)C
MOL010639	0.1328	0.8672	0.8217	Meliae Cortex	nimbolin B	Not Available	FALSE	O1C2C3C(C4C(C2OC(=O)/C=C/c2ccccc2)(C2=C(C(CC2OC(O)C4)c2ccoc2)C)C)(C(OC(=O)C)CC(OC(=O)C)C3(C1)C)C
MOL010641	0.1012	0.8988	0.8415	Meliae Cortex	Ohchinolide B	Not Available	FALSE	O1CC2(C3C1C(C1(C(C3(C(CC2OC(=O)C)OC(=O)C)C)CC(=O)OC2C1=C(C(C2)c1cocc1)C)C)OC(=O)/C(=C/C)/C)C
MOL010642	0.0901	0.9099	0.8345	Meliae Cortex	Ohchinolide C	Not Available	FALSE	O1C2C3C(C4C(C2OC(=O)/C(=C/C)/C)(C2=C(C(CC2OC(=O)C4)c2ccoc2)C)C)(C(OC(=O)C)CC(OC(=O)C(C)C)C3(C1)C)C
MOL010643	0.2185	0.7815	0.7557	Meliae Cortex	sendanolactone	Not Available	FALSE	C1(=O)C(C2C(O1)CC1C2CCC2C1=CC(=O)C1C2CCC(=O)C1)CCC=C(C)C
MOL010644	0.6372	0.3628	0.6656	Meliae Cortex	toosendain	Not Available	FALSE	O1C23C4(C(C56C(CC4O)C(C(OC(=O)C)CC5O)(C(OC6)O)C)C(=O)C(OC(=O)C)C2(C(CC13)c1ccoc1)C)C
MOL010645	0.2838	0.7162	0.7586	Meliae Cortex	toosendanone A	Not Available	FALSE	C12(C(C3=CCC4C(C3CC2)(CCC(=O)C4(C)C)C)(CC(C1C1C(C(CC1)C(O)(C)C)O)O)C)C
MOL010646	0.4785	0.5215	0.7087	Meliae Cortex	trichilin A	Not Available	FALSE	O1C23C4(C(C56C(C(C(OC(=O)C)C(OC(=O)C)C5O)(C(OC6)OC(=O)C(CC)C)C)CC4O)C(=O)C(O)C2(C(CC13)c1cocc1)C)C
MOL010647	0.1157	0.8843	0.7988	Meliae Cortex	trichilinin B	Not Available	FALSE	O1CC2(C3C1C(C1(C(C3(C(CC2OC(=O)C)OC(=O)/C(=C/C)/C)C)CC(C2(C1=CCC2c1cocc1)C)OC(=O)C)C)O)C
MOL010648	0.1981	0.8019	0.7766	Meliae Cortex	trichilinin D	Not Available	FALSE	O1CC2(C3C1C(C1(C(C3(C(CC2O)OC(=O)/C=C\c2ccccc2)C)CC(C2(C1=CCC2c1cocc1)C)OC(=O)C)C)O)C
MOL010649	0.1856	0.8144	0.7658	Meliae Cortex	(3R,6S)-3-[(5R,9R,10R,13S,14S,16S,17S)-16-hydroxy-4,4,10,13,14-pentamethyl-3-oxo-1,2,5,6,9,11,12,15,16,17-decahydrocyclopenta[a]phenanthren-17-yl]-6-prop-1-en-2-yloxan-2-one	10950762	FALSE	OC1C(C2(C(C(C3=CCC4C(C3CC2)(CCC(=O)C4(C)C)C)(C1)C)C)C1CCC(OC1=O)C(=C)C

MOL010650	0.2537	0.7463	0.7643	Meliae Cortex	SMR000232316	Not Available	FALSE	C123C4(C(C5(C(CC4OC(=O)C)C(C(=O)C=C5)(C)C)C)CCC1(C(c1ccoc1)OC(=O)C2O3)C)C
MOL010651	0.8834	0.1166	0.9663	Meliae Azedarach Fructus	3-Cycloheptenone	70722	FALSE	O=C1CCCC=CC1
MOL010652	0.8791	0.1209	0.9083	Meliae Azedarach Fructus	3-Thiotolene	12024	FALSE	c1(ccsc1)C
MOL010654	0.5769	0.4231	0.6142	Meliae Azedarach Fructus	9-OCTADECENAL	5283381	FALSE	C(=O)CCCCCCC/C=C/CCCCCCCC
MOL010655	0.6395	0.3605	0.6568	Meliae Azedarach Fructus	azadirachtin	Not Available	FALSE	C123C(C(OC3)(OC3(C1(C1CC3C3(C(O1)OC=C3)O)O)C)C(=O)OC)C1(C3C(C2O)OCC3(C(CC1OC(=O)/C(=C/C)/C)OC(=O)C)C(=O)OC)C
MOL010656	0.8598	0.1402	0.6769	Meliae Azedarach Fructus	Bicyclogermacrene	Not Available	FALSE	C12/C=C(\CC/C=C(\CCC1C2(C)C)/C)/C
MOL010657	0.1714	0.8286	0.8000	Meliae Azedarach Fructus	meldenin	Not Available	FALSE	O(C1C2C(C3C(C1O)C1=CCC(C1(CC3)C)c1ccoc1)(CCC(=O)C2(C)C)C)C(=O)C
MOL010658	0.2051	0.7949	0.7776	Meliae Azedarach Fructus	melialactone	Not Available	FALSE	OC1C2(C(C3(C(C1)C(C(O)CC3)(C)C)C)CCC1(C2CCC1C1CC(OC1=O)CC(C)C)C)C
MOL010659	0.2320	0.7680	0.6837	Meliae Azedarach Fructus	melianodiol	Not Available	FALSE	O1C(O)C(C2C3(C(C4=CCC5C(C4CC3)(CCC(=O)C5(C)C)C)(CC2)C)C)CC1C(O)C(O)(C)C
MOL010660	0.2237	0.7763	0.7800	Meliae Azedarach Fructus	melianol	Not Available	FALSE	O1C(O)C(C2C3(C(C4=CCC5C(C4CC3)(CCC(O)C5(C)C)C)(CC2)C)C)CC1C1OC1(C)C
MOL010661	0.1938	0.8062	0.7828	Meliae Azedarach Fructus	melianone	Not Available	FALSE	O1C(O)C(C2C3(C(C4=CCC5C(C4CC3)(CCC(=O)C5(C)C)C)(CC2)C)C)CC1C1OC1(C)C
MOL010662	0.4844	0.5156	0.8852	Meliae Azedarach Fructus	melianoninol	Not Available	FALSE	O1C(C(c2c1ccc(OC)c2)CO)c1c(OC)cc(C(O)c1)/C=C\C=O
MOL010663	0.0837	0.9163	0.8195	Meliae Azedarach Fructus	salannin	Not Available	FALSE	C12(C(C3(C4C(C1OC1C2=C(C(C1)c1ccoc1)C)OCC4(C(CC3OC(=O)/C(=C/C)/C)OC(=O)C)C)C)CC(=O)OC)C
MOL010664	0.8525	0.1475	0.7799	Meliae Azedarach Fructus	Tetradecanol	36690390	FALSE	C(CCC(CC(C)C)O)(CCCC)CC
MOL010665	0.9310	0.0690	0.9622	Meliae Azedarach Fructus	ZINC02037591	6999854	FALSE	C(CCC)(C=C)O
MOL010666	0.8998	0.1002	0.8810	Raphani Semen	1,1-DIMETHOXY-2-METHYLPROPANE	15619	FALSE	C(C(C)C)(OC)OC
MOL010667	0.8944	0.1056	0.9517	Raphani Semen	1,3-DIMETHYLCYCLOHEXANE (TRANS)	16629	FALSE	C1C(CCCC1C)C
MOL010668	0.9409	0.0591	0.9624	Raphani Semen	4-butoxybutan-1-ol	20111	FALSE	C(CCCOCCCC)O
MOL010669	0.8764	0.1236	0.8268	Raphani Semen	4-Tridecanol	Not Available	FALSE	C(CCCCCCCC)C(CCC)O

MOL010670	0.8900	0.1100	0.8115	Raphani Semen	5-methyl-2-Undecene	Not Available	FALSE	C/C=C/CC(CCCCCC)C
MOL010671	0.6689	0.3311	0.6618	Raphani Semen	methyl (E)-hexadec-7-enoate	5364431	FALSE	O(C(=O)CCCCC/C=C/CCCCCCCC)C
MOL010674	0.8963	0.1037	0.8237	Raphani Semen	9-methyl-3-Undecene	Not Available	FALSE	CC/C=C\CCCCC(CC)C
MOL010675	0.8341	0.1659	0.7645	Raphani Semen	Dimetilsolfato	6497	FALSE	S(=O)(=O)(OC)OC
MOL010678	0.8529	0.1471	0.6688	Raphani Semen	MEE	878	FALSE	CS
MOL010678	0.8529	0.1471	0.6688	Eriobotryae Folium	MEE	878	FALSE	CS
MOL010679	0.8451	0.1549	0.8315	Raphani Semen	raphanin	Not Available	FALSE	C(=C\S(=O)C)/CCN=C=S
MOL010680	0.9388	0.0612	0.7274	Raphani Semen	sinapine	Not Available	FALSE	O(c1c(O)c(OC)cc(c1)/C=C/C(=O)OCC[N+](C)(C)C)C
MOL010681	0.9283	0.0717	0.7067	Raphani Semen	sinapine thiocyanate	Not Available	FALSE	C(C[N+](C)(C)C)OC(=O)/C=C/c1cc(c(cc1OC)O)OC
MOL010683	0.9329	0.0671	0.9772	Raphani Semen	Cyclohexylethanol	20508	FALSE	C1(CCCCC1)CCO
MOL010684	0.5427	0.4573	0.6183	Raphani Semen	2-Methylhexadecanoic acid methyl ester	Not Available	FALSE	C(=O)(C(CCCCCCCCCCCCCCC)C)OC
MOL010685	0.9271	0.0729	0.8951	Raphani Semen	3-methyl-5-ETHYLHEPTANE	59099756	FALSE	C(CC(CC)C)(CC)CC
MOL010686	0.9271	0.0729	0.9612	Panacis Japonici Rhizoma	2-Ethoxypropane	12256	FALSE	O(C(C)C)CC
MOL010686	0.9271	0.0729	0.9612	Litchi Semen	2-Ethoxypropane	12256	FALSE	O(C(C)C)CC
MOL010686	0.9271	0.0729	0.9612	Capsellae Herba	2-Ethoxypropane	12256	FALSE	O(C(C)C)CC
MOL010687	0.9211	0.0789	0.9657	Cucurbitae Moschatae Semen	LEUCINOL	2724272	FALSE	C(CC)(CN)C
MOL010687	0.9211	0.0789	0.9657	Litchi Semen	LEUCINOL	2724272	FALSE	C(CC)(CN)C
MOL010688	0.7239	0.2761	0.6855	Litchi Semen	LAMA	8906	FALSE	C(CCCCCCCCCCC)OC(=O)C(=C)C
MOL010689	0.9316	0.0684	0.9649	Litchi Semen	ZINC01598471	6993004	FALSE	C(C(C)O)(CC)C
MOL010691	0.5682	0.4318	0.6386	Litchi Semen	Ethyl palmitelaidate	5364759	FALSE	C(=O)(CCCCCCC/C=C/CCCCCC)OCC

MOL010692	0.8867	0.1133	0.8419	Litchi Semen	(2S,3S,4R,5R,6R)-3-[(2S,3R,5S,6R)-3-acetamido-5-hydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4,5,6-trihydroxyoxane-2-carboxylic acid	6852395	FALSE	C1(C(CC(C(O1)CO)O)NC(=O)C)OC1C(OC(C(C1O)O)O)C(=O)O
MOL010693	0.9285	0.0715	0.9262	Litchi Semen	Hyaluronic acid_qt	50904881	FALSE	C1(C(CC(C(O1)CO)O)NC(=O)C)O
MOL010694	0.9239	0.0761	0.9381	Litchi Semen	Dibutyl acetal	79117	FALSE	C(C)(OCCCC)OCCCC
MOL010695	0.9347	0.0653	0.9651	Litchi Semen	[(2S)-4-acetyloxybutan-2-yl] acetate	6994406	FALSE	C(CCOC(=O)C)(OC(=O)C)C
MOL010696	0.9292	0.0708	0.9531	Mume Flos	Hex-2-enyl acetate	2733294	FALSE	C(/C=C/CCC)OC(=O)C
MOL010697	0.9374	0.0626	0.9451	Mume Flos	Phenylpropyl acetate	31226	FALSE	c1(CCCOC(=O)C)ccccc1
MOL010698	0.9530	0.0470	0.9631	Mume Flos	Benzyl butyrate	7650	FALSE	c1(COC(=O)CCC)ccccc1
MOL010699	0.9465	0.0535	0.9656	Mume Flos	Isocreosol	14519	FALSE	c1(c(cc(cc1)C)O)OC
MOL010700	0.9248	0.0752	0.9220	Mume Flos	cis-3-Hexenyl butyrate	5352438	FALSE	C(=O)(OCC/C=C\CC)CCC
MOL010701	0.9199	0.0801	0.9618	Mume Flos	2-hydroxy-1-phenylethanone	68490	FALSE	c1(C(=O)CO)ccccc1
MOL010702	0.9363	0.0637	0.9510	Mume Flos	Acetate C-7	8159	FALSE	C(CCCCC)COC(=O)C
MOL010703	0.9402	0.0598	0.9595	Mume Flos	Pear oil	12348	FALSE	C(OC(=O)C)CCCC
MOL010704	0.9519	0.0481	0.9608	Mume Flos	p-Methylanisole	7731	FALSE	c1(ccc(cc1)C)OC
MOL010705	0.9221	0.0779	0.9223	Mume Flos	2-Decenol	5364942	FALSE	C(CCCCC)C/C=C/CO
MOL010706	0.9374	0.0626	0.9513	Mume Flos	4-Pentenyl acetate	74096	FALSE	C(OC(=O)C)CCC=C
MOL010707	0.9061	0.0939	0.9724	Mume Flos	Placcel M	10401	FALSE	C1(=O)CCCCCO1
MOL010708	0.8778	0.1222	0.6737	Rose Rugosae Flos	1,2,3-tri-O-galloyl-β-D-glucose	Not Available	FALSE	O1C(C(O)C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C1OC(=O)c1cc(O)c(O)c(O)c1)CO

MOL010709	0.5903	0.4097	0.6039	Rose Rugosae Flos	2-Heptodecanone	18027	FALSE	C(CCCCCCCCCC)CCCCC(=O)C
MOL010709	0.5903	0.4097	0.6039	Ginseng Folium	2-Heptodecanone	18027	FALSE	C(CCCCCCCCCC)CCCCC(=O)C
MOL010710	0.6816	0.3184	0.7170	Rose Rugosae Flos	rugosin E	Not Available	FALSE	O1C2C(OC(=O)c3c(c4c(C(=O)OC2)cc(O)c(O)c4O)c(O)c(O)c(O)c3)C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C1OC(=O)c1c(Oc2cc3c(c(O)c2O)c2c(C(=O)OC(C(OC(=O)c4cc(O)c(O)c(O)c4)C(OC(=O)c4cc(O)c(O)c(O)c4)C=O)C(O)COC3=O)cc(O)c(O)c2O)c(O)c(O)c(O)c1
MOL010711	0.8614	0.1386	0.7399	Rose Rugosae Flos	rugosin E_qt	Not Available	FALSE	OC(=O)c1c(Oc2cc3c(c(O)c2O)c2c(C(=O)OC(C(OC(=O)c4cc(O)c(O)c(O)c4)C(OC(=O)c4cc(O)c(O)c(O)c4)C=O)C(O)COC3=O)cc(O)c(O)c2O)c(O)c(O)c(O)c1
MOL010712	0.8706	0.1294	0.6775	Rose Rugosae Flos	strictinin	Not Available	FALSE	O1C2C(OC(=O)c3c(c4c(C(=O)OC2)cc(O)c(O)c4O)c(O)c(O)c(O)c3)C(O)C(O)C1OC(=O)c1cc(O)c(O)c(O)c1
MOL010713	0.8543	0.1457	0.7253	Rose Rugosae Flos	tellimagrandinI	Not Available	FALSE	OC1C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C2OC(=O)c3c(c(c(c(c3O)O)O)O)c3c(c(cc3C(=O)OCC2O1)O)O)O
MOL010714	0.8205	0.1795	0.7430	Rose Rugosae Flos	tellimagrandinII	Not Available	FALSE	O1C2C(OC(=O)c3c(c4c(C(=O)OC2)cc(O)c(O)c4O)c(O)c(O)c(O)c3)C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C1OC(=O)c1cc(O)c(O)c(O)c1
MOL010715	0.9174	0.0826	0.9292	Rose Rugosae Flos	2-Methylheptan-4-one	69378	FALSE	C(C(=O)CCC)C(C)C
MOL010716	0.8619	0.1381	0.8046	Rose Rugosae Flos	XAN	1188	FALSE	c12c(c(=O)[nH]c(=O)[nH]1)[nH]cn2
MOL010717	0.9257	0.0743	0.9207	Rose Rugosae Flos	ZINC02166569	7004908	FALSE	C(=O)(C(CCC)C)C(CC)C
MOL010718	0.8833	0.1167	0.6500	Rose Rugosae Flos	1,2,6-tri-O-galloyl-β-D-glucose	Not Available	FALSE	O1C(C(OC(=O)c2cc(O)c(O)c(O)c2)C(O)(C1O)COC(=O)c1cc(O)c(O)c(O)c1)COC(=O)c1cc(O)c(O)c(O)c1
MOL010720	0.9301	0.0699	0.9481	Rose Rugosae Flos	Leaf acetate	5363388	FALSE	O(CC/C=C\CC)C(=O)C
MOL010720	0.9301	0.0699	0.9481	Capsellae Herba	Leaf acetate	5363388	FALSE	O(CC/C=C\CC)C(=O)C
MOL010721	0.8369	0.1631	0.7830	Rose Rugosae Flos	3-Tridecyne	143685	FALSE	CCC#CCCCCCCCCC
MOL010722	0.9256	0.0744	0.8989	Rose Rugosae Flos	4,5-Dimethyloctane, threo	6430929	FALSE	C(C(CCC)C)(CCC)C
MOL010723	0.9296	0.0704	0.9687	Rose Rugosae Flos	()-Styrene glycol	643312	FALSE	C(CO)(O)c1ccccc1
MOL010724	0.8942	0.1058	0.7146	Rose Rugosae Flos	6,6-Dimethylundecane	28474	FALSE	CCCCCC(CCCCC)(C)C

MOL010726	0.6278	0.3722	0.7258	Rose Rugosae Flos	Casuarictin	Not Available	FALSE	O1C2C(OC(=O)c3c(c4c(C1=O)cc(O)c(O)c4O)c(O)c(O)c(O)c3)C(OC1C2OC(=O)c2c(c3c(C(=O)OC1)cc(O)c(O)c3O)c(O)c(O)c(O)c2)OC(=O)c1cc(O)c(O)c(O)c
MOL010726	0.6278	0.3722	0.7258	Rosae Laevigatae Fructus	Casuarictin	Not Available	FALSE	O1C2C(OC(=O)c3c(c4c(C1=O)cc(O)c(O)c4O)c(O)c(O)c(O)c3)C(OC1C2OC(=O)c2c(c3c(C(=O)OC1)cc(O)c(O)c3O)c(O)c(O)c(O)c2)OC(=O)c1cc(O)c(O)c(O)c
MOL010726	0.6278	0.3722	0.7258	Juglandis Semen	Casuarictin	Not Available	FALSE	O1C2C(OC(=O)c3c(c4c(C1=O)cc(O)c(O)c4O)c(O)c(O)c(O)c3)C(OC1C2OC(=O)c2c(c3c(C(=O)OC1)cc(O)c(O)c3O)c(O)c(O)c(O)c2)OC(=O)c1cc(O)c(O)c(O)c1
MOL010728	0.8695	0.1305	0.8866	Rose Rugosae Flos	Ethyl 2-methyllactate	6653	FALSE	C(=O)(C(C)(C)O)OCC
MOL010729	0.8426	0.1574	0.8275	Rose Rugosae Flos	germacrone	54121414	FALSE	C1(=O)CCC(C)CCC(C(C)C)CCC1C
MOL010730	0.8184	0.1816	0.6440	Rose Rugosae Flos	isodaucene	Not Available	FALSE	C12(C(C(CC1)C(=C)C)CCC(=CC2)C)C
MOL010732	0.9202	0.0798	0.9269	Rose Rugosae Flos	Isodecanol	32898	FALSE	C(CCCCO)CCC(C)C
MOL010733	0.9324	0.0676	0.9402	Rose Rugosae Flos	linalyl formate	36690112	FALSE	C(CCC=C(C)C)(OC=O)(C=C)C
MOL010734	0.9204	0.0796	0.9270	Rose Rugosae Flos	557986_ALDRICH	2737541	FALSE	C(CCCCC)CCC(C)O
MOL010735	0.9427	0.0573	0.9612	Rose Rugosae Flos	(2S,4S)-4-methyl-2-(2-methylprop-1-enyl)oxane	1712086	FALSE	C1(CC(CCO1)C)C=C(C)C
MOL010735	0.9427	0.0573	0.9612	Ephedra Herba	(2S,4S)-4-methyl-2-(2-methylprop-1-enyl)oxane	1712086	FALSE	C1(CC(CCO1)C)C=C(C)C
MOL010736	0.4653	0.5347	0.6118	Rose Rugosae Flos	rubixanthin	Not Available	FALSE	C1(=C(CC(CC1(C)C)O)C)/C=C\C(=C\C=C\C(=C\C=C\C=C(\C=C\C=C(\C=C\C=C(\CCC=C(C)C)/C)/C)/C)\C)\C
MOL010737	0.8334	0.1666	0.7411	Rose Rugosae Flos	rugosin A	Not Available	FALSE	O1C2C(OC(=O)c3c(c4c(C(=O)OC2)cc(Oc2c(cc(O)c(O)c2O)C(=O)O)c(O)c4O)c(O)c(O)c(O)c3)C(OC(=O)c2cc(O)c(O)c(O)c2)C(OC(=O)c2cc(O)c(O)c(O)c2)C1OC(=O)c1cc(O)c(O)c(O)c1
MOL010738	0.8863	0.1137	0.7756	Rose Rugosae Flos	rugosin D_qt	12444662	FALSE	OC(=O)c1c(c2c(C(=O)O)cc(Oc3c(cc(O)c(O)c3O)C(=O)O)c(O)c2O)c(O)c(O)c(O)c1
MOL010739	0.8472	0.1528	0.7555	Rose Rugosae Flos	rugosin B	Not Available	FALSE	O1C2C(OC(=O)C3C(=C(O)C(=C(O)C3)O)C3c(C(=O)OC2)cc(Oc2c(cc(O)c(O)c2O)C(=O)O)c(O)c3O)C(OC(=O)c2cc(O)c(O)c(O)c2)C(C1O)CC(=O)c1cc(O)c(O)c(O)c1
MOL010740	0.8950	0.1050	0.7938	Rose Rugosae Flos	rugosin B_qt	Not Available	FALSE	OC(=O)C1C(=C(O)C(=C(O)C1O)O)c1c(C(=O)O)cc(Oc2c(cc(O)c(O)c2O)C(=O)O)c(O)c1O

MOL010741	0.5342	0.4658	0.7224	Rose Rugosae Flos	rugosin D	Not Available	FALSE	O(c1c(O)c(O)c2c3c(C(=O)OC4C(OC(=O)c5cc(O)c(O)c(O)c5)C(OC(=O)c5cc(O)c(O)c(O)c5)C(OC4COC(=O)c2c1)OC(=O)c1cc(O)c(O)c(O)c1)cc(O)c(O)c3O)c1c(C(=O)OC2OC3C(OC(=O)c4c(c5c(C(=O)OC3)cc(O)c(O)c5O)c(O)c(O)c(O)c4)C(OC(=O)c3cc(O)c(O)c(O)c3)C2OC(=O)c2cc(O)c(O)c(O)c2)cc(O)c(O)c1O
MOL010742	0.9243	0.0757	0.8885	Ephedra Herba	2,3,4-Trimethyl-5-phenyloxazolidine	Not Available	FALSE	O1C(N(C(C1c1ccccc1)C)C)C
MOL010743	0.9584	0.0416	0.8279	Ephedra Herba	19889-94-2	88295	FALSE	C1(CC2CC(C2(C)C)C1C)O
MOL010744	0.9254	0.0746	0.9612	Ephedra Herba	2-Methylpent-2-en-1-ol	5362851	FALSE	C(/C(=C/CC)/C)O
MOL010745	0.9048	0.0952	0.9046	Ephedra Herba	(E)-oct-3-en-1-yne	5362862	FALSE	C#C/C=C/CCCC
MOL010746	0.9395	0.0605	0.9520	Ephedra Herba	1,2,3-trimethylcyclohexane	6432164	FALSE	C1(C(CCCC1C)C)C
MOL010747	0.9362	0.0638	0.9653	Ephedra Herba	(2S)-heptane-1,2-diol	10606775	FALSE	C(CCCCC)(CO)O
MOL010748	0.9585	0.0415	0.9706	Ephedra Herba	1,3,4-trimethyl-3-cyclohexene-1-carboxaldehyde	57473007	FALSE	C1(CC(=C(CC1)C)C)(C=O)C
MOL010749	0.8730	0.1270	0.9599	Ephedra Herba	2,5-Dimethylpyrazole	79096	FALSE	c1(nn(cc1)C)C
MOL010750	0.9308	0.0692	0.9184	Ephedra Herba	1Ph5SHTetrazol	690730	FALSE	n1(nnnc1S)c1ccccc1
MOL010752	0.9311	0.0689	0.9478	Ephedra Herba	p-Nitrosotoluene	12166	FALSE	c1(ccc(cc1)C)N=O
MOL010753	0.9092	0.0908	0.9409	Ephedra Herba	(2R)-1-ethoxypropan-2-ol	6999922	FALSE	C(C(C)O)OCC
MOL010754	0.9195	0.0805	0.9546	Ephedra Herba	Ethyltrimethylethylene	25403	FALSE	C(=C(C)C)(CC)C
MOL010756	0.9272	0.0728	0.9696	Ephedra Herba	2-methyl-butanol-1-ol	53684422	FALSE	C(C(CC)C)(O)O
MOL010757	0.9054	0.0946	0.9655	Ephedra Herba	Tiglaldehyde	5321950	FALSE	C(=C\C)(/C=O)\C

MOL010757	0.9054	0.0946	0.9655	Lysimachiae Foenigraeci Herba	Tiglaldehyde	5321950	FALSE	C(=C\C)(/C=O)\C
MOL010759	0.8983	0.1017	0.9635	Ephedra Herba	C2H5CH=CH COOH	638122	FALSE	C(=O)(/C=C/CC)O
MOL010760	0.9165	0.0835	0.9220	Ephedra Herba	2-ethylidene-1,1-dimethyl-cyclopentane	21160395	FALSE	C1(/C(=C\C)/CCC1)(C)C
MOL010761	0.9254	0.0746	0.8356	Ephedra Herba	3,7-dimethyl-cyclopenta cyclooctene	Not Available	FALSE	C12C(=CC=C2C)C=CC(=CC=C1)C
MOL010762	0.9573	0.0427	0.9559	Ephedra Herba	3,8-menthadiene	71386448	FALSE	C1=C(CCC(C1)C)C(=C)C
MOL010763	0.9148	0.0852	0.9416	Ephedra Herba	3-methylhexa-2,4-diene	5367612	FALSE	C(=C\C)(/C=C/C)\C
MOL010764	0.9295	0.0705	0.8118	Ephedra Herba	2-Methyl-1-naphthol	24055	FALSE	c1cc(c(c2ccccc12)O)C
MOL010765	0.9579	0.0421	0.9565	Ephedra Herba	3-methyl-6-(1-methylethyl-idene)-cyclohexene	15564402	FALSE	C1=CC(CCC1=C(C)C)C
MOL010766	0.7075	0.2925	0.6037	Typhonii Rhizoma	3-METHYLPHENANTHRENE	13258	FALSE	c12c3c(ccc1cccc2)ccc(c3)C
MOL010766	0.7075	0.2925	0.6037	Ephedra Herba	3-METHYLPHENANTHRENE	13258	FALSE	c12c3c(ccc1cccc2)ccc(c3)C
MOL010766	0.7075	0.2925	0.6037	Ginseng Folium	3-METHYLPHENANTHRENE	13258	FALSE	c12c3c(ccc1cccc2)ccc(c3)C
MOL010767	0.9506	0.0494	0.9613	Ephedra Herba	p-Toluyl chloride	13405	FALSE	c1(C(=O)Cl)ccc(cc1)C
MOL010768	0.9400	0.0600	0.7782	Ephedra Herba	KYNA	3845	FALSE	c12c(c(cc(n1)C(=O)O)O)cccc2
MOL010769	0.9373	0.0627	0.9582	Ephedra Herba	Methyl 5-methylhexanoate	519894	FALSE	C(=O)(CCCC(C)C)OC
MOL010770	0.8690	0.1310	0.8661	Ephedra Herba	3-Undecyne	143689	FALSE	C(CCCCC)CC#CCC

MOL010771	0.9114	0.0886	0.9348	Ephedra Herba	(S)-1-Boc-3-methylpiperazine	7023035	FALSE	N1(C(=O)OC(C)(C)C)CC(NCC1)C
MOL010772	0.9497	0.0503	0.9528	Ephedra Herba	Methylbenzylamine	7669	FALSE	c1(ccccc1)CNC
MOL010773	0.9554	0.0446	0.9774	Ephedra Herba	1,3-p-Menthadien-7-al	526762	FALSE	C1=C(CCC(=C1)C=O)C(C)C
MOL010774	0.9281	0.0719	0.9413	Ephedra Herba	[(2S)-6-methylhept-5-en-2-yl] acetate	11263749	FALSE	C(=O)(C)OC(CCC=C(C)C)C
MOL010775	0.9271	0.0729	0.9149	Ephedra Herba	Allyloxybenzene	74458	FALSE	C(Oc1ccccc1)C=C
MOL010776	0.9463	0.0537	0.9220	Ephedra Herba	2-Butene, 2-phenyl-, (Z)-	5358306	FALSE	c1(/C(=C\C)/C)ccccc1
MOL010777	0.8434	0.1566	0.6701	Ephedra Herba	WLN: G1G	6344	FALSE	C(Cl)Cl
MOL010778	0.9485	0.0515	0.9152	Ephedra Herba	m-Ethylacetophenone	31493	FALSE	c1(cc(ccc1)CC)C(=O)C
MOL010779	0.8639	0.1361	0.9078	Ephedra Herba	DS	6163	FALSE	S(=O)(=O)(OCC)OCC
MOL010780	0.9631	0.0369	0.9156	Ephedra Herba	Ephedroxane	161171	FALSE	O1C(=O)N(C(C1c1ccccc1)C)C
MOL010781	0.8888	0.1112	0.8803	Ephedra Herba	Ethyl 2-decenoate	5463904	FALSE	C(=O)(/C=C/CCCCCCC)OCC
MOL010782	0.9110	0.0890	0.9056	Ephedra Herba	Methyl 2-decenoate	5368064	FALSE	C(=O)(/C=C/CCCCCCC)OC
MOL010783	0.9639	0.0361	0.9745	Ephedra Herba	carvenone	Not Available	FALSE	C1(=O)C=C(C(=C)C)CCC1C
MOL010784	0.8861	0.1139	0.9675	Campsis Flos	isobutyric acid	6590	FALSE	C(=O)(C(C)C)O
MOL010784	0.8861	0.1139	0.9675	Ephedra Herba	isobutyric acid	6590	FALSE	C(=O)(C(C)C)O
MOL010785	0.9570	0.0430	0.9684	Ephedra Herba	()-N-Methylephedrine	102023	FALSE	c1(C(C(N(C)C)C)O)ccccc1
MOL010786	0.8476	0.1524	0.8675	Ephedra Herba	O-benzoyl-L-(+)-pseudoephedrine	Not Available	FALSE	O(C(C(NC)C)c1ccccc1)C(=O)c1ccccc1
MOL010787	0.8968	0.1032	0.8864	Ephedra Herba	Trans-ionone	Not Available	FALSE	O=C(C)/C=C\C1C(=CCCC1(C)C)C
MOL010788	0.9341	0.0659	0.8808	Ephedra Herba	leucopelargonidin	Not Available	FALSE	c12c(OC(C(C1O)O)c1ccc(cc1)O)cc(cc2O)O
MOL010789	0.9212	0.0788	0.7653	Ephedra Herba	1,5,8-trimethyl-1,2-dihydro-naphthalene	Not Available	FALSE	C1(CC=Cc2c(ccc(c12)C)C)C

MOL010792	0.8980	0.1020	0.7703	Ephedra Herba	1,5-dimethyl-4-(2-hexenyl)benzene	Not Available	FALSE	c1(ccc(c(c1)C)C/C=C/CCC)C
MOL010793	0.9628	0.0372	0.9726	Ephedra Herba	[(1S,4S)-4-isopropyl-1-cyclohex-2-enyl]methanol	13747942	FALSE	C1=CC(CCC1C(C)C)CO
MOL010795	0.9078	0.0922	0.8164	Ephedra Herba	1-propenyl-2-vinyl-4-methylcycloheptane	Not Available	FALSE	C1(C(CC(CCC1)C)C=C)/C=C/C
MOL010796	0.6598	0.3402	0.6553	Ephedra Herba	Promyr	8042	FALSE	C(CCCCCCCCCCCC)C(=O)OC(C)C
MOL010797	0.9491	0.0509	0.9228	Ephedra Herba	Dehydroxylinalool oxide A	6430803	FALSE	C1(OC(CCC1)(C)C)(C=C)C
MOL010799	0.8095	0.1905	0.7647	Aristolochiae Fructus	Ariskanin A	5320068	FALSE	O(C)c1c(OC)c2c(c(c1)C(=O)OC)c([N+](=O)O)cc1c2cccc1
MOL010799	0.8095	0.1905	0.7647	Caulis Akebiae	Ariskanin A	5320068	FALSE	O(C)c1c(OC)c2c(c(c1)C(=O)OC)c([N+](=O)O)cc1c2cccc1
MOL010800	0.7235	0.2765	0.7786	Caulis Akebiae	serratagenic acid	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C)(C(=O)O)CC4C3=CCC21)C)O
MOL010801	0.3982	0.6018	0.7218	Caulis Akebiae	β-amyrin	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C)(C)CC4C3=CCC21)C)O
MOL010802	0.8951	0.1049	0.7036	Caulis Akebiae	Aristoloside	128576	FALSE	O1COc2c1c1c3cc(cc(c3cc(c1c(c2)C(=O)O)[N+](=O)O)OC)OC1C(O)C(O)C(O)C(O1)CO
MOL010803	0.8382	0.1618	0.6991	Caulis Akebiae	aristolochic acid A	46184319	FALSE	c1cc(c2c(c1)c1c(c(c2)C(=O)O)c(cc2c1OCO2)C(=O)O)OC
MOL010804	0.9139	0.0861	0.6728	Aristolochiae Fructus	aristolochic acid Ⅱ	108168	FALSE	O1COc2c1c1c3ccccc3cc(c1c(c2)C(=O)O)[N+](=O)O
MOL010804	0.9139	0.0861	0.6728	Caulis Akebiae	aristolochic acid Ⅱ	108168	FALSE	O1COc2c1c1c3ccccc3cc(c1c(c2)C(=O)O)[N+](=O)O
MOL010806	0.7130	0.2870	0.7745	Caulis Akebiae	quinatic acid	Not Available	FALSE	C1(CCC2(C(C1(CO)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(=C)CC4C3=CCC21)C)O
MOL010807	0.8764	0.1236	0.7547	Caulis Akebiae	Cyanin	Not Available	FALSE	C1(C(C(C(C(O1)Oc1cc(cc2c1cc(c([o+]2)c1ccc(c(c1)O)O)OC1C(C(C(C(O1)CO)O)O)O)O)O)O)O)CO
MOL010808	0.7297	0.2703	0.8856	Caulis Akebiae	oleanonic acid	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C)(C)CC4C3=CCC21)C
MOL010809	0.7470	0.2530	0.8231	Caulis Akebiae	mesembryanthemoidigenic acid	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)CO)C(=O)O)C)C)(C)C)O
MOL010810	0.7200	0.2800	0.8305	Caulis Akebiae	akebonoic acid	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(=C)CC4C3=CCC21)C)O

MOL010811	0.7676	0.2324	0.7873	Caulis Akebiae	Akeboside sth	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)OC1OC(C(C(C1O)O)O)C)CO)C)C)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)C)O)O
MOL010812	0.7788	0.2212	0.7326	Aucklandiae Radix	(Z)6,(Z)9-Pentadecadien-1-ol	5365570	FALSE	CCCCC/C=C\C/C=C\CCCCCO
MOL010813	0.7849	0.2151	0.6392	Aucklandiae Radix	Benzo[a]carbazole	9196	FALSE	c12c(c3c([nH]2)cccc3)ccc2c1cccc2
MOL010814	0.8656	0.1344	0.8089	Aucklandiae Radix	2-(4a,8-dimethyl-1,2,3,4,4a,5,6,7-octahydro-napthalen-2-yl)-prop-2en-1-ol	Not Available	FALSE	C1CC(=C2C(C1)(CCC(C2)C(=C)CO)C)C
MOL010815	0.9268	0.0732	0.9488	Aucklandiae Radix	2,4-Hexadiene, 3,4-dimethyl-, (E,Z)-	5368977	FALSE	C/C=C(\C(=C\C)\C)/C
MOL010816	0.8810	0.1190	0.8451	Aucklandiae Radix	7-methylocta-3,4-diene	142131	FALSE	CC(CC=C=CCC)C
MOL010817	0.8138	0.1862	0.6654	Aucklandiae Radix	7-methyl-4-(1-methylethylidene)-bicyclo[5.3.1]undec-1-en-8-ol	Not Available	FALSE	C1(CC=CC2(C1(O2)/C(=C/C(=C)C)/C)C)(C)C
MOL010818	0.7633	0.2367	0.8183	Aucklandiae Radix	(3aS,5R,8aS,9aS)-5,8a-dimethyl-3-methylene-5,6,7,8,9,9a-hexahydro-3aH-benzo[f]benzofuran-2-one	6540817	FALSE	C12(C(=CC3C(C1)OC(=O)C3=C)C(CCC2)C)C
MOL010819	0.8499	0.1501	0.8156	Aucklandiae Radix	Ambrosin	Not Available	FALSE	C12(C3C(C(=C)C(=O)O3)CCC(C1C=CC2=O)C)C
MOL010820	0.2568	0.7432	0.7854	Aucklandiae Radix	Methyl betulinate	73493	FALSE	C12(C(C3C(CC1)(C1(C(CC3)C3(C(CC1)C(C(CC3)O)(C)C)C)C)C)C(CC2)C(=C)C)C(=O)OC
MOL010820	0.2568	0.7432	0.7854	Eriobotryae Folium	Methyl betulinate	73493	FALSE	C12(C(C3C(CC1)(C1(C(CC3)C3(C(CC1)C(C(CC3)O)(C)C)C)C)C)C(CC2)C(=C)C)C(=O)OC

MOL010821	0.8394	0.1606	0.6701	Aucklandiae Radix	Caryophyllene-(I3)	Not Available	FALSE	C1C/C=C(\CC2C(/C(=C\1)/C)CC2(C)C)/C
MOL010822	0.8853	0.1147	0.6236	Aucklandiae Radix	ZINC04026824	Not Available	FALSE	C123C(C(C(C1)C(=C)C(C2)O)(C)C)CCC3C
MOL010823	0.9235	0.0765	0.9618	Aucklandiae Radix	ETA	700	FALSE	C(CO)N
MOL010824	0.9142	0.0858	0.8242	Aucklandiae Radix	2-[(2R,4aR,8aS)-4a-methyl-8-methylene-decalin-2-yl]acrylic acid	6451579	FALSE	C12C(CCC(C1)C(=C)C(=O)O)(CCCC2=C)C
MOL010825	0.8088	0.1912	0.7241	Aucklandiae Radix	Costunolide	5281437	FALSE	C12C(C(=C)C(=O)O1)CC/C(=C/CC/C(=C/2)/C)/C
MOL010826	0.8088	0.1912	0.7241	Aucklandiae Radix	costuslactone	Not Available	FALSE	C12C(C(=C)C(=O)O1)CC/C(=C/CC/C(=C/2)/C)/C
MOL010827	0.9155	0.0845	0.9589	Aucklandiae Radix	1,2-Dimethylcyclohexene	15480	FALSE	C1(=C(CCCC1)C)C
MOL010828	0.4965	0.5035	0.6164	Aucklandiae Radix	cynaropicrin	Not Available	FALSE	C12C3C(C(=C)CC(C1C(=C)C(=O)O2)OC(=O)/C(=C/O)/C)CC(C3=C)O
MOL010829	0.9213	0.0787	0.8840	Citri Sarcodactylis Fructus	4-[(1R)-2,6,6-trimethyl-1-cyclohex-2-enyl]butan-2-one	12858404	FALSE	C1(C(CCC=C1C)(C)C)CCC(=O)C
MOL010829	0.9213	0.0787	0.8840	Aucklandiae Radix	4-[(1R)-2,6,6-trimethyl-1-cyclohex-2-enyl]butan-2-one	12858404	FALSE	C1(C(CCC=C1C)(C)C)CCC(=O)C
MOL010830	0.7907	0.2093	0.7169	Aucklandiae Radix	dihydrocostuslactone	Not Available	FALSE	C\1(=C\CC/C(=C/C2C(CC1)C(C(=O)O2)C)/C)/C
MOL010831	0.8012	0.1988	0.7422	Aucklandiae Radix	Ermanthin	100572	FALSE	C1CC(=C)C2C1C(=CCC1C2OC(=O)C1=C)C
MOL010832	0.8009	0.1991	0.6810	Aucklandiae Radix	Eremophilene	52319950	FALSE	C1C(CC2(C(=CCCC2C)C1)C)C(=C)C
MOL010833	0.7633	0.2367	0.8183	Aucklandiae Radix	eudesma-5,11(13)-dien-8,12-olide	6326704	FALSE	C1CCC2(C(=CC3C(C2)OC(=O)C3=C)C1C)C
MOL010834	0.9591	0.0409	0.8802	Caryophylliflos	Aceteugenol	7136	FALSE	c1(c(cc(cc1)CC=C)OC)OC(=O)C
MOL010834	0.9591	0.0409	0.8802	Aucklandiae Radix	Aceteugenol	7136	FALSE	c1(c(cc(cc1)CC=C)OC)OC(=O)C
MOL010835	0.6686	0.3314	0.6174	Aucklandiae Radix	humulane-1,6-dien-3-ol	Not Available	FALSE	C\1=C(\CCCC(/C=C/C(CC1C)C)(C)C)/C
MOL010836	0.7716	0.2284	0.7605	Aucklandiae Radix	Isoalantolactone	73285	FALSE	C1(=O)C(=C)C2C(O1)CC1(C(C2)C(=C)CCC1)C

MOL010837	0.8483	0.1517	0.7253	Aucklandiae Radix	isodihydrocostunolide	Not Available	FALSE	C1CC(CCC2C(/C=C(/C1)\C)OC(=O)C2=O)C
MOL010838	0.8440	0.1560	0.8002	Aucklandiae Radix	3-Epizaluzanin C	470970	FALSE	C12C(C3C(C(=C)CC1)CC(C3=C)O)OC(=O)C2=C
MOL010839	0.1527	0.8473	0.7283	Aucklandiae Radix	lappadilactone	Not Available	FALSE	C12C(C(C(=O)O1)(CC1(C3C(C(=O)CC1)(CCC1C3OC(=O)C1=C)C)C)O)CCC(=C)C1C2CC(=C)C1
MOL010841	0.8454	0.1546	0.7269	Aucklandiae Radix	picriside B_qt	Not Available	FALSE	C12C(/C=C/CC/C=C(/CC1)\C)OC(=O)C2=C
MOL010842	0.8310	0.1690	0.8002	Aucklandiae Radix	Naphthol[1,2-b]furan-2(3H)-one,decahydro-6-hydroxy-5a-methyl-3,9-bis(methylene)-,[3as-(3aalpha,5abeta,6beta,9aalpha,9bbeta)]	482788	FALSE	O1C(=O)C(=C)C2C1C1C(CC2)(C(CCC1=C)O)C
MOL010843	0.8431	0.1569	0.8016	Aucklandiae Radix	Balchanin	188297	FALSE	C1(=CCC(C2(C1C1C(CC2)C(=C)C(=O)O1)C)O)C
MOL010844	0.8895	0.1105	0.6520	Aucklandiae Radix	spathulenol	13854252	FALSE	C12C3C(C(=C)CCC1C2(C)C)CCC3(C)O
MOL010845	0.9555	0.0445	0.9399	Hordei Fructus Germinatus	candicine	23135	FALSE	[N+](CCc1ccc(cc1)O)(C)(C)C
MOL010846	0.9097	0.0903	0.7865	Hordei Fructus Germinatus	deoxynivalenol standard	Not Available	FALSE	C12(C3(C4(C(OC1C(C3)O)C=C(C(=O)C4O)C)CO)C)OC2
MOL010847	0.9186	0.0814	0.9578	Hordei Fructus Germinatus	EG	174	FALSE	C(CO)O
MOL010848	0.6990	0.3010	0.6061	Hordei Fructus Germinatus	gliadin	Not Available	FALSE	O=C(NC(CCC1)C(=O)NC(CCC(=O)N)C(=O)O)C(NC(=O)C1N(CCC1)C(=O)C(N)Cc1ccc(O)cc1)CCC(=O)N
MOL010851	0.9235	0.0765	0.9545	Hordei Fructus Germinatus	PG	10442	FALSE	C(CCO)O
MOL010854	0.9081	0.0919	0.9705	Hordei Fructus Germinatus	D-Prolin	6971012	FALSE	C1(C(=O)O)CCCN1
MOL010855	0.9357	0.0643	0.9677	Hordei Fructus Germinatus	Sucol B	8064	FALSE	C(CCO)CO
MOL010856	0.9152	0.0848	0.9665	Hordei Fructus Germinatus	putrescine	1045	FALSE	C(CCN)CN
MOL010856	0.9152	0.0848	0.9665	Citri Grandis Exocarpium	putrescine	1045	FALSE	C(CCN)CN
MOL010857	0.8361	0.1639	0.7112	Hordei Fructus Germinatus	Sterigmatocystin	Not Available	FALSE	c12c3c(OC4C3C=CO4)cc(c1c(=O)c1c(o2)cccc1O)OC
MOL010858	0.8887	0.1113	0.7229	Hordei Fructus Germinatus	tianshic acid	Not Available	FALSE	OC(CCCCCC)C(O)/C=C/C(O)CCCCCCC(=O)O
MOL010858	0.8887	0.1113	0.7229	Semen Aesculi	tianshic acid	Not Available	FALSE	OC(CCCCCC)C(O)/C=C/C(O)CCCCCCC(=O)O
MOL010859	0.9495	0.0505	0.9321	Hordei Fructus Germinatus	TSS	1150	TRUE	NCCc1c[nH]c2ccccc12
MOL010860	0.8729	0.1271	0.7977	Hordei Fructus Germinatus	violanthin	Not Available	FALSE	c1(cc(=O)c2c(c(c(c(c2o1)C1OC(C(C(C1O)O)O)C)O)C1OC(C(C(C1O)O)O)CO)O)c1ccc(cc1)O

MOL010863	0.8232	0.1768	0.7505	Hordei Fructus Germinatus	3-ACETYLDEOXYNIVALENOL	Not Available	FALSE	C12(C3(C4(C(OC1C(C3)C(=O)C)C=C(C(=O)C4O)C)CO)C)CO2
MOL010864	0.8645	0.1355	0.9354	Hordei Fructus Germinatus	5,7-Dihydroxy-3',4',5'-trimethoxyflavon	5379265	FALSE	c12c(c(=O)cc(o1)c1cc(c(c(c1)OC)OC)OC)c(cc(c2)O)O
MOL010866	0.2950	0.7050	0.7943	Fructus Arctii	Arctignan E	Not Available	FALSE	O1C(=O)C(C(C1)Cc1cc2C(C(Oc2c(c1)OC)c1cc(c(cc1)O)OC)CO)Cc1cc(c(c(c1)OC)O)C(C(c1cc(c(cc1)O)OC)O)CO
MOL010867	0.3562	0.6438	0.7319	Fructus Arctii	lappaol H	Not Available	FALSE	O1C(=O)C(C(C1)Cc1cc(c(c(c1)OC)O)C(C(c1cc(c(cc1)O)OC)O)CO)Cc1cc(c(c(c1)OC)O)C(C(c1cc(c(cc1)O)OC)O)CO
MOL010868	0.1039	0.8961	0.7035	Fructus Arctii	neoarctin A	Not Available	FALSE	O1CC(C(Cc2cc(OC)c(Oc3c(OC)cc(CC4C(COC4=O)Cc4cc(OC)c(OC)cc4)cc3)cc2)C1=O)Cc1cc(OC)c(O)c(OC)c1
MOL010869	0.1788	0.8212	0.6786	Fructus Arctii	neoarctin B	Not Available	FALSE	O1CC(C(Cc2cc(OC)c(O)c(OC)c2)C1=O)Cc1cc(OC)c(c2c(OC)cc(CC3C(Cc4cc(OC)c(O)c(OC)c4)C(=O)OC3)cc2)cc1
MOL010870	0.9324	0.0676	0.9685	Fructus Arctii	TERPINEOL	Not Available	FALSE	C1=CCC(CC1)C(C)(C)O
MOL010871	0.0868	0.9132	0.6741	Fructus Arctii	isolappaol C	Not Available	FALSE	O1C(=O)C(C(C1)Cc1cc(c(cc1)O)OC)Cc1cc2C(C(Oc2c(c1)OC)c1cc(c(cc1)O)OC)CO
MOL010872	0.1601	0.8399	0.6792	Fructus Arctii	lappaol A	Not Available	FALSE	O1C(=O)C(C(C1)Cc1cc2C(C(Oc2c(c1)OC)c1cc(c(cc1)O)OC)CO)Cc1cc(c(cc1)O)OC
MOL010873	0.0827	0.9173	0.6623	Fructus Arctii	Lappaol B	46173977	FALSE	O1CC(C(Cc2cc3C(C(Oc3c(OC)c2)c2cc(OC)c(O)cc2)CO)C1=O)Cc1cc(OC)c(OC)cc1
MOL010877	0.2274	0.7726	0.8019	Fructus Arctii	lappaol F	Not Available	FALSE	O1C(=O)C(C(C1)Cc1cc2C(C(Oc2c(c1)OC)c1cc(c(cc1)O)OC)CO)Cc1cc2C(C(Oc2c(c1)OC)c1cc(c(cc1)O)OC)CO
MOL010878	0.9129	0.0871	0.9624	Cucurbitae Moschatae Semen	Cucurbitine	28405994	FALSE	C1(C(=O)O)(N)CCNC1
MOL010879	0.9303	0.0697	0.9686	Cucurbitae Moschatae Semen	PKA	12332	FALSE	C(CCCC)C(=O)N
MOL010880	0.9212	0.0788	0.9418	Cucurbitae Moschatae Semen	3-OCTENOIC ACID	5282716	FALSE	C(=C\CCCC)/CC(=O)O
MOL010881	0.9319	0.0681	0.9737	Cucurbitae Moschatae Semen	Valeramide	12298	FALSE	C(C(=O)N)CCC
MOL010883	0.9145	0.0855	0.9315	Cucurbitae Moschatae Semen	Triglyzerid	5460048	FALSE	O(C(COC=O)COC=O)C=O
MOL010884	0.9342	0.0658	0.9237	Cucurbitae Moschatae Semen	2-Hexylpyridine	70797	FALSE	c1(CCCCCC)ccccn1
MOL010885	0.8799	0.1201	0.9695	Cucurbitae Moschatae Semen	(1S,2R)-2-methylcyclopentanol	642631	FALSE	C1(C(CCC1)O)C
MOL010886	0.6742	0.3258	0.6002	Benincasae Semen	Sphingoid	5280335	FALSE	C(=C\CCCCCCCCCCCCC)/C(C(CO)N)O

MOL010886	0.6742	0.3258	0.6002	Cucurbitae Moschatae Semen	Sphingoid	5280335	FALSE	C(=C\CCCCCCCCCCCCC)/C(C(CO)N)O
MOL010887	0.7552	0.2448	0.7883	Kaki Calyx	Barbinervic acid	194183	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3(O)C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C
MOL010889	0.8305	0.1695	0.7441	Quisqualis Indica	5-desgalloylstachyurin	Not Available	FALSE	O1C2C(OC(=O)c3c(c4c(c(C2O)c(O)c(O)c4O)C1=O)c(O)c(O)c(O)c3)C1OC(=O)c2c(c3c(C(=O)OCC1O)cc(O)c(O)c3O)c(O)c(O)c(O)c2
MOL010891	0.8639	0.1361	0.7198	Quisqualis Indica	Punicalagin_qt	Not Available	FALSE	c12c3c4c(c(c5c(C(=O)O)cc(c(c5O)O)O)c(c(c46c2=O)O)O)c(=O)oc3c(c(c1c1c(C(=O)O)cc(c(c1O)O)O)O)O
MOL010892	0.8729	0.1271	0.9238	Quisqualis Indica	quisqualic acid	6971145	FALSE	n1(c(=O)[nH]c(=O)o1)CC(C(=O)O)N
MOL010893	0.9050	0.0950	0.8606	Quisqualis Indica	brevioflin carboxylic acid	Not Available	FALSE	o1c2c(C(CC2=O)C(=O)O)c2c(c1=O)cc(O)c(O)c2O
MOL010894	0.5214	0.4786	0.7168	Quisqualis Indica	castalagin	Not Available	FALSE	O1C2C3OC(=O)c4c(c5c(c(C2O)c(O)c(O)c5O)C1=O)c(O)c(O)c(O)c4c1c(C(=O)OC2C3OC(=O)c3c(c4c(C(=O)OC2)cc(O)c(O)c4O)c(O)c(O)c(O)c3)cc(O)c(O)c1O
MOL010895	0.8305	0.1695	0.7441	Quisqualis Indica	Casuariin	Not Available	FALSE	O1C2C(OC(=O)c3c(c4c(c(C2O)c(O)c(O)c4O)C1=O)c(O)c(O)c(O)c3)C1OC(=O)c2c(c3c(C(=O)OCC1O)cc(O)c(O)c3O)c(O)c(O)c(O)c2
MOL010896	0.5680	0.4320	0.7004	Semen Aesculi	aescigenin	Not Available	FALSE	O1C2C3(C(C4=CCC5C(C4(C2)C)(CCC2C5(CCC(O)C2(CO)C)C)C)CC(C1C3O)(C)C)CO
MOL010897	0.6577	0.3423	0.7060	Semen Aesculi	protoaescigenin	Not Available	FALSE	OC1C2(C(C3=CCC4C(C3(C1)C)(CCC1C4(CCC(O)C1(CO)C)C)C)CC(C(O)C2O)(C)C)CO
MOL010898	0.7424	0.2576	0.8128	Semen Aesculi	escin	Not Available	FALSE	O(C1C2(C(C3=CCC4C(C3(CC2O)C)(CCC2C4(CCC(OC3OC(C(OC4OC(C(O)C(O)C4O)CO)C(O)C3OC3OC(C(O)C(O)C3O)CO)C(=O)O)C2(CO)C)C)C)CC(C1OC(=O)/C(=C\C)/C)(C)C)CO)C(=O)C
MOL010899	0.4006	0.5994	0.7667	Semen Aesculi	aescin	Not Available	FALSE	O(C1C2(C(C3=CCC4C(C3(CC2O)C)(CCC2C4(CCC(O)C2(CO)C)C)C)CC(C1OC(=O)/C(=C\C)/C)(C)C)CO)C(=O)C
MOL010900	0.2168	0.7832	0.6260	Semen Aesculi	spinastenol	Not Available	FALSE	C1CC(CC2C1(C1C(=CC2)C2C(CC1)(C(CC2)C(/C=C\C(C(C)C)CC)C)C)C)O
MOL010901	0.5667	0.4333	0.7162	Semen Aesculi	Escinidin	185465	FALSE	OC1C2(C(C3=CCC4C(C3(C1)C)(CCC1C4(CCC(O)C1(C)C)C)C)CC(C(O)C2O)(C)C)CO
MOL010902	0.9343	0.0657	0.7292	Semen Aesculi	wilsonic acid	Not Available	FALSE	c1cccc2c1C1(C2C(=C)N1)C(=O)O
MOL010904	0.9092	0.0908	0.6397	Linderae Radix	Dimethulen	10719	FALSE	c12c(ccc2C)c(ccc(c1)CC)C
MOL010905	0.8091	0.1909	0.7517	Linderae Radix	linderalactone	Not Available	FALSE	c12c(occ2C)C/C(=C/CCC2=CC1OC2=O)/C
MOL010906	0.9126	0.0874	0.8807	Linderae Radix	isolinderoxide	Not Available	FALSE	CCCC1C(CCCCC(C)C)O1
MOL010907	0.8030	0.1970	0.8197	Linderae Radix	Norboldine	22179	FALSE	c12c3c4c(CC1NCCc2cc(c3OC)O)cc(c(c4)OC)O
MOL010908	0.8142	0.1858	0.7732	Linderae Radix	Lindenenol	Not Available	FALSE	C12C3(C(C(=C)C1C2)C(c1c(C3)occ1C)O)C
MOL010909	0.8938	0.1062	0.8625	Linderae Radix	dodeca-1,4-dien-3-one	5971051	FALSE	C=CC(=O)/C=C/CCCCCCC
MOL010910	0.8823	0.1177	0.8100	Linderae Radix	(4E)-dodeca-1,4-diene	5326948	FALSE	C=CC/C=C/CCCCCCC

MOL010911	0.9515	0.0485	0.9302	Linderae Radix	3,4,5-Hemimelliten ol	10696	FALSE	c1(c(cc(cc1C)O)C)C
MOL010912	0.9076	0.0924	0.8700	Linderae Radix	Linderic acid	5282730	FALSE	C(=O)(CC/C=C/CCCCCCC)O
MOL010913	0.8382	0.1618	0.7352	Linderae Radix	C09495	Not Available	FALSE	C123C(O1)C(c1c(occ1C)C/C(=C/CC3)/C)OC2=O
MOL010914	0.9146	0.0854	0.8845	Linderae Radix	linderoxide	Not Available	FALSE	CCCC1C(CCCCCCC)O1
MOL010915	0.8657	0.1343	0.7855	Linderae Radix	neolinderalact one	Not Available	FALSE	O1C2c3c(/C(=C\CCC(C1=O)C2)/C)occ3C
MOL010916	0.8942	0.1058	0.8291	Linderae Radix	nubigenol	Not Available	FALSE	C(=O)(C(Cc1ccc(cc1)O)O)c1c(cc(cc1O)O)O
MOL010917	0.7465	0.2535	0.8784	Linderae Radix	Boldine	10154	TRUE	c12c3c4c(CC1N(CCc2cc(c3OC)O)C)cc(c(c4)OC)O
MOL010918	0.8930	0.1070	0.7836	Lysimachiae Foenigraeci Herba	Aseanostatin P1	520298	FALSE	C(CCCCCCCCCCC(=O)O)(C)C
MOL010918	0.8930	0.1070	0.7836	Amygdalus Communis Vas	Aseanostatin P1	520298	FALSE	C(CCCCCCCCCCC(=O)O)(C)C
MOL010919	0.6771	0.3229	0.9532	Amygdalus Communis Vas	17-beta-estradiol	5757	TRUE	C12C3C(c4c(CC3)cc(cc4)O)CCC1(C(CC2)O)C
MOL010920	0.9264	0.0736	0.9591	Amygdalus Communis Vas	6-Oxooctanoic acid	77914	FALSE	C(=O)(CCCCC(=O)O)CC
MOL010921	0.6491	0.3509	0.9391	Amygdalus Communis Vas	estrone	6918970	FALSE	C12C3C(c4c(CC3)cc(cc4)O)CCC1(C(=O)CC2)C
MOL010922	0.4912	0.5088	0.6259	Amygdalus Communis Vas	Diisooctyl succinate	120074	FALSE	C(=O)(CCC(=O)OCCCCCC(C)C)OCCCCCC(C)C
MOL010925	0.7655	0.2345	0.6041	Amygdalus Communis Vas	Isooleic acid	5282760	FALSE	C(CC/C=C/CCCCCCC)CCCCCC(=O)O
MOL010925	0.7655	0.2345	0.6041	Foeniculi Fructus	Isooleic acid	5282760	FALSE	C(CC/C=C/CCCCCCC)CCCCCC(=O)O
MOL010925	0.7655	0.2345	0.6041	Arisaematis Rhizoma	Isooleic acid	5282760	FALSE	C(CC/C=C/CCCCCCC)CCCCCC(=O)O
MOL010926	0.8834	0.1166	0.6953	Amygdalus Communis Vas	2-Hydroxy-hexadecanoic acid	12575964	FALSE	C(CCCCCCCCCCCC)CC(C(=O)O)O
MOL010927	0.9150	0.0850	0.9004	Amygdalus Communis Vas	2-undecenoic acid	5282728	FALSE	C(=O)(/C=C/CCCCCCCC)O
MOL010930	0.8287	0.1713	0.6709	Eriobotryae Folium	10,10-dimethyl-2,6-bis(methylene)-dicyclo[7.2.0]undecane	Not Available	FALSE	C12C(=C)CCCC(=C)CCC1C(C2)(C)C
MOL010930	0.8287	0.1713	0.6709	Ardisiae Japonicae Herba	10,10-dimethyl-2,6-bis(methylene)-dicyclo[7.2.0]undecane	Not Available	FALSE	C12C(=C)CCCC(=C)CCC1C(C2)(C)C

MOL010931	0.8508	0.1492	0.7032	Eriobotryae Folium	(4R)-3,5,5-trimethyl-4-[(E,3R)-3-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybut-1-enyl]cyclohex-2-en-1-one	9820702	FALSE	C1C(=O)C=C(C(C1(C)C)/C=C/C(C)OC1C(O)C(O)C(O)C(O1)CO)C
MOL010931	0.8508	0.1492	0.7032	Ardisiae Japonicae Herba	(4R)-3,5,5-trimethyl-4-[(E,3R)-3-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybut-1-enyl]cyclohex-2-en-1-one	9820702	FALSE	C1C(=O)C=C(C(C1(C)C)/C=C/C(C)OC1C(O)C(O)C(O)C(O1)CO)C
MOL010931	0.8508	0.1492	0.7032	Daturae Flos	(4R)-3,5,5-trimethyl-4-[(E,3R)-3-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybut-1-enyl]cyclohex-2-en-1-one	9820702	FALSE	C1C(=O)C=C(C(C1(C)C)/C=C/C(C)OC1C(O)C(O)C(O)C(O1)CO)C
MOL010932	0.9299	0.0701	0.7515	Daturae Flos	(4R)-4-[(E,3R)-3-hydroxybut-1-enyl]-3,5,5-trimethylcyclohex-2-en-1-one	13857510	FALSE	C1C(=O)C=C(C(C1(C)C)/C=C/C(C)O)C

MOL010932	0.9299	0.0701	0.7515	Eriobotryae Folium	(4R)-4-[(E,3R)-3-hydroxybut-1-enyl]-3,5,5-trimethylcyclohex-2-en-1-one	13857510	FALSE	C1C(=O)C=C(C(C1(C)C)/C=C/C(C)O)C
MOL010932	0.9299	0.0701	0.7515	Ardisiae Japonicae Herba	(4R)-4-[(E,3R)-3-hydroxybut-1-enyl]-3,5,5-trimethylcyclohex-2-en-1-one	13857510	FALSE	C1C(=O)C=C(C(C1(C)C)/C=C/C(C)O)C
MOL010933	0.7748	0.2252	0.8167	Ardisiae Japonicae Herba	ardisianoside K	Not Available	FALSE	O1C2C3(C4(C(C5(C(CC4)C(C(OC4OCC(OC6OC(C(O)C(O)C6OC6OC(C(O)C(O)C6O)C)CO)C(O)C4OC4OC(C(O)C(O)C4O)CO)CC5)(C)C)C)CC=C3C3C(C12)(CCC(C3)(CO)C)CO)C)C
MOL010934	0.4585	0.5415	0.7710	Ardisiae Japonicae Herba	ardisianoside K_qt	Not Available	FALSE	O1C2C3(C4(C(C5(C(CC4)C(C)(C(O)CC5)C)C)CC=C3C3C(C12)(CCC(C3)(CO)C)CO)C)C
MOL010935	0.7740	0.2260	0.8218	Ardisiae Japonicae Herba	ardisicrenoside A	Not Available	FALSE	O1C23C(C4(C(C5(C(CC4)C(C(OC4OCC(OC6OC(C(O)C(O)C6OC6OC(C(O)C(O)C6O)C)CO)C(O)C4OC4OC(C(O)C(O)C4O)CO)CC5)(C)C)C)CC3)C)(CC(O)C3(C2CC(CC3)(CO)C)C1)C
MOL010936	0.4598	0.5402	0.7867	Ardisiae Japonicae Herba	ardisianoside F_qt	Not Available	FALSE	O1C23C(C4(C(C5(C(CC4)C(C(O)CC5)(C)C)C)CC3)C)(CC(O)C3(C2CC(CC3)(CO)C)C1)C
MOL010937	0.7704	0.2296	0.8114	Ardisiae Japonicae Herba	ardisicrenoside G	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C(=O)O)CO)C)C)(C)C)OC1OCC(C(C1OC1C(O)C(O)C(O)C(O1)CO)O)OC1OC(C(C(C1OC1C(O)C(O)C(O)C(O1)C)O)O)CO
MOL010938	0.7175	0.2825	0.7670	Ardisiae Japonicae Herba	ardisicrenoside G_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C(=O)O)CO)C)C)(C)C)O
MOL010939	0.4874	0.5126	0.6377	Ardisiae Japonicae Herba	2-methyl-5-[(Z)-tridec-8-enyl]resorcinol	6440454	FALSE	Oc1c(c(O)cc(c1)CCCCCCC/C=C\CCCC)C
MOL010940	0.4874	0.5126	0.6377	Ardisiae Japonicae Herba	Ardisinol I	5319846	FALSE	Oc1cc(CCCCCCC/C=C/CCCC)cc(O)c1C
MOL010941	0.5854	0.4146	0.7182	Ardisiae Japonicae Herba	Ardisinol II	5319856	FALSE	Oc1cc(CCCCCCC/C=C/CCCC)cc(O)c1
MOL010942	0.4449	0.5551	0.6733	Ardisiae Japonicae Herba	ardisinol	Not Available	FALSE	c1(c(c(c(cc1)C(CCCCC)C/C=C/CCCC)O)C)O

MOL010943	0.7014	0.2986	0.8310	Ardisiae Japonicae Herba	1-(4-Hydroxy-3-methoxyphenyl)-3,5-diacetoxytane	Not Available	FALSE	c1(c(ccc(c1)CCC(OC(=O)C)CC(OC(=O)C)CCC)O)OC
MOL010944	0.9014	0.0986	0.9637	Ardisiae Japonicae Herba	phenylmethanediol	427890	FALSE	C(c1ccccc1)(O)O
MOL010945	0.9095	0.0905	0.9514	Ardisiae Japonicae Herba	(2-hydroxyphenyl)methyl benzoate	12731045	FALSE	C(=O)(c1ccccc1)OCc1c(cccc1)O
MOL010946	0.9463	0.0537	0.9380	Ardisiae Japonicae Herba	PHENYLACETONE	7678	FALSE	C(=O)(C)Cc1ccccc1
MOL010946	0.9463	0.0537	0.9380	Panacis Quinquefolii Radix	PHENYLACETONE	7678	FALSE	C(=O)(C)Cc1ccccc1
MOL010947	0.8644	0.1356	0.6151	Campsis Flos	(Z)-calamenene	6429077	FALSE	C1(CCC(c2c1cc(cc2)C)C)C(C)C
MOL010947	0.8644	0.1356	0.6151	Ardisiae Japonicae Herba	(Z)-calamenene	6429077	FALSE	C1(CCC(c2c1cc(cc2)C)C)C(C)C
MOL010948	0.7692	0.2308	0.7362	Ardisiae Japonicae Herba	caryophyllenyl alcohol	Not Available	FALSE	C1(C2C(C1)C(CCCC(/C=C/2\O)C)C)(C)C
MOL010949	0.7679	0.2321	0.8085	Ardisiae Japonicae Herba	Cyclamin	Not Available	FALSE	O1C23C(C4(C(C5(C(CC4)C(C(OC4OCC(OC6OC(C(O)C(OC7OC(C(O)C(O)C7O)CO)C6OC6OCC(O)C(O)C6O)CO)C(O)C4OC4OC(C(O)C(O)C4O)CO)CC5)(C)C)C)CC3)C)(CC(O)C3(C2CC(CC3)(C)C=O)C1)C
MOL010950	0.4161	0.5839	0.7965	Ardisiae Japonicae Herba	cyclamin_qt	Not Available	FALSE	O1C23C(C4(C(C5(C(CC4)C(C(O)CC5)(C)C)C)CC3)C)(CC(O)C3(C2CC(C=O)(CC3)C)C1)C
MOL010951	0.9636	0.0364	0.9171	Ardisiae Japonicae Herba	Methylsyringol	12462	FALSE	c1(c(OC)cccc1OC)OC
MOL010952	0.7546	0.2454	0.8206	Ardisiae Japonicae Herba	triterpenoid glycoside 1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C3(CC1)C1C(C(C2)O)(CCC(C1)(C)C=O)CO3)C)C)C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)OC1OC(C(C(C1O)O)O)C)CO)O)OC1OC(C(C(C1O)O)O)CO
MOL010953	0.4161	0.5839	0.7965	Ardisiae Japonicae Herba	triterpenoid glycoside 1_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C3(CC1)C1C(C(C2)O)(CCC(C1)(C)C=O)CO3)C)C)C)C)O
MOL010954	0.8814	0.1186	0.9500	Ardisiae Japonicae Herba	Tropyliden	11000	FALSE	C1C=CC=CC=C1
MOL010954	0.8814	0.1186	0.9500	Maydis Seigma	Tropyliden	11000	FALSE	C1C=CC=CC=C1
MOL010955	0.8444	0.1556	0.6645	Ardisiae Japonicae Herba	decahydro-2,2,4,8-tetramethyl-4,8-methano-azulen-9-ol	Not Available	FALSE	C1C(CC2C3(CCCC(C12)(C3O)C)C)(C)C

MOL010956	0.9134	0.0866	0.9703	Ardisiae Japonicae Herba	(3R,5S)-3,5-dimethyltetrahydrofuran-2-one	5324164	FALSE	O1C(=O)C(CC1C)C
MOL010957	0.9352	0.0648	0.9211	Ardisiae Japonicae Herba	(Z)-Ethyl cinnamate	5284656	FALSE	O(CC)C(=O)/C=C\c1ccccc1
MOL010957	0.9352	0.0648	0.9211	Cinnamomi Ramulus	(Z)-Ethyl cinnamate	5284656	FALSE	O(CC)C(=O)/C=C\c1ccccc1
MOL010958	0.8601	0.1399	0.7575	Ardisiae Japonicae Herba	(-)-Gallocatechol gallate	199472	FALSE	O1C(C(OC(=O)c2cc(O)c(O)c(O)c2)Cc2c1cc(O)cc2O)c1cc(O)c(O)c(O)c1
MOL010959	0.3966	0.6034	0.6969	Ardisiae Japonicae Herba	ilexol	Not Available	FALSE	OC1C(C2C(C3C(=CC2)C2(C(C4C(CC2)(CCC(C4C)C)C)(CC3)C)C)(CC1)C)(C)C
MOL010961	0.8822	0.1178	0.8398	Ginkgo Folium	Kaempferol 3-O-rhamnoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)C
MOL010961	0.8822	0.1178	0.8398	Ardisiae Japonicae Herba	Kaempferol 3-O-rhamnoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)C
MOL010962	0.8822	0.1178	0.8398	Ardisiae Japonicae Herba	kaempferol rhamnose	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1C(O)C(O)C(O)C(O1)C)c1ccc(cc1)O)O)O
MOL010963	0.8468	0.1532	0.8032	Ardisiae Japonicae Herba	5-hydroxy-2-(4-hydroxyphenyl)-3,7-bis[[(2R,3S,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy]chromone	11444588	FALSE	C1(C(C(C(OC1C)Oc1cc(c2c(c1)oc(c(c2=O)OC1OC(C(C(C1O)O)O)C)c1ccc(cc1)O)O)O)O)O
MOL010964	0.3711	0.6289	0.7063	Ardisiae Japonicae Herba	MAESANIN	5384838	FALSE	OC1=C(CCCCCCCCC/C=C\CCCC)C(=O)C(=CC1=O)OC
MOL010965	0.8981	0.1019	0.8770	Saxifraga Stolonifera	Norbergenin	73192	FALSE	O1C2C(OC(=O)c3c2c(O)c(O)c3)C(O)C(O)C1C
MOL010965	0.8981	0.1019	0.8770	Ardisiae Japonicae Herba	Norbergenin	73192	FALSE	O1C2C(OC(=O)c3c2c(O)c(O)c3)C(O)C(O)C1CO
MOL010966	0.3555	0.6445	0.8409	Ardisiae Japonicae Herba	Phthalic acid, isobutyl octyl ester	6423815	FALSE	C(=O)(c1c(C(=O)OCCCCCCCC)cccc1)OCC(C)C
MOL010968	0.7137	0.2863	0.8478	Ardisiae Japonicae Herba	primulanin	Not Available	FALSE	O1C23C(C4(C(C5(C(CC4)C(C(OC4OCC(OC6OC(C(O)C(O)C6OC6OCC(O)C(O)C6O)CO)C(O)C4O)CC5)(C)C)C)CC3)C)(CC(O)C3(C2CC(CC3)(C)C=O)C1)C

MOL010969	0.8917	0.1083	0.8797	Ardisiae Japonicae Herba	Propyl isothiocyanate	69403	FALSE	S=C=NCCC
MOL010970	0.8788	0.1212	0.8674	Ardisiae Japonicae Herba	(2S)-2-methylthiirane	21766881	FALSE	S1C(C1)C
MOL010972	0.8717	0.1283	0.7621	Ardisiae Japonicae Herba	Quercitrin-2'-gallate	5320864	FALSE	O1C(C(O)C(O)C(OC(=O)c2cc(O)c(O)c(O)c2)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1)C
MOL010973	0.6772	0.3228	0.7758	Ardisiae Japonicae Herba	Rapanone	100659	FALSE	OC1=C(CCCCCCCCCCCCC)C(=O)C(=CC1=O)O
MOL010974	0.8789	0.1211	0.7510	Ardisiae Japonicae Herba	tri-O-methylnorberberin	44584185	FALSE	c1(c(c(c2c(c1)C(=O)OC1C2OC(C(C1O)O)CO)OC)OC)OC
MOL010975	0.7553	0.2447	0.8075	Ardisiae Japonicae Herba	triterpene glycoside 4	Not Available	FALSE	C1C2C3(CCC1(C)C=O)C(CC1(C2(CCC2C1(CCC1C2(CCC(C1(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)OC1C(C(C(C(O1)C)O)O)O)CO)O)OC1OC(C(C(C1O)O)OC1OCC(C(C1O)O)O)CO)C)C)OC3)C)O
MOL010976	0.4161	0.5839	0.7965	Ardisiae Japonicae Herba	triterpene glycoside 4_qt	Not Available	FALSE	C1C2C3(CCC1(C=O)C)C(CC1(C2(CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)OC3)C)O
MOL010977	0.7066	0.2934	0.8163	Ardisiae Japonicae Herba	triterpenoid glycoside 2	Not Available	FALSE	C1C2C3(CCC1(C)OC(C)C)C(CC1(C2(CCC2C1(CCC1C2(CCC(C1(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)OC1C(C(C(C(O1)C)O)O)O)CO)O)OC1OC(C(C(C1O)O)O)CO)C)C)OC3)C)O
MOL010978	0.3904	0.6096	0.7786	Ardisiae Japonicae Herba	triterpenoid glycoside 2_qt	Not Available	FALSE	C1C2C3(CCC1(OC(C)C)C)C(CC1(C2(CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)OC3)C)O
MOL010979	0.9268	0.0732	0.9143	Ardisiae Japonicae Herba	2,4-Dimethylpentan-2-ol	12235	FALSE	CC(CC(C)C)(O)C
MOL010980	0.7567	0.2433	0.8164	Ardisiae Japonicae Herba	triterpenoid glycoside 3	Not Available	FALSE	C1C2C3(CCC1(C)C(=O)O)C(CC1(C2(CCC2C1(CCC1C2(CCC(C1(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)OC1C(C(C(C(O1)C)O)O)O)CO)O)OC1OC(C(C(C1O)O)O)CO)C)C)OC3)C)O
MOL010981	0.7184	0.2816	0.7787	Ardisiae Japonicae Herba	triterpenoid glycoside 3_qt	Not Available	FALSE	C1C2C3(CCC1(C)C(=O)O)C(CC1(C2(CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)OC3)C)O
MOL010983	0.4373	0.5627	0.7257	Ardisiae Japonicae Herba	2,5-Dihydroxy-3-[(10Z)-pentadec-10-en-1-yl]cyclohexa-2,5-diene-1,4-dione	Not Available	FALSE	C1(=O)C(=C(C(=O)C(=C1)O)CCCCCCCCC/C=C\CCC)O

MOL010984	0.9035	0.0965	0.7876	Ardisiae Japonicae Herba	2H-benz[e]indol-2-one,1,3,3a,4,5,9b-hexahydro-	Not Available	FALSE	N1C(=O)CC2c3c(CCC12)cccc3
MOL010985	0.4223	0.5777	0.7330	Ardisiae Japonicae Herba	2-hydroxy-5-methoxy-3-pentadecaenyl benzoquinone	Not Available	FALSE	C1(=O)C(=CC(=O)C=C1)CC(/C=C/C(CCCCCCCCCCC)OC)O
MOL010986	0.8508	0.1492	0.7032	Ardisiae Japonicae Herba	(7E)-9-hydroxymegastigma-4, 7-dien-3-on-9-O-beta-D-glucopyranoside	38346679	FALSE	C1(OC(C(C(C1O)O)O)CO)OC(/C=C/C1C(=CC(=O)CC1(C)C)C)C
MOL010987	0.9299	0.0701	0.7515	Ardisiae Japonicae Herba	(7E)-9-hydroxymegastigma-4, 7-dien-3-on-9-O-beta-D-glucopyranoside_qt	Not Available	FALSE	OC(C)/C=C/C1C(=CC(=O)CC1(C)C)C
MOL010988	0.9535	0.0465	0.9776	Ardisiae Japonicae Herba	2-methyl-5-(1-methylethylidene)-cyclo-hexanone	14440745	FALSE	C1(=O)C(CCC(=C(C)C)C1)C
MOL010990	0.9305	0.0695	0.9453	Ardisiae Japonicae Herba	Isomatsutakeol	5318599	FALSE	C(/C=C/CCCCC)O
MOL010991	0.9353	0.0647	0.9686	Ardisiae Japonicae Herba	(2S)-pentan-2-ol	2724896	FALSE	CC(CCC)O
MOL010992	0.9516	0.0484	0.8956	Ardisiae Japonicae Herba	3,4,5-Trimethoxybenzaldehyde	6858	FALSE	C(=O)c1cc(c(c(c1)OC)OC)OC
MOL010993	0.9217	0.0783	0.9611	Ardisiae Japonicae Herba	(E)-3,4-dimethylhex-3-en-2-one	5363236	FALSE	CC(=O)/C(=C(/CC)\C)/C

MOL010994	0.7136	0.2864	0.8426	Ardisiae Japonicae Herba	3beta-O-(alpha-L-rhamnopyranosyl-(1-2)-beta-D-glucopyranosyl-(1-4)-alpha-L-arabinopynanosyl)cyclamiretin A	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C3(CC1)C1C(C(C2)O)(CCC(C1)(C)C=O)C(=C)O3)C)C)(C)C)OC1OCC(C(C1O)O)OC1OC(C(C(C1OC1C(O)C(O)C(O)C(O1)C)O)O)CO
MOL010995	0.4123	0.5877	0.7956	Ardisiae Japonicae Herba	3beta-O-(alpha-L-rhamnopyranosyl-(1-2)-beta-D-glucopyranosyl-(1-4)-alpha-L-arabinopynanosyl)cyclamiretin A_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C3(CC1)C1C(C(C2)O)(CCC(C1)(C)C=O)C(=C)O3)C)C)(C)C)O
MOL010996	0.9188	0.0812	0.9388	Ardisiae Japonicae Herba	3-hexen-2-one(E)	5367744	FALSE	CC(=O)/C=C/CC
MOL010997	0.8999	0.1001	0.8964	Ardisiae Japonicae Herba	3-Hexynol	66083	FALSE	C(CC#CCC)O
MOL010998	0.9133	0.0867	0.9613	Ardisiae Japonicae Herba	3-methoxy-1-ethenyl-cyclopentene	Not Available	FALSE	C1(=CC(CC1)OC)C=C
MOL010999	0.9534	0.0466	0.8859	Ardisiae Japonicae Herba	2-isopropyl-3-methyl-1-cyclohex-2-enone	10103344	FALSE	C1(=O)C(=C(CCC1)C)C(C)C
MOL011000	0.8363	0.1637	0.7550	Ardisiae Japonicae Herba	(E,Z)-alpha-farnesene	5353086	FALSE	C=C/C(=C/C/C=C(/C)\CCC=C(C)C)/C
MOL011001	0.9135	0.0865	0.9324	Ardisiae Japonicae Herba	Mesityloxid	8858	FALSE	CC(=O)C=C(C)C
MOL011001	0.9135	0.0865	0.9324	Rhododendri Daurici Folium	Mesityloxid	8858	FALSE	CC(=O)C=C(C)C
MOL011001	0.9135	0.0865	0.9324	Caulis Akebiae	Mesityloxid	8858	FALSE	CC(=O)C=C(C)C
MOL011001	0.9135	0.0865	0.9324	Mahoniae Caulis	Mesityloxid	8858	FALSE	CC(=O)C=C(C)C

MOL011002	0.2986	0.7014	0.6353	Ardisiae Japonicae Herba	5-ethoxy-2-hydroxy-3-[(10Z)-pentadec-10-en-1-yl][1,4]benzoquinone	Not Available	FALSE	C1(=O)C(=C(C(=O)C(=C1)OCC)CCCCCCCCC/C=C\CCCC)O
MOL011003	0.3748	0.6252	0.7158	Ardisiae Japonicae Herba	5-ethoxy-2-hydroxy-3-[(8Z)-tridec-8-en-1-yl][1,4]benzoquinone	Not Available	FALSE	C1(=O)C(=C(C(=O)C(=C1)OCC)CCCCCCC/C=C\CCCC)O
MOL011004	0.9261	0.0739	0.9336	Ardisiae Japonicae Herba	(E)-5-methyloct-5-en-1-ol	6536854	FALSE	C(CCC/C(=C/CC)/C)O
MOL011005	0.9025	0.0975	0.8107	Ardisiae Japonicae Herba	6-O-Methyl catalpol	Not Available	FALSE	O1C2(C1C(OC)C1C2C(OC=C1)OC1OC(C(O)C(O)C1O)CO)CO
MOL011006	0.9255	0.0745	0.7725	Ardisiae Japonicae Herba	6-O-Methyl catalpol_qt	Not Available	FALSE	O1C2(C1C(OC)C1C2C(OC=C1)O)CO
MOL011007	0.9225	0.0775	0.9254	Ardisiae Japonicae Herba	1-(1-ethoxyethoxy)hexane	Not Available	FALSE	O(CCCCCC)C(OCC)C
MOL011008	0.8587	0.1413	0.9256	Ardisiae Japonicae Herba	8-oxabicyclo[5.1.0]octane	642973	FALSE	O1C2C1CCCCC2
MOL011010	0.7923	0.2077	0.7639	Ardisiae Japonicae Herba	ardimerin digallate	Not Available	FALSE	O1C(C(O)C(O)C(O)C1COC(=O)c1cc(O)c(O)c(O)c1)c1c(OC)c(O)c2OC(=O)c3cc(C4OC(C(O)C(O)C4O)COC(=O)c4cc(O)c(O)c(O)c4)c(OC)c(O)c3OC(=O)c2c1
MOL011011	0.8809	0.1191	0.7598	Ardisiae Japonicae Herba	ardimerin	44423020	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(OC)c(O)c2OC(=O)c3cc(C4OC(C(O)C(O)C4O)CO)c(OC)c(O)c3OC(=O)c2c1
MOL011012	0.9348	0.0652	0.9445	Ardisiae Japonicae Herba	1-(1-ethoxyethoxy)pentane	Not Available	FALSE	O(CCCCC)C(OCC)C
MOL011012	0.9348	0.0652	0.9445	Panacis Japonici Rhizoma	1-(1-ethoxyethoxy)pentane	Not Available	FALSE	O(CCCCC)C(OCC)C
MOL011013	0.7842	0.2158	0.8151	Ardisiae Japonicae Herba	ardisiamamilloside C	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)CO)CO)C)C)(C)C)OC1OCC(C(C1OC1C(O)C(O)C(O)C(O1)CO)O)OC1OC(C(C(C1OC1C(O)C(O)C(O)C(O1)C)O)O)CO
MOL011014	0.4484	0.5516	0.7679	Ardisiae Japonicae Herba	ardisiamamilloside C_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)CO)CO)C)C)(C)C)O

MOL011015	0.7618	0.2382	0.8168	Ardisiae Japonicae Herba	ardisiamamilloside F	Not Available	FALSE	O(C1CCC2(C(C1(C)C)CCC1(C2CCC23C1(CC(C1(C2CC(CC1)(C(=O)O)C)CO3)O)C)C)C1C(OC2C(O)C(O)C(O)C(O2)CO)C(C(OC2OC(C(C(C2OC2OC(C(C(C2O)O)O)C)O)O)CO)CO1)O
MOL011016	0.7184	0.2816	0.7787	Ardisiae Japonicae Herba	ardisiamamilloside F_qt	Not Available	FALSE	OC1CCC2(C(C1(C)C)CCC1(C2CCC23C1(CC(C1(C2CC(CC1)(C(=O)O)C)CO3)O)C)C)C
MOL011017	0.7066	0.2934	0.8477	Ardisiae Japonicae Herba	ardisiamamilloside H	Not Available	FALSE	O1C23C(C4(C(C5(C(CC4)C(C(OC4OCC(OC6OC(C(O)C(O)C6OC6OC(C(O)C(O)C6O)C)CO)C(O)C4O)CC5)(C)C)C)CC3)C)(CC(=O)C3(C2CC(CC3)(C)C=O)C1)C
MOL011018	0.3755	0.6245	0.7837	Ardisiae Japonicae Herba	ardisiamamilloside H_qt	Not Available	FALSE	O1C23C(C)(C4(C(C5(C(CC4)C(C(O)CC5)(C)C)C)C3)C)CC(=O)C3(C2CC(C=O)(CC3)C)C1
MOL011019	0.3856	0.6144	0.7603	Ardisiae Japonicae Herba	ardisianone A	Not Available	FALSE	O=C1C(=CC(=O)C=C1)C(CCCCC)CC/C=C/CCCC
MOL011020	0.4153	0.5847	0.7426	Ardisiae Japonicae Herba	ardisianone B	Not Available	FALSE	O(C(CCC(CCCCC)C1=C(O)C(=O)C=CC1=O)C=C/CCC)C
MOL011021	0.7782	0.2218	0.7960	Ardisiae Japonicae Herba	ardisianoside A	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C3(CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=C)O3)C)C)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)CO)O)OC1OC(C(C(C1OC1OCC(C(C1O)O)O)O)OC1OC(C(C(C1O)OC1C(O)C(O)C(O)C(O)C(O1)CO)OC1C(O)C(O)C(O)C(O1)CO)CO)O)CO
MOL011022	0.4578	0.5422	0.7949	Ardisiae Japonicae Herba	ardisianoside C_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C3(CC1)C1C(C(C2)O)(CCC(C1)(C)C)CO3)C)C)(C)C)O
MOL011023	0.7793	0.2207	0.8021	Ardisiae Japonicae Herba	ardisianoside B	Not Available	FALSE	O1C23C(C4(C(C5(C(CC4)C(C(OC4OCC(OC6OC(C(O)C(OC7OC(C(O)C(OC8OC(C(O)C(O)C8O)CO)C7O)CO)C6OC6OCC(O)C(O)C6O)CO)C(O)C4OC4OC(C(O)C(O)C4O)CO)CC5)(C)C)C)CC3)C)(CC(O)C3(C2CC(CC3)(C)C)C1)C
MOL011024	0.7325	0.2675	0.8445	Ardisiae Japonicae Herba	ardisianoside C	Not Available	FALSE	O1C23C(C4(C(C5(C(CC4)C(C(OC4OCC(OC6OC(C(O)C(O)C6OC6OC(C(O)C(O)C6O)C)CO)C(O)C4O)CC5)(C)C)C)CC3)C)(CC(O)C3(C2CC(CC3)(C)C)C1)C
MOL011025	0.7085	0.2915	0.8351	Ardisiae Japonicae Herba	ardisianoside D	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C3(CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=C)O3)C)C)(C)C)OC1OCC(C(C1O)O)OC1OC(C(C(C1OC1C(O)C(O)C(O)CO1)O)O)CO
MOL011026	0.4413	0.5587	0.7983	Ardisiae Japonicae Herba	ardisianoside D_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C3(CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=C)O3)C)C)(C)C)O
MOL011027	0.7479	0.2521	0.8452	Ardisiae Japonicae Herba	ardisianoside E	Not Available	FALSE	O1C23C(C4(C(C5(C(CC4)C(C(OC4OCC(OC6OC(C(O)C(O)C6O)CO)C(O)C4OC4OC(C(O)C(O)C4O)CO)CC5)(C)C)C)CC3)C)(CC(O)C3(C2CC(CC3)(CO)C)C1)C
MOL011028	0.9572	0.0428	0.8982	Ardisiae Japonicae Herba	1(2H)-naphthalenone,3,4,4a,5,8,8a-hexahydro-8a-methyl-,trans-	12512776	FALSE	C1(=O)CCCC2CC=CCC12C

MOL011029	0.7756	0.2244	0.8086	Ardisiae Japonicae Herba	ardisianoside F	Not Available	FALSE	O1C23C(C4(C(C5(C(CC4)C(C(OC4OCC(OC6OC(C(O)C(OC7OC(C(O)C(O)C7O)CO)C6OC6OCC(O)C(O)C6O)CO)C(O)C4OC4OC(C(O)C(O)C4O)CO)CC5)(C)C)C)CC3)C)(CC(O)C3(C2CC(CC3)(CO)C)C1)C
MOL011030	0.7522	0.2478	0.8247	Ardisiae Japonicae Herba	ardisianoside G	Not Available	FALSE	O1C23C(C4(C(C5(C(CC4)C(C(OC4OCC(OC6OC(C(O)C(O)C6OC6OC(C(O)C(O)C6O)C)CO)C(O)C4OC4OC(C(O)C(O)C4O)CO)CC5)(C)C)C)CC3)C)(CC(O)C3(C2CC(O)(CC3)C)C1)C
MOL011031	0.4977	0.5023	0.7641	Ardisiae Japonicae Herba	ardisianoside G_qt	Not Available	FALSE	O1C23C(C4(C(C5(C(CC4)C(C(O)CC5)(C)C)C)CC3)C)(CC(O)C3(C2CC(O)(CC3)C)C1)C
MOL011032	0.7853	0.2147	0.8004	Ardisiae Japonicae Herba	ardisianoside H	Not Available	FALSE	O1C23C(C4(C(C5(C(CC4)C(C(OC4OCC(OC6OC(C(O)C(OC7OC(C(OC8OC(C(O)C(O)C8O)CO)C(OC8OC(C(O)C(O)C8O)CO)C7O)CO)C6OC6OCC(O)C(O)C6O)CO)C(O)C4OC4OC(C(O)C(O)C4O)CO)CC5)(C)C)C)CC3)C)(CC(O)C3(C2CC(CC3)(C)C)C1=O)C
MOL011033	0.4557	0.5443	0.7995	Ardisiae Japonicae Herba	ardisianoside H_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C3(CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)O3)C)C)(C)C)O
MOL011034	0.7535	0.2465	0.8208	Ardisiae Japonicae Herba	ardisianoside I	Not Available	FALSE	O1C23C(C4(C(C5(C(CC4)C(C(OC4OCC(OC6OC(C(O)C(O)C6OC6OC(C(O)C(O)C6O)C)CO)C(O)C4OC4OC(C(O)C(O)C4O)CO)CC5)(C)C)C)CC3)C)(CC(O)C3(C2CC(CC3)(CO)C)C1=O)C
MOL011035	0.4974	0.5026	0.7682	Ardisiae Japonicae Herba	ardisianoside I_qt	Not Available	FALSE	O1C(=O)C23C(C41C(C1(C(C5(C(CC1)C(C(O)CC5)(C)C)C)CC4)C)(CC2O)C)CC(CC3)(CO)C
MOL011036	0.7411	0.2589	0.8208	Ardisiae Japonicae Herba	ardisianoside J	Not Available	FALSE	O1C23C(C4(C(C5(C(CC4)C(C(OC4OCC(OC6OC(C(O)C(O)C6OC6OC(C(O)C(O)C6O)C)CO)C(O)C4OC4OC(C(O)C(O)C4O)CO)CC5)(C)C)C)CC3)C)(CC(O)C3(C2CC(CC3)(C)C=O)C1=O)C
MOL011037	0.4610	0.5390	0.7718	Ardisiae Japonicae Herba	ardisianoside J_qt	Not Available	FALSE	O1C(=O)C23C(C41C(C1(C(C5(C(CC1)C(C(O)CC5)(C)C)C)CC4)C)(CC2O)C)CC(C=O)(CC3)C
MOL011038	0.8979	0.1021	0.8011	Ginkgo Semen	(+)-Catechin-5-O-glucoside	6324898	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1cc(c(cc1)O)O)OC1OC(C(C(C1O)O)O)CO)O
MOL011038	0.8979	0.1021	0.8011	Jujubae Fructus	(+)-Catechin-5-O-glucoside	6324898	FALSE	c1(cc(c2c(c1)OC(C(C2)O)c1cc(c(cc1)O)O)OC1OC(C(C(C1O)O)O)CO)O
MOL011039	0.7654	0.2346	0.6033	Oroxyli Semen	Vaccenic acid	5281127	FALSE	OC(=O)CCCCCCCCC/C=C/CCCCCC
MOL011039	0.7654	0.2346	0.6033	Ginkgo Semen	Vaccenic acid	5281127	FALSE	OC(=O)CCCCCCCCC/C=C/CCCCCC
MOL011039	0.7654	0.2346	0.6033	Jujubae Fructus	Vaccenic acid	5281127	FALSE	OC(=O)CCCCCCCCC/C=C/CCCCCC
MOL011039	0.7654	0.2346	0.6033	Cucurbitae Moschatae Semen	Vaccenic acid	5281127	FALSE	OC(=O)CCCCCCCCC/C=C/CCCCCC
MOL011041	0.4833	0.5167	0.7038	Ginkgo Semen	16-Propoxystrychnine	Not Available	FALSE	O(C12N3CCC41C1N(c5c4cccc5)C(=O)CC4OCC=C(C(C14)C2)C3)CCC

MOL011042	0.6778	0.3222	0.7415	Ginkgo Semen	18alpha-Hydroglycyrrhetic acid	Not Available	FALSE	OC12C3=CC(=O)C4C(C3(CCC1(CCC(O)(C2)C(=O)O)C)C)(CCC1C4(CCC(O)C1(C)C)C)C
MOL011043	0.2762	0.7238	0.8330	Ginkgo Semen	20(R)-Ginsenoside-Rh2	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3O)CO)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL011044	0.2305	0.7695	0.7376	Ginkgo Semen	20(R)-Ginsenoside-Rh2_qt	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL011045	0.9428	0.0572	0.9504	Ginkgo Semen	4-Methoxypyridoxine	76581	FALSE	O(Cc1c(CO)cnc(c1O)C)C
MOL011046	0.9122	0.0878	0.8532	Ginkgo Semen	4-Nitrophenyl α-D-mannopyranoside	449023	FALSE	O1C(C(O)C(O)C(O)C1Oc1ccc([N+](=O)O)cc1)CO
MOL011047	0.9189	0.0811	0.9378	Ginkgo Semen	4-Nitrophenyl α-D-mannopyranoside_qt	980	FALSE	Oc1ccc([N+](=O)O)cc1
MOL011048	0.7987	0.2013	0.7028	Ginkgo Semen	6-Tridecylresorcylic acid	162958	FALSE	Oc1c(c(CCCCCCCCCCCCC)cc(O)c1)C(=O)O
MOL011049	0.4817	0.5183	0.8412	Ginkgo Semen	7-Epicephalomannine	Not Available	FALSE	O1C2C(OC(=O)C)(C3C(C(O)C2)(C(=O)C(OC(=O)C)C2=C(C(OC(=O)C(O)C(NC(=O)/C(=C/C)/C)c4ccccc4)CC(O)(C3OC(=O)c3ccccc3)C2(C)C)C)C)C1
MOL011051	0.6915	0.3085	0.6099	Anemarrhenae Rhizoma	Ginkgoic acid	5281858	FALSE	c1(cccc(c1C(=O)O)CCCCCCC/C=C\CCCCCC)O
MOL011051	0.6915	0.3085	0.6099	Ginkgo Folium	Ginkgoic acid	5281858	FALSE	c1(cccc(c1C(=O)O)CCCCCCC/C=C\CCCCCC)O
MOL011051	0.6915	0.3085	0.6099	Ginkgo Semen	Ginkgoic acid	5281858	FALSE	c1(cccc(c1C(=O)O)CCCCCCC/C=C\CCCCCC)O
MOL011052	0.6935	0.3065	0.6185	Ginkgo Semen	Anacardic acid C	5318418	FALSE	c1(cccc(c1C(=O)O)CCCCCCC/C=C\C/C=C/CCC)O
MOL011052	0.6935	0.3065	0.6185	Ginkgo Folium	Anacardic acid C	5318418	FALSE	c1(cccc(c1C(=O)O)CCCCCCC/C=C\C/C=C/CCC)O
MOL011053	0.6877	0.3123	0.6189	Ginkgo Semen	Anacaridic acid D	Not Available	FALSE	c1(cccc(c1C(=O)O)CCCCCCC/C=C\C/C=C/CC=C)O
MOL011053	0.6877	0.3123	0.6189	Ginkgo Folium	Anacaridic acid D	Not Available	FALSE	c1(cccc(c1C(=O)O)CCCCCCC/C=C\C/C=C/CC=C)O
MOL011054	0.3809	0.6191	0.6351	Ginkgo Folium	Bilobol	5281852	FALSE	Oc1cc(CCCCCCC/C=C\CCCCCC)cc(O)c1
MOL011054	0.3809	0.6191	0.6351	Ginkgo Semen	Bilobol	5281852	FALSE	Oc1cc(CCCCCCC/C=C\CCCCCC)cc(O)c1
MOL011055	0.9083	0.0917	0.9410	Ginkgo Semen	Cardiospermin	179647	FALSE	O1C(C(O)C(O)C(O)C1OC(C(=C)CO)C#N)CO
MOL011056	0.9182	0.0818	0.9596	Ginkgo Semen	Cardiospermin_qt	Not Available	FALSE	OC(C(=C)CO)C#N

MOL011058	0.9101	0.0899	0.6890	Ginkgo Semen	Ginkgolid A	Not Available	FALSE	C1(C(=O)OC2C1(C13C4(C2)C2(C(O1)OC(=O)C2O)C(CC4OC3=O)C(C)(C)C)O)C
MOL011059	0.9140	0.0860	0.6790	Ginkgo Semen	Ginkgolid B	Not Available	FALSE	C1(C(=O)OC2C1(C13C4(C2O)C2(C(O1)OC(=O)C2O)C(CC4OC3=O)C(C)(C)C)O)C
MOL011060	0.9101	0.0899	0.6890	Ginkgo Semen	ginkgolide a	Not Available	FALSE	C12C(C(C(=O)O1)C)(C13C4(C2)C2(C(O1)OC(=O)C2O)C(CC4OC3=O)C(C)(C)C)O
MOL011060	0.9101	0.0899	0.6890	Ginkgo Folium	ginkgolide a	Not Available	FALSE	C12C(C(C(=O)O1)C)(C13C4(C2)C2(C(O1)OC(=O)C2O)C(CC4OC3=O)C(C)(C)C)O
MOL011061	0.9140	0.0860	0.6790	Ginkgo Semen	Ginkgolide B	Not Available	FALSE	C12C(C(C(=O)O1)C)(C13C4(C2O)C2(C(O1)OC(=O)C2O)C(CC4OC3=O)C(C)(C)C)O
MOL011062	0.7710	0.2290	0.6585	Ginkgo Semen	6-Tridecylsalicylic acid	161306	FALSE	c1(c(c(ccc1)O)C(=O)O)CCCCCCCCCCCCC
MOL011064	0.8226	0.1774	0.6743	Ginkgo Semen	16-heptadecynoic acid	5312626	FALSE	OC(=O)CCCCCCCCCCCCCCCC#C
MOL011065	0.8573	0.1427	0.7229	Ginkgo Semen	(7Z,10Z)-hexadeca-7,10-dienoic acid	13932172	FALSE	OC(=O)CCCCC/C=C\C/C=C\CCCCC
MOL011066	0.8587	0.1413	0.8070	Ginkgo Semen	Isorhamnetin-3-arabinoglucoside	Not Available	FALSE	C1(C(C(C(OC1)OC1C(C(C(OC1CO)Oc1c(=O)c2c(oc1c1cc(c(cc1)O)OC)cc(cc2O)O)O)O)O)O)O
MOL011067	0.7985	0.2015	0.8862	Arisaematis Rhizoma	LACTONE	5585	TRUE	c12c(cc3c(c1C)oc(c3)C)c(cc(=O)o2)C
MOL011067	0.7985	0.2015	0.8862	Gleditsiae Spina	LACTONE	5585	TRUE	c12c(cc3c(c1C)oc(c3)C)c(cc(=O)o2)C
MOL011067	0.7985	0.2015	0.8862	Ginkgo Semen	LACTONE	5585	TRUE	c12c(cc3c(c1C)oc(c3)C)c(cc(=O)o2)C
MOL011070	0.8571	0.1429	0.7519	Ginkgo Semen	5,10-Pentadecadienoic acid, (Z,Z)-	5362874	FALSE	OC(=O)CCC/C=C/CCC/C=C/CCCC
MOL011071	0.9589	0.0411	0.8882	Ginkgo Semen	pinol	Not Available	FALSE	C1(OC2C=CC1CC2)(C)C
MOL011072	0.3399	0.6601	0.7603	Ginkgo Semen	Quinicine	Not Available	FALSE	c1(ccc2c(c1)c(ccn2)C(=O)CCC1C(C=C)CNCC1)OC
MOL011073	0.6297	0.3703	0.8452	Ginkgo Semen	Scillaren A	Not Available	FALSE	C1C(C=C2C(C1)(C1C(CC2)C2(C(CC1)(C(CC2)c1ccc(=O)oc1)C)O)C)OC1OC(C(C(C1O)O)OC1OC(C(C(C1O)O)O)CO)C
MOL011074	0.2549	0.7451	0.7653	Ginkgo Semen	Scillaren A_qt	Not Available	FALSE	C1C(C=C2C(C1)(C1C(CC2)C2(C(C)(CC1)C(c1ccc(=O)oc1)CC2)O)C)O
MOL011075	0.6996	0.3004	0.7855	Ginkgo Semen	Shikodonin	Not Available	FALSE	C1C2(C(C3(CC1)COC(=O)C14C3C(CC(C1)C(=C)C4=O)O)C(OC2)O)C
MOL011076	0.8402	0.1598	0.7410	Hedysari Radix	(+)-Medicarpin	73067	FALSE	O1C2C(c3c1cc(OC)cc3)COc1c2ccc(O)c1

MOL011077	0.9654	0.0346	0.8646	Hedysari Radix	methyl (Z)-3-(3,4,5-trimethoxyphenyl)prop-2-enoate	6431041	FALSE	O(c1c(OC)cc(cc1OC)/C=C\C(=O)OC)C
MOL011078	0.8594	0.1406	0.8929	Hedysari Radix	3',7-dihydroxy-4'-methoxy-isoflavone	46881076	FALSE	C1C(C(=O)c2ccc(cc2O1)O)c1cc(c(cc1)OC)O
MOL011079	0.9487	0.0513	0.9197	Hedysari Radix	2-[4-(methoxymethyl)phenyl]acetic acid	22988428	FALSE	c1(ccc(cc1)COC)CC(=O)O
MOL011081	0.5096	0.4904	0.6647	Hedysari Radix	Linolenic acid methyl ester	5367462	FALSE	O(C(=O)CCCCCCC/C=C/C/C=C/C/C=C/CC)C
MOL011083	0.7985	0.2015	0.9488	Hedysari Radix	2-methoxy-3-phenyl-chromone	20111922	FALSE	c1ccc2c(c1)oc(c(c2=O)c1ccccc1)OC
MOL011085	0.8143	0.1857	0.7360	Hedysari Radix	trioleic glyceride	56604910	FALSE	O(C(=O)CCCCCCCCCCCC)CC(O)CO
MOL011087	0.9288	0.0712	0.9706	Physochlainae Radix	2,3-Butanediol, meso-	220010	FALSE	CC(C(C)O)O
MOL011087	0.9288	0.0712	0.9706	Citri Sarcodactylis Fructus	2,3-Butanediol, meso-	220010	FALSE	CC(C(C)O)O
MOL011088	0.9116	0.0884	0.8842	Physochlainae Radix	2-Nitrobenzoic acid	11087	FALSE	OC(=O)c1c([N+](=O)O)cccc1
MOL011089	0.9527	0.0473	0.9705	Physochlainae Radix	Homoveratrole	68126	FALSE	O(c1c(OC)ccc(c1)C)C
MOL011089	0.9527	0.0473	0.9705	Mume Flos	Homoveratrole	68126	FALSE	O(c1c(OC)ccc(c1)C)C
MOL011090	0.9614	0.0386	0.9467	Physochlainae Radix	3-Methoxy-4-propoxybenzaldehyde	592110	FALSE	O(CCC)c1c(OC)cc(cc1)C=O

MOL011091	0.8768	0.1232	0.7744	Physochlainae Radix	[(1S,3S,5S,7S)-7-hydroxy-8-methyl-8-azabicyclo[3.2.1]octan-3-yl] (2S)-3-hydroxy-2-phenylpropanoate	183088	FALSE	OC1C2N(C(C1)CC(OC(=O)C(c1ccccc1)CO)C2)C
MOL011092	0.8158	0.1842	0.8815	Physochlainae Radix	apohyoscine	Not Available	FALSE	O1C2C1C1N(C2CC(OC(=O)C(=C)c2ccccc2)C1)C
MOL011093	0.8158	0.1842	0.8815	Daturae Flos	apohyoscine	Not Available	FALSE	O1C2C1C1N(C2CC(OC(=O)C(=C)c2ccccc2)C1)C
MOL011093	0.8158	0.1842	0.8815	Physochlainae Radix	apohyoscine	Not Available	FALSE	O1C2C1C1N(C2CC(OC(=O)C(=C)c2ccccc2)C1)C
MOL011094	0.8845	0.1155	0.6821	Physochlainae Radix	6-methoxy-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[[(2S,3R,4S,5R)-3,4,5-trihydroxytetrahydropyran-2-yl]oxymethyl]tetrahydropyran-2-yl]oxy-coumarin	10994544	FALSE	C1(C(C(OC(C1O)Oc1c(cc2c(c1)oc(=O)cc2)OC)COC1C(C(C(CO1)O)O)O)O)O
MOL011096	0.9410	0.0590	0.7714	Physochlainae Radix	scopoline	Not Available	FALSE	O1C2C3N(C(C2O)CC1C3)C
MOL011097	0.8985	0.1015	0.7865	Polygoni Tinctorii Foliu	3,5,4'-trihydroxy-6,7-methylenedioxyflavone-3-O-β-D-glucopyranoside	Not Available	FALSE	c12c(c(c3c(c1)oc(c(c3=O)OC1OC(CO)C(C(C1O)O)O)c1ccc(cc1)O)O)OCO2
MOL011098	0.5803	0.4197	0.7027	Polygoni Tinctorii Foliu	9alpha,13alpha-dihydroxylisopropylidenylisatisine,a	Not Available	FALSE	c12ccccc1[nH]cc2C12N(c3ccccc3C1=O)C(=O)C13C2OC(C1OC(O3)(C)C)CO

MOL011098	0.5803	0.4197	0.7027	Indigo Naturalis	9alpha,13alpha-dihydroxylisopropylidenylisatisine,a	Not Available	FALSE	c12ccccc1[nH]cc2C12N(c3ccccc3C1=O)C(=O)C13C2OC(C1OC(O3)(C)C)CO
MOL011099	0.9273	0.0727	0.9000	Polygoni Tinctorii Foliu	Adenosine	Not Available	FALSE	n1cnc2c(c1N)ncn2C1C(C(C(O1)CO)O)O
MOL011100	0.2484	0.7516	0.6402	Indigo Naturalis	bisindigotin	Not Available	FALSE	c1ccc2c(c1)C(=O)C(=N2)c1c(c2c([nH]1)cccc2)C1=c2c(=N/C/1=C\1/Nc3c(C1=O)cccc3)cccc2
MOL011100	0.2484	0.7516	0.6402	Polygoni Tinctorii Foliu	bisindigotin	Not Available	FALSE	c1ccc2c(c1)C(=O)C(=N2)c1c(c2c([nH]1)cccc2)C1=c2c(=N/C/1=C\1/Nc3c(C1=O)cccc3)cccc2
MOL011103	0.7499	0.2501	0.6019	Polygoni Tinctorii Foliu	Glucobrassicin-1-Sulfonate	Not Available	FALSE	S(/C(=N\OS(=O)(=O)O)/Cc1cn(c2c1cccc2)S(=O)(=O)O)C1OC(C(C(C1O)O)O)CO
MOL011105	0.9219	0.0781	0.8199	Indigo Naturalis	indican	Not Available	FALSE	c1ccc2c(c1)c(c[nH]2)OC1C(C(C(C(O1)CO)O)O)O
MOL011105	0.9219	0.0781	0.8199	Polygoni Tinctorii Foliu	indican	Not Available	FALSE	c1ccc2c(c1)c(c[nH]2)OC1C(C(C(C(O1)CO)O)O)O
MOL011106	0.9102	0.0898	0.8643	Indigo Naturalis	indican_qt	Not Available	FALSE	c1ccc2c(c1)C(C=[NH+]2)O
MOL011106	0.9102	0.0898	0.8643	Polygoni Tinctorii Foliu	indican_qt	Not Available	FALSE	c1ccc2c(c1)C(C=[NH+]2)O
MOL011107	0.9206	0.0794	0.8045	Polygoni Tinctorii Foliu	isatan B	Not Available	FALSE	O1C(C(O)C(=O)C(O)C1Oc1c2c([nH]c1)cccc2)CO
MOL011107	0.9206	0.0794	0.8045	Indigo Naturalis	isatan B	Not Available	FALSE	O1C(C(O)C(=O)C(O)C1Oc1c2c([nH]c1)cccc2)CO
MOL011108	0.7951	0.2049	0.7064	Polygoni Tinctorii Foliu	isatisine,a	Not Available	FALSE	c12ccccc1[nH]cc2C12N(c3ccccc3C1=O)C(=O)C1(C2OC(C1O)CO)O
MOL011108	0.7951	0.2049	0.7064	Indigo Naturalis	isatisine,a	Not Available	FALSE	c12ccccc1[nH]cc2C12N(c3ccccc3C1=O)C(=O)C1(C2OC(C1O)CO)O
MOL011109	0.9267	0.0733	0.8015	Polygoni Tinctorii Foliu	isoorientin	Not Available	FALSE	c1(ccc(c(c1)O)O)c1oc2c(c(=O)c1)c(c(c(c2)O)C1OC(C(C(C1O)O)O)O)O
MOL011109	0.9267	0.0733	0.8015	Indigo Naturalis	isoorientin	Not Available	FALSE	c1(ccc(c(c1)O)O)c1oc2c(c(=O)c1)c(c(c(c2)O)C1OC(C(C(C1O)O)O)O)O
MOL011110	0.9011	0.0989	0.8297	Indigo Naturalis	isoscoparin	Not Available	FALSE	c1(ccc(c(c1)OC)O)c1oc2c(c(=O)c1)c(c(c(c2)O)C1OC(C(C(C1O)O)O)O)O
MOL011110	0.9011	0.0989	0.8297	Polygoni Tinctorii Foliu	isoscoparin	Not Available	FALSE	c1(ccc(c(c1)OC)O)c1oc2c(c(=O)c1)c(c(c(c2)O)C1OC(C(C(C1O)O)O)O)O
MOL011111	0.9140	0.0860	0.8198	Polygoni Tinctorii Foliu	isovitexin	Not Available	FALSE	c1(ccc(cc1)O)c1oc2c(c(=O)c1)c(c(c(c2)O)C1OC(C(C(C1O)O)O)O)O
MOL011111	0.9140	0.0860	0.8198	Indigo Naturalis	isovitexin	Not Available	FALSE	c1(ccc(cc1)O)c1oc2c(c(=O)c1)c(c(c(c2)O)C1OC(C(C(C1O)O)O)O)O
MOL011114	0.8857	0.1143	0.7667	Polygoni Tinctorii Foliu	saponarin	Not Available	FALSE	c1(ccc(cc1)O)c1oc2c(c(=O)c1)c(c(c(c2)OC1C(O)C(O)C(O)C(O1)CO)C1OC(C(C(C1O)O)O)O)O
MOL011115	0.9155	0.0845	0.8198	Polygoni Tinctorii Foliu	saponarin_qt	Not Available	FALSE	c1(ccc(cc1)O)C1=[O+]c2c(C(=O)C1)c(c(c(c2)O)C1OC(C(C(C1O)O)O)O)O
MOL011116	0.4365	0.5635	0.7464	Polygoni Tinctorii Foliu	TR-saponin A_qt	Not Available	FALSE	OC1CCC2(C(C1(C(=O)OC)C)CCC1(C2CC=C2C1(C)C(O)C(O)C1(C2CC(C)(C(C1OC(=O)/C(=C\C)/C)OC(=O)/C(=C\C)/C)C)CO)C)C
MOL011117	0.4503	0.5497	0.6070	Wikstroemiae Indicae Rasix	Thymelol	5281406	FALSE	O(c1cc2c(oc1=O)cc(O)c(OC)c2)c1cc2oc(=O)ccc2cc1

MOL011118	0.8875	0.1125	0.8421	Wikstroemiae Indicae Rasix	Kaempferol 3-O-.beta.-D-glucopyranoside	5481218	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)ccc2)c1ccc(O)cc1)CO
MOL011120	0.2532	0.7468	0.6272	Wikstroemiae Indicae Rasix	stigmastan-3,7-diol	Not Available	FALSE	C1(CCC2(C(C1)CC(C1C3CCC(C(CCC(CC)C(C)C)C)C3(C)CCC21)O)C)O
MOL011121	0.8283	0.1717	0.7840	Trigonellae Semen	Tricin 7-O-glucopyranoside	5322022	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2oc(cc(=O)c2c(O)c1)c1cc(OC)c(O)c(OC)c1)CO
MOL011121	0.8283	0.1717	0.7840	Wikstroemiae Indicae Rasix	Tricin 7-O-glucopyranoside	5322022	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2oc(cc(=O)c2c(O)c1)c1cc(OC)c(O)c(OC)c1)CO
MOL011121	0.8283	0.1717	0.7840	Phragmitis Rhizoma	Tricin 7-O-glucopyranoside	5322022	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2oc(cc(=O)c2c(O)c1)c1cc(OC)c(O)c(OC)c1)CO
MOL011122	0.8511	0.1489	0.8723	Wikstroemiae Indicae Rasix	wikstroemin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(oc(cc2=O)c2ccc(O)cc2)cc(OC)c1)COC1OC(C(O)C(O)C1O)CO
MOL011123	0.7705	0.2295	0.6931	Wikstroemiae Indicae Rasix	WIKSTROMOL	321311	FALSE	c1(c(ccc(c1)CC1C(C(=O)OC1)(Cc1ccc(c(c1)OC)O)O)O)OC
MOL011124	0.4090	0.5910	0.6119	Wikstroemiae Indicae Rasix	Wikstrosin	Not Available	FALSE	c1c(cc2c(c1)cc(c(=O)o2)Oc1cc2c(cc1c1c3c(ccc1O)ccc(=O)o3)ccc(=O)o2)O
MOL011125	0.5270	0.4730	0.7662	Ganoderma	(+)-Ganodericacid Mf	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC=C1C3(C)C(CC(C(CC/C=C(/C(=O)O)\C)C)C3(C)CC=C21)O)C)OC(=O)C
MOL011126	0.1836	0.8164	0.6862	Ganoderma	(+)-Methyl ganoderate E	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CC(=O)C1=C2C(=O)CC2(C1(C(=O)CC2C(CC(=O)CC(C(=O)OC)C)C)C)C)C
MOL011127	0.1463	0.8537	0.7432	Ganoderma	(+)-Methyl ganolucidate A	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1=C2C(=O)CC2(C1(C(CC2C(CC(=O)CC(C(=O)OC)C)C)O)C)C)C
MOL011128	0.1754	0.8246	0.7080	Ganoderma	(+)-Methyl ganolucidate B	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1=C2C(=O)CC2(C1(C(CC2C(CC(=O)CC(C(=O)OC)C)C)O)C)C)C)O

MOL011129	0.2252	0.7748	0.6902	Ganoderma	methyl (4R)-4-[(5R,10S,13R,14R,17R)-4,4,10,13,14-pentamethyl-3,7,11,15-tetraoxo-2,5,6,12,16,17-hexahydro-1H-cyclopenta[a]phenanthren-17-yl]pentanoate	21633085	FALSE	C1(=O)CCC2(C(C1(C)C)CC(=O)C1=C2C(=O)CC2(C1(C(=O)CC2C(CCC(=O)OC)C)C)C)C
MOL011130	0.8270	0.1730	0.7439	Ganoderma	(E)-beta-Farnesene	Not Available	FALSE	CCC(=C)CC/C=C(\C)/CCC=C(C)C
MOL011131	0.4977	0.5023	0.7224	Ganoderma	(R,E)-6-((3S,10S,13R,14R,15S,17R)-3,15-diacetoxy-4,4,10,13,14-pentamethyl-2,3,4,5,6,7,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl)-2-methylhept-2-enoic acid	Not Available	FALSE	C(=O)(/C(=C/CCC(C)C1CC(C2(C3=C(CCC12C)C1(CCC(C(C1CC3)C)OC(=O)C)C)C)OC(=O)C)/C)O
MOL011132	0.9662	0.0338	0.8544	Ganoderma	1,8-Cineole	Not Available	FALSE	C1CC2COC1(CC2(C)C)C
MOL011133	0.5399	0.4601	0.6884	Ganoderma	12-Deacetylganoderic acid H	Not Available	FALSE	C1C(C(C2C(C1)(C1=C(C(=O)C2)C2(C(C(C1=O)O)(C(CC2=O)C(CC(=O)CC(C)C(=O)O)C)C)C)(C)C)O
MOL011134	0.6273	0.3727	0.6679	Ganoderma	20-Hydroxylganoderic acid G	637000	FALSE	C1C(C(C2C(C1)(C1=C(C(C2)O)C2(C(C(C1=O)O)(C(CC2=O)C(CC(=O)CC(C(=O)O)C)(C)O)C)C)(C)C)O

MOL011135	0.4847	0.5153	0.7246	Ganoderma	22,23-dimethylene ganodermic acid S	Not Available	FALSE	O=C(OC1CCC2(C(C1(C)C)CC=C1C2=CCC2(C1(C(CC2C(C)C(=C)C(=C)/C=C(\C)/C(=O)O)OC(=O)C)C)C)C)C
MOL011136	0.2137	0.7863	0.6762	Ganoderma	22β-acetoxy-3α,15α-dihydroxylanosta-7,9(11),24-trien-26-oic acid	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1C2CCC2(C1(C(CC2C(C)C(OC(=O)C)C/C=C(\C)/C(=C)O)O)C)C)C)C
MOL011138	0.5905	0.4095	0.6839	Ganoderma	3α,15α,22α-trihydroxylanosta-7,9(11),24-trien-26-oic acid	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC=C1C2=CCC2(C1(C(CC2C(C)C(O)C/C=C(\C)/C(=O)O)O)C)C)C)O
MOL011139	0.5095	0.4905	0.7309	Ganoderma	3α,15α-diacetoxy-22α-hydroxylanosta-7,9(11),24-trien-26-oic acid	Not Available	FALSE	CC(=O)OC1CCC2(C(C1(C)C)CC=C1C2=CCC2(C1(C(CC2C(C)C(O)C/C=C(\C)/C(=O)O)OC(=O)C)C)C)C
MOL011140	0.2084	0.7916	0.7359	Ganoderma	5alpha-Lanosta-7,9(11),24-triene-15alpha,26-dihydroxy-3-one	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=CCC3(C(C1=CC2)(C(CC3C(CC/C=C(/C)\CO)C)O)C)C)(C)C
MOL011141	0.1912	0.8088	0.6841	Ganoderma	6α-hydroxyergosta-4,7,22-trien-3-one	Not Available	FALSE	C1CC(=O)C=C2C(C=C3C4CCC(C4(CCC3C12C)C)C(C)/C=C\C(C(C)C)C)O
MOL011142	0.1912	0.8088	0.6841	Ganoderma	6β-hydroxyergosta-4,7,22-trien-3-one	Not Available	FALSE	C1CC(=O)C=C2C(C=C3C4CCC(C4(CCC3C12C)C)C(C)/C=C\C(C(C)C)C)O
MOL011143	0.4424	0.5576	0.6104	Ganoderma	7-O-Methyl-ganoderic acid O	Not Available	FALSE	C1C(C(C2C(C1)(C1=C(C(C2)OC)C2(C(CC1)(C(CC2OC(=O)C)C(C(C/C=C(\C)/C(=O)O)OC(=O)C)C)C)C)(C)C)OC(=O)C

MOL011144	0.5856	0.4144	0.7014	Ganoderma	8beta,9alpha-Dihydroganoderic acid J	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(C(=O)C2)C2(C(CC1=O)(C(CC2O)C(CC(=O)CC(C)C(=O)O)C)C)C)(C)C
MOL011145	0.9273	0.0727	0.9000	Ganoderma	alpha-D-Arabinofuranosyladenine	96368	FALSE	O1C(C(C(C1CO)O)O)n1cnc2c1ncnc2N
MOL011146	0.9569	0.0431	0.7844	Ganoderma	ST5330609	Not Available	FALSE	C12C3(C)C(CC(C1)C2(C)C)O3
MOL011147	0.9055	0.0945	0.9293	Ganoderma	alpha-Terpineol	Not Available	FALSE	C1C(=CCC(C1)C(C)(C)C)C
MOL011149	0.8502	0.1498	0.6123	Ganoderma	beta-Bazzanene	12444487	FALSE	C1(=CCC(CC1)(C1(C(=C)CCC1)C)C)C
MOL011150	0.9110	0.0890	0.8572	Ganoderma	beta-Irone	Not Available	FALSE	O=C(C)/C=C\C1=C(C)CCC(C)C1(C)C
MOL011152	0.1903	0.8097	0.7391	Ganoderma	butyl ganoderate A	46184561	FALSE	C1C(=O)C(C2C(C1)(C1=C(C(C2)O)C2(C(CC1=O)(C(CC2O)C(CC(=O)CC(C)C(=O)OCCCC)C)C)C)(C)C
MOL011153	0.2043	0.7957	0.7087	Ganoderma	butyl lucidenate N	46184563	FALSE	C1C(C(C2C(C1)(C1=C(C(C2)O)C2(C(CC1=O)(C(CC2=O)C(CCC(=O)OCCCC)C)C)C)C)(C)C)O
MOL011155	0.8525	0.1475	0.7298	Ganoderma	Daucene	Not Available	FALSE	C1C(=C2C(C1)(C=C(CC2)C)C)C(C)C
MOL011156	0.1924	0.8076	0.7222	Ganoderma	epoxyganoderiol A	Not Available	FALSE	C1CC(=O)C(C2CC(C3=C(CCC4(C3(CCC4C(C)CCC3OC3(C)CO)C)C)C12C)O)(C)C
MOL011157	0.1735	0.8265	0.7100	Ganoderma	epoxyganoderiol B	14015437	FALSE	C1CC(=O)C(C2CC=C3C4(CCC(C4(CC=C3C12C)C)C)CCC1OC1(C)CO)C)(C)C
MOL011158	0.2036	0.7964	0.7158	Ganoderma	epoxyganoderiol C	Not Available	FALSE	C1CC(C(C2CC=C3C4(CCC(C4(CC=C3C12C)C)C(C)CCC1OC1(C)CO)C)(C)C)O
MOL011159	0.1613	0.8387	0.6920	Ganoderma	ergosta-4,6,8(14),22-tetraene-3-one	Not Available	FALSE	C1(=O)CCC2(C(=C1)C=CC1=C3CCC(C3(C)CCC21)C(/C=C/C(C)C(C)C)(C)C)C
MOL011160	0.1776	0.8224	0.6963	Ganoderma	ergosta-4,7,22-trien-3,6-dione	11177299	FALSE	C1(=O)CCC2(C(=C1)C(=O)C=C1C3CCC(C(/C=C/C(C)C(C)C)C)C3(C)CCC21)C
MOL011161	0.2495	0.7505	0.6098	Ganoderma	ergosta-7,22-dien-2β,3α,9α-triol	Not Available	FALSE	C1(C(CC2(C(C1)CC=C1C2(CCC2(C1CCC2C(C)/C=C/C(C(C)C)C)C)O)C)O)O
MOL011163	0.1926	0.8074	0.6142	Ganoderma	Ergosta-7,22-dien-3-one	Not Available	FALSE	C1(=O)CCC2(C(C1)CC=C1C3CCC(C(/C=C/C(C(C)C)C)C)C3(C)CCC21)C
MOL011164	0.2521	0.7479	0.6554	Ganoderma	ergosta-7,22-dien-3β,5α,6α-triol	Not Available	FALSE	C1(CCC2(C(C1)(C(C=C1C2CCC2(C1CCC2C(C)/C=C/C(C(C)C)C)C)O)O)C)O
MOL011168	0.2055	0.7945	0.7163	Ganoderma	ergosta-7,9(11),22-trien-3β,5α,6α-triol	Not Available	FALSE	C1(CCC2(C(C1)(C(C=C1C3CCC(C3(C)CC=C21)C(/C=C/C(C)C(C)C)(C)C)O)O)C)O

MOL011169	0.2819	0.7181	0.7257	Corayceps	Peroxyergosterol	Not Available	FALSE	C1(CCC2(C3(C1)C=CC1(C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC21)OO3)C)O
MOL011169	0.2819	0.7181	0.7257	Ganoderma	Peroxyergosterol	Not Available	FALSE	C1(CCC2(C3(C1)C=CC1(C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC21)OO3)C)O
MOL011169	0.2819	0.7181	0.7257	Omphalia	Peroxyergosterol	Not Available	FALSE	C1(CCC2(C3(C1)C=CC1(C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC21)OO3)C)O
MOL011169	0.2819	0.7181	0.7257	Polyporus Umbellatus(Pers)Fr.	Peroxyergosterol	Not Available	FALSE	C1(CCC2(C3(C1)C=CC1(C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC21)OO3)C)O
MOL011169	0.2819	0.7181	0.7257	Viticis Fructus	Peroxyergosterol	Not Available	FALSE	C1(CCC2(C3(C1)C=CC1(C4CCC(C(/C=C/C(C)C(C)C)C)C4(C)CCC21)OO3)C)O
MOL011170	0.1720	0.8280	0.7193	Ganoderma	(E,6R)-2-methyl-6-[(5R,10S,13R,14R,17R)-4,4,10,13,14-pentamethyl-3-oxo-1,2,5,6,12,15,16,17-octahydrocyclopenta[a]phenanthren-17-yl]hept-2-enal	13934282	FALSE	O=C1C(C2C(C3=CCC4(C(CCC4C(CC/C=C(\C)/C=O)C)(C3=CC2)C)C)(CC1)C)(C)C
MOL011171	0.1897	0.8103	0.7264	Ganoderma	ganoderal B	Not Available	FALSE	C(=O)/C(=C/CCC(C)C1CCC2(C3=C(CCC12C)C1(CCC(=O)C(C1CC3O)C)C)C)/C
MOL011172	0.1833	0.8167	0.7477	Ganoderma	ganoderan B	Not Available	FALSE	C(=O)/C(=C/CCC(C)C1CCC2(C3=C(CCC12C)C1(CCC(=O)C(C1CC3O)(C)C)C)C)/C
MOL011173	0.5601	0.4399	0.7054	Ganoderma	ganoderenic acid a	Not Available	FALSE	OC1C2(C(C(C1)/C(=C/C(=O)CC(C)C(=O)O)/C)(CC(=O)C1=C2C(O)CC2C1(CCC(=O)C2(C)C)C)C)C
MOL011174	0.5812	0.4188	0.6893	Ganoderma	ganoderenic acid c	Not Available	FALSE	C(=O)(C(CC(=O)/C=C(\C)/C1CC(C2(C3=C(C(=O)CC12C)C1(CCC(C(C1CC3O)(C)C)O)C)C)O)C)O
MOL011175	0.5329	0.4671	0.7022	Ganoderma	Ganoderenic acid D	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=C(C(C2)O)C2(C(CC1=O)(C(CC2=O)/C(=C\C(=O)CC(C(=O)O)C)/C)C)C)C)(C)C
MOL011176	0.5213	0.4787	0.6989	Ganoderma	Ganoderenic acid G	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=C(C(=O)C)C2(C(CC1=O)(C(CC2=O)/C(=C\C(=O)CC(C(=O)O)C)/C)C)C)C)(C)C
MOL011177	0.5317	0.4683	0.7058	Ganoderma	ganoderenic acid H	Not Available	FALSE	C(=O)(C(CC(=O)/C=C(\C)/C1CC(=O)C2(C3=C(C(=O)CC12C)C1(CCC(C(C1CC3=O)(C)C)O)C)C)C)O
MOL011178	0.5663	0.4337	0.7002	Ganoderma	ganoderenic acid I	Not Available	FALSE	C(=O)(C(CC(=O)/C=C(\C)/C1CC(C2(C3=C(C(=O)CC12C)C1(CCC(C(C1CC3=O)(C)C)O)C)C)O)C)O
MOL011179	0.5661	0.4339	0.7001	Ganoderma	ganoderic acid A	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CC(C1=C2C(=O)CC2(C1(C)C(CC2C(CC(=O)CC(C(=O)O)C)C)O)C)O)C
MOL011180	0.5459	0.4541	0.7276	Ganoderma	Ganoderic acid alpha	Not Available	FALSE	C1C(C(C2C(C1)(C1=C(C(=O)C2)C2(C(CC1=O)OC(=O)C)(C(C(C2)O)C(CC(=O)CC(C)C(=O)O)C)C)C)(C)C)O

MOL011181	0.5538	0.4462	0.6958	Ganoderma	Ganoderic acid AM1	Not Available	FALSE	C1C(C(C2C(C1)(C1=C(C(=O)C2)C2(C(CC1=O)(C(CC2=O)C(CC(=O)CC(C)C(=O)O)C)C)C)(C)C)O
MOL011182	0.5669	0.4331	0.6937	Ganoderma	ganoderic acid B	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC(C1=C2C(=O)CC2(C1(C)C(=O)CC2C(CC(=O)CC(C(=O)O)C)C)C)O)C)O
MOL011183	0.5650	0.4350	0.7259	Ganoderma	(E,6R)-6-[(3S,5R,7S,10S,13R,14R,17R)-3,7-dihydroxy-4,4,10,13,14-pentamethyl-11,15-dioxo-2,3,5,6,7,12,16,17-octahydro-1H-cyclopenta[a]phenanthren-17-yl]-2-methylhept-2-enoic acid	10097521	FALSE	C1C(C(C2C(C1)(C1=C(C(C2)O)C2(C(CC1=O)(C(CC2=O)C(CC/C=C(\C)/C(=O)O)C)C)C)(C)C)O
MOL011184	0.5468	0.4532	0.7058	Ganoderma	(2S,6R)-6-[(5R,7S,10S,13R,14R,17R)-7-hydroxy-4,4,10,13,14-pentamethyl-3,11,15-trioxo-1,2,5,6,7,12,16,17-octahydrocyclopenta[a]phenanthren-17-yl]-2-methyl-4-oxoheptanoic acid	10481601	FALSE	C1(=O)CCC2(C(C1(C)C)CC(C1=C2C(=O)CC2(C1(C)C(=O)CC2C(CC(=O)CC(C(=O)O)C)C)C)O)C
MOL011185	0.6144	0.3856	0.6866	Ganoderma	ganoderic acid C2	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC(C1=C2C(=O)CC2(C1(C(CC2C(C)CC(=O)CC(C)C(=O)O)O)C)C)O)C)O
MOL011186	0.5399	0.4601	0.6884	Ganoderma	Ganoderic acid C6	Not Available	FALSE	C1C(C(C2C(C1)(C1=C(C(=O)C2)C2(C(CC1=O)O)(C(CC2=O)C(CC(=O)CC(C)C(=O)O)C)C)C)(C)C)O

MOL011187	0.5669	0.4331	0.6937	Ganoderma	ganoderic acid D	Not Available	FALSE	C1C(C(C2C(C1)(C1=C(C(C2)O)C2(C(CC1=O)(C(C2=O)C(CC(=O)CC(C)C(=O)O)C)C)C)(C)C)O
MOL011188	0.5915	0.4085	0.7034	Ganoderma	Ganoderic acid delta	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=C(C(C2)O)C2(C(CC1=O)(C(CC2O)C(CC(/C=C(\C)/C(=O)O)O)C)C)C)(C)C
MOL011189	0.5618	0.4382	0.7430	Ganoderma	Ganoderic acid DM	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=C(C(=O)C2)C2(C(CC1)(C(CC2)C(C)CC/C=C(\C)/C(=O)O)C)C)(C)C
MOL011190	0.5196	0.4804	0.6995	Ganoderma	ganoderic acid E	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CC(=O)C1=C2C(=O)CC2(C1(C)C(=O)CC2C(CC(=O)CC(C(=O)O)C)C)C)C
MOL011191	0.5925	0.4075	0.6929	Ganoderma	Ganoderic acid epsilon	Not Available	FALSE	C1C(C(C2C(C1)(C1=C(C(C2)O)C2(C(CC1=O)(C(CC2=O)C(CC(/C=C(\C)/C(=O)O)O)C)C)C)(C)C)O
MOL011192	0.5867	0.4133	0.6832	Ganoderma	(E,4S,6R)-4-hydroxy-2-methyl-6-[(3S,5R,7S,10S,12S,13R,14R,17R)-3,7,12-trihydroxy-4,4,10,13,14-pentamethyl-11,15-dioxo-2,3,5,6,7,12,16,17-octahydro-1H-cyclopenta[a]phenanthren-17-yl]hept-2-enoic acid	10721020	FALSE	C1C(C(C2C(C1)(C1=C(C(C2)O)C2(C(C(C1=O)O)(C(CC2=O)C(CC(/C=C(\C)/C(=O)O)O)C)C)C)(C)C)O
MOL011193	0.5255	0.4745	0.7142	Ganoderma	ganoderic acid F	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CC(=O)C1=C2C(=O)C(C2(C1(C)C(=O)CC2C(CC(=O)CC(C(=O)O)C)C)C)OC(=O)C)C
MOL011194	0.5542	0.4458	0.6804	Ganoderma	ganoderic acid G	Not Available	FALSE	C1(C2CC(C3=C(C2(CCC1O)C)C(=O)C(C1(C3(C(=O)CC1C(CC(=O)CC(C)C(=O)O)C)C)C)O)O)(C)C
MOL011195	0.5915	0.4085	0.7034	Ganoderma	Ganoderic acid gamma	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=C(C(C2)O)C2(C(CC1=O)(C(CC2O)C(CC(/C=C(\C)/C(=O)O)O)C)C)C)(C)C
MOL011196	0.5297	0.4703	0.7169	Ganoderma	ganoderic acid H	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC(=O)C1=C2C(=O)C(C2(C1(C)C(=O)CC2C(CC(=O)CC(C(=O)O)C)C)C)OC(=O)C)C)O
MOL011197	0.5747	0.4253	0.6901	Ganoderma	ganoderic acid I	Not Available	FALSE	C1(C2CC(C3=C(C2(CCC1O)C)C(=O)CC1(C3(C(=O)CC1C(O)(CC(=O)CC(C)C(=O)O)C)C)C)O)(C)C
MOL011198	0.5529	0.4471	0.6977	Ganoderma	ganoderic acid J	Not Available	FALSE	C12(C(CC(C1(C1=C(C3(C(CC1=O)C(C(=O)CC3)(C)C)C)C(=O)C2)C)O)C(CC(=O)CC(C)C(=O)O)C)C
MOL011199	0.5926	0.4074	0.6959	Ganoderma	ganoderic acid K	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC(=O)C1=C2C(=O)CC2(C1(C)C(CC2C(CC(=O)CC(C(=O)O)C)C)O)C)C)O

MOL011200	0.6194	0.3806	0.6889	Ganoderma	ganoderic acid L	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC(C1=C2C(=O)CC2(C1(C)C(CC2C(CC(=O)CC(C(=O)O)C)(C)O)O)C)O)C)O
MOL011201	0.5331	0.4669	0.6851	Ganoderma	ganoderic acid M	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CC(C1=C2C(=O)C(C2(C1(C)C(=O)CC2C(CC(=O)CC(C(=O)O)C)C)C)O)O)C
MOL011202	0.5063	0.4937	0.7433	Ganoderma	ganoderic acid Ma	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC(C1=C2CCC2(C1(C)C(CC2C(CC/C=C(/C(=O)O)\C)C)O)C)OC(=O)C)C)OC(=O)C
MOL011203	0.4773	0.5227	0.6765	Ganoderma	ganoderic acid Mb	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC(C1=C2CCC2(C1(C)C(CC2C(C(C/C=C(/C(=O)O)\C)OC(=O)C)C)OC(=O)C)C)O)C)OC(=O)C
MOL011204	0.4760	0.5240	0.6743	Ganoderma	ganoderic acid Mc	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC(C1=C2CCC2(C1(C)C(CC2C(C(C/C=C(/C(=O)O)\C)OC(=O)C)C)O)C)OC(=O)C)C)OC(=O)C
MOL011205	0.4466	0.5534	0.6337	Ganoderma	ganoderic acid Md	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC(C1=C2CCC2(C1(C)CCC2C(C(C/C=C(/C(=O)O)\C)OC(=O)C)C)C)OC)OC(=O)C
MOL011206	0.4911	0.5089	0.7362	Ganoderma	(E,6R)-6-[(3R,5R,10S,13R,14R,15S,17R)-3,15-diacetoxy-4,4,10,13,14-pentamethyl-2,3,5,6,12,15,16,17-octahydro-1H-cyclopenta[a]phenanthren-17-yl]-2-methylhept-2-enoic acid	9985134	FALSE	C1(CCC2(C(C1(C)C)CC=C1C3(C)C(CC(C(CC/C=C(/C(=O)O)\C)C)C3(C)CC=C21)OC(=O)C)C)OC(=O)C
MOL011207	0.4705	0.5295	0.6610	Ganoderma	ganoderic acid Mg	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC(C1=C2CCC2(C1(C)C(CC2C(C(C/C=C(/C(=O)O)\C)OC(=O)C)C)O)C)OC)C)O
MOL011208	0.4984	0.5016	0.7039	Ganoderma	ganoderic acid Mh	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC(C1=C2CCC2(C1(C)C(CC2C(C(C/C=C(/C(=O)O)\C)OC(=O)C)C)O)C)O)C)OC(=O)C
MOL011209	0.4864	0.5136	0.7244	Ganoderma	ganoderic acid Mi	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC(C1=C2CCC2(C1(C)CCC2C(CC/C=C(/C(=O)O)\C)C)C)OC)C)OC(=O)C
MOL011210	0.4871	0.5129	0.6759	Ganoderma	ganoderic acid Mk	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC=C1C3(C)C(CC(C(CCC(C(=O)O)C)OC(=O)C)C)C3(C)CC=C21)O)C)OC(=O)C
MOL011211	0.5512	0.4488	0.6954	Ganoderma	Ganoderic acid N	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CC(C1=C2C(=O)CC2(C1(C)C(=O)CC2C(CC(=O)CC(C(=O)O)C)(C)O)C)O)C
MOL011212	0.4906	0.5094	0.6577	Ganoderma	Ganoderic acid P	Not Available	FALSE	C1C(C(C2C(C1)(C1=CC(=O)C3(C(C1=CC2)(C(CC3C(C(C/C=C(\C)/C(=O)O)OC(=O)C)C)OC(=O)C)C)C)(C)C)O

MOL011213	0.4932	0.5068	0.6759	Ganoderma	ganoderic acid Q	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC=C1C3(C)C(CC(C(C(OC(=O)C)C/C=C(/C(=O)O)\C)C)C3(C)CC=C21)O)C)OC(=O)C
MOL011214	0.4690	0.5310	0.6506	Ganoderma	(E,5S,6S)-5-acetoxy-6-[(3R,5R,10S,13R,14R,17R)-3-acetoxy-4,4,10,13,14-pentamethyl-2,3,5,6,12,15,16,17-octahydro-1H-cyclopenta[a]phenanthren-17-yl]-2-methylhept-2-enoic acid	21637706	FALSE	C1(CCC2(C(C1(C)C)CC=C1C3(C)CCC(C(C(C/C=C(/C(=O)O)\C)OC(=O)C)C)C3(C)CC=C21)C)OC(=O)C
MOL011215	0.5077	0.4923	0.6534	Ganoderma	(E,5S,6S)-5-acetoxy-6-[(3R,5R,10S,13R,14R,17R)-3-hydroxy-4,4,10,13,14-pentamethyl-2,3,5,6,12,15,16,17-octahydro-1H-cyclopenta[a]phenanthren-17-yl]-2-methylhept-2-enoic acid	21637705	FALSE	C1(CCC2(C(C1(C)C)CC=C1C3(C)CCC(C(C(C/C=C(/C(=O)O)\C)OC(=O)C)C)C3(C)CC=C21)C)O
MOL011216	0.4528	0.5472	0.6384	Ganoderma	Ganoderic acid T	21637704	FALSE	C1(CCC2(C(C1(C)C)CC=C1C3(C)C(CC(C(C(C/C=C(/C(=O)O)\C)OC(=O)C)C)C3(C)CC=C21)OC(=O)C)C)OC(=O)C
MOL011217	0.5715	0.4285	0.6872	Ganoderma	Ganoderic acid theta	Not Available	FALSE	C1C(C(C2C(C1)(C1=C(C(=O)C2)C2(C(C(C1=O)O)(C(CC2=O)C(CC(/C=C(\C)/C(=O)O)O)C)C)C)(C)C)O
MOL011218	0.5452	0.4548	0.7412	Ganoderma	ganoderic acid TQ	Not Available	FALSE	C1C(=O)C(C2(C(C1)(C1=CCC3(C(C1=CC2)(C(CC3C(C)CC/C=C(\C)/C(=O)O)OC(=O)C)C)C)C)(C)C
MOL011219	0.5544	0.4456	0.7385	Ganoderma	Ganoderic acid TR	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=CCC3(C(C1=CC2)(C(CC3C(CC/C=C(\C)/C(=O)O)C)O)C)C)C)(C)C

MOL011220	0.5920	0.4080	0.7618	Ganoderma	Ganoderic acid U	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC(C1=C2CCC2(C1(C)CCC2C(CC/C=C(\C)/C(=O)O)C)C)O)C)O
MOL011221	0.5290	0.4710	0.7448	Ganoderma	ganoderic acid V	Not Available	FALSE	C(=O)(/C(=C/CCC(C)C1CC(C2(C3=C(CCC12C)C1(CCC(=O)C(C1CC3O)(C)C)C)C)OC(=O)C)/C)O
MOL011222	0.5563	0.4437	0.7393	Ganoderma	Ganoderic acid V1	Not Available	FALSE	C1C(C(C2C(C1)(C1=C(C(=O)C2)C2(C(CC1=O)(CCC2=O)C(CC/C=C(\C)/C(=O)O)(C)C)C)C)(C)C)
MOL011223	0.5254	0.4746	0.7411	Ganoderma	ganoderic acid W	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC(C1=C2CCC2(C1(C(CC2C(C)CC/C=C(/C(=O)O)\C)OC(=O)C)C)O)C)OC(=O)C
MOL011224	0.5274	0.4726	0.7486	Ganoderma	Ganoderic acid X	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC=C1C3(C)C(CC(C(CC/C=C(\C)/C(=O)O)C)C3(C)CC=C21)OC(=O)C)C)O
MOL011225	0.5861	0.4139	0.7646	Ganoderma	Ganoderic acid Y	57397445	FALSE	C1(CCC2(C(C1(C)C)CC=C1C3(C)CCC(C(CC/C=C(/C(=O)O)\C)C)C3(C)CC=C21)C)O
MOL011226	0.5849	0.4151	0.7658	Ganoderma	ganoderic acid Z	Not Available	FALSE	C(=O)(/C(=C/CCC(C)C1CCC2(C3=C(CCC12C)C1(CCC(C(C1CC3)(C)C)O)C)C)/C)O
MOL011227	0.5782	0.4218	0.7060	Ganoderma	Ganoderic acid zeta	Not Available	FALSE	C1C(C(C2C(C1)(C1=C(C(=O)C2)C2(C(CC1=O)(CCC2=O)C(CC(/C=C(\C)/C(=O)O)O)C)C)C)(C)C)
MOL011228	0.5867	0.4133	0.6832	Ganoderma	Ganoderic acid zta	Not Available	FALSE	C1C(C(C2C(C1)(C1=C(C(C2)O)C2(C(CC1=O)(CCC2=O)C(CC(/C=C(\C)/C(=O)O)O)C)C)C)(C)C)
MOL011229	0.1820	0.8180	0.7484	Ganoderma	Ganoderic aldehyde A	14484704	FALSE	C1C(C(C2C(C1)(C1=C(CC2)C2(C(CC1=O)C(CC2)C(CC/C=C(\C)/C=O)C)C)C)(C)C)O
MOL011231	0.2327	0.7673	0.7222	Ganoderma	AIDS070764	471007	FALSE	C1(=O)CCC2(C(C1(C)C)CC=C1C3(C)C(CC(C(CCC=C(CO)CO)C)C3(C)CC=C21)O)C
MOL011233	0.2800	0.7200	0.6035	Ganoderma	ganoderiol D	Not Available	FALSE	C1CC(=O)C(C2CC(=O)C3=C(CCC4(C3(CCC4C(C)CCC(C(CO)(C)O)O)C)C)C12C)(C)C
MOL011234	0.2317	0.7683	0.7216	Ganoderma	ganoderiol E	15602281	FALSE	C1CC(C(C2CC(=O)C3=C(CCC4(C3(CCC4C(C)CCC=C(CO)CO)C)C)C12C)(C)C)O
MOL011235	0.2164	0.7836	0.7261	Ganoderma	Ganoderiol F	471008	FALSE	O=C1C(C2C(C3=CCC4(C(CCC4C(CCC=C(CO)CO)C)(C3=CC2)C)C)(CC1)C)(C)C
MOL011238	0.1998	0.8002	0.7002	Ganoderma	ganoderiol I	Not Available	FALSE	C1CC(=O)C(C2CC(C3=C(CCC4(C3(C(CC4C(C)CCC=C(CO)CO)O)C)C)C12C)OC)C
MOL011239	0.2280	0.7720	0.7345	Ganoderma	ganodermadiol	Not Available	FALSE	OC1C(C2C(C3=CCC4(C(CCC4C(CC/C=C(/CO)\C)C)(C3=CC2)C)C)(CC1)C)(C)C
MOL011240	0.2356	0.7644	0.6735	Ganoderma	Ganodermanodiol	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=CCC3(C(C1=CC2)(CCC3C(CCC(C(C)(C)O)O)C)C)C)(C)C
MOL011241	0.2356	0.7644	0.6735	Ganoderma	Ganodermanondiol	73294	FALSE	C1(=O)CCC2(C(C1(C)C)CC=C1C3(C)CCC(C(CCC(C(C)(C)O)O)C)C3(C)CC=C21)C
MOL011243	0.2407	0.7593	0.7407	Ganoderma	ganodermatriol	Not Available	FALSE	OC1C(C2C(C3=CCC4(C(CCC4C(CCC=C(CO)CO)C)(C3=CC2)C)C)(CC1)C)(C)C
MOL011244	0.1923	0.8077	0.7215	Ganoderma	ganodermenonol	Not Available	FALSE	O=C1C(C2C(C3=CCC4(C(CCC4C(CC/C=C(/CO)\C)C)(C3=CC2)C)C)(CC1)C)(C)C
MOL011245	0.4911	0.5089	0.7362	Ganoderma	Ganodermic acid R	5317517	FALSE	O(C1C2(C(C(C1)C(CC/C=C(/C)\C(=O)O)C)(CC=C1C3(C(C(C(OC(=O)C)CC3)(C)C)CC=C21)C)C)C(=O)C

MOL011246	0.5221	0.4779	0.6951	Ganoderma	ganodermic acid O	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CC(=O)C1=C2C(=O)CC2(C1(C)C(=O)CC2C(CC(=O)CC(C(=O)O)C)(C)O)C)C
MOL011247	0.5274	0.4726	0.7486	Ganoderma	ganodermic acid T- Q	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC=C1C2=CCC2(C1(C(CC2C(C)CC/C=C(\C)/C(=O)O)OC(=O)C)C)C)O
MOL011248	0.5270	0.4730	0.7662	Ganoderma	ganodermic acid T- O	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC=C1C2=CCC2(C1(C(CC2C(C)CC/C=C(\C)/C(=O)O)O)C)C)OC(=O)C
MOL011249	0.4906	0.5094	0.6577	Ganoderma	ganodermic acidP2	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC=C1C2=CCC2(C1(C(CC2C(C)C(C/C=C(\C)/C(=O)O)OC(=O)C)OC(=O)C)C)C)O
MOL011250	0.1923	0.8077	0.7215	Ganoderma	Ganodermnonol	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=CCC3(C(C1=CC2)(CCC3C(CC/C=C(\C)/CO)C)C)C)C)(C)C
MOL011251	0.1923	0.8077	0.7215	Ganoderma	(5R,10S,13R,14R,17R)-17-[(E,2R)-7-hydroxy-6-methylhept-5-en-2-yl]-4,4,10,13,14-pentamethyl-1,2,5,6,12,15,16,17-octahydrocyclopenta[a]phenanthren-3-one	13934284	FALSE	C12(C(CCC1(C1=CCC3C(C(=O)CCC3(C1=CC2)C)(C)C)C)C(CC/C=C(/CO)\C)C)C
MOL011252	0.5317	0.4683	0.7215	Ganoderma	Ganolucidic acid A	475412	FALSE	OC1C2(C(C(C1)C(CC(=O)CC(C)C(=O)O)C)(CC(=O)C1=C2CCC2C1(CCC(=O)C2(C)C)C)C)C
MOL011253	0.5759	0.4241	0.7274	Ganoderma	ganolucidic acid B	Not Available	FALSE	C1(C2CCC3=C(C2(CCC1O)C)C(=O)CC1(C3(C(CC1C(CC(=O)CC(C)C(=O)O)C)O)C)C)(C)C
MOL011254	0.5931	0.4069	0.6805	Ganoderma	ganolucidic acid C	Not Available	FALSE	C1(CCC2(C(C1(C)CO)CCC1=C2C(=O)CC2(C1(C)C(CC2C(CC(=O)CC(C(=O)O)C)C)O)C)C)O
MOL011255	0.5554	0.4446	0.7332	Ganoderma	ganolucidic acid D	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1=C2C(=O)CC2(C1(C)C(CC2C(CC(/C=C(/C(=O)O)\C)O)C)O)C)C
MOL011256	0.5495	0.4505	0.7307	Ganoderma	ganolucidic acid E	15602283	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1=C2C(=O)CC2(C1(C)C(CC2C(CC/C=C(/C(=O)O)\C)C)O)C)C
MOL011257	0.6695	0.3305	0.6939	Ganoderma	ganosporelactone A	Not Available	FALSE	OC12C3C(C4(C(C3=O)(C3=C(C5(C(CC3O)C(C(=O)CC5)(COC(=O)C(C2)C)C)C)C(=O)C4O)C)C)C(C1)C
MOL011258	0.6812	0.3188	0.6836	Ganoderma	ganosporelactone B	132113	FALSE	O[C@@]12[C@@H]3[C@H]([C@@]4([C@@](C3=O)(C3=C([C@@]5([C@@H]([C@@]([C@@H](O)CC5)(COC(=O)[C@@H](C2)C)C[C@H]3O)C)C(=O)[C@H]4O)C)C)[C@@H](C1)C
MOL011259	0.4945	0.5055	0.6870	Ganoderma	ganosporericacid A	Not Available	FALSE	C(=O)(C(CC(=O)CC(C)C1CC(=O)C2(C3=C(C(=O)C(=O)C12C)C1(CCC(=O)C(C1CC3=O)(C)C)C)C)C)O
MOL011260	0.9390	0.0610	0.9679	Capsellae Herba	GCS	441477	FALSE	O1C(C(O)C(O)C(N)C1O)CO

MOL011260	0.9390	0.0610	0.9679	Ganoderma	GCS	441477	FALSE	O1C(C(O)C(O)C(N)C1O)CO
MOL011261	0.8545	0.1455	0.6441	Ganoderma	Isobazzanene	15923394	FALSE	C1=C(CCC(C1)(C1=CCCC1(C)C)C)C
MOL011262	0.5216	0.4784	0.7427	Ganoderma	lanosta-7,9(11),24-trien-15α-acetoxy-3α-hydroxy-23-oxo-26-oic acid	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC=C1C2=CCC2(C1(C(CC2C(C)CC(=O)/C=C(\C)/C(=O)O)OC(=O)C)C)C)O
MOL011263	0.5034	0.4966	0.7323	Ganoderma	lanosta-7,9(11),24-trien-3α,15α-diacetoxy-23-oxo-26-oic acid	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC=C1C2=CCC2(C1(C(CC2C(C)CC(=O)/C=C(\C)/C(=O)O)OC(=O)C)C)C)OC(=O)C
MOL011264	0.5228	0.4772	0.7593	Ganoderma	lanosta-7,9(11),24-trien-3α-acetoxy-15α-hydroxy-23-oxo-26-oic acid	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC=C1C2=CCC2(C1(C(CC2C(C)CC(=O)/C=C(\C)/C(=O)O)O)C)C)OC(=O)C
MOL011265	0.5026	0.4974	0.7448	Ganoderma	lanosta-7,9(11),24-trien-3α-acetoxy-26-oic acid	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC=C1C2=CCC2(C1(CCC2C(C)CC/C=C(\C)/C(=O)O)C)C)OC(=O)C
MOL011266	0.2054	0.7946	0.7185	Ganoderma	Lucialdehyde A	Not Available	FALSE	C1C(C(C2C(C1)(C1=CCC3(C(C1=CC2)(CCC3C(CC/C=C(\C)/C=O)C)C)C)(C)C)O
MOL011267	0.1661	0.8339	0.7422	Ganoderma	Lucialdehyde B	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=C(C(=O)C2)C2(C(CC1)(C(CC2)C(CC/C=C(\C)/C=O)C)C)C)(C)C
MOL011268	0.1849	0.8151	0.7440	Ganoderma	Lucialdehyde C	Not Available	FALSE	C1C(C(C2C(C1)(C1=C(C(=O)C2)C2(C(CC1)(C(CC2)C(CC/C=C(\C)/C=O)C)C)C)(C)C)O

MOL011269	0.5360	0.4640	0.6559	Ganoderma	(4R)-4-[(3S,5R,7S,10S,12S,13R,14R,17R)-12-acetoxy-3,7-dihydroxy-11,15-diketo-4,4,10,13,14-pentamethyl-2,3,5,6,7,12,16,17-octahydro-1H-cyclopenta[a]phenanthren-17-yl]valeric acid	11203160	FALSE	C1C(C(C2C(C1)(C1=C(C(C2)O)C2(C(C(C1=O)OC(=O)C)(C(CC2=O)C(C)CCC(=O)O)C)C)(C)C)O
MOL011270	0.5409	0.4591	0.6853	Ganoderma	(4R)-4-[(5R,7S,10S,13R,14R,17R)-7-hydroxy-3,11,15-triketo-4,4,10,13,14-pentamethyl-1,2,5,6,7,12,16,17-octahydrocyclopenta[a]phenanthren-17-yl]valeric acid	14109375	FALSE	OC1C2=C(C3(C(C1)C(C(=O)CC3)(C)C)C)C(=O)CC1(C2(C(=O)CC1C(CCC(=O)O)C)C)C
MOL011271	0.6194	0.3806	0.6891	Ganoderma	lucidenic acid B	Not Available	FALSE	C(=O)(CCC(C)C1CC(=O)C2(C3=C(C(=O)C(C12C)O)C1(CCC(=O)C(C1CC3O)(C)C)C)C)O

MOL011272	0.6524	0.3476	0.6764	Ganoderma	(4R)-4-[(3S,5R,7S,10S,12S,13R,14R,17R)-3,7,12-trihydroxy-11,15-diketo-4,4,10,13,14-pentamethyl-2,3,5,6,7,12,16,17-octahydro-1H-cyclopenta[a]phenanthren-17-yl]valeric acid	20056103	FALSE	C1(C2CC(C3=C(C2(CCC1O)C)C(=O)C(C1(C3(C(=O)CC1C(CCC(=O)O)C)C)C)O)O)(C)C
MOL011273	0.5749	0.4251	0.6693	Ganoderma	lucidenic acid D1	Not Available	FALSE	C(=O)(CCC(C)C1CC(=O)C2(C3=C(C(=O)C(=O)C12C)C1(CCC(=O)C(C1CC3=O)(C)C)C)C)O
MOL011274	0.5136	0.4864	0.6549	Ganoderma	Lucidenic acid D2	23247891	FALSE	C12(C(CC(=O)C1(C1=C(C3(C(CC1=O)C(C(=O)CC3)(C)C)C)C(=O)C2OC(=O)C)C)C(CCC(=O)O)C)C
MOL011275	0.6194	0.3806	0.6891	Ganoderma	lucidenic acid E1	Not Available	FALSE	C(=O)(CCC(C)C1CC(=O)C2(C3=C(C(=O)C(C12C)O)C1(CCC(=O)C(C1CC3O)(C)C)C)C)O
MOL011276	0.5231	0.4769	0.6550	Ganoderma	lucidenic acid E2	Not Available	FALSE	C1(C2C(CCC1O)(C1=C(C(=O)C2)C2(C(C(CC2=O)C(CCC(=O)O)C)(C(C1=O)OC(=O)C)C)C)(C)C
MOL011277	0.5231	0.4769	0.6781	Ganoderma	(4R)-4-[(5R,10S,13R,14R,17R)-3,7,11,15-tetraketo-4,4,10,13,14-pentamethyl-2,5,6,12,16,17-hexahydro-1H-cyclopenta[a]phenanthren-17-yl]valeric acid	23247893	FALSE	C12(C(CC(=O)C1(C1=C(C3(C(CC1=O)C(C(=O)CC3)(C)C)C)C(=O)C2)C)C(CCC(=O)O)C)C
MOL011278	0.6598	0.3402	0.6906	Ganoderma	lucidenic acid G	14109386	FALSE	C12(C(CC(C1(C1=C(C3(C(CC1O)C(C(=O)CC3)(CO)C)C)C(=O)C2)C)O)C(CCC(=O)O)C)C
MOL011279	0.6620	0.3380	0.6867	Ganoderma	lucidenic acid H	Not Available	FALSE	C(=O)(CCC(C)C1CC(=O)C2(C3=C(C(=O)CC12C)C1(CCC(C(C1CC3O)(CO)C)O)C)C)O

MOL011280	0.6449	0.3551	0.6936	Ganoderma	lucidenic acid I	Not Available	FALSE	C(=O)(CCC(C)C1CC(=O)C2(C3=C(C(=O)CC12C)C1(CCC(C(C1CC3=O)(CO)C)O)C)C)O
MOL011281	0.7130	0.2870	0.6996	Ganoderma	lucidenic acid J	Not Available	FALSE	C1(CCC2(C(C1(C)CO)CC(=O)C1=C2C(=O)C(C2(C1(C(=O)CC2C(C)CCC(=O)O)C)C)O)C)O
MOL011282	0.5964	0.4036	0.6838	Ganoderma	Lucidenic acid K	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=C(C(=O)C2)C2(C(C(C1=O)O)(C(CC2=O)C(C)CCC(=O)O)C)C)(C)C
MOL011283	0.6348	0.3652	0.6811	Ganoderma	lucidenic acid L	Not Available	FALSE	C(=O)(CCC(C)C1CC(=O)C2(C3=C(C(=O)C(C12C)O)C1(CCC(C(C1CC3=O)(C)C)O)C)C)O
MOL011284	0.6060	0.3940	0.6814	Ganoderma	lucidenic acid M	Not Available	FALSE	C(=O)(CCC(C)C1CC(C2(C3=C(C(=O)CC12C)C1(CCC(C(C1CC3O)(C)C)O)C)C)O)O
MOL011285	0.5753	0.4247	0.6802	Ganoderma	(4R)-4-[(3S,5R,7S,10S,13R,14R,17R)-3,7-dihydroxy-11,15-diketo-4,4,10,13,14-pentamethyl-2,3,5,6,7,12,16,17-octahydro-1H-cyclopenta[a]phenanthren-17-yl]valeric acid	21592283	FALSE	C1C(C(C2C(C1)(C1=C(C(C2)O)C2(C(CC1=O)(C(CC2=O)C(CCC(=O)O)C)C)C)(C)C)O
MOL011286	0.3632	0.6368	0.7269	Ganoderma	lucidenolactone	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=C(C(C2)O)C2(C(CC1=O)(C(CC2=O)C1(CC(=O)CC1)C)C)C)(C)C
MOL011287	0.4933	0.5067	0.7999	Ganoderma	lucidone A	Not Available	FALSE	C1C(C(C2C(C1)(C1=C(C(C2)O)C2(C(CC1=O)(C)C(CC2=O)C(=O)C)C)C)(C)C)O
MOL011288	0.5520	0.4480	0.8453	Ganoderma	lucidone B	Not Available	FALSE	C1CC(=O)C(C2CC(C3=C(C(=O)CC4(C3(C(=O)CC4C(=O)C)C)C)C12C)O)C
MOL011289	0.5361	0.4639	0.7758	Ganoderma	lucidone C	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC(C1=C2C(=O)CC2(C1(C(CC2C(=O)C)O)C)C)O)C)O
MOL011290	0.2321	0.7679	0.6659	Ganoderma	Lucidumol A	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=C(CC2)C2(C(CC1)(C(CC2)C(CCC(C(C)(C)O)O)C)C)C)(C)C
MOL011291	0.2328	0.7672	0.6765	Ganoderma	Lucidumol B	Not Available	FALSE	C1C(C(C2C(C1)(C1=CCC3(C(C1=CC2)(CCC3C(C)CCC(C(C)(C)CO)O)C)C)C)(C)C)O

MOL011292	0.5231	0.4769	0.6550	Ganoderma	(4R)-4-[(3S,5R,10S,12S,13R,14R,17R)-12-acetoxy-3-hydroxy-7,11,15-triketo-4,4,10,13,14-pentamethyl-1,2,3,5,6,12,16,17-octahydrocyclopenta[a]phenanthren-17-yl]valeric acid	23247892	FALSE	C1C(C(C2C(C1)(C1=C(C(=O)C2)C2(C(C(C1=O)OC(=O)C)(C(CC2=O)C(C)CCC(=O)O)C)C)(C)C)O
MOL011293	0.3788	0.6212	0.6778	Ganoderma	methly lucidenate L	44566900	FALSE	C1C(C(C2C(C1)(C1=C(C(=O)C2)C2(C(C(C1=O)O)(C(CC2=O)C(C)CCC(=O)OC)C)C)(C)C)O
MOL011294	0.2030	0.7970	0.6931	Ganoderma	Methyl 8beta,9alpha-dihydroganoderate J	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(C(=O)C2)C2(C(CC1=O)(C(CC2O)C(C)CC(=O)CC(C)C(=O)OC)C)C)(C)C
MOL011295	0.2168	0.7832	0.7056	Ganoderma	methyl ganoderate A	49865664	FALSE	C1C(=O)C(C2C(C1)(C1=C(C(C2)O)C2(C(CC1=O)(C(CC2O)C(CC(=O)CC(C)C(=O)OC)C)C)C)(C)C
MOL011296	0.2183	0.7817	0.6968	Ganoderma	methyl ganoderate B	71459521	FALSE	C1C(C(C2C(C1)(C1=C(C(C2)O)C2(C(CC1=O)(C(CC2=O)C(CC(=O)CC(C)C(=O)OC)C)C)C)(C)C)O
MOL011297	0.2051	0.7949	0.7073	Ganoderma	methyl ganoderate D	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=C(C(C2)O)C2(C(CC1=O)(C(CC2=O)C(CC(=O)CC(C)C(=O)OC)C)C)C)(C)C
MOL011298	0.2150	0.7850	0.7072	Ganoderma	methyl ganoderate F	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=C(C(=O)C2)C2(C(C(C1=O)OC(=O)C)(C(CC2=O)C(C)CC(=O)CC(C)C(=O)OC)C)C)(C)C
MOL011299	0.3579	0.6421	0.6998	Ganoderma	Methyl ganoderate G	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC(C1=C2C(=O)C(C2(C1(C(=O)CC2C(CC(=O)CC(C(=O)OC)C)C)C)O)O)C)O
MOL011300	0.2294	0.7706	0.7159	Ganoderma	methyl ganoderate H	Not Available	FALSE	C1C(C(C2C(C1)(C1=C(C(=O)C2)C2(C(C(C1=O)OC(=O)C)(C(CC2=O)C(CC(=O)CC(C)C(=O)OC)C)C)C)(C)C)O
MOL011301	0.4114	0.5886	0.6909	Ganoderma	Methyl ganoderate I	Not Available	FALSE	C1(CCC2(C(C1(C)C)CC(C1=C2C(=O)C(C2(C1(C(=O)CC2C(CC(=O)CC(C(=O)OC)C)(O)C)C)C)O)O)C)O
MOL011302	0.1993	0.8007	0.7075	Ganoderma	Methyl ganoderate K	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CC(=O)C1=C2C(=O)CC2(C1(C(CC2C(CC(=O)CC(C(=O)OC)C)C)O)C)C)C
MOL011303	0.1459	0.8541	0.7103	Ganoderma	methyl Ganoderic acid DM	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=C(C(=O)C2)C2(C(CC1)(C(CC2)C(C)CC/C=C(\C)/C(=O)OC)C)C)(C)C

MOL011304	0.1440	0.8560	0.7198	Ganoderma	methyl Ganoderic acid TR	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1=CCC3(C(C1=CC2)(C(CC3C(CC/C=C(\C)/C(=O)OC)C)O)C)C)(C)C
MOL011305	0.2395	0.7605	0.7063	Ganoderma	methyl (4R)-4-[(5R,7S,10S,13R,14R,17R)-7-hydroxy-4,4,10,13,14-pentamethyl-3,11,15-trioxo-1,2,5,6,7,12,16,17-octahydrocyclopenta[a]phenanthren-17-yl]pentanoate	21636089	FALSE	C1C(=O)C(C2C(C1)(C1=C(C(C2)O)C2(C(CC1=O)(C(CC2=O)C(CCC(=O)OC)C)C)C)(C)C
MOL011306	0.2143	0.7857	0.6720	Ganoderma	methyl (4R)-4-[(5R,10S,12S,13R,14R,17R)-12-acetoxy-4,4,10,13,14-pentamethyl-3,7,11,15-tetraoxo-2,5,6,12,16,17-hexahydro-1H-cyclopenta[a]phenanthren-17-yl]pentanoate	21633083	FALSE	C1C(=O)C(C2C(C1)(C1=C(C(=O)C2)C2(C(C(C1=O)OC(=O)C)(C(CC2=O)C(C)CCC(=O)OC)C)C)(C)C
MOL011307	0.2157	0.7843	0.6828	Ganoderma	methyl lucidenate E2	Not Available	FALSE	C1C(C(C2C(C1)(C1=C(C(=O)C2)C2(C(C(C1=O)OC(=O)C)(C(CC2=O)C(CCC(=O)OC)C)C)C)(C)C)O
MOL011308	0.2355	0.7645	0.6953	Ganoderma	methyl lucidenate P	Not Available	FALSE	C1C(C(C2C(C1)(C1=C(C(C2)O)C2(C(C(C1=O)OC(=O)C)(C(CC2=O)C(CCC(=O)OC)C)C)C)(C)C)O

MOL011309	0.2643	0.7357	0.7030	Ganoderma	methyl (4R)-4-[(5R,7S,10S,13R,14R,15S,17R)-7,15-dihydroxy-4,4,10,13,14-pentamethyl-3,11-dioxo-2,5,6,7,12,15,16,17-octahydro-1H-cyclopenta[a]phenanthren-17-yl]pentanoate	11271456	FALSE	C1C(=O)C(C2C(C1)(C1=C(C(C2)O)C2(C(CC1=O)(C(CC2O)C(C)CCC(=O)OC)C)C)C)(C)C
MOL011310	0.9559	0.0441	0.8307	Ganoderma	(1R,3S,5R)-6,6-dimethyl-2-methylene-3-norpinanol	88302	FALSE	C1(CC2CC(C1=C)C2(C)C)O
MOL011311	0.9055	0.0945	0.9345	Ganoderma	γ-butyrobetaine	134	FALSE	[N+](C)(C)(C)CCCC(=O)O
MOL011315	0.9491	0.0509	0.9310	Ranunculi Ternati Radix	Etilevodopa	170345	FALSE	C(=O)(C(Cc1cc(c(cc1)O)O)N)OCC
MOL011316	0.9397	0.0603	0.9312	Ranunculi Ternati Radix	Melevodopa	23497	FALSE	c1(cc(c(cc1)O)O)CC(C(=O)OC)N
MOL011318	0.9071	0.0929	0.9601	Ranunculi Ternati Radix	5-methylol-3H-furan-2-one	14639470	FALSE	C1C=C(OC1=O)CO
MOL011319	0.4251	0.5749	0.8298	Ranunculi Ternati Radix	Truflex OBP	66540	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCCCCCC
MOL011319	0.4251	0.5749	0.8298	Allii Fistulost Bulbus	Truflex OBP	66540	FALSE	c1(c(C(=O)OCCCC)cccc1)C(=O)OCCCCCCCC
MOL011320	0.7654	0.2346	0.6033	Mahoniae Caulis	VCA	5282761	FALSE	C(CCC/C=C\CCCCCC)CCCCCC(=O)O
MOL011320	0.7654	0.2346	0.6033	Typhonii Rhizoma	VCA	5282761	FALSE	C(CCC/C=C\CCCCCC)CCCCCC(=O)O
MOL011320	0.7654	0.2346	0.6033	Ranunculi Ternati Radix	VCA	5282761	FALSE	C(CCC/C=C\CCCCCC)CCCCCC(=O)O
MOL011321	0.9248	0.0752	0.9378	Ranunculi Ternati Radix	Ethyl succinate	31249	FALSE	O(C(=O)CCC(=O)OCC)CC
MOL011322	0.8752	0.1248	0.7823	Ranunculi Ternati Radix	Diisobutyl succinate	70214	FALSE	O(CC(C)C)C(=O)CCC(=O)OCC(C)C

MOL011323	0.1728	0.8272	0.6887	Ranunculi Ternati Radix	8-[5-(5,7-dihydroxy-4-keto-chromen-2-yl)-2-methoxy-phenyl]-5-hydroxy-7-methoxy-2-(4-methoxyphenyl)chromone	9894522	FALSE	o1c2c(c3cc(c4oc5c(c(=O)c4)c(O)cc(O)c5)ccc3OC)c(OC)cc(O)c2c(=O)cc1c1ccc(OC)cc1
MOL011324	0.9363	0.0637	0.9641	Ranunculi Ternati Radix	methyl 5-hydroxy-4-oxopentanoate	10464455	FALSE	O(C(=O)CCC(=O)CO)C
MOL011326	0.8982	0.1018	0.9700	Ranunculi Ternati Radix	L-Pantolactone	736053	FALSE	O1CC(C(O)C1=O)(C)C
MOL011327	0.3973	0.6027	0.6167	Ranunculi Ternati Radix	Podocarpusflavone A	5320644	FALSE	o1c2c(c3cc(c4oc5c(c(=O)c4)c(O)cc(O)c5)ccc3O)c(O)cc(O)c2c(=O)cc1c1ccc(OC)cc1
MOL011328	0.2413	0.7587	0.6497	Ranunculi Ternati Radix	Stigmasta-4,6,8	Not Available	FALSE	C1=C2C(CCC1=C)(C1(C(=C3C(CC1)C(CC3)(C)C(C)(C)CC/C(=C/C)/C(C)C)C=C2)C)C
MOL011331	0.6433	0.3567	0.6306	Indigo Naturalis	(+)-isolariciresinol	Not Available	FALSE	C1(C(Cc2c(C1C1=CC(=C(CC1)O)OC)cc(c(c2)OC)O)CO)CO
MOL011332	0.7957	0.2043	0.6575	Indigo Naturalis	10h-indolo,[3,2-b],quinoline	Not Available	FALSE	n1c2c(cc3ccccc13)[nH]c1c2cccc1
MOL011333	0.9352	0.0648	0.7040	Indigo Naturalis	2,3-dihydropyrrolo,[2,1-b],quinazolin-9(1h)-one	Not Available	FALSE	n1c2n(c(=O)c3ccccc13)CCC2
MOL011334	0.8990	0.1010	0.8832	Indigo Naturalis	4,(3h)-quinazolinone	Not Available	FALSE	n1c[nH]c(=O)c2ccccc12
MOL011335	0.8233	0.1767	0.7268	Indigo Naturalis	Isoindigo	5318575	FALSE	O=C1Nc2c(/C/1=C\1/c3c(NC1=O)cccc3)cccc2
MOL011336	0.9281	0.0719	0.9659	Indigo Naturalis	5,6-dioxocyclohexa-1,3-diene-1-carboxylic acid	20154716	FALSE	C(=O)(C1=CC=CC(=O)C1=O)O
MOL011337	0.8833	0.1167	0.7957	Gentianae Radix Et Rhozima	Saponarin	441381	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(OC2OC(C(O)C(O)C2O)CO)cc2oc(cc(=O)c2c1O)c1ccc(O)cc1

MOL011337	0.8833	0.1167	0.7957	Indigo Naturalis	Saponarin	441381	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(OC2OC(C(O)C(O)C2O)CO)cc2oc(cc(=O)c2c1O)c1ccc(O)cc1
MOL011338	0.5013	0.4987	0.7652	Semiaquilegiae Radix	4,4'-tetrahydro-1H,3H-furo[3,4-c]furan-1,4-diylbis(2-methoxyphenol)	637584	FALSE	C1(OCC2C1COC2c1cc(c(cc1)O)OC)c1cc(c(cc1)O)OC
MOL011339	0.9297	0.0703	0.9659	Semiaquilegiae Radix	(1E,4α,5β,6α)-4,5,6-trihydroxy-2-cyclohexen-1-ylideneacetonitrile	Not Available	FALSE	C\1(=C\C#N)/C=CC(C(C1O)O)O
MOL011341	0.9216	0.0784	0.9159	Semiaquilegiae Radix	(2S,3R,4S,5S,6R)-2-((2-hydroxy-4-(2-hydroxyethyl)phenoxy)methyl)-6-(hydroxymethyl)tetrahydro-2H-pyran-3,4,5-triol	Not Available	FALSE	c1(c(ccc(c1)CCO)OCC1OC(C(C(C1O)O)O)CO)O
MOL011342	0.9255	0.0745	0.8900	Semiaquilegiae Radix	(6R,7aR)-6-hydroxy-7,7a-dihydro-6H-benzofuran-2-one	639165	FALSE	C1(CC2C(=CC(=O)O2)C=C1)O
MOL011343	0.9255	0.0745	0.8900	Semiaquilegiae Radix	(6S,7aR)-6-hydroxy-7,7a-dihydro-6H-benzofuran-2-one	155054	FALSE	C1(CC2C(=CC(=O)O2)C=C1)O
MOL011344	0.9644	0.0356	0.9625	Semiaquilegiae Radix	(R)-1-(3,4-dimethoxyphenyl)ethane-1,2-diol	11183213	FALSE	c1cc(c(cc1C(O)CO)OC)OC
MOL011345	0.9115	0.0885	0.9701	Semiaquilegiae Radix	Polymethylglutamate	6998933	FALSE	C(CC(N)C(=O)O)C(=O)OC

MOL011346	0.9360	0.0640	0.8881	Semiaquilegiae Radix	(Z)-2-((4R,5R,6S)-4,5-dihydroxy-6-((2S,3S,4R,5R,6S)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yloxy)cyclohex-2-enylidene)acetonitrile	Not Available	FALSE	C\1(=C\C#N)/C=CC(C(C1OC1OC(C(C(C1O)O)O)CO)O)O
MOL011347	0.9297	0.0703	0.9659	Semiaquilegiae Radix	(Z)-2-((4R,5R,6S)-4,5-dihydroxy-6-((2S,3S,4R,5R,6S)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yloxy)cyclohex-2-enylidene)acetonitrile_qt	Not Available	FALSE	C\1(=C\C#N)/C=CC(C(C1O)O)O
MOL011348	0.9359	0.0641	0.8832	Semiaquilegiae Radix	2-(3,4-dihydroxy-2-((2R,3S,4R,5R,6S)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yloxy)phenyl)acetonitrile	Not Available	FALSE	c1(ccc(c(c1OC1OC(C(C(C1O)O)O)CO)O)O)CC#N
MOL011349	0.9357	0.0643	0.9558	Semiaquilegiae Radix	2-(2,3,4-trihydroxyphenyl)acetonitrile	19107661	FALSE	c1(ccc(c(c1O)O)O)CC#N

MOL011350	0.9278	0.0722	0.8055	Semiaquilegiae Radix	2-(4-((2S,3R,4S,5S,6R)-6-(((2R,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)tetrahydrofuran-2-yloxy)methyl)-3,4,5-trihydroxytetrahydro-2H-pyran-2-yloxy)phenyl)acetonitrile	Not Available	FALSE	C1(C(C(OC1)OCC1C(C(C(C(O1)Oc1ccc(cc1)CC#N)O)O)O)O)(O)CO
MOL011351	0.9351	0.0649	0.9727	Semiaquilegiae Radix	4-HYDROXYBENZYLCYANIDE	26548	FALSE	Oc1ccc(cc1)CC#N
MOL011352	0.9276	0.0724	0.9050	Semiaquilegiae Radix	2-[4-hydroxy-2-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]acetonitrile	10425556	FALSE	C1(C(C(C(OC1CO)Oc1cc(ccc1CC#N)O)O)O)O
MOL011353	0.9329	0.0671	0.9604	Semiaquilegiae Radix	4-hydroxy-2-β-D-glucopyranosyl oxypheylacetonitrile_qt	14970422	FALSE	Oc1cc(ccc1CC#N)O
MOL011354	0.9276	0.0724	0.9050	Semiaquilegiae Radix	2-(β-D-glucopyranosyloxy)-4-hydroxy-benzeneacetonirtile	Not Available	FALSE	c1(cc(ccc1CC#N)O)OC1OC(C(O)C(O)C1O)CO

MOL011355	0.9514	0.0486	0.9709	Semiaquilegiae Radix	Methyl 2,4-dihydroxyphenylacetate	105727	FALSE	C(=O)(Cc1c(cc(cc1)O)O)OC
MOL011356	0.9251	0.0749	0.8034	Semiaquilegiae Radix	2-propenoic acid,3-(4'-hydroxyphenyl)-(4-carboxyl)-phenyl ester	Not Available	FALSE	C1(CCC(CC1)C(=O)O)OC(=O)/C=C/c1ccc(cc1)O
MOL011357	0.9507	0.0493	0.9468	Semiaquilegiae Radix	Ethyl vanillate	12038	FALSE	c1(cc(c(cc1)O)OC)C(=O)OCC
MOL011358	0.9382	0.0618	0.9578	Semiaquilegiae Radix	4-(bromomethyl)-2-hydroxybenzoic acid	19069090	FALSE	c1cc(c(cc1CBr)O)C(=O)O
MOL011359	0.9125	0.0875	0.6852	Semiaquilegiae Radix	4-[β-D-xylopyranosyl-(1→6)-0-b-D-glucopyranosyloxy]-1-(2-nitroethyl)benzene	Not Available	FALSE	C1(C(C(OC1O)OCC1C(C(C(C(O1)Oc1ccc(cc1)CC[N+](=O)O)O)O)O)O)O
MOL011360	0.9305	0.0695	0.7740	Semiaquilegiae Radix	4-hydroxy-1-(2-nitroethyl)benene-4-0-(6'-0-β-D-xylopyranosy)-β-D-glucopyranoside	Not Available	FALSE	C1(C(C(OC1O)OCC1C(C(C(C(O1)Oc1ccc(cc1)CCC#N)O)O)O)O)O
MOL011361	0.8977	0.1023	0.7804	Semiaquilegiae Radix	4-hydroxy-1-(2-nitroethyl)benzene-4-O-(6'-O-β-D-xylopyranosyl)-β-D-glucopyranoside	Not Available	FALSE	C1C(CCC(C1)CC[N+](=O)O)OC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O

MOL011362	0.8652	0.1348	0.8470	Semiaquilegiae Radix	acacetin-(1→2)-O-α-L-rhamnosy1-6-C-β-D-glucopyranoside	Not Available	FALSE	C1(C(C(C(OC1C)OOC1C(OC(C(C1O)O)CO)c1c(c2c(cc1O)oc(cc2=O)c1ccc(cc1)OC)O)O)O)O
MOL011363	0.9465	0.0535	0.8948	Semiaquilegiae Radix	4-(beta-D-glucosyloxy)benzoic acid	440186	FALSE	C1(C(C(C(OC1CO)Oc1ccc(cc1)C(=O)O)O)O)O
MOL011364	0.9339	0.0661	0.9261	Semiaquilegiae Radix	butyl-β-D-mannopyranoside	67412812	FALSE	C1(C(C(C(OC1CO)OCCCC)O)O)O
MOL011365	0.9079	0.0921	0.7601	Semiaquilegiae Radix	caffeic acid twenty-four ester	Not Available	FALSE	c1(ccc(cc1C)/C=C/C(=C)CC)C
MOL011366	0.8476	0.1524	0.9143	Semiaquilegiae Radix	DIBUTYL TEREPHTHALATE	16066	FALSE	c1(C(=O)OCCCC)ccc(cc1)C(=O)OCCCC
MOL011367	0.4408	0.5592	0.6682	Semiaquilegiae Radix	E-semiaquilegin A	Not Available	FALSE	c1(c(cc(cc1)/C=C/C(=O)OCC12C(CC3C4C1CCC(C4)C(C3)(COC(=O)/C=C/c1cc(c(cc1)O)O)O)C(CCC2)(C)C)O)O
MOL011368	0.9163	0.0837	0.8986	Semiaquilegiae Radix	griffonilide	Not Available	FALSE	O1C2C(O)C(O)C=CC2=CC1=O
MOL011369	0.9360	0.0640	0.8881	Semiaquilegiae Radix	griffonin	Not Available	FALSE	O1C(OC2C(O)C(O)C=C/C/2=C/C#N)C(O)C(O)C(O)C1CO
MOL011370	0.9297	0.0703	0.9659	Semiaquilegiae Radix	griffonin_qt	Not Available	FALSE	OC1C(O)C(O)C=C/C/1=C\C#N
MOL011371	0.9275	0.0725	0.8973	Semiaquilegiae Radix	menisdaurin	Not Available	FALSE	C1(C(C(C(C(O1)CO)O)O)O)OC1/C(=C/C#N)/C=CC(C1)O
MOL011372	0.9236	0.0764	0.9612	Semiaquilegiae Radix	menisdaurin_qt	Not Available	FALSE	OC1/C(=C/C#N)/C=CC(C1)O
MOL011372	0.9236	0.0764	0.9612	Menispermi Rhizoma	menisdaurin_qt	Not Available	FALSE	OC1/C(=C/C#N)/C=CC(C1)O
MOL011373	0.9395	0.0605	0.9490	Semiaquilegiae Radix	methyl 3-hydroxy-4-methoxybenzoate	4056967	FALSE	c1(cc(c(cc1)OC)O)C(=O)OC
MOL011374	0.9312	0.0688	0.9331	Semiaquilegiae Radix	n butyl-0-β-D-fructopyranoside	Not Available	FALSE	C1C(C(C(C(O1)(OCCCC)O)O)O)O
MOL011375	0.9358	0.0642	0.9195	Semiaquilegiae Radix	n-butyl-α-D-fructopyranoside	70499994	FALSE	C1C(C(C(C(O1)(CO)OCCCC)O)O)O
MOL011375	0.9358	0.0642	0.9195	Lobeliae Chinensis Herba	n-butyl-α-D-fructopyranoside	70499994	FALSE	C1C(C(C(C(O1)(CO)OCCCC)O)O)O

MOL011377	0.6906	0.3094	0.7986	Semiaquilegiae Radix	semiaquilegoside A	Not Available	FALSE	C1C(C(C2C(C1)(c1c(CC2=O)cc(c(c1O)OC1OC(C(C(C1O)O)O)CO)C(C)C)C)(C)C)O
MOL011378	0.6009	0.3991	0.7977	Semiaquilegiae Radix	semiaquilegoside A_qt	Not Available	FALSE	C1C(C(C2C(C1)(c1c(CC2=O)cc(c(c1O)O)C(C)C)C)(C)C)O
MOL011379	0.8983	0.1017	0.6950	Semiaquilegiae Radix	Thalictricoside	45359754	FALSE	C1(C(C(C(OC1)OCC1C(C(C(C(O1)Oc1ccc(cc1)CC[N+](=O)O)O)O)O)O)O)O
MOL011380	0.4519	0.5481	0.6799	Semiaquilegiae Radix	Z-semiaquilegin A	Not Available	FALSE	c1c(c(cc(c1)/C=C\C(=O)OCC12C(CCC34C1CCC(C3)C(C4)(O)COC(=O)/C=C\c1cc(c(cc1)O)O)C(CCC2)(C)C)O)O
MOL011381	0.9058	0.0942	0.9289	Pseudostellariae Radix	PYC	12473	FALSE	OC(=O)c1[nH]ccc1
MOL011382	0.9228	0.0772	0.8882	Pseudostellariae Radix	3-furylmethyl 1H-pyrrole-2-carboxylate	189695	FALSE	[nH]1c(ccc1)C(=O)OCc1cocc1
MOL011383	0.9410	0.0590	0.8684	Pseudostellariae Radix	3-Furfuryl 2-pyrrolecarboxylate	71307283	FALSE	[nH]1c(ccc1)C(=O)Oc1c(C)occ1
MOL011384	0.5746	0.4254	0.6277	Panacis Quinquefolii Radix	6-phenyldodecane	Not Available	FALSE	c1(ccccc1)C(CCCCC)CCCCCC
MOL011385	0.6704	0.3296	0.6591	Panacis Quinquefolii Radix	6-PHENYLUNDECANE	20660	FALSE	c1(ccccc1)C(CCCCC)CCCCC
MOL011387	0.6944	0.3056	0.6813	Panacis Quinquefolii Radix	heptadeca-1,8-dien-4,6-diyn-3,10-diol	Not Available	FALSE	C=CC(C#CC#C/C=C/C(CCCCCCC)O)O
MOL011387	0.6944	0.3056	0.6813	Saposhnikoviae Radix	heptadeca-1,8-dien-4,6-diyn-3,10-diol	Not Available	FALSE	C=CC(C#CC#C/C=C/C(CCCCCCC)O)O
MOL011388	0.7637	0.2363	0.8232	Panacis Quinquefolii Radix	Chrysosplenetin	5281608	FALSE	c1(c(c(c2c(c1)oc(c(c2=O)OC)c1cc(c(cc1)O)OC)O)OC)OC
MOL011389	0.7331	0.2669	0.7154	Panacis Quinquefolii Radix	chikusetsusaponin Ⅳa	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C)C1OC(C(O)C(O)C1O)C(=O)O
MOL011389	0.7331	0.2669	0.7154	Achyranthis Bidentatae Radix	chikusetsusaponin Ⅳa	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C)C1OC(C(O)C(O)C1O)C(=O)O
MOL011389	0.7331	0.2669	0.7154	Panacis Japonici Rhizoma	chikusetsusaponin Ⅳa	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C)C1OC(C(O)C(O)C1O)C(=O)O
MOL011390	0.7553	0.2447	0.9079	Panacis Quinquefolii Radix	3-epioleanolic acid	7061302	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3CC(CCC3(C(=O)O)CC4)(C)C)C)(CC2)C)(CC1)C)(C)C
MOL011390	0.7553	0.2447	0.9079	Achyranthis Bidentatae Radix	3-epioleanolic acid	7061302	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3CC(CCC3(C(=O)O)CC4)(C)C)C)(CC2)C)(CC1)C)(C)C

MOL011392	0.9137	0.0863	0.9617	Panacis Quinquefolii Radix	galacturonic acid	46173899	FALSE	OC(C(O)C(O)C=O)C(O)C(=O)O
MOL011393	0.7446	0.2554	0.8121	Panacis Quinquefolii Radix	gensenoside-Rb1	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3(OC(C(O)C(O)C3OC3(C(C(C(OO)O3)O)O)O)C)CO)C)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(C(O)C(O)C1O)COC1OC(C(O)C(O)C1O)CO)(CCC=C(C)C)C)C
MOL011394	0.5928	0.4072	0.7475	Panacis Quinquefolii Radix	(2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[[(3S,5R,8R,9R,10R,12R,13R,14R,17S)-12-hydroxy-4,4,8,10,14-pentamethyl-17-[(2S)-6-methyl-2-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhept-5-en-2-yl]-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-c	9918692	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3O)CO)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(C(O)C(O)C1O)CO)(CCC=C(C)C)C)C

MOL011395	0.6384	0.3616	0.8211	Panacis Quinquefolii Radix	(2S,3R,4S,5S,6R)-2-[(2S)-2-[(3S,5R,8R,9R,10R,12R,13R,14R,17S)-3,12-dihydroxy-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-17-yl]-6-methylhept-5-en-2-yl]oxy-6-[[(2S,3R,4S,5S)-3,4,5-trihydroxyoxan-2-yl]oxymet	21672570	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(C(O)C(O)C1O)COC1C(C(CO1)O)O)O)(C)CCC=C(C)C)C
MOL011396	0.7282	0.2718	0.8093	Panacis Quinquefolii Radix	ginsenoside-Rb2	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(C(O)C(O)C1O)COC1OCC(O)C(O)C1O)(CCC=C(C)C)C)C
MOL011397	0.7331	0.2669	0.8151	Panacis Quinquefolii Radix	ginsenoside-Rc	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(C(O)C(O)C1O)COC1OC(C(O)C1O)CO)(CCC=C(C)C)C)C
MOL011398	0.7390	0.2610	0.8303	Panacis Quinquefolii Radix	ginsenoside-Re	Not Available	FALSE	O(C1C(OC2C(O)C(O)C(O)C(O2)C)C(O)C(O)C(O1)CO)C1C2C(C(CCC2(C2C(C1)C1(C)CCC(C(CCC=C(C)C)(C)OC3C(O)C(O)C(O)C(O3)CO)C1C(C2)O)C)O)(C)C
MOL011399	0.2511	0.7489	0.7078	Panacis Quinquefolii Radix	ginsenoside-Re_qt	Not Available	FALSE	OC1C2C(C(CCC2(C2C(C1)C1(C)CCC(C(CCC=C(C)C)(C)O)C1C(C2)O)C)O)(C)C
MOL011400	0.6702	0.3298	0.8663	Panacis Quinquefolii Radix	ginsenoside rf	441922	FALSE	O(C1C2C(C3C(C4(C(C(CC4)C(O)(CCC=C(C)C)C)C(O)C3)C)(C1)C)(CCC(O)C2(C)C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)CO)CO

MOL011400	0.6702	0.3298	0.8663	Ginsen Radix Et Rhizoma Rubra	ginsenoside rf	441922	FALSE	O(C1C2C(C3C(C4(C(C(CC4)C(O)(CCC=C(C)C)C)C(O)C3)C)(C1)C)(CCC(O)C2(C)C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)CO)CO
MOL011400	0.6702	0.3298	0.8663	Panax Ginseng C. A. Mey.	ginsenoside rf	441922	FALSE	O(C1C2C(C3C(C4(C(C(CC4)C(O)(CCC=C(C)C)C)C(O)C3)C)(C1)C)(CCC(O)C2(C)C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)CO)CO
MOL011401	0.6724	0.3276	0.7238	Panacis Quinquefolii Radix	ginsenoside-Rg1	Not Available	FALSE	O(C1C2C(C3C(C4(C(C(CC4)C(OC4OC(C(O)C(O)C4O)CO)(CCC=C(C)C)C)C(O)C3)C)(C1)C)(CCC(O)C2(C)C)C)C1OC(C(O)C(O)C1O)CO
MOL011402	0.2494	0.7506	0.7336	Panacis Quinquefolii Radix	ginsenoside-Rg1_qt	44583955	FALSE	OC(C1C2C(C3(C(C4(C(C(O)C3)C(C(O)CC4)(C)C)C)CC2O)C)(CC1)C)(CCC=C(C)C)C
MOL011403	0.6562	0.3438	0.8505	Panacis Quinquefolii Radix	ginsenoside-Rg2	Not Available	FALSE	O(C1C2C(C3C(C4(C(C(CC4)C(O)(CC/C=C(/CC)\C)C)C(O)C3)C)C1)(CCC(O)C2(C)C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)C)CO
MOL011403	0.6562	0.3438	0.8505	Ginseng Folium	ginsenoside-Rg2	Not Available	FALSE	O(C1C2C(C3C(C4(C(C(CC4)C(O)(CC/C=C(/CC)\C)C)C(O)C3)C)C1)(CCC(O)C2(C)C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)C)CO
MOL011404	0.2415	0.7585	0.6898	Ginseng Folium	ginsenoside-Rg2_qt	Not Available	FALSE	OC1C2C(C3C(C4(C(C(CC4)C(O)(CC/C=C(/CC)\C)C)C(O)C3)C)C1)(CCC(O)C2(C)C)C
MOL011404	0.2415	0.7585	0.6898	Achyranthis Bidentatae Radix	ginsenoside-Rg2_qt	Not Available	FALSE	OC1C2C(C3C(C4(C(C(CC4)C(O)(CC/C=C(/CC)\C)C)C(O)C3)C)C1)(CCC(O)C2(C)C)C
MOL011404	0.2415	0.7585	0.6898	Panacis Quinquefolii Radix	ginsenoside-Rg2_qt	Not Available	FALSE	OC1C2C(C3C(C4(C(C(CC4)C(O)(CC/C=C(/CC)\C)C)C(O)C3)C)C1)(CCC(O)C2(C)C)C
MOL011405	0.6798	0.3202	0.8580	Ginseng Folium	ginsenoside-Rg3	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL011405	0.6798	0.3202	0.8580	Panacis Quinquefolii Radix	ginsenoside-Rg3	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL011406	0.2305	0.7695	0.7376	Panacis Quinquefolii Radix	ginsenoside-Rg3_qt	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL011406	0.2305	0.7695	0.7376	Ginseng Folium	ginsenoside-Rg3_qt	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL011407	0.4038	0.5962	0.7568	Panacis Quinquefolii Radix	ginsenoside-Rh1	Not Available	FALSE	O(C1C2C(C3C(C4(C(C(CC4)C(O)(CCC=C(C)C)C)C(O)C3)C)(C1)C)(CCC(O)C2(C)C)C)C1OC(C(O)C(O)C1O)CO
MOL011408	0.2494	0.7506	0.7336	Panacis Quinquefolii Radix	ginsenoside-Rh1_qt	Not Available	FALSE	OC1C2C(C3C(C4(C(C(CC4)C(O)(C)CCC=C(C)C)C(O)C3)C)(C1)C)(CCC(O)C2(C)C)C
MOL011409	0.7794	0.2206	0.7964	Panacis Quinquefolii Radix	ginsenoside-Ra0	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(C(O)C(O)C1O)COC1OC(C(O)C(O)C1O)CO)(CCC=C(C)C)C)C

MOL011410	0.7319	0.2681	0.8231	Panacis Quinquefolii Radix	gypenoside XI	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3O)COC3OC(C(O)C(O)C3O)C)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(C(O)C(O)C1O)CO)(CCC=C(C)C)C)C
MOL011411	0.7083	0.2917	0.8460	Panacis Quinquefolii Radix	gypenosideⅧ	Not Available	FALSE	OC1C2C(C3C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)CC4)(C)C)C)C1)(CCC2C(OC1OC(C(O)C(O)C1O)CO)(CC(C)C=C(C)C)C)C
MOL011412	0.7207	0.2793	0.8439	Panacis Quinquefolii Radix	gypenosideIII	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3(OC(C(O)C(O)C3OC3(C(C(C(OO)O3)O)O)O)C)CC(=O)C)C)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(C(O)C(O)C1O)CO)(CCC=C(C)C)C)C
MOL011413	0.6944	0.3056	0.6813	Panacis Quinquefolii Radix	(3S,8E,10S)-heptadeca-1,8-dien-4,6-diyne-3,10-diol	10467801	FALSE	OC(CCCCCCC)/C=C/C#CC#CC(O)C=C
MOL011414	0.3761	0.6239	0.6596	Panacis Quinquefolii Radix	Isofernene	12311007	FALSE	C1CC(C2C(C1)(C1=C(CC2)C2(C(CC1)(C1C(CC2)(C(CC1)C(C)C)C)C)C)(C)C
MOL011416	0.7423	0.2577	0.6752	Panacis Quinquefolii Radix	Lindenene	Not Available	FALSE	C1C2C(=C)C3C(C12)(Cc1c(C3)c(co1)C)C
MOL011419	0.2235	0.7765	0.7203	Panacis Quinquefolii Radix	malonyl ginsenoside Rd	12309018	FALSE	OC1C(C2C(C3C(C4(C(C(CC4)C(O)(CCC=C(C)C)CC3)C)(CC2)C)(CC1)C)(C)C
MOL011420	0.7323	0.2677	0.7999	Panacis Quinquefolii Radix	malonyl-ginsenoside Rb1	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)COC(=O)CC(=O)O)CO)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(C(O)C(O)C1O)COC1OC(C(O)C(O)C1O)CO)(CCC=C(C)C)C)C
MOL011421	0.2305	0.7695	0.7376	Panacis Quinquefolii Radix	malonyl-ginsenoside Rb1_qt	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL011422	0.7122	0.2878	0.7980	Panacis Quinquefolii Radix	malonyl-ginsenoside Rb2	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)COC(=O)CC(=O)O)CO)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(C(O)C(O)C1O)COC1OCC(O)C(O)C1O)(CCC=C(C)C)C)C
MOL011423	0.2305	0.7695	0.7376	Panacis Quinquefolii Radix	malonyl-ginsenoside Rb2_qt	Not Available	FALSE	OC1C2C(C3(C(C4(C(C(C(O)CC4)(C)C)CC3)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL011424	0.6881	0.3119	0.8245	Panacis Quinquefolii Radix	malonyl-ginsenoside Rd	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)COC(=O)CC(=O)O)CO)CC4)(C)C)C)C1)C)(CCC2C(OC1OC(C(O)C(O)C1O)CO)(CCC=C(C)C)C)C
MOL011425	0.2305	0.7695	0.7376	Panacis Quinquefolii Radix	malonyl-ginsenoside Rd_qt	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)C)(CCC2C(O)(C)CCC=C(C)C)C
MOL011426	0.7893	0.2107	0.7333	Panacis Quinquefolii Radix	panaxytriol	46184189	FALSE	C=CC(C#CC#CCC(C(CCCCCCC)O)O)O

MOL011427	0.9197	0.0803	0.9185	Panacis Quinquefolii Radix	Phenyl isothiocyanate	Not Available	FALSE	c1(ccccc1)/N=C/C=S
MOL011428	0.9482	0.0518	0.9685	Panacis Quinquefolii Radix	Phenethyl acetate	7654	FALSE	c1cccc(c1)CCOC(=O)C
MOL011429	0.9275	0.0725	0.8379	Panacis Quinquefolii Radix	Phlegmariuine -N	195484	FALSE	c1(c(cc2c(c1C)cccn2)C)O
MOL011432	0.9559	0.0441	0.8307	Panacis Quinquefolii Radix	(1R,3R,5R)-6,6-dimethyl-2-methylene-3-norpinanol	10931630	FALSE	OC1CC2C(C(C2)C1=C)(C)C
MOL011432	0.9559	0.0441	0.8307	Nardostachyos Radix Et Rhizoma	(1R,3R,5R)-6,6-dimethyl-2-methylene-3-norpinanol	10931630	FALSE	OC1CC2C(C(C2)C1=C)(C)C
MOL011433	0.6985	0.3015	0.6504	Panacis Quinquefolii Radix	polyacetylene PQ-1	Not Available	FALSE	O(C(CCCCCCC)C(O)CC#CC#CC(O)C=C)C
MOL011434	0.7518	0.2482	0.7322	Panacis Quinquefolii Radix	polyacetylene PQ-2	Not Available	FALSE	O1C(C1C(O)C(O)C#CC#CC(O)C=C)CCCCCCC
MOL011435	0.7518	0.2482	0.7322	Panacis Quinquefolii Radix	PQ-2	Not Available	FALSE	C=CC(O)C#CC#CC(C(O)C1C(CCCCCCC)O1)O
MOL011436	0.3249	0.6751	0.7812	Panacis Quinquefolii Radix	Praeruptorin A	Not Available	FALSE	c12c(c3c(cc1)ccc(=O)o3)C(C(C(O2)(C)C)C/C=C\C)OC(=O)C

MOL011437	0.6264	0.3736	0.8641	Panacis Quinquefolii Radix	(2S,3R,4R,5R,6S)-2-[[(2R,3R,4S,5S,6R)-2-[[(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-3,12-dihydroxy-17-[(2S,5R)-5-(1-hydroxy-1-methylethyl)-2-methyl-2-tetrahydrofuranyl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthr	21633072	FALSE	O1C(CCC1C(O)(C)C)(C1C2C(C3(C(C4(C(C(CC4)O)(C)C)C(C3)OC3OC(C(C(C3OC3OC(C(C(C3O)O)O)C)O)O)CO)C)CC2O)C)(CC1)C)C
MOL011438	0.2516	0.7484	0.7079	Panacis Quinquefolii Radix	pseudoginsenoside RT5_qt	15886258	FALSE	O1C(CCC1C(O)(C)C)(C1C2C(C3(C(C4(C(C(CC4)O)(C)C)C(C3)O)C)CC2O)C)(CC1)C)C

MOL011439	0.4203	0.5797	0.7763	Panacis Quinquefolii Radix	(2R,3R,4S,5S,6R)-2-[[(3S,5R,6S,8R,9R,10R,12R,13R,14R,17S)-3,12-dihydroxy-17-[(2S,5R)-5-(2-hydroxypropan-2-yl)-2-methyloxolan-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-6-yl]oxy]-6-(hydroxymethyl)oxa	21633075	FALSE	O1C(CCC1C(O)(C)C)(C1C2C(C3(C(C4(C(C(C(CC4)O)(C)C)C(C3)OC3OC(C(C(C3O)O)O)CO)C)CC2O)C)(CC1)C)C
MOL011440	0.9193	0.0807	0.9318	Panacis Quinquefolii Radix	vitamin b6	1054	TRUE	Oc1c(c(CO)cnc1C)CO
MOL011440	0.9193	0.0807	0.9318	Hordei Fructus Germinatus	vitamin b6	1054	TRUE	Oc1c(c(CO)cnc1C)CO
MOL011441	0.9462	0.0538	0.9703	Panacis Quinquefolii Radix	Sorbin	6904	FALSE	OC(C(O)CO)C(O)C(=O)CO
MOL011442	0.2050	0.7950	0.6384	Panacis Quinquefolii Radix	(8S,9S,10R,13R,14S,17R)-17-[(1R,4R)-4-ethyl-1,5-dimethylhexyl]-10,13-dimethyl-1,2,8,9,11,12,14,15,16,17-decahydrocyclopenta[a]phenanthren-7-one	12444466	FALSE	C1=CC2=CC(=O)C3C4CCC(C(CCC(CC)C(C)C)C)C4(C)CCC3C2(CC1)C
MOL011447	0.9116	0.0884	0.8866	Panacis Quinquefolii Radix	Amyltoluene	14109	FALSE	c1(ccccc1)CCCCCC

MOL011448	0.8355	0.1645	0.8890	Panacis Quinquefolii Radix	2-(4-cyclohexylphenoxy)ethanol	160168	FALSE	C1CCC(CC1)c1ccc(cc1)OCCO
MOL011449	0.6600	0.3400	0.8606	Panacis Quinquefolii Radix	20-(R)-Ginsenoside-Rg2	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)OC2C(C(C(C(O2)C)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL011450	0.2494	0.7506	0.7336	Panacis Quinquefolii Radix	20-(R)-Ginsenoside-Rg2_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL011451	0.4038	0.5962	0.7568	Panacis Quinquefolii Radix	20(R)-Ginsenoside-Rh1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)O)C)C)(C)C)O
MOL011452	0.2494	0.7506	0.7336	Panacis Quinquefolii Radix	20(R)-Ginsenoside-Rh1_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL011453	0.6798	0.3202	0.8580	Panacis Quinquefolii Radix	20-(S)-Ginsenoside-Rg3	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)O
MOL011454	0.2305	0.7695	0.7376	Panacis Quinquefolii Radix	20-(S)-Ginsenoside-Rg3_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL011455	0.4144	0.5856	0.7459	Panacis Quinquefolii Radix	20-Hexadecanoylingenol	Not Available	FALSE	C123C(=O)C(C4C(CC1C)C4(C)C)C=C(COC(=O)CCC)C(C2(C(C(=C3)C)O)O)O
MOL011457	0.8993	0.1007	0.9037	Panacis Quinquefolii Radix	3-Methoxyherbacetin	5319442	FALSE	c1(cc(c2c(c1O)oc(c(c2=O)OC)c1ccc(cc1)O)O)O
MOL011458	0.7759	0.2241	0.7991	Panacis Quinquefolii Radix	3-O-beta-D-Xylopyranosyl-(1-6)-beta-D-glucopyranosyl-(1-6)-beta-D-glucopyranosyl oleanolic acid 28-O-beta-D-glucopyranosyl ester	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1OC(C(C(C1O)O)O)O)CO)C)C)(C)C)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)COC1OCC(C(C1O)O)O

MOL011459	0.7553	0.2447	0.9079	Panacis Quinquefolii Radix	3-O-beta-D-Xylopyranosyl-(1-6)-beta-D-glucopyranosyl-(1-6)-beta-D-glucopyranosyl oleanolic acid 28-O-beta-D-glucopyranosyl ester_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)C)(C)C)O
MOL011460	0.7369	0.2631	0.6810	Panacis Quinquefolii Radix	3-phenyldecane	Not Available	FALSE	C(CCCCCCC)(CC)c1ccccc1
MOL011461	0.5797	0.4203	0.6799	Panacis Quinquefolii Radix	3-phenyldodecane	Not Available	FALSE	C(CCCCCCCCC)(CC)c1ccccc1
MOL011462	0.8992	0.1008	0.8665	Panacis Quinquefolii Radix	3-phenylhexane	12411130	FALSE	c1(ccccc1)C(CC)CCC
MOL011463	0.5665	0.4335	0.6499	Panacis Quinquefolii Radix	4-phenyldodecane	Not Available	FALSE	C(CCCCCCCC)(CCC)c1ccccc1
MOL011464	0.4695	0.5305	0.6390	Panacis Quinquefolii Radix	4-phenyltridecane	Not Available	FALSE	c1(ccccc1)C(CCC)CCCCCCCCC
MOL011465	0.6682	0.3318	0.6683	Panacis Quinquefolii Radix	4-phenylundecane	Not Available	FALSE	c1(ccccc1)C(CCC)CCCCCCC
MOL011466	0.5720	0.4280	0.6365	Panacis Quinquefolii Radix	5-phenyldodecane	Not Available	FALSE	c1(ccccc1)C(CCCC)CCCCCCC
MOL011467	0.4763	0.5237	0.6229	Panacis Quinquefolii Radix	5-phenyltridecane	Not Available	FALSE	c1(ccccc1)C(CCCC)CCCCCCCC
MOL011468	0.5866	0.4134	0.6647	Daturae Flos	Pinoresinol diglucoside	174003	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(OC3OC(C(O)C(O)C3O)CO)cc2)C1)c1cc(OC)c(OC2OC(C(O)C(O)C2O)CO)cc1
MOL011468	0.5866	0.4134	0.6647	Eucommiae Folium	Pinoresinol diglucoside	174003	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(OC3OC(C(O)C(O)C3O)CO)cc2)C1)c1cc(OC)c(OC2OC(C(O)C(O)C2O)CO)cc1
MOL011469	0.8398	0.1602	0.7249	Daturae Flos	trans-p-hydroxyphenylethanol-p-β-coumarate	Not Available	FALSE	c1c(ccc(c1)CCOC(=O)/C=C\c1ccc(cc1)O)O

MOL011470	0.3371	0.6629	0.7540	Daturae Flos	12-Deoxywithastramonolide	Not Available	FALSE	C1CCC2(C(C1=O)(C1C(C3C2O3)C2C(CC1)(C(CC2)C(C1OC(=O)C(=C(C1)C)CO)C)C)C)O
MOL011471	0.8888	0.1112	0.9611	Daturae Flos	MCT	9958	FALSE	Oc1cc(ccc1O)C
MOL011472	0.8718	0.1282	0.8031	Daturae Flos	/-O-β-D-glucopyranosyl-KaempPferol	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1C(C(C(C(O1)COC1C(C(C(C(O1)C)O)O)O)O)O)O)c1ccc(cc1)O)O)OC1C(C(C(C(O1)CO)O)O)O
MOL011473	0.8670	0.1330	0.7544	Daturae Flos	7—O—α-L—ramnopyranosyl—KaempferoL	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OCC1C(C(C(C(O1)O)OCC1C(C(C(C(O1)O)O)O)O)O)O)c1ccc(cc1)O)O)OC1C(C(C(C(O1)O)O)O)O
MOL011474	0.8688	0.1312	0.7986	Daturae Flos	3-O-β-D-glueopyranosyl-(1→2)glueoPyranosyl-Kaempferol	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OCC1C(C(C(C(O1)O)OCC1C(C(C(C(O1)O)O)O)O)O)O)c1ccc(cc1)O)O)O
MOL011475	0.8687	0.1313	0.8095	Daturae Flos	7-O-β-D-glueopyranosyl-Kaempferol	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1C(C(C(C(O1)CO)O)O)OC1C(C(C(C(O1)CO)O)O)O)c1ccc(cc1)O)O)OC1C(C(C(C(O1)C)O)O)O
MOL011476	0.8813	0.1187	0.7652	Daturae Flos	3-O-β-D-glueopyranosyl	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OCC1C(C(C(C(O1)O)O)O)O)c1ccc(cc1)O)O)OC1OC(C(C(C1O)O)O)O
MOL011477	0.8945	0.1055	0.7862	Daturae Flos	7-O-α-L-rhamnopyranosyl-Kaempferol	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(cc1)O)O)OCC1C(C(C(C(O1)O)O)O)O
MOL011478	0.8768	0.1232	0.7744	Daturae Flos	Anisodamine	929216	FALSE	OC1C2N(C(C1)CC(OC(=O)C(c1ccccc1)CO)C2)C
MOL011479	0.9298	0.0702	0.8903	Daturae Flos	Cuscohygrine	6552019	FALSE	O=C(CC1N(CCC1)C)CC1N(CCC1)C
MOL011480	0.4586	0.5414	0.6308	Daturae Flos	Datuarmetelin e C	Not Available	FALSE	C1CCC2(C(C1=O)(C1C(CC2O)C2C(C(C1)O)(C(CC2)C(C1OC(=O)C(=C(C1)C)COC)CO)C)C)O
MOL011481	0.4778	0.5222	0.6301	Daturae Flos	Datuarmetelin e E	Not Available	FALSE	C1CCC2(C(C1=O)(C1C(CC2O)C2C(C(C1)O)(C(CC2)C(C1OC(=O)C(=C(C1)C)C)CO)C)C)O
MOL011482	0.6391	0.3609	0.6839	Daturae Flos	Daturametelin e M	Not Available	FALSE	C1=CCC2(C(C1=O)(C1C(CC2O)C2C(C(C1)O)(C(CC2)C1C2OC(=O)C(C(C2)(OC1)C)CO)C)C)O
MOL011484	0.5990	0.4010	0.7981	Daturae Flos	Datuarmetelos ide A	Not Available	FALSE	C1CCC2(C(C1=O)(C1C(C3C2O3)C2C(C(C1)O)(C(CC2)C(C1OC(=O)C(=C(C1)C)COC1C(C(C(C(O1)CO)O)O)O)O)C)C)O
MOL011485	0.4858	0.5142	0.7216	Daturae Flos	Datuarmetelos ide A_qt	Not Available	FALSE	C1CCC2(C(C1=O)(C1C(C3C2O3)C2C(C(C1)O)(C(CC2)C(C1OC(=O)C(=C(C1)C)CO)C)C)C)O
MOL011486	0.5705	0.4295	0.8180	Daturae Flos	Datuarmetelos ide B	Not Available	FALSE	C1=CCC2(C(C1=O)(C1C(C3C2O3)C2C(CC1)(C(CC2)C(C1OC(=O)C(=C(C1)C)COC1C(C(C(C(O1)CO)O)O)O)O)C)C)O

MOL011487	0.3433	0.6567	0.7627	Daturae Flos	Datuarmetelos ide B_qt	Not Available	FALSE	C1=CCC2(C(C1=O)(C1C(C3C2O3)C2C(CC1)(C(CC 2)C(C1OC(=O)C(=C(C1)C)CO)C)C)C)O
MOL011488	0.6036	0.3964	0.8030	Daturae Flos	Datuarmetelos ide C	Not Available	FALSE	C1=CCC2(C(C1=O)(C1C(C3C2O3)C2C(C(C1)O)(C(CC2)C(C1OC(=O)C(=C(C1)C)COC1C(C(C(C(O1)C O)O)O)O)C)C)C)O
MOL011489	0.4934	0.5066	0.7232	Daturae Flos	Datuarmetelos ide C_qt	Not Available	FALSE	C1=CCC2(C(C1=O)(C1C(C3C2O3)C2C(C(C1)O)(C(CC2)C(C1OC(=O)C(=C(C1)C)CO)C)C)C)O
MOL011490	0.2101	0.7899	0.6768	Daturae Flos	Datumetelin	Not Available	FALSE	O1CC(C2C3(C(C4C(CC3)C3(C(=CC4)CC=CC3=O) C)CC2)C)C2OC(=O)C(C1(C2)C)COC
MOL011491	0.9159	0.0841	0.8585	Daturae Flos	Datumetine	12451106	FALSE	O(C1CC2N(C(CC2)C1)C)C(=O)c1ccc(OC)cc1
MOL011492	0.9205	0.0795	0.7873	Daturae Flos	Daturametela mdie A	60714421	FALSE	c1c(ccc(c1)/C=C/C(=O)N(CCCC(=O)OC)C)O
MOL011493	0.9205	0.0795	0.7873	Daturae Flos	Daturametela mdie B	Not Available	FALSE	c1c(ccc(c1)/C=C\C(=O)N(CCCC(=O)OC)C)O
MOL011494	0.3977	0.6023	0.7607	Daturae Flos	Daturametelin A	Not Available	FALSE	O1C(C(C2C3(C(C4C(CC3)C3(C(=CC4)CC=CC3=O)C)CC2)C)C)CC(=C(C1=O)COC1OC(C(O)C(O)C1O)CO)C
MOL011495	0.2114	0.7886	0.7261	Daturae Flos	Daturametelin A_qt	Not Available	FALSE	O1C(C(C2CCC3C2(CCC2C3CC=C3C2(C)C(=O)C= CC3)C)C)CC(=C(C1=O)CO)C
MOL011496	0.5149	0.4851	0.8131	Daturae Flos	(6R)-6-[(1R)-1-[(8S,9S,10R,13S,14S,17R)-10,13-dimethyl-1-oxo-4,7,8,9,11,12,14,15,16,17-decahydrocyclopenta[a]phenanthren-17-yl]-2-hydroxyethyl]-4-methyl-3-[[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]-5,6-dihydropyran-2-one	14428176	FALSE	O1C(C(C(C(C1CO)O)O)O)OCC1=C(CC(OC1=O)C(C1C2(C(C3C(CC2)C2(C(=CC3)CC=CC2=O)C)CC1)C)CO)C

MOL011497	0.2998	0.7002	0.6221	Daturae Flos	(6R)-6-[(1R)-2-hydroxy-1-[(8S,9S,10R,13S,14S,17R)-1-keto-10,13-dimethyl-4,7,8,9,11,12,14,15,16,17-decahydrocyclopenta[a]phenanthren-17-yl]ethyl]-4-methyl-3-methylol-5,6-dihydropyran-2-one	14428178	FALSE	OCC1=C(CC(OC1=O)C(C1C2(C(C3C(CC2)C2(C(=CC3)CC=CC2=O)C)CC1)C)CO)C
MOL011498	0.2101	0.7899	0.6768	Daturae Flos	(1R,2R,5R,6S)-2-[(8S,9S,10R,13S,14S,17R)-10,13-dimethyl-1-oxo-4,7,8,9,11,12,14,15,16,17-decahydrocyclopenta[a]phenanthren-17-yl]-6-(methoxymethyl)-5-methyl-4,8-dioxabicyclo[3.3.1]nonan-7-one	14428167	FALSE	O1C2(CC(OC(=O)C2COC)C(C1)C1C2(C(C3C(CC2)C2(C(=CC3)CC=CC2=O)C)CC1)C)C
MOL011499	0.5318	0.4682	0.7179	Daturae Flos	Daturametelin e A	Not Available	FALSE	C1=CCC2(C(C1=O)(C1C(C3C2O3)C2C(C(C1)O)(C(CC2O)C(C1OC(=O)C(=C(C1)C)C)C)C)C)O
MOL011500	0.5021	0.4979	0.6373	Daturae Flos	Daturametelin e B	Not Available	FALSE	C1CCC2(C(C1=O)(C1C(CC2O)C2C(CC1)(C(CC2O)C(C1OC(=O)C(=C(C1)C)C)CO)C)C)O
MOL011501	0.4951	0.5049	0.6848	Daturae Flos	Daturametelin e F	Not Available	FALSE	C1=CCC2(C(C1=O)(C1C(CC2O)C2C(C(C1)O)(C(CC2)C1C2OC(=O)C(C(C2)(OC1)C)COC)C)C)O
MOL011502	0.5922	0.4078	0.6310	Daturae Flos	Daturametelin e K	Not Available	FALSE	C1=CCC2(C(C1=O)(C1C(CC2O)C2C(C(C1)O)(C(CC2)C(CO)C1OC(=O)C(C(C1)(C)O)CC(O)C)C)C)O

MOL011503	0.6638	0.3362	0.6475	Daturae Flos	Daturametelin e L	Not Available	FALSE	C1=CCC2(C(C1=O)(C1C(CC2O)C2C(C(C1)O)(C(C C2)C(CO)C1OC(=O)C(C(C1)(C)O)(CC(O)C)O)C)C) O
MOL011504	0.9101	0.0899	0.7830	Daturae Flos	Daturametelin e N	Not Available	FALSE	C1C(CC(C(C1(C)C)(O)/C(=C/C(=O)C)/O)(C)O)O
MOL011505	0.6299	0.3701	0.8046	Daturae Flos	Daturametelos ide E	Not Available	FALSE	C1=CCC2(C(C1=O)(C1C(C(C2O)O)C2C(CC1)(C(C C2)C(C1OC(=O)C(=C(C1)C)COC1C(C(C(C(O1)CO)O)O)O)C)C)C)O
MOL011506	0.4675	0.5325	0.6667	Daturae Flos	Daturametelos ide E_qt	Not Available	FALSE	C1=CCC2(C(C1=O)(C1C(C(C2O)O)C2C(CC1)(C(C C2)C(C1OC(=O)C(=C(C1)C)CO)C)C)C)O
MOL011507	0.6840	0.3160	0.7809	Daturae Flos	Daturametelos ide F	Not Available	FALSE	C1=CCC2(C(C1=O)(C1C(C(C2O)O)C2C(C(C1)O)(C(CC2)C(C1OC(=O)C(=C(C1)C)COC1C(C(C(C(O1)CO)O)O)O)C)C)C)O
MOL011508	0.6084	0.3916	0.6486	Daturae Flos	Daturametelos ide F_qt	Not Available	FALSE	C1=CCC2(C(C1=O)(C1C(C(C2O)O)C2C(C(C1)O)(C(CC2)C(C1OC(=O)C(=C(C1)C)CO)C)C)C)O
MOL011509	0.5803	0.4197	0.7975	Daturae Flos	Daturametelos ide G	Not Available	FALSE	C1CCC2(C(C1=O)(C1C(CC2O)C2C(CC1)(C(CC2)C (C1OC(=O)C(=C(C1)C)COC1C(C(C(C(O1)CO)O)O) O)C)C)C)O
MOL011510	0.3131	0.6869	0.6492	Daturae Flos	Daturametelos ide G_qt	Not Available	FALSE	C1CCC2(C(C1=O)(C1C(CC2O)C2C(CC1)(C(CC2)C (C1OC(=O)C(=C(C1)C)CO)C)C)C)O
MOL011511	0.6129	0.3871	0.7820	Daturae Flos	Daturametelos ide H	Not Available	FALSE	C1CCC2(C(C1=O)(C1C(CC2O)C2C(C(C1)O)(C(CC 2)C(C1OC(=O)C(=C(C1)C)COC1C(C(C(C(O1)CO) O)O)O)C)C)C)O
MOL011512	0.4738	0.5262	0.6385	Daturae Flos	Daturametelos ide H_qt	Not Available	FALSE	C1CCC2(C(C1=O)(C1C(CC2O)C2C(C(C1)O)(C(CC 2)C(C1OC(=O)C(=C(C1)C)CO)C)C)C)O
MOL011513	0.6027	0.3973	0.7332	Daturae Flos	Daturametelos ide I	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1O)C)CC(C1(C3CCC1C(C 1OC(=O)C(=C(C1)C)CO)C)C)O)OC1OC(C(C(C1O) O)O)CO
MOL011514	0.3672	0.6328	0.6331	Daturae Flos	Daturametelos ide I_qt	Not Available	FALSE	C1C(CC2=CCC3C(C2(C1O)C)CC(C1(C3CCC1C(C 1OC(=O)C(=C(C1)C)CO)C)C)O)O
MOL011515	0.6364	0.3636	0.8273	Daturae Flos	Daturametelos ide J	Not Available	FALSE	C1C(CC2(C(C1O)(C1C(=CC2O)C2C(CC1)(C(CC2) C(C1OC(=O)C(=C(C1)C)CO)C)C)C)O)OC1OC(C(C (C1O)O)O)CO
MOL011516	0.5223	0.4777	0.6595	Daturae Flos	Daturametelos ide J_qt	Not Available	FALSE	C1C(CC2(C(C1O)(C1C(=CC2O)C2C(CC1)(C(CC2) C(C1OC(=O)C(=C(C1)C)CO)C)C)C)O)O
MOL011517	0.9145	0.0855	0.8184	Daturae Flos	Daturametelos ide N	Not Available	FALSE	C1C(CC(C(C1(C)C)(O)/C(=C/C(=O)C)/O)(C)O)OC1 C(C(C(C(O1)CO)O)O)O
MOL011518	0.9070	0.0930	0.8047	Daturae Flos	Guaiaeol-O-β-D-diglucopyranoside	Not Available	FALSE	c1cc(c(cc1)OC)OC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)CO)O)O)O)O)O
MOL011519	0.8182	0.1818	0.7586	Daturae Flos	hyoscine	Not Available	FALSE	C12C(O2)C2N(C1CC(C2)OC(=O)C(c1ccccc1)CO)C
MOL011520	0.2991	0.7009	0.7372	Daturae Flos	hypaconitine	23337	FALSE	O([C@@]12C3[C@@H]4N(CC5([C@H](C4([C@H]4[C@@H]1C(OC(=O)c1ccccc1)[C@](O)(C4)C(OC) C2O)C(OC)CC5)C3OC)COC)C)C(=O)C

MOL011521	0.8734	0.1266	0.8086	Daturae Flos	KaemPferol-3	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(=O)c2c(oc1c1ccc(O)cc1)cc(OC1OC(C(O)C(O)C1O)CO)cc2O)CO
MOL011521	0.8734	0.1266	0.8086	Equiseti Hiemalis Herba	KaemPferol-3	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(=O)c2c(oc1c1ccc(O)cc1)cc(OC1OC(C(O)C(O)C1O)CO)cc2O)CO
MOL011522	0.4608	0.5392	0.6772	Daturae Flos	litorin	5486808	FALSE	S(CCC(NC(=O)C(NC(=O)C(NC(=O)CNC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C(NC(=O)C1NC(=O)CC1)CCC(=O)N)Cc1c2c([nH]c1)cccc2)C)C(C)C)Cc1[nH]cnc1)Cc1ccccc1)C(=O)N)C
MOL011523	0.9535	0.0465	0.8758	Daturae Flos	Meteloidine	Not Available	FALSE	OC1C2N(C(C1O)CC(OC(=O)/C(=C/C)/C)C2)C
MOL011524	0.9491	0.0509	0.9628	Daturae Flos	methyl (2S)-3-hydroxy-2-phenylpropanoate	11008522	FALSE	OCC(c1ccccc1)C(=O)OC
MOL011525	0.9000	0.1000	0.8182	Daturae Flos	Norhyoscyamine	12442861	FALSE	O(C1CC2NC(CC2)C1)C(=O)C(c1ccccc1)CO
MOL011526	0.9100	0.0900	0.8102	Daturae Flos	Phenethyl alcohol-O-β-D-glucopyranosyl-(2→1)-O-β-D-glucopyranoside	Not Available	FALSE	c1cccc(c1)CCOC1C(C(C(C(O1)CO)OC1C(C(C(C(O1)CO)O)O)O)O)O)O
MOL011527	0.9363	0.0637	0.9526	Daturae Flos	phenylpropyl acetate	66598934	FALSE	c1c(ccc(c1)CCCC(=O)C)O
MOL011528	0.9088	0.0912	0.9173	Daturae Flos	p-hydroxyphenethyl-p-hydroxybenzoate	Not Available	FALSE	c1c(ccc(c1)CCOC(=O)c1ccc(cc1)O)O
MOL011529	0.9510	0.0490	0.9132	Daturae Flos	pseudotropine	449293	FALSE	OC1CC2N(C(CC2)C1)C
MOL011530	0.8884	0.1116	0.8046	Daturae Flos	Quercetin-3	Not Available	FALSE	C1(C(C(C(OC1CO)Oc1cc(c2c(c1)oc(c(c2=O)OC1C(C(C(C(O1)CO)O)O)O)c1ccc(c(c1)O)O)O)O)O)O
MOL011531	0.1732	0.8268	0.6636	Daturae Flos	Secowithamerclin	Not Available	FALSE	C1=CCC2=CCC3C(C2(C1=O)C)CCC1(C3CCC1C(CO)C1OC(=O)C(=C(C1)C)COC)C
MOL011532	0.9279	0.0721	0.8994	Daturae Flos	Tigloidine	Not Available	FALSE	O(C1CC2N(C(CC2)C1)C)C(=O)/C(=C\C)/C
MOL011533	0.9448	0.0552	0.8859	Daturae Flos	troPane-3α	13855894	FALSE	C1(C2CC(CC(C1)N2C)O)O
MOL011534	0.9435	0.0565	0.9557	Daturae Flos	(S)-tropic acid	785356	FALSE	OCC(c1ccccc1)C(=O)O
MOL011535	0.4806	0.5194	0.6287	Daturae Flos	Withafastuosin F	Not Available	FALSE	C1CCC2(C(C1=O)(C1C(CC2O)C2C(CC1)(C(CC2)C(C1OC(=O)C(=C(C1)C)CO)CO)C)C)O
MOL011536	0.3225	0.6775	0.6282	Daturae Flos	Withametelin C	Not Available	FALSE	C1CCC2(C(C1=O)(C1C(CC2O)C2C(CC1)(C(CC2)C(C1OC(=O)C(=C(C1)C)C)CO)C)C)O

MOL011537	0.4858	0.5142	0.7216	Daturae Flos	Withametelin E	Not Available	FALSE	C1CCC2(C(C1=O)(C1C(C3C2O3)C2C(C(C1)O)(C(CC2)C(C1OC(=O)C(=C(C1)C)CO)C)C)C)O
MOL011538	0.3631	0.6369	0.7215	Daturae Flos	Withametelin G	Not Available	FALSE	C1=CCC2(C(C1=O)(C1C(CC2O)C2C(CC1)(C(CC2)C1C2OC(=O)C(=C)C(C2)(OC1)C)C)C)O
MOL011539	0.2148	0.7852	0.7044	Daturae Flos	Withametelin	Not Available	FALSE	O1CC(C2C3(C(C4C(CC3)C3(C(=CC4)CC=CC3=O)C)CC2)C)C2OC(=O)C(=C)C1(C2)C
MOL011540	0.3088	0.6912	0.7741	Daturae Flos	withanolide D	Not Available	FALSE	C1=CC(C23C(C1=O)(C1C(CC2O3)C2C(CC1)(C(CC2)C(C)C1OC(=O)C(=C(C1)C)C)C)C)O
MOL011541	0.6207	0.3793	0.8136	Daturae Flos	withanoside III	Not Available	FALSE	C1C(CC2(C(C1O)(C1C(C3C2O3)C2C(CC1)(C(CC2)C(C1OC(=O)C(=C(C1)C)CO)C)C)C)O)OC1OC(CO)C(C(C1O)O)O
MOL011542	0.4717	0.5283	0.6987	Daturae Flos	withanoside III_qt	Not Available	FALSE	C1C(CC2(C(C1O)(C1C(C3C2O3)C2C(CC1)(C(CC2)C(C1OC(=O)C(=C(C1)C)CO)C)C)C)O)O
MOL011543	0.9279	0.0721	0.8322	Jujubae Fructus	Zizybeoside I	11972301	FALSE	O(C1C(O)C(O)C(OC1OCc1ccccc1)CO)C1OC(C(O)C(O)C1O)CO
MOL011543	0.9279	0.0721	0.8322	Daturae Flos	Zizybeoside I	11972301	FALSE	O(C1C(O)C(O)C(OC1OCc1ccccc1)CO)C1OC(C(O)C(O)C1O)CO
MOL011545	0.9336	0.0664	0.7646	Ginkgo Folium	(1R,2R)-1,2-Diphenylethylenediamine	2724998	FALSE	c1(C(C(c2ccccc2)N)N)ccccc1
MOL011546	0.8948	0.1052	0.9726	Ligustici Rhizoma Et Radix	4-Methyl-2,3-dihydrofuran	36744	FALSE	O1C=C(CC1)C
MOL011546	0.8948	0.1052	0.9726	Ginkgo Folium	4-Methyl-2,3-dihydrofuran	36744	FALSE	O1C=C(CC1)C
MOL011547	0.8925	0.1075	0.9090	Eriobotryae Folium	lutidine	7937	FALSE	n1c(cccc1C)C
MOL011547	0.8925	0.1075	0.9090	Ginkgo Folium	lutidine	7937	FALSE	n1c(cccc1C)C
MOL011548	0.9006	0.0994	0.9305	Ginkgo Folium	Hexamethylethane	11675	FALSE	C(C(C)(C)C)(C)(C)C
MOL011548	0.9006	0.0994	0.9305	Peucedanidecursivi Radix	Hexamethylethane	11675	FALSE	C(C(C)(C)C)(C)(C)C
MOL011548	0.9006	0.0994	0.9305	Peucedani Radix	Hexamethylethane	11675	FALSE	C(C(C)(C)C)(C)(C)C
MOL011548	0.9006	0.0994	0.9305	Viticis Fructus	Hexamethylethane	11675	FALSE	C(C(C)(C)C)(C)(C)C
MOL011549	0.9475	0.0525	0.8532	Ginkgo Folium	2,3-dihydro-7-hydroxy-3-methyl-1H-inden-1-one	Not Available	FALSE	C1(=O)CC(c2cccc(c12)O)C
MOL011550	0.1556	0.8444	0.6788	Ginkgo Folium	sciadopitysin	5281696	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)OC)c1c(cc(c2c1oc(cc2=O)c1ccc(cc1)OC)O)O)O)OC
MOL011551	0.9171	0.0829	0.9021	Ginkgo Folium	2,3-dimethyloctane	Not Available	FALSE	C(CCCCC)(C(C)C)C

MOL011553	0.9141	0.0859	0.7095	Ginkgo Folium	2-butyl-1,1,3-trimethyl cyclohexane	Not Available	FALSE	C1(C(C(CCC1)C)CCCC)(C)C
MOL011554	0.9341	0.0659	0.9441	Ginkgo Folium	2-isopropyl-2,5-dimethyl-cyclohexanone	Not Available	FALSE	O=C1C(CCC(C1)C)(C(C)C)C
MOL011555	0.9510	0.0490	0.9215	Ginkgo Folium	DMBC	7531	FALSE	OC(Cc1ccccc1)(C)C
MOL011558	0.9464	0.0536	0.9312	Ginkgo Folium	3-(2-pentenyl)-1,2,4-cyclopentanetrione	Not Available	FALSE	C1(=O)C(=O)C(C(=O)C1)C/C=C/CC
MOL011559	0.8917	0.1083	0.9014	Ginkgo Folium	Sym-m-xylenol	7948	FALSE	Cc1cc(O)cc(C)c1
MOL011559	0.8917	0.1083	0.9014	Eucommiae Folium	Sym-m-xylenol	7948	FALSE	Cc1cc(O)cc(C)c1
MOL011560	0.9260	0.0740	0.8413	Ginkgo Folium	3,4,4a,5,6,7-hexahydro-1,1,4a-trimethyl-2(1H)-napthalenone	55263459	FALSE	O=C1C(C2=CCCCC2(CC1)C)(C)C
MOL011561	0.9209	0.0791	0.9598	Ginkgo Folium	Maleimide, 2-ethyl-3-methyl-	29995	FALSE	O=C1NC(=O)C(=C1CC)C
MOL011562	0.9243	0.0757	0.9324	Ginkgo Folium	3-Ethylhexane	12096	FALSE	C(CCC)(CC)CC
MOL011563	0.9244	0.0756	0.9493	Paederiae Scandentis Herba	gamma-Hexenol	5284503	FALSE	OCC/C=C/CC
MOL011563	0.9244	0.0756	0.9493	Ginkgo Folium	gamma-Hexenol	5284503	FALSE	OCC/C=C/CC
MOL011563	0.9244	0.0756	0.9493	Citri Grandis Exocarpium	gamma-Hexenol	5284503	FALSE	OCC/C=C/CC
MOL011563	0.9244	0.0756	0.9493	Scutellariae Barbatae Herba	gamma-Hexenol	5284503	FALSE	OCC/C=C/CC
MOL011563	0.9244	0.0756	0.9493	Rose Rugosae Flos	gamma-Hexenol	5284503	FALSE	OCC/C=C/CC
MOL011564	0.9246	0.0754	0.9709	Ginkgo Folium	HBR	439314	FALSE	OC(C(=O)C)C
MOL011564	0.9246	0.0754	0.9709	Litchi Semen	HBR	439314	FALSE	OC(C(=O)C)C
MOL011565	0.8729	0.1271	0.9602	Ginkgo Folium	3-Methylcyclopent-2-enone	17691	FALSE	O=C1CCC(=C1)C

MOL011566	0.9166	0.0834	0.9258	Ginkgo Folium	m-Tolyl carbinol	11476	FALSE	Cc1cccc(CO)c1
MOL011567	0.7929	0.2071	0.8959	Ginkgo Folium	3,3'-dimethoxy-cis-stilbene-4,4'-diol	9548762	FALSE	c1(c(ccc(c1)/C=C\c1ccc(c(c1)OC)O)O)OC
MOL011568	0.9458	0.0542	0.9166	Ginkgo Folium	5,6,7,7a-tetrahydro-4,4,7a-trimethy-2(4H)-benzofuranone	Not Available	FALSE	C12C(=CCC(C2)C)C(C(=O)O1)C
MOL011569	0.3874	0.6126	0.6278	Ginkgo Folium	5 -Methoxy-bilobetin	5319411	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1cc(c(c(c1)OC)OC)c1c(cc(c2c1oc(cc2=O)c1ccc(cc1)O)O)O)O)O
MOL011569	0.3874	0.6126	0.6278	Solidaginis Herba	5 -Methoxy-bilobetin	5319411	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1cc(c(c(c1)OC)OC)c1c(cc(c2c1oc(cc2=O)c1ccc(cc1)O)O)O)O)O
MOL011570	0.5720	0.4280	0.6365	Ginkgo Folium	5-phenyldodecane	Not Available	FALSE	C(CCCCCCC)(CCCC)c1ccccc1
MOL011571	0.4558	0.5442	0.6568	Ginkgo Folium	methyl 5-[(2R,3S)-3-undecyloxiran-2-yl]pentanoate	15591293	FALSE	C(=O)(CCCCC1C(CCCCCCCCCCC)O1)OC
MOL011573	0.9213	0.0787	0.7077	Ephedra Herba	6-Hydroxykynurenate	440752	FALSE	O=c1c2c([nH]c(c1)C(=O)O)ccc(O)c2
MOL011573	0.9213	0.0787	0.7077	Ginkgo Folium	6-Hydroxykynurenate	440752	FALSE	O=c1c2c([nH]c(c1)C(=O)O)ccc(O)c2
MOL011574	0.9346	0.0654	0.9495	Ginkgo Folium	Ethylheptenone	5363290	FALSE	C(=C\CCC(=O)C)(/CC)\C
MOL011575	0.5746	0.4254	0.6277	Ginkgo Folium	6-phenyldodecane	Not Available	FALSE	C(CCCCCC)(CCCCC)c1ccccc1
MOL011576	0.9281	0.0719	0.9530	Campsis Flos	1-PHENYL-ETHANOL	637516	FALSE	OC(c1ccccc1)C
MOL011576	0.9281	0.0719	0.9530	Ginkgo Folium	1-PHENYL-ETHANOL	637516	FALSE	OC(c1ccccc1)C
MOL011577	0.9285	0.0715	0.9442	Paederiae Scandentis Herba	o-Tolualdehyde	10722	FALSE	c1(c(cccc1)C)C=O

MOL011577	0.9285	0.0715	0.9442	Lysimachiae Foenigraeci Herba	o-Tolualdehyde	10722	FALSE	c1(c(cccc1)C)C=O
MOL011577	0.9285	0.0715	0.9442	Ginkgo Folium	o-Tolualdehyde	10722	FALSE	c1(c(cccc1)C)C=O
MOL011578	0.8879	0.1121	0.7546	Ginkgo Folium	Bilobalide	Not Available	FALSE	O1C2OC(=O)C(O)C32C2(C(OC(=O)C2)CC3(O)C(C)(C)C)C1=O
MOL011579	0.9173	0.0827	0.9067	Ginkgo Folium	Bilobanone	5315457	FALSE	o1c(CC(C)C)cc(C2CC(=O)C(=CC2)C)c1
MOL011580	0.8493	0.1507	0.8356	Chrysanthemi Flos	5-hydroxy-2-(4-hydroxy-3-methoxyphenyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	11294177	FALSE	c12c(=O)cc(oc1cc(OC1C(C(C(C(O1)CO)O)O)O)cc2O)c1cc(c(cc1)O)OC
MOL011580	0.8493	0.1507	0.8356	Polygoni Orientalis Fructus	5-hydroxy-2-(4-hydroxy-3-methoxyphenyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	11294177	FALSE	c12c(=O)cc(oc1cc(OC1C(C(C(C(O1)CO)O)O)O)cc2O)c1cc(c(cc1)O)OC
MOL011580	0.8493	0.1507	0.8356	Ginkgo Folium	5-hydroxy-2-(4-hydroxy-3-methoxyphenyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	11294177	FALSE	c12c(=O)cc(oc1cc(OC1C(C(C(C(O1)CO)O)O)O)cc2O)c1cc(c(cc1)O)OC
MOL011581	0.8667	0.1333	0.8009	Ginkgo Folium	Cycloundecene(E)	5362790	FALSE	C1CCCC/C=C/CCCC1

MOL011582	0.9110	0.0890	0.7611	Ginkgo Folium	(2R,8aS)-2,5,5,8a-tetramethyl-3,6-dihydro-2H-chromene	22211686	FALSE	O1C2(C(=CCC1C)C(CC=C2)(C)C)C
MOL011584	0.7764	0.2236	0.7665	Ginkgo Folium	(2R,3R,4R)-4-[(2R,3R)-2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxychroman-8-yl]-2-(3,4,5-trihydroxyphenyl)chroman-3,5,7-triol	13831064	FALSE	c1c(c(c2c(c1O)CC(C(O2)c1cc(c(cc1)O)O)O)C1c2c(cc(cc2O)O)OC(C1O)c1cc(c(c(c1)O)O)O)O
MOL011585	0.3533	0.6467	0.6526	Ginkgo Folium	Cardanol monoene	5281854	FALSE	Oc1cc(CCCCCCC/C=C\CCCCCC)ccc1
MOL011586	0.9140	0.0860	0.6790	Ginkgo Folium	ginkgolide B	Not Available	FALSE	O1C23C4(C5(C(CC4OC3=O)C(C)(C)C)C1OC(=O)C5O)C(O)C1OC(=O)C(C21O)C
MOL011587	0.9130	0.0870	0.6937	Ginkgo Folium	ginkgolide C	Not Available	FALSE	O1C23C4(C5(C(C(O)C4OC3=O)C(C)(C)C)C1OC(=O)C5O)C(O)C1OC(=O)C(C21O)C
MOL011588	0.9157	0.0843	0.6969	Ginkgo Folium	ginkgolide J	Not Available	FALSE	C123C4(C5(C(O3)OC(=O)C5O)C(C(C4OC2=O)O)C(C)(C)C)CC2C1(C(C(=O)O2)C)O
MOL011589	0.9175	0.0825	0.6929	Ginkgo Folium	Ginkgolide M	Not Available	FALSE	C12C(C(C(=O)O1)C)C13C4(C2O)C2(C(O1)OC(=O)C2O)C(C(C4OC3=O)O)C(C)(C)C
MOL011591	0.9125	0.0875	0.9561	Ginkgo Folium	saccharic acid	33037	FALSE	OC(C(O)C(O)C(=O)O)C(O)C(=O)O
MOL011592	0.9362	0.0638	0.9636	Ginkgo Folium	Isoamyl butyrate	7795	FALSE	O(CCC(C)C)C(=O)CCC
MOL011593	0.8662	0.1338	0.8317	Ginkgo Folium	Isoflavon	72304	FALSE	o1c2c(c(=O)c(c3ccccc3)c1)cccc2
MOL011594	0.7098	0.2902	0.7425	Ginkgo Folium	Isogoycyrol	Not Available	FALSE	c1(ccc2c(c1)oc1c2c(=O)oc2c1c1c(c(c2)OC)CCC(O1)(C)C)O
MOL011595	0.9185	0.0815	0.9712	Ginkgo Folium	Allo-L-isoleucine	6950182	FALSE	OC(=O)C(N)C(CC)C
MOL011596	0.9160	0.0840	0.8429	Ginkgo Folium	Luteolin-3′-glucoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc(ccc1O)c1oc2c(c(=O)c1)c(O)cc(O)c2)CO
MOL011597	0.9096	0.0904	0.8497	Ginkgo Folium	Luteolin-4′-glucoside	26235513	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(O)cc(cc1)c1oc2c(c(=O)c1)c(O)cc(O)c2)CO
MOL011598	0.9069	0.0931	0.8812	Ginkgo Folium	Nerylacetone	1713001	FALSE	O=C(CC/C=C(\CCC=C(C)C)/C)C
MOL011598	0.9069	0.0931	0.8812	Rose Rugosae Flos	Nerylacetone	1713001	FALSE	O=C(CC/C=C(\CCC=C(C)C)/C)C
MOL011600	0.6819	0.3181	0.6312	Ginseng Folium	METHYLPHENANTHRENE	13256	FALSE	c12c3c(ccc1cccc2)cccc3C

MOL011600	0.6819	0.3181	0.6312	Ginkgo Folium	METHYLPHENANTHRENE	13256	FALSE	c12c3c(ccc1cccc2)cccc3C
MOL011600	0.6819	0.3181	0.6312	Tamaricis Cacumen	METHYLPHENANTHRENE	13256	FALSE	c12c3c(ccc1cccc2)cccc3C
MOL011601	0.8958	0.1042	0.8699	Ginkgo Folium	Phthalide	6885	FALSE	O1Cc2c(C1=O)cccc2
MOL011602	0.8820	0.1180	0.9300	Ginkgo Folium	py	1049	FALSE	n1ccccc1
MOL011603	0.9355	0.0645	0.9489	Ginkgo Folium	sequoyitol	439990	FALSE	O(C1C(O)C(O)C(O)C(O)C1O)C
MOL011604	0.8841	0.1159	0.8727	Ginkgo Folium	Syringetin	5281953	FALSE	o1c(c2cc(OC)c(O)c(OC)c2)c(O)c(=O)c2c1cc(O)cc2O
MOL011605	0.8536	0.1464	0.7891	Ginkgo Folium	syringetin-3-rutinoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(OC)c(O)c(OC)c1)COC1OC(C(O)C(O)C1O)C
MOL011606	0.9133	0.0867	0.8626	Ginkgo Folium	(E)-4-[(1R,5R)-2,5,6,6-tetramethyl-1-cyclohex-2-enyl]but-3-en-2-one	10219918	FALSE	O=C(/C=C/C1C(C(CC=C1C)C)(C)C)C
MOL011607	0.8836	0.1164	0.6061	Ginkgo Folium	alpha-santalol	Not Available	FALSE	C12(C3C1CC(C2(CC/C=C(\CO)/C)C)C3)C
MOL011608	0.7390	0.2610	0.6967	Menthae Herba	1,3-bis-[2-(3,4-dihydroxyphenyl)-1-carboxy]ethoxycarbonyl-2-(3,4-dihydroxyphenyl)-7,8-dihydroxy-1,2-dihydronaphthalene	Not Available	FALSE	c1(ccc2c(c1O)C(C(C(=C2)C(=O)OC(C(=O)O)Cc1cc(c(cc1)O)O)c1ccc(c(c1)O)O)C(=O)OC(C(=O)O)Cc1ccc(c(c1)O)O)O

MOL011609	0.4872	0.5128	0.6894	Menthae Herba	1,3-bis[2-(3,4-dihydroxyphenyl)-1-methoxycarbonyl]ethoxycarbonyl-2-(3,4-dihydroxyphenyl)-7,8-dihydroxy-1,2-dihydronaphthalene	Not Available	FALSE	c1(ccc2c(c1O)C(C(C(=C2)C(=O)OC(C(=O)OC)Cc1ccc(c(c1)O)O)c1ccc(c(c1)O)O)C(=O)OC(C(=O)OC)Cc1cc(c(cc1)O)O)O
MOL011610	0.8068	0.1932	0.7243	Menthae Herba	3-[2-(3,4-dihydroxyphenyl)-1-carboxy]ethoxycarbonyl-2-(3,4-dihydroxyphenyl)-7,8-dihydroxy-1,2-dihydronaphthalene-1-carboxylic acid	Not Available	FALSE	C1(C(C(=Cc2ccc(c(c12)O)O)C(=O)OC(Cc1ccc(c(c1)O)O)C(=O)O)c1ccc(c(c1)O)O)C(=O)O
MOL011611	0.9495	0.0505	0.9419	Menthae Herba	PTBP	7393	FALSE	C(c1ccc(cc1)O)(C)(C)C
MOL011612	0.8566	0.1434	0.7953	Menthae Herba	7,8-dihydroxy-2-(3,4-dihydroxyphenyl)-1,2-dihydronaphthalene-1,3-dicarboxylic acid	Not Available	FALSE	c1cc2c(c(c1O)O)C(C(C(=C2)C(=O)O)c1ccc(c(c1)O)O)C(=O)O

MOL011613	0.9348	0.0652	0.9261	Menthae Herba	2-[(1S)-4-methyl-5-oxo-1-cyclohex-3-enyl]propan-2-yl acetate	2728764	FALSE	C1C=C(C(=O)CC1C(C)(C)OC(=O)C)C
MOL011614	0.8034	0.1966	0.7066	Menthae Herba	1-(3,4-dihydroxyphenyl)-3-[2-(3,4-dihydroxyphenyl)-1-carboxy]ethoxycarbonyl-6,7-dihydroxy-1,2-dihydronaphthalene-2-carboxylic acid	Not Available	FALSE	C1(C(C(=Cc2cc(c(cc12)O)O)C(=O)OC(Cc1cc(c(cc1)O)O)C(=O)O)C(=O)O)c1cc(c(cc1)O)O
MOL011615	0.9580	0.0420	0.9776	Menthae Herba	(1R,4S)-Iso-dihydrocarvone	443181	FALSE	C1(=O)CC(C(=C)C)CCC1C
MOL011616	0.7949	0.2051	0.8436	Menthae Herba	Fortunellin	5317385	FALSE	c12c(c(=O)cc(o1)c1ccc(cc1)OC)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL011617	0.8591	0.1409	0.8073	Menthae Herba	(1S,2R)-1-(3,4-dihydroxyphenyl)-6,7-dihydroxy-1,2-dihydronaphthalene-2,3-dicarboxylic acid	21602019	FALSE	c1(cc2c(cc1O)C(C(C(=C2)C(=O)O)C(=O)O)c1cc(c(cc1)O)O)O
MOL011618	0.9370	0.0630	0.9316	Menthae Herba	cis-Ocimene, 8-oxo-	5369951	FALSE	O=C/C(=C/CC=C(C)C)/C=C

MOL011619	0.7390	0.2610	0.6967	Menthae Herba	1-[2-(3,4-dihydroxyphenyl)-1-methoxycarbonyl]ethoxycarbonyl-2-(3,4-dihydroxyphenyl)-3-[2-(3,4-dihydroxyphenyl)-1-carboxy] ethoxycarbonyl-7,8-dihydroxy-1,2-dihydronaphthalene	Not Available	FALSE	C1(C(C(=Cc2ccc(c(c12)O)O)C(=O)OC(Cc1cc(c(cc1)O)O)C(=O)O)c1cc(c(cc1)O)O)C(=O)OC(Cc1ccc(c(c1)O)O)C(=O)O
MOL011620	0.8767	0.1233	0.8513	Aurantii Fructus Immaturus	Eriocitrin	83489	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(O)cc1)COC1OC(C(O)C(O)C1O)C
MOL011620	0.8767	0.1233	0.8513	Menthae Herba	Eriocitrin	83489	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(O)cc1)COC1OC(C(O)C(O)C1O)C
MOL011621	0.8659	0.1341	0.8673	Menthae Herba	5-hydroxy-2-(4-hydroxyphenyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxymethyl] tetrahydropyran-2-yl]oxy-chromone	9851181	FALSE	c12c(c(=O)cc(o1)c1ccc(cc1)O)c(cc(c2)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)O

MOL011623	0.6405	0.3595	0.6917	Menthae Herba	1-[2-(3,4-dihydroxyphenyl)-1-carboxy]ethoxycarbonyl-2-(3,4-dihydroxyphenyl)-3-[2-(3,4-dihydroxyphenyl)-1-methoxycarbonyl]ethoxycarbonyl-7,8-dihydrox-1,2-dihydronaphthalene	Not Available	FALSE	C1(C(C(=Cc2ccc(c(c12)O)O)C(=O)OC(Cc1cc(c(cc1)O)O)C(=O)OC)c1cc(c(cc1)O)O)C(=O)OC(Cc1cc(c(cc1)O)O)C(=O)O
MOL011624	0.8049	0.1951	0.7417	Menthae Herba	1-[2-(3,4-dihydroxyphenyl)-1-carboxy]ethoxycarbonyl-2-(3,4-dihydroxyphenyl)-7,8-dihydroxy-1,2-dihydronaphthalene-3-carboxylic acid	Not Available	FALSE	C1(C(C(=Cc2ccc(c(c12)O)O)C(=O)O)c1cc(c(cc1)O)O)C(=O)OC(Cc1cc(c(cc1)O)O)C(=O)O
MOL011626	0.9621	0.0379	0.9585	Menthae Herba	(3R)-3-phenylbutanal	10877278	FALSE	c1(C(CC=O)C)ccccc1
MOL011627	0.8103	0.1897	0.7209	Allii Fistulost Bulbus	1-hexoxyoctane	519362	FALSE	O(CCCCCCCC)CCCCCC
MOL011628	0.2054	0.7946	0.6534	Allii Fistulost Bulbus	Kaur-16-ene	Not Available	FALSE	C123C(C4(C(CC1)C(CCC4)(C)C)C)CCC(C2)C(=C)C3
MOL011629	0.9555	0.0445	0.9758	Allii Fistulost Bulbus	Methoxyacetic acid,1-cyclopentylethyl ester	Not Available	FALSE	O(C(C1CCCC1)C)C(=O)COC

MOL011630	0.7396	0.2604	0.6738	Allii Fistulost Bulbus	Methoxyacetic acid,2-tetradecyl ester	Not Available	FALSE	O(C(CCCCCCCCCCCC)C)C(=O)COC
MOL011631	0.8033	0.1967	0.7377	Allii Fistulost Bulbus	Methoxyacetic acid,2-tridecyl ester	Not Available	FALSE	O(C(CCCCCCCCCCC)C)C(=O)COC
MOL011632	0.8029	0.1971	0.7399	Allii Fistulost Bulbus	Methoxyacetic acid,3-tridecyl ester	Not Available	FALSE	O(C(CCCCCCCCCC)CC)C(=O)COC
MOL011633	0.9373	0.0627	0.9510	Allii Fistulost Bulbus	Methylamine, N-(1-ethylpentylidene)	Not Available	FALSE	N(=C(\CCCC)/CC)/C
MOL011634	0.9171	0.0829	0.8471	Allii Fistulost Bulbus	Benethamine	65055	FALSE	c1(CCNCc2ccccc2)ccccc1
MOL011634	0.9171	0.0829	0.8471	Equiseti Hiemalis Herba	Benethamine	65055	FALSE	c1(CCNCc2ccccc2)ccccc1
MOL011635	0.9356	0.0644	0.8447	Allii Fistulost Bulbus	Tetranap	8404	FALSE	c12c(cccc1)CCCC2
MOL011636	0.9384	0.0616	0.7783	Allii Fistulost Bulbus	5-METHYLTETRALIN	17768	FALSE	c12c(c(ccc1)C)CCCC2
MOL011639	0.9074	0.0926	0.8068	Allii Fistulost Bulbus	Propanoic acid,3-mercapto-,2-ethylhexyl ester	Not Available	FALSE	C(COC(=O)CCS)(CCCC)CC
MOL011641	0.9389	0.0611	0.9656	Allii Fistulost Bulbus	ethenoxycyclohexane	75129	FALSE	C1(CCCCC1)OC=C
MOL011643	0.9130	0.0870	0.9453	Allii Fistulost Bulbus	pectin	441476	FALSE	O1C(C(O)C(O)C(O)C1O)C(=O)O
MOL011643	0.9130	0.0870	0.9453	Citri Fructus	pectin	441476	FALSE	O1C(C(O)C(O)C(O)C1O)C(=O)O
MOL011646	0.9329	0.0671	0.9436	Allii Fistulost Bulbus	(6S)-6-methyloctan-1-ol	13548104	FALSE	C(CCCCCO)(CC)C
MOL011647	0.8953	0.1047	0.9145	Allii Fistulost Bulbus	2,2,4-Trimethylpentanol	31258	FALSE	OCC(CC(C)C)(C)C
MOL011648	0.4695	0.5305	0.6119	Allii Fistulost Bulbus	METHYL 10-OCTADECENOATE	5364425	FALSE	O(C(=O)CCCCCCCC/C=C/CCCCCCC)C
MOL011649	0.5590	0.4410	0.6648	Allii Fistulost Bulbus	11,13-Dimethyl-12-tetradecen-1-ol acetate	Not Available	FALSE	O(CCCCCCCCCCC(C)C=C(C)C)C(=O)C

MOL011650	0.8769	0.1231	0.7002	Allii Fistulost Bulbus	11-Dodecenyl trifluoroacetate	543399	FALSE	FC(F)(F)C(=O)OCCCCCCCCCCC=C
MOL011651	0.5783	0.4217	0.6114	Allii Fistulost Bulbus	13-Octadecenal	5364497	FALSE	C(CCC/C=C\CCCC)CCCCCCCC=O
MOL011652	0.8585	0.1415	0.9639	Allii Fistulost Bulbus	2-Aminoimidazole	82140	FALSE	c1(ncc[nH]1)N
MOL011653	0.8648	0.1352	0.9681	Allii Fistulost Bulbus	3,3-dimethyl-2,4-dihydropyrazole	557772	FALSE	N1N=CCC1(C)C
MOL011654	0.9619	0.0381	0.9615	Allii Fistulost Bulbus	2-Butenoic acid,4-nitrophenyl ester	Not Available	FALSE	O(c1ccc([N+](=O)O)cc1)C(=O)/C=C/C
MOL011655	0.8591	0.1409	0.7763	Allii Fistulost Bulbus	2-hexyloctan-1-ol	545551	FALSE	C(CCCCCC)(CCCCCC)CO
MOL011656	0.8917	0.1083	0.8887	Allii Fistulost Bulbus	2,4-Dimethylpent-2-ene	12260	FALSE	C(C=C(C)C)(C)C
MOL011657	0.8305	0.1695	0.7561	Allii Fistulost Bulbus	2-Tetradecanol	25113578	FALSE	OC(CCCCCCCCCCCC)C
MOL011658	0.9411	0.0589	0.9473	Allii Fistulost Bulbus	3(2H)-Furanone,2-hexyl-5-methyl-	Not Available	FALSE	O1C(CCCCCC)C(=O)C=C1C
MOL011659	0.9138	0.0862	0.9424	Allii Fistulost Bulbus	3-Acetonylcyclopentanone	59079064	FALSE	O=C1CC(CC1)CC(=O)C
MOL011660	0.8887	0.1113	0.9572	Allii Fistulost Bulbus	5-methylisoxazol-3-amine	66172	FALSE	c1(cc(on1)C)N
MOL011661	0.9254	0.0746	0.9604	Allii Fistulost Bulbus	3-Pentanol,2,3-dimethyl-	38988826	FALSE	OC(C(C)C)(CC)C
MOL011662	0.9225	0.0775	0.9231	Allii Fistulost Bulbus	(2R)-2-amino-3-(4-aminophenyl) propionic acid	7135682	FALSE	C(C(=O)O)(Cc1ccc(cc1)N)N
MOL011663	0.5816	0.4184	0.6766	Allii Fistulost Bulbus	4-heptadecyl-3-henicosenol	Not Available	FALSE	CCCCCCCCCCCCCCCCCC(=CCCO)CCCCCCCCCCCCCCCCC

MOL011664	0.7010	0.2990	0.6803	Allii Fistulost Bulbus	7,11-Hexadecadienal	13532956	FALSE	C(=O)CCCCC/C=C\CC/C=C\CCCC
MOL011665	0.9015	0.0985	0.8398	Allii Fistulost Bulbus	9-Undecenoic acid,2,6,10-trimethyl-	Not Available	FALSE	OC(=O)C(CCCC(CCC=C(C)C)C)C
MOL011666	0.9172	0.0828	0.9780	Allii Fistulost Bulbus	Acetone (4-hydroxy-6-methyl-2-pyrimidinyl)hydrazone	253221	FALSE	O=c1nc([nH]c(c1)C)NN=C(C)C
MOL011668	0.8811	0.1189	0.8474	Allii Fistulost Bulbus	Citronellyl isobutyrate	37888402	FALSE	C(=O)(C(C)C)OCCC(C)CCC=C(C)C
MOL011669	0.9315	0.0685	0.9776	Allii Fistulost Bulbus	1-Vinylcyclohexanol	74741	FALSE	OC1(CCCCC1)C=C
MOL011670	0.9170	0.0830	0.7951	Allii Fistulost Bulbus	2,2,3,3-Tetramethylcyclopropanemethanol	544179	FALSE	OCC1C(C1(C)C)(C)C
MOL011671	0.8928	0.1072	0.8093	Allii Fistulost Bulbus	Decyl dichloroacetate	522796	FALSE	ClC(Cl)C(=O)OCCCCCCCCCC
MOL011673	0.9192	0.0808	0.9557	Allii Fistulost Bulbus	Vinyl sulfide	12321	FALSE	S(C=C)C=C
MOL011674	0.7039	0.2961	0.6474	Allii Fistulost Bulbus	E-14-Hexadecenal	5363106	FALSE	O=CCCCCCCCCCCCC/C=C/C
MOL011675	0.5682	0.4318	0.6193	Xanthii Fructus	1,3,5-tri-o-caffeoylquinic acid	Not Available	FALSE	C1C(CC(C(C1OC(=O)/C=C/c1ccc(c(c1)O)O)O)OC(=O)/C=C\c1ccc(c(c1)O)O)(O)C(=O)OC(=O)/C=C/c1ccc(c(c1)O)O
MOL011677	0.8533	0.1467	0.7196	Xanthii Fructus	1,4-di-o-caffeoylquinic acid	Not Available	FALSE	C1C(CC(C(C1O)OC(=O)/C=C/c1ccc(c(c1)O)O)O)(OC(=O)/C=C/c1ccc(c(c1)O)O)C(=O)O
MOL011683	0.9539	0.0461	0.9519	Cicadae Periostracum	N-Acetyldopamine	100526	FALSE	c1(cc(c(cc1)O)O)CCNC(=O)C
MOL011684	0.9087	0.0913	0.8456	Cicadae Periostracum	(3Z)-3-(2-amino-4,6-dioxo-5,8-dihydro-1H-pteridin-7-ylidene)-2-oxopropanoic acid	6437642	FALSE	C(=c\1/c(=O)[nH]c2c([nH]1)[nH]c(nc2=O)N)\C(=O)C(=O)O

MOL011685	0.8793	0.1207	0.8581	Cicadae Periostracum	Ranachrome 4	10729	FALSE	O=c1c2ncc(=O)[nH]c2[nH]c(N)n1
MOL011686	0.6328	0.3672	0.6782	Sojae Semen Praeparatum	6''-O-Acetyldaidzin	156155	FALSE	c12c(c(=O)c(co2)c2ccc(cc2)O)ccc(c1)OC1OC(C(C(C1O)O)O)COC(=O)C
MOL011687	0.8006	0.1994	0.7960	Sojae Semen Praeparatum	6'-O-Acetylgenistin	5315831	FALSE	c12c(c(=O)c(co2)c2ccc(cc2)O)c(cc(c1)OC1OC(C(C(C1O)O)O)COC(=O)C)O
MOL011688	0.6310	0.3690	0.6895	Sojae Semen Praeparatum	[(2R,3S,4S,5R,6S)-3,4,5-trihydroxy-6-[3-(4-hydroxyphenyl)-6-methoxy-4-oxochromen-7-yl]oxyoxan-2-yl]methyl acetate	10228095	FALSE	c12c(cc(c(c2)OC)OC2OC(C(C(C2O)O)O)COC(=O)C)occ(c1=O)c1ccc(cc1)O
MOL011689	0.8331	0.1669	0.7289	Sojae Semen Praeparatum	6'-O-malonyldaidzin	Not Available	FALSE	c12c(c(=O)c(co2)c2ccc(cc2)O)cccc1OC1OC(C(C(C1O)O)O)COC(=O)CC(=O)O
MOL011690	0.8623	0.1377	0.7430	Sojae Semen Praeparatum	6'-O-malonylgenistin	Not Available	FALSE	c12c(c(=O)c(co2)c2ccc(cc2)O)c(ccc1OC1OC(C(C(C1O)O)O)COC(=O)CC(=O)O)O
MOL011691	0.8037	0.1963	0.6973	Sojae Semen Praeparatum	6'-O-malonylglycitin	Not Available	FALSE	c12c(c(OC3OC(C(C(C3O)O)O)COC(=O)CC(=O)O)cc(c2)OC)occ(c1=O)c1ccc(cc1)O
MOL011693	0.9325	0.0675	0.8285	Centipedae Herba	10-hydroxy-8,9-dioxyisopropylidene-thymol	Not Available	FALSE	c1(cc(c(cc1)C1(OC(OC1)(C)C)CO)O)C
MOL011694	0.8762	0.1238	0.8132	Centipedae Herba	Plenolin	442294	FALSE	C12(C(C(CC3C(C1O)C(C(=O)O3)C)C)C=CC2=O)C
MOL011695	0.7414	0.2586	0.8453	Centipedae Herba	11alpha-Methoxysaikosaponin f	Not Available	FALSE	C1C2C(CCC1)(CO)C(CC1(C2=CC(C2C1(CCC1C2(CCC(C1(C)C)OC1OC(C(C(C1O)O)O)OC1OC(C(C(C1O)O)O)C)COC1OC(C(C(C1O)O)O)CO)C)C)OC)C)O
MOL011696	0.3920	0.6080	0.7136	Centipedae Herba	11alpha-Methoxysaikosaponin f_qt	Not Available	FALSE	C1C2C(CCC1)(CO)C(CC1(C2=CC(C2C1(CCC1C2(CCC(C1(C)C)O)C)C)OC)C)O

MOL011697	0.6417	0.3583	0.7489	Centipedae Herba	1α,3β,19α,23-tetrahydroxyurs-12-ene-28-oicacid-28-O-β-D-xylopyranoside	Not Available	FALSE	C1C(C(C(C(O1)OC(=O)C12CCC(C(C1C1=CCC3C(C1(CC2)C)(CCC1C3(CC(C(C1(C)CO)O)O)C)C)(C)O)C)O)O)O
MOL011698	0.7394	0.2606	0.7373	Centipedae Herba	1α,3β,19α,23-tetrahydroxyurs-12-ene-28-oicacid-28-O-β-D-xylopyranoside_qt	Not Available	FALSE	OC(=O)C12CCC(C(C1C1=CCC3C(C1(CC2)C)(CCC1C3(CC(C(C1(C)CO)O)O)C)C)(C)O)C
MOL011699	0.6002	0.3998	0.8210	Centipedae Herba	1β,2β,3β,19α-tetrahydroxyurs-12-ene-28-oate-3-O-β-D-xylopyranoside	Not Available	FALSE	O(C(=O)C12CCC(C(C1C1=CCC3C(C1(CC2)C)(CCC1C3(C(C(C(C1(C)C)OC1C(C(C(CO1)O)O)O)O)O)C)C)(C)O)C)C
MOL011700	0.4541	0.5459	0.7252	Centipedae Herba	1β,2β,3β,19α-tetrahydroxyurs-12-ene-28-oate	Not Available	FALSE	O(C(=O)C12CCC(C(C1C1=CCC3C(C1(CC2)C)(CCC1C3(C(C(C(C1(C)C)O)O)O)C)C)(C)O)C)C
MOL011701	0.5778	0.4222	0.7460	Centipedae Herba	2α,3β,23,19α-tetrahydroxyurs-12-ene-28-oicacid-28-O-β-D-xylopyranoside	Not Available	FALSE	C1C(C(C(C(O1)OC(=O)C12CCC(C(C1C1=CCC3C(C1(CC2)C)(CCC1C3(C(CC(C1(C)CO)O)O)C)C)C)(C)O)C)O)O)O
MOL011702	0.7647	0.2353	0.7977	Centipedae Herba	2α,3β,23,19α-tetrahydroxyurs-12-ene-28-oicacid-28-O-β-D-xylopyranoside_qt	Not Available	FALSE	OC(=O)C12CCC(C(C1C1=CCC3C(C1(CC2)C)(CCC1C3(C(CC(C1(C)CO)O)C)C)C)(C)O)C

MOL011704	0.7586	0.2414	0.8937	Centipedae Herba	1-[(Z)-2-(3,5-dimethoxyphenyl)vinyl]-3,5-dimethoxybenzene	11472105	FALSE	c1(cc(cc(c1)/C=C\c1cc(cc(c1)OC)OC)OC)OC
MOL011705	0.6388	0.3612	0.8237	Centipedae Herba	3α,16α,21β,22α,28-pentahydroxyolean-12-ene-28-O-β-D-xylopyranoside	Not Available	FALSE	C1C(C(C(C(O1)OCC12C(C(C(CC1C1=CCC3C(C1(CC2O)C)(CCC1C3(CCC(C1(C)C)O)C)C)(C)C)O)O)O)O)O
MOL011706	0.5667	0.4333	0.7162	Centipedae Herba	3α,16α,21β,22α,28-pentahydroxyolean-12-ene-28-O-β-D-xylopyranoside_qt	Not Available	FALSE	OCC12C(C(C(CC1C1=CCC3C(C1(CC2O)C)(CCC1C3(CCC(C1(C)C)O)C)C)(C)C)O)O
MOL011707	0.5604	0.4396	0.7871	Centipedae Herba	3α,21β,22α,28-tetrahydroxyolean-12-ene-28-O-β-D-xylopyranoside	Not Available	FALSE	C1C(C(C(C(O1)OCC12C(C(C(CC1C1=CCC3C(C1(CC2)C)(CCC1C3(CCC(C1(C)C)O)C)C)(C)C)O)O)O)O)O
MOL011708	0.5667	0.4333	0.7162	Centipedae Herba	3α,21β,22α,28-tetrahydroxyolean-12-ene	Not Available	FALSE	OCC12C(C(C(CC1C1=CCC3C(C1(CC2O)C)(CCC1C3(CCC(C1(C)C)O)C)C)(C)C)O)O
MOL011709	0.5604	0.4396	0.7871	Centipedae Herba	3α,21α,22α,28-tetrahydroxyolean-12-ene-28-O-β-D-xylopyranoside	Not Available	FALSE	C1C(C(C(C(O1)OCC12C(C(C(CC1C1=CCC3C(C1(CC2)C)(CCC1C3(CCC(C1(C)C)O)C)C)(C)C)O)O)O)O)O

MOL011710	0.4768	0.5232	0.7308	Centipedae Herba	3α,21α,22α,28-tetrahydroxyolean-12-ene-28-O-β-D-xylopyranoside_qt	Not Available	FALSE	OCC12C(C(C(CC1C1=CCC3C(C1(CC2)C)(CCC1C3(CCC(C1(C)C)O)C)C)(C)C)O)O
MOL011711	0.6525	0.3475	0.8396	Centipedae Herba	3β,16α,21β,22α,28-penahydroxyolean-12-ene-28-O-β-D-xylopyranoside	Not Available	FALSE	C1C(C(C(C(O1)OC(=O)C12C(C(C(CC1C1=CCC3C(C1(CC2O)C)(CCC1C3(CCC(C1(C)C)O)C)C)(C)C)O)O)O)O)O
MOL011712	0.7297	0.2703	0.7444	Centipedae Herba	3β,16α,21β,22α,28-penahydroxyolean-12-ene-28-O-β-D-xylopyranoside_qt	Not Available	FALSE	OC(=O)C12C(C(C(CC1C1=CCC3C(C1(CC2O)C)(CCC1C3(CCC(C1(C)C)O)C)C)(C)C)O)O
MOL011713	0.9250	0.0750	0.8682	Centipedae Herba	8,10-dihydroxy-9(2)-methylbutyryloxythymol	Not Available	FALSE	c1(cc(c(cc1)C(O)(CCC(=O)CCC)CO)O)C
MOL011714	0.9488	0.0512	0.9202	Centipedae Herba	8,10-dihydroxy-9-isobutyryloxythymol	Not Available	FALSE	c1(cc(c(cc1)C(O)(CO)COC(=O)C(C)C)O)C
MOL011715	0.9463	0.0537	0.9312	Centipedae Herba	2-(2-hydroxy-4-methylphenyl)propane-1,2,3-triol	14543617	FALSE	OCC(c1ccc(cc1O)C)(CO)O

MOL011716	0.6970	0.3030	0.7520	Centipedae Herba	[2-hydroxy-2-(2-hydroxy-4-methylphenyl)-3-(2-methylpropanoyloxy)propyl] 2-methylpropanoate	16196971	FALSE	c1(cc(c(cc1)C(O)(COC(=O)C(C)C)COC(=O)C(C)C)O)C
MOL011717	0.9524	0.0476	0.9580	Centipedae Herba	9-hydroxythymol	Not Available	FALSE	c1(c(ccc(c1)C)C(CO)C)O
MOL011718	0.4379	0.5621	0.7683	Centipedae Herba	Arnicolide D	Not Available	FALSE	O1C2C(C(OC(=O)C(=C)C)C3(C(C(C2)C)C=CC3=O)C)C(C1=O)C
MOL011719	0.9249	0.0751	0.7897	Centipedae Herba	Bicyclo[2.2.2]octa-2,5-diene, 1,2,3,6-tetramethyl-	Not Available	FALSE	C12(CCC(C(=C1C)C)C=C2C)C
MOL011720	0.3798	0.6202	0.7291	Centipedae Herba	Brevilin A	Not Available	FALSE	C12C(C(C3C(CC1C)OC(=O)C3C)OC(=O)/C(=C/C)/C)(C(=O)C=C2)C
MOL011721	0.8984	0.1016	0.8255	Centipedae Herba	Parthenin	442288	FALSE	C12(C3C(C(=C)C(=O)O3)CCC(C1(C=CC2=O)O)C)C
MOL011722	0.4355	0.5645	0.7393	Centipedae Herba	arnicolide C	14656910	FALSE	C12(C(C(CC3C(C1OC(=O)C(C)C)C(C(=O)O3)C)C)C=CC2=O)C
MOL011723	0.3601	0.6399	0.6019	Centipedae Herba	florilenalin angelic acid	Not Available	FALSE	C12C(CC3C(CC1=C)OC(=O)C3=C)C(CC2OC(=O)/C(=C/C)/C)(O)C
MOL011724	0.3493	0.6507	0.6182	Centipedae Herba	florilenalin isobutyrate	Not Available	FALSE	C12C(CC3C(CC1=C)OC(=O)C3=C)C(CC2OC(=O)C(C)(C)C)(O)C
MOL011726	0.4354	0.5646	0.7195	Centipedae Herba	senecioylplenolin	Not Available	FALSE	C12C(C(C3C(CC1C)OC(=O)C3=C)OC(=O)C=C(C)C)(C(=O)C=C2)C

MOL011727	0.5925	0.4075	0.6247	Centipedae Herba	[(3S,4aR,6aR,6aR,6bR,8aR,12S,12aR,14aR,14bR)-4,4,6a,6b,8a,12,14b-heptamethyl-11-methylene-1,2,3,4a,5,6,6a,7,8,9,10,12,12a,13,14,14a-hexadecahydropicen-3-yl] hexadecanoate	14055767	FALSE	C1(C2C(C3C(C4(C(C5C(CC4)(CCC(=C)C5C)C)CC3)C)(CC2)C)(CCC1OC(=O)CCCCCCCCCCCCCCC)C)(C)C
MOL011728	0.8745	0.1255	0.7655	Centipedae Herba	(1R,3aR,5R,5aS,8aR,9S,9aS)-9-hydroxy-1,5,8a-trimethyl-3a,4,5,5a,6,7,9,9a-octahydro-1H-azuleno[7,6-d]furan-2,8-dione	14996421	FALSE	O1C2C(C(O)C3(C(C(C2)C)CCC3=O)C)C(C1=O)C
MOL011729	0.8952	0.1048	0.6944	Saposhnikoviae Radix	11-hydroxy-sec-o-beta-d-glucosylhamaudol	Not Available	FALSE	c12c(cc3c(c1O)c(=O)cc(o3)CO)OC(C(C2)OOCC(O)C(O)C(O)C(O)CO)(C)C
MOL011730	0.8774	0.1226	0.8203	Saposhnikoviae Radix	11-hydroxy-sec-o-beta-d-glucosylhamaudol_qt	Not Available	FALSE	c12c(cc3c(c1O)c(=O)cc(o3)CO)OC(C(C2)O)(C)C
MOL011731	0.7134	0.2866	0.7942	Saposhnikoviae Radix	3'-O-Acetylhamaudol	5315865	FALSE	O1C(C(OC(=O)C)Cc2c1cc1oc(cc(=O)c1c2O)C)(C)C
MOL011734	0.8111	0.1889	0.8183	Saposhnikoviae Radix	Cimifugin	441960	FALSE	c12c(cc3c(c1OC)c(=O)cc(o3)CO)OC(C2)C(O)(C)C
MOL011734	0.8111	0.1889	0.8183	Cimicifugae Rhizoma	Cimifugin	441960	FALSE	c12c(cc3c(c1OC)c(=O)cc(o3)CO)OC(C2)C(O)(C)C

MOL011735	0.3880	0.6120	0.7427	Saposhnikoviae Radix	deltoin	Not Available	FALSE	c12c(cc3c(c1)ccc(=O)o3)OC(C2)C(C)(OC(=O)/C(=C/C)/C)C
MOL011736	0.4193	0.5807	0.7273	Saposhnikoviae Radix	3'-O-angeloylhamaudol	56643444	FALSE	O1C(C(OC(=O)/C(=C\C)/C)Cc2c1cc1oc(cc(=O)c1c2O)C)(C)C
MOL011737	0.8698	0.1302	0.8142	Saposhnikoviae Radix	divaricatacid	Not Available	FALSE	c12c(cc3c(c1OC)c(=O)cc(o3)C(=O)O)OC(C2)C(O)(C)C
MOL011738	0.8962	0.1038	0.7603	Saposhnikoviae Radix	divaricataester,a	Not Available	FALSE	c1oc(cc1)C(=O)CC1C(=O)CCC1C(=O)OCC
MOL011739	0.4163	0.5837	0.8497	Saposhnikoviae Radix	divaricataester,b	Not Available	FALSE	c12c(cc3c(c1OC)C(=C)C=C(O3)C(=O)OCC)OC(C2)C(C)(O)C
MOL011740	0.7660	0.2340	0.7470	Saposhnikoviae Radix	divaricatol	Not Available	FALSE	c12c(cc3c(c1O)c(=O)cc(o3)CO)OC(C(C2)OC(=O)C)(C)C
MOL011741	0.9278	0.0722	0.8095	Saposhnikoviae Radix	fangfengalpyrimidine	Not Available	FALSE	C12CC(=O)N(C3=NC(=O)C(C13)CC(C(O)CO)O)CCC2
MOL011742	0.9428	0.0572	0.8571	Saposhnikoviae Radix	fraxidin	Not Available	FALSE	c1(c(c(c2c(c1)C=CC(=O)C2)O)OC)OC
MOL011743	0.8214	0.1786	0.8206	Saposhnikoviae Radix	hamaudol	Not Available	FALSE	c12c(cc3c(c1O)c(=O)cc(o3)C)OC(C(C2)O)(C)C
MOL011745	0.9270	0.0730	0.8328	Saposhnikoviae Radix	isofraxidin	Not Available	FALSE	c1(c(c(c2c(c1)C=CC(=O)C2)OC)O)OC
MOL011746	0.8969	0.1031	0.7556	Saposhnikoviae Radix	isopimpinellin	Not Available	FALSE	c12c(c(c3c(c1OC)ccc(=O)o3)OC)occ2
MOL011747	0.4766	0.5234	0.6853	Saposhnikoviae Radix	ledebouriellol	Not Available	FALSE	c12c(cc3c(c1O)c(=O)cc(o3)CO)OC(C(C2)OC(=O)/C(=C\C)/C)(C)C
MOL011748	0.8921	0.1079	0.8280	Notopterygii Rhizoma Et Radix	nodakenetin	Not Available	FALSE	c12c(cc3c(c1)OC(C3)C(C)C)ccc(=O)o2
MOL011748	0.8921	0.1079	0.8280	Saposhnikoviae Radix	nodakenetin	Not Available	FALSE	c12c(cc3c(c1)OC(C3)C(C)C)ccc(=O)o2
MOL011749	0.7034	0.2966	0.8354	Saposhnikoviae Radix	phelloptorin	Not Available	FALSE	c12c(c(c3c(c1OC)ccc(=O)o3)OCC=C(C)C)occ2
MOL011750	0.8519	0.1481	0.7486	Saposhnikoviae Radix	prim-o-beta-d-glucosylcimifugin	Not Available	FALSE	c12c(cc3c(c1OC)c(=O)cc(o3)COOCC(O)C(O)C(O)C(O)CO)OC(C2)C(C)(O)C
MOL011752	0.8828	0.1172	0.7158	Saposhnikoviae Radix	sec-o-beta-d-glucosylhamaudol	Not Available	FALSE	c12c(cc3c(c1O)c(=O)cc(o3)C)OC(C(C2)OOCC(O)C(O)C(O)C(O)CO)(C)C
MOL011753	0.7630	0.2370	0.7959	Saposhnikoviae Radix	5-O-Methylvisaminol	441970	FALSE	c12c(c3c(OC(C3)C(O)(C)C)cc2oc(cc1=O)C)OC
MOL011754	0.9302	0.0698	0.7449	Saposhnikoviae Radix	4-hydroxy-9-methoxyfuro[3,2-g]chromen-7-one	5385192	FALSE	o1c2c(c(O)c3c(oc(=O)cc3)c2OC)cc1
MOL011755	0.8719	0.1281	0.7606	Saposhnikoviae Radix	5-methoxy-8-hydroxypsoralen	Not Available	FALSE	c12c(c(c3c(c1OC)ccc(=O)o3)O)occ2
MOL011756	0.9316	0.0684	0.9497	Gnaphalii Affinis Herba	7-octen-4-ol	Not Available	FALSE	C=CCCC(CCC)O
MOL011756	0.9316	0.0684	0.9497	Saposhnikoviae Radix	7-octen-4-ol	Not Available	FALSE	C=CCCC(CCC)O

MOL011758	0.8631	0.1369	0.7529	Spirodelae Herba	(R,7E,11Z,13Z)-10-hydroxyhexadeca-7,11,13-trienoic acid	Not Available	FALSE	C(=O)(CCCCC/C=C/CC(/C=C\C=C/CC)O)O
MOL011762	0.9085	0.0915	0.8281	Spirodelae Herba	luteolin-7-monoglucoside	13093776	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL011763	0.9085	0.0915	0.8281	Spirodelae Herba	luteolin-7-o-beta-d-galactopyranoside	Not Available	FALSE	c1c(cc(c2c1oc(cc2=O)c1ccc(c(c1)O)O)O)OC1C(O)C(O)C(O)C(O1)CO
MOL011764	0.5670	0.4330	0.7286	Spirodelae Herba	Lycopersene	5365816	FALSE	C(C/C=C(/CC/C=C(/CCC=C(C)C)\C)\C)/C(=C/CC/C=C(/CC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C)\C)/C
MOL011768	0.8421	0.1579	0.7052	Spirodelae Herba	7Z,10Z,13Z-hexadecatrienoic acid	21158969	FALSE	C(=O)(/C=C/C=C/C=C\CCCCCCCCC)O
MOL011769	0.9563	0.0437	0.8701	Ligustici Rhizoma Et Radix	(3E,6S,7S)-3-butylidene-6,7-dihydroxy-4,5,6,7-tetrahydroisobenzofuran-1-one	10036566	FALSE	C1(=O)O/C(=C/CCC)/C2=C1C(C(CC2)O)O
MOL011770	0.9518	0.0482	0.8822	Ligustici Rhizoma Et Radix	senkyunolide J	15138553	FALSE	C1(=O)OC(C2=C1C(C(CC2)O)O)CCCC
MOL011771	0.9221	0.0779	0.8117	Ligustici Rhizoma Et Radix	senkyunolide L	Not Available	FALSE	C1(=O)O/C(=C/CCC)/C2=C1C(C(CC2)O)Cl
MOL011772	0.8358	0.1642	0.7643	Ligustici Rhizoma Et Radix	senkyunolide M	Not Available	FALSE	C1(=O)O/C(=C/CCC)/C2=C1C(C(CC2)C(=O)CCC)O
MOL011773	0.8556	0.1444	0.7010	Ligustici Rhizoma Et Radix	(3S,3aR)-5-isopropylidene-3,8-dimethyl-2,3,3a,4,6,7-hexahydro-1H-azulene	10932599	FALSE	C12C(CCC1=C(CCC(=C(C)C)C2)C)C
MOL011775	0.8888	0.1112	0.8570	Ligustici Rhizoma Et Radix	undeca-1,4-diene	5358328	FALSE	C=CC/C=C/CCCCCC
MOL011776	0.9542	0.0458	0.9605	Ligustici Rhizoma Et Radix	p-Ethoxytoluene	73955	FALSE	c1(ccc(cc1)C)OCC

MOL011777	0.9735	0.0265	0.8288	Ligustici Rhizoma Et Radix	4-methoxy-6-[(E)-prop-1-enyl]-1,3-benzodioxole	6436484	FALSE	c12c(cc(cc1OC)/C=C/C)OCO2
MOL011778	0.8790	0.1210	0.7414	Ligustici Rhizoma Et Radix	ligusinenoside A	Not Available	FALSE	c1(c(cc(cc1)/C=C/CO)OC)OC1OC(C(C(C1O)O)O)COC1OC(C(C1O)O)CO
MOL011779	0.5981	0.4019	0.6153	Ligustici Rhizoma Et Radix	ligusinenoside B	Not Available	FALSE	c1(c(cc(cc1)C(C(Oc1ccc(cc1OC)/C=C/COC1OC(C(C(C1O)O)O)CO)CO)O)OC)OC1OC(C(C(C1O)O)O)CO
MOL011780	0.7110	0.2890	0.7133	Ligustici Rhizoma Et Radix	ligusinenoside B_qt	Not Available	FALSE	c1(c(cc(cc1)C(C(Oc1ccc(cc1OC)/C=C/CO)CO)O)OC)O
MOL011781	0.6565	0.3435	0.6851	Ligustici Rhizoma Et Radix	ligusinenoside C	Not Available	FALSE	c1(c(cc(cc1)C(C(Oc1ccc(cc1OC)/C=C/COC1OC(C(C(C1O)O)O)COC1OC(C(C1O)O)CO)CO)O)OC)O
MOL011782	0.9594	0.0406	0.8564	Ligustici Rhizoma Et Radix	Ligustilide	5319022	FALSE	C12=C(C(=O)O/C/1=C\CCC)C=CCC2
MOL011783	0.9548	0.0452	0.9677	Ligustici Rhizoma Et Radix	Vananote	7476	FALSE	c1(ccc(cc1)OC)C(=O)C
MOL011783	0.9548	0.0452	0.9677	Polygoni Cuspidati Rhizoma Et Radix	Vananote	7476	FALSE	c1(ccc(cc1)OC)C(=O)C
MOL011783	0.9548	0.0452	0.9677	Oroxyli Semen	Vananote	7476	FALSE	c1(ccc(cc1)OC)C(=O)C
MOL011784	0.9588	0.0412	0.9109	Ligustici Rhizoma Et Radix	senkyunolide B	68776935	FALSE	C1(=O)O/C(=C/CCC)/c2c(cccc12)O
MOL011785	0.9217	0.0783	0.8550	Ligustici Rhizoma Et Radix	senkyunolide D	Not Available	FALSE	C1(=O)OC(C2=C1C=CCC2)(C(=O)CCC)O
MOL011786	0.9533	0.0467	0.8887	Ligustici Rhizoma Et Radix	senkyunolide E	Not Available	FALSE	C1(=O)O/C(=C/C(CC)O)/c2ccccc12
MOL011787	0.7464	0.2536	0.7894	Puerariae Flos	Glycitin	187808	FALSE	c12c(cc(c(c2)OC)OC2OC(C(C(C2O)O)O)CO)occ(c1=O)c1ccc(cc1)O
MOL011787	0.7464	0.2536	0.7894	Sojae Semen Praeparatum	Glycitin	187808	FALSE	c12c(cc(c(c2)OC)OC2OC(C(C(C2O)O)O)CO)occ(c1=O)c1ccc(cc1)O
MOL011789	0.7306	0.2694	0.8368	Puerariae Flos	kaikasaponin I	Not Available	FALSE	C1(CC(C2(C(C1)C1=CCC3C(C1(CC2)C)(CCC1C3(CCC(C1(C)C)OC1OC(C(C(C1OC1C(C(C(C(O1)CO)O)O)O)O)O)C(=O)O)C)C)O)(C)C

MOL011790	0.7667	0.2333	0.8416	Puerariae Flos	(2S,3S,4S,5R,6R)-6-[[(3S,4aR,6aR,6bS,8aR,9R,12aS,14aR,14bR)-9-hydroxy-4,4,6a,6b,8a,11,11,14b-octamethyl-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydropicen-3-yl]oxy]-5-[[(2S,3R,4S,5R,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[[(2S,3R,4R,5R,6S)-3,4,5-trihy	21629874	FALSE	O1C(C(C(C(C1C)O)O)O)OC1C(C(C(OC1OC1C(C(C(OC1OC1C(C2C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(C(CC(C3)(C)C)O)C)C)C)(CC1)C)(C)C)C(=O)O)O)O)CO)O)O
MOL011791	0.8084	0.1916	0.7915	Puerariae Flos	Kakkalide	5490351	FALSE	c12c(=O)c(coc2cc(c(c1O)OC)OC1C(C(C(C(O1)COC1C(C(C(CO1)O)O)O)O)O)O)c1ccc(cc1)OC
MOL011792	0.7699	0.2301	0.7630	Puerariae Flos	4'-Methyltectorigenin 7-glucoside	10027948	FALSE	c1c(c(=O)c2c(o1)cc(c(c2O)OC)OC1C(C(C(C(O1)CO)O)O)O)c1ccc(cc1)OC
MOL011793	0.8634	0.1366	0.8846	Puerariae Flos	kakkatin	Not Available	FALSE	c12c(cc(c(c2)O)OC)OC=C(C1O)c1ccc(cc1)O
MOL011794	0.9366	0.0634	0.9766	Puerariae Flos	Methyl isovalerate	11160	FALSE	C(=O)(CC(C)C)OC
MOL011796	0.7767	0.2233	0.8305	Puerariae Flos	sissotrin	25200563	FALSE	c12c(c(=O)c(co2)c2ccc(cc2)OC)c(cc(c1)OC1OC(C(C(C1O)O)O)O)CO)O

MOL011797	0.4108	0.5892	0.7532	Abri Herba	(3S,4aR,6aR,6bS,8aR,9R,12aS,14aR,14bR)-4,4,6a,6b,8a,11,11,14b-octamethyl-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydropicene-3,9-diol	9846221	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(O)CC(C3)(C)C)C)C)(CC2)C)(CC1)C)(C)C
MOL011797	0.4108	0.5892	0.7532	Radix Puerariae	(3S,4aR,6aR,6bS,8aR,9R,12aS,14aR,14bR)-4,4,6a,6b,8a,11,11,14b-octamethyl-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydropicene-3,9-diol	9846221	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(O)CC(C3)(C)C)C)C)(CC2)C)(CC1)C)(C)C
MOL011797	0.4108	0.5892	0.7532	Puerariae Flos	(3S,4aR,6aR,6bS,8aR,9R,12aS,14aR,14bR)-4,4,6a,6b,8a,11,11,14b-octamethyl-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydropicene-3,9-diol	9846221	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(O)CC(C3)(C)C)C)C)(CC2)C)(CC1)C)(C)C
MOL011798	0.7719	0.2281	0.8201	Puerariae Flos	Soyasaponin VI	164453	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(OC4OC(=C(O)C(=O)C4)C)CC(C3)(C)C)C)C)(CC2)C)(CC1)C)(CO)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)C)CO)C(=O)O

MOL011800	0.2716	0.7284	0.6841	Chrysanthemi Flos	(24r)-cycloart-25-en-3beta,24-diol	Not Available	FALSE	C1C(C(C2C(C1)(C1(C(CC2)C2(C(CC1)(C(CC2)C(C)CCC(C(=C)C)O)C)C)C)(C)C)O
MOL011801	0.3022	0.6978	0.6313	Chrysanthemi Flos	(24r)-cycloartane-3beta,24,25-triol	54764687	FALSE	C1C(C(C2C(C1)(C1(C(CC2)C2(C(CC1)(C(CC2)C(C)CCC(C(C)(C)O)O)C)C)C)(C)C)O
MOL011805	0.2978	0.7022	0.6156	Chrysanthemi Flos	(24s)-29-norcycloartane-3,beta,24,25-triol	Not Available	FALSE	C1C(C(C2C(C1)(C1(C(CC2)C2(C(CC1)(C(CC2)C(C)CCC(C(C)(O)C)O)C)C)C)C)O
MOL011806	0.3022	0.6978	0.6313	Chrysanthemi Flos	(24s)-cycloartane-3beta,24,25-triol	Not Available	FALSE	C1C(C(C2C(C1)(C1(C(CC2)C2(C(CC1)(C(CC2)C(C)CCC(C(C)(C)O)O)C)C)C)(C)C)O
MOL011807	0.2758	0.7242	0.6571	Chrysanthemi Flos	(24s)-lanost-9(11)-ene-3,beta,24,25-triol	Not Available	FALSE	C1C(C(C2C(C1)(C1=CCC3(C(C1CC2)(CCC3C(C)CCC(C(C)(C)O)O)C)C)C)(C)C)O
MOL011809	0.2305	0.7695	0.7250	Chrysanthemi Flos	(3S,5R,8R,9R,10R,13R,14R,17S)-17-[(2S,5S)-5-(2-hydroxypropan-2-yl)-2-methyloxolan-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol	21575463	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C1(CCC(O1)C(C)(O)C)C)C)C)(C)C)O
MOL011810	0.4295	0.5705	0.8059	Chrysanthemi Flos	Faradiol alpha-epoxide	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(C(C2)O)(CC2C(C1C)(O2)C)C)C)C)(C)C)O
MOL011811	0.7631	0.2369	0.8444	Chrysanthemi Flos	Tilianine	5321954	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(OC)cc1

MOL011812	0.4376	0.5624	0.7637	Chrysanthemi Flos	arnidiol	Not Available	FALSE	C1C(C(C2C(C1)(C1(C(CC2)(C2(C(CC1)C1C(C(C2)O)(CCC(=C)C1C)C)C)C)C)(C)C)O
MOL011813	0.3918	0.6082	0.7524	Chrysanthemi Flos	(3S,4aR,6aR,6bS,8S,8aS,11R,12S,12aS,14aR,14bR)-4,4,6a,6b,8a,11,12,14b-octamethyl-2,3,4a,5,6,7,8,9,10,11,12,12a,14,14a-tetradecahydro-1H-picene-3,8-diol	9803424	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1C)C)C)C)C)(C)C)O
MOL011814	0.3616	0.6384	0.7981	Chrysanthemi Flos	Calenduladiol	461835	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(C(C2)O)(C)CCC1C(=C)C)C)C)(C)C)O
MOL011814	0.3616	0.6384	0.7981	Calendula Officinalis	Calenduladiol	461835	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(C(C2)O)(C)CCC1C(=C)C)C)C)(C)C)O
MOL011815	0.9005	0.0995	0.8433	Chrysanthemi Flos	chrysanthediol A	Not Available	FALSE	C1C/C(=C\CC(C(=C)C(CC1C(=C)C)O)O)/C
MOL011816	0.5452	0.4548	0.6778	Chrysanthemi Flos	[(1S,5S,7S)-7-acetoxy-5-isopropenyl-2,8-dimethylene-cyclodecyl] acetate	11688333	FALSE	C1CC(=C)C(CCC(=C)C(CC1C(=C)C)OC(=O)C)OC(=O)C
MOL011817	0.5452	0.4548	0.6778	Chrysanthemi Flos	chrysanthediol C	Not Available	FALSE	C1CC(=C)C(CCC(=C)C(CC1C(=C)C)OC(=O)C)OC(=O)C
MOL011818	0.3823	0.6177	0.8143	Chrysanthemi Flos	Coflodiol	5273648	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=C3C(C(C2)O)(C)CCC(C3)(C)C)CC1)C)C)(C)C)O
MOL011819	0.2235	0.7765	0.7203	Chrysanthemi Flos	dammarenediol II	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C(CC2)C(CCC=C(C)C)(C)O)C)C)(C)C)O

MOL011820	0.3932	0.6068	0.7541	Chrysanthemi Flos	(3S,4aR,6aR,6aR,6bR,8S,8aS,12S,12aR,14aR,14bR)-4,4,6a,6b,8a,11,12,14b-octamethyl-2,3,4a,5,6,6a,7,8,9,12,12a,13,14,14a-tetradecahydro-1H-picene-3,8-diol	9846222	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(C(C2)O)(CC=C(C1C)C)C)C)C)(C)C)O
MOL011821	0.4103	0.5897	0.8098	Chrysanthemi Flos	heliantriol a1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=C3C(C(C2)O)(CCC(C3)(C)C)CO)CC1)C)C)(C)C)O
MOL011822	0.3818	0.6182	0.8142	Chrysanthemi Flos	heliantriol b2	9890381	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(C(C2)O)(CCC1C(=C)C)CO)C)C)(C)C)O
MOL011823	0.4326	0.5674	0.7659	Chrysanthemi Flos	(3S,4aR,6aR,6aR,6bR,8S,8aS,9S,12S,12aR,14aR,14bR)-4,4,6a,6b,8a,11,12,14b-octamethyl-2,3,4a,5,6,6a,7,8,9,12,12a,13,14,14a-tetradecahydro-1H-picene-3,8,9-triol	9890380	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1C(C(C2)O)(C(C=C(C1C)C)O)C)C)C)(C)C)O
MOL011824	0.4130	0.5870	0.7830	Chrysanthemi Flos	longispinogenin	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)CO)C)C)(C)C)O
MOL011825	0.3959	0.6041	0.7936	Chrysanthemi Flos	NSC707002	397934	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C)C)C)(C)C)O
MOL011826	0.8880	0.1120	0.8707	Campsis Flos	psi-Ionone	1757003	FALSE	C(=C\C=C\C(=O)C)(/CCC=C(C)C)\C
MOL011826	0.8880	0.1120	0.8707	Chrysanthemi Flos	psi-Ionone	1757003	FALSE	C(=C\C=C\C(=O)C)(/CCC=C(C)C)\C
MOL011827	0.9243	0.0757	0.9408	Chrysanthemi Flos	pulegene	Not Available	FALSE	C1(=CC(CC1)C)C(C)C
MOL011828	0.8397	0.1603	0.8039	Chrysanthemi Flos	robinin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(OC1OC(C(O)C(O)C1O)C)c2)c1ccc(O)cc1)COC1OC(C(O)C(O)C1O)C

MOL011829	0.7853	0.2147	0.6520	Schizonepetae Herba	(E)-3-{3-[1-carboxy-2-(3,4-dihydroxyphenyl)ethoxycarbonyl]-7-hydroxy-2-(3,4-dihydroxyphenyl)benzofuran-5-yl}propenoic acid	Not Available	FALSE	c1(c(cc(cc1)c1oc2c(c1C(=O)OC(C(=O)O)Cc1cc(c(cc1)O)O)cc(cc2O)/C=C/C(=O)O)O)O
MOL011830	0.9622	0.0378	0.8112	Schizonepetae Herba	(Z)-(1S,5R)-beta-Pinen-10-yl-beta-vicianoside_qt	Not Available	FALSE	C12CC(CC/C/1=C\O)C2(C)C
MOL011831	0.9498	0.0502	0.9677	Schizonepetae Herba	(1R,2R,4S)-4-isopropenyl-1-methylcyclohexane-1,2-diol	11217495	FALSE	C1CC(CC(C1(O)C)O)C(=C)C
MOL011832	0.6960	0.3040	0.6404	Schizonepetae Herba	1-carboxy-2-(3,4-dihydroxyphenyl)erhyl-(E)-3-{3-[1-carboxy-2-(3,4-dihydroxyphenyl)ethoxycarboayl]-7-hydroxy-2-(3,4-dihydroxyphenyl)-benzofuran-5-yl} propenoate	Not Available	FALSE	c1(c(cc(cc1)c1oc2c(c1C(=O)OC(C(=O)O)Cc1cc(c(cc1)O)O)cc(cc2O)/C=C/C(=O)OC(Cc1cc(c(cc1)O)O)C(=O)O)O)O

MOL011833	0.6081	0.3919	0.6391	Schizonepetae Herba	1-carboxy-2-(3,4-dihydroxyphenyl)ethyl-(E)-3-{3-[1-methoxycarbonyl-2-(3,4-dihydroxyphenyl)ethoxycarbonyl]-7-hydroxy-2-(3,4-dihydroxyphenyl)benzofuran--5-yl}propenoate	Not Available	FALSE	c1(c(cc(cc1)c1oc2c(c1C(=O)OC(C(=O)OC)Cc1cc(c(cc1)O)O)cc(cc2O)/C=C/C(=O)OC(Cc1cc(c(cc1)O)O)C(=O)O)O)O
MOL011835	0.9386	0.0614	0.9531	Schizonepetae Herba	1-Ethoxypentane	87370	FALSE	C(COCC)CCC
MOL011836	0.9069	0.0931	0.9029	Schizonepetae Herba	1,3-Heptadiene, 3-ethyl-2-methyl-	5365718	FALSE	C(CC)/C=C(\CC)/C(=C)C
MOL011837	0.9535	0.0465	0.8433	Schizonepetae Herba	3,5-diformyl-2,4-dihydroxy-6-methylbenzoic acid	Not Available	FALSE	C(=O)(c1c(c(c(c(c1C)C=O)O)C=O)O)O
MOL011838	0.8946	0.1054	0.9506	Schizonepetae Herba	(5S)-3,5-dimethylcyclohex-2-en-1-one	642465	FALSE	C1(CC(=CC(=O)C1)C)C
MOL011839	0.8928	0.1072	0.9707	Schizonepetae Herba	(1R,2R,3S)-3-methylcyclopentane-1,2-diol	11893928	FALSE	C1(C(CCC1C)O)O
MOL011840	0.9361	0.0639	0.9487	Schizonepetae Spica	EAK	246728	FALSE	CCCCCC(=O)CC
MOL011840	0.9361	0.0639	0.9487	Schizonepetae Herba	EAK	246728	FALSE	CCCCCC(=O)CC
MOL011841	0.8996	0.1004	0.9720	Schizonepetae Herba	(3S)-3-methylcyclohexan-1-one	7057964	FALSE	C1C(CCCC1=O)C

MOL011842	0.8791	0.1209	0.9666	Schizonepetae Herba	(R)-()-3-Methylcyclopentanone	637894	FALSE	C1(CC(=O)CC1)C
MOL011843	0.9661	0.0339	0.8850	Schizonepetae Herba	3B-hydroxy-4(8)-ene-P-mentllane-3(9)-lactone	Not Available	FALSE	C1CC2=C(C(=O)CC2(CC1C)O)C
MOL011843	0.9661	0.0339	0.8850	Schizonepetae Spica	3B-hydroxy-4(8)-ene-P-mentllane-3(9)-lactone	Not Available	FALSE	C1CC2=C(C(=O)CC2(CC1C)O)C
MOL011844	0.8728	0.1272	0.7892	Schizonepetae Herba	cis,trans-4,5-Diethyl-3,5-octadiene	5358324	FALSE	CC/C=C(/C(=C\CC)/CC)\CC
MOL011845	0.8574	0.1426	0.8224	Schizonepetae Herba	Hesperetin-5-glucoside	Not Available	FALSE	C1(C(C(OC(C1O)CO)Oc1cc(cc2c1C(=O)CC(O2)c1ccc(c(c1)O)OC)O)O)O
MOL011846	0.8921	0.1079	0.8732	Schizonepetae Herba	Menthyl acetate, dl-	62335	FALSE	C1CC(C(CC1C)OC(=O)C)C(C)C
MOL011847	0.9223	0.0777	0.9599	Schizonepetae Herba	Octophilic acid	Not Available	FALSE	C(C(C(=O)O)NC(C)C(=O)O)CCN
MOL011848	0.9615	0.0385	0.9600	Schizonepetae Herba	d-Piperitone	61362	FALSE	C1CC(C(=O)C=C1C)C(C)C
MOL011848	0.9615	0.0385	0.9600	Schizonepetae Spica	d-Piperitone	61362	FALSE	C1CC(C(=O)C=C1C)C(C)C
MOL011849	0.9257	0.0743	0.7819	Schizonepetae Herba	Schizonepetoside B	Not Available	FALSE	C1(C2C(OC(C1O)CO)OCC(C1C(=O)CC(CC1)C)(O2)C)O
MOL011849	0.9257	0.0743	0.7819	Schizonepetae Spica	Schizonepetoside B	Not Available	FALSE	C1(C2C(OC(C1O)CO)OCC(C1C(=O)CC(CC1)C)(O2)C)O
MOL011850	0.9238	0.0762	0.8419	Schizonepetae Herba	Schizonepetoside C	Not Available	FALSE	C1C(CC/C(=C(\C)/COC2OC(C(C(C2O)O)O)CO)/C1=O)C
MOL011851	0.9501	0.0499	0.9778	Schizonepetae Herba	Schizonepetoside C_qt	Not Available	FALSE	C1C(CC/C(=C(/C)\CO)/C1=O)C
MOL011852	0.9242	0.0758	0.8404	Schizonepetae Herba	Schizonepetoside D	Not Available	FALSE	O1C(C(O)C(O)C(O)C1OCC(=C)C1CCC(CC1=O)C)CO
MOL011853	0.9510	0.0490	0.9769	Schizonepetae Herba	Schizonepetoside D_qt	Not Available	FALSE	OCC(=C)C1CCC(CC1=O)C
MOL011854	0.9450	0.0550	0.9209	Schizonepetae Herba	Schizonodiol	Not Available	FALSE	C1(C=C(C(=O)CC1C)C(C)(C)O)O
MOL011855	0.9391	0.0609	0.9046	Schizonepetae Herba	Schizonol	Not Available	FALSE	C1C=C(C(=O)CC1C)C(C)(C)O
MOL011858	0.8948	0.1052	0.9610	Schizonepetae Herba	2-Cyclooctenone	5367523	FALSE	C1=CC(=O)CCCCC1
MOL011859	0.7225	0.2775	0.8528	Schizonepetae Herba	deoxyoleanolic acid	Not Available	FALSE	OC(=O)C12C(C3=CCC4C(C3(CC1)C)(CCC1C4(CCCC1(C)C)C)C)CC(CC2)(C)C
MOL011860	0.9580	0.0420	0.9776	Coriandri Sativi Herba	d-Dihydrocarvone	22227	FALSE	C1(=O)CC(C(=C)C)CCC1C

MOL011860	0.9580	0.0420	0.9776	Schizonepetae Herba	d-Dihydrocarvone	22227	FALSE	C1(=O)CC(C(=C)C)CCC1C
MOL011861	0.9588	0.0412	0.9571	Schizonepetae Herba	(+)-cis-Isopulegone	443529	FALSE	O=C1C(CCC(C1)C)C(=C)C
MOL011862	0.9545	0.0455	0.9035	Schizonepetae Herba	(1S,4aS,8aR)-1-methyldecalin-2-one	21122297	FALSE	C12C(CCCC1)CCC(=O)C2C
MOL011863	0.8223	0.1777	0.7176	Schizonepetae Herba	octahydro-4α,5-dimethyl-3-(1-methylethyl)naphthalenone	Not Available	FALSE	C1CC(C2(C(C1)C(=O)CC(C2)C(C)C)C)C
MOL011864	0.9285	0.0715	0.9327	Schizonepetae Herba	2-Octenyl acetate	5463875	FALSE	C(=O)(C)OC/C=C/CCCCC
MOL011865	0.9136	0.0864	0.8056	Glechomae Herba	rosmarinic acid	5281792	FALSE	OC(=O)C(Cc1ccc(O)c(O)c1)OC(=O)/C=C/c1ccc(O)c(O)c1
MOL011865	0.9136	0.0864	0.8056	Schizonepetae Herba	rosmarinic acid	5281792	FALSE	OC(=O)C(Cc1ccc(O)c(O)c1)OC(=O)/C=C/c1ccc(O)c(O)c1
MOL011865	0.9136	0.0864	0.8056	Menthae Herba	rosmarinic acid	5281792	FALSE	OC(=O)C(Cc1ccc(O)c(O)c1)OC(=O)/C=C/c1ccc(O)c(O)c1
MOL011865	0.9136	0.0864	0.8056	Perilla Frutescens	rosmarinic acid	5281792	FALSE	OC(=O)C(Cc1ccc(O)c(O)c1)OC(=O)/C=C/c1ccc(O)c(O)c1
MOL011866	0.9244	0.0756	0.8399	Schizonepetae Herba	(2R,5S)-5-methyl-2-[(E)-1-methyl-2-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]oxy-vinyl]cyclohexan-1-one	21636052	FALSE	O1C(C(C(C(C1CO)O)O)O)O/C=C(/C1CCC(CC1=O)C)\C
MOL011867	0.9379	0.0621	0.8719	Schizonepetae Herba	schizonepetoside E	Not Available	FALSE	O1C(C(C(C(C1CO)O)O)O)OCC(O)(C1CCC(CC1=O)C)C
MOL011868	0.9403	0.0597	0.9637	Schizonepetae Herba	schizonepetoside E_qt	Not Available	FALSE	OCC(O)(C1CCC(CC1=O)C)C
MOL011869	0.6960	0.3040	0.6404	Schizonepetae Herba	schizotenuin A	46224244	FALSE	c1(c(ccc(c1)c1c(C(=O)OC(C(=O)O)Cc2ccc(c(c2)O)O)c2cc(cc(c2o1)O)/C=C/C(=O)OC(Cc1ccc(c(c1)O)O)C(=O)O)O)O

MOL011870	0.9232	0.0768	0.9169	Schizonepetae Spica	[(1S)-1-vinylhexyl] acetate	22805587	FALSE	C(=O)(C)OC(C=C)CCCCC
MOL011872	0.9586	0.0414	0.9571	Schizonepetae Spica	()-Menthone	443159	FALSE	C1(=O)C(CCC(C1)C)C(C)C
MOL011872	0.9586	0.0414	0.9571	Echinopsis Radix	()-Menthone	443159	FALSE	C1(=O)C(CCC(C1)C)C(C)C
MOL011873	0.9580	0.0420	0.9615	Schizonepetae Spica	cinerolon	Not Available	FALSE	C1(=O)C(=C(C(C1)O)C)C/C=C\C
MOL011874	0.9499	0.0501	0.9530	Schizonepetae Spica	cis-2-methyl-5-(1-methylvinyl)cyclohex-2-en-1-yl acetate	Not Available	FALSE	C(=O)(CC)OC1C=CCC(C1)C(=C)C
MOL011875	0.8295	0.1705	0.8301	Schizonepetae Spica	Eriodictiol-7-glucoside	147394	FALSE	O1C(C(C(C(C1Oc1cc2c(C(=O)CC(c3cc(O)c(cc3)OC)O2)c(c1)O)O)O)O)CO
MOL011876	0.9588	0.0412	0.9571	Schizonepetae Spica	(2S,5R)-2-isopropenyl-5-methyl-1-cyclohexanone	10534862	FALSE	C1(=O)CC(C)CCC1C(=C)C
MOL011877	0.9413	0.0587	0.9134	Schizonepetae Spica	(6S,7aS)-3,6-dimethyl-5,6,7,7a-tetrahydro-4H-benzofuran-2-one	10986613	FALSE	O1C2CC(CCC2=C(C1=O)C)C
MOL011878	0.7631	0.2369	0.8444	Moslae Herba	tilianin	Not Available	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(OC)cc1
MOL011878	0.7631	0.2369	0.8444	Schizonepetae Spica	tilianin	Not Available	FALSE	c1(cc(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(OC)cc1
MOL011879	0.9244	0.0756	0.7452	Lysimachiae Foenigraeci Herba	1,4,6-trimethyl-1,2-dihydro-naphthalene	Not Available	FALSE	C1(CC=C(c2cc(ccc12)C)C)C
MOL011880	0.9254	0.0746	0.7701	Lysimachiae Foenigraeci Herba	1,6,8-trimethyl-1,2,3,4-tetrahydronaphthalene	Not Available	FALSE	C1(CCCc2c1c(cc(c2)C)C)C
MOL011881	0.8265	0.1735	0.7673	Lysimachiae Foenigraeci Herba	13-Tetradecenal	522841	FALSE	C(=O)CCCCCCCCCCCC=C

MOL011883	0.9171	0.0829	0.9715	Lysimachiae Foenigraeci Herba	(1S,2S,5S)-2,5-dimethylcyclohexan-1-ol	10920530	FALSE	C1(C(CCC(C1)C)C)O
MOL011884	0.9272	0.0728	0.9211	Lysimachiae Foenigraeci Herba	3,7-Dimethyloct-1,5,7-trien-3-ol	40510009	FALSE	C=CC(C/C=C/C(=C)C)(O)C
MOL011884	0.9272	0.0728	0.9211	Campsis Flos	3,7-Dimethyloct-1,5,7-trien-3-ol	40510009	FALSE	C=CC(C/C=C/C(=C)C)(O)C
MOL011885	0.6911	0.3089	0.7873	Lysimachiae Foenigraeci Herba	lysiflavonoide A	Not Available	FALSE	C12C(C(=O)C(C(O1)C1CCC(CC1)O)OC1OC(C(C(C1OC1OC(C(C(C1O)O)OC1OC(C(C(C1O)O)O)CO)CO)O)O)O)CO)c(cc(c2)OC1OC(C(C(C1O)O)OC(=O)/C=C/c1ccc(cc1)O)C)O
MOL011886	0.3886	0.6114	0.7570	Lysimachiae Foenigraeci Herba	lysimachigenin A	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(C(C(C(C1)(C)C)OC(=O)/C(=C/C)/C)O)CO)C)C)C)(C)C)O
MOL011887	0.7340	0.2660	0.8035	Lysimachiae Foenigraeci Herba	lysimachigenoside B	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(C(C(C(C1)(C)C)OC(=O)/C(=C/C)/C)O)COC(=O)C)C)C)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)CO)O)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO
MOL011888	0.3351	0.6649	0.7499	Lysimachiae Foenigraeci Herba	lysimachigenoside B_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(C(C(C(C1)(C)C)OC(=O)/C(=C/C)/C)O)COC(=O)C)C)C)(C)C)O
MOL011889	0.7725	0.2275	0.8116	Lysimachiae Foenigraeci Herba	lysimachigenoside C	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(C(C(C(C1)(C)C)OC(=O)/C(=C/C)/C)O)CO)C)C)C)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)CO)O)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO
MOL011890	0.7985	0.2015	0.8187	Lysimachiae Foenigraeci Herba	lysimachigenoside D	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(C(C(C(C1)(C)C)O)O)CO)C)C)C)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)CO)O)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO
MOL011891	0.5667	0.4333	0.7162	Lysimachiae Foenigraeci Herba	lysimachigenoside D_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(C(C(C(C1)(C)C)O)O)CO)C)C)C)(C)C)O
MOL011892	0.7097	0.2903	0.7668	Lysimachiae Foenigraeci Herba	lysimachigenoside E	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)OC(=O)C)(C(CC(C1)(C)C)O)COC(=O)/C(=C/C)/C)C)C)C)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)CO)O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)COC(=O)C)OC1C(C(C(C(O1)CO)O)O)O)O)O)O
MOL011893	0.3012	0.6988	0.7589	Lysimachiae Foenigraeci Herba	lysimachigenoside E_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)OC(=O)C)(C(CC(C1)(C)C)O)COC(=O)/C(=C\C)/C)C)C)C)(C)C)O

MOL011894	0.7339	0.2661	0.7722	Lysimachiae Foenigraeci Herba	lysimachigenoside F	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)OC(=O)C)(C(CC(C1)(C)C)OC1OC(C(C(C1O)O)O)CO)COC(=O)/C(=C/C)/C)C)C)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)CO)O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)CO)O)O)O
MOL011896	0.8540	0.1460	0.8371	Viticis Negundo Folium	1-hydroxy-1,7-dimethyl-4-isopropyl-2,7-cyclodecadiene	Not Available	FALSE	C1(/C=C\C(CC/C(=C\CC1)/C)C(C)C)(C)O
MOL011897	0.8125	0.1875	0.8225	Viticis Negundo Folium	2,5-furandione,3-dodecenyl-	Not Available	FALSE	C1(CC(=O)OC1=O)C/C=C/CCCCCCCCC
MOL011898	0.8265	0.1735	0.6775	Viticis Negundo Folium	cadinol	12302226	FALSE	OC1(C2C(C(CC1)C(C)C)C=C(CC2)C)C
MOL011899	0.8009	0.1991	0.6810	Viticis Negundo Folium	eremophilene	12309744	FALSE	C1(CCC=C2C1(CC(CC2)C(=C)C)C)C
MOL011900	0.2239	0.7761	0.6014	Viticis Fructus	[(1R,3R,4R,4aS,5'E,8aS)-3,4a,8,8-tetramethyl-5'-(2-oxoethylidene)spiro[decalin-4,2'-tetrahydrofuran]-1-yl] acetate	11462191	FALSE	C1CC(C2C(C1)(C1(C(CC2OC(=O)C)C)CC/C(=C\C=O)/O1)C)(C)C
MOL011901	0.3709	0.6291	0.6094	Viticis Fructus	(2E)-2-[(1R,2R,4aS,8aS)-2,5,5,8a-tetramethylspiro[decalin-1,5'-tetrahydrofuran]-2'-ylidene]acetaldehyde	11208535	FALSE	C1CC(C2C(C1)(C1(C(CC2)C)CC/C(=C\C=O)/O1)C)(C)C
MOL011902	0.8002	0.1998	0.7090	Viticis Fructus	10-O-vanilloyaucubin	Not Available	FALSE	C12C(OC3OC(C(C(C3O)O)O)CO)OC=CC1C(C=C2COC(=O)c1ccc(c(c1)OC)O)O

MOL011903	0.3817	0.6183	0.7350	Viticis Fructus	12s,16s(r)-dihydroxy-ent-labda-7,13-dien-15,16-olide	Not Available	FALSE	C1CCC(C2C1(C(C(=CC2)C)CC(C1=CC(=O)OC1O)O)C)(C)C
MOL011904	0.9198	0.0802	0.9082	Viticis Fructus	2,6-Diethylpyridine	136745	FALSE	n1c(CC)cccc1CC
MOL011905	0.8767	0.1233	0.8479	Viticis Fructus	3,6,7-Trimethylquercetagenin	5280699	FALSE	c1(c(c(=O)c2c(o1)cc(c(c2O)OC)OC)OC)c1cc(c(cc1)O)O
MOL011907	0.2428	0.7572	0.7099	Viticis Fructus	(2S,4aS,10aR)-7-isopropyl-1,1,4a-trimethyl-2,3,4,9,10,10a-hexahydrophenanthren-2-ol	13996029	FALSE	C1C(C(C2C(C1)(c1c(CC2)cc(cc1)C(C)C)C)(C)C)O
MOL011908	0.2865	0.7135	0.6815	Viticis Fructus	Dihydrosolidagenone	Not Available	FALSE	C1CC(C2C(C1)(C(C(CC2=O)C)(CCc1cocc1)O)C)(C)C
MOL011909	0.2988	0.7012	0.6734	Viticis Fructus	(3R)-5-[(1S,4aS,8aS)-5,5,8a-trimethyl-2-methylene-1-decalinyl]-3-methylpent-1-en-3-ol	3034394	FALSE	C12(C(C(CCC2)(C)C)CCC(=C)C1CCC(C=C)(C)O)C
MOL011912	0.2598	0.7402	0.6983	Viticis Fructus	(2R,4aS,10aR)-7-isopropyl-2,4a-dimethyl-1-methylene-4,9,10,10a-tetrahydro-3H-phenanthren-2-ol	11033408	FALSE	OC1(C(=C)C2C(CC1)(c1c(CC2)cc(cc1)C(C)C)C)C

MOL011913	0.4991	0.5009	0.6584	Viticis Fructus	[(1S,3R,4R,4aS,8aS)-3,4a,8,8-tetramethyl-5'-oxo-spiro[decalin-4,2'-tetrahydrofuran]-1-yl] acetate	11834250	FALSE	O1C2(C3(C(C(CCC3)(C)C)C(OC(=O)C)CC2C)C)CCC1=O
MOL011914	0.3219	0.6781	0.6343	Viticis Fructus	[(1R,3R,4R,4aS,8aS)-3,4a,8,8-tetramethyl-6'-oxo-spiro[decalin-4,2'-tetrahydropyran]-1-yl] acetate	21668660	FALSE	O1C2(C3(C(C(CCC3)(C)C)C(CC2C)OC(=O)C)C)CCCC1=O
MOL011917	0.7803	0.2197	0.7235	Viticis Fructus	eurostoside	Not Available	FALSE	O(C1OC=CC2C1C(=CC2O)COC(=O)/C=C\c1ccc(O)cc1)C1OC(C(O)C(O)C1O)CO
MOL011918	0.7467	0.2533	0.6468	Viticis Fructus	eurostoside_qt	Not Available	FALSE	O(C1OC=CC2C1C(=CC2O)COC(=O)/C=C\c1ccc(O)cc1)C1OC(C(O)C(O)C1O)CO
MOL011919	0.4991	0.5009	0.6584	Viticis Fructus	[(1R,3R,4R,4aS,8aS)-3,4a,8,8-tetramethyl-5'-oxo-spiro[decalin-4,2'-tetrahydrofuran]-1-yl] acetate	21668661	FALSE	C1CC(C2C(C1)(C1(C(CC2OC(=O)C)C)OC(=O)CC1)C)(C)C
MOL011920	0.8026	0.1974	0.7066	Viticis Fructus	nishindaside	Not Available	FALSE	O1C(CC2C(C=C(C2C1OC1OC(C(C(C1O)O)O)O)CO)COC(=O)c1ccc(cc1)O)O)OC
MOL011921	0.8451	0.1549	0.7054	Viticis Fructus	nishindaside_qt	Not Available	FALSE	O1C(CC2C(C=C(C2C1O)COC(=O)c1ccc(cc1)O)O)OC
MOL011922	0.5117	0.4883	0.7061	Viticis Fructus	paulownin	3084131	FALSE	O1C(C2(O)C(C(OC2)c2cc3OCOc3cc2)C1)c1cc2OCOc2cc1

MOL011924	0.9467	0.0533	0.9373	Viticis Fructus	(5R)-2-methyl-5-(2-oxoethyl)cyclopentene-1-carbaldehyde	11105549	FALSE	O=CC1=C(CCC1CC=O)C
MOL011926	0.4831	0.5169	0.6654	Viticis Fructus	[(2S,4aS,5R,6R,8aS)-1,1,4a,6-tetramethyl-5'-oxo-spiro[decalin-5,2'-tetrahydrofuran]-2-yl] acetate	11771639	FALSE	O1C2(C3(C(C(C(OC(=O)C)CC3)(C)C)CCC2C)C)CCC1=O
MOL011927	0.4442	0.5558	0.7732	Viticis Fructus	4H-1-benzopyran-4-one, 3-[[O--6-deoxyhexopyranosyl-(1->6)-O-[hexopyranosyl-(1->2)]hexopyranosyl]oxy]-5,7-dihydroxy-2-(4-methoxyphenyl)-	Not Available	FALSE	C1C(C(C2C(C1)(C13C(CC2)CC2(C(C1O3)O2)C(C)C)C)(C)C)O
MOL011929	0.1896	0.8104	0.6862	Viticis Fructus	vitetrifolin c	15543012	FALSE	C1CC(C2=CC(C(C(C2(C1)C)(CCc1cocc1)O)C)OC(=O)C)(C)C
MOL011933	0.3246	0.6754	0.7152	Viticis Fructus	vitetrifolin g	Not Available	FALSE	C1CC(C2=CC(C(C(C2=C1)(C)CCC(C=C)(C)O)C)O)(C)C
MOL011934	0.2988	0.7012	0.6734	Viticis Fructus	vitexifolin A	Not Available	FALSE	OC(CCC1C2(C(C(CCC2)(C)C)CCC1=C)C)(C)C=C
MOL011938	0.5413	0.4587	0.6739	Viticis Fructus	4-(3,4-dimethoxyphenyl)-6-hydroxy-5-methoxynaphthalene-2-carbaldehyde	21592421	FALSE	c1(c(ccc(c1)c1cc(cc2ccc(c(c12)OC)O)C=O)OC)OC
MOL011939	0.5693	0.4307	0.7330	Viticis Fructus	vitrofolal B	44584755	FALSE	C1(C(C(C2(C1)CCC(C2OC)O)C1CCC(C(OC)C1)OC)O)C=O

MOL011940	0.6871	0.3129	0.7695	Viticis Fructus	vitrofolal C	Not Available	FALSE	OC1c2c(c3c1cc(OC)c(OC)c3)C1(CC2C=O)ccc(O)c1OC
MOL011942	0.9387	0.0613	0.7458	Equiseti Hiemalis Herba	1-Methoxynaphthalene	16668	FALSE	c12c(cccc1OC)cccc2
MOL011943	0.8969	0.1031	0.9728	Equiseti Hiemalis Herba	4,5-Dihydrosylvan	15145	FALSE	C1(=CCCO1)C
MOL011944	0.9178	0.0822	0.9182	Equiseti Hiemalis Herba	IPZ	33166	FALSE	c1(c(nccn1)C(C)C)OC
MOL011944	0.9178	0.0822	0.9182	Achyranthis Bidentatae Radix	IPZ	33166	FALSE	c1(c(nccn1)C(C)C)OC
MOL011945	0.8835	0.1165	0.7909	Equiseti Hiemalis Herba	ISODODECANE	23459	FALSE	CC(CCCCCCCCC)C
MOL011946	0.9110	0.0890	0.9361	Equiseti Hiemalis Herba	3,3-Dimethylhexane	11233	FALSE	C(CCC)(CC)(C)C
MOL011947	0.9324	0.0676	0.9636	Equiseti Hiemalis Herba	3-Butynol	13566	FALSE	C(C#C)CO
MOL011948	0.9441	0.0559	0.9227	Equiseti Hiemalis Herba	p-tert-Butylaniline	69861	FALSE	C(c1ccc(cc1)N)(C)(C)C
MOL011949	0.8239	0.1761	0.7568	Equiseti Hiemalis Herba	Allopseudocain	638023	FALSE	C1(C2N(C(CC1OC(=O)c1ccccc1)CC2)C)C(=O)OC
MOL011950	0.9208	0.0792	0.7835	Equiseti Hiemalis Herba	Gossypitrin	Not Available	FALSE	c1c(c(c2c(c1O)c(=O)c(c(o2)c1ccc(c(c1)O)O)O)O)OC1OC(C(C(C1O)O)O)CO
MOL011951	0.8981	0.1019	0.9663	Equiseti Hiemalis Herba	Methyl glutarate	73917	FALSE	C(=O)(CCCC(=O)O)OC
MOL011952	0.8797	0.1203	0.7712	Equiseti Hiemalis Herba	gossypetin-3-β-D-(2-O-β-D-glucopyranosidoglucopyranoside)-8-β-D-glucopyranoside	Not Available	FALSE	c1(=O)c2c(oc(c1OC1OC(C(C(C1OC1C(C(C(C(O1)CO)O)O)O)O)O)CO)c1cc(c(cc1)O)O)c(c(cc2O)O)OC1OC(C(C(C1O)O)O)CO
MOL011953	0.8706	0.1294	0.7818	Equiseti Hiemalis Herba	Herbacetin-3-beta-D-(2-O-beta-D-glucopyranosidoglucopyranoside)-8-beta-D-glucopyranoside	11968590	FALSE	c1(=O)c2c(oc(c1OC1OC(C(C(C1OC1C(C(C(C(O1)CO)O)O)O)O)O)CO)c1ccc(cc1)O)c(c(cc2O)O)OC1OC(C(C(C1O)O)O)CO
MOL011954	0.9235	0.0765	0.8000	Equiseti Hiemalis Herba	Herbacetrin	5318021	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(O)c2oc(c(O)c(=O)c2c(O)c1)c1ccc(O)cc1)CO

MOL011955	0.8709	0.1291	0.7902	Equiseti Hiemalis Herba	kaempferol-3-diglucoside-7-glucoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)CO)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL011956	0.8722	0.1278	0.7853	Equiseti Hiemalis Herba	kaempferol-3-glucoside-7-diglucoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(cc2o1)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)CO)OC1C(O)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL011957	0.9319	0.0681	0.9590	Equiseti Hiemalis Herba	m-Hba	7420	FALSE	C(=O)(c1cc(ccc1)O)O
MOL011957	0.9319	0.0681	0.9590	Glechomae Herba	m-Hba	7420	FALSE	C(=O)(c1cc(ccc1)O)O
MOL011958	0.9521	0.0479	0.9422	Equiseti Hiemalis Herba	m-methoxycinnamic acid	12185542	FALSE	C(=O)(/C=C\c1cc(ccc1)OC)O
MOL011960	0.5656	0.4344	0.6060	Notopterygii Rhizoma Et Radix	14-methylhexadecaoic acid methyl ester	Not Available	FALSE	O(C(=O)CCCCCC/C=C\CCCCC(C)CC)C
MOL011961	0.6637	0.3363	0.6081	Notopterygii Rhizoma Et Radix	4,8,12-trimethyltridecanoic acid methyl ester	Not Available	FALSE	C(=O)(CCC(CCCC(CCCC(C)C)C)C)OC
MOL011963	0.1572	0.8428	0.7303	Notopterygii Rhizoma Et Radix	8-geranoxy-5-methoxypsoralen	Not Available	FALSE	c12c(c(c3c(c1OC)ccc(=O)o3)OC/C=C(/CCC=C(C)C)\C)occ2
MOL011964	0.9337	0.0663	0.7471	Notopterygii Rhizoma Et Radix	Bergaptol-O-β-D-glucopyranoside	14704101	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(occ2)cc2oc(=O)ccc12)CO
MOL011965	0.4953	0.5047	0.7821	Notopterygii Rhizoma Et Radix	anisocoumarin,h	Not Available	FALSE	c1c(cc2c(c1)ccc(=O)o2)OC/C=C(/CC(C=C(C)C)O)\C
MOL011967	0.8611	0.1389	0.8933	Notopterygii Rhizoma Et Radix	chrysoeriol,7-rutinoside	Not Available	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1cc(c(cc1)O)OC)O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL011968	0.5132	0.4868	0.6642	Notopterygii Rhizoma Et Radix	coumarin,glycoside	Not Available	FALSE	c12c(cc3c(c1OC/C=C(/CCC(C(C)(C)O)OCC1C(C(C(C(O1)O)O)O)O)\C)ccc(=O)o3)occ2
MOL011969	0.8021	0.1979	0.8727	Notopterygii Rhizoma Et Radix	Demethylfuropinnarin	5316520	FALSE	o1c2c(C(C)(C)C=C)c3oc(=O)ccc3c(O)c2cc1
MOL011969	0.8021	0.1979	0.8727	Rhododendri Daurici Folium	Demethylfuropinnarin	5316520	FALSE	o1c2c(C(C)(C)C=C)c3oc(=O)ccc3c(O)c2cc1
MOL011970	0.4761	0.5239	0.6598	Notopterygii Rhizoma Et Radix	diversoside	Not Available	FALSE	c1c(cc2c(c1)ccc(=O)o2)OC/C=C(/CCC(C(C)(C)O)OC1OC(C(C(C1O)O)O)CO)\C
MOL011971	0.5970	0.4030	0.7428	Notopterygii Rhizoma Et Radix	diversoside_qt	15560114	FALSE	c1c(cc2c(c1)ccc(=O)o2)OC/C=C(/CCC(C(C)(C)O)O)\C
MOL011972	0.6408	0.3592	0.8667	Notopterygii Rhizoma Et Radix	isoimperatorin	Not Available	FALSE	c12c(cc3c(c1OCCC=C(C)C)ccc(=O)o3)occ2

MOL011973	0.7905	0.2095	0.7355	Notopterygii Rhizoma Et Radix	marmesinin	Not Available	FALSE	c1c2c(cc3c1OC(C3)C(C)(OC1C(O)C(O)C(O)C(O1)CO)C)ccc(=O)o2
MOL011974	0.1064	0.8936	0.8358	Notopterygii Rhizoma Et Radix	notopterol	Not Available	FALSE	c12c(cc3c(c1OC/C=C(/CC(C=C(C)C)C)\C)ccc(=O)o3)occ2
MOL011975	0.1380	0.8620	0.6004	Notopterygii Rhizoma Et Radix	notoptol	Not Available	FALSE	c12c(cc3c(c1OC/C=C(/C/C=C/C(C)(C)O)\C)ccc(=O)o3)occ2
MOL011976	0.8913	0.1087	0.9320	Notopterygii Rhizoma Et Radix	2-(4-hydroxyphenyl)ethyl 4-methoxybenzoate	14704104	FALSE	c1c(ccc(c1)C(=O)OCCc1ccc(cc1)O)OC
MOL011977	0.7630	0.2370	0.8295	Polygoni Orientalis Fructus	p-Hydroxyphenethyl trans-ferulate	637308	FALSE	c1(c(ccc(c1)/C=C/C(=O)OCCc1ccc(cc1)O)O)OC
MOL011977	0.7630	0.2370	0.8295	Notopterygii Rhizoma Et Radix	p-Hydroxyphenethyl trans-ferulate	637308	FALSE	c1(c(ccc(c1)/C=C/C(=O)OCCc1ccc(cc1)O)O)OC
MOL011978	0.7492	0.2508	0.7971	Notopterygii Rhizoma Et Radix	Phenyethyl 3-methylcaffeate	5284444	FALSE	c1(c(ccc(c1)/C=C/C(=O)OCCc1ccccc1)O)OC
MOL011979	0.8539	0.1461	0.9426	Notopterygii Rhizoma Et Radix	phenethyl,vanillate	Not Available	FALSE	c1(c(ccc(c1)C(=O)OCCc1ccc(cc1)OC)O)OC
MOL011980	0.8466	0.1534	0.8792	Notopterygii Rhizoma Et Radix	Pterostilbene	5281727	FALSE	c1(cc(cc(c1)/C=C/c1ccc(cc1)O)OC)OC
MOL011981	0.9466	0.0534	0.7861	Notopterygii Rhizoma Et Radix	cis-Verbenyl acetate	6427494	FALSE	C1(C2C(=CC(C1C2)OC(=O)C)C)(C)C
MOL011983	0.4769	0.5231	0.7750	Prinsepiae Nux	balnoaphonin	Not Available	FALSE	C1C(C(C(C1)C1OC2(C1CO)CC(CC2OC)/C=C\C=O)OC)O
MOL011984	0.2389	0.7611	0.6482	Prinsepiae Nux	stigmast-4-ene-3β,6β-diol	Not Available	FALSE	C1C(C=C2C(C1)(C1C(CC2O)C2C(CC1)(C(CC2)C(C)CCC(C(C)C)CC)C)C)O
MOL011985	0.6740	0.3260	0.7127	Cimicifugae Rhizoma	12beta-hydroxylcimigenol,3-o-alpha-l-arabinopyranoside	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(C(C1)O)(C1C4(C2O)OC(CC1C)C(C(C)(C)O)O4)C)C)C3)(C)C)OC1C(O)C(O)C(O)CO1

MOL011986	0.6416	0.3584	0.7119	Cimicifugae Rhizoma	12beta-hydroxylcimigenol,3-o-alpha-l-arabinopyranoside_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(C(C1)O)(C1C4(C2O)OC(CC1C)C(C(C)(C)O)O4)C)C)C3)(C)C)O
MOL011987	0.3387	0.6613	0.6966	Cimicifugae Rhizoma	15-O-acetylacerinol	Not Available	FALSE	C1C2C(C3C(C1)(CC1=C(CC3)C3(C(CC1)(C1C4(C3OC(=O)C)OC(CC1C)C(C(C)(C)O)O4)C)C)O2)(C)C
MOL011988	0.6474	0.3526	0.7100	Cimicifugae Rhizoma	16alpha,24alpha-dihydroxy-12beta-acetoxy-25,26,27-trinor-16,24-cyclocycloartan-23-one,3beta-o-alpha-l-arabinopyranoside	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(C(C1)OC(=O)C)(C1C(C2)(C(C(=O)CC1C)O)O)C)C)C3)(C)C)OC1OCC(C(C1O)O)O
MOL011989	0.8850	0.1150	0.7533	Cimicifugae Rhizoma	MBT	697993	FALSE	c12c(sc(n1)S)cccc2
MOL011990	0.4437	0.5563	0.6302	Cimicifugae Rhizoma	23-epi-26-deoxyactein	Not Available	FALSE	C1(C(COC(C1O)OC1CCC23C(C1(C)C)CCC1C2(CCC2(C1(CC1C2C(CC2(O1)OCC1(C2O1)C)C)C)C)C3)O)O
MOL011991	0.4266	0.5734	0.7503	Cimicifugae Rhizoma	23-epi-26-deoxyactein_qt	Not Available	FALSE	OC1CCC23C(C1(C)C)CCC1C2(CCC2(C1(CC1C2C(CC2(O1)OCC1(C2O1)C)C)C)C)C3
MOL011992	0.3461	0.6539	0.7025	Cimicifugae Rhizoma	23-o-acetylcimigenol-3-o-beta-d-xylopyranoside	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C(C(=O)C2O)C(CC(C1OC1(C)C)OC(=O)C)C)C)C3)(C)C)OC1C(C(C(CO1)O)O)O
MOL011993	0.3018	0.6982	0.7231	Cimicifugae Rhizoma	23-o-acetylcimigenol-3-o-beta-d-xylopyranoside_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C(C(=O)C2O)C(CC(C1OC1(C)C)OC(=O)C)C)C)C3)(C)C)O
MOL011994	0.3461	0.6539	0.7025	Cimicifugae Rhizoma	23-o-acetylshengmanol-3-o-alpha-l-arabinopyranoside	Not Available	FALSE	C1C(C(C(C(O1)OC1CCC23C(C1(C)C)CCC1C2(CCC2(C1(C(C(=O)C2C(CC(C1C(C)(C)O1)OC(=O)C)C)O)C)C)C3)O)O)O

MOL011995	0.3018	0.6982	0.7231	Cimicifugae Rhizoma	23-o-acetylshengmanol-3-o-alpha-l-arabinopyranoside_qt	Not Available	FALSE	OC1CCC23C(C1(C)C)CCC1C2(CCC2(C1(C(C(=O)C2C(CC(C1C(C)(C)O1)OC(=O)C)C)O)C)C)C3
MOL011996	0.5934	0.4066	0.7149	Cimicifugae Rhizoma	24-O-acetyl-7,8-didehydrocimigenol-3-β-D-xyloside	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C1C(C2O)(OC(CC1C)C(C(C)(C)O)OC(=O)C)O)C)C)C3)(C)C)OC1OCC(C(C1O)O)O
MOL011997	0.5421	0.4579	0.7447	Cimicifugae Rhizoma	24-O-acetyl-7,8-didehydrocimigenol-3-β-D-xyloside_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C1C(C2O)(OC(CC1C)C(C(C)(C)O)OC(=O)C)O)C)C)C3)(C)C)O
MOL011998	0.5670	0.4330	0.7289	Cimicifugae Rhizoma	24-epi-7,8-didehydrocimigenol	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C1C4(C2O)OC(CC1C)C(C(C)(C)O)O4)C)C)C3)(C)C)O
MOL011999	0.4424	0.5576	0.7704	Cimicifugae Rhizoma	24-epi-acerinol	Not Available	FALSE	C1C2C(C3C(C1)(CC1=C(CC3)C3(C(CC1)(C1C4(C3O)OC(CC1C)C(C(C)(C)O)O4)C)C)O2)(C)C
MOL012000	0.4785	0.5215	0.6924	Cimicifugae Rhizoma	24-hydroxy-12beta-acetoxy-25,26,27-trinorcycloartan-16,23-dione,3beta-o-alpha-l-arabinopyranoside	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(C(C1)OC(=O)C)(C(C(=O)C2)C(CC(=O)CO)C)C)C)C3)(C)C)OC1OCC(C(C1O)O)O
MOL012001	0.4495	0.5505	0.7057	Cimicifugae Rhizoma	24-hydroxy-12beta-acetoxy-25,26,27-trinorcycloartan-16,23-dione,3beta-o-alpha-l-arabinopyranoside_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(C(C1)OC(=O)C)(C(C(=O)C2)C(CC(=O)CO)C)C)C)C3)(C)C)O

MOL012002	0.5868	0.4132	0.7145	Cimicifugae Rhizoma	24-o-acetylcimigenol-3-o-beta-d-xylopyranoside	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C1C(C2O)(OC(CC1C)C(OC(=O)C)C(C)(C)O)O)C)C)C3)(C)C)OC1C(C(C(CO1)O)O)O
MOL012003	0.5440	0.4560	0.7390	Cimicifugae Rhizoma	24-o-acetylcimigenol-3-o-beta-d-xylopyranoside_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C1C(C2O)(OC(CC1C)C(OC(=O)C)C(C)(C)O)O)C)C)C3)(C)C)O
MOL012004	0.5934	0.4066	0.7149	Cimicifugae Rhizoma	24R-O-acetyl-7,8-didehydrocimigenol-3-β-D-araloside	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C1C(C2O)(OC(CC1C)C(C(C)(C)O)OC(=O)C)O)C)C)C3)(C)C)OC1OCC(C(C1O)O)O
MOL012005	0.5501	0.4499	0.6935	Cimicifugae Rhizoma	25-O-acetyl-7,8-didehydrocimigenol-3-O-α-L-araloside	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C1C4(C2O)OC(CC1C)C(C(C)(C)OC(=O)C)O4)C)C)C3)(C)C)OC1OCC(C(C1O)O)O
MOL012006	0.4573	0.5427	0.7303	Cimicifugae Rhizoma	25-O-acetyl-7,8-didehydrocimigenol-3-β-D-xyloside_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C1C4(C2O)OC(CC1C)C(C(C)(C)OC(=O)C)O4)C)C)C3)(C)C)O
MOL012007	0.5501	0.4499	0.6935	Cimicifugae Rhizoma	25-O-acetyl-7,8-didehydrocimigenol-3-β-D-xyloside	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C1C4(C2O)OC(CC1C)C(C(C)(C)OC(=O)C)O4)C)C)C3)(C)C)OC1OCC(C(C1O)O)O
MOL012008	0.5859	0.4141	0.7054	Cimicifugae Rhizoma	25-o-acetylcimigenol-3-o-beta-d-galactoyranoside	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C1C4(C2O)OC(CC1C)C(C(C)(C)OC(=O)C)O4)C)C)C3)(C)C)OC1C(C(C(C(O1)CO)O)O)O
MOL012009	0.4557	0.5443	0.7219	Cimicifugae Rhizoma	25-o-acetylcimigenol-3-o-beta-d-galactoyranoside_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C1C4(C2O)OC(CC1C)C(C(C)(C)OC(=O)C)O4)C)C)C3)(C)C)O

MOL012010	0.6464	0.3536	0.8117	Cimicifugae Rhizoma	25-o-acetylcimigenol-3-o-beta-d-glc(1-2)beta-d-xylopyranoside	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C1C4(C2O)OC(CC1C)C(C(C)(C)OC(=O)C)O4)C)C)C3)(C)C)OC1C(C(C(CO1)O)O)OC1C(C(C(C(O1)CO)O)O)O
MOL012011	0.4557	0.5443	0.7219	Cimicifugae Rhizoma	25-o-acetylcimigenol-3-o-beta-d-glc(1-2)beta-d-xylopyranoside_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C1C4(C2O)OC(CC1C)C(C(C)(C)OC(=O)C)O4)C)C)C3)(C)C)O
MOL012012	0.4780	0.5220	0.7321	Cimicifugae Rhizoma	25-o-acetylcimigenol	Not Available	FALSE	C1CC(C(C2C31C1(C(CC2)C2(C(CC1)(C1C4(C2O)CC(C(C)(C)OC(=O)C)C(CC1C)O4)C)C)C3)(C)C)O
MOL012013	0.5485	0.4515	0.6583	Cimicifugae Rhizoma	25-o-anhydrocimigenol-3-beta-d-xylopyranoside	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C1C4(C2O)OC(CC1C)C(C(=C)C)O4)C)C)C3)(C)C)OC1C(C(C(CO1)O)O)O
MOL012014	0.5062	0.4938	0.7370	Cimicifugae Rhizoma	25-o-anhydrocimigenol-3-beta-d-xylopyranoside_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C1C4(C2O)OC(CC1C)C(C(=C)C)O4)C)C)C3)(C)C)O
MOL012015	0.4415	0.5585	0.6508	Cimicifugae Rhizoma	26-deoxyactein	Not Available	FALSE	C1(C(COC(C1O)OC1CCC23C(C1(C)C)CCC1C2(CC(C2(C1(CC1C2C(CC2(O1)OCC1(C2O1)C)C)C)C)OC(=O)C)C3)O)O
MOL012016	0.3671	0.6329	0.7226	Cimicifugae Rhizoma	26-deoxyactein_qt	Not Available	FALSE	OC1CCC23C(C1(C)C)CCC1C2(CC(C2(C1(CC1C2C(CC2(O1)OCC1(C2O1)C)C)C)C)OC(=O)C)C3
MOL012017	0.5591	0.4409	0.7188	Cimicifugae Rhizoma	3'-O-acetyl-24-epi-7,8-didehydrocimigenol-3-O-β-D-xyloside	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C1C4(C2O)OC(CC1C)C(C(C)(C)O)O4)C)C)C3)(C)C)OC1OCC(C(C1O)OC(=O)C)O
MOL012018	0.5305	0.4695	0.7330	Cimicifugae Rhizoma	3-keto-24-epi-7,8-didehydrocimi genol	Not Available	FALSE	C1C(=O)C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C1C4(C2O)OC(CC1C)C(C(C)(C)O)O4)C)C)C3)(C)C

MOL012019	0.9420	0.0580	0.8862	Cimicifugae Rhizoma	4-o-acetyl-caffeic acid	Not Available	FALSE	C(=O)(/C=C/c1cc(O)c(OC(=O)C)cc1)O
MOL012020	0.4712	0.5288	0.6516	Cimicifugae Rhizoma	7,8-Didehydro-27-deoxyactein	Not Available	FALSE	C123C4(C2)C(C(C(OC2C(C(C(CO2)O)O)O)CC4)(C)C)CC=C1C1(C(C(C3)OC(=O)C)(C2C(OC3(C4C(O4)(CO3)C)CC2C)C1)C)C
MOL012021	0.3745	0.6255	0.7310	Cimicifugae Rhizoma	7,8-Didehydro-27-deoxyactein_qt	Not Available	FALSE	C123C4(C2)C(C(C(O)CC4)(C)C)CC=C1C1(C(C(C3)OC(=O)C)(C2C(OC3(C4C(O4)(CO3)C)CC2C)C1)C)C
MOL012022	0.6199	0.3801	0.6735	Cimicifugae Rhizoma	7,8-didehydrocimigenol-3-O-β-D-xyloside	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C1C4(C2O)OC(CC1C)C(C(C)(C)O)O4)C)C)C3)(C)C)OC1OCC(C(C1O)O)O
MOL012023	0.5670	0.4330	0.7289	Cimicifugae Rhizoma	7,8-didehydrocimigenol	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C1C4(C2O)OC(CC1C)C(C(C)(C)O)O4)C)C)C3)(C)C)O
MOL012024	0.7300	0.2700	0.7949	Cimicifugae Rhizoma	Cimiside C	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C1C(C2OC2C(C(C(O2)CO)O)O)O)(OC(CC1C)C(C(C)(C)O)OC(=O)C)O)C)C3)(C)C)OC1OCC(C(C1O)O)O
MOL012025	0.5440	0.4560	0.7390	Cimicifugae Rhizoma	Cimiside D_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C1C(C2O)(OC(CC1C)C(C(C)(C)O)OC(=O)C)O)C)C3)(C)C)O
MOL012026	0.7300	0.2700	0.7949	Cimicifugae Rhizoma	Cimiside D	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C1C(C2OC2C(C(C(O2)CO)O)O)O)(OC(CC1C)C(C(C)(C)O)OC(=O)C)O)C)C3)(C)C)OC1OCC(C(C1O)O)O
MOL012027	0.9300	0.0700	0.8281	Cimicifugae Rhizoma	Ferulic acid-β-D-glucoside	Not Available	FALSE	c1(c(ccc(c1)/C=C\C(=O)OC1C(C(C(C(O1)CO)O)O)O)OC)O
MOL012028	0.7321	0.2679	0.8115	Cimicifugae Rhizoma	Heracleifolinoside A	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C(C(=O)C2O)C(CC(=O)C(C(C)(C)OC1C(C(C(C(O1)CO)O)O)O)O)C)C)C3)(C)C)OC1OCC(C(C1O)O)O
MOL012029	0.5250	0.4750	0.7364	Cimicifugae Rhizoma	Heracleifolinoside A_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C(C(=O)C2O)C(CC(=O)C(C(C)(C)O)O)O)C)C)C3)(C)C)O
MOL012030	0.7215	0.2785	0.8143	Cimicifugae Rhizoma	Heracleifolinoside B	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C(C(=O)C2)C(CC(=O)C(C(C)(C)OC1C(C(C(C(O1)CO)O)O)O)O)O)C)C)C3)(C)C)OC1OCC(C(C1O)O)O
MOL012031	0.4327	0.5673	0.6857	Cimicifugae Rhizoma	Heracleifolinoside B_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C(C(=O)C2)C(CC(=O)C(C(C)(C)O)O)O)C)C)C3)(C)C)O
MOL012032	0.7706	0.2294	0.8118	Cimicifugae Rhizoma	Heracleifolinoside C	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C1C(C2O)(O)OC(CC1C)C(C(C)(C)O)OC1OC(C(C(C1O)O)O)CO)C)C)C3)(C)C)OC1OCC(C(C1O)O)O
MOL012033	0.6546	0.3454	0.7161	Cimicifugae Rhizoma	Heracleifolinoside C_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C1C(C2O)(O)OC(CC1C)C(C(C)(C)O)O)O)C)C)C3)(C)C)O

MOL012034	0.7706	0.2294	0.8118	Cimicifugae Rhizoma	Heracleifolinoside D	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C1C(C2O)(O)OC(CC1C)C(C(C)(C)O)OC1OC(C(C(C1O)O)O)CO)C)C3)(C)C)OC1OCC(C(C1O)O)O
MOL012035	0.6546	0.3454	0.7161	Cimicifugae Rhizoma	Heracleifolinoside D_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C1C(C2O)(O)OC(CC1C)C(C(C)(C)O)O)C)C)C3)(C)C)O
MOL012036	0.7332	0.2668	0.7941	Cimicifugae Rhizoma	Heracleifolinoside E	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C1C(C2OC2C(C(C(O2)CO)O)O)O)(O)OC(CC1C)C(C(C)(C)O)OC(=O)C)C)C3)(C)C)OC1OCC(C(C1O)O)O
MOL012037	0.5421	0.4579	0.7447	Cimicifugae Rhizoma	Heracleifolinoside E_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C1C(C2O)(O)OC(CC1C)C(C(C)(C)O)OC(=O)C)C)C3)(C)C)O
MOL012038	0.7248	0.2752	0.8192	Cimicifugae Rhizoma	Heracleifolinoside F	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C(C(=O)C2O)C(CC(=O)C(C(C)(C)O)OC1C(C(C(C(O1)COC1C(C(C(CO1)O)O)O)O)O)O)O)C)C)C3)(C)C)O
MOL012039	0.5250	0.4750	0.7364	Cimicifugae Rhizoma	Heracleifolinoside F_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1)(C(C(=O)C2O)C(CC(=O)C(C(C)(C)O)O)C)C)C3)(C)C)O
MOL012040	0.9020	0.0980	0.6697	Cimicifugae Rhizoma	Norkhelloside	Not Available	FALSE	c1c2c(c(c3c1occ3)O)c(=O)cc(o2)COC1C(C(C(C(O1)COC1C(C(CO1)(O)CO)O)O)O)O
MOL012041	0.9019	0.0981	0.7774	Cimicifugae Rhizoma	Norkhelloside_qt	Not Available	FALSE	c1c2c(c(c3c1occ3)O)c(=O)cc(o2)CO
MOL012042	0.4424	0.5576	0.7704	Cimicifugae Rhizoma	acerinol	Not Available	FALSE	C1C2C(C3C(C1)(CC1=C(CC3)C3(C(CC1)(C1C4(C3O)OC(CC1C)C(C(C)(C)O)O4)C)C)O2)(C)C
MOL012043	0.5159	0.4841	0.6682	Cimicifugae Rhizoma	actein	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(C(C1)OC(=O)C)(C1C(C2)OC2(CC1C)OC(C1(C2O1)C)O)C)C)C3)(C)C)OC1C(C(C(CO1)O)O)O
MOL012044	0.4438	0.5562	0.7209	Cimicifugae Rhizoma	actein_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(C(C1)OC(=O)C)(C1C(C2)OC2(CC1C)OC(C1(C2O1)C)O)C)C)C3)(C)C)O
MOL012045	0.6091	0.3909	0.6664	Cimicifugae Rhizoma	cimicifoetisidе a	Not Available	FALSE	O(C1C(C(O)C(O)CO1)O)C(=O)OC1CCC23C(C1(C)C)CCC1C2(CCC2(C1(C(C14C2C(CC(O1)C(C(C)(C)O)O4)C)O)C)C)C3
MOL012046	0.5216	0.4784	0.7272	Cimicifugae Rhizoma	cimicifoetisidе a_qt	Not Available	FALSE	OC(=O)OC1CCC23C(C1(C)C)CCC1C2(CCC2(C1(C(C14C2C(CC(O1)C(C(C)(C)O)O4)C)O)C)C)C3
MOL012047	0.5153	0.4847	0.6762	Cimicifugae Rhizoma	cimicifoetisidе b	Not Available	FALSE	O(C1C(C(O)C(O)CO1)O)C(=O)OC1CCC23C(C1(C)C)CCC1C2(CCC2(C1(C(C14C2C(CC(O1)C(C(C)(C)OC(=O)C)O4)C)O)C)C)C3
MOL012048	0.4114	0.5886	0.7140	Cimicifugae Rhizoma	cimicifoetisidе b_qt	Not Available	FALSE	OC(=O)OC1CCC23C(C1(C)C)CCC1C2(CCC2(C1(C(C14C2C(CC(O1)C(C(C)(C)OC(=O)C)O4)C)O)C)C)C2
MOL012049	0.6120	0.3880	0.6220	Cimicifugae Rhizoma	cimicifugadine	Not Available	FALSE	C1CC(C2C3(C1)C1(C(CC2)C2(C(CC1O)(c1c(C2)nc(cc1C)C(C(C)(C)O)O)C)C)C3)(OC1C(C(C(CO1)O)O)O)C
MOL012050	0.6236	0.3764	0.6208	Cimicifugae Rhizoma	cimicifugadine_qt	Not Available	FALSE	C1CC(C2C3(C1)C1(C(CC2)C2(C(CC1O)(c1c(C2)nc(cc1C)C(C(C)(C)O)O)C)C)C3)(O)C
MOL012052	0.8074	0.1926	0.7746	Cimicifugae Rhizoma	Tuberosine A	5322166	FALSE	c1(c(ccc(c1)/C=C\C(=O)NCCc1cc(c(cc1O)OC)O)OC
MOL012053	0.8304	0.1696	0.7363	Cimicifugae Rhizoma	cimicifugic acid	Not Available	FALSE	c1(cc(cc(c1)O)C1Oc2c(C1CO)cc(cc2OC)/C=C/C(=O)O)OC

MOL012054	0.4436	0.5564	0.6918	Cimicifugae Rhizoma	cimicifugoside	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1O)(C(C(=O)C2)C(CC(=O)C1C(C)(C)O1)C)C)C3)(C)C)OC1C(C(C(CO1)O)O)O
MOL012055	0.3802	0.6198	0.7349	Cimicifugae Rhizoma	cimicifugoside_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1O)(C(C(=O)C2)C(CC(=O)C1C(C)(C)O1)C)C)C3)(C)C)O
MOL012056	0.6139	0.3861	0.6759	Cimicifugae Rhizoma	cimicifugoside h-1	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C1C4(C2O)OC(C(O4)CC1C)C(O)(C)C)C)C)C3)(C)C)OC1C(C(C(CO1)O)O)O
MOL012057	0.5602	0.4398	0.7239	Cimicifugae Rhizoma	cimicifugoside h-1_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C1C4(C2O)OC(C(O4)CC1C)C(O)(C)C)C)C)C3)(C)C)O
MOL012058	0.9387	0.0613	0.9038	Cimicifugae Rhizoma	Cimidahurine	5315869	FALSE	C1(C(C(C(C(O1)Oc1c(ccc(c1)CCO)O)O)O)O)CO
MOL012060	0.6139	0.3861	0.6759	Cimicifugae Rhizoma	cimigenol-3-O-B-D-xylopyranoside	Not Available	FALSE	C123C4(C2)C(C(C(CC4)OC2C(C(C(CO2)O)O)O)(C)C)CCC1C1(C(CC3)(C2C3(C1O)OC(C(O3)CC2C)C(C)(C)O)C)C
MOL012061	0.6600	0.3400	0.6971	Cimicifugae Rhizoma	cimigenol-3-O-beta-d-galactopyranoside	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C1C4(C2O)OC(CC1C)C(C(O)(C)C)O4)C)C)C3)(C)C)OC1C(O)C(O)C(O)C(O1)CO
MOL012062	0.5602	0.4398	0.7239	Cimicifugae Rhizoma	cimigenol	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C1C4(C2O)OC(CC1C)C(C(C)(C)O)O4)C)C)C3)(C)C)O
MOL012063	0.5149	0.4851	0.6397	Cimicifugae Rhizoma	cimilactone a	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(C(C1)OC(=O)C)(C1C(C2)OC(=O)CC1C)C)C)C3)(C)C)OC1C(C(C(CO1)O)O)O
MOL012064	0.5110	0.4890	0.7379	Cimicifugae Rhizoma	cimilactone a_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(C(C1)OC(=O)C)(C1C(C2)OC(=O)CC1C)C)C)C3)(C)C)O
MOL012065	0.5380	0.4620	0.6382	Cimicifugae Rhizoma	cimilactone b	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(C(C1)OC(=O)C)(C1C(C2)OC(=O)CC1C)C)C)C3)(C)C)OC1C(C(C(CO1)O)O)O
MOL012066	0.5367	0.4633	0.7404	Cimicifugae Rhizoma	cimilactone b_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(C(C1)OC(=O)C)(C1C(C2)OC(=O)CC1C)C)C)C3)(C)C)O
MOL012067	0.5485	0.4515	0.6583	Cimicifugae Rhizoma	cimiside e	Not Available	FALSE	C1(C(C(C(OC1)OC1CCC23C(C1(C)C)CCC1C2(CCC2(C1(C(C14C2C(CC(C(O1)C(=C)C)O4)C)O)C)C)C3)O)O)O
MOL012068	0.5062	0.4938	0.7370	Cimicifugae Rhizoma	cimiside e_qt	Not Available	FALSE	OC1CCC23C(C1(C)C)CCC1C2(CCC2(C1(C(C14C2C(CC(C(O1)C(=C)C)O4)C)O)C)C)C3
MOL012069	0.5534	0.4466	0.6935	Cimicifugae Rhizoma	dahurinol	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C1C(C2=O)OC(CC1C)C(O)C(C)(C)O)C)C)C3)(C)C)O
MOL012070	0.6450	0.3550	0.6006	Cimicifugae Rhizoma	demethoxycimicifugamide	Not Available	FALSE	c1(c(ccc(c1)/C=C\C(=O)NCCc1ccc(cc1)O)OC1OC(C(C(C1O)O)O)CO)OC
MOL012071	0.3827	0.6173	0.7665	Cimicifugae Rhizoma	heracleifolinol	Not Available	FALSE	C1C2C(C3C(C1)(CC1=C(CC3)C3(C(CC1)(C1C(C3O)(OC(CC1C)C(C(C)(C)O)OC(=O)C)O)C)C)O2)(C)C
MOL012072	0.4378	0.5622	0.6345	Cimicifugae Rhizoma	methylcimicifugoside	Not Available	FALSE	O1C2C(C3(C(C4=CCC5C6(C4(C6)CC3OC(=O)C)CCC(OC3OCC(O)C(O)C3O)C5(C)C)(C2)C)C)C(CC21OC(OC)C1(OC21)C)C

MOL012073	0.3409	0.6591	0.7128	Cimicifugae Rhizoma	methylcimicifugoside_qt	Not Available	FALSE	O1C2C(C3(C(C4=CCC5C6(C4(C6)CC3OC(=O)C)C CC(O)C5(C)C)(C2)C)C)C(CC21OC(OC)C1(OC21)C)C
MOL012074	0.7075	0.2925	0.6942	Cimicifugae Rhizoma	neocimiside	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1O)(C1C(C2)(C(C(=O)CC1C)O)O)C)C)C3)(C)C)OC1C(C(C(CO1)O)O)O
MOL012075	0.7270	0.2730	0.7012	Cimicifugae Rhizoma	neocimiside_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(=CC2)C2(C(CC1O)(C1C(C2)(C(C(=O)CC1C)O)O)C)C)C3)(C)C)O
MOL012076	0.9455	0.0545	0.7888	Cimicifugae Rhizoma	Norvisnagin	612239	FALSE	o1c2c(c(O)c3c(occ3)c2)c(=O)cc1C
MOL012077	0.9226	0.0774	0.9257	Cimicifugae Rhizoma	(2R,3S)-2,3-dihydroxy-2-(4-hydroxybenzyl)succinic acid	10038020	FALSE	C(C(C(=O)O)O)(Cc1ccc(cc1)O)(C(=O)O)O
MOL012078	0.8694	0.1306	0.7933	Cimicifugae Rhizoma	visamminol	Not Available	FALSE	c1(cc(=O)c2c(o1)cc1c(c2O)CC(O1)C(C)(C)O)C
MOL012079	0.7143	0.2857	0.7629	Cimicifugae Rhizoma	(+)-Isolariciresinol-3α-O-β-D-glucopyranoside	Not Available	FALSE	c1(c(cc2c(c1)CC(C(C2c1ccc(c(c1)OC)O)COC1C(C(C(C(O1)CO)O)O)O)CO)O)OC
MOL012080	0.3577	0.6423	0.6561	Cimicifugae Rhizoma	(20r,24r)-24,25-epoxy-3-beta-(beta-d-xylopyranosyloxy)-9,19-cyclolanost-7-ene-16,23-dione	Not Available	FALSE	C1(CCC23C(C1(C)C)CC=C1C4(C)CC(=O)C(C(CC(=O)C5C(C)(C)O5)C)C4(C)CCC21C3)OC1C(O)C(O) C(O)CO1
MOL012081	0.3060	0.6940	0.7376	Cimicifugae Rhizoma	(20r,24r)-24,25-epoxy-3-beta-(beta-d-xylopyranosyloxy)-9,19-cyclolanost-7-ene-16,23-dione_qt	Not Available	FALSE	C1(CCC23C(C1(C)C)CC=C1C4(C)CC(=O)C(C(CC(=O)C5C(C)(C)O5)C)C4(C)CCC21C3)O
MOL012082	0.9312	0.0688	0.8381	Cimicifugae Rhizoma	3-(3-methylbut-2-enylidene)oxindole	Not Available	FALSE	O=C1Nc2c(/C/1=C/C=C(C)C)cccc2
MOL012083	0.6872	0.3128	0.7035	Cimicifugae Rhizoma	12beta-hydroxycimigenol	Not Available	FALSE	C1(C(C(C(OC1)OC1CCC23C(C1(C)C)CCC1C2(CC(C2(C1(C(C1(C2CCC(O1)C(C)(C)O)O)O)C)C)O)C3) O)O)O

MOL012084	0.7214	0.2786	0.6902	Cimicifugae Rhizoma	12beta-hydroxycimigenol_qt	Not Available	FALSE	OC1CCC23C(C1(C)C)CCC1C2(CC(C2(C1(C(C1(C2CCC(O1)C(C)(C)O)O)O)C)C)O)C3
MOL012085	0.6665	0.3335	0.6663	Tamaricis Cacumen	1-METHYLPHENANTHRENE	13257	FALSE	c12c3c(ccc1cccc2)c(ccc3)C
MOL012087	0.9562	0.0438	0.9269	Tamaricis Cacumen	3-(2-hydroxy-4-methoxy-phenyl)acrylic acid	12840862	FALSE	c1(c(cc(cc1)OC)O)/C=C/C(=O)O
MOL012088	0.3675	0.6325	0.6896	Tamaricis Cacumen	24-methylene-cycloartanol	Not Available	FALSE	C12(C(C(CC2)C(CCC(=C)C(C)C)C)(CCC23C4(C(CCC12)C(CCC4O)(C)C)C3)C)C
MOL012089	0.6850	0.3150	0.6105	Tamaricis Cacumen	9-METHYLPHENANTHRENE	13438	FALSE	c12c3c(c(cc1cccc2)C)cccc3
MOL012090	0.8680	0.1320	0.7453	Tamaricis Cacumen	(Z)-9-Pentadecenoic acid	6365140	FALSE	OC(=O)CCCCCCC/C=C/CCCCC
MOL012091	0.3593	0.6407	0.7204	Tamaricis Cacumen	Tamarixol	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2=CCC3(C(C2(CC1)C)C(CC3)C)C)CO)C)(C)C)O
MOL012092	0.3390	0.6610	0.7233	Tamaricis Cacumen	Tamarixone	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2=CCC3(C(C2(CC1)C)C(CC3)C)C)CO)C)(C)C
MOL012093	0.7812	0.2188	0.7270	Tamaricis Cacumen	ambrettolide	Not Available	FALSE	CC(O)CCCC/C=C/CCCCCCCCO
MOL012094	0.8621	0.1379	0.6441	Tamaricis Cacumen	calacorene	71353669	FALSE	C1(C(C)C)CC=C(c2c1cc(cc2)C)C
MOL012096	0.3576	0.6424	0.7664	Tamaricis Cacumen	myricadiol	Not Available	FALSE	OC1C(C2C(C3C(C4=CCC5(C(C4(CC3)C)CC(CC5)(C)C)CO)(CC2)C)(CC1)C)(C)C
MOL012097	0.9060	0.0940	0.8649	Tamaricis Cacumen	2-(3,4-dimethoxyphenyl)-3,5,7-trihydroxy-chromone	5487855	FALSE	c12c(oc(c(c1=O)O)c1cc(c(cc1)OC)OC)cc(cc2O)O
MOL012098	0.8804	0.1196	0.7109	Tamaricis Cacumen	Trimethylnaphthalene	28226	FALSE	c12c(cc(cc1C)C)cccc2C
MOL012100	0.8212	0.1788	0.7725	Moslae Herba	5,7-Dimethoxy-4'-hydroxyflavone	161172	FALSE	c1(cc(=O)c2c(cc(cc2o1)OC)OC)c1ccc(cc1)O
MOL012101	0.6615	0.3385	0.9766	Moslae Herba	Mosloflavone	471722	TRUE	o1c2c(c(O)c(OC)c(OC)c2)c(=O)cc1c1ccccc1
MOL012101	0.6615	0.3385	0.9766	Oroxyli Semen	Mosloflavone	471722	TRUE	o1c2c(c(O)c(OC)c(OC)c2)c(=O)cc1c1ccccc1

MOL012102	0.7841	0.2159	0.8051	Moslae Herba	5-hydroxy-6-methoxyflavanone-7-O-α-D-galactopyranoside	Not Available	FALSE	c1(c(cc2c(c1O)C(=O)CC(O2)c1ccccc1)OC1C(C(C(C(O1)CO)O)O)O)OC
MOL012104	0.6556	0.3444	0.6843	Moslae Herba	9-epi-(e)-caryophyllene	Not Available	FALSE	C\1(=C\CCC(=C)C2C(CC1)C(C2C)CC)/C
MOL012105	0.9172	0.0828	0.8113	Moslae Herba	MORIN-7-O-β-D-glucoside	45269053	FALSE	c12c(oc(c(c1=O)O)c1ccc(cc1O)O)cc(cc2O)OC1OC(C(C(C1O)O)O)CO
MOL012106	0.9351	0.0649	0.8856	Moslae Herba	Carvacryl acetate	80792	FALSE	c1(ccc(cc1OC(=O)C)C(C)C)C
MOL012106	0.9351	0.0649	0.8856	Asari Radix Et Rhizoma	Carvacryl acetate	80792	FALSE	c1(ccc(cc1OC(=O)C)C(C)C)C
MOL012107	0.8291	0.1709	0.7593	Kaempferiae Rhizoma	delta-selinene	12308846	FALSE	C1(=CC2=C(CCCC2(CC1)C)C)C(C)C
MOL012107	0.8291	0.1709	0.7593	Moslae Herba	delta-selinene	12308846	FALSE	C1(=CC2=C(CCCC2(CC1)C)C)C(C)C
MOL012108	0.8459	0.1541	0.8528	Moslae Herba	Negletein	471719	FALSE	c12c(oc(cc2=O)c2ccccc2)cc(c(c1O)O)OC
MOL012108	0.8459	0.1541	0.8528	Oroxyli Semen	Negletein	471719	FALSE	c12c(oc(cc2=O)c2ccccc2)cc(c(c1O)O)OC
MOL012110	0.9459	0.0541	0.7522	Moslae Herba	tricyclene	14744268	FALSE	C12CC(CC1)C(C2(C)C)C
MOL012110	0.9459	0.0541	0.7522	Coriandri Sativi Herba	tricyclene	14744268	FALSE	C12CC(CC1)C(C2(C)C)C
MOL012111	0.1554	0.8446	0.8603	Magnoliae Flos	(-)-galbacin	Not Available	FALSE	O1C(C(C(C1c1cc2c(cc1OCO2)C)C)c1ccc2c(c1)OCO2
MOL012112	0.3441	0.6559	0.7628	Magnoliae Flos	36150-23-9	182278	FALSE	C12C(COC1c1ccc(c(c1)OC)OC)C(OC2)c1ccc2c(c1)OCO2
MOL012113	0.9267	0.0733	0.9198	Magnoliae Flos	2,4,6-Octatriene, 3,4-dimethyl-	5371124	FALSE	C/C=C(/C(=C/C=C/C)/C)\C
MOL012114	0.7049	0.2951	0.6685	Asari Radix Et Rhizoma	Dodecatetraenamide, N-(2-methylpropyl)-	6440406	FALSE	O=C(NCC(C)C)/C=C/C=C/C=C/C=C/CCC
MOL012114	0.7049	0.2951	0.6685	Magnoliae Flos	Dodecatetraenamide, N-(2-methylpropyl)-	6440406	FALSE	O=C(NCC(C)C)/C=C/C=C/C=C/C=C/CCC
MOL012115	0.2392	0.7608	0.8648	Magnoliae Flos	(2S,3S)-5-allyl-2-(3,4-dimethoxyphenyl)-7-methoxy-3-methyl-2,3-dihydrobenzofuran	21722968	FALSE	c1cc(cc(c1OC)OC)C1Oc2c(C1C)cc(cc2OC)CC=C
MOL012116	0.9683	0.0317	0.8181	Asari Radix Et Rhizoma	Sarisan	95289	FALSE	O1COc2c1cc(c(c2)CC=C)OC

MOL012116	0.9683	0.0317	0.8181	Magnoliae Flos	Sarisan	95289	FALSE	O1COc2c1cc(c(c2)CC=C)OC
MOL012117	0.3256	0.6744	0.6992	Magnoliae Flos	burcellin a	Not Available	FALSE	c1(cc(cc(c1OC)OC)C1OC2=CC(=O)C(C=C2C1C)(CC=C)OC)OC
MOL012118	0.3869	0.6131	0.8826	Magnoliae Flos	burcellin b	Not Available	FALSE	c1cc(cc2c1OCO2)C1OC2=CC(=O)C(C=C2C1C)(CC=C)OC
MOL012119	0.4942	0.5058	0.7379	Magnoliae Flos	(1R,5R,6R,7R)-3-allyl-6-(3,4-dimethoxyphenyl)-1-methoxy-7-methylbicyclo[3.2.1]oct-2-ene-4,8-dione	10713269	FALSE	c1(cc(c(cc1)OC)OC)C1C2C(=O)C(=CC(C1C)(C2=O)OC)CC=C
MOL012120	0.5301	0.4699	0.7957	Magnoliae Flos	(1R,5R,6R,7R)-3-allyl-6-(1,3-benzodioxol-5-yl)-1-methoxy-7-methylbicyclo[3.2.1]oct-2-ene-4,8-dione	10569137	FALSE	c12c(cc(cc1)C1C3C(=O)C(=CC(C1C)(C3=O)OC)CC=C)OCO2
MOL012121	0.4881	0.5119	0.7639	Magnoliae Flos	denudadione c	Not Available	FALSE	c1(cc2c(cc1)OCO2)C1C2C(=O)C(=CC(C1C)(CC=C)C2=O)OC
MOL012122	0.5489	0.4511	0.8278	Magnoliae Flos	denudalide	Not Available	FALSE	c1(cc(c2c(c1)CC(=O)O2)C/C=C(/CCC=C(C)C)\C)O
MOL012123	0.2858	0.7142	0.7990	Magnoliae Flos	denudanolide a	Not Available	FALSE	c1(cc2c(cc1)OCO2)C1C2C(=C)C(=CC(C1C)(OC2=O)OC)CC=C
MOL012124	0.4050	0.5950	0.6185	Magnoliae Flos	denudanolide b	Not Available	FALSE	c1(cc(c(cc1)O)OC)C1C2C(=C)C(=CC(C1C)(OC2=O)OC)CC=C
MOL012125	0.2362	0.7638	0.7393	Magnoliae Flos	denudanolide c	Not Available	FALSE	c1(cc(c(cc1)OC)OC)C1C2C(=C)C(=CC(C1C)(OC2=O)OC)CC=C
MOL012126	0.2501	0.7499	0.6006	Magnoliae Flos	denudanolide d	Not Available	FALSE	c1(cc(c(c(c1)OC)OC)OC)C1C2C(=C)C(=CC(C1C)(OC2=O)OC)CC=C
MOL012127	0.6026	0.3974	0.7500	Magnoliae Flos	denudaquinol	Not Available	FALSE	c1(cc(c(c(c1)CC(=O)OC)O)C/C=C(/CCC=C(C)C)\C)O
MOL012128	0.9486	0.0514	0.7984	Magnoliae Flos	epicamphor	12309505	FALSE	C1C(=O)C2CCC1(C2(C)C)C
MOL012128	0.9486	0.0514	0.7984	Asari Radix Et Rhizoma	epicamphor	12309505	FALSE	C1C(=O)C2CCC1(C2(C)C)C

MOL012129	0.3441	0.6559	0.7628	Magnoliae Flos	5-[(1R,3aR,4S,6aR)-4-(3,4-dimethoxyphenyl)-1,3,3a,4,6,6a-hexahydrofuro[4,3-c]furan-1-yl]-1,3-benzodioxole	11210905	FALSE	C12C(COC1c1ccc(c(c1)OC)OC)C(OC2)c1ccc2c(c1)OCO2
MOL012130	0.3600	0.6400	0.6745	Magnoliae Flos	(2S,3R,3aR,7R,7aS)-7-allyl-2-(1,3-benzodioxol-5-yl)-3a,4-dimethoxy-3-methyl-2,3,7,7a-tetrahydrobenzofuran-6-one	21629911	FALSE	c12c(ccc(c1)C1OC3C(C1C)(C(=CC(=O)C3CC=C)OC)OC)OCO2
MOL012131	0.3018	0.6982	0.7941	Magnoliae Flos	isodihydrofutoquinol a	25774970	FALSE	c12ccc(cc1OCO2)CC(C1(C(=CC(=O)C(=C1)CC=C)OC)OC)C
MOL012132	0.3018	0.6982	0.7941	Magnoliae Flos	isodihydrofutoquinol b	25774968	FALSE	c12ccc(cc1OCO2)CC(C1(C(=CC(=O)C(=C1)CC=C)OC)OC)C
MOL012133	0.9467	0.0533	0.8359	Magnoliae Flos	Kakoul	596894	FALSE	C(=O)(CC)c1cc2OCOc2cc1O
MOL012133	0.9467	0.0533	0.8359	Asari Radix Et Rhizoma	Kakoul	596894	FALSE	C(=O)(CC)c1cc2OCOc2cc1O
MOL012134	0.1737	0.8263	0.7024	Magnoliae Flos	lariciresinol	Not Available	FALSE	c12c(ccc(c1)C1CC3(C(C1C)(C=C(C(=O)C3)/C=C\C)OC)OC)OCO2
MOL012135	0.2721	0.7279	0.8903	Magnoliae Flos	licarin b	52316243	FALSE	c1cc(cc2c1OCO2)C1Oc2c(C1C)cc(cc2OC)CC=C
MOL012136	0.3098	0.6902	0.8428	Magnoliae Flos	5-[(2S,3S,4R,5R)-5-(3,4-dimethoxyphenyl)-3,4-dimethyl-2-tetrahydrofuranyl]-1,3-benzodioxole	10450921	FALSE	c1(c(ccc(c1)C1C(C(C(O1)c1ccc2c(c1)OCO2)C)C)OC)OC

MOL012138	0.4645	0.5355	0.8320	Magnoliae Flos	(1S,5R,6R,7R)-3-allyl-6-(1,3-benzodioxol-5-yl)-1-methoxy-7-methyl-8-oxabicyclo[3.2.2]non-2-ene-4,9-dione	10618232	FALSE	c12cc(ccc1OCO2)C1C2C(=O)C(=CC(C1C)(OC2=O)OC)CC=C
MOL012139	0.3403	0.6597	0.7051	Magnoliae Flos	nirandin a	Not Available	FALSE	c1c(c(c(cc1C1OC2=CC(=O)C(=CC2(C1C)OC)CC=C)OC)OC)OC
MOL012140	0.7927	0.2073	0.7153	Asari Radix Et Rhizoma	4,9-dimethoxy-1-vinyl-$b-carboline	5316876	FALSE	c1cc2c(cc1)c1c(n2OC)c(ncc1OC)C=C
MOL012141	0.7866	0.2134	0.6760	Asari Radix Et Rhizoma	Caribine	Not Available	FALSE	c12c(cc3c(c1)C1C4N(C3)CC(C4=CC3C1NCCC3)O)OCO2
MOL012142	0.7871	0.2129	0.9036	Asari Radix Et Rhizoma	Estriol	40488277	FALSE	c1c(cc2c(c1)C1C(CC2)C2C(CC1)(C(C(C2)O)O)C)O
MOL012142	0.7871	0.2129	0.9036	Peucedani Radix	Estriol	40488277	FALSE	c1c(cc2c(c1)C1C(CC2)C2C(CC1)(C(C(C2)O)O)C)O
MOL012143	0.8861	0.1139	0.8103	Asari Radix Et Rhizoma	ACon1_002321	9960512	FALSE	c1(c(oc2c(c1=O)c(cc(c2)O)O)c1ccc(cc1)O)OC1C(C(C(C(O1)COC1C(C(C(C(O1)CO)O)O)O)O)O)O
MOL012144	0.8934	0.1066	0.7934	Asari Radix Et Rhizoma	Myristelaidic acid	5312402	FALSE	CCCC/C=C/CCCCCCCC(=O)O
MOL012145	0.9508	0.0492	0.7928	Asari Radix Et Rhizoma	DHNQ	10141	FALSE	c1cc(c2c(c1O)C(=O)C=CC2=O)O
MOL012146	0.7245	0.2755	0.7056	Asari Radix Et Rhizoma	Sarmentolosid e	Not Available	FALSE	C1C(CC2(C(C1)(C1C(CC2)C2(C(CC1O)(C(CC2)C1=CC(=O)OC1)C)O)CO)O)OC1OC(C(C(C1O)O)O)C
MOL012147	0.9326	0.0674	0.9636	Coriandri Sativi Herba	ZINC02013201	638098	FALSE	OC(CCC)CC
MOL012148	0.9216	0.0784	0.9273	Coriandri Sativi Herba	Phenoxyacetone	69313	FALSE	c1(OCC(=O)C)ccccc1
MOL012149	0.8937	0.1063	0.9706	Coriandri Sativi Herba	3-methyl-2,3-dihydro-furan	12218405	FALSE	O1CC(C=C1)C
MOL012150	0.9580	0.0420	0.9776	Coriandri Sativi Herba	cis-Dihydrocarvone	443167	FALSE	C1C(=O)C(CCC1C(=C)C)C
MOL012151	0.9311	0.0689	0.9653	Coriandri Sativi Herba	cis-linalool,oxide	12978150	FALSE	C1(C(OC(CC1)C=C)(C)C)O
MOL012152	0.9092	0.0908	0.8311	Coriandri Sativi Herba	Coriandrin	119586	FALSE	o1c2c(c(OC)c3c(c2)cc(oc3=O)C)cc1
MOL012153	0.7981	0.2019	0.8053	Coriandri Sativi Herba	coriandrone A	Not Available	FALSE	c12c(c(cc3c1C(=O)OC(C3)C)OC)CC(O2)C(C)(C)O
MOL012154	0.7626	0.2374	0.8120	Coriandri Sativi Herba	coriandrone B	Not Available	FALSE	c12c(c(cc3c1C(=O)OC(C3)C)OC)CC(C(O2)(C)C)O
MOL012155	0.9355	0.0645	0.9387	Coriandri Sativi Herba	trans-linalool,oxide	Not Available	FALSE	C1C(OC(CC1)(C=C)C)C(=C)C

MOL012156	0.9211	0.0789	0.7609	Coriandri Sativi Herba	trans-sabinenehydrate	Not Available	FALSE	C1(CC2C(C1)(C2)C(C)C)(C)O
MOL012157	0.9599	0.0401	0.7620	Coriandri Sativi Herba	α-fenchene	12309838	FALSE	C1(C2CCC1C(=C)C2)(C)C
MOL012158	0.8477	0.1523	0.7512	Solidaginis Herba	2-Methoxybenzyl-2,3,6-trimethoxybenzoate	5319409	FALSE	c1(ccc(c(c1OC)C(=O)OCc1ccccc1OC)OC)OC
MOL012159	0.9327	0.0673	0.8903	Solidaginis Herba	6-Methoxysalicylic acid	591524	FALSE	c1(c(cccc1O)OC)C(=O)O
MOL012160	0.9112	0.0888	0.8151	Solidaginis Herba	2-hydroxy-6-methoxybenzyl-2-methoxybenzoate	Not Available	FALSE	O(Cc1c(cccc1OC)O)C(=O)c1c(OC)cccc1
MOL012161	0.8961	0.1039	0.8288	Solidaginis Herba	2-Methoxybenzyl-2,6-dimethoxybenzoate	5319408	FALSE	c1(c(cccc1OC)OC)C(=O)OCc1ccccc1OC
MOL012162	0.7800	0.2200	0.8323	Solidaginis Herba	3,5-dimethoxy-4-acetoxycinnamylangelate	Not Available	FALSE	c1(c(cc(cc1OC)/C=C/COC(=O)/C(=C\C)/C)OC)OC(=O)C
MOL012163	0.7936	0.2064	0.8647	Solidaginis Herba	3-methoxy-4-acetoxycinnamyl angelate	Not Available	FALSE	O(c1cc(ccc1OC(=O)C)/C=C\COC(=O)/C(=C\C)/C)C
MOL012164	0.5499	0.4501	0.6159	Solidaginis Herba	3-methoxy-5-acetyl-31-tritriacontene	Not Available	FALSE	CCC(OC)CC(C(=O)C)CCCCCCCCCCCCCCCCCCCCCCCCCC/C=C/C
MOL012165	0.2155	0.7845	0.7519	Solidaginis Herba	Methyl dehydro-15-hydroxy-abietan-18-oate	11573479	FALSE	c1cc2c(cc1C(C)(C)O)CCC1C2(CCCC1(C)C(=O)OC)C
MOL012166	0.9190	0.0810	0.8415	Solidaginis Herba	Methyl(2Z,8Z)-decadien-4,6-diynoate	Not Available	FALSE	COC(=O)/C=C\C#CC#C/C=C/C

MOL012167	0.8411	0.1589	0.7003	Solidaginis Herba	(5R,8S,8aS)-5-isopropenyl-3,8-dimethyl-1,2,4,5,6,7,8,8a-octahydroazulene	24766093	FALSE	C12C(CCC(CC1=C(CC2)C)C(=C)C)C
MOL012169	0.8903	0.1097	0.8817	Solidaginis Herba	Benzyl 2,6-methoxybenzoate	370912	FALSE	O(Cc1ccccc1)C(=O)c1c(OC)cccc1OC
MOL012170	0.9255	0.0745	0.9194	Solidaginis Herba	Benzyl 2-hydroxy-6-methoxybenzoate	6430728	FALSE	O(Cc1ccccc1)C(=O)c1c(OC)cccc1O
MOL012171	0.8630	0.1370	0.7036	Solidaginis Herba	cadala-1(10),3,8-triene	Not Available	FALSE	C12C(C(C)C)C=CC(=C2C=CC(C1)C)C
MOL012172	0.8332	0.1668	0.7238	Solidaginis Herba	leiocarposide	Not Available	FALSE	c1(c(c(c(cc1)C(=O)OCc1c(OC2OC(C(C(C2O)O)O)CO)cccc1)O)OC)OC1OC(C(C(C1O)O)O)CO
MOL012173	0.9064	0.0936	0.8832	Solidaginis Herba	leiocarposide_qt	Not Available	FALSE	c1(c(c(c(cc1)C(=O)OCc1c(O)cccc1)O)OC)O
MOL012174	0.9410	0.0590	0.9210	Solidaginis Herba	o-Anisic acid	11370	FALSE	c1(c(cccc1)OC)C(=O)O
MOL012175	0.7405	0.2595	0.8469	Benzoinum	19α-hydroxy-3-oxo-olean-12-en-28-oic acid	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1O)(C)C)C(=O)O)C)C)(C)C
MOL012176	0.4109	0.5891	0.7068	Benzoinum	3β-hydroxy-12-oxo-13Hα-olean-28,19β-olide	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(=O)C1)C1C3(CC2)CCC(C1OC3=O)(C)C)C)C)(C)C)O
MOL012177	0.9380	0.0620	0.9193	Benzoinum	4-[(E)-3-ethoxyprop-1-enyl]-2-methoxyphenol	13436179	FALSE	c1(c(cc(cc1)/C=C/COCC)OC)O
MOL012178	0.5308	0.4692	0.7652	Benzoinum	6β-hydroxy-3-oxo-11α,12α-epoxyolean-28,13β-olide	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2O)(C2(C3(C4C1O4)C1C(CC2)(CCC(C1)(C)C)C(=O)C3)C)C)(C)C

MOL012179	0.7289	0.2711	0.8440	Benzoinum	6β-hydroxy-3-oxo-olean-12-en-28-oic acid	Not Available	FALSE	C1C(=O)C(C2C(C1)(C1C(CC2O)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)C)(C)C
MOL012180	0.9284	0.0716	0.9073	Benzoinum	Acrylophenone	13028	FALSE	C(=O)(C=C)c1ccccc1
MOL012181	0.9287	0.0713	0.8927	Benzoinum	Allyl cinnamate	641423	FALSE	O(CC=C)C(=O)/C=C/c1ccccc1
MOL012182	0.9071	0.0929	0.8981	Benzoinum	Amyl cinnamate	5355854	FALSE	C(=O)(/C=C/c1ccccc1)OCCCCC
MOL012183	0.9513	0.0487	0.9394	Benzoinum	ALLYLBENZOATE	11406	FALSE	c1c(cccc1)C(=O)OCC=C
MOL012184	0.8315	0.1685	0.6446	Benzoinum	Cedrene-V6	Not Available	FALSE	C12C(CCC1=C(C(CC2)(C)C)C)(C)C=C
MOL012185	0.9149	0.0851	0.9208	Benzoinum	2-propenoic acid-3-phenyl-Butyl ester	Not Available	FALSE	C(=O)(C=C)OCCC(C)c1ccccc1
MOL012186	0.3425	0.6575	0.7615	Benzoinum	Cinobufagin	Not Available	FALSE	C1C(CC2C(C1)(C1C(CC2)C23C(CC1)(C(C(C3O2)OC(=O)C)c1ccc(=O)oc1)C)C)O
MOL012187	0.7354	0.2646	0.8493	Benzoinum	Phenol, 4-(3-(benzoyloxy)-1-propenyl)-2-methoxy-	6441293	FALSE	C(=O)(c1ccccc1)OC/C=C/c1cc(OC)c(O)cc1
MOL012188	0.5400	0.4600	0.7807	Benzoinum	[(E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enyl] (E)-3-phenylprop-2-enoate	11978003	FALSE	C(=O)(/C=C/c1ccccc1)OC/C=C/c1cc(OC)c(O)cc1
MOL012189	0.6305	0.3695	0.7953	Benzoinum	Coniferyl diangelate	5316044	FALSE	C/C=C(\C(=O)Oc1ccc(cc1OC)/C=C/COC(=O)/C(=C\C)/C)/C
MOL012190	0.8293	0.1707	0.7821	Benzoinum	5,5'-Bivanillin	95086	FALSE	c1c(c(c(cc1C=O)c1cc(cc(c1O)OC)C=O)O)OC
MOL012191	0.7408	0.2592	0.8735	Benzoinum	3-(4-hydroxy-3-methoxyphenyl)-2-oxopropylbenzoate	Not Available	FALSE	c1(ccccc1)C(=O)OCC(=O)Cc1ccc(c(c1)OC)O
MOL012192	0.8855	0.1145	0.8797	Benzoinum	Labdanol	778574	FALSE	O(CC(C)C)C(=O)/C=C/c1ccccc1
MOL012194	0.9142	0.0858	0.9459	Benzoinum	PPY	997	FALSE	c1cccc(c1)CC(=O)C(=O)O

MOL012195	0.6908	0.3092	0.7626	Benzoinum	3-benzoylsiaresinolic acid	Not Available	FALSE	O(C(=O)c1ccccc1)C1CCC2(C(C1(C)C)CCC1(C2CC=C2C1(CCC1(C2C(C(CC1)(C)C)O)C(=O)O)C)C)C
MOL012196	0.6027	0.3973	0.7651	Benzoinum	3-phenylpropyl 3-phenylprop-2-enoate	5320530	FALSE	C(=O)(/C=C/c1ccccc1)OCCCc1ccccc1
MOL012197	0.9346	0.0654	0.9388	Benzoinum	(S)-1-Phenyl-2-propen-1-ol	10197720	FALSE	OC(c1ccccc1)C=C
MOL012198	0.7614	0.2386	0.8330	Benzoinum	siaresinolic acid	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1O)(C)C)C(=O)O)C)C)(C)C)O
MOL012200	0.4635	0.5365	0.7230	Benzoinum	Sumatrol	Not Available	FALSE	c1c(c2c(c3c1OC(C3)C(=C)C)OC1C(C2=O)c2c(OC1)cc(c(c2)OC)OC)O
MOL012201	0.5625	0.4375	0.7220	Benzoinum	trans-(tetrahydro-2-(4-hydroxy-3-methoxyphenyl)-5-oxofuran-3-yl)methylbenzoate	Not Available	FALSE	O(c1cc(ccc1O)C1C(CC(=O)O1)COC(=O)c1ccccc1)C
MOL012202	0.6998	0.3002	0.7452	Benzoinum	3-cinnamoyl sumaresinolic acid	Not Available	FALSE	O(C(=O)/C=C/c1ccccc1)C1CCC2(C(C1(C)C)C(CC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C)C(=O)O)C)C)O)C
MOL012203	0.7222	0.2778	0.7720	Benzoinum	3β,6β-dihydroxy-11-oxo-olean-12-en-28-oic acid	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(=CC1=O)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)C)(C)C)O
MOL012204	0.5514	0.4486	0.7560	Benzoinum	3β,6β-dihydroxy-11α,12α-epoxyolean-28,13β-olide	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C3(C4C1O4)C1C(CC2)(CCC(C1)(C)C)C(=O)C3)C)C)C)(C)C)O
MOL012205	0.8498	0.1502	0.7404	Lobeliae Chinensis Herba	ethyl rosmarinate	44437692	FALSE	c1(c(ccc(c1)/C=C/C(=O)OC(Cc1ccc(c(c1)O)O)C(=O)OCC)O)O
MOL012207	0.2223	0.7777	0.6638	Lobeliae Chinensis Herba	lobelanidine	Not Available	FALSE	OC(CC1N(C(CCC1)CC(O)c1ccccc1)C)c1ccccc1
MOL012208	0.2615	0.7385	0.9070	Lobeliae Chinensis Herba	Lobelanine	442647	FALSE	O=C(CC1N(C(CCC1)CC(=O)c1ccccc1)C)c1ccccc1

MOL012209	0.2400	0.7600	0.9470	Lobeliae Chinensis Herba	2-[(2R,6S)-6-[(2R)-2-hydroxy-2-phenylethyl]-1-methylpiperidin-2-yl]-1-phenylethanone	688025	FALSE	OC(CC1N(C(CCC1)CC(=O)c1ccccc1)C)c1ccccc1
MOL012210	0.7933	0.2067	0.6823	Lobeliae Chinensis Herba	lobetyolin	Not Available	FALSE	C/C=C/C#CC#CCC(/C=C/CCCO)OC1OC(C(C(C1O)O)O)CO
MOL012211	0.8205	0.1795	0.7340	Lobeliae Chinensis Herba	lobetyolin_qt	Not Available	FALSE	C/C=C/C#CC#CCC/C=C/CCCO
MOL012212	0.7321	0.2679	0.7935	Lobeliae Chinensis Herba	luteolin 3',4'-dimethylether-7-O-β-D-glucoside	Not Available	FALSE	c1c(cc2c(c1O)c(=O)cc(o2)c1ccc(c(c1)OC)OC)OC1OC(C(C(C1O)O)O)CO
MOL012213	0.8950	0.1050	0.9596	Lobeliae Chinensis Herba	Kampferol-3,4'-dimethyl ether	5351234	FALSE	c1c(cc2c(c1O)c(=O)cc(o2)c1ccc(c(c1)OC)OC)O
MOL012214	0.9362	0.0638	0.9149	Lobeliae Chinensis Herba	n-butyl-O-β-D-fructopyranoside	Not Available	FALSE	C1(C(OCC(C1O)O)(CO)OCCC)O
MOL012215	0.9170	0.0830	0.9638	Lobeliae Chinensis Herba	POL	1031	FALSE	OCCC
MOL012216	0.4044	0.5956	0.8065	Lobeliae Chinensis Herba	norlobelanine	36689182	FALSE	O=C(CC1NC(CCC1)CC(=O)c1ccccc1)c1ccccc1
MOL012218	0.9333	0.0667	0.8768	Lobeliae Chinensis Herba	rel-(2R,4R,6S)-N-methyl-4-hydroxyl-2-(2-butanone)-6-(2-hydroxybutyl)-piperidine	Not Available	FALSE	CCC(O)CC1N(C(CC(C1)O)CC(=O)CC)C
MOL012219	0.9322	0.0678	0.9170	Lobeliae Chinensis Herba	salicin	439503	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(cccc1)CO)CO
MOL012220	0.9031	0.0969	0.9635	Lobeliae Chinensis Herba	Saligenol	5146	FALSE	Oc1c(cccc1)CO
MOL012221	0.9347	0.0653	0.8386	Lobeliae Chinensis Herba	trans-10-ethyl-8-methyl-lobelidiol	Not Available	FALSE	CCC(CC1N(C(CCC1)CC(C)O)C)O
MOL012222	0.9370	0.0630	0.8579	Lobeliae Chinensis Herba	trans-8,10-diethyl lobelionol	Not Available	FALSE	CCC(=O)CC1N(C(CCC1)CC(C)O)C

MOL012223	0.9331	0.0669	0.8315	Lobeliae Chinensis Herba	trans-N-methyl-2,6-bis(2-hydroxybutyl)-△3-piperideine	Not Available	FALSE	CCC(O)CC1N(C(CCC1)CC(O)CC)C
MOL012224	0.1673	0.8327	0.6917	Lobeliae Chinensis Herba	(-)(2R,3S)-2,3-dihydro-2-(4-hydroxy-3-methoxy phenyl)-3-hydroxy-methyl-7-methoxy-5-benzofuran propanoic acid ethyl ester	Not Available	FALSE	CCCC(=O)CCc1cc(c2c(c1)C(C(O2)c1cc(c(cc1)O)OC)CO)OC
MOL012225	0.2638	0.7362	0.7031	Lobeliae Chinensis Herba	3-[(2S,3R)-2-(4-hydroxy-3-methoxy-phenyl)-3-(hydroxymethyl)-7-methoxy-2,3-dihydrobenzofuran-5-yl]propyl acetate	11281091	FALSE	CC(=O)OCCCc1cc(c2c(c1)C(C(O2)c1cc(c(cc1)O)OC)CO)OC
MOL012226	0.1673	0.8327	0.6917	Lobeliae Chinensis Herba	(+)(2R,3S)-2,3-dihydro-2-(4-hydroxy-3-methoxy phenyl)-3-hydroxy-methyl-7-methoxy-5-benzofuran propanoic acid ethyl ester	Not Available	FALSE	CCCC(=O)CCc1cc(c2c(c1)C(C(O2)c1cc(c(cc1)O)OC)CO)OC

MOL012227	0.2638	0.7362	0.7031	Lobeliae Chinensis Herba	(+)(2S,3R)-2,3-dihydro-2-(4-hydroxy-3-methoxy-phenyl)-3-hydroxy-methyl-7-methoxy-5-benzofuran propanoic acid ethyl ester	Not Available	FALSE	CC(=O)OCCCc1cc(c2c(c1)C(C(O2)c1cc(c(cc1)O)OC)CO)OC
MOL012228	0.9463	0.0537	0.8915	Lobeliae Chinensis Herba	(2R,4R,6R,2'S)-N-methyl-4-hydroxyl-2-(2-butanone)-6-(2-hydroxybutyl)-piperidine	Not Available	FALSE	CCC(O)CC1NC(CC(C1)O)CC(=O)CC
MOL012229	0.8400	0.1600	0.7305	Lobeliae Chinensis Herba	2,3,10-trihydroxy-4,9-dimethyl-dodee-6-enedioic acid diethyl ester	Not Available	FALSE	CCOC(=O)C(C(C(C)C/C=C/CC(C(CC(=O)OCC)O)C)O)O
MOL012231	0.9289	0.0711	0.7798	Lobeliae Chinensis Herba	Leptodactylone	442134	FALSE	o1c(=O)ccc2c(cc(c(c12)O)OC)OC
MOL012232	0.9399	0.0601	0.8121	Lobeliae Chinensis Herba	5-hydroxy-6,7-dimethoxycoumarin	14059525	FALSE	c1(c(cc2c(c1O)ccc(=O)o2)OC)OC
MOL012233	0.9520	0.0480	0.8382	Lobeliae Chinensis Herba	5-Hydroxy-7-methoxycoumarin	5748603	FALSE	o1c2c(c(O)cc(OC)c2)ccc1=O
MOL012234	0.9333	0.0667	0.8886	Lobeliae Chinensis Herba	cis-2-(2-butan-one)-6-(2-hydroxybutyl)-Piperidine	Not Available	FALSE	CCC(O)CC1NC(CCC1)CC(=O)CC

MOL012235	0.9034	0.0966	0.7360	Lobeliae Chinensis Herba	cis-N-methyl-2-(2-hydroxybutyl)-6-[2-[(1,3)-dioxolan-4-yl-methanol]-propyl]-piperidine	Not Available	FALSE	CC1(CC2N(C(CCC2)CC(CC)O)C)OC(CO1)CO
MOL012238	0.9311	0.0689	0.8486	Scutellariae Barbatae Herba	p-Hydroxycinnamic acid, ethyl ester	676946	FALSE	C(=O)(/C=C/c1ccc(cc1)O)OCC
MOL012239	0.9511	0.0489	0.9568	Scutellariae Barbatae Herba	()-p-Menth-1-ene	70954	FALSE	C1(=CCC(CC1)C(C)C)C
MOL012240	0.9035	0.0965	0.8742	Scutellariae Barbatae Herba	2',3',5,7-tetrahydroxyflavone	5321864	FALSE	c1(cc(=O)c2c(cc(cc2o1)O)O)c1c(c(ccc1)O)O
MOL012241	0.9595	0.0405	0.9468	Scutellariae Barbatae Herba	3-Methyl-6-(1-methylethyl)-cyclohexene	12504268	FALSE	C1=CC(CCC1C(C)C)C
MOL012242	0.7969	0.2031	0.8019	Scutellariae Barbatae Herba	5-hydroxy-2-(4-hydroxy-3,5-dimethoxy-phenyl)-6,7-dimethoxy-chromone	16681753	FALSE	c1(cc(=O)c2c(c(c(cc2o1)OC)OC)O)c1cc(c(c(c1)OC)O)OC
MOL012243	0.8555	0.1445	0.8684	Scutellariae Barbatae Herba	5,6,2'-trihydroxy-7,8-dimethoxyflavone	15100720	FALSE	c1(cc(=O)c2c(c(c(c(c2o1)OC)OC)O)O)c1c(cccc1)O
MOL012244	0.9413	0.0587	0.9134	Scutellariae Barbatae Herba	(6R,7aS)-3,6-dimethyl-5,6,7,7a-tetrahydro-4H-benzofuran-2-one	642876	FALSE	O1C(=O)C(=C2C1CC(CC2)C)C

MOL012245	0.8763	0.1237	0.9147	Scutellariae Barbatae Herba	5,7,4'-trihydroxy-6-methoxyflavanone	26213330	FALSE	C1(CC(=O)c2c(c(c(cc2O1)O)OC)O)c1ccc(cc1)O
MOL012246	0.8777	0.1223	0.8886	Scutellariae Barbatae Herba	5,7,4'-trihydroxy-8-methoxyflavanone	Not Available	FALSE	C1(CC(=O)c2c(cc(c(c2O1)OC)O)O)c1ccc(cc1)O
MOL012247	0.7009	0.2991	0.8988	Scutellariae Barbatae Herba	5,7-dihydroxy-8-methoxy-2-(2-methoxyphenyl)chromone	13889021	FALSE	c1(cc(=O)c2c(cc(c(c2o1)OC)O)O)c1c(cccc1)OC
MOL012248	0.8057	0.1943	0.9573	Scutellariae Barbatae Herba	5-hydroxy-7,8-dimethoxy-2-(4-methoxyphenyl)chromone	14353376	FALSE	c1(cc(=O)c2c(cc(c(c2o1)OC)OC)O)c1ccc(cc1)OC
MOL012249	0.6865	0.3135	0.8218	Scutellariae Barbatae Herba	7,2'-dihydroxy-5,8-dimethoxyflavone	Not Available	FALSE	c1(cc(=O)c2c(cc(c(c2o1)OC)O)OC)c1c(cccc1)O
MOL012250	0.6280	0.3720	0.9552	Scutellariae Barbatae Herba	7-hydroxy-5,8-dimethoxy-2-phenyl-chromone	14825644	FALSE	c1(cc(=O)c2c(cc(c(c2o1)OC)O)OC)c1ccccc1
MOL012251	0.8287	0.1713	0.9568	Scutellariae Barbatae Herba	Chrysin-5-methylether	5490127	FALSE	c1(cc(=O)c2c(cc(cc2o1)O)OC)c1ccccc1
MOL012252	0.3361	0.6639	0.7070	Scutellariae Barbatae Herba	9,19-cyclolanost-24-en-3-ol	Not Available	FALSE	C1(CCC23C(C1(C)C)CCC1C4(C)CCC(C(CCC=C(C)C)C)C4(C)CCC21C3)O
MOL012255	0.8035	0.1965	0.6474	Scutellariae Barbatae Herba	Caryophyllene oxide	Not Available	FALSE	O1C2(C1CCC(=C)C1C(C(C1)(C)C)CC2)C
MOL012258	0.9336	0.0664	0.8585	Scutellariae Barbatae Herba	p-Hydroxybenzalacetone	796857	FALSE	C(=C\C(=O)C)/c1ccc(cc1)O
MOL012262	0.8267	0.1733	0.7925	Scutellariae Barbatae Herba	ombuoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(OC)c2)c1cc(OC)c(O)cc1)COC1OC(C(O)C(O)C1O)C

MOL012263	0.9503	0.0497	0.8808	Scutellariae Barbatae Herba	p-Acetoxycinnamic acid	5373941	FALSE	C(=O)(/C=C/c1ccc(cc1)OC(=O)C)O
MOL012264	0.9419	0.0581	0.9471	Scutellariae Barbatae Herba	1-(4-hydroxyphenyl)acetone	7019274	FALSE	c1(ccc(cc1)O)CC(=O)C
MOL012266	0.8030	0.1970	0.7113	Scutellariae Barbatae Herba	rivularin	13889022	FALSE	c1(cc(=O)c2c(cc(c(c2o1)OC)OC)O)c1c(cccc1OC)O
MOL012267	0.8514	0.1486	0.8360	Scutellariae Barbatae Herba	Scutevulin	5321205	FALSE	c1(cc(=O)c2c(cc(c(c2o1)OC)O)O)c1c(cccc1)O
MOL012267	0.8514	0.1486	0.8360	Oroxyli Semen	Scutevulin	5321205	FALSE	c1(cc(=O)c2c(cc(c(c2o1)OC)O)O)c1c(cccc1)O
MOL012269	0.1892	0.8108	0.6375	Scutellariae Barbatae Herba	Stigmasta-5,22-dien-3-ol-acetate	Not Available	FALSE	C1(CCC2(C(=CCC3C4CCC(C(/C=C/C(CC)C(C)C)C)C4(C)CCC23)C1)C)OC(=O)C
MOL012272	0.3299	0.6701	0.7500	Cyathulae Radix	2,3-isopropylidene cyasterone	Not Available	FALSE	OC12C(C(CC2)C(O)(C(O)CC2C(C(=O)OC2C)C)C)(CCC2C3(C(CC4OC(OC4C3)(C)C)C(=O)C=C12)C)C
MOL012273	0.3299	0.6701	0.7500	Cyathulae Radix	2,3-isopropylidene isocyasterone	Not Available	FALSE	OC12C(C(CC2)C(O)(C(O)CC2C(C(=O)OC2C)C)C)(CCC2C3(C(CC4OC(OC4C3)(C)C)C(=O)C=C12)C)C
MOL012274	0.5972	0.4028	0.6688	Cyathulae Radix	24-hydroxycyasterone	Not Available	FALSE	OC12C(C(CC2)C(O)(C(O)CC2(C(C(=O)OC2C)C)O)C)(CCC2C3(C(CC(O)C(O)C3)C(=O)C=C12)C)C
MOL012275	0.7366	0.2634	0.8529	Cyathulae Radix	3-O-β-D-glucopyranosyl oleanolic acid	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(O)CCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)CO)C)C)OC1OC(C(C(C1O)O)OC1OC(C(C(C1O)O)O)CO)CO
MOL012276	0.7613	0.2387	0.8412	Cyathulae Radix	3-O-β-D-glucopyranosyl oleanolic acid_qt	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(O)CCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)CO)C)C)O
MOL012277	0.6409	0.3591	0.6997	Achyranthis Bidentatae Radix	3-O-(β-D-glucopyranosiduronic acid) oleanolic acid	14314623	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(OC6OC(C(C(C6O)O)O)C(=O)OC)CCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)C)C)C)O
MOL012277	0.6409	0.3591	0.6997	Cyathulae Radix	3-O-(β-D-glucopyranosiduronic acid) oleanolic acid	14314623	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(OC6OC(C(C(C6O)O)O)C(=O)OC)CCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)C)C)C)O

MOL012278	0.6842	0.3158	0.6969	Cyathulae Radix	3-O-[methyl-β-D-glucopyranosiduronate]-28-O-β-D-glucopyranosyl oleanolic acid	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(OC6OC(C(C(C6O)O)O)C(=O)OC)CCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)C)C)C)OC1C(O)C(O)C(O)C(O1)CO
MOL012279	0.7412	0.2588	0.8165	Cyathulae Radix	3-O-[α-L-rhamnopyranosyl-(1→3)-(n-butyl-β-D-glucopyranosiduronate}-28-O-β-D-glucopyranosyl oleanolic acid	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(OC6C(C(C(C(O6)C(=O)OCCCC)O)OC6OC(C)C(O)C(O)C6O)O)CCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)C)C)C)OC1C(O)C(O)C(O)C(O1)CO
MOL012280	0.6411	0.3589	0.8142	Cyathulae Radix	3-O-[α-L-rhamnopyranosyl-(1→3)β-D-glucopyranosiduronic acid] oleanolic acid	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(OC6C(C(C(C(O6)C(=O)OC)O)OC6OC(C)C(O)C(O)C6O)O)CCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)C)C)C)O
MOL012281	0.7454	0.2546	0.8375	Cyathulae Radix	3-O-[α-L-rhamnopyranosyl-(1→3)β-D-glucopyranosiduronic acid]-28-O-β-D-glucopyranosyl oleanolic acid	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(OC6C(C(C(C(O6)C(=O)O)O)OC6OC(C)C(O)C(O)C6O)O)CCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)C)C)C)OC1C(O)C(O)C(O)C(O1)CO
MOL012282	0.7331	0.2669	0.7154	Cyathulae Radix	3-O-[β-D-glucopyranosiduronic acid]-28-O-β-D-glucopyranosyl oleanolic acid	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(OC6OC(C(C(C6O)O)O)C(=O)O)CCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)C)C)C)OC1C(O)C(O)C(O)C(O1)CO

MOL012283	0.7607	0.2393	0.8121	Cyathulae Radix	3-O-[β-D-glucopyranosyl-(1→2)-α-L-rhamnopyranosyl-(1→3)β-D-glucopyranosiduronic acid]-28-O-β-D-glucopyranosyl oleanolic acid	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(OC6C(C(C(C(O6)C(=O)O)O)OC6OC(C)C(O)C(O)C6O)OC6C(O)C(O)C(O)C(O6)CO)CCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)C)C)C)OC1C(O)C(O)C(O)C(O1)CO
MOL012284	0.9502	0.0498	0.9705	Cyathulae Radix	4-((1-ethoxy-2-hydroxy)ethyl)phenol	Not Available	FALSE	c1(ccc(cc1)C(CO)OCC)O
MOL012285	0.4754	0.5246	0.6342	Cyathulae Radix	amararterone A	Not Available	FALSE	OC12C(C(CC2)C(O)(C(O)CC(C(C)CO)CC)C)(CCC2C3(C(CC(O)C(O)C3)C(=O)C=C12)C)C
MOL012286	0.7714	0.2286	0.7657	Cyathulae Radix	Betavulgarin	442668	FALSE	o1c2c(c(OC)c3OCOc3c2)c(=O)c(c2c(O)cccc2)c1
MOL012287	0.3899	0.6101	0.6874	Cyathulae Radix	capitasterone	Not Available	FALSE	OC12C(C(CC2)C(O)(C2OC(=O)C(C(C2)CC)C)C)(CCC2C3(C(CC(O)C(O)C3)C(=O)C=C12)C)C
MOL012288	0.5100	0.4900	0.6917	Ajugae Decumbentis Herba	Cyasteron	119444	FALSE	OC12C(C(CC2)C(O)(C(O)CC2C(C(=O)OC2C)C)C)(CCC2C3(C(CC(O)C(O)C3)C(=O)C=C12)C)C
MOL012288	0.5100	0.4900	0.6917	Cyathulae Radix	Cyasteron	119444	FALSE	OC12C(C(CC2)C(O)(C(O)CC2C(C(=O)OC2C)C)C)(CCC2C3(C(CC(O)C(O)C3)C(=O)C=C12)C)C
MOL012289	0.9241	0.0759	0.9607	Cyathulae Radix	Cycasin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1OC/N=[N+](/O)\C)CO
MOL012290	0.8866	0.1134	0.9444	Cyathulae Radix	Cycasin_qt	Not Available	FALSE	OC/N=[N+](/O)\C
MOL012291	0.5100	0.4900	0.6917	Cyathulae Radix	isocyasterone	Not Available	FALSE	OC12C(C(CC2)C(O)(C(O)CC2C(C(=O)OC2C)C)C)(CCC2C3(C(CC(O)C(O)C3)C(=O)C=C12)C)C
MOL012292	0.5211	0.4789	0.6260	Cyathulae Radix	makisterone B	Not Available	FALSE	OC12C(C(CC2)C(O)(C(O)CC(C(CO)C)C)C)(CCC2C3(C(CC(O)C(O)C3)C(=O)C=C12)C)C
MOL012293	0.9561	0.0439	0.8638	Cyathulae Radix	N-(3,4,5-trimethoxyphenyl)formamide	11052941	FALSE	C(=O)Nc1cc(c(c(c1)OC)OC)OC
MOL012294	0.9336	0.0664	0.8977	Cyathulae Radix	Phenylglucoside	65080	FALSE	c1(ccccc1)OC1OC(C(C(C1O)O)O)CO
MOL012295	0.7696	0.2304	0.9184	Cyathulae Radix	Poststerone	441835	FALSE	OC12C(C(CC2)C(=O)C)(CCC2C3(C(CC(O)C(O)C3)C(=O)C=C12)C)C
MOL012296	0.5273	0.4727	0.6808	Cyathulae Radix	precyasterone	Not Available	FALSE	OC12C(C(CC2)C(O)(C2OC(=O)C(C(C2)C(O)C)C)C)(CCC2C3(C(CC(O)C(O)C3)C(=O)C=C12)C)C
MOL012297	0.8133	0.1867	0.7847	Radix Bupleuri	puerarin	5281807	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2occ(c(=O)c2ccc1O)c1ccc(O)cc1

MOL012297	0.8133	0.1867	0.7847	Cyathulae Radix	puerarin	5281807	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2occ(c(=O)c2ccc1O)c1ccc(O)cc1
MOL012297	0.8133	0.1867	0.7847	Radix Puerariae	puerarin	5281807	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2occ(c(=O)c2ccc1O)c1ccc(O)cc1
MOL012297	0.8133	0.1867	0.7847	Hemerocallis Radix	puerarin	5281807	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c2occ(c(=O)c2ccc1O)c1ccc(O)cc1
MOL012298	0.8575	0.1425	0.9072	Cyathulae Radix	Rubrosterone	Not Available	FALSE	OC12C(CCC3C4(C(CC(O)C(O)C4)C(=O)C=C13)C)(C(=O)CC2)C
MOL012299	0.6008	0.3992	0.6802	Cyathulae Radix	Sengosterone	Not Available	FALSE	OC12C(C(CC2)C(O)(C(O)CC2C(C(=O)OC2C)C)C)(CCC2C3(C(O)(CC(O)C(O)C3)C(=O)C=C12)C)C
MOL012300	0.9069	0.0931	0.7258	Eucommiae Folium	(1R,3S,6R)-1,3,7,7-Tetramethyl-2-Oxabicyclo[4,4,0]dec-9-ene	Not Available	FALSE	C12(OC(CCC1C(CC=C2)(C)C)C)C
MOL012301	0.9364	0.0636	0.8850	Eucommiae Folium	(2R,3R,4S,5S,6R)-2-[[(1S,4aR,5S,7aS)-5-hydroxy-7-methylol-1,4a,5,7a-tetrahydrocyclopenta[c]pyran-1-yl]oxy]-6-methylol-tetrahydropyran-3,4,5-triol	11875891	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)C1C2C(C=CO1)C(C=C2CO)O
MOL012302	0.9426	0.0574	0.9267	Eucommiae Folium	2-bromoethylcyclohexane	15440	FALSE	C1(CCCCC1)CCBr
MOL012303	0.9114	0.0886	0.7183	Eucommiae Folium	(Z,E)-2-(2-Butenylidene)-1,3,3-trimethyl-7-Oxabicyclo[2,2,1]heptane	Not Available	FALSE	C12(/C(=C/C=C\C)/C(C(CC1)O2)(C)C)C
MOL012304	0.8944	0.1056	0.9517	Eucommiae Folium	cis-1,3-Dimethylcyclohexane	252361	FALSE	C1(CC(CCC1)C)C

MOL012305	0.9390	0.0610	0.9147	Eucommiae Cortex	1-Deoxyeucommiol	5316559	FALSE	C1(=C(C(CC1)CCO)CO)CO
MOL012305	0.9390	0.0610	0.9147	Eucommiae Folium	1-Deoxyeucommiol	5316559	FALSE	C1(=C(C(CC1)CCO)CO)CO
MOL012306	0.9168	0.0832	0.9385	Eucommiae Folium	2,3,4-Trimethylpentane	11269	FALSE	CC(C(C(C)C)C)C
MOL012307	0.9190	0.0810	0.9219	Eucommiae Folium	2,4-Dimethylhexane	56983219	FALSE	CC(CC(CC)C)C
MOL012308	0.9136	0.0864	0.7039	Eucommiae Folium	2-Cyclopropylidene-1,7,7-trimethylbicyclo[2,2,1]heptane	Not Available	FALSE	C12(C(=C3CC3)CC(CC1)C2(C)C)C
MOL012309	0.9260	0.0740	0.8413	Eucommiae Folium	(4aR)-1,1,4a-trimethyl-4,5,6,7-tetrahydro-3H-naphthalen-2-one	21717982	FALSE	C1(C(=O)CCC2(CCCC=C12)C)(C)C
MOL012310	0.9069	0.0931	0.7258	Eucommiae Folium	3,4,4a,5,6,8a-Hexahydro-2,5,5,8a-tetramethyl-(2a,4a,8a)-2H-1-Benzopyran	Not Available	FALSE	C1(CCC2C(O1)(C=CCC2(C)C)C)C
MOL012311	0.9087	0.0913	0.9292	Eucommiae Folium	2-Pentene, 3-ethyl-4,4-dimethyl-	5369078	FALSE	C/C=C(/C(C)(C)C)\CC
MOL012312	0.8792	0.1208	0.9421	Eucommiae Folium	3-Furylmethyl acetate	566611	FALSE	C(=O)(C)OCc1cocc1
MOL012313	0.9173	0.0827	0.9486	Eucommiae Folium	3-methylhex-2-ene	5352660	FALSE	C/C=C(/CCC)\C
MOL012314	0.8912	0.1088	0.8871	Eucommiae Folium	Dehydrodihydroionone	577126	FALSE	CC(=O)CCC1=C(C=CCC1(C)C)C

MOL012315	0.8993	0.1007	0.8927	Eucommiae Folium	6,7-DODECANEDIONE	26257	FALSE	CCCCCC(=O)C(=O)CCCCC
MOL012316	0.9075	0.0925	0.7741	Eucommiae Folium	ajugoside	Not Available	FALSE	O(C1(C2C(CC1)C=COC2OC1OC(O)(C(O)C(O)C1O)CO)C)C(=O)C
MOL012317	0.9609	0.0391	0.8480	Eucommiae Folium	ajugoside_qt	Not Available	FALSE	O(C1(C2C(CC1)C=COC2O)C)C(=O)C
MOL012318	0.9292	0.0708	0.9347	Eucommiae Folium	(2S,3R,4S,5S,6R)-2-ethoxy-6-(hydroxymethyl)tetrahydropyran-3,4,5-triol	9815668	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)CC
MOL012319	0.9444	0.0556	0.9545	Eucommiae Folium	guaiacyl glycerol	12310250	FALSE	c1c(c(cc(c1)C(C(CO)O)O)OC)O
MOL012320	0.9086	0.0914	0.8108	Eucommiae Folium	harpagide acetate	Not Available	FALSE	C(=O)(C)OC1(C2C(OC=CC2(C(C1)O)O)OC1C(O)C(O)C(O)C(O1)CO)C
MOL012321	0.9495	0.0505	0.8267	Eucommiae Folium	harpagide acetate_qt	Not Available	FALSE	C(=O)(C)OC1(C2COC=CC2(C(C1)O)O)C
MOL012322	0.5932	0.4068	0.6751	Eucommiae Folium	liriodendrin	Not Available	FALSE	O1C(C2C(C(OC2)c2cc(OC)c(OC3OC(C(O)C(O)C3O)CO)c(OC)c2)C1)c1cc(OC)c(OC2OC(C(O)C(O)C2O)CO)c(OC)c1
MOL012324	0.9418	0.0582	0.9706	Eucommiae Folium	trans-4-hydroxycyclohexanc-1-carboxylic acid	151138	FALSE	C1(CCC(CC1)O)C(=O)O
MOL012325	0.9154	0.0846	0.6875	Ginsen Radix Et Rhizoma Rubra	(butylsulfonyl)ethynylbenzene	Not Available	FALSE	c1(c(cccc1)S(=O)(=O)CCCC)C#C
MOL012326	0.8472	0.1528	0.6078	Ginsen Radix Et Rhizoma Rubra	1-ethenyl-1-methyl-2-(1-methylethenyl)-4-(isopropyl)-cyclohexane	Not Available	FALSE	C1(C(CC(CC1)C(C)C)C(=C)C)(C)C=C
MOL012327	0.1789	0.8211	0.6048	Ginsen Radix Et Rhizoma Rubra	Agidol 7	6928	FALSE	C(c1c(c(cc(c1)CC)C(C)(C)C)O)c1c(c(cc(c1)CC)C(C)(C)C)O
MOL012328	0.6798	0.3202	0.8580	Ginsen Radix Et Rhizoma Rubra	20(S)-ginsenoside Rg3	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C

MOL012329	0.2305	0.7695	0.7376	Ginsen Radix Et Rhizoma Rubra	20(S)-ginsenoside Rg3_qt	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(O)CC4)(C)C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL012330	0.7658	0.2342	0.8295	Ginsen Radix Et Rhizoma Rubra	ginsenoside R0	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)C(CC(C1)(C)C)C(=O)OC1OC(C(C(C1O)O)O)CO)C)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)O)O)O)C(=O)O
MOL012331	0.7188	0.2812	0.8295	Ginsen Radix Et Rhizoma Rubra	ginsenoside R0_qt	Not Available	FALSE	OC1CCC2(C(C1(C)C)CCC1(C2CC=C2C1(CCC1C2CC(CC1C(=O)O)(C)C)C)C)C
MOL012332	0.6562	0.3438	0.8505	Panacis Japonici Rhizoma	ginsenoside Rg2	Not Available	FALSE	O(C1C2C(C3C(C4(C(C(CC4)C(O)(CC/C=C(/CC)\C)C)C(O)C3)C)C1)(CCC(O)C2(C)C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)C)CO
MOL012332	0.6562	0.3438	0.8505	Ginsen Radix Et Rhizoma Rubra	ginsenoside Rg2	Not Available	FALSE	O(C1C2C(C3C(C4(C(C(CC4)C(O)(CC/C=C(/CC)\C)C)C(O)C3)C)C1)(CCC(O)C2(C)C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)C)CO
MOL012333	0.2415	0.7585	0.6898	Ginsen Radix Et Rhizoma Rubra	ginsenoside Rg2_qt	Not Available	FALSE	OC1C2C(C3C(C4(C(C(CC4)C(O)(CC/C=C(/CC)\C)C)C(O)C3)C)C1)(CCC(O)C2(C)C)C
MOL012333	0.2415	0.7585	0.6898	Panacis Japonici Rhizoma	ginsenoside Rg2_qt	Not Available	FALSE	OC1C2C(C3C(C4(C(C(CC4)C(O)(CC/C=C(/CC)\C)C)C(O)C3)C)C1)(CCC(O)C2(C)C)C
MOL012334	0.6798	0.3202	0.8580	Ginsen Radix Et Rhizoma Rubra	ginsenoside Rg3	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL012335	0.2305	0.7695	0.7376	Ginsen Radix Et Rhizoma Rubra	ginsenoside Rg3_qt	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL012336	0.3220	0.6780	0.7810	Ginsen Radix Et Rhizoma Rubra	ginsenoside Rh4	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(O2)CO)O)O)O)(C2(C(C(C1)O)C(CC2)/C(=C\CC=C(C)C)/C)C)C)C)O
MOL012336	0.3220	0.6780	0.7810	Ginseng Folium	ginsenoside Rh4	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(O2)CO)O)O)O)(C2(C(C(C1)O)C(CC2)/C(=C\CC=C(C)C)/C)C)C)C)O
MOL012337	0.2389	0.7611	0.7561	Ginseng Folium	ginsenoside Rh4_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)/C(=C\CC=C(C)C)/C)C)C)C)(C)C)O
MOL012337	0.2389	0.7611	0.7561	Ginsen Radix Et Rhizoma Rubra	ginsenoside Rh4_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)/C(=C\CC=C(C)C)/C)C)C)C)(C)C)O
MOL012338	0.6970	0.3030	0.8056	Ginsen Radix Et Rhizoma Rubra	ginsenoside Rs1	Not Available	FALSE	C1CC2(C(C(C1OC1C(C(C(C(O1)COC(=O)C)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)(C)C)CCC1(C2CC(C2C1(CCC2C(CCC=C(C)C)(C)OC1C(C(C(CO1)O)O)O)O)O)C)O)C)C
MOL012339	0.2622	0.7378	0.7312	Ginsen Radix Et Rhizoma Rubra	ginsenoside Rs1_qt	Not Available	FALSE	C1CC2(C(C(C1OC1C(C(C(C(O1)COC(=O)C)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)(C)C)CCC1(C2CC(C2C1(CCC2C(CCC=C(C)C)(O)C)C)O)C)C
MOL012340	0.8608	0.1392	0.6197	Ginsen Radix Et Rhizoma Rubra	globulol	Not Available	FALSE	OC1(C2C(C3C(C3CC1)(C)C)C(CC2)C)C
MOL012341	0.6662	0.3338	0.8108	Ginsen Radix Et Rhizoma Rubra	O-isoprenyl benzophenone	69247242	FALSE	C(=O)(c1c(cccc1)CC=C(C)C)c1ccccc1
MOL012342	0.9436	0.0564	0.9379	Ginsen Radix Et Rhizoma Rubra	p-tert-Butylanisole	94750	FALSE	COc1ccc(cc1)C(C)(C)C

MOL012343	0.7893	0.2107	0.7333	Ginsen Radix Et Rhizoma Rubra	(3R,9R,10R)-heptadec-1-en-4,6-diyne-3,9,10-triol	10540577	FALSE	OC(CCCCCCC)C(O)CC#CC#CC(O)C=C
MOL012344	0.8331	0.1669	0.6734	Ginsen Radix Et Rhizoma Rubra	(4aR,9aS)-2,9,9-trimethyl-5-methylene-4,4a,6,7,8,9a-hexahydro-3H-benzo[7]annulene	11830551	FALSE	C12C(CCCC(=C)C1CCC(=C2)C)(C)C
MOL012346	0.7408	0.2592	0.7565	Campsis Flos	(4aS,6aR,6aS,6bR,8aR,9R,10S,11R,12aR,14bS)-10,11-dihydroxy-2,2,6a,6b,9,12a-hexamethyl-9-methylol-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	11504083	FALSE	C1(O)C(CC2(C(C1(C)CO)CCC1(C)C3(C)CCC4(CCC(C)(C)CC4C3=CCC21)C(=O)O)C)O
MOL012347	0.9212	0.0788	0.9359	Campsis Flos	83861-75-0	6440743	FALSE	C(/C=C/C/C=C/CC)O
MOL012348	0.9221	0.0779	0.9371	Campsis Flos	3-Octenol, cis-	5364475	FALSE	C(C/C=C/CCCC)O
MOL012349	0.9534	0.0466	0.9682	Campsis Flos	Perillyl acetate	Not Available	FALSE	C(=O)(C)OCC1=CCC(C(=C)C)CC1
MOL012350	0.9616	0.0384	0.8504	Campsis Flos	Spiroxabovolide	Not Available	FALSE	O1C(=O)C(=C(C21OC(CCC2)C)C)C
MOL012351	0.9057	0.0943	0.9034	Campsis Flos	Undec-5-en-2-one	6365436	FALSE	CC(=O)CC/C=C/CCCCC
MOL012352	0.3675	0.6325	0.7362	Campsis Flos	ursolic aldehyde	Not Available	FALSE	C(=O)C12CCC3(C4(CCC5C(C(O)CCC5(C4CC=C3C2C(C(CC1)C)C)C)(C)C)C)C
MOL012353	0.8782	0.1218	0.9104	Campsis Flos	3-(2-furyl)-2-methyl-acrolein	6210220	FALSE	C(=O)/C(=C/c1occc1)/C

MOL012354	0.8986	0.1014	0.9731	Campsis Flos	(2S)-2-methyloxolan-3-one	7060523	FALSE	O1C(C(=O)CC1)C
MOL012355	0.9552	0.0448	0.9208	Campsis Flos	1-(2-furylmethyl)pyrrole-2-carbaldehyde	529880	FALSE	n1(c(ccc1)C=O)Cc1ccco1
MOL012356	0.9598	0.0402	0.9374	Campsis Flos	2-Phenylbutenal	6429333	FALSE	C(=O)/C(=C/C)/c1ccccc1
MOL012357	0.7408	0.2592	0.7565	Campsis Flos	2α,3α,24-trihydroxy olean-12 en-28 oic acid	51922488	FALSE	C1(C(CC2(C(C1(C)CO)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C)(C)CC4C3=CCC21)C)O)O
MOL012358	0.7472	0.2528	0.7763	Campsis Flos	2α,3α-dihydroxyurs-12-en-28-oic acid	Not Available	FALSE	C1(C(CC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C)C(C)C4C3=CCC21)C)O)O
MOL012359	0.9069	0.0931	0.9730	Campsis Flos	3-Cyclohexen-1-methanol	12299190	FALSE	C1(CC=CCC1)CO
MOL012360	0.7574	0.2426	0.9071	Campsis Flos	3-Epiursolic Acid	Not Available	FALSE	CC1CCC2(CCC3(C(=CCC4C3(CCC3C4(CCC(C3(C)C)O)C)C)C2C1C)C)C(=O)O
MOL012361	0.9258	0.0742	0.9638	Campsis Flos	2,3,5-Trimethylcyclopent-en-1-one	Not Available	FALSE	C1(=O)C(=C(CC1C)C)C
MOL012364	0.8624	0.1376	0.7025	Campsis Flos	Elemol	69648000	FALSE	C(C)(C)(C1CC(C(=C)C)C(C)(C=C)CC1)O
MOL012365	0.7652	0.2348	0.6065	Momordicae Semen	13Z-octadecenoic acid	5312441	FALSE	C(=O)(CCCCCCCCCCC/C=C\CCCC)O
MOL012367	0.8573	0.1427	0.6940	Momordicae Semen	11-hexadecenoic acid	5312413	FALSE	C(=O)(CCCCCCCCC/C=C/CCCC)O
MOL012368	0.5610	0.4390	0.6180	Momordicae Semen	Stearone	10440	FALSE	CCCCCCCCCCCCCCCCC(=O)CCCCCCCCCCCCCCCCC
MOL012369	0.9379	0.0621	0.9135	Momordicae Semen	2-ethyl-cyclopropane octanoic acid	Not Available	FALSE	C1(C(C1)CC)CCCCCCCC(=O)O
MOL012370	0.3849	0.6151	0.7430	Momordicae Semen	25-Nor-5(10)-dehydroisokarounidiol	489922	FALSE	C1C(C(c2c(C1)c1c(cc2)C2(C(CC1)(C1C(CC2)(CCC(C1)(C)CO)C)C)C)(C)C)O

MOL012371	0.3819	0.6181	0.8127	Momordicae Semen	7-Oxydihydrokarounidiol	122881	FALSE	O=C1C2=C(C3(C(C(C(O)CC3)(C)C)C1)C)CCC1(C3C(CCC21C)(CCC(C3)(CO)C)C)C
MOL012372	0.3821	0.6179	0.7822	Momordicae Semen	(3R,4aR,6aS,6bS,8aS,11R,12aR,14bS)-4,4,6a,6b,8a,11,14b-heptamethyl-11-methylol-1,2,3,4a,7,8,9,10,12,12a,13,14-dodecahydropicen-3-ol	10003399	FALSE	C1C(C(C2C(C1)(C1=C(C=C2)C2(C(CC1)(C1C(CC2)(CCC(C1)(C)CO)C)C)C)(C)C)O
MOL012374	0.6832	0.3168	0.8241	Momordicae Semen	momordic acid	Not Available	FALSE	C1(C(C2C(C(=O)C1)(C)C1C(CC2)(C2C(=CC1)C1C(CC2C)(CCC(C1)(C)C)C(=O)O)C)(C)C)O
MOL012377	0.2168	0.7832	0.6260	Momordicae Semen	bessisterol	Not Available	FALSE	OC1CC2C(C3C(=CC2)C2C(C(C(/C=C/C(C(C)C)CC)C)CC2)(CC3)C)(CC1)C
MOL012378	0.7672	0.2328	0.6482	Momordicae Semen	(9Z,11Z,13E)-octadeca-9,11,13-trienoic acid	5322021	FALSE	O=C(O)CCCCCCC/C=C\C=C/C=C/CCCC
MOL012379	0.9114	0.0886	0.6544	Aristolochiae Fructus	1,2,3,7-Tetramethylindole	599503	FALSE	n1(c(c(c2cccc(c12)C)C)C)C
MOL012380	0.8591	0.1409	0.7996	Aristolochiae Fructus	1,6,10-dodecatrien-4-ol,3,7,11-trimethyl-	Not Available	FALSE	C=CC(C(C/C=C(/CCC=C(C)C)\C)O)C
MOL012381	0.8344	0.1656	0.7505	Aristolochiae Fructus	5-tert-Butyl-3,3-dimethyl-1-indanone	608582	FALSE	C1(=O)CC(c2cc(ccc12)C(C)(C)C)(C)C
MOL012382	0.9478	0.0522	0.8515	Aristolochiae Fructus	3-methoxy-1H-quinazoline-2,4-dione	303855	FALSE	[nH]1c(=O)n(c(=O)c2ccccc12)OC
MOL012383	0.9044	0.0956	0.8200	Aristolochiae Fructus	2-oxo-calarene	Not Available	FALSE	C1(=O)CC(C2(C(=C1)C(CC1C2C1(C)C)OO)C)C

MOL012384	0.9189	0.0811	0.7917	Aristolochiae Fructus	3-(4-Methylpent-3-enyl)thiophene	566107	FALSE	c1c(ccs1)CCC=C(C)C
MOL012385	0.8140	0.1860	0.7632	Aristolochiae Fructus	3beta-Hydroxy-atractylon	Not Available	FALSE	C1C(C(=C)C2C(C1)(Cc1c(C2)c(co1)C)C)O
MOL012386	0.8762	0.1238	0.7376	Aristolochiae Fructus	aristolactam Ⅰa-N-β-D-glucopyanoside	Not Available	FALSE	O1c2c3c4c(cc5c3cccc5OO)n(c(=O)c4cc2OC1)C1OC(C(O)C(O)C1O)CO
MOL012387	0.9226	0.0774	0.6505	Aristolochiae Fructus	aristolactam Ⅰa-N-β-D-glucopyanoside_qt	Not Available	FALSE	O1c2c3c4c(cc5c3cccc5OO)[nH]c(=O)c4cc2OC1
MOL012388	0.8673	0.1327	0.6478	Aristolochiae Fructus	aristolactam-N-β-D-glucopyanoside	Not Available	FALSE	O1c2c3c4c(cc5c3cccc5OOC)n(c(=O)c4cc2OC1)C1OC(C(O)C(O)C1O)CO
MOL012389	0.8843	0.1157	0.7821	Aristolochiae Fructus	aristolactam-N-β-D-glucopyanoside_qt	Not Available	FALSE	O1c2c3c4c(cc5c3cccc5OOC)[nH]c(=O)c4cc2OC1
MOL012390	0.9185	0.0815	0.6510	Aristolochiae Fructus	aristolochic acid Ⅲ	3084007	FALSE	O1c2c3c(c(cc2OC1)C(=O)O)c([N+](=O)O)cc1c3cc(cc1)OC
MOL012391	0.9078	0.0922	0.6481	Aristolochiae Fructus	aristolochic acid Ⅲa	165274	FALSE	O1c2c3c(c(cc2OC1)C(=O)O)c([N+](=O)O)cc1c3cc(cc1)O
MOL012392	0.9167	0.0833	0.6518	Aristolochiae Fructus	aristolochic acid Ⅳ	167493	FALSE	O1c2c3c(c(cc2OC1)C(=O)O)c([N+](=O)O)cc1c3cc(cc1OC)OC
MOL012393	0.9138	0.0862	0.6537	Aristolochiae Fructus	aristolochic acid Ⅶ	5319403	FALSE	O1c2c3c(c([N+](=O)O)cc4c3ccc(c4OC)OC)c(cc2OC1)C(=O)O
MOL012394	0.8787	0.1213	0.6636	Aristolochiae Fructus	aristolochic acid Ⅶa	1941	FALSE	O1c2c3c(c([N+](=O)O)cc4c3ccc(c4OC)O)c(cc2OC1)C(=O)O
MOL012395	0.8914	0.1086	0.6627	Aristolochiae Fructus	aristolochic acid Ⅷa	147113	FALSE	O1c2c3c(c([N+](=O)O)cc4c3ccc(c4O)OC)c(cc2OC1)C(=O)O
MOL012396	0.8933	0.1067	0.6702	Aristolochiae Fructus	3,4-Methylenedioxy-10-hydroxy aristololactam	Not Available	FALSE	O1c2c3c4c(cc2OC1)c(=O)[nH]c4cc1c3cc(cc1)O

MOL012397	0.9248	0.0752	0.9617	Aristolochiae Fructus	4-aminobenzaldoxime	6436931	FALSE	C(=N\O)/c1ccc(cc1)N
MOL012398	0.9624	0.0376	0.8944	Aristolochiae Fructus	4-Ethyl-m-xylene	13403	FALSE	c1(c(cc(cc1)C)C)CC
MOL012399	0.9484	0.0516	0.8549	Aristolochiae Fructus	p-tert-Butylthiophenol	75454	FALSE	c1(ccc(cc1)C(C)(C)C)S
MOL012400	0.9613	0.0387	0.8133	Eriobotryae Folium	(S)-cis-Verbenol	87839	FALSE	C12C(C=C(C(C1(C)C)C2)C)O
MOL012400	0.9613	0.0387	0.8133	Peucedanidecursivi Radix	(S)-cis-Verbenol	87839	FALSE	C12C(C=C(C(C1(C)C)C2)C)O
MOL012400	0.9613	0.0387	0.8133	Aristolochiae Fructus	(S)-cis-Verbenol	87839	FALSE	C12C(C=C(C(C1(C)C)C2)C)O
MOL012400	0.9613	0.0387	0.8133	Caryophylliflos	(S)-cis-Verbenol	87839	FALSE	C12C(C=C(C(C1(C)C)C2)C)O
MOL012400	0.9613	0.0387	0.8133	Citri Sarcodactylis Fructus	(S)-cis-Verbenol	87839	FALSE	C12C(C=C(C(C1(C)C)C2)C)O
MOL012400	0.9613	0.0387	0.8133	Peucedani Radix	(S)-cis-Verbenol	87839	FALSE	C12C(C=C(C(C1(C)C)C2)C)O
MOL012401	0.9037	0.0963	0.7251	Aristolochiae Fructus	calarene	Not Available	FALSE	C1CC(C2(C(=C1)C(CC1C2C1(C)C)OO)C)C
MOL012403	0.9401	0.0599	0.7628	Aristolochiae Fructus	[(1S,2S,4S)-1,7,7-trimethylnorbornan-2-yl] propanoate	23617863	FALSE	C(=O)(CC)OC1CC2CCC1(C2(C)C)C
MOL012404	0.8856	0.1144	0.8074	Aristolochiae Fructus	oxidized aristolane A	Not Available	FALSE	C1CC(C2(C(=CC(=O)C3C2C3(C)C)C1O)C)C
MOL012405	0.8616	0.1384	0.7429	Aristolochiae Fructus	oxidized aristolane B	Not Available	FALSE	C1CC(C2(C(=C1)CCC1C2C1(C=O)C)C)C
MOL012406	0.9044	0.0956	0.8200	Aristolochiae Fructus	oxidized aristolane C	Not Available	FALSE	C1(=O)CC(C2(C(=C1)C(CC1C2C1(C)C)OO)C)C
MOL012407	0.9355	0.0645	0.9489	Aristolochiae Fructus	Pinitol	7020271	FALSE	O(C1C(O)C(O)C(O)C(O)C1O)C
MOL012408	0.9548	0.0452	0.9742	Aristolochiae Fructus	BETA,4-BIS(METHYLENE)CYCLOHEXANEETHANOL	34627	FALSE	C1C(CCC(=C)C1)C(=C)CO

MOL012409	0.8362	0.1638	0.7638	Rhododendri Daurici Folium	(2R-cis)-1,2,3,4,4a,5,6,7-Octahydro-alpha,alpha,4a,8-tetramethyl-2-naphthalenemethanol	6432005	FALSE	C1C(CCC2(CCCC(=C12)C)C)C(O)(C)C
MOL012410	0.8484	0.1516	0.6928	Rhododendri Daurici Folium	(1R,3E,7E,11R)-1,5,5,8-tetramethyl-12-oxabicyclo[9.1.0]dodeca-3,7-diene	10704181	FALSE	C12(C/C=C/C(C/C=C(/CCC1O2)\C)(C)C)C
MOL012411	0.9268	0.0732	0.7855	Rhododendri Daurici Folium	1,2,3,6-tetramethyldicyclo[2.2.2]oct-2-ene	Not Available	FALSE	C12(C(=C(C(CC1C)CC2)C)C)C
MOL012412	0.8642	0.1358	0.7426	Rhododendri Daurici Folium	1,5,5,8-tetramethyl-3,7-cycloundecadien-1-ol	Not Available	FALSE	C1(C/C=C/C(C/C=C(\CCC1)/C)(C)C)(O)C
MOL012413	0.9249	0.0751	0.6397	Rhododendri Daurici Folium	1,5-dimethyl-6-methylethenylspiro[2.4]heptane	Not Available	FALSE	C1(CC21CC(C(C2)C)C)(C)C=C
MOL012414	0.8671	0.1329	0.7847	Rhododendri Daurici Folium	10,10-Dimethyl-2,6-dimethylenebicyclo[7.2.0]undecan-5beta-ol	Not Available	FALSE	C12C(=C)CCC(C(=C)CCC1C(C2)(C)C)O
MOL012415	0.8684	0.1316	0.8662	Rhododendri Daurici Folium	1-cis,5-trans Germacrone	5317572	FALSE	C\1=C(\CC(=O)C(=C(C)C)C/C=C(/CC1)\C)/C
MOL012416	0.9537	0.0463	0.8406	Rhododendri Daurici Folium	2,3,4-Trimethoxyacetophenone	83810	FALSE	C(=O)(C)c1c(c(c(cc1)OC)OC)OC
MOL012417	0.8970	0.1030	0.9347	Rhododendri Daurici Folium	Picoline	7975	FALSE	c1(ccccn1)C

MOL012418	0.9532	0.0468	0.9673	Rhododendri Daurici Folium	Amyl cyclopentenone	117549	FALSE	C1(=O)C(=CCC1)CCCCC
MOL012419	0.5509	0.4491	0.6279	Rhododendri Daurici Folium	4a,8-dimethyl-2-(1-methylethenylethyl)-1,2,3,4,4a,5,6,8a-octahydronaphthalene	Not Available	FALSE	C1C(CCC2(CCC=C(C12)C)C)CCC(=C)C
MOL012420	0.3431	0.6569	0.6333	Rhododendri Daurici Folium	4a-methyl-1-methylethenyl-7-(1-methylethenylethyl)decahydronaphthalene	Not Available	FALSE	C1(CCCC2(CCC(CC12)CCC(=C)C)C)C(=C)C
MOL012421	0.9068	0.0932	0.8140	Rhododendri Daurici Folium	5-methyl kaempferol	Not Available	FALSE	c1(c(O)c(=O)c2c(cc(O)cc2o1)C)c1ccc(O)cc1
MOL012422	0.9324	0.0676	0.9380	Rhododendri Daurici Folium	2-Ethyl-5-methylpyridine	519519	FALSE	c1(ccc(cn1)C)CC
MOL012423	0.4772	0.5228	0.7511	Rhododendri Daurici Folium	5-methyl-2-isopropyl-9-methylethenyl dicyclo[4.4.0]dec-1-ene	Not Available	FALSE	C12=C(C(CC(C1CCC(C2)C)C)C=C)C(C)C
MOL012424	0.8385	0.1615	0.7785	Rhododendri Daurici Folium	6-Tetradecanone	81277	FALSE	CCCCCC(=O)CCCCCCCC
MOL012425	0.6452	0.3548	0.6271	Rhododendri Daurici Folium	7,11-dimethyl-3-methylethenyl-1,6,10-dodecatriene	Not Available	FALSE	C(=C\C(CC/C=C(/CCC=C(C)C)\C)C)/C=C

MOL012426	0.8661	0.1339	0.7121	Rhododendri Daurici Folium	7-methyl-4-methylethenyl-1,2,3,4,4a,5,6,8a-octahydronaphthalene	Not Available	FALSE	C1CCC(C2CCC(=CC12)C)C(=C)C
MOL012427	0.9165	0.0835	0.7769	Rhododendri Daurici Folium	8-demethyl farrerol	59072631	FALSE	c1(cc2c(c(c1C)O)C(=O)CC(O2)c1ccc(cc1)O)O
MOL012428	0.8336	0.1664	0.7829	Rhododendri Daurici Folium	Weedout	31677	FALSE	ClCC(=O)N(c1c(CC)cccc1CC)COCCCC
MOL012430	0.8704	0.1296	0.8267	Rhododendri Daurici Folium	eriodictin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(O)cc1)C
MOL012431	0.8400	0.1600	0.7606	Rhododendri Daurici Folium	(2E,4E,6E)-3,7,11-trimethyldodeca-2,4,6,10-tetraene	11637048	FALSE	C/C=C(\C)/C=C/C=C(\C)/CCC=C(C)C
MOL012432	0.8607	0.1393	0.7560	Rhododendri Daurici Folium	Farrerol	442396	FALSE	O1C(CC(=O)c2c1c(c(O)c(c2O)C)C)c1ccc(O)cc1
MOL012433	0.4923	0.5077	0.6526	Rhododendri Daurici Folium	Fastigilin B	442241	FALSE	C12C(C(C3C(C(C1C)O)OC(=O)C3C)OC(=O)C=C(C)C)(C(=O)C=C2)C
MOL012434	0.3972	0.6028	0.7164	Rhododendri Daurici Folium	Germanicol	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1=CC(CCC1(CC2)C)(C)C)C)C)C)(C)C)O
MOL012435	0.8876	0.1124	0.7728	Rhododendri Daurici Folium	Gossypetin-3-beta-D-(2-O-beta-D-glucopyranosidoglucopyranoside)-8-beta-D-glucopyranoside	Not Available	FALSE	c1(=O)c2c(oc(c1OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)c1ccc(c(c1)O)O)c(c(cc2O)O)OC1OC(C(C(C1O)O)O)CO
MOL012436	0.7017	0.2983	0.7446	Rhododendri Daurici Folium	Grayanotoxin I	Not Available	FALSE	O(C1C23C(C(O)(C4C(O)(C(O)C3)C(C(O)C4)(C)C)C)CCC1C(O)(C2)C)C(=O)C
MOL012437	0.7211	0.2789	0.7511	Rhododendri Daurici Folium	graynotoxin II	Not Available	FALSE	OC1C23C(CCC1C(O)(C2)C)C(=C)C1C(O)(C(O)C3)C(C(O)C1)(C)C
MOL012438	0.9144	0.0856	0.9213	Rhododendri Daurici Folium	Hexyl isovalerate	61455	FALSE	C(=O)(CC(C)C)OCCCCCC

MOL012439	0.8318	0.1682	0.7018	Rhododendri Daurici Folium	(1Z,4E,8E)-2,6,6,9-tetramethylcycloundeca-1,4,8-triene	5318101	FALSE	C\1=C/C/C(=C\CC/C(=C/CC1(C)C)/C)/C
MOL012440	0.9208	0.0792	0.8007	Rhododendri Daurici Folium	Isohyperoside acetate	5748375	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)OC1C(O)C(O)C(O1)C(O)CO)c1cc(c(cc1)O)O
MOL012441	0.8487	0.1513	0.7300	Rhododendri Daurici Folium	(1S,4aS,8aS)-7-isopropylidene-1,4a-dimethyl-1-decalinol	1715323	FALSE	C1C(=C(C)C)CC2C(C1)(CCCC2(C)O)C
MOL012442	0.2054	0.7946	0.6534	Rhododendri Daurici Folium	kaur-16-ene	Not Available	FALSE	C1CCC2(C(C1(C)C)CCC13C2CCC(C(=C)C1)C3)C
MOL012444	0.9165	0.0835	0.7769	Rhododendri Daurici Folium	poriol	Not Available	FALSE	O1C(CC(=O)c2c1cc(O)c(c2O)C)c1ccc(O)cc1
MOL012445	0.9462	0.0538	0.8833	Rhododendri Daurici Folium	4-[(3R)-3-hydroxybutyl] phenol	919205	FALSE	OC(CCc1ccc(O)cc1)C
MOL012446	0.6189	0.3811	0.7340	Rhododendri Daurici Folium	Rhodojaponin IV	Not Available	FALSE	C12C(C(CC34C(C1(C)O)CCC(C3OC(=O)C)C(C4)(C)O)OC(=O)C)(C(C(C2)O)(C)C)O
MOL012447	0.8651	0.1349	0.8602	Rhododendri Daurici Folium	santolina triene	12315283	FALSE	C(C=C(C)C)(C(=C)C)C=C
MOL012449	0.9029	0.0971	0.7816	Rhododendri Daurici Folium	β-lonene	53249763	FALSE	C1(CCc2c(C1)ccc(c2)C)(C)C
MOL012450	0.8264	0.1736	0.6799	Rhododendri Daurici Folium	γ-selinene	Not Available	FALSE	C1(=C)CCCC2(CCC(=C(C)C)CC12)C
MOL012451	0.4577	0.5423	0.6224	Achyranthis Bidentatae Radix	(20r,22r)-2beta,3beta,20,22,26-pentahydroxy-cholestan-7,12-dien-6-one	Not Available	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(=CC1)C(CC2)C(C(CCC(CO)C)O)(O)C)C)O)O
MOL012452	0.4577	0.5423	0.6224	Achyranthis Bidentatae Radix	(20R,22R)-2β,3β,20,22,26-pentahydroxy-cholestan-7,12-dien-6-one	Not Available	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(=CC1)C(CC2)C(C)(C(CCC(CO)C)O)O)C)C)O)O

MOL012453	0.7278	0.2722	0.8382	Achyranthis Bidentatae Radix	18-(β-D-Oxyglucose)-28-Oxo-12-oleanolic acid-3β-3-O-(β-D-glucose)-β-D-glucuronic acid methylester	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1OC(C(C(C1O)OC1OC(C(C(C1O)O)O)CO)O)C(=O)OC)C)C)C(=O)OC1OC(C(C(C1O)O)O)CO
MOL012454	0.7553	0.2447	0.9079	Achyranthis Bidentatae Radix	18-(β-D-Oxyglucose)-28-Oxo-12-oleanolic acid-3β-3-O-(β-D-glucose)-β-D-glucuronic acid methylester_qt	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)O)C)C)C)C(=O)O
MOL012455	0.9324	0.0676	0.9460	Achyranthis Bidentatae Radix	oct-1-en-2-ol	15372159	FALSE	C=C(CCCCCC)O
MOL012456	0.5740	0.4260	0.6635	Achyranthis Asperae Herba	Inokosterone	441828	FALSE	OC12C(C(CC2)C(O)(C(O)CCC(CO)C)C)(CCC2C3(C(CC(O)C(O)C3)C(=O)C=C12)C)C
MOL012456	0.5740	0.4260	0.6635	Mori Follum	Inokosterone	441828	FALSE	OC12C(C(CC2)C(O)(C(O)CCC(CO)C)C)(CCC2C3(C(CC(O)C(O)C3)C(=O)C=C12)C)C
MOL012456	0.5740	0.4260	0.6635	Achyranthis Bidentatae Radix	Inokosterone	441828	FALSE	OC12C(C(CC2)C(O)(C(O)CCC(CO)C)C)(CCC2C3(C(CC(O)C(O)C3)C(=O)C=C12)C)C
MOL012457	0.5436	0.4564	0.7869	Achyranthis Bidentatae Radix	28-deglucosyl achyranthoside D methyl ester	Not Available	FALSE	O(C1CCC2(C(C1(C)C)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C)C(=O)O)C)C)C)C1C(C(C(C(O1)C(=O)OC)O)OC(OCC(=O)OC)C(O)C(=O)OC)OC1C(O)C(O)C(O)C(O1)CO
MOL012458	0.5050	0.4950	0.7378	Achyranthis Bidentatae Radix	achyranthoside D trimethyl ester_qt	Not Available	FALSE	O(C1CCC2(C(C1(C)C)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C)C(=O)O)C)C)C)C1C(C(C(C(O1)C(=O)OC)O)OC(OCC(=O)OC)C(O)C(=O)OC)O
MOL012459	0.7181	0.2819	0.7212	Achyranthis Bidentatae Radix	28-deglucosyl-chikusetsusaponin iva	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)OC1C(C(C(C(O1)C(=O)O)O)O)O
MOL012460	0.7553	0.2447	0.9079	Achyranthis Bidentatae Radix	28-deglucosyl-chikusetsusaponin iva_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O
MOL012461	0.3707	0.6293	0.7225	Achyranthis Bidentatae Radix	28-norolean-17-en-3-ol	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(CC1)C1=C(CC2)CCC(C1)(C)C)C)C)(C)C)O

MOL012462	0.9070	0.0930	0.8762	Achyranthis Bidentatae Radix	2-Octenal, 2-butyl-	5362697	FALSE	C(=O)/C(=C\CCCCC)/CCCC
MOL012462	0.9070	0.0930	0.8762	Polygoni Orientalis Fructus	2-Octenal, 2-butyl-	5362697	FALSE	C(=O)/C(=C\CCCCC)/CCCC
MOL012463	0.4728	0.5272	0.6716	Achyranthis Bidentatae Radix	2β,3β,20α,22α,25-pentahydroxycholesta-8,14-dien-6-one	Not Available	FALSE	C1(C(CC2C(C1)(C1=C(CC2=O)C2=CCC(C2(CC1)C)C(C)(O)C(CCC(O)(C)C)O)C)O)O
MOL012464	0.7043	0.2957	0.7081	Achyranthis Bidentatae Radix	3-O-(β-D-glucose)-oleanolic acid-28-O-(β-D-glucose)	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(OC5OC(C(O)C(O)C5O)CO)(CC4)CCC(C3)(C)C)C)(CC2)C)(CC1)C)(C)C)C1OC(C(O)C(O)C1O)CO
MOL012465	0.3862	0.6138	0.7602	Achyranthis Bidentatae Radix	(3S,4aR,6aR,6bS,8aS,12aS,14aR,14bR)-4,4,6a,6b,11,11,14b-heptamethyl-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydropicene-3,8a-diol	21633445	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(O)(CC4)CCC(C3)(C)C)C)(CC2)C)(CC1)C)(C)C
MOL012466	0.7343	0.2657	0.7120	Achyranthis Bidentatae Radix	3-O-(β-D-glucuronic acid)-oleanolic acid-28-O-(β-D-glucose)	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(OC5OC(C(O)C(O)C5O)CO)(CC4)CCC(C3)(C)C)C)(CC2)C)(CC1)C)(C)C)C1OC(C(O)C(O)C1O)C(=O)O
MOL012468	0.6692	0.3308	0.6792	Achyranthis Bidentatae Radix	3-O-β-D-glucuronopyranoside-6-O-butyl ester	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(OC6C(C(C(C(O6)C(=O)OCCCC)O)O)O)CCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)C)C)O
MOL012469	0.6409	0.3591	0.6997	Achyranthis Bidentatae Radix	3-O-β-D-glucuronopyranoside-6-O-methyl ester	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(OC6C(C(C(C(O6)C(=O)OC)O)O)O)CCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)C)C)O
MOL012470	0.8912	0.1088	0.8747	Achyranthis Bidentatae Radix	6-Dodecanone	80165	FALSE	CCCCCC(=O)CCCCCC

MOL012471	0.7490	0.2510	0.8333	Achyranthis Bidentatae Radix	achybidensaponin,i	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C=C1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1C(C(C(C(O1)CO)O)O)O)C)C)(C)C)OC1C(C(C(OC2C(C(C(C(O2)C)O)O)O)O)(C(O1)C(=O)O)O)O)O
MOL012472	0.7475	0.2525	0.6936	Achyranthis Bidentatae Radix	achybidensaponin,i_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C=C1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)OC1C(C(C(O)(C(O1)C(=O)O)O)O)O
MOL012473	0.7367	0.2633	0.7117	Achyranthis Bidentatae Radix	achybidensaponin,ii	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C=C1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1C(C(C(C(O1)C(=O)O)O)O)O)C)C)(C)C)OC1C(C(C(C(O1)C(=O)O)O)O)O
MOL012474	0.7550	0.2450	0.8954	Achyranthis Bidentatae Radix	achybidensaponin,ii_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C=C1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O
MOL012475	0.6479	0.3521	0.6935	Achyranthis Bidentatae Radix	achyranthesterone A	Not Available	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C(CC2)C(C(CCC(O)(C)C)O)(O)CO)C)O)C)O)O
MOL012476	0.7098	0.2902	0.8308	Achyranthis Bidentatae Radix	achyranthoside Ⅱ	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1C(C(C(C(O1)COC1OC(C(C(C1O)O)O)CO)OC(COCC(=O)O)C(O)C(=O)O)O)O)C)C)C(=O)O
MOL012477	0.6747	0.3253	0.8058	Achyranthis Bidentatae Radix	achyranthoside Ⅱ_qt	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1C(C(C(C(O1)CO)OC(COCC(=O)O)C(O)C(=O)O)O)O)C)C)C(=O)O
MOL012478	0.6934	0.3066	0.8235	Achyranthis Bidentatae Radix	achyranthoside Ⅲ	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1C(C2C(C(O1)C(=O)O)OC(C(O2)OCC(=O)O)(O)C(=O)O)O)C)C)C)C(=O)OC1OC(C(C(C1O)O)O)CO
MOL012479	0.6572	0.3428	0.8067	Achyranthis Bidentatae Radix	achyranthoside Ⅳ	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1C(C2C(C(O1)C(=O)O)OC(C(O2)OCC(=O)O)(O)C(=O)O)O)C)C)C(=O)O
MOL012480	0.6934	0.3066	0.8235	Achyranthis Bidentatae Radix	achyranthoside A	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1OC(C2C(C1O)OC(C(O2)(C(=O)O)O)OCC(=O)O)C(=O)O)C)C)C(=O)OC1OC(C(C(C1O)O)O)CO
MOL012481	0.6572	0.3428	0.8067	Achyranthis Bidentatae Radix	achyranthoside A_qt	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1OC(C2C(C1O)OC(C(O2)(C(=O)O)O)OCC(=O)O)C(=O)O)C)C)C(=O)O
MOL012482	0.5499	0.4501	0.6690	Achyranthis Bidentatae Radix	achyranthoside A trimethyl ester	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1OC(C2C(C1O)OC(C(O2)(C(=O)OC)O)OCC(=O)OC)C(=O)OC)C)C)C(=O)OC1OC(C(C(C1O)O)O)CO
MOL012483	0.5317	0.4683	0.6688	Achyranthis Bidentatae Radix	achyranthoside A trimethyl ester_qt	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1OC(C2C(C1O)OC(C(O2)(C(=O)OC)O)OCC(=O)OC)C(=O)OC)C)C)C(=O)O
MOL012484	0.7142	0.2858	0.8342	Achyranthis Bidentatae Radix	achyranthoside c	Not Available	FALSE	C1(C(O)C(O)C(O)C(O1)CO)OC(=O)C12CCC3(C4(CCC5C(C(OC6C(C(C(C(O6)C(=O)O)O)O)OC(OCC(=O)O)C(O)C(=O)O)O)CCC5(C4CC=C3C1CC(CC2)(C)C)C)(C)C)C

MOL012485	0.6670	0.3330	0.8206	Achyranthis Bidentatae Radix	achyranthoside c_qt	Not Available	FALSE	O(C1CCC2(C(C1(C)C)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C)C(=O)O)C)C)C)C1C(C(C(C(O1)C(=O)O)O)OC(OCC(=O)O)C(O)C(=O)O)O
MOL012486	0.5674	0.4326	0.7520	Achyranthis Bidentatae Radix	achyranthoside C butyl dimethyl ester	Not Available	FALSE	C1(C(O)C(O)C(O)C(O1)CO)OC(=O)C12CCC3(C4(CCC5C(C(OC6C(C(C(C(O6)C(=O)OCCCC)O)OC(OCC(=O)OC)C(O)C(=O)OC)O)CCC5(C4CC=C3C1CC(CC2)(C)C)C)(C)C)C)C
MOL012487	0.5254	0.4746	0.7118	Achyranthis Bidentatae Radix	achyranthoside C butyl dimethyl ester_qt	Not Available	FALSE	O(C1CCC2(C(C1(C)C)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C)C(=O)O)C)C)C)C1C(C(C(C(O1)C(=O)OCCCC)O)OC(OCC(=O)OC)C(O)C(=O)OC)O
MOL012488	0.6184	0.3816	0.7993	Achyranthis Bidentatae Radix	achyranthoside C dimethyl ester	Not Available	FALSE	C1(C(O)C(O)C(O)C(O1)CO)OC(=O)C12CCC3(C4(CCC5C(C(OC6C(C(C(C(O6)C(=O)O)O)OC(OCC(=O)OC)C(O)C(=O)OC)O)CCC5(C4CC=C3C1CC(CC2)(C)C)C)(C)C)C)C
MOL012489	0.5451	0.4549	0.7809	Achyranthis Bidentatae Radix	achyranthoside C dimethyl ester_qt	Not Available	FALSE	O(C1CCC2(C(C1(C)C)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C)C(=O)O)C)C)C)C1C(C(C(C(O1)C(=O)O)O)OC(OCC(=O)OC)C(O)C(=O)OC)O
MOL012490	0.5915	0.4085	0.7604	Achyranthis Bidentatae Radix	achyranthoside C trimethyl ester	Not Available	FALSE	C1(C(O)C(O)C(O)C(O1)CO)OC(=O)C12CCC3(C4(CCC5C(C(OC6C(C(C(C(O6)C(=O)OC)O)OC(OCC(=O)OC)C(O)C(=O)OC)O)CCC5(C4CC=C3C1CC(CC2)(C)C)C)(C)C)C)C
MOL012491	0.7306	0.2694	0.8025	Achyranthis Bidentatae Radix	achyranthoside D	Not Available	FALSE	C1(C(O)C(O)C(O)C(O1)CO)OC(=O)C12CCC3(C4(CCC5C(C(OC6C(C(C(C(O6)C(=O)O)O)OC(OCC(=O)O)C(O)C(=O)O)OC6C(O)C(O)C(O)C(O6)CO)CCC5(C4CC=C3C1CC(CC2)(C)C)C)(C)C)C)C
MOL012492	0.6091	0.3909	0.7605	Achyranthis Bidentatae Radix	achyranthoside D trimethyl ester	Not Available	FALSE	C1(C(O)C(O)C(O)C(O1)CO)OC(=O)C12CCC3(C4(CCC5C(C(OC6C(C(C(C(O6)C(=O)OC)O)OC(OCC(=O)OC)C(O)C(=O)OC)OC6C(O)C(O)C(O)C(O6)CO)CCC5(C4CC=C3C1CC(CC2)(C)C)C)(C)C)C)C
MOL012493	0.7041	0.2959	0.8380	Achyranthis Bidentatae Radix	achyranthoside E	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1OC(C(C(C1O)OC(OCC(=O)O)C(=O)O)O)C(=O)O)C)C)C(=O)OC1OC(C(C(C1O)O)O)CO
MOL012494	0.6340	0.3660	0.8069	Achyranthis Bidentatae Radix	achyranthoside E_qt	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1OC(C(C(C1O)OC(OCC(=O)O)C(=O)O)O)C(=O)O)C)C)C(=O)O
MOL012495	0.4232	0.5768	0.6929	Achyranthis Bidentatae Radix	achyranthoside E butyl dimethyl ester	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1OC(C(C(C1O)OC(OCC(=O)OC)C(=O)OC)O)C(=O)OCCCCC)C)C)C(=O)OC1OC(C(C(C1O)O)O)CO
MOL012496	0.5250	0.4750	0.6508	Achyranthis Bidentatae Radix	achyranthoside E butyl dimethyl ester_qt	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1OC(C(C(C1O)OC(OCC(=O)OC)C(=O)OC)O)C(=O)OCCCCC)C)C)C(=O)O

MOL012497	0.5849	0.4151	0.8040	Achyranthis Bidentatae Radix	achyranthoside E dimethyl ester	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1OC(C(C(C1O)OC(OCC(=O)OC)C(=O)OC)O)C(=O)O)C)C)C(=O)OC1OC(C(C(C1O)O)O)CO
MOL012498	0.5202	0.4798	0.7639	Achyranthis Bidentatae Radix	achyranthoside E dimethyl ester_qt	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1OC(C(C(C1O)OC(OCC(=O)OC)C(=O)OC)O)C(=O)O)C)C)C(=O)O
MOL012499	0.4518	0.5482	0.7298	Achyranthis Bidentatae Radix	achyranthoside E trimethyl ester	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1OC(C(C(C1O)OC(OCC(=O)OC)C(=O)OC)O)C(=O)OC)C)C)C(=O)OC1OC(C(C(C1O)O)O)CO
MOL012500	0.5147	0.4853	0.6938	Achyranthis Bidentatae Radix	achyranthoside E trimethyl ester_qt	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1OC(C(C(C1O)OC(OCC(=O)OC)C(=O)OC)O)C(=O)OC)C)C)C(=O)O
MOL012501	0.7332	0.2668	0.7926	Achyranthis Bidentatae Radix	achyranthoside I	Not Available	FALSE	C1C2C(CCC1(C)C)(CCC1(C2=CCC2C1(CCC1C2(CCC(C1(C)C)OC1C(C(C(O1)COC1OC(C(C(C1O)O)O)CO)OC(COCC(=O)O)C(O)C(=O)O)O)O)C)C)C(=O)OC1OC(C(C(C1O)O)O)CO
MOL012502	0.7116	0.2884	0.8347	Achyranthis Bidentatae Radix	bidentatoside, i	Not Available	FALSE	O1C(C(C(C(C1CO)O)O)O)OC(=O)C12CCC(CC1C1=CCC3C(C1(CC2)C)(CCC1C3(CCC(C1(C)C)OC1OC(C(C2OC(C(OC12)OCC(=O)O)(O)C(=O)O)O)O)C(=O)O)C)(C)C
MOL012503	0.6786	0.3214	0.8143	Achyranthis Bidentatae Radix	bidentatoside, i_qt	Not Available	FALSE	OC(=O)C12CCC(CC1C1=CCC3C(C1(CC2)C)(CCC1C3(CCC(C1(C)C)OC1OC(C(C2OC(C(OC12)OCC(=O)O)(O)C(=O)O)O)C(=O)O)C)(C)C
MOL012504	0.4077	0.5923	0.6843	Achyranthis Bidentatae Radix	bidentatoside, ii	Not Available	FALSE	C(=O)COC(C=O)OC1CCC2(C(C1(C)C)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C)C(=O)OC1C(O)C(O)C(O)C(O1)CO)C)C)C
MOL012505	0.6008	0.3992	0.7695	Achyranthis Bidentatae Radix	bidentatoside, ii_qt	Not Available	FALSE	C(=O)COC(C=O)OC1CCC2(C(C1(C)C)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C)C(=O)O)C)C)C
MOL012506	0.7375	0.2625	0.8410	Panacis Japonici Rhizoma	chikusetsusaponin Ⅳ	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C)C1OC(C(OC2OC(C(O)C2O)CO)C(O)C1O)C(=O)O
MOL012506	0.7375	0.2625	0.8410	Achyranthis Bidentatae Radix	chikusetsusaponin Ⅳ	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C)C1OC(C(OC2OC(C(O)C2O)CO)C(O)C1O)C(=O)O
MOL012507	0.6562	0.3438	0.8505	Achyranthis Bidentatae Radix	chikusetsusaponin I	Not Available	FALSE	O(C1C2C(C3C(C4(C(C(CC4)C(O)(CC/C=C(/CC)\C)C)C(O)C3)C)C1)(CCC(O)C2(C)C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)C)CO
MOL012508	0.6699	0.3301	0.6830	Achyranthis Bidentatae Radix	chikusetsusaponin IVA butyl ester	44566502	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C)C1OC(C(O)C(O)C(O)C1O)C(=O)OCCCC
MOL012509	0.6842	0.3158	0.6969	Achyranthis Bidentatae Radix	Chikusetsusaponin IVa methyl ester	637855	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C)C1OC(C(O)C(O)C1O)C(=O)OC

MOL012510	0.7518	0.2482	0.8286	Achyranthis Bidentatae Radix	Chikusetsusaponin V butyl ester	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)CO)C(=O)OCCCC
MOL012511	0.7408	0.2592	0.8379	Achyranthis Bidentatae Radix	Chikusetsusaponin V methyl ester	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)CO)C(=O)OC
MOL012512	0.7181	0.2819	0.7212	Achyranthis Bidentatae Radix	deglucose chikusetsusaponin Iva	Not Available	FALSE	O(C1CCC2(C(C1(C)C)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C)C(=O)O)C)C)C)C1C(C(C(C(O1)C(=O)O)O)O)O
MOL012513	0.7553	0.2447	0.9079	Achyranthis Bidentatae Radix	deglucose chikusetsusaponin Iva_qt	Not Available	FALSE	OC1CCC2(C(C1(C)C)CCC1(C2CC=C2C1(CCC1(C2CC(CC1)(C)C)C(=O)O)C)C)C
MOL012514	0.7038	0.2962	0.8024	Achyranthis Bidentatae Radix	Ecdysterone-3-O-beta-D-glucopyranoside	Not Available	FALSE	OC12C(C(CC2)C(O)C(O)CCC(O)(C)C)(CCC2C3(C(CC(OC4OC(C(O)C(O)C4O)CO)C(O)C3)C(=O)C=C12)C)C
MOL012515	0.6426	0.3574	0.7202	Achyranthis Bidentatae Radix	Ecdysterone-3-O-beta-D-glucopyranoside_qt	Not Available	FALSE	OC12C(C(CC2)C(O)C(O)CCC(O)(C)C)(CCC2C3(C(CC(O)C(O)C3)C(=O)C=C12)C)C
MOL012516	0.9323	0.0677	0.8667	Achyranthis Bidentatae Radix	geniposide	29927668	FALSE	C1(=COC(OC2C(C(C(C(O2)CO)O)O)O)C2C1CC=C2CO)C(=O)CO
MOL012517	0.5447	0.4553	0.7251	Achyranthis Bidentatae Radix	hederagenin-28-O-β-D-glucopyranosyl ester	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(CO)C
MOL012518	0.7613	0.2387	0.8412	Achyranthis Bidentatae Radix	hederagenin-28-O-β-D-glucopyranosyl ester_qt	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(CO)C
MOL012519	0.7181	0.2819	0.7212	Achyranthis Bidentatae Radix	Monoglucuronide F	176079	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(C)C)C1OC(C(O)C(O)C1O)C(=O)O
MOL012520	0.3134	0.6866	0.7500	Achyranthis Bidentatae Radix	niuxixinsterone A	Not Available	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C(CC2)C1(C(CC(C(O)C)C)OC(O1)c1oc(cc1)CO)C)C)O)C)O)O
MOL012521	0.2572	0.7428	0.7500	Achyranthis Bidentatae Radix	niuxixinsterone B	Not Available	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(=CC1)C(CC2)C1(C(CCC(C)(O)C)OC(O1)c1oc(cc1)CO)C)C)O)C)O
MOL012522	0.3367	0.6633	0.7383	Achyranthis Bidentatae Radix	niuxixinsterone C	Not Available	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C(CC2)C1(C(CCC(CO)C)OC(O1)c1oc(cc1)CO)C)C)O)C)O)C)O)O

MOL012523	0.6037	0.3963	0.6248	Achyranthis Bidentatae Radix	N-trans-feruloyl-3-methoxytyramine-4'-O-β-D-glucopyranoside	Not Available	FALSE	c1cc(cc(c1O)OC)/C=C/C(=O)NCCc1cc(c(cc1)OC1OC(C(O)C(O)C1O)CO)OC
MOL012524	0.8074	0.1926	0.7746	Achyranthis Bidentatae Radix	Hmp-hmpep	5352115	FALSE	c1cc(cc(c1O)OC)/C=C/C(=O)NCCc1cc(c(cc1)O)OC
MOL012526	0.6699	0.3301	0.6830	Achyranthis Bidentatae Radix	oleanolic acid 3-O-[β-D-glucuronopyranoside-6-O-butyl ester]-28-O-β-D-glucopyranoside	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C)C1OC(C(O)C(O)C1O)C(=O)OCCCC
MOL012527	0.6754	0.3246	0.6941	Achyranthis Bidentatae Radix	oleanolic acid 3-O-[β-D-glucuronopyranoside-6-O-ethyl ester]-28-O-β-D-glucopyranoside	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C)C1OC(C(O)C(O)C1O)C(=O)OCC
MOL012528	0.6842	0.3158	0.6969	Achyranthis Bidentatae Radix	oleanolic acid 3-O-[β-D-glucuronopyranoside-6-O-methyl ester]-28-O-β-D-glucopyranoside	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC3OC(C(O)C(O)C3O)CO)C)(CC2)C)(CC1)C)(C)C)C1OC(C(O)C(O)C1O)C(=O)OC
MOL012529	0.6692	0.3308	0.6792	Achyranthis Bidentatae Radix	oleanolic acid-3-O-β-D-(6'-butyl)-glucuronopyranoside	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(OC6C(C(C(C(=O)OCCCC)O6)O)O)O)CCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)C)C)C)O
MOL012530	0.7181	0.2819	0.7212	Achyranthis Bidentatae Radix	oleanolic acid-3-O-β-D-glucuronopyranoside	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(OC6C(C(C(C(O6)C(=O)O)O)O)O)O)CCC5(C4CC=C3C2CC(CC1)(C)C)C)(C)C)C)C)O

MOL012531	0.4426	0.5574	0.7474	Achyranthis Bidentatae Radix	pjs-1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1C(C(C(C(O1)CO)O)O)O)C)C)(C)C)O
MOL012532	0.6455	0.3545	0.6990	Achyranthis Bidentatae Radix	Polypodine B	441833	FALSE	OC12C(C(CC2)C(O)(C(O)CCC(O)(C)C)C)(CCC2C3(C(O)(CC(O)C(O)C3)C(=O)C=C12)C)C
MOL012533	0.8865	0.1135	0.8282	Achyranthis Bidentatae Radix	quercetin-3-O-rutinoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1OC(C(O)C(O)C1O)COC1OC(C(O)C(O)C1O)C)c1cc(O)c(O)cc1
MOL012534	0.5469	0.4531	0.6933	Achyranthis Bidentatae Radix	rhapontisterone B	Not Available	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C(CC2)C(C(CCC(O)(C)C)O)(C)O)C)O)C)O)O
MOL012535	0.8575	0.1425	0.9072	Achyranthis Bidentatae Radix	rubrosterone	Not Available	FALSE	OC12C(CCC3C4(C(CC(O)C(O)C4)C(=O)C=C13)C)(C(=O)CC2)C
MOL012536	0.2957	0.7043	0.6490	Achyranthis Bidentatae Radix	Rubschisantherin	Not Available	FALSE	O(C1C(C(Cc2c(c3c1cc(OC)c(OC)c3OC)c(OC)c1OCOc1c2)C)C)C(=O)C
MOL012537	0.2853	0.7147	0.8101	Achyranthis Bidentatae Radix	Spinoside A	5281325	FALSE	O(C1C(C2(C(C3C(CC2)(C2C(=CC3)C(C(=O)C(=C2)O)(C)C)C)(C1)C)C)C(O)(C)C(=O)/C=C/C(O)(C)C)C1OCC(OC(=O)C)C(O)C1OC(=O)C
MOL012539	0.3960	0.6040	0.7070	Achyranthis Bidentatae Radix	stachysterone D	Not Available	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C(CC2)C(C1CCC(O1)(C)C)(C)O)C)O)C)O)O
MOL012540	0.7273	0.2727	0.8492	Achyranthis Bidentatae Radix	zingiberoside r1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)OC1C(C(C(C(O1)C(=O)O)O)O)OC1C(C(C(C(O1)CO)O)O)O)O
MOL012541	0.7553	0.2447	0.9079	Achyranthis Bidentatae Radix	zingiberoside r1_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)C)O
MOL012542	0.5469	0.4531	0.6933	Achyranthis Bidentatae Radix	β-ecdysterone	27545171	FALSE	C1(C(CC2C(C1)(C1C(=CC2=O)C2(C(CC1)(C(CC2)C(C)(C(CCC(C)(O)C)O)O)C)O)C)O)O
MOL012543	0.8676	0.1324	0.8430	Eriobotryae Folium	(2R)-8-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-6-methylol-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-tetrahydropyran-2-yl]-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	10507459	FALSE	c1c(c2c(c(c1O)C1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO)OC(CC2=O)c1ccc(cc1)O)O

MOL012544	0.8613	0.1387	0.8486	Eriobotryae Folium	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)-8-[(2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]chroman-4-one	23514988	FALSE	OC1C(c2c3c(c(cc2O)O)C(=O)CC(O3)c2ccc(cc2)O)OC(C(C1O)O)CO
MOL012545	0.8676	0.1324	0.8430	Eriobotryae Folium	(2S)-8-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-6-methylol-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl-tetrahydropyran-2-yl]oxy-tetrahydropyran-2-yl]-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	10603320	FALSE	c1c(c2c(c(c1O)C1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO)OC(CC2=O)c1ccc(cc1)O)O
MOL012546	0.8613	0.1387	0.8486	Eriobotryae Folium	(2S)-naringenin 8-C-α-L-rhamnopyranosyl-(1→2)-β-D-glucopyranoside_qt	42607891	FALSE	OC1C(c2c3c(c(cc2O)O)C(=O)CC(O3)c2ccc(cc2)O)OC(C(C1O)O)CO

MOL012547	0.8217	0.1783	0.7075	Eriobotryae Folium	(6S,9R)-Vomifoliol-9-O-β-apiofuranosyl-(1'→6')O-β-gluopyranoside	Not Available	FALSE	C1(=O)C=C(C(C(C1)(C)C)(/C=C/C(C)OC1OC(C(O)C(O)C1O)COC1OCC(O)(C1O)CO)O)C
MOL012548	0.8828	0.1172	0.7871	Eriobotryae Folium	(4R)-4-hydroxy-4-[(E,3R)-3-hydroxybut-1-enyl]-3,5,5-trimethylcyclohex-2-en-1-one	11229837	FALSE	C1(=O)C=C(C(C(C1)(C)C)(/C=C/C(C)O)O)C
MOL012549	0.8113	0.1887	0.7053	Eriobotryae Folium	(6S,9R)-Vomifoliol-9-O-β-xylopyranosyl-(1'→6')O-β-gluopyranoside	Not Available	FALSE	C1(=O)C=C(C(C(C1)(C)C)(/C=C/C(C)OC1OC(C(O)C(O)C1O)COC1C(O)C(O)C(O)CO1)O)C
MOL012550	0.9231	0.0769	0.8103	Eriobotryae Folium	(E)-2-Hexenyl-gamma-L-arabinopyranosyl-(1-2)-beta-D-glucopyranoside	Not Available	FALSE	C(=C\CCC)/COC1OCC(C(C1OC1OC(C(C(C1O)O)O)CO)O)O
MOL012551	0.9719	0.0281	0.9588	Eriobotryae Folium	1,4-Dimethoxy-2,3-dimethylbenzene	148299	FALSE	c1(c(ccc(c1C)OC)OC)C
MOL012552	0.7290	0.2710	0.7293	Eriobotryae Folium	1β-hydroxyeuscaphic acid	Not Available	FALSE	C1(C(C(C2C(C1O)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1(C)O)C)C(=O)O)C)C)(C)C)O)O
MOL012553	0.9058	0.0942	0.8997	Eriobotryae Folium	2,2,3,3-TETRAMETHYLHEXANE	26057	FALSE	CC(C(CCC)(C)C)(C)C

MOL012554	0.8519	0.1481	0.6449	Eriobotryae Folium	2,3,5,8-tetramethyldecane	Not Available	FALSE	CC(C(CC(CCC(CC)C)C)C)C
MOL012555	0.6851	0.3149	0.6954	Eriobotryae Folium	23-cis-p-coumaryhormentic acid	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1(C)O)C)C(=O)O)C)C)(COC(=O)/C=C\c1ccc(cc1)O)C)O)O
MOL012556	0.6851	0.3149	0.6954	Eriobotryae Folium	23-trans-p-coumaryhormentic acid	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1(C)O)C)C(=O)O)C)C)(COC(=O)/C=C/c1ccc(cc1)O)C)O)O
MOL012557	0.7007	0.2993	0.7598	Eriobotryae Folium	2α,19α-dihydroxy-3-oxo-urs-12-en-28-oic acid	Not Available	FALSE	C1(=O)C(CC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C)C(C)(C4C3=CCC21)O)C)O
MOL012558	0.7218	0.2782	0.7370	Eriobotryae Folium	2α,3α,19α,23-tetrahydroxy-olean-12-en-28-oic acid	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(O)C(CC5(C4CC=C3C2C(C(CC1)(C)C)O)C)O)(CO)C)C)C)O
MOL012559	0.7405	0.2595	0.7570	Eriobotryae Folium	2α,3α,19α-trihydroxy-olean-12-en-28-oic acid	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(O)C(CC5(C4CC=C3C2C(C(CC1)(C)C)O)C)O)(C)C)C)C)O
MOL012560	0.7472	0.2528	0.7763	Eriobotryae Folium	2α,3α-dihydroxyursolic acid	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1C)C)C(=O)O)C)C)(C)C)O)O
MOL012561	0.7430	0.2570	0.7461	Eriobotryae Folium	2α,3β,13β-trihydroxyurs-11-en-28-oic acid	Not Available	FALSE	C1(C(CC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)O)CCC(C)C(C)(C4C3(C=CC21)O)O)C)O)O
MOL012562	0.2747	0.7253	0.7749	Eriobotryae Folium	2α,3β-dihydroxy-lup-20(29)-en-28-oic acid methyl ester	14059617	FALSE	C1(C(CC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)OC)CCC(C(=C)C)C4C3CCC21)C)O)O
MOL012563	0.9049	0.0951	0.8009	Perillae Fructus	3,6-dimethyldecane	Not Available	FALSE	CCC(CCC(CCCC)C)C
MOL012563	0.9049	0.0951	0.8009	Eriobotryae Folium	3,6-dimethyldecane	Not Available	FALSE	CCC(CCC(CCCC)C)C
MOL012564	0.9055	0.0945	0.8579	Eriobotryae Folium	3,7-dimethylnonane	Not Available	FALSE	CCC(CCCC(CC)C)C

MOL012565	0.6963	0.3037	0.7383	Eriobotryae Folium	3-0-trans-cafeoyhormentic acid	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1(C)O)C)C(=O)O)C)C)(C)C)OC(=O)/C=C/c1ccc(c(c1)O)O)O
MOL012566	0.6818	0.3182	0.6685	Eriobotryae Folium	3-0-trans-p-coumarylrotundic acid	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1(C)O)C)C(=O)O)C)C)(CO)C)OC(=O)/C=C/c1ccc(cc1)O
MOL012567	0.9227	0.0773	0.8903	Eriobotryae Folium	3-Ethyloctane	79985	FALSE	CCC(CCCCC)CC
MOL012568	0.7019	0.2981	0.6350	Eriobotryae Folium	3-oxo-α–ionyl-9-o-β-D-apiofuranosyl(1→6)-β-D-glucopyransidse	Not Available	FALSE	C1(=O)C=C(C(C(C1)(C)C)CCC(C)OC1OC(C(O)C(O)C1O)COC1OCC(OC)(O)C1O)C
MOL012569	0.9053	0.0947	0.7874	Eriobotryae Folium	(4R)-4-[(3R)-3-hydroxybutyl]-3,5,5-trimethylcyclohex-2-en-1-one	14135400	FALSE	C1(=O)C=C(C(C(C1)(C)C)CCC(C)O)C
MOL012570	0.6492	0.3508	0.6824	Eriobotryae Folium	3α-trans-Feruloyloxy-2α-hydroxyurs-12-en-28-oic	Not Available	FALSE	C1(C2C(CCC1C)(CCC1(C2CCC2C1(CCC1C2(CC(C(C1(C)C)OC(=O)/C=C/c1ccc(c(c1)OC)O)O)C)C)C)C(=O)O)C
MOL012571	0.7531	0.2469	0.7823	Eriobotryae Folium	(1R,2R,4aS,6aR,6aS,6bR,8S,8aR,10S,12aR,14bS)-1,8,10-trihydroxy-1,2,6a,6b,9,9,12a-heptamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid	21672636	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(=CC1)C1C(CC2)(CCC(C1(C)O)C)C(=O)O)C)C)(C)C)O

MOL012572	0.7531	0.2469	0.7823	Eriobotryae Folium	3β,6β,19α-trihydroxyurs-12-en-29-oic acid	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(=CC1)C1C(CC2)(CCC(C1(C)O)C)C(=O)O)C)C)(C)C)O
MOL012573	0.8785	0.1215	0.7055	Eriobotryae Folium	4,6-dimethylundecane	Not Available	FALSE	CCCC(CC(CCCCC)C)C
MOL012574	0.9242	0.0758	0.9522	Eriobotryae Folium	6E-octenoic acid	5282721	FALSE	C(=O)(CCCC/C=C/C)O
MOL012575	0.8933	0.1067	0.7144	Eriobotryae Folium	5,6-dimethylundecane	Not Available	FALSE	CCCCC(C(CCCCC)C)C
MOL012576	0.7531	0.2469	0.7823	Eriobotryae Folium	6α,19α-dihydroxyursolic acid	Not Available	FALSE	C1(CCC2(C(C1(C)C)C(CC1(C2CC=C2C1(CCC1(C2C(C(CC1)C)(O)C)C(=O)O)C)C)O)C)O
MOL012577	0.6820	0.3180	0.8339	Eriobotryae Folium	(2R,3R,10S)-2,10-bis(3,4-dihydroxyphenyl)-3,5-dihydroxy-3,4,9,10-tetrahydro-2H-pyrano[6,5-h]chromen-8-one	10456516	FALSE	c1c(c2c(c3c1OC(=O)CC3c1ccc(c(c1)O)O)OC(C(C2)O)c1cc(c(cc1)O)O)O
MOL012578	0.6820	0.3180	0.8339	Eriobotryae Folium	Cinchonain 1a	442675	FALSE	c1c(c2c(c3c1OC(=O)CC3c1ccc(c(c1)O)O)OC(C(C2)O)c1cc(c(cc1)O)O)O
MOL012579	0.6989	0.3011	0.8301	Eriobotryae Folium	(4R,8R,9R)-4,8-bis(3,4-dihydroxyphenyl)-5,9-dihydroxy-4,8,9,10-tetrahydro-3H-pyrano[6,5-h]chromen-2-one	21676383	FALSE	c12c(c3c(cc1O)OC(C(C3)O)c1cc(c(cc1)O)O)OC(=O)CC2c1cc(c(cc1)O)O
MOL012580	0.7851	0.2149	0.7660	Eriobotryae Folium	Cinchonain Id 7-O-β-Glucopyranoside	Not Available	FALSE	c12c(c3c(cc1OC1C(C(C(C(O1)CO)O)O)O)OC(C(C3)O)c1cc(c(cc1)O)O)OC(=O)CC2c1ccc(c(c1)O)O

MOL012581	0.6989	0.3011	0.8301	Eriobotryae Folium	(4S,8R,9R)-4,8-bis(3,4-dihydroxyphenyl)-5,9-dihydroxy-4,8,9,10-tetrahydro-3H-pyrano[6,5-h]chromen-2-one	21676382	FALSE	c12c(c3c(cc1O)OC(C(C3)O)c1cc(c(cc1)O)O)OC(=O)CC2c1ccc(c(c1)O)O
MOL012582	0.8265	0.1735	0.6775	Eriobotryae Folium	delta-Cadinol	Not Available	FALSE	C1C(=CC2C(C1)C(CCC2C(C)C)(C)O)C
MOL012583	0.7774	0.2226	0.8232	Eriobotryae Folium	(2R,3R,4S)-2-(3,4-dihydroxyphenyl)-4-(2,4,6-trihydroxyphenyl)chroman-3,5,7-triol	14009028	FALSE	c1c(c2c(cc1O)OC(C(C2c1c(cc(cc1O)O)O)O)c1cc(c(cc1)O)O)O
MOL012584	0.8124	0.1876	0.8094	Eriobotryae Folium	Eriobofuran	178939	FALSE	o1c2c(c3c1cccc3)cc(OC)c(O)c2OC
MOL012585	0.7542	0.2458	0.6926	Eriobotryae Folium	eriojaposides A	Not Available	FALSE	C1(=O)C=C(C(C(C1)(C)C)/C=C/C(C)OC1OC(C(O)C(O)C1O)COC1C(O)C(O)C(O)CO1)C
MOL012586	0.6923	0.3077	0.6583	Eriobotryae Folium	eriojaposides B	Not Available	FALSE	C1(=O)C=C(C(C(C1)(C)C)/C=C/C(C)OC1OC(C(O)C(O)C1O)COC1C(O)C(O)C(O)C(O1)C)C
MOL012587	0.8219	0.1781	0.7508	Eriobotryae Folium	CHEBI:42362	444108	FALSE	C/C=C(\C)/CC/C=C(\C)/CCC=C(C)C
MOL012589	0.6845	0.3155	0.7103	Eriobotryae Folium	Farnesyl acetate	1551481	FALSE	CC(=CCC/C(=C\CC/C(=C/COC(=O)C)/C)/C)C
MOL012590	0.9371	0.0629	0.9521	Eriobotryae Folium	Neric acid	5275520	FALSE	C(=O)(/C=C(\C)/CCC=C(C)C)O
MOL012590	0.9371	0.0629	0.9521	Litseae Fructus	Neric acid	5275520	FALSE	C(=O)(/C=C(\C)/CCC=C(C)C)O
MOL012591	0.9406	0.0594	0.8635	Eriobotryae Folium	meliotine	660	FALSE	O1C(=O)CCc2ccccc12
MOL012592	0.9133	0.0867	0.9254	Eriobotryae Folium	BIHEPTADIENECARBOXYLIC ACID	6433689	FALSE	C(C)/C=C/C=C/C(=O)O

MOL012593	0.5429	0.4571	0.6942	Eriobotryae Folium	isohumbertiol-3-o-{α-L-rhamnopyranosyl(1→4)-α-L-rhamnopyranosyl(1→2)-[α-L-rhamnopyranosyl(1→6)]}-β-D-glucopyranoside	Not Available	FALSE	O(C1C(C(C(C(O1)CO)O)O)OC1OC(C(OC2OC(C(O)C(O)C2O)C)C(O)C1O)C)OC(C=C)(C)CC1C=C(CCC1=C(C)C)C
MOL012594	0.9183	0.0817	0.8593	Eriobotryae Folium	isohumbertiol-3-o-{α-L-rhamnopyranosyl(1→4)-α-L-rhamnopyranosyl(1→2)-[α-L-rhamnopyranosyl(1→6)]}-β-D-glucopyranoside_qt	Not Available	FALSE	OOC(C=C)(C)CC1C=C(CCC1=C(C)C)C
MOL012595	0.8977	0.1023	0.8170	Eriobotryae Folium	isorhamnetin-3-O-glucoside	Not Available	FALSE	c1(c(oc2c(c1=O)c(cc(c2)O)O)c1cc(c(cc1)O)OC)OC1C(C(C(C(O1)CO)O)O)O
MOL012596	0.3207	0.6793	0.6085	Eriobotryae Folium	kaempferol 3-O-α-L-(2″,4″-di-Z-p-coumaroyl)-rhamnoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(C(C(C(O1)C)OC(=O)/C=C\c1ccc(cc1)O)O)OC(=O)/C=C\c1ccc(cc1)O)c1ccc(O)cc1
MOL012597	0.8679	0.1321	0.8424	Eriobotryae Folium	kaempferol-3-O-neohesperidoside	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)C)CO)c1ccc(cc1)O)O)O
MOL012598	0.3229	0.6771	0.7521	Eriobotryae Folium	kaempferol-3-O-α-L-(2″,4″-di-E-feruloyl)-rhamnoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(C(C(C(O1)C)OC(=O)/C=C/c1cc(c(cc1)O)OC)O)OC(=O)/C=C/c1cc(c(cc1)O)OC)c1ccc(O)cc1

MOL012599	0.3207	0.6793	0.6085	Eriobotryae Folium	kaempferol-3-O-α-L-(2″,4″-di-E-p-coumaroyl)-rhamnoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(C(C(C(O1)C)OC(=O)/C=C/c1ccc(cc1)O)O)OC(=O)/C=C/c1ccc(cc1)O)c1ccc(O)cc1
MOL012600	0.8735	0.1265	0.8633	Eriobotryae Folium	Kaemp-7-neohesperidoside	5483905	FALSE	O(C1C(O)C(O)C(OC1Oc1cc2oc(c(O)c(=O)c2c(O)c1)c1ccc(O)cc1)CO)C1OC(C(O)C(O)C1O)C
MOL012601	0.3229	0.6771	0.7521	Eriobotryae Folium	kaempherol-3-O-α-L-(2',4'-di-E-feruloyl)-rhamnoside	Not Available	FALSE	c1c(c2c(cc1O)oc(c(c2=O)OC1C(C(C(C(O1)C)OC(=O)/C=C/c1cc(c(cc1)O)OC)O)OC(=O)/C=C/c1cc(c(cc1)O)OC)c1ccc(cc1)O)O
MOL012602	0.3207	0.6793	0.6085	Eriobotryae Folium	kaempherol-3-O-α-L-(2',4'-di-E-p-coumaroyl)-rhamnoside	Not Available	FALSE	c1c(c2c(cc1O)oc(c(c2=O)OC1C(C(C(C(O1)C)OC(=O)/C=C/c1ccc(cc1)O)O)OC(=O)/C=C/c1ccc(cc1)O)c1ccc(cc1)O)O
MOL012603	0.3207	0.6793	0.6085	Eriobotryae Folium	kaempherol-3-O-α-L-(2',4'-di-Z-p-coumaroyl)-rhamnoside	49822436	FALSE	c1c(c2c(cc1O)oc(c(c2=O)OC1C(C(C(C(O1)C)OC(=O)/C=C\c1ccc(cc1)O)O)OC(=O)/C=C\c1ccc(cc1)O)c1ccc(cc1)O)O
MOL012604	0.4725	0.5275	0.6566	Eriobotryae Folium	loquatifolin A	Not Available	FALSE	C(CC=C(C)C)/C(=C\CCC(OC1C(C(C(C(O1)COC1OC(C(O)C(O)C1O)C)O)O)OC1OC(C(O)C(O)C1O)C)(C)C=C)/C
MOL012605	0.3061	0.6939	0.7473	Eriobotryae Folium	methyl corosolate	Not Available	FALSE	C1(C(CC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C(=O)OC)CCC(C)C(C)C4C3=CCC21C)O)O
MOL012606	0.3107	0.6893	0.7655	Eriobotryae Folium	methyl maslinate	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)OC)C)(CC2)C)(CC1O)C)(C)C
MOL012608	0.4864	0.5136	0.6651	Eriobotryae Folium	nerolido-3-O-α-L-rhamnopyranosyl(1→4)-α-L-rhamnopyranosyl(1→2)-β-D-glucopyranoside	Not Available	FALSE	C(CC=C(C)C)/C(=C\CCC(OC1C(C(C(C(O1)COC1OC(C(OC2OC(C(O)C(O)C2O)C)C(O)C1O)C)O)O)O)(C)C=C)/C
MOL012609	0.8642	0.1358	0.7920	Zanthoxyli Pericarpium	cis-nerolidol	12227246	FALSE	C(CC=C(C)C)/C(=C\CCC(O)(C)C=C)/C
MOL012609	0.8642	0.1358	0.7920	Eriobotryae Folium	cis-nerolidol	12227246	FALSE	C(CC=C(C)C)/C(=C\CCC(O)(C)C=C)/C

MOL012610	0.4672	0.5328	0.6577	Eriobotryae Folium	nerolido-3-O-α-L-rhamnopyranosyl(1→6)-α-L-rhamnopyranosyl(1→2)-β-D-glucopyranoside	Not Available	FALSE	C(CC=C(C)C)/C(=C\CCC(OC1C(C(C(C(O1)CO)O)O)OC1OC(C(OC2OC(C(O)C(O)C2O)C)C(O)C1O)C)(C)C=C)/C
MOL012611	0.4855	0.5145	0.7084	Eriobotryae Folium	nerolido-3-α-L-rhamnopyranosyl(1→4)-α-L-rhamnopyranosyl(1→2)-[α-L-rhamnopyranosyl(1→6)]-β-D-glucopyranoside	Not Available	FALSE	C(CC=C(C)C)/C(=C\CCC(OC1C(C(C(C(O1)COC1OC(C(O)C(O)C1O)C)O)O)OC1OC(C(OC2OC(C(O)C(O)C2O)C)C(O)C1O)C)(C)C=C)/C
MOL012613	0.9583	0.0417	0.8247	Eriobotryae Folium	pinocarvone	12314319	FALSE	O=C1CC2C(C(C2)C1=C)(C)C
MOL012614	0.8801	0.1199	0.7898	Eriobotryae Folium	Quercetin 3-sambubioside	5487635	FALSE	O(C1C(O)C(O)C(OC1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1)CO)C1OCC(O)C(O)C1O
MOL012615	0.9196	0.0804	0.8020	Eriobotryae Folium	quercetin-4'-O-β-D-galactoside	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)O)c1ccc(c(c1)O)OC1C(C(C(C(O1)CO)O)O)O)O)O
MOL012616	0.8949	0.1051	0.7916	Eriobotryae Folium	7-((6-Deoxy-alpha-L-mannopyranosyl)oxy)-2-(3,4-dihydroxyphenyl)-3,5-dihydroxy-4H-benzopyran-4-one	5748601	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2oc(c(O)c(=O)c2c(O)c1)c1cc(O)c(O)cc1)C
MOL012617	0.4988	0.5012	0.6355	Eriobotryae Folium	Torulene	Not Available	FALSE	C1CCC(=C(C1(C)C)/C=C\C(=C\C=C\C(=C\C=C\C=C(\C=C\C=C(\C=C\C=C(\C=C\C=C(C)C)/C)/C)/C)\C)\C

MOL012618	0.9339	0.0661	0.8034	Eriobotryae Folium	(E)-linalool oxide acetate pyr	6427501	FALSE	O1C(C(OC(=O)C)CCC1(C)C=C)(C)C
MOL012618	0.9339	0.0661	0.8034	Zanthoxyli Pericarpium	(E)-linalool oxide acetate pyr	6427501	FALSE	O1C(C(OC(=O)C)CCC1(C)C=C)(C)C
MOL012619	0.3953	0.6047	0.7329	Eriobotryae Folium	uvaol	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(CO)CCC(C)C(C)C4C3=CCC21)C)O
MOL012620	0.7605	0.2395	0.6611	Eriobotryae Folium	vomifoliol-9-o-β-D-apiofuranosyl(1→6)-β-D-glucopyransside	Not Available	FALSE	C1(=O)C=C(C(C(C1)(C)C)(CCC(C)OC1OC(C(O)C(O)C1O)COC1OCC(OC)(O)C1O)O)C
MOL012621	0.8858	0.1142	0.7938	Eriobotryae Folium	(4S)-4-hydroxy-4-[(3R)-3-hydroxybutyl]-3,5,5-trimethylcyclohex-2-en-1-one	14135402	FALSE	C1(=O)C=C(C(C(C1)(C)C)(CCC(C)O)O)C
MOL012622	0.8905	0.1095	0.8395	Eriobotryae Folium	515-69-5	1201551	FALSE	OC(C1CCC(=CC1)C)(CCC=C(C)C)C
MOL012623	0.9214	0.0786	0.9739	Eriobotryae Folium	(5R)-5-ethyloxolan-2-one	7173971	FALSE	O1C(CCC1=O)CC
MOL012624	0.6699	0.3301	0.7637	Ginseng Folium	DIMETHYL ANTHRAQUINONE	317828	FALSE	c1(c(ccc2C(=O)c3ccccc3C(=O)c12)C)C
MOL012625	0.8781	0.1219	0.7942	Ginseng Folium	WLN: R2R	7647	FALSE	C(Cc1ccccc1)c1ccccc1
MOL012627	0.9276	0.0724	0.9028	Ginseng Folium	Phenyl isobutyrate	519756	FALSE	C(=O)(C(C)C)Oc1ccccc1
MOL012628	0.9130	0.0870	0.7162	Typhonii Rhizoma	2,3,6-Trimethylnaphthalene	13237	FALSE	c1c(c(cc2cc(ccc12)C)C)C
MOL012628	0.9130	0.0870	0.7162	Ginseng Folium	2,3,6-Trimethylnaphthalene	13237	FALSE	c1c(c(cc2cc(ccc12)C)C)C
MOL012629	0.9410	0.0590	0.9713	Ginseng Folium	2,3-dimethoxy-2-methylbutane	Not Available	FALSE	CC(C(C)OC)(C)OC

MOL012631	0.2801	0.7199	0.7187	Ginseng Folium	20(R)-dammarane-3β,6α,12β,20,25-pentol	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C(C)(CCCC(C)(C)O)O)C)C)(C)C)O
MOL012632	0.2762	0.7238	0.8330	Ginseng Folium	20-(R)-ginsenoside Rh2	Not Available	FALSE	C1C2C(C3(C(C1O)C(CC3)C(CCC=C(C)C)(C)O)C)(CCC1C2(CCC(C1(C)C)OC1OC(C(C(C1O)O)O)CO)C)C
MOL012633	0.2305	0.7695	0.7376	Ginseng Folium	20-(R)-ginsenoside Rh2_qt	Not Available	FALSE	C1C2C(C3(C(C1O)C(CC3)C(CCC=C(C)C)(C)O)C)(CCC1C2(CCC(C1(C)C)O)C)C
MOL012634	0.7236	0.2764	0.8399	Ginseng Folium	20-gluc-ginsenoside Rf	Not Available	FALSE	C1C2C(C3C(C1O)C(CC3)C(CCC=C(C)C)(C)OC1OC(C(C(C1O)O)O)CO)(CC(C1C2(CCC(C1(C)C)O)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO)C
MOL012635	0.2429	0.7571	0.7151	Ginseng Folium	20-gluc-ginsenoside Rf_qt	Not Available	FALSE	C1C2C(C3C(C1O)C(CC3)C(CCC=C(C)C)(C)O)(CC(C1C2(CCC(C1(C)C)O)C)O)C
MOL012636	0.8858	0.1142	0.6975	Ginseng Folium	2-cyclohexyl-octane	Not Available	FALSE	CC(CCCCCC)C1CCCCC1
MOL012638	0.9513	0.0487	0.9265	Ginseng Folium	2-isopentanyl-4-methylcyclopenta-1,3-dione	Not Available	FALSE	C1(=O)C(C(=O)C(C1)C)CCC(C)C
MOL012640	0.3963	0.6037	0.7069	Ginseng Folium	3β,6α,12β-triol-22,23,24,25,26,27-hexanordammaran-20-one	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C(=O)C)C)C)(C)C)O
MOL012643	0.9161	0.0839	0.9654	Ginseng Folium	(S)-2-butanol	444683	FALSE	CC(CC)O
MOL012644	0.8418	0.1582	0.6717	Ginseng Folium	caryophellene	5498518	FALSE	C12CC/C(=C\CCC(=C)C1CC2(C)C)/C
MOL012644	0.8418	0.1582	0.6717	Aurantii Fructus Immaturus	caryophellene	5498518	FALSE	C12CC/C(=C\CCC(=C)C1CC2(C)C)/C
MOL012645	0.2389	0.7611	0.7561	Ginseng Folium	dammar-20(22),24-diene-3β,6α,12β-triol	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)/C(=C/CC=C(C)C)/C)C)C)(C)C)O

MOL012646	0.7494	0.2506	0.8097	Ginseng Folium	(2S,3R,4S,5S,6R)-2-[(2S)-2-[(3S,5R,8R,9R,10R,12R,13R,14R,17S)-3-[(2R,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]oxy-12-hydroxy-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,1	9898279	FALSE	C12C(C3(C(C(C2)O)C(CC3)C(OC2OC(C(C(C2O)O)O)COC2OC(C(C(C2O)O)O)CO)(CCC=C(C)C)C)C)(CCC2C1(CCC(C2(C)C)OC1C(OC2OC(C(C(C2O)O)O)CO)C(C(C(O1)CO)O)O)C)C
MOL012647	0.7118	0.2882	0.8238	Ginseng Folium	Ginsenoside Rd2	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(OC1OC(COC2OCC(C(C2O)O)O)C(C(C1O)O)O)(CCC=C(C)C)C)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)O)O
MOL012648	0.6769	0.3231	0.7566	Ginseng Folium	ginsenoside Rg7	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(OC1C(C(C(C(O1)CO)O)O)O)O)(CCC(C(=C)C)O)C)C)C)(C)C)OC1OC(C(C(C1O)O)O)CO
MOL012649	0.2433	0.7567	0.6631	Ginseng Folium	majoroside F2_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(O)(CCC(C(=C)C)O)C)C)C)(C)C)O
MOL012649	0.2433	0.7567	0.6631	Panacis Japonici Rhizoma	majoroside F2_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(O)(CCC(C(=C)C)O)C)C)C)(C)C)O
MOL012650	0.4608	0.5392	0.7848	Ginseng Folium	ginsenoside Rh5	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2OC(C(C(C2O)O)O)C)O)(C2(C(C(C1)O)C(CC2)/C(=C\CC(C(=C)C)O)/C)C)C)(C)C)O
MOL012651	0.2445	0.7555	0.6685	Ginseng Folium	ginsenoside Rh5_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)/C(=C\CC(C(=C)C)O)/C)C)C)(C)C)O
MOL012652	0.4722	0.5278	0.7048	Ginseng Folium	ginsenoside Rh6	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C(C/C=C/C(C)(C)OO)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)(C)C)O
MOL012653	0.2968	0.7032	0.7046	Ginseng Folium	ginsenoside Rh6_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C(C/C=C/C(C)(C)OO)(C)O)C)C)(C)C)O

MOL012654	0.3761	0.6239	0.7850	Ginseng Folium	ginsenoside Rh7	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(=O)C1)C(CC2)C(CCC=C(C)C)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)C)(C)C)O
MOL012655	0.2321	0.7679	0.7354	Ginseng Folium	ginsenoside Rh7_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(=O)C1)C(CC2)C(CCC=C(C)C)(C)O)C)C)(C)C)O
MOL012656	0.4255	0.5745	0.7327	Ginseng Folium	ginsenoside Rh8	Not Available	FALSE	C1C(C(C2=CC(C3(C(C2(C1)C)CC(C1C3CCC1C(CCC=C(C)C)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)O)(C)C)O
MOL012657	0.2240	0.7760	0.6937	Ginseng Folium	ginsenoside Rh8_qt	Not Available	FALSE	C1C(C(C2=CC(C3(C(C2(C1)C)CC(C1C3CCC1C(CCC=C(C)C)(C)O)O)C)O)(C)C)O
MOL012658	0.4743	0.5257	0.7755	Ginseng Folium	ginsenoside Rh9	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C3C(C1)OC(CC(C3CC2)(C)OC1C(C(C(C(O1)CO)O)O)O)C=C(C)C)C)C)(C)C)O
MOL012659	0.3202	0.6798	0.7894	Ginseng Folium	ginsenoside Rh9_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C3C(C1)OC(CC(C3CC2)(C)O)C=C(C)C)C)C)(C)C)O
MOL012660	0.3337	0.6663	0.7205	Ginseng Folium	ginsenoside RS-9	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(O)(CCC=C(C)C)C)C)C)(C)C)OC1CC(C(C(C1O)O)O)COC(=O)C
MOL012661	0.3368	0.6632	0.7398	Ginseng Folium	ginsenoside-F1	Not Available	FALSE	OC1C2C(C3C(C4(C(C(O)C3)C(C(O)CC4)(C)C)C)C1)(CCC2(C(OC1OC(C(O)C(O)C1O)CO)(CCC=C(C)C)C)C)C
MOL012662	0.2623	0.7377	0.7176	Ginseng Folium	ginsenoside-F1_qt	Not Available	FALSE	OC1C2C(C3C(C4(C(C(O)C3)C(C(O)CC4)(C)C)C)C1)(CCC2(C(O)(CCC=C(C)C)C)C)C
MOL012663	0.6284	0.3716	0.8544	Ginseng Folium	ginsenoside-F3	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(OC1C(C(C(C(O1)CO)O)O)OC1C(O)C(O)C(O)CO1)C)C)C)(C)C)O
MOL012664	0.2494	0.7506	0.7336	Ginseng Folium	ginsenoside-F3_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL012665	0.6211	0.3789	0.8510	Ginseng Folium	ginsenoside-Rg4	Not Available	FALSE	O(C1C2C(C3C(C4(C(C(O)C3)C(CC4)/C(=C\CC=C(C)C)/C)C)C1)(CCC(O)C2(CC)C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)C)CO
MOL012666	0.2191	0.7809	0.7358	Ginseng Folium	ginsenoside-Rg4_qt	Not Available	FALSE	OC1C2C(C3C(C4(C(C(O)C3)C(CC4)/C(=C\CC=C(C)C)/C)C)C1)(CCC(O)C2(CC)C)C
MOL012667	0.3019	0.6981	0.7126	Ginseng Folium	ginsenoside-Rh3	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CCC2)/C(=C\CC=C(C)C)/C)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)O
MOL012668	0.2289	0.7711	0.7349	Ginseng Folium	ginsenoside-Rh3_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CCC2)/C(=C\CC=C(C)C)/C)C)C)(C)C)O
MOL012669	0.6769	0.3231	0.7566	Ginseng Folium	majoroside F2	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC(C(=C)C)O)(C)OC1C(C(C(C(O1)CO)O)O)O)O)C)C)(C)C)OC1OC(C(C(C1O)O)O)CO
MOL012669	0.6769	0.3231	0.7566	Panacis Japonici Rhizoma	majoroside F2	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC(C(=C)C)O)(C)OC1C(C(C(C(O1)CO)O)O)O)O)C)C)(C)C)OC1OC(C(C(C1O)O)O)CO

MOL012670	0.7011	0.2989	0.7172	Ginseng Folium	majoroside F4	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C(C/C=C/C(C)(O)C)(C)OC1C(C(C(C(O1)CO)O)O)O)C)C)(C)C)OC1OC(C(C(C1O)O)O)CO
MOL012671	0.2659	0.7341	0.7211	Ginseng Folium	majoroside F4_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C(C/C=C/C(C)(O)C)(C)O)C)C)(C)C)O
MOL012672	0.5427	0.4573	0.6183	Ginseng Folium	methyl 2-methyl-hexadecanoate	Not Available	FALSE	C(=O)(C(CCCCCCCCCCCCCC)C)OC
MOL012673	0.6788	0.3212	0.6963	Ginseng Folium	methyl 7,10,12-hexadecatrienoate	Not Available	FALSE	C(=O)(CCCCC/C=C/C/C=C/C=C/CCC)OC
MOL012674	0.7136	0.2864	0.8383	Ginseng Folium	Notoginseoside Fe	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(OC1OC(COC2OC(C(C2O)O)CO)C(C(C1O)O)O)(CCC=C(C)C)C)C)C)(C)C)OC1C(C(C(C(O1)CO)O)O)O
MOL012675	0.8763	0.1237	0.8257	Ginseng Folium	panasenoside	Not Available	FALSE	O(C1C(O)C(O)C(OC1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)CO)C1OC(C(O)C(O)C1O)CO
MOL012676	0.2305	0.7695	0.7376	Ginseng Folium	protopanaxadiol	71463826	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(O)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL012677	0.4203	0.5797	0.7763	Ginseng Folium	pseudo-ginsenosideRT5	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)CO)O)O)O)O)(C2(C(C(C1)O)C(CC2)C1(C)CCC(O1)C(C)(C)O)C)C)(C)C)O
MOL012678	0.2516	0.7484	0.7079	Ginseng Folium	pseudo-ginsenosideRT5_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C1(C)CCC(O1)C(C)(C)O)C)C)(C)C)O
MOL012679	0.8447	0.1553	0.7844	Ginseng Folium	3-Tetradecanone	69418	FALSE	CCC(=O)CCCCCCCCCC
MOL012680	0.9536	0.0464	0.8987	Mahoniae Caulis	Antiarol	69505	FALSE	c1(cc(c(c(c1)OC)OC)OC)O
MOL012680	0.9536	0.0464	0.8987	Mori Cortex	Antiarol	69505	FALSE	c1(cc(c(c(c1)OC)OC)OC)O
MOL012681	0.8481	0.1519	0.6393	Mori Cortex	Dimethyl (methylenedi-4,1-phenylene)biscarbamate	99337	FALSE	c1c(ccc(c1)Cc1ccc(cc1)NC(=O)OC)NC(=O)OC
MOL012682	0.9395	0.0605	0.8220	Mori Cortex	5,7-Dihydroxycoumarin	5324654	FALSE	o1c(=O)ccc2c(cc(cc12)O)O

MOL012683	0.9325	0.0675	0.8769	Mori Cortex	6-hydroxy coumarin-7-O-β-D-glucopyranoside	Not Available	FALSE	o1c(=O)ccc2cc(c(cc12)OC1OC(C(C(C1O)O)O)CO)O
MOL012684	0.9086	0.0914	0.7391	Mori Cortex	6-hydroxycoumarin-6-O-α-rhamnopyranosyl-(1→6)-O-β-D-glucopyranoside	Not Available	FALSE	o1c(=O)ccc2cc(c(cc12)O)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)C
MOL012685	0.9091	0.0909	0.7589	Mori Cortex	6-hydroxycoumarin-7-O-β-D-apiofuranosyl-(1→6)-O-β-D-glucopyranoside	Not Available	FALSE	o1c(=O)ccc2c(cc(cc12)OC1OC(C(C(C1O)O)O)COC1OCC(C1O)(O)CO)O
MOL012686	0.9030	0.0970	0.7970	Mori Cortex	7-methoxy-5,4'-dihydroxyflavanonol	Not Available	FALSE	C1(CC(=O)c2c(cc(cc2O1)OC)O)(c1ccc(cc1)O)O
MOL012687	0.8641	0.1359	0.7627	Mori Cortex	cis-mulberroside A	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc(cc(O)c1)/C=C/c1c(O)cc(OC2OC(C(O)C(O)C2O)CO)cc1)CO
MOL012688	0.9056	0.0944	0.7355	Smilax China	Cudranin	5281717	FALSE	Oc1cc(cc(O)c1)/C=C/c1c(O)cc(O)cc1
MOL012688	0.9056	0.0944	0.7355	Ramulus Mori	Cudranin	5281717	FALSE	Oc1cc(cc(O)c1)/C=C/c1c(O)cc(O)cc1
MOL012688	0.9056	0.0944	0.7355	Mori Cortex	Cudranin	5281717	FALSE	Oc1cc(cc(O)c1)/C=C/c1c(O)cc(O)cc1
MOL012689	0.4305	0.5695	0.6788	Mori Cortex	cyclomulberrochromene	Not Available	FALSE	c12c(c(=O)c3c(o1)c1C=CC(Oc1cc3O)(C)C)C(Oc1c2ccc(c1)O)C=C(C)C
MOL012690	0.2078	0.7922	0.6167	Mori Cortex	kuwanon A	44258296	FALSE	c1(c(c(=O)c2c(cc(cc2o1)O)O)CC=C(C)C)c1ccc(c2C=CC(Oc12)(C)C)O
MOL012692	0.4651	0.5349	0.6519	Mori Cortex	kuwanon D	Not Available	FALSE	O1C2(C3C(C(C3c3c1cc(O)c(c3)C1Oc3c(C(=O)C1)c(O)cc(O)c3)(C)C)CC2)C
MOL012695	0.4730	0.5270	0.6988	Mori Cortex	kuwanon G	Not Available	FALSE	O1C2(C3C(C(CC(=C3)C)c3c(O)cc(O)cc3)C(=O)c3c(O)cc(O)cc3)c(O)cc(O)c2c(=O)c(c1c1c(O)cc(O)cc1)CC=C(C)C

MOL012697	0.4590	0.5410	0.6017	Mori Cortex	(E)-1-[3-[(1S,5R,6S)-6-[2,4-dihydroxy-3-(3-methylbut-2-enyl)benzoyl]-5-(2,4-dihydroxyphenyl)-3-methyl-1-cyclohex-2-enyl]-2,4-dihydroxyphenyl]-3-(2,4-dihydroxyphenyl)prop-2-en-1-one	6440670	FALSE	C(=O)(/C=C/c1c(cc(cc1)O)O)c1c(c(c(cc1)O)C1C=C(CC(C1C(=O)c1c(c(c(cc1)O)CC=C(C)C)O)c1c(cc(cc1)O)O)C)O
MOL012699	0.4775	0.5225	0.6993	Mori Cortex	kuwanon K	Not Available	FALSE	c1(c(c(=O)c2c(cc(cc2o1)O)O)CC=C(C)C)c1c(c(c(cc1)O)C1C=C(CC(C1C(=O)c1c(cc(cc1)O)O)c1c(cc(cc1)O)O)C)O
MOL012700	0.4660	0.5340	0.6510	Mori Cortex	(2S)-2-[3-[(1S,5R,6S)-6-(2,4-dihydroxybenzoyl)-5-(2,4-dihydroxyphenyl)-3-methyl-1-cyclohex-2-enyl]-2,4-dihydroxyphenyl]-5,7-dihydroxychroman-4-one	184877	FALSE	O=C(C1C(CC(=CC1c1c(O)c(C2Oc3c(C(=O)C2)c(O)cc(O)c3)ccc1O)C)c1c(O)cc(O)cc1)c1c(O)cc(O)cc1
MOL012701	0.6218	0.3782	0.6580	Mori Cortex	Kuwanon M	Not Available	FALSE	O1C(C2C(CC(=CC2c2c1cc(O)c1c2oc(c(c1=O)CC=C(C)C)c1c(O)cc(O)cc1)C)(C)C)c1c2oc(c(c(=O)c2c(O)cc1O)CC=C(C)C)c1c(O)cc(O)cc1

MOL012702	0.5337	0.4663	0.6618	Mori Cortex	2-[3-[(1S,5R,6S)-6-[2,4-dihydroxy-3-(3-methylbut-2-enyl)benzoyl]-5-(2,4-dihydroxyphenyl)-3-methyl-1-cyclohex-2-enyl]-2,4-dihydroxy-phenyl]-5,7-dihydroxy-3-(3-methylbut-2-enyl)chromone	21636210	FALSE	c1(c(c(=O)c2c(o1)cc(cc2O)O)CC=C(C)C)c1c(c(cc1)O)C1C=C(CC(C1C(=O)c1c(c(cc1)O)CC=C(C)C)O)c1c(cc(cc1)O)O)C)O
MOL012710	0.4287	0.5713	0.7156	Mori Cortex	limonianin	14162621	FALSE	O1C(C=Cc2c1cc(O)c1c2oc(cc1=O)c1ccc(O)cc1)(C)C
MOL012711	0.5021	0.4979	0.6758	Mori Cortex	moracenin C	Not Available	FALSE	c1(c(c(=O)c2c(cc(c(c2o1)C1C=C(CC(C1c1c(cc(cc1)O)O)C(=O)c1c(c2CCC(Oc2cc1)(C)C)O)C)O)O)CC=C(C)C)c1c(cc(cc1)O)O
MOL012712	0.4768	0.5232	0.7016	Mori Cortex	moracenin D	Not Available	FALSE	c1(c(c(=O)c2c(o1)c(c(cc2O)O)C1C=C(CC(C1C(=O)c1c(cc(cc1)O)O)c1c(cc(cc1)O)O)C)CCC(C)(C)O)c1c(cc(cc1)O)O
MOL012713	0.8800	0.1200	0.7738	Mori Cortex	Moracetin	5319886	FALSE	C1(C(C(C(OC1CO)OCC1C(C(C(C(O1)OCC1C(C(C(C(O1)Oc1c(=O)c2c(oc1c1cc(c(cc1)O)O)cc(cc2O)O)O)O)O)O)O)O)O)O)O
MOL012714	0.9010	0.0990	0.7501	Mori Cortex	Moracin A	441839	FALSE	c1(cc(cc(c1)c1oc2c(c1)c(cc(c2)OC)OC)O)O
MOL012715	0.8877	0.1123	0.7989	Mori Cortex	moracin M-3'-O-β-D-glucopyranoside	Not Available	FALSE	c1c2c(ccc1)cc(o2)c1cc(cc(c1)OC1OC(C(C(C1O)O)O)CO)O
MOL012716	0.9307	0.0693	0.8210	Mori Cortex	5-(benzofuran-2-yl)resorcinol	641363	FALSE	c1c2c(ccc1)cc(o2)c1cc(cc(c1)O)O
MOL012717	0.8786	0.1214	0.7178	Mori Cortex	moracin M-6,3'-di-O-β-D-glucopyranoside	Not Available	FALSE	c1c2c(ccc1OC1OC(C(C(C1O)O)O)CO)cc(o2)c1cc(cc(c1)OC1OC(C(C(C1O)O)O)CO)O

MOL012718	0.9080	0.0920	0.6912	Mori Cortex	moracin M-6-O-β-D-glucopyranoside	Not Available	FALSE	c1c2c(ccc1OC1OC(C(C(C1O)O)O)CO)cc(o2)c1cc(cc(c1)O)O
MOL012719	0.5691	0.4309	0.8074	Mori Cortex	moracin O	42603436	FALSE	O1C(C(O)(C)C)Cc2c1cc1oc(cc1c2)c1cc(O)cc(O)c1
MOL012720	0.5040	0.4960	0.6288	Mori Cortex	morusignin L	44258298	FALSE	O1C(C=Cc2c1cc1oc(c(CCC(O)(C)C)c(=O)c1c2O)c1c(O)cc(O)cc1)(C)C
MOL012721	0.4623	0.5377	0.7428	Mori Cortex	Morusin-4-glucoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc(O)c(c2oc3c4c(OC(C=C4)(C)C)cc(O)c3c(=O)c2CC=C(C)C)cc1)CO
MOL012722	0.5248	0.4752	0.6386	Mori Cortex	Oxydihydromorusin	5481968	FALSE	O1C(C=Cc2c3oc(c(CCC(O)(C)C)c(=O)c3c(O)cc12)c1c(O)cc(O)cc1)(C)C
MOL012723	0.4118	0.5882	0.6655	Mori Cortex	mulberranol	Not Available	FALSE	c1(c(c(=O)c2c(o1)cc1c(c2O)CC(O1)C(C)(C)O)CC=C(C)C)c1c(cc(cc1)O)O
MOL012724	0.0978	0.9022	0.7023	Mori Cortex	5-[7-[(2E)-3,7-dimethylocta-2,6-dienyl]-6-methoxy-benzofuran-2-yl]resorcinol	6440635	FALSE	o1c2c(C/C=C(/CCC=C(C)C)\C)c(OC)ccc2cc1c1cc(O)cc(O)c1
MOL012725	0.4416	0.5584	0.6108	Mori Cortex	Mulberrofuran C	157143	FALSE	O=C(C1C(CC(=CC1c1c(O)cc(cc1O)c1oc2c(c1)ccc(O)c2)C)c1c(O)cc(O)cc1)c1c(O)cc(O)cc1
MOL012726	0.5705	0.4295	0.6618	Mori Cortex	mulberrofuran G	Not Available	FALSE	O1C2(Oc3c(C4C2C(CC(=C4)C)c2c1cc(O)cc2)c(O)cc(c3)c1oc2c(c1)ccc(O)c2)c1c(O)cc(O)cc1
MOL012727	0.3887	0.6113	0.7512	Mori Cortex	mulberrofuran K	Not Available	FALSE	c1cc(cc2c1CC(O2)c1cc(c2c(c1)OC1(C3C2C=C(CC3c2c(O1)cc(cc2)O)C)Cc1ccc(c2c1OC(C=C2)(C)C)O)O)O
MOL012728	0.4861	0.5139	0.6721	Mori Cortex	mulberrofuran M	Not Available	FALSE	c1cc(cc2c1cc(o2)c1cc(c2c(c1)OC1C2C(=O)C2(Oc3c(C1=C2)ccc(c3)O)C)OC(=O)c1ccc(cc1O)O)O
MOL012729	0.1748	0.8252	0.6521	Mori Cortex	Mulberrofuran N	5319929	FALSE	c12ccc(cc1oc(c2)c1c(c(cc(c1CC=C(C)C)OC)O)CC=C(C)C)O
MOL012730	0.4264	0.5736	0.6450	Mori Cortex	Mulberrofuran O	Not Available	FALSE	c1cc(cc2c1cc(o2)c1cc(c(c(c1)O)C1C(C(=O)c2ccc3c(c2O)C=CC(O3)(C)C)C(CC(=C1)C)c1ccc(cc1O)O)O)O
MOL012731	0.5926	0.4074	0.6477	Mori Cortex	Mulberrofuran P	Not Available	FALSE	c1cc(cc2c1cc(o2)c1cc(c2c(c1)OC1(c3c2cc(c(c3c2c(O1)cc(cc2)O)O)C)c1c(cc(cc1)O)O)O)O
MOL012732	0.6378	0.3622	0.6808	Mori Cortex	mulberrofuran Q	Not Available	FALSE	c1cc(cc2c1cc(o2)c1cc(c2c(c1)OC1(C3(C2C(=O)C2(CC3c3c(O2)cc(cc3)O)C)O1)c1ccc(cc1O)O)O)O

MOL012733	0.8641	0.1359	0.7627	Mori Cortex	(2S,3R,4S,5S,6R)-2-[3-hydroxy-5-[(E)-2-[2-hydroxy-4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]oxy-phenyl]vinyl]phenoxy]-6-methylol-tetrahydropyran-3,4,5-triol	6443484	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc(cc(O)c1)/C=C/c1c(O)cc(OC2OC(C(O)C(O)C2O)CO)cc1)CO
MOL012734	0.7288	0.2712	0.6808	Mori Cortex	mulberroside C	Not Available	FALSE	C1C(C(C(C(O1)Oc1cc(cc(c1)c1oc2c(c1)cc1c(c2)OC(C(C1)O)(C)C)O)O)O)O
MOL012735	0.6351	0.3649	0.7966	Mori Cortex	mulberroside C_qt	Not Available	FALSE	Oc1cc(cc(c1)c1oc2c(c1)cc1c(c2)OC(C(C1)O)(C)C)O
MOL012736	0.4198	0.5802	0.7067	Mori Cortex	Multiflor-7-ene	Not Available	FALSE	C1CCC(C2C1(C1C(=CC2)C2(C(CC1)(C1C(CC2)(CCC(C1)(C)C)C)C)C)(C)C
MOL012737	0.8980	0.1020	0.7887	Mori Cortex	oxyresveratrol-2-O-β-D-glucopyranoside	Not Available	FALSE	c1(ccc(c(c1)OC1OC(C(C(C1O)O)O)CO)/C=C/c1cc(cc(c1)O)O)O
MOL012738	0.8712	0.1288	0.7508	Mori Cortex	oxyresveratrol-3'-O-β-D-glucopyranosyl-4-O-β-D-glucopyranosyl-(1→6)-O-β-D-glucopyranoside	Not Available	FALSE	c1(cc(c(cc1)/C=C/c1c(cc(cc1)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)O)O)OC1C(C(C(C(CO)O1)O)O)O
MOL012739	0.9348	0.0652	0.8572	Mori Cortex	4-[(E)-2-(2,4-dihydroxyphenyl)vinyl]resorcinol	9881314	FALSE	c1(cc(c(cc1)/C=C/c1c(cc(cc1)O)O)O)O
MOL012740	0.8999	0.1001	0.8037	Mori Cortex	oxyresveratrol-3'-O-β-glucopyranoside	Not Available	FALSE	c1(ccc(c(c1)O)/C=C/c1cc(cc(c1)O)OC1OC(C(C(C1O)O)O)CO)O

MOL012741	0.8629	0.1371	0.7650	Mori Cortex	oxyresveratrol-4-O-β-D-glucopyranosyl-3'-O-β-D-apiofuranosyl-(1→6)-O-β-D-glucopyranoside	Not Available	FALSE	c1(cc(c(cc1)/C=C/c1cc(cc(c1)O)OC1OC(C(C(C1O)O)O)COC1OCC(C1O)(CO)O)O)OC1C(C(C(C(CO)O1)O)O)O
MOL012742	0.8665	0.1335	0.7565	Mori Cortex	oxyresveratrol-4-O-β-D-glucopyranosyl-3'-O-β-D-glucopyranosyl-(1→6)-O-β-D-glucopyranoside	Not Available	FALSE	c1(cc(c(cc1)/C=C/c1cc(cc(c1)O)OC1OC(C(C(C1O)O)O)COC1OC(C(C(C1O)O)O)CO)O)OC1C(C(C(C(CO)O1)O)O)O
MOL012743	0.7801	0.2199	0.6879	Mori Cortex	resveratrol-3,4'-di-O-β-D-glucopyranoside	Not Available	FALSE	c1(ccc(cc1)/C=C/c1cc(cc(c1)O)OC1OC(C(C(C1O)O)O)CO)OC1C(C(C(C(CO)O1)O)O)O
MOL012744	0.9051	0.0949	0.9491	Smilacis Glabrae Rhixoma	resveratrol	445154	TRUE	c1(ccc(cc1)/C=C/c1cc(cc(c1)O)O)O
MOL012744	0.9051	0.0949	0.9491	Polygoni Cuspidati Rhizoma Et Radix	resveratrol	445154	TRUE	c1(ccc(cc1)/C=C/c1cc(cc(c1)O)O)O
MOL012744	0.9051	0.0949	0.9491	Mori Cortex	resveratrol	445154	TRUE	c1(ccc(cc1)/C=C/c1cc(cc(c1)O)O)O
MOL012748	0.4903	0.5097	0.7662	Mori Cortex	76464-71-6	Not Available	FALSE	C12(C(C(=O)c3c(O1)cc1c(c3O)C=CC(O1)(C)C)(Oc1c2ccc(c1)O)O)CC=C(C)C
MOL012749	0.4448	0.5552	0.7208	Mori Cortex	sanggenone B	Not Available	FALSE	C12(C(C(=O)c3c(O1)cc(c(c3O)C1=CC3(Oc4c(C(C1)C3)ccc(c4)O)C)O)(Oc1c2ccc(c1)O)CC=C(C)C)O
MOL012750	0.5166	0.4834	0.7384	Mori Cortex	sanggenone C	Not Available	FALSE	C12(C(c3c(O2)cc(cc3)O)(Oc2c(C1=O)c(c(C1C(C(=O)c3c(cc(cc3)O)O)C(c3c(cc(cc3)O)O)CC(=C1)C)c(c2)O)O)O)CC=C(C)C
MOL012751	0.5166	0.4834	0.7382	Mori Cortex	sanggenone D	Not Available	FALSE	c1(c(c(c2c(c1)OC1(C(C2=O)(Oc2c1ccc(c2)O)CC=C(C)C)O)O)C1C=C(CC(C1C(=O)c1ccc(cc1O)O)c1c(cc(cc1)O)O)C)O
MOL012752	0.5208	0.4792	0.7514	Mori Cortex	sanggenone E	Not Available	FALSE	C12(C(C(=O)c3c(O1)cc(c(c3O)C1C=C(CC(C1)(c1c(cc(cc1)O)O)C(=O)c1c(c(c(cc1)O)CC=C(C)C)O)C)O)(Oc1c2ccc(c1)O)CC=C(C)C)O
MOL012753	0.5580	0.4420	0.6457	Mori Cortex	sanggenone F	Not Available	FALSE	C1(CC(=O)c2c(O1)cc(cc2O)O)c1ccc2c(C=CC(O2)(C)C)c1O
MOL012754	0.4386	0.5614	0.6782	Mori Cortex	sanggenone G	Not Available	FALSE	C1(CC(=O)c2c(O1)cc(c(c2O)C1C=C(CC(C1C(=O)c1c(cc(cc1)O)O)c1c(cc(cc1)O)O)CCC=C(C)C)O)c1c(cc(cc1)O)O

MOL012755	0.4887	0.5113	0.6732	Mori Cortex	sanggenone H	Not Available	FALSE	C1(CC(=O)c2c(O1)cc(cc2O)O)c1c2c(C=CC(O2)(C)C)c(cc1)O
MOL012759	0.2765	0.7235	0.7588	Mori Cortex	sanggenone L	Not Available	FALSE	C12(C(C(=O)c3c(O1)c(c1c(c3O)C=CC(O1)(C)C)CC=C(C)C)(Oc1c2ccc(c1)O)CC=C(C)C)O
MOL012760	0.5096	0.4904	0.7618	Mori Cortex	sanggenone M	Not Available	FALSE	C12(C(C(=O)c3c(O1)c1c(cc3O)OC(C=C1)(C)C)(Oc1c2ccc(c1)O)O)CC=C(C)C
MOL012762	0.5335	0.4665	0.7570	Mori Cortex	sanggenone O	15479637	FALSE	C12(C(C(=O)c3c(O1)cc(c(c3O)C1C=C(CC(C1C(=O)c1c(cc(cc1)O)O)c1c(cc(cc1)O)O)C)O)(Oc1c2ccc(c1)O)O)CC=C(C)C
MOL012763	0.4484	0.5516	0.6711	Mori Cortex	ursane	9548870	FALSE	C12(C3(C(C4C(CC3)(CCC(C4C)C)C)CCC1C1(C(CC2)C(CCC1)(C)C)C)C)C
MOL012765	0.8948	0.1052	0.6963	Polygoni Orientalis Fructus	1,3,3-Trimethyl-2-(2-methyl-cyclo-propyl)-cyclohexene	Not Available	FALSE	C1(=C(C(CCC1)(C)C)C1C(C1)C)C
MOL012766	0.8330	0.1670	0.6860	Polygoni Orientalis Fructus	ZINC05063142	11906485	FALSE	C1(C(=CCC2C(CCCC12C)(C)C)C)CO
MOL012767	0.9153	0.0847	0.8109	Polygoni Orientalis Fructus	1,4,5,6,7,7a-hexahydro-4-methyl-7-(1-methylethyl)-2H-inden-2-one	Not Available	FALSE	C1C(=O)C=C2C(CCC(C12)C(C)C)C
MOL012768	0.9133	0.0867	0.9039	Polygoni Orientalis Fructus	Hendecynoic acid	31039	FALSE	C(=O)(CCCCCCCCC#C)O
MOL012769	0.8889	0.1111	0.8064	Polygoni Orientalis Fructus	2,5,9-Trimethylcycloundeca-4,8-dienone	Not Available	FALSE	C1(=O)C(C/C=C(/CC/C=C(\CC1)/C)\C)C
MOL012770	0.6277	0.3723	0.7395	Polygoni Orientalis Fructus	28-O-β-D-glucopyranosyl-3β,7β-dihydroxy-lup-20(29)-en-28-oate	Not Available	FALSE	C1C(C(C2C(C1)(C1C(C(C2)O)(C2(C(CC1)C1C(CC2)CC2(C(C1)C(CC2)C(=C)C)C(=O)OC1C(C(C(C(O1)CO)O)O)O)C)C)(C)C)O
MOL012771	0.8206	0.1794	0.7962	Polygoni Orientalis Fructus	28-O-β-D-glucopyranosyl-3β,7β-dihydroxy-lup-20(29)-en-28-oate_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(C(C2)O)(C2(C(CC1)C1C(CC2)CC2(C(C1)C(CC2)C(=C)C)C(=O)O)C)C)(C)C)O

MOL012772	0.9178	0.0822	0.7556	Polygoni Orientalis Fructus	3,3'-di-O-methylellagic acid-4'-O-β-D-glucopyranoside	Not Available	FALSE	c1(c(c2c3c(c1)c(=O)oc1c3c(c(=O)o2)cc(c1OC)O)OC)OC1OC(CO)C(C(C1O)O)O
MOL012773	0.9420	0.0580	0.7897	Polygoni Orientalis Fructus	3,5,7-Trihydroxy chromone	46886154	FALSE	c1c(c(=O)c2c(cc(cc2o1)O)O)O
MOL012774	0.9213	0.0787	0.8840	Polygoni Orientalis Fructus	4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-2-butanone	38988368	FALSE	CC(=O)CCC1C(=CCCC1(C)C)C
MOL012777	0.8754	0.1246	0.8448	Polygoni Orientalis Fructus	kaempferol-3-O-α-L-rhamnoside	Not Available	FALSE	c1c(c2c(cc1O)OC(C(C2=O)OC1C(C(C(C(C)O1)O)O)O)c1cccc(c1)O)O
MOL012778	0.9077	0.0923	0.8618	Polygoni Orientalis Fructus	kaempferol-3-O-α-L-rhamnoside_qt	Not Available	FALSE	c1c(c2c(cc1O)OC(C(C2=O)O)c1cccc(c1)O)O
MOL012779	0.9187	0.0813	0.8119	Polygoni Orientalis Fructus	taxifolin-3-O-β-D-glucoside	14187089	FALSE	c1c(c2c(cc1O)OC(C(C2=O)OC1C(C(C(C(CO)O1)O)O)O)c1ccc(c(c1)O)O)O
MOL012781	0.9208	0.0792	0.7851	Mori Cortex	quercetin 3-O-arabinoside	12309865	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)CO1)c1cc(O)c(O)cc1
MOL012782	0.9265	0.0735	0.8040	Mori Cortex	Isohyperoside	10813969	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(=O)c2c(oc1c1cc(O)c(O)cc1)cc(O)cc2O)CO
MOL012783	0.8149	0.1851	0.7409	Mori Cortex	quercetin-3-O-(2',6'-digalloyl)-β-D-glucoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(OC(=O)c2cc(O)c(O)c(O)c2)C(O)C(O)C(O1)COC(=O)c1cc(O)c(O)c(O)c1)c1cc(c(O)cc1)O
MOL012784	0.8683	0.1317	0.7577	Mori Cortex	quercetin-3-O-2'-galloyl-β-D-glucoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(OC(=O)c2cc(O)c(O)c(O)c2)C(O)C(O)C(O1)CO)c1cc(c(O)cc1)O
MOL012785	0.7171	0.2829	0.7214	Mori Cortex	quercetin-3-O-6'-trans-coumaroyl-β-D-glucoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)COC(=O)/C=C/c1ccc(cc1)O)c1cc(c(O)cc1)O
MOL012786	0.9265	0.0735	0.8040	Mori Cortex	quercetin-3-O-α-L-galactoside	25079947	FALSE	o1c(c(c(=O)c2c1cc(O)cc2O)OC1OC(C(O)C(O)C1O)CO)c1cc(O)c(O)cc1

MOL012787	0.9065	0.0935	0.8319	Mori Cortex	quercetin-7-O-β-D-gentiobioside	Not Available	FALSE	c1(c(O)c(=O)c2c(O)cc(OC3OC(C(C(C3O)O)O)COC3OC(C(C(C3O)O)O)CO)cc2o1)c1cc(O)c(O)cc1
MOL012788	0.6114	0.3886	0.6920	Flos Genkwa	Tiliroside	5320686	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)COC(=O)/C=C/c1ccc(O)cc1
MOL012788	0.6114	0.3886	0.6920	Leonuri Herba	Tiliroside	5320686	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)COC(=O)/C=C/c1ccc(O)cc1
MOL012788	0.6114	0.3886	0.6920	Rosae Laevigatae Fructus	Tiliroside	5320686	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)COC(=O)/C=C/c1ccc(O)cc1
MOL012788	0.6114	0.3886	0.6920	Potentillae Chinensis Herba	Tiliroside	5320686	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)COC(=O)/C=C/c1ccc(O)cc1
MOL012788	0.6114	0.3886	0.6920	Mori Cortex	Tiliroside	5320686	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)COC(=O)/C=C/c1ccc(O)cc1
MOL012788	0.6114	0.3886	0.6920	Rubi Fructus	Tiliroside	5320686	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)COC(=O)/C=C/c1ccc(O)cc1
MOL012789	0.9379	0.0621	0.9553	Mori Cortex	2,3,4-Trihydroxybenzoate	11874	FALSE	C(=O)(c1c(c(c(cc1)O)O)O)O
MOL012790	0.9323	0.0677	0.9615	Mori Cortex	DBH	19	FALSE	C(=O)(c1c(c(ccc1)O)O)O
MOL012791	0.9174	0.0826	0.8475	Mori Cortex	3,4,8,9,10-pentahydroxybenzo[c]chromen-6-one	18504424	FALSE	c1(ccc2c(c1O)oc(=O)c1c2c(c(c(c1)O)O)O)O
MOL012792	0.5001	0.4999	0.6509	Mori Cortex	Acbglu	6439941	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(O)cc1)COC(=O)/C=C/c1ccc(cc1)O
MOL012793	0.8764	0.1236	0.7549	Mori Cortex	cyanidin 3,5-di-O-glycoside	Not Available	FALSE	c1(c(cc2c(cc(O)cc2[o+]1)OC1C(O)C(O)C(O)C(O1)CO)OC1C(O)C(O)C(O)C(O1)CO)c1cc(O)c(O)cc1
MOL012794	0.8953	0.1047	0.8185	Polygoni Avicularis Herba	Juglanin	5318717	FALSE	O1C(C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)CO
MOL012794	0.8953	0.1047	0.8185	Juglandis Semen	Juglanin	5318717	FALSE	O1C(C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)CO
MOL012794	0.8953	0.1047	0.8185	Mori Cortex	Juglanin	5318717	FALSE	O1C(C(O)C(O)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)CO
MOL012795	0.7529	0.2471	0.7382	Mori Cortex	Kaempferol-3-O-(2',6'-digalloyl)-β-D-glucoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(OC(=O)c2cc(O)c(O)c(O)c2)C(O)C(O)C(O1)COC(=O)c1cc(O)c(O)c(O)c1)c1ccc(O)cc1
MOL012796	0.8806	0.1194	0.7596	Mori Cortex	Kaempferol-3-O-(6'-galloyl)-β-D-glucoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)COC(=O)c1cc(O)c(O)c(O)c1)c1ccc(O)cc1

MOL012797	0.8631	0.1369	0.7641	Mori Cortex	Kaempferol-3-O-2'-galloyl-β-D-glucoside	Not Available	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(OC(=O)c2cc(O)c(O)c(O)c2)C(O)C(O)C(O1)CO)c1ccc(O)cc1
MOL012798	0.6114	0.3886	0.6920	Mori Cortex	Kaempferol-3-O-6'-trans-coumaroyl-β-D-glucoside	12775852	FALSE	c1(c(c(=O)c2c(O)cc(O)cc2o1)OC1C(O)C(O)C(O)C(O1)COC(=O)/C=C/c1ccc(cc1)O)c1ccc(O)cc1
MOL012799	0.8611	0.1389	0.8422	Mori Cortex	Kaempferol-3-O-α-L-rhamnoside	Not Available	FALSE	o1c(c(c(=O)c2c1cc(O)cc2O)OC1OC(C(O)C(O)C1O)C)c1cc(O)ccc1
MOL012800	0.9423	0.0577	0.8798	Mori Cortex	3,5,7-trihydroxy-2-(3-hydroxyphenyl)chromone	9860659	FALSE	o1c(c(c(=O)c2c1cc(O)cc2O)O)c1cc(O)ccc1
MOL012801	0.8930	0.1070	0.9621	Mori Cortex	Monomethyl succinate	77487	FALSE	C(=O)(CCC(=O)O)OC
MOL012802	0.7553	0.2447	0.9079	Mori Cortex	myrianthic acid	Not Available	FALSE	C(=O)(C12CCC3(C4(CCC5C(C(CCC5(C4CC=C3C2CC(CC1)(C)C)C)O)(C)C)C)C)O
MOL012803	0.9392	0.0608	0.8273	Coriolus	(2R,3R,4S,5S,6R)-2-(3,4-dimethoxybenzyl)oxy-6-methylol-tetrahydropyran-3,4,5-triol	21581594	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)Cc1cc(c(cc1)OC)OC
MOL012804	0.9325	0.0675	0.8911	Coriolus	(2R,3R,4S,5S,6R)-2-(4-hydroxy-3-methoxy-benzyl)oxy-6-methylol-tetrahydropyran-3,4,5-triol	21627672	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)Cc1cc(c(cc1)O)OC
MOL012805	0.9514	0.0486	0.9181	Coriolus	o-Veratryl alcohol	79738	FALSE	c1(c(c(ccc1)OC)OC)CO
MOL012806	0.9589	0.0411	0.9681	Coriolus	2,4-Dimethoxybenzyl alcohol	81750	FALSE	c1(c(cc(cc1)OC)OC)CO
MOL012807	0.9600	0.0400	0.9651	Coriolus	2,5-Dimethoxybenzyl alcohol	118495	FALSE	C(c1c(ccc(c1)OC)OC)O

MOL012808	0.9189	0.0811	0.9553	Coriolus	3-cyanopropanamide	3017295	FALSE	C(CC#N)C(=O)N
MOL012812	0.2521	0.7479	0.6554	Coriolus	ergosta-7,22-dien-3β,5α,6β-triol	Not Available	FALSE	C1C(CC2(C(C1)(C1C(=CC2O)C2C(CC1)(C(CC2)C(C)/C=C/C(C(C)C)C)C)C)O)O
MOL012815	0.2471	0.7529	0.6241	Coriolus	ergosta-7-ene-3β,5α,6β-triol	Not Available	FALSE	C1C(CC2(C(C1)(C1C(=CC2O)C2C(CC1)(C(CC2)C(C)CCC(C(C)C)C)C)C)O)O
MOL012816	0.2504	0.7496	0.6683	Coriolus	ergosterol peroxide	Not Available	FALSE	C1C(CC2(C(C1)(C1C(C=C2)(C2C(CC1)(C(CC2)C(C)/C=C/C(C(C)C)C)C)C)C)C)O
MOL012821	0.8517	0.1483	0.6286	Echinopsis Radix	2-(3,4-diacetoxybutyn-1)-5-(propyn-1)thiophene	Not Available	FALSE	c1(ccc(s1)C#CC(OC(=O)C)COC(=O)C)C#CC
MOL012822	0.9034	0.0966	0.7373	Echinopsis Radix	2-(3,4-dihydroxybutyn-1)-5-(propyn-1)thiophene	Not Available	FALSE	c1(ccc(s1)C#CC(O)CO)C#CC
MOL012823	0.8651	0.1349	0.7036	Echinopsis Radix	2-(pentadiyn-1,3)-5-(3,4-dihydroxybutyn-1)thiophene	Not Available	FALSE	c1(ccc(s1)C#CC(O)CO)C#CC#CC
MOL012825	0.8917	0.1083	0.6362	Echinopsis Radix	5-(3,4-dihydroxybutyn-1)-bithiophene	Not Available	FALSE	c1(cccs1)c1cc(cs1)C#CC(O)CO
MOL012829	0.9115	0.0885	0.6620	Echinopsis Radix	5-(4-Hydroxybut-1-ynyl)-2,2'-bithiophene	440357	FALSE	c1(cccs1)c1ccc(s1)C#CCCO
MOL012831	0.8804	0.1196	0.6948	Sinapis Semen	5-But-3-en-1-ynyl-[2,2']bithiophenyl	70813	FALSE	c1(cccs1)c1sc(cc1)C#CC=C
MOL012831	0.8804	0.1196	0.6948	Echinopsis Radix	5-But-3-en-1-ynyl-[2,2']bithiophenyl	70813	FALSE	c1(cccs1)c1sc(cc1)C#CC=C
MOL012832	0.8105	0.1895	0.8620	Echinopsis Radix	5,5″-dichlorine-α-terthiophene	Not Available	FALSE	C1(=CC=C(C1)Cl)C1=CC=C(C1)C1=CC=C(C1)Cl

MOL012833	0.8871	0.1129	0.6984	Echinopsis Radix	2-Acetylthiophene, 5-(2-thienyl)-	606422	FALSE	c1(cccs1)c1ccc(s1)C(=O)C
MOL012834	0.6956	0.3044	0.7146	Echinopsis Radix	5-acetyl-α-terthiophene	Not Available	FALSE	C1(=CC=C(C1)C(=O)C)C1=CC=C(C1)C1=CC=CC1
MOL012835	0.8587	0.1413	0.8426	Echinopsis Radix	5-chloro-α-terthiophene	Not Available	FALSE	C1(=CC=C(C1)Cl)C1=CC=C(C1)C1=CC=CC1
MOL012836	0.9243	0.0757	0.8029	Echinopsis Radix	5-hydroxy-α-terthiophene	Not Available	FALSE	C1(=CC=C(C1)C(=O)O)C1=CC=C(C1)C1=CC=CC1
MOL012839	0.8800	0.1200	0.7221	Echinopsis Radix	echinothiophene	Not Available	FALSE	c1c2c(c3c(c1OC1OC(C(C(C1O)O)O)CO)C(OC3=O)/C=C/C=C/CCO)sc(c2)CO
MOL012840	0.7801	0.2199	0.6738	Echinopsis Radix	echinothiophene_qt	Not Available	FALSE	c1c2c(c3c(c1O)C(OC3=O)/C=C/C=C/CCO)sc(c2)CO
MOL012841	0.8185	0.1815	0.7713	Echinopsis Radix	echinoynethiophene	Not Available	FALSE	C1(=CC=C(C1)C#CC#CC(O)CO)C#CC
MOL012843	0.3926	0.6074	0.7224	Echinopsis Radix	olean-3-one	Not Available	FALSE	C1(=O)CCC2(C(C1(C)C)CCC1(C)C3(C)CCC4(C)CCC(C)(C)CC4C3CCC21)C
MOL012844	0.8581	0.1419	0.8103	Echinopsis Radix	(4R)-4-[(1Z)-1,5-dimethylhexa-1,4-dienyl]-1-methylcyclohexene	13252683	FALSE	C1(CCC(=CC1)C)/C(=C\CC=C(C)C)/C
MOL012845	0.7181	0.2819	0.7212	Panacis Japonici Rhizoma	chikusetsusaponin Ⅳa_qt	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(C)C)C1OC(C(O)C(O)C1O)C(=O)O
MOL012846	0.6593	0.3407	0.8252	Panacis Japonici Rhizoma	Chikusetsusaponin Ia	Not Available	FALSE	OC1C2C(C3(C(C4(C(CC3)C(C(OC3OC(C(O)C(O)C3O)COC3OCC(O)C(O)C3O)CC4)(C)C)C)C1)C)(CCC2C(O)(CCC=C(C)C)C)C
MOL012847	0.7285	0.2715	0.8448	Panacis Japonici Rhizoma	Chikusetsusaponin Ib	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(C)C)C1OC(C(OC2OC(C(O)C2O)CO)C(O)C1O)C(=O)OC1OC(O)C(O)C(O)C1CO
MOL012848	0.6743	0.3257	0.8468	Panacis Japonici Rhizoma	chikusetsusaponin III	Not Available	FALSE	OC1C2C(C3C(C4(C(C(C3)C)C(CC4)C3(OC(C(O)C(O)C3OC3OC(C(O)C(O)C3O)CO)CO)OC3OCC(O)C(O)C3O)(C)C)C)C1)(CCC2C(O)(CCC=C(C)C)C)
MOL012849	0.3824	0.6176	0.7268	Panacis Japonici Rhizoma	chikusetsusaponin III_qt	Not Available	FALSE	OC1(OC(C(O)C(O)C1O)CO)C1C(C2C(C3C(C4(C(CC4)C(O)(CCC=C(C)C)C)C(O)C3)C)CC2C)(CC1)C)(C)C
MOL012850	0.9191	0.0809	0.9196	Panacis Japonici Rhizoma	Isopropyl ethyl ether	13843578	FALSE	O(C(C)C(C)C)C(C)C(C)C
MOL012851	0.7341	0.2659	0.8385	Panacis Japonici Rhizoma	notoginsenoside r1	441934	FALSE	O(C1C2C(C3C(C4(C(C(CC4)C(OC4OC(C(O)C(O)C4O)CO)(CCC=C(C)C)C)C(O)C3)C)(C1)C)(CCC(O)C2(C)C)C)C1OC(C(O)C(O)C1OC1OCC(O)C(O)C1O)CO

MOL012852	0.7622	0.2378	0.7951	Panacis Japonici Rhizoma	Notoginsenoside R4	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(OC1C(O)C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)CO1)C)C)C)(C)C)OC1C(OC2C(O)C(O)C(O)C(O)C(O2)CO)C(O)C(O)C(O1)CO
MOL012853	0.2305	0.7695	0.7376	Panacis Japonici Rhizoma	Notoginsenoside R4_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(O)C)C)C)(C)C)O
MOL012854	0.7518	0.2482	0.8246	Panacis Japonici Rhizoma	Notoginsenoside R6	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(O)C(O)C(O)C(O2)CO)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)CO)C)C)C)(C)C)O
MOL012855	0.2494	0.7506	0.7336	Panacis Japonici Rhizoma	Notoginsenoside R6_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2O)(C2(C(C(C1)O)C(CC2)C(CCC=C(C)C)(C)O)C)C)C)(C)C)O
MOL012856	0.6264	0.3736	0.8641	Panacis Japonici Rhizoma	Pseudo-ginsenoside F11	Not Available	FALSE	O(C1C2C(C3C(C4(C(C(CC4)C4(OC(CC4)C(O)(C)C)C)C(O)C3)C)(C1)C)(CCC(O)C2(C)C)C)C1OC(C(O)C(O)C1OC1OC(C(O)C(O)C1O)C)CO
MOL012857	0.2516	0.7484	0.7079	Panacis Japonici Rhizoma	Pseudo-ginsenoside F11_qt	Not Available	FALSE	OC1C2C(C3C(C4(C(C(CC4)C4(OC(CC4)C(O)(C)C)C)C(O)C3)C)(C1)C)(CCC(O)C2(C)C)C
MOL012858	0.5589	0.4411	0.8588	Panacis Japonici Rhizoma	Vina-ginsenoside R1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)COC(=O)C)O)O)OC2C(C(C(C(O2)C)O)O)O)(C2(C(C(C1)O)C(CC2)C1(OC(CC1)C(O)(C)C)C)C)C)C)O
MOL012859	0.3621	0.6379	0.7877	Panacis Japonici Rhizoma	Vina-ginsenoside R1_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(C(C(C(O2)COC(=O)C)O)O)O)(C2(C(C(C1)O)C(CC2)C1(OC(CC1)C(O)(C)C)C)C)C)C)O
MOL012860	0.5597	0.4403	0.8592	Panacis Japonici Rhizoma	Vina-ginsenoside R2	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(OC3C(O)C(O)C(O)CO3)C(O)C(O)C(O2)COC(=O)C)(C2(C(C(C1)O)C(CC2)C1(CCC(O1)C(O)(C)C)C)C)C)C)O
MOL012861	0.3621	0.6379	0.7877	Panacis Japonici Rhizoma	Vina-ginsenoside R2_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2OC2C(O)C(O)C(O)C(O2)COC(=O)C)(C2(C(C(C1)O)C(CC2)C1(CCC(O1)C(O)(C)C)C)C)C)C)O
MOL012862	0.8850	0.1150	0.8550	Perillae Fructus	methyl (E)-dodec-9-enoate	5362755	FALSE	C(=O)(CCCCCCC/C=C/CC)OC
MOL012864	0.8946	0.1054	0.8530	Perillae Fructus	Cellon	6591	FALSE	C(C(Cl)Cl)(Cl)Cl
MOL012865	0.9392	0.0608	0.8630	Perillae Fructus	1,4-diethyl-1,4-dimethyl-2,5-cyclohexadiene	572347	FALSE	C1(C=CC(C=C1)(C)CC)(C)CC
MOL012866	0.8932	0.1068	0.8265	Perillae Fructus	linalyl anthranilate	Not Available	FALSE	C=CC(CCC=C(C)C)(C)OC(=O)c1c(cccc1)N
MOL012866	0.8932	0.1068	0.8265	Zanthoxyli Pericarpium	linalyl anthranilate	Not Available	FALSE	C=CC(CCC=C(C)C)(C)OC(=O)c1c(cccc1)N

MOL012867	0.8964	0.1036	0.7971	Perillae Fructus	1.3-dimethyl-4.8-dioxatricyclo[5.1.0.0(3.5)]octane-2,6-diol	Not Available	FALSE	C12(C(C3(OC3C(C1O2)O)C)O)C
MOL012868	0.8477	0.1523	0.8267	Perillae Fructus	Methyl 12-tridecynoate	554090	FALSE	C(=O)(CCCCCCCCCCC#C)OC
MOL012869	0.8693	0.1307	0.8401	Perillae Fructus	1-chloro-4-mesyl-benzene	7395	FALSE	c1(ccc(cc1)S(=O)(=O)C)Cl
MOL012870	0.9120	0.0880	0.8052	Perillae Fructus	2-(1-Hydroxyethyl) norbornadiene	Not Available	FALSE	C12C(=CC(C=C1)C2)C(C)O
MOL012872	0.8901	0.1099	0.8634	Perillae Fructus	WLN: Q1XGGG	8259	FALSE	C(C(Cl)(Cl)Cl)O
MOL012873	0.9060	0.0940	0.9223	Perillae Fructus	(3R)-2,2-dimethyl-3-propyloxirane	21720138	FALSE	O1C(C1CCC)(C)C
MOL012874	0.8956	0.1044	0.9092	Perillae Fructus	2,5-dimethyl-3-methylenehexa-1,5-diene	535055	FALSE	C=C(C(=C)CC(=C)C)C
MOL012875	0.9301	0.0699	0.9766	Perillae Fructus	(1S,2S)-2-ethylcyclohexan-1-ol	6994303	FALSE	C1(C(CCCC1)CC)O
MOL012876	0.5447	0.4553	0.7013	Perillae Fructus	2-hexyl-cyclopropane octanoic acid methyl ester	14325746	FALSE	C1(C(C1)CCCCCC)CCCCCCCC(=O)OC
MOL012877	0.8485	0.1515	0.9739	Perillae Fructus	3,4-Dichlorobutane nitrile	Not Available	FALSE	C(#N)CC(CCl)Cl
MOL012878	0.8538	0.1462	0.8425	Perillae Fructus	3-Chloropropylsulfonyl chloride	15410	FALSE	C(CCCl)S(=O)(=O)Cl
MOL012879	0.9472	0.0528	0.7994	Perillae Fructus	3-oxiranyl-7-oxabicyclo[4.1.0]heptane	Not Available	FALSE	C12(CCCCC1O2)C1OC1
MOL012880	0.9482	0.0518	0.9563	Perillae Fructus	()-Isopulegol	1268090	FALSE	C1(C(CCC(C1)C)C(=C)C)O
MOL012881	0.8775	0.1225	0.6827	Perillae Fructus	5-Methyl-2-phenylindole	83247	FALSE	[nH]1c(cc2cc(ccc12)C)c1ccccc1

MOL012882	0.9433	0.0567	0.8796	Perillae Fructus	Benzylidenemalonaldehyde	583063	FALSE	C(=O)C(=Cc1ccccc1)C=O
MOL012884	0.2184	0.7816	0.7185	Perillae Fructus	butyrospermol	12302190	FALSE	OC1C(C2C(C3C(=CC2)C2(C(C(CC2)C(CCC=C(C)C)C)(CC3)C)C)(CC1)C)(C)C
MOL012885	0.9244	0.0756	0.9442	Perillae Fructus	Propyl chloroacetate	79378	FALSE	C(=O)(CCl)OCCC
MOL012886	0.9202	0.0798	0.9721	Perillae Fructus	Chloroethyl acetate	10959	FALSE	C(=O)(C)OCCCl
MOL012887	0.8375	0.1625	0.7490	Perillae Fructus	Chloromesyl chloride	77054	FALSE	C(S(=O)(=O)Cl)Cl
MOL012888	0.2190	0.7810	0.6457	Perillae Fructus	citrostadienol	Not Available	FALSE	OC1C(C2C(C3C(=CC2)C2C(C(CC2)C(CC/C(=C/C)/C(C)C)C)(CC3)C)(CC1)C)C
MOL012889	0.8619	0.1381	0.6520	Perillae Fructus	(-)-cis-.beta.-Elemene	6431151	FALSE	C1(C(CC(CC1)C(=C)C)C(=C)C)(C)C=C
MOL012890	0.8971	0.1029	0.9661	Perillae Fructus	HAI	7965	FALSE	NC1CCCCC1
MOL012892	0.9302	0.0698	0.9484	Perillae Fructus	methyl hept-2-enoate	5368087	FALSE	C(=O)(/C=C/CCCC)OC
MOL012893	0.9327	0.0673	0.6123	Perillae Fructus	(E)-(4-methylbenzylidene)-(4-phenyltriazol-1-yl)amine	9602469	FALSE	n1(nnc(c1)c1ccccc1)/N=C/c1ccc(cc1)C
MOL012895	0.9544	0.0456	0.9777	Perillae Fructus	()-Perillaaldehyde	1548901	FALSE	C(=O)C1=CCC(C(=C)C)CC1
MOL012896	0.7243	0.2757	0.9157	Perillae Fructus	Phthalic acid, butyl isohexyl ester	6423865	FALSE	C(=O)(c1c(C(=O)OCCCC)cccc1)OCCCC(C)C
MOL012897	0.8638	0.1362	0.8099	Perillae Fructus	O-propyl aminosulfanyl methanethioate	536887	FALSE	NSC(=S)OCCC
MOL012899	0.9646	0.0354	0.8415	Perillae Fructus	Tricyclo[5.2.1.0(2,6)]decan-10-one	Not Available	FALSE	C12C3CCCC3C(CC1)C2=O
MOL012900	0.8231	0.1769	0.6193	Perillae Fructus	Trimethylphosphine oxide	69609	FALSE	P(=O)(C)(C)C
MOL012901	0.9200	0.0800	0.9775	Lablab Semen Album	D-Homoproline	6931662	FALSE	OC(=O)C1NCCCC1
MOL012902	0.1117	0.8883	0.8603	Menispermi Rhizoma	6'-dauricinoline	Not Available	FALSE	c1c(cc(c(c1)O)Oc1ccc(cc1)CC1c2c(CCN1C)cc(c(c2)OC)OC)CC1N(CCc2c1cc(c(c2)O)OC)C
MOL012903	0.7821	0.2179	0.6798	Menispermi Rhizoma	Dauricumidine	Not Available	FALSE	ClC1C2(C34C(NCC3)(C1)C(=C(OC)C(=O)C4)OC)C(O)C(=CC2=O)OC

MOL012905	0.1885	0.8115	0.8352	Menispermi Rhizoma	Disinomenine	Not Available	FALSE	Oc1c2C34C(C(N(CC3)C)Cc2c(c2c3c(C56C(C(N(CC5)C)C3)C=C(OC)C(=O)C6)c(O)c(OC)c2)cc1OC)C=C(OC)C(=O)C4
MOL012906	0.9275	0.0725	0.8973	Menispermi Rhizoma	Menisdaurin	Not Available	FALSE	O1C(OC2CC(O)C=C/C2=C\C#N)C(O)C(O)C(O)C1CO
MOL012907	0.7821	0.2179	0.6798	Caulis Sinomenii	Acutumidine	Not Available	FALSE	ClC1C2(C34C(NCC3)(C1)C(=C(OC)C(=O)C4)OC)C(O)C(=CC2=O)OC
MOL012907	0.7821	0.2179	0.6798	Menispermi Rhizoma	Acutumidine	Not Available	FALSE	ClC1C2(C34C(NCC3)(C1)C(=C(OC)C(=O)C4)OC)C(O)C(=CC2=O)OC
MOL012910	0.7444	0.2556	0.7780	Menispermi Rhizoma	Bianfugecine	Not Available	FALSE	O(c1cc2c3c(nccc3c1)c1c(C2=O)cc(OC)cc1)C
MOL012911	0.7830	0.2170	0.7654	Menispermi Rhizoma	Bianfugedine	Not Available	FALSE	O1c2c3c4c(nccc4cc2OC1)c1c(C3=O)cc(OC)cc1
MOL012912	0.6200	0.3800	0.8275	Menispermi Rhizoma	Bianfugenine	Not Available	FALSE	O(c1c2c3c(nccc3c(OC)c1OC)c1c(C2=O)cc(OC)cc1)C
MOL012913	0.9462	0.0538	0.8626	Menispermi Rhizoma	Corypalline	280225	FALSE	O(c1cc2CCN(Cc2cc1O)C)C
MOL012914	0.1117	0.8883	0.8603	Menispermi Rhizoma	dauricinoline	71463990	FALSE	c12C(N(CCc1cc(c(c2)OC)O)C)Cc1cc(Oc2ccc(CC3c4c(cc(c(c4)OC)OC)CCN3C)cc2)c(cc1)O
MOL012915	0.1234	0.8766	0.8485	Menispermi Rhizoma	dauricline	Not Available	FALSE	c1c(cc(c(c1)O)Oc1ccc(cc1)CC1c2c(CCN1C)cc(c(c2)O)OC)CC1N(CCc2c1cc(c(c2)OC)C)C
MOL012916	0.0855	0.9145	0.7720	Menispermi Rhizoma	dauricoline	Not Available	FALSE	O(c1cc2C(N(CCc2cc1O)C)Cc1cc(Oc2ccc(CC3N(CCc4c3cc(OC)c(O)c4)C)cc2)c(O)cc1)C
MOL012917	0.1116	0.8884	0.8601	Menispermi Rhizoma	daurinoline	12309092	FALSE	c12C(N(CCc1cc(c(c2)OC)OC)C)Cc1cc(Oc2ccc(CC3c4c(cc(c(c4)OC)O)CCN3C)cc2)c(cc1)O
MOL012918	0.7337	0.2663	0.7819	Menispermi Rhizoma	dauriporphinoline	Not Available	FALSE	n1c2c3c(cc1)c(c(c(c3C(=O)c1c2ccc(c1)OC)O)OC)OC
MOL012919	0.1142	0.8858	0.8615	Menispermi Rhizoma	Daurisoline	51106	FALSE	O(c1cc2C(N(CCc2cc1OC)C)Cc1ccc(Oc2cc(CC3N(CCc4c3cc(O)c(OC)c4)C)ccc2O)cc1)C
MOL012920	0.6305	0.3695	0.7766	Menispermi Rhizoma	sinomenine	Not Available	FALSE	O(C1=CC2C3(CCN(C2CC2c3c(O)c(OC)cc2)C)CC1=O)C
MOL012921	0.6284	0.3716	0.8021	Jujubae Fructus	stepharine	Not Available	FALSE	O(c1c2C3(CC4NCCc(c24)cc1OC)C=CC(=O)C=C3)C
MOL012921	0.6284	0.3716	0.8021	Menispermi Rhizoma	stepharine	Not Available	FALSE	O(c1c2C3(CC4NCCc(c24)cc1OC)C=CC(=O)C=C3)C
MOL012922	0.6130	0.3870	0.8073	Menispermi Rhizoma	l-SPD	6917970	FALSE	O(c1c2CN3C(Cc2ccc1O)c1c(CC3)cc(OC)c(O)c1)C
MOL012923	0.6400	0.3600	0.6468	Typhonii Rhizoma	2,7-DIMETHYLPHENANTHRENE	15305	FALSE	c12c3c(ccc1cc(cc2)C)cc(cc3)C
MOL012924	0.9442	0.0558	0.9072	Typhonii Rhizoma	(5R)-5-(benzyl)hydantoin	703702	FALSE	C1(C(=O)NC(=O)N1)Cc1ccccc1
MOL012926	0.9204	0.0796	0.8843	Typhonii Rhizoma	(5S)-5-(4-hydroxybenzyl)hydantoin	233111	FALSE	C1(Cc2ccc(cc2)O)NC(=O)NC1=O
MOL012927	0.7749	0.2251	0.7284	Typhonii Rhizoma	6-METHYL-2-PHENYLQUINOLINE	33792	FALSE	n1c2c(cc(cc2)C)ccc1c1ccccc1

MOL012928	0.9181	0.0819	0.7723	Typhonii Rhizoma	2-METHYBENZOTHIAZOLE	8446	FALSE	c12c(sc(n1)C)cccc2
MOL012929	0.3441	0.6559	0.7454	Cynanchistauntonii Rhizoma Et Radix	glaucoside C	Not Available	FALSE	O1CC2OC(=O)C3C(CCC4=COC1(C24)C)C1(C(=CC3)CC(C(C1)O)OC1OC(C(C(C1)OC)OC1OC(C(C(C1)O)OC1OC(C(C(C1)OC)O)C)C)C)C
MOL012931	0.5169	0.4831	0.7660	Cynanchistauntonii Rhizoma Et Radix	Glaucoside H	Not Available	FALSE	O1C2C3C(=COC3(OC2)C)CCC2C3(CC(O)C(OC4OC(C(OC5OC(C(OC6OC(C(OC7OC(C(O)C(O)C7O)CO)C(OC)C6)C)C(O)C5)C)C(OC)C4)C)CC3=CCC2C1=O)C
MOL012932	0.7316	0.2684	0.7409	Cynanchistauntonii Rhizoma Et Radix	glaucoside H_qt	Not Available	FALSE	O1C2C3C(=COC3(OC2)C)CCC2C3(CC(O)C(CC3=CCC2C1=O)O)C
MOL012933	0.5868	0.4132	0.7090	Cynanchistauntonii Rhizoma Et Radix	Tylophorinidine	161749	FALSE	OC1C2N(CCC2)Cc2c1c1c(c3c2cc(OC)c(O)c3)cc(OC)cc1
MOL012934	0.8163	0.1837	0.7291	Iridis Tectori Rhizoma	Iridin	5281777	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(OC)c(O)c2c(occ(c2=O)c2cc(OC)c(OC)c(O)c2)c1)CO
MOL012935	0.8928	0.1072	0.7527	Iridis Tectori Rhizoma	tectoruside	Not Available	FALSE	C1=CC(C(=CC1C(=O)C)OC)OC1OC(C(OC2OC(C(C(C2O)O)O)CO)C(C1O)O)CO
MOL012936	0.9247	0.0753	0.9658	Iridis Tectori Rhizoma	tectoruside_qt	Not Available	FALSE	C1=CC(C(=CC1C(=O)C)OC)O
MOL012937	0.7686	0.2314	0.6053	Benincasae Semen	2,4-octadecadienoic acid	5312457	FALSE	OC(=O)/C=C/C=C/CCCCCCCCCCCCC
MOL012939	0.0464	0.9536	0.6407	Jujubae Fructus	Scutianine C	Not Available	FALSE	C(=O)(C(C(CC)C)N(C)C)NC1C(Oc2ccc(/C=C\NC(=O)C(NC1=O)Cc1ccccc1)cc2)C(C)C
MOL012940	0.6785	0.3215	0.8353	Jujubae Fructus	Spiradine A	Not Available	FALSE	C1CC2(C3C4(C1)C1C56CC3(N(C4C6CC(C(=C)C5)C1=O)C2)O)C
MOL012941	0.9364	0.0636	0.9451	Jujubae Fructus	Sylvestrene	Not Available	FALSE	C1CCC(C=C1C)C(=C)C
MOL012942	0.8748	0.1252	0.6694	Jujubae Fructus	Tannin	Not Available	FALSE	O1C(C(O)C(OC(=O)c2cc(O)c(O)c(O)c2)C(O)C1OC(=O)c1cc(O)c(O)c(O)c1)COC(=O)c1cc(O)c(O)c(O)c1
MOL012943	0.5684	0.4316	0.7869	Jujubae Fructus	Ziziphin	Not Available	FALSE	O1C23OC(CC(OC4OC(C(O)C(OC(=O)C)C4OC(=O)C)C)(C2C2C(C4(C(C5(C(CC4)C(C(OC4OCC(OC6OC(C(O)C(O)C6O)C)C(O)C4O)CC5)(C)C)C)CC2)C)(C3)C1)C)C=C(C)C
MOL012945	0.6888	0.3112	0.8226	Jujubae Fructus	Zizyphus saponin III	Not Available	FALSE	C(=CC1OC23C(C(C1)(C)O)C1C(C2)(C2(C(CC1)C1(C(CC2)C(C(CC1)OC1OCC(C(C1OC1OC(C(C(C1OO)O)O)C)OC1OC(C(C(C1OC1OCC(C(C1O)O)O)O)O)CO)O)(C)C)C)C)CO3)(C)C
MOL012946	0.3975	0.6025	0.7953	Jujubae Fructus	zizyphus saponin I_qt	Not Available	FALSE	OC1CCC2(C3CCC4C5C(CC(C=C(C)C)OC65CC4(C3(CCC2C1(C)C)C)CO6)(C)O)C
MOL012947	0.6888	0.3112	0.8398	Jujubae Fructus	Zizyphus saponin II	Not Available	FALSE	C(=CC1OC23C(C(C1)(C)O)C1C(C2)(C2(C(CC1)C1(C(CC2)C(C(CC1)OC1OCC(C(C1OC1OC(C(C(C1OO)(O)O)O)C)OC1OC(C(C(C1O)O)O)CO)O)(C)C)C)C)CO3)(C)C

MOL012948	0.7840	0.2160	0.6896	Jujubae Fructus	Zuztvisude I	Not Available	FALSE	C1C(=O)C=C(C(C1(C)C)(O)/C=C/C(C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO)C
MOL012949	0.8828	0.1172	0.7871	Jujubae Fructus	(4S)-4-hydroxy-4-[(E,3S)-3-hydroxybut-1-enyl]-3,5,5-trimethylcyclohex-2-en-1-one	10537120	FALSE	C1C(=O)C=C(C(C1(C)C)(O)/C=C/C(C)O)C
MOL012952	0.8843	0.1157	0.8990	Jujubae Fructus	Daechualkaloid A	5316289	FALSE	O1CC2=C(NC1)C(=O)CC2
MOL012954	0.0784	0.9216	0.7114	Jujubae Fructus	daechuine S3	Not Available	FALSE	C1C2CC(C(C1)OC)/C=C\NC(=O)C(NC(=O)C1C(O2)CCN1C(=O)C(CC(=O)C(N(C)C)C(C)CC)C(C)CC)C(C)CC
MOL012955	0.2099	0.7901	0.6334	Jujubae Fructus	24-Dehydrocholesterol	439577	FALSE	OC1CC2=CCC3C4C(C(CC4)C(CCC=C(C)C)C)(CCC3C2(CC1)C)C
MOL012957	0.9130	0.0870	0.9453	Jujubae Fructus	ADA	445929	FALSE	O1C(C(O)C(O)C(O)C1O)C(=O)O
MOL012958	0.6847	0.3153	0.8420	Jujubae Fructus	jujubasaponin IV	Not Available	FALSE	O1C23OC(C(O)(C2C2C(C4(C(C5(C(CC4)C(C(OC4OC(C(O)C(OC6OC(C(O)C(O)C6O)CO)C4OC4OC(C(O)C(O)C4O)C)CO)CC5)(C)C)C)CC2)C)(C3)C1)CC=C(C)C
MOL012959	0.3634	0.6366	0.7758	Jujubae Fructus	jujubasaponin IV_qt	Not Available	FALSE	O1C23OC(C(O)(C2C2C(C4(C(C5(C(CC4)C(C(O)CC5)(C)C)C)CC2)C)(C3)C1)C)CC=C(C)C
MOL012960	0.7399	0.2601	0.8072	Jujubae Fructus	jujuboside A	Not Available	FALSE	O1C23OC(CC(O)(C2C2C(C4(C(C5(C(CC4)C(C(OC4OCC(O)C(OC6OC(C(O)C(O)C6OC6OCC(O)C(O)C6O)COC6OC(C(O)C(O)C6O)CO)C4OC4OC(C(O)C(O)C4O)C)CC5)(C)C)C)CC2)C)(C3)C1)C)C=C(C)C
MOL012961	0.3975	0.6025	0.7953	Jujubae Fructus	jujuboside A_qt	Not Available	FALSE	O1C23OC(CC(O)(C2C2C(C4(C(C5(C(CC4)C(C(O)CC5)(C)C)C)CC2)C)(C3)C1)C)C=C(C)C
MOL012962	0.7963	0.2037	0.8488	Jujubae Fructus	swertisin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1OC
MOL012963	0.8688	0.1312	0.7433	Jujubae Fructus	zizybeoside II	46173942	FALSE	O(C1C(OC2OC(C(O)C(O)C2O)CO)C(OC(C1O)CO)OCc1ccccc1)C1OC(C(O)C(O)C1O)CO
MOL012964	0.6776	0.3224	0.8442	Jujubae Fructus	zizyphus saponin I	Not Available	FALSE	C(=CC1OC23C(C(C1)(C)O)C1C(C2)(C2(C(CC1)C1(C(CC2)C(C(CC1)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)C)OC1OC(C(C(C1O)O)O)CO)O)(C)C)C)CO3)(C)C
MOL012965	0.8062	0.1938	0.7706	Jujubae Fructus	zizyvoside II	Not Available	FALSE	O(C1C(OC2OC(C(O)C(O)C2O)CO)C(OC(C1O)CO)OC(/C=C/C1(O)C(CC(=O)C=C1C)(C)C)C1OC(C(O)C(O)C1O)CO

MOL012966	0.8828	0.1172	0.7871	Jujubae Fructus	(4R)-4-hydroxy-4-[(E,3S)-3-hydroxybut-1-enyl]-3,5,5-trimethylcyclohex-2-en-1-one	11816951	FALSE	OC(/C=C/C1(O)C(CC(=O)C=C1C)(C)C)C
MOL012967	0.7840	0.2160	0.6896	Jujubae Fructus	zizyvoside I	Not Available	FALSE	O(C1C(O)C(O)C(OC1OC(/C=C/C1(O)C(CC(=O)C=C1C)(C)C)C)CO)C1OC(C(O)C(O)C1O)C
MOL012968	0.9398	0.0602	0.9314	Jujubae Fructus	1-(4-Coumaroyl)alpha-rhamnopyranose	6438942	FALSE	C1(C(C(C(OC1C)OC(=O)/C=C/c1ccc(cc1)O)O)O)O
MOL012969	0.7451	0.2549	0.7902	Jujubae Fructus	2α-hydroxyoleanolic acid	Not Available	FALSE	OC1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C
MOL012970	0.7472	0.2528	0.7763	Jujubae Fructus	2α-hydroxyursolic acid	Not Available	FALSE	C1(CCC2(C(C1C)C1=CCC3C(C1(CC2)C)(CCC1C3(CC(C(C1(C)C)O)O)C)C)C(=O)O)C
MOL012971	0.6782	0.3218	0.6676	Jujubae Fructus	3-O-cis-p-coumaroyl alphitolic acid	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)C(=O)O)(CC3)C)C)(CC2)C)(CC1O)C)(C)C)C(=O)/C=C\c1ccc(O)cc1
MOL012972	0.7151	0.2849	0.7136	Jujubae Fructus	6'-O-p-Coumaroylgenipingentiobioside	6324973	FALSE	c1(ccc(cc1)/C=C/C(=O)OCC1C(C(C(C(O1)OCC1C(C(C(C(O1)OC1OC=C(C2C1C(=CC2)CO)C(=O)OC)O)O)O)O)O)O)O
MOL012974	0.7691	0.2309	0.7881	Jujubae Fructus	Asimilobine	160875	FALSE	O(c1c2c3C(NCCc3cc1O)Cc1c2cccc1)C
MOL012975	0.3729	0.6271	0.8531	Jujubae Fructus	Catharanthamine	Not Available	FALSE	O(C1C2(C3N(CCC43C(N(c3c4cc(C4(C5OC6(CC5CN(C6)CCc5c4[nH]c4c5cccc4)CC)C(=O)OC)c(OC)c3)C)C1(O)C(=O)OC)CC=C2)CC)C(=O)C
MOL012976	0.9273	0.0727	0.7510	Jujubae Fructus	coumestrol	5281707	FALSE	c12oc(=O)c3c(c1ccc(c2)O)oc1c3ccc(c1)O
MOL012977	0.1007	0.8993	0.6978	Jujubae Fructus	Daechuine S10	Not Available	FALSE	c1(ccc(cc1)CC(N(C)C)C(=O)N1C2C(CC1)Oc1cc(c(cc1)OC)/C=C/NC(=O)C(NC2=O)C(CC)C)O
MOL012978	0.0762	0.9238	0.6680	Jujubae Fructus	Daechuine S26	Not Available	FALSE	c1c2cc(c(c1)O)/C=C\NC(=O)C(NC(=O)C1C(O2)CCN1C(=O)C(N(C)C)Cc1ccccc1)C(C)CC
MOL012980	0.0670	0.9330	0.7438	Jujubae Fructus	Daechuine S6	Not Available	FALSE	c1c2cc(c(c1)OC)/C=C\NC(=O)C(NC(=O)C1C(O2)CCN1C(=O)C(N(C)C)Cc1ccccc1)C(C)CC
MOL012982	0.1083	0.8917	0.7153	Jujubae Fructus	Daechuine S8-1	Not Available	FALSE	c1c2cc(c(c1)OC)/C=C\NC(=O)C(NC(=O)C1C(O2)CCN1C(=O)C(CC(=O)C(N(C)C)CC(C)C)CC(C)C)CC(C)C

MOL012983	0.6863	0.3137	0.8302	Jujubae Fructus	Jujubasaponin VI	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C23C(CC1)C1C(OC2)(C3)OC2C1(OC(C2)C(C)(O)C)C)C)(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)O)O)CO
MOL012984	0.4844	0.5156	0.7397	Jujubae Fructus	Jujubasaponin VI_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C23C(CC1)C1C(OC2)(C3)OC2C1(OC(C2)C(C)(O)C)C)C)(C)C)O
MOL012985	0.6847	0.3153	0.8420	Jujubae Fructus	Jujubasaponin V	Not Available	FALSE	C1C2C(C34C(C1)C1C(C3)(OC(C1(O)C)CC=C(C)C)OC4)(CCC1C2(CCC(C1(C)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)OC1OC(C(C(C1O)O)O)CO)O)C)C
MOL012986	0.3634	0.6366	0.7758	Jujubae Fructus	Jujubasaponin V_qt	Not Available	FALSE	C1C2C(C34C(C1)C1C(C3)(OC(C1(O)C)CC=C(C)C)OC4)(CCC1C2(CCC(C1(C)C)O)C)C
MOL012987	0.3975	0.6025	0.7953	Jujubae Fructus	Jujubogenin	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C23C(CC1)C1C(C2)(OC(CC1(C)O)C=C(C)C)OC3)C)C)(C)C)O
MOL012988	0.7399	0.2601	0.8072	Jujubae Fructus	Jujuboside A1	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C23C(CC1)C1C(C2)(OC(CC1(C)O)C=C(C)C)OC3)C)C)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)C)OC1OC(C(C(C1OC1OCC(C(C1O)O)O)O)O)COC1OC(C(C(C1O)O)O)CO)O
MOL012989	0.3975	0.6025	0.7953	Jujubae Fructus	Jujuboside C_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C23C(CC1)C1C(C2)(OC(CC1(C)O)C=C(C)C)OC3)C)C)(C)C)O
MOL012990	0.7547	0.2453	0.8068	Jujubae Fructus	Jujuboside C	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C23C(CC1)C1C(C2)(OC(CC1(O)C)C=C(C)C)OC3)C)C)(C)C)OC1OCC(C(C1OC1OC(C(C(C1O)O)O)C)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)COC1OC(C(C(C1O)O)O)CO)O
MOL012991	0.6888	0.3112	0.8226	Jujubae Fructus	Jujuboside	Not Available	FALSE	C123C(C4C(C2)(OC3)OC(CC4(C)O)C=C(C)C)CCC2C1(CCC1C2(CCC(C1(C)C)OC1C(C(OC2C(OC3C(C(C(CO3)O)O)O)C(C(C(O2)CO)O)O)C(CO1)O)OC1C(C(C(O1)C)O)O)O)C)C
MOL012993	0.0587	0.9413	0.7338	Jujubae Fructus	Mauritine A	Not Available	FALSE	O1C2C(N(CC2)C(=O)C(NC(=O)C(N(C)C)C)C(C)C)C(=O)NC(Cc2ccccc2)C(=O)N/C=C\c2ccc1cc2
MOL012994	0.0982	0.9018	0.6767	Gleditsiae Fructus	1beta,5alpha,11-Triacetoxy-7beta-benzoyl-4alpha-hydroxy-8beta-nicotinoyl-dihydroagarofuran	Not Available	FALSE	c1cc(cnc1)C(=O)OC1C(C2C(C3(C1(C(CCC3(O)C)OC(=O)C)COC(=O)C)OC2(C)C)OC(=O)C)OC(=O)c1ccccc1
MOL012995	0.7025	0.2975	0.8401	Jujubae Fructus	zizyberanalic acid	Not Available	FALSE	C1(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)C(=O)O)CC3)C)(CC2)C)(C(C1O)C=O)C)(C)C
MOL012995	0.7025	0.2975	0.8401	Gleditsiae Fructus	zizyberanalic acid	Not Available	FALSE	C1(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)C(=O)O)CC3)C)(CC2)C)(C(C1O)C=O)C)(C)C

MOL012995	0.7025	0.2975	0.8401	Gleditsiae Spina	zizyberanalic acid	Not Available	FALSE	C1(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)C(=O)O)CC3)C)(CC2)C)(C(C1O)C=O)C)(C)C
MOL012996	0.7330	0.2670	0.8031	Gleditsiae Spina	alphitolic acid	Not Available	FALSE	C1(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)C(=O)O)CC3)C)(CC2)C)(CC(C1O)O)C)(C)C
MOL012996	0.7330	0.2670	0.8031	Gleditsiae Fructus	alphitolic acid	Not Available	FALSE	C1(C2C(C3C(C4(C(C5C(CC4)(CCC5C(=C)C)C(=O)O)CC3)C)(CC2)C)(CC(C1O)O)C)(C)C
MOL012997	0.9718	0.0282	0.8717	Gleditsiae Fructus	N6-(2-Isopentenyl)adenine	45070	FALSE	c12c(c(ncn1CC=C(C)C)N)ncn2
MOL013000	0.9500	0.0500	0.8993	Mahoniae Caulis	1-[4-(1-methyl-2-propenyl) phenyl]-ethanone	Not Available	FALSE	O=C(c1ccc(C(C)C=C)cc1)C
MOL013001	0.8594	0.1406	0.6508	Mahoniae Caulis	ISOPALMITIC ACID	36247	FALSE	OC(=O)CCCCCCCCCCCCCC(C)C
MOL013004	0.5284	0.4716	0.6200	Mahoniae Caulis	4-[(1R,3aR,4R,6aR)-4-(4-hydroxy-3,5-dimethoxyphenyl)-1,3,3a,4,6,6a-hexahydrofuro[4,3-c]furan-1-yl]-2,6-dimethoxyphenol	11796268	FALSE	c1(c(cc(cc1OC)C1C2C(CO1)C(OC2)c1cc(c(c(c1)OC)O)OC)OC)O
MOL013005	0.2404	0.7596	0.6152	Mahoniae Caulis	4b,5,6,7,8,8a,9,10-octahydro-4b,8-dimethyl-2-Isopropylphenanthrene	Not Available	FALSE	C12(C(C(CCC1)C)CCc1c2ccc(c1)C(C)C)C
MOL013006	0.9312	0.0688	0.8306	Mahoniae Caulis	(2S,3S,4R,5R,6R)-6-(3,4,5-trimethoxyphenoxy)tetrahydro-2H-pyran-2,3,4,5-tetraol	Not Available	FALSE	c1(cc(cc(c1OC)OC)OC1OC(C(C(C1O)O)O)O)OC

MOL013008	0.9264	0.0736	0.8833	Mahoniae Caulis	WLN: L6TJ AR	13229	FALSE	C1(CCCCC1)c1ccccc1
MOL013009	0.9396	0.0604	0.7999	Mahoniae Caulis	Decahydro-2,3-dimethyl-naphthalene	Not Available	FALSE	C12C(CC(C(C1)C)C)CCCC2
MOL013010	0.9309	0.0691	0.8321	Mahoniae Caulis	erythrosyringoylglycerol 8-O-β-D-glucoside	Not Available	FALSE	c1(cc(c(c(c1)OC)O)OC)C(O)C(OC1OC(O)C(C(C1O)O)O)CO
MOL013011	0.9415	0.0585	0.9382	Mahoniae Caulis	erythrosyringoylglycerol 8-O-β-D-glucoside_qt	14237631	FALSE	c1(cc(c(c(c1)OC)O)OC)C(O)C(O)CO
MOL013012	0.2118	0.7882	0.7014	Mahoniae Caulis	Oxyacanthine	Not Available	FALSE	O1c2c3C(N(CCc3cc(OC)c2OC)C)Cc2ccc(Oc3cc(CC4N(CCc5c4cc1c(OC)c5)C)ccc3O)cc2
MOL013014	0.8931	0.1069	0.8863	Inulae Herba	Tomentosin	155173	FALSE	O1C2C(CC=C(C(C2)C)CCC(=O)C)C(=C)C1=O
MOL013015	0.9297	0.0703	0.7721	Inulae Herba	Quercetagitrin	5320826	FALSE	c12c(=O)c(c(oc1cc(c(c2O)O)OC1C(C(C(C(O1)CO)O)O)O)c1cc(c(cc1)O)O)O
MOL013016	0.8899	0.1101	0.8142	Inulae Herba	Nepitrin	120742	FALSE	c12c(cc(c(c1O)OC)OC1OC(C(C(C1O)O)O)CO)oc(cc2=O)c1cc(c(cc1)O)O
MOL013017	0.8141	0.1859	0.7202	Inulae Herba	Ivalin	65156	FALSE	C12(C(CC3C(C1)OC(=O)C3=C)C(=C)CC(C2)O)C
MOL013018	0.0536	0.9464	0.6103	Inulae Herba	Toonacilin	Not Available	FALSE	C1=CC(C(C(C1=O)(C)C)CC(=O)OC)(C1C(=C)C23C(C(C1OC(=O)C)OC(=O)C)(C(CC2O3)c1cocc1)C)C
MOL013019	0.6867	0.3133	0.6659	Inulae Herba	inuchinenolide A	Not Available	FALSE	O1C2C(C(=C)C1=O)C(C=C(C(C2)C)CCC(=O)C)OC(=O)C
MOL013020	0.6118	0.3882	0.6941	Inulae Herba	Gaillardin	267247	FALSE	OC1(C2C(C(OC(=O)C)C1)C(=CC1OC(=O)C(=C)C1C2)C)C
MOL013021	0.9022	0.0978	0.7901	Inulae Herba	Patulitrin	5320435	FALSE	c1(c(c(=O)c2c(o1)cc(c(c2O)OC)OC1C(O)C(O)C(O)C(O1)CO)O)c1cc(c(cc1)O)O
MOL013022	0.9002	0.0998	0.9065	Sinapis Semen	3,5-Octadien-2-one, (E,E)-	5352876	FALSE	C(=C\C(=O)C)/C=C/CC
MOL013023	0.9522	0.0478	0.9004	Sinapis Semen	Biosol	18597	FALSE	c1(c(cc(cc1)O)C)C(C)C
MOL013024	0.9193	0.0807	0.9448	Sinapis Semen	Diallyl	11598	FALSE	C(CC=C)C=C
MOL013025	0.8612	0.1388	0.8311	Sinapis Semen	3-Methylthiopropyl	62351	FALSE	C(CN=C=S)CSC
MOL013026	0.9657	0.0343	0.9572	Sinapis Semen	4-hydroxybenzoylcholine	151252	FALSE	O(CC[N+](C)(C)C)C(=O)c1ccc(cc1)O
MOL013027	0.8928	0.1072	0.8654	Sinapis Semen	i-Butyl isothiocyanate	68960	FALSE	C(C(C)C)N=C=S

MOL013028	0.9227	0.0773	0.9567	Sinapis Semen	Butyl mustard oil	11613	FALSE	C(CCC)N=C=S
MOL013029	0.9044	0.0956	0.9632	Sinapis Semen	3-Methylbutyl isothiocyanate	79086	FALSE	C(CN=C=S)C(C)C
MOL013030	0.8948	0.1052	0.9402	Sinapis Semen	Pentyl isothiocyanate	69415	FALSE	C(CN=C=S)CCC
MOL013031	0.9338	0.0662	0.9414	Sinapis Semen	Phenethyl cyanide	12581	FALSE	c1(ccccc1)CCC#N
MOL013033	0.9033	0.0967	0.9450	Sinapis Semen	Butyl isthiocyanate	Not Available	FALSE	C(CC/N=C/C=S)C
MOL013034	0.9310	0.0690	0.9497	Sinapis Semen	(+)-(Z)-Methyl epijasmonate	6428089	FALSE	C(=O)(CC1C(C(=O)CC1)C/C=C\CC)OC
MOL013036	0.9291	0.0709	0.9678	Sinapis Semen	ZINC02034403	6999774	FALSE	CCC(C=C)O
MOL013037	0.1791	0.8209	0.6213	Sinapis Semen	2-(2-phenylethyl)-6-[[(5S,6R,7R,8S)-5,6,7-trihydroxy-4-keto-2-(2-phenylethyl)-5,6,7,8-tetrahydrochromen-8-yl]oxy]chromone	14283395	FALSE	c1cc(ccc1)CCc1cc(=O)c2c(o1)C(C(C(C2O)O)O)Oc1cc2c(cc1)oc(cc2=O)CCc1ccccc1
MOL013038	0.8277	0.1723	0.6890	Sinapis Semen	2-phenyl-1H-isoquinoline	5320529	FALSE	c1ccc2c(c1)CN(C=C2)c1ccccc1
MOL013039	0.5244	0.4756	0.7581	Sinapis Semen	6' -Sinapoylspinosin	Not Available	FALSE	c1(c(c(cc(c1)/C=C/C(=O)OCC1C(C(C(C(O1)OC1C(OC(C(C1O)O)CO)C1Cc2c(C=C1OC)oc(cc2=O)c1ccc(cc1)O)O)O)O)OC)O)OC
MOL013040	0.9427	0.0573	0.9070	Lasiosphaera Seu Calvatia	Coenzyme Q0	69068	FALSE	C1(=C(C(=O)C(=CC1=O)C)OC)OC
MOL013041	0.9456	0.0544	0.9689	Lasiosphaera Seu Calvatia	hexitol	120700	FALSE	C(O)C(O)C(O)C(O)C(O)CO
MOL013042	0.8973	0.1027	0.8114	Lasiosphaera Seu Calvatia	Illudins I	Not Available	FALSE	C1(C2(C(C3=C(C1=O)CC(C3)(C)CO)(C)O)CC2)C
MOL013043	0.9426	0.0574	0.9742	Lasiosphaera Seu Calvatia	N-Methyl-L-phenylalanine hydrochloride	6951135	FALSE	OC(=O)C(NC)Cc1ccccc1

MOL013044	0.9392	0.0608	0.9509	Lasiosphaera Seu Calvatia	N,N-Dimethyl-L-phenylalanine	40475207	FALSE	OC(=O)C(N(C)C)Cc1ccccc1
MOL013046	0.8400	0.1600	0.6322	Lasiosphaera Seu Calvatia	UR	1176	TRUE	O=C(N)N
MOL013047	0.8827	0.1173	0.8559	Lasiosphaera Seu Calvatia	Uric acid	Not Available	FALSE	N1C(=O)NC2C(=NC(=O)N2)C1=O
MOL013050	0.9219	0.0781	0.9493	Lasiosphaera Seu Calvatia	calvatic acid	Not Available	FALSE	OC(=O)c1ccc(/[N+](=N/C#N)/O)cc1
MOL013051	0.1926	0.8074	0.6142	Lasiosphaera Seu Calvatia	ergosta-7,22-dien-3-one	Not Available	FALSE	C1C(=O)CC2C(C1)(C1C(=CC2)C2C(CC1)(C(CC2)C(/C=C/C(C(C)C)C)C)C)C
MOL013052	0.9336	0.0664	0.9759	Lasiosphaera Seu Calvatia	2-(4-hydroxyphenyl)ethyl acetate	637753	FALSE	c1(ccc(cc1)CCOC(=O)C)O
MOL013053	0.8931	0.1069	0.6043	Lasiosphaera Seu Calvatia	melanin	Not Available	FALSE	O=c1c2c3c(c4c5c2c[nH]c5c(c(=O)c4=O)C)c[nH]c3c(c1=O)C
MOL013054	0.9534	0.0466	0.9461	Lasiosphaera Seu Calvatia	methyl calvatate	Not Available	FALSE	O(C(=O)c1ccc(/[N+](=N/C#N)/O)cc1)C
MOL013057	0.9340	0.0660	0.9484	Oroxyli Semen	COLLIDINE	15100	FALSE	c1(c(ccc(n1)C)C)C
MOL013058	0.8331	0.1669	0.8868	Oroxyli Semen	2,5-dihydroxy-6,7-dimethoxyflavone	Not Available	FALSE	c1(c(c(c2c(c1)OC(CC2=O)(c1ccccc1)O)O)OC)OC
MOL013059	0.8054	0.1946	0.7689	Oroxyli Semen	3,7,3',5'-tetramethoxy-2hydrochroxy flavone	Not Available	FALSE	c1(ccc2c(c1)OC(C(C2=O)OC)(c1cc(c(c(c1)OC)O)OC)O)OC
MOL013060	0.7705	0.2295	0.6297	Oroxyli Semen	7,10-Octadecadienoic acid	46190394	FALSE	CCCCCCC/C=C/C/C=C/CCCCCC(=O)O
MOL013061	0.8845	0.1155	0.8262	Oroxyli Semen	Baicalein-6-glucuronide	5321472	FALSE	C1(C(C(OC(C1O)C(=O)O)Oc1c(O)cc2c(c1O)c(=O)cc(o2)c1ccccc1)O)O
MOL013062	0.9115	0.0885	0.8244	Oroxyli Semen	BZQ	3102	TRUE	O=C(c1ccccc1)c1ccccc1
MOL013063	0.8368	0.1632	0.8480	Oroxyli Semen	Chrysin-7-O-β-D-glucuronide	Not Available	FALSE	c1(cc(c2c(c1)oc(cc2=O)c1ccccc1)O)OC1OC(C(C(C1)O)O)C(=O)O
MOL013064	0.9014	0.0986	0.8096	Oroxyli Semen	Scutellarein-5-galactoside	Not Available	FALSE	c1cc(ccc1O)c1cc(=O)c2c(o1)cc(c(c2OC1OC(C(C(C1O)O)O)CO)O)O
MOL013065	0.5144	0.4856	0.7573	Oroxyli Semen	Teucvin	Not Available	FALSE	C1CC2=C3C(C1)C1(C(CC3OC2=O)C)CC(OC1=O)c1cocc1
MOL013066	0.8127	0.1873	0.9128	Oroxyli Semen	chrysin-7-O-glucuronide	15558426	FALSE	c12c(c(=O)cc(o1)c1ccccc1)c(cc(c2)OC1OC(C(C(C1O)O)O)CO)O
MOL013067	0.8553	0.1447	0.8478	Oroxyli Semen	Tecomin	3884	FALSE	OC1=C(CC=C(C)C)C(=O)C(=O)c2c1cccc2

MOL013068	0.8437	0.1563	0.8479	Forsythiae Fructus	Oroxindin	3084961	FALSE	O1C(Oc2c(OC)c3oc(cc(=O)c3c(O)c2)c2ccccc2)C(O)C(O)C(O)C1C(=O)O
MOL013068	0.8437	0.1563	0.8479	Scutellariae Radix	Oroxindin	3084961	FALSE	O1C(Oc2c(OC)c3oc(cc(=O)c3c(O)c2)c2ccccc2)C(O)C(O)C(O)C1C(=O)O
MOL013068	0.8437	0.1563	0.8479	Oroxyli Semen	Oroxindin	3084961	FALSE	O1C(Oc2c(OC)c3oc(cc(=O)c3c(O)c2)c2ccccc2)C(O)C(O)C(O)C1C(=O)O
MOL013068	0.8437	0.1563	0.8479	Atractylodes Lancea (Thunb.)Dc.	Oroxindin	3084961	FALSE	O1C(Oc2c(OC)c3oc(cc(=O)c3c(O)c2)c2ccccc2)C(O)C(O)C(O)C1C(=O)O
MOL013069	0.8761	0.1239	0.8097	Oroxyli Semen	quercetin-3-O-α-L-arabinopyranoside	Not Available	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1CCC(C(C1O)O)O)c1ccc(c(c1)O)O)O)O
MOL013070	0.9208	0.0792	0.7851	Oroxyli Semen	quercetin-3-O-β-D-arabinopyranoside	51692880	FALSE	c1(cc(c2c(c1)oc(c(c2=O)OC1OCC(C(C1O)O)O)c1ccc(c(c1)O)O)O)O
MOL013071	0.8624	0.1376	0.8407	Oroxyli Semen	Scutellarein-7-rutinoside	5321203	FALSE	c12c(oc(cc2=O)c2ccc(cc2)O)cc(c(c1O)O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL013072	0.8803	0.1197	0.8487	Oroxyli Semen	5,7-dihydroxy-2-phenyl-6-[(2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	22524531	FALSE	O1C(C(O)C(O)C(O)C1Oc1c(O)c2c(oc(cc2=O)c2ccccc2)cc1O)CO
MOL013073	0.7652	0.2348	0.8862	Oroxyli Semen	beta-Lapachone	3885	FALSE	O1C(CCC2=C1c1c(C(=O)C2=O)cccc1)(C)C
MOL013074	0.9190	0.0810	0.8272	Peucedani Radix	6-methoxy-2-oxo-2H-chromen-7-yl beta-D-glucopyranoside	439514	FALSE	c1(c(cc2c(c1)oc(=O)cc2)OC)OC1OC(C(C(C1O)O)O)CO
MOL013075	0.8670	0.1330	0.8303	Peucedani Radix	apterin	57459455	FALSE	CC(C)(OC1OC(CO)C(O)C(O)C1O)C1Oc2ccc3ccc(=O)oc3c2C1O

MOL013076	0.9008	0.0992	0.8316	Peucedani Radix	(8S,9R)-9-hydroxy-8-(2-hydroxypropan-2-yl)-8,9-dihydrofuro[2,3-h]chromen-2-one	11817856	FALSE	CC(C)(O)C1Oc2ccc3ccc(=O)oc3c2C1O
MOL013077	0.3759	0.6241	0.8145	Peucedani Radix	Decursin	442126	FALSE	c12c(cc3c(c1)ccc(=O)o3)OC(C(C2)OC(=O)C=C(C)C)(C)C
MOL013077	0.3759	0.6241	0.8145	Peucedanidecursivi Radix	Decursin	442126	FALSE	c12c(cc3c(c1)ccc(=O)o3)OC(C(C2)OC(=O)C=C(C)C)(C)C
MOL013078	0.1262	0.8738	0.6606	Peucedani Radix	praeruptorin E	Not Available	FALSE	O1C(C(OC(=O)/C(=C\C)/C)C(OC(=O)CC(C)C)c2c1ccc1c2oc(=O)cc1)(C)C
MOL013079	0.3190	0.6810	0.7975	Peucedani Radix	dl-praeruptorin a	38347601	FALSE	c12C(C(C(Oc2ccc2c1oc(=O)cc2)(C)C)OC(=O)/C(=C\C)/C)OC(=O)C
MOL013081	0.5398	0.4602	0.7117	Peucedani Radix	Decussine	Not Available	FALSE	c1ccc2c(c1)c1c3n2C(c2c(C=C3N(CC1)C)ccnc2)C
MOL013082	0.9288	0.0712	0.7687	Peucedani Radix	p-Toluquinaldine	13414	FALSE	c12c(nc(cc2)C)ccc(c1)C
MOL013083	0.9269	0.0731	0.7989	Peucedani Radix	Skimmin (8CI)	99693	FALSE	c12c(cc(cc1)OC1OC(C(C(C1O)O)O)CO)oc(=O)cc2
MOL013084	0.8042	0.1958	0.7743	Peucedani Radix	sinodielides A	Not Available	FALSE	C12=C(CCC3C(C2C(=CC1)C)OC(=O)C3C)C
MOL013085	0.8041	0.1959	0.7333	Peucedani Radix	(9aS,9bR)-3,6,9-trimethyl-5,7,9a,9b-tetrahydro-4H-azuleno[5,4-d]furan-2-one	11117870	FALSE	C1C=C(C2C1=C(CCC1=C(C(=O)OC21)C)C)C
MOL013086	0.7444	0.2556	0.7364	Peucedani Radix	3'(S)-Acetoxy-4'(R)-hydroxy-3',4'-dihydroxanthyletin	5320881	FALSE	C1(C(Oc2c(C1O)cc1c(c2)oc(=O)cc1)(C)C)OC(=O)C
MOL013087	0.3194	0.6806	0.7969	Peucedani Radix	Peucedanocoumarin II	5320509	FALSE	c1c2c(c3c(c1)ccc(=O)o3)C(C(C(O2)(C)C)OC(=O)C)OC(=O)/C(=C/C)/C
MOL013088	0.9311	0.0689	0.7722	Peucedanidecursivi Radix	(+)-trans-Decursidinol	Not Available	FALSE	C1(COc2c(C1O)cc1c(c2)oc(=O)cc1)O
MOL013088	0.9311	0.0689	0.7722	Peucedani Radix	(+)-trans-Decursidinol	Not Available	FALSE	C1(COc2c(C1O)cc1c(c2)oc(=O)cc1)O

MOL013089	0.9038	0.0962	0.7426	Peucedani Radix	apiosylskimmin	Not Available	FALSE	C1(C(C(C(C(O1)COC1C(C(CO1)(O)CO)O)O)O)O)Oc1cc2oc(=O)ccc2cc1
MOL013090	0.8340	0.1660	0.7776	Peucedani Radix	praerosideIV	44144278	FALSE	O(C1C(Oc2c(C1)c1oc(=O)ccc1cc2)(C)C)C1OC(C(O)C(O)C1O)CO
MOL013091	0.8875	0.1125	0.8500	Peucedani Radix	Lomatin	759302	FALSE	OC1C(Oc2c(C1)c1oc(=O)ccc1cc2)(C)C
MOL013092	0.3194	0.6806	0.7969	Peucedani Radix	Pteryxin	5281425	FALSE	c12C(C(C(Oc2ccc2c1oc(=O)cc2)(C)C)OC(=O)C)OC(=O)/C(=C\C)/C
MOL013093	0.7749	0.2251	0.6774	Peucedani Radix	rubricauloside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1OC(C(O)Cc1c2oc(=O)ccc2c(OC)cc1OC)(C)C)COC1OCC(O)(C1O)CO
MOL013094	0.8826	0.1174	0.8305	Peucedani Radix	8-[(2R)-2,3-dihydroxy-3-methyl-butyl]-5,7-dimethoxy-coumarin	176970	FALSE	OC(C(O)Cc1c2oc(=O)ccc2c(OC)cc1OC)(C)C
MOL013096	0.4456	0.5544	0.7264	Peucedani Radix	3'-Hydroxy-4'-tigloyloxy-3',4'-dihydroseslin	6444285	FALSE	O1C(C(O)C(OC(=O)/C(=C/C)/C)c2c1ccc1c2oc(=O)cc1)(C)C
MOL013097	0.8574	0.1426	0.9397	Peucedani Radix	Coumurrayin	176911	FALSE	c1(=O)ccc2c(o1)c(c(cc2OC)OC)CC=C(C)C
MOL013098	0.3675	0.6325	0.7654	Peucedani Radix	[(9R)-8,8-dimethyl-2-oxo-9,10-dihydropyrano[6,5-h]chromen-9-yl] (Z)-2-methylbut-2-enoate	668081	FALSE	O1C(C(OC(=O)/C(=C\C)/C)Cc2c1ccc1c2oc(=O)cc1)(C)C
MOL013099	0.9450	0.0550	0.8521	Peucedani Radix	6-[(2S)-2,3-dihydroxy-3-methyl-butyl]-7-hydroxy-coumarin	11149722	FALSE	o1c(=O)ccc2cc(c(cc12)O)CC(C(C)(C)O)O

MOL013100	0.8820	0.1180	0.8294	Peucedani Radix	(2S)-2-(1-hydroxy-1-methyl-ethyl)-9-[(2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]oxy-2,3-dihydrofuro[3,2-g]chromen-7-one	21733113	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2OC(Cc2cc2c1oc(=O)cc2)C(O)(C)C)CO
MOL013101	0.8933	0.1067	0.8399	Peucedani Radix	rutarin_qt	44146779	FALSE	O1C(Cc2c1c(O)c1oc(=O)ccc1c2)C(O)(C)C
MOL013102	0.8900	0.1100	0.8029	Peucedani Radix	Decursinol	442127	FALSE	C1(C(Oc2c(C1)cc1c(c2)oc(=O)cc1)(C)C)O
MOL013103	0.1766	0.8234	0.6962	Peucedanidecursivi Radix	532-16-1	1781413	FALSE	c1(=O)ccc2c(o1)cc(cc2)OC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C
MOL013103	0.1766	0.8234	0.6962	Peucedani Radix	532-16-1	1781413	FALSE	c1(=O)ccc2c(o1)cc(cc2)OC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C
MOL013105	0.2097	0.7903	0.8464	Peucedani Radix	Sesibiricin	12315487	FALSE	c1(=O)ccc2c(o1)c(c(cc2OCC=C(C)C)OC)CC=C(C)C
MOL013106	0.8837	0.1163	0.8772	Peucedani Radix	NORBORNANE	9233	FALSE	C12CC(CC1)CC2
MOL013106	0.8837	0.1163	0.8772	Peucedanidecursivi Radix	NORBORNANE	9233	FALSE	C12CC(CC1)CC2
MOL013107	0.9235	0.0765	0.7799	Peucedani Radix	Sphondin	108104	FALSE	c1(c2c(c3c(c1)ccc(=O)o3)cco2)OC
MOL013108	0.9528	0.0472	0.9765	Mahoniae Folum	ISOCYCLOCITRAL	Not Available	FALSE	O=CC1C(C(C=C(C1)C)C)C
MOL013109	0.6522	0.3478	0.6191	Mahoniae Folum	METHYL 13-METHYLPENTADECANOATE	Not Available	FALSE	O(C(=O)CCCCCCCCCCCC(CC)C)C
MOL013110	0.6170	0.3830	0.7913	Gnaphalii Affinis Herba	kaurenoic acid	Not Available	FALSE	C123C(C4(C(C(C(=O)O)(CCC4)C)CC3)C)CCC(C(=C)C1)C2
MOL013111	0.3493	0.6507	0.6168	Gnaphalii Affinis Herba	SBB005938	7093249	FALSE	OC1(C(C2(C(C(CCC2)(C)C)CC1)C)CCC(O)(C)C=C)C
MOL013112	0.2011	0.7989	0.6449	Gnaphalii Affinis Herba	4-Cholesten-3-one	91477	FALSE	C12C3C(C4(C(=CC(=O)CC4)CC3)C)CCC1(C(CC2)C(CCCC(C)C)C)C
MOL013113	0.5475	0.4525	0.6838	Gnaphalii Affinis Herba	Gnaphalin	Not Available	FALSE	O1C2(C3(C(C4(C(CC3=O)C)CC(OC4=O)c3ccoc3)CCC2)CO)C1
MOL013114	0.9313	0.0687	0.9575	Gnaphalii Affinis Herba	trans-4-Hexen-1-ol	641248	FALSE	C(CC/C=C/C)O

MOL013115	0.5790	0.4210	0.7048	Gnaphalii Affinis Herba	(1S,4aS,4bR,7R,10aS)-1,4a,7-trimethyl-7-vinyl-3,4,4b,5,6,9,10,10a-octahydro-2H-phenanthrene-1-carboxylic acid	24721193	FALSE	C12C(C3C(=CC(CC3)(C=C)C)CC2)(CCCC1(C(=O)O)C)C
MOL013116	0.9513	0.0487	0.9184	Smilacis Glabrae Rhixoma	3-O-caffeoylshikimic acid	Not Available	FALSE	O(C(=O)/C=C/c1cc(c(cc1)O)O)C1CC(=CC(C1O)O)C(=O)O
MOL013117	0.5516	0.4484	0.9114	Smilacis Glabrae Rhixoma	4,7-Dihydroxy-5-methoxyl-6-methyl-8-formyl-flavan	Not Available	FALSE	c1(c(c2c(c(c1O)C=O)OC(CC2O)c1ccccc1)OC)C
MOL013118	0.9114	0.0886	0.8248	Smilacis Glabrae Rhixoma	Neoastilbin	442437	FALSE	C1(C(C(OC(C1O)C)OC1C(Oc2c(C1=O)c(cc(c2)O)O)c1ccc(c(c1)O)O)O)O
MOL013121	0.3620	0.6380	0.6843	Smilacis Glabrae Rhixoma	[(2S,3S,4R,5R)-2-[(2R,3R,4S,5S,6R)-3-acetyloxy-6-(acetyloxymethyl)-4,5-dihydroxyoxan-2-yl]oxy-4-hydroxy-2,5-bis[[(E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]oxymethyl]oxolan-3-yl] (E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoate	11658052	FALSE	c1(cc(c(cc1)O)OC)/C=C/C(=O)OC1C(C(OC1(COC(=O)/C=C/c1cc(c(cc1)O)OC)OC1OC(C(C(C1OC(=O)C)O)O)COC(=O)C)COC(=O)/C=C/c1ccc(c(c1)OC)O)O

MOL013123	0.3340	0.6660	0.6619	Smilacis Glabrae Rhixoma	Smiglaside D	Not Available	FALSE	C1(C(C(OC1(COC(=O)/C=C/c1ccc(cc1)O)OC1OC(C(C(C1OC(=O)C)O)OC(=O)C)COC(=O)C)COC(=O)/C=C/c1ccc(c(c1)OC)O)O)OC(=O)/C=C/c1cc(c(cc1)O)OC
MOL013124	0.3498	0.6502	0.6822	Smilacis Glabrae Rhixoma	Smiglaside E	11764506	FALSE	C1(C(C(OC1(COC(=O)/C=C/c1ccc(cc1)O)OC1OC(C(C(C1OC(=O)C)O)O)COC(=O)C)COC(=O)/C=C/c1ccc(c(c1)OC)O)O)OC(=O)/C=C/c1cc(c(cc1)O)OC
MOL013127	0.8891	0.1109	0.9729	Smilacis Glabrae Rhixoma	Tulipane	68352	FALSE	C1CC(=C)C(=O)O1
MOL013128	0.9026	0.0974	0.8377	Smilacis Glabrae Rhixoma	isoastilbin	Not Available	FALSE	O1C(OC2C(Oc3c(C2=O)c(O)cc(O)c3)c2cc(O)cc(O)c2)C(O)C(O)C(O)C1C
MOL013129	0.9139	0.0861	0.8286	Smilacis Glabrae Rhixoma	(2R,3R)-2-(3,5-dihydroxyphenyl)-3,5,7-trihydroxychroman-4-one	5320468	FALSE	OC1C(Oc2c(C1=O)c(O)cc(O)c2)c1cc(O)cc(O)c1
MOL013130	0.9285	0.0715	0.7800	Arisaematis Rhizoma	1-methyl-1H-indene	12337159	FALSE	c12c(cccc2)C=CC1C
MOL013131	0.4775	0.5225	0.6362	Arisaematis Rhizoma	12,15-Octadecadienoic acid, methyl ester	5365571	FALSE	C(=O)(CCCCCCCCCC/C=C/C/C=C/CC)OC
MOL013132	0.9249	0.0751	0.9351	Arisaematis Rhizoma	1-isopentylpyrrole	19863974	FALSE	c1cccn1CCC(C)C
MOL013133	0.8952	0.1048	0.9294	Arisaematis Rhizoma	2-Allylfuran	530402	FALSE	c1coc(c1)CC=C
MOL013134	0.9404	0.0596	0.8859	Arisaematis Rhizoma	2-(2-furylmethyl)-5-methylfuran	595524	FALSE	o1c(ccc1C)Cc1ccco1
MOL013135	0.9249	0.0751	0.9270	Arisaematis Rhizoma	1-Phenylbutene-2	5356732	FALSE	c1(ccccc1)C/C=C/C
MOL013136	0.8953	0.1047	0.9698	Arisaematis Rhizoma	Furfuryl acetate	12170	FALSE	c1(COC(=O)C)ccco1
MOL013137	0.9593	0.0407	0.8747	Arisaematis Rhizoma	2-methyl-3-(z-methylpropenoateyl)-6-metyleneureido-3,ene-hydropyran	Not Available	FALSE	N(C(=O)N=C)C1CC=C(C(O1)C)/C=C/C(=O)OC
MOL013138	0.8640	0.1360	0.9075	Arisaematis Rhizoma	2,7-Dimethyloxepine	578868	FALSE	O1C(=CC=CC=C1C)C

MOL013139	0.9281	0.0719	0.9625	Arisaematis Rhizoma	3-acetamino-2-piperidone	68907166	FALSE	C1(C(=O)NCCC1)NC(=O)C
MOL013140	0.9315	0.0685	0.8856	Arisaematis Rhizoma	3-isopropyl-6-isobutyl-2,5-piperazinedione	Not Available	FALSE	N1C(=O)C(NC(=O)C1CC(C)C)C(C)C
MOL013141	0.9215	0.0785	0.9573	Arisaematis Rhizoma	3-methyl-6-sec-butyl-2,5-piperazinedione	25765999	FALSE	N1C(=O)C(NC(=O)C1C(CC)C)C
MOL013142	0.9264	0.0736	0.9373	Arisaematis Rhizoma	3,4-DI-O-Methyl-1-arabinopyranose	14337662	FALSE	C1(O)C(O)C(OC)C(OC)CO1
MOL013143	0.8540	0.1460	0.7184	Arisaematis Rhizoma	(+)-3,8-dimethyl-5(1-methylethylethylidene)-1,2,3,4,5,6,7,8-octahydroazulene-6-one	Not Available	FALSE	C1(=O)CC2C3C(C1)CC(C(=C3CC2C)C)C
MOL013144	0.4749	0.5251	0.6400	Arisaematis Rhizoma	Methyl (6E,9E)-6,9-octadecadienoate	5365662	FALSE	C(=O)(CCCC/C=C/C/C=C/CCCCCCCC)OC
MOL013145	0.4753	0.5247	0.6402	Arisaematis Rhizoma	Methyl-7,10-octadecadienoate	5365663	FALSE	C(=O)(CCCCC/C=C/C/C=C/CCCCCCC)OC
MOL013147	0.9382	0.0618	0.9452	Arisaematis Rhizoma	2-propionamido benzoic acid	3264674	FALSE	c1(c(NC(=O)CC)cccc1)C(=O)O
MOL013148	0.8847	0.1153	0.9060	Arisaematis Rhizoma	2,2-Methylenebisfuran	70972	FALSE	c1ccoc1Cc1occc1
MOL013149	0.5645	0.4355	0.6185	Arisaematis Rhizoma	Heptatriacontane	23598	FALSE	C(CCCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCCC
MOL013150	0.9152	0.0848	0.9527	Arisaematis Rhizoma	(2S)-2-amyl-2-methyl-oxirane	11062413	FALSE	O1C(C1)(C)CCCCC

MOL013151	0.5288	0.4712	0.6067	Arisaematis Rhizoma	Z-24-Tritriaconten-2-one	5364607	FALSE	O=C(CCCCCCCCCCCCCCCCCCCCCC/C=C/CCCCCCCC)C
MOL013152	0.8425	0.1575	0.7950	Arisaematis Rhizoma	apigenin-6-c-arabinosyl-8-c-galactoside	Not Available	FALSE	C1(COC(C(C1O)O)c1c(c(c2c(c1O)c(=O)cc(o2)c1ccc(cc1)O)C1C(C(C(C(O1)CC)O)O)O)O)O
MOL013153	0.8732	0.1268	0.7542	Arisaematis Rhizoma	apigenin-6-c-galactosyl-8-c-arabinoside	Not Available	FALSE	C1(C(OC(C(C1O)O)c1c(c(c2c(c1O)c(=O)cc(o2)c1ccc(cc1)O)C1C(C(C(CO1)O)O)O)O)O)O
MOL013154	0.8807	0.1193	0.7688	Arisaematis Rhizoma	apigenin-6,8-di-c-β-D-galactoside	Not Available	FALSE	C1(C(OC(C(C1O)O)c1c(c(c2c(c1O)c(=O)cc(o2)c1ccc(cc1)O)C1C(C(C(C(O1)CO)O)O)O)O)O)O
MOL013155	0.8807	0.1193	0.7688	Arisaematis Rhizoma	apigenin-6,8-di-c-β-D-glucopyranoside	Not Available	FALSE	C1(C(OC(C(C1O)O)c1c(c(c2c(c1O)c(=O)cc(o2)c1ccc(cc1)O)C1C(C(C(C(O1)CO)O)O)O)O)O)O
MOL013157	0.9160	0.0840	0.8537	Arisaematis Rhizoma	betonicine	164643	FALSE	C1([N+](CC(C1)O)(C)C)C(=O)O
MOL013159	0.8632	0.1368	0.7755	Arisaematis Rhizoma	gammaeudesmane	Not Available	FALSE	C1(C2C(C(=O)CC1)(CCC1C2OC(=O)C1C)C)(O)C
MOL013162	0.8871	0.1129	0.7372	Arisaematis Rhizoma	(S)-3-hydroxypalmitic acid	10989404	FALSE	C(CCCCCCCCCCCCC)C(CC(=O)O)O
MOL013163	0.9225	0.0775	0.8203	Arisaematis Rhizoma	Inden	7219	FALSE	c12c(C=CC1)cccc2
MOL013165	0.5151	0.4849	0.6037	Arisaematis Rhizoma	octadecanoic acid,2-hydroxy-,methyl ester	Not Available	FALSE	C(CCCCCCCCCCCCCCCC)C(C(=O)OC)O
MOL013167	0.9631	0.0369	0.7579	Arisaematis Rhizoma	penylglucosazone	Not Available	FALSE	c1ccc(cc1)N/N=C\C(=N/Nc1ccccc1)\C(O)C(O)C(CO)O
MOL013168	0.8728	0.1272	0.7911	Arisaematis Rhizoma	schaftoside	Not Available	FALSE	c12c(C3OC(C(C(C3O)O)O)CO)c(c(c(c1c(=O)cc(o2)c1ccc(cc1)O)O)C1OC(C(C(C1O)O)O)CO)O
MOL013169	0.9082	0.0918	0.9154	Arisaematis Rhizoma	2-methyl-5-propylfuran	5191689	FALSE	c1cc(oc1CCC)C
MOL013171	0.8581	0.1419	0.7632	Sapindi Mukorossi Semen	1,6-Dihydroxy-3,7-dimethoxyxanthone	5316766	FALSE	o1c2c(c(=O)c3c1cc(O)c(OC)c3)c(O)cc(OC)c2
MOL013172	0.5258	0.4742	0.7369	Sapindi Mukorossi Semen	Mukuroziside I	Not Available	FALSE	O1C(C(C(C(C1OC1C(OC(C(C1O)O)CO)OC/C(=C\C/C(=C/CC/C(=C/OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)OC1OC(C(C(C1O)O)O)C)O)CO)/C)/C)/C)O)O)O)C

MOL013173	0.4960	0.5040	0.7485	Sapindi Mukorossi Semen	Mukuroziosid e II	Not Available	FALSE	O1C(C(C(C(C1OC1C(C(OC(C1OC1OC(C(C(C1O)O)O)C)OCC(CCC/C(=C/CC/C(=C/OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)C)OC1OC(C(C(C1O)O)O)C)O)CO)/C)/C)C)CO)O)O)O)C
MOL013174	0.6885	0.3115	0.8370	Sapindi Mukorossi Semen	Mukurozisapo nin E	Not Available	FALSE	C1(C(C(OC(C1O)C)OC1C(OCC(C1O)O)OC1C(C2C(CC1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)O)C)C)(C)CO)O)OC1OCC(C(C1O)O)OC(=O)C
MOL013175	0.7708	0.2292	0.7944	Sapindi Mukorossi Semen	Mukurozisapo nin Y	Not Available	FALSE	C1C(C(C(C(O1)OC1C(C(OC(C1O)C)OC1C(OCC(C1O)O)OC1C(C2C(CC1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(CCC(C1)(C)C)C(=O)OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)CO)O)O)CO)C)C)C)(C)CO)O)O)O)O
MOL013176	0.3880	0.6120	0.7427	Peucedanidecursivi Radix	2-[(2S)-7-oxo-2,3-dihydrofuro[4,5-g]chromen-2-yl]propan-2-yl (E)-2-methylbut-2-enoate	906525	FALSE	C(=O)(/C(=C/C)/C)OC(C)(C)C1Oc2cc3c(ccc(=O)o3)cc2C1
MOL013177	0.1295	0.8705	0.6315	Peucedanidecursivi Radix	[(6R,7S)-8,8-dimethyl-7-(3-methylbut-2-enoyloxy)-2-oxo-6,7-dihydropyrano[5,6-g]chromen-6-yl] 3-methylbut-2-enoate	15521791	FALSE	O1C(C(C(c2c1cc1oc(=O)ccc1c2)OC(=O)C=C(C)C)OC(=O)C=C(C)C)(C)C
MOL013179	0.9109	0.0891	0.8696	Gleditsiae Spina	fisetin	5281614	TRUE	Oc1cc2c(cc1)c(=O)c(O)c(o2)c1ccc(O)c(O)c1
MOL013181	0.6160	0.3840	0.7432	Gleditsiae Fructus Abnormalis	gleditsioside N	Not Available	FALSE	O1CC(C(C(C1OC1C(C(COC1OCC1OC(C(C(C1O)O)O)OC1C(C2C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3)(C)C)C(=O)OC2OC(C(C(C2OC2OC(C(C(C2O)O)O)OC2OCC(C(C2O)OC2OCC(C(C2O)O)O)O)O)C)OC(=O)/C(=C/CCC(O)(C)C=C)/CO)O)COC(=O)/C(=C\CCC(O)(C)C=C)/C)C)C)(CC1)C)(C)C)O)O)O)O)O
MOL013182	0.5972	0.4028	0.7375	Gleditsiae Fructus Abnormalis	gleditsioside O	Not Available	FALSE	O1CC(C(C(C1OC1C(C(COC1OCC1OC(C(C(C1O)O)O)OC1C(C2C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3)(C)C)C(=O)OC2OC(C(C(C2OC2OC(C(C(C2O)O)O)OC2OCC(C(C2O)OC2OCC(C(C2O)O)O)O)O)C)OC(=O)/C(=C/CCC(O)(C)C=C)/C)O)COC(=O)/C(=C\CCC(O)(C)C=C)/C)C)C)(CC1)C)(C)C)O)O)O)O)O

MOL013183	0.4995	0.5005	0.7195	Gleditsiae Fructus Abnormalis	gleditsioside P	Not Available	FALSE	O1CC(C(C(C1OC1C(C(COC1OCC1OC(C(C(C1O)O)O)OC1C(C2C(C3C(CC2)(C2(C(=CC3)C3C(CC2)(CCC(C3)(C)C)C(=O)OC2OC(C(C(C2OC2OC(C(C(C2O)O)OC2OCC(C(C2O)OC2OCC(C(C2O)O)O)O)O)C)OC(=O)/C(=C/CCC(O)(C)C=C)/C)O)COC(=O)/C(=C\CCC(OC2OCC(C(C2OC(=O)/C(=C/CCC(O)(C)C=C)/C)O)O)(C)C=C)/C)C)C)(CC1)C)(C)C)O)O)O)O)O
MOL013184	0.6192	0.3808	0.7531	Gleditsiae Fructus Abnormalis	gleditsioside Q	Not Available	FALSE	O1CC(C(C(C1OC1C(C(COC1OCC1OC(C(C(C1O)O)O)OC1C(C2C(C3C(CC2)(C2(C(=CC3)C3C(C(C2)O)(CCC(C3)(C)C)C(=O)OC2OC(C(C(C2OC2OC(C(C(C2O)O)OC2OCC(C(C2O)OC2OCC(C(C2O)O)O)O)O)C)O)O)COC(=O)/C(=C/CCC(O)(C)C=C)/CO)C)C)(CC1)C)(C)C)O)O)O)O)O
MOL013186	0.8664	0.1336	0.6358	Litseae Fructus	cubeben camphor	Not Available	FALSE	C12C3(C(CCC1C(C)C)C)C2C(CC3)(O)C
MOL013195	0.6774	0.3226	0.7976	Litseae Fructus	Litsoeine	31415	FALSE	O(c1c2c3C(NCCc3cc1OC)Cc1c2cc(OC)c(O)c1)C
MOL013197	0.6702	0.3298	0.6623	Litseae Fructus	piperenol B	Not Available	FALSE	C1(C(C(C(C=C1)OC(=O)c1ccccc1)O)O)(O)COC(=O)c1ccccc1
MOL013198	0.5589	0.4411	0.7536	Litseae Fructus	Tephrosin	Not Available	FALSE	C12(c3c(cc(c(c3)OC)OC)OCC1Oc1c(C2=O)ccc2c1C=CC(O2)(C)C)O
MOL013200	0.6664	0.3336	0.6711	Litseae Fructus	zeylenol	51693478	FALSE	C1(C(C(C(C=C1)OC(=O)c1ccccc1)O)(O)COC(=O)c1ccccc1)O
MOL013201	0.8566	0.1434	0.6486	Litseae Fructus	bicyclosesquiphellandrene	15694800	FALSE	C1(CCC(C2CCC(=C)C=C12)C)C(C)C
MOL013202	0.9499	0.0501	0.8968	Anisi Stellati Fructus	3-O-Feruloylquinic acid	25175592	FALSE	O(C1CC(O)(CC(O)C1O)C(=O)O)C(=O)/C=C\c1cc(OC)c(O)cc1
MOL013203	0.9542	0.0458	0.9531	Anisi Stellati Fructus	Anisketone	31231	FALSE	c1(ccc(cc1)OC)CC(=O)C
MOL013203	0.9542	0.0458	0.9531	Foeniculi Fructus	Anisketone	31231	FALSE	c1(ccc(cc1)OC)CC(=O)C
MOL013204	0.9315	0.0685	0.9571	Anisi Stellati Fructus	WLN: VHR DVH	12173	FALSE	c1(ccc(cc1)C=O)C=O
MOL013205	0.9412	0.0588	0.9348	Anisi Stellati Fructus	p-Methoxycinnamaldehyde	641294	FALSE	c1(ccc(cc1)OC)/C=C/C=O
MOL013206	0.8741	0.1259	0.7549	Polygoni Avicularis Herba	desmanthin-1	Not Available	FALSE	O1C(C(O)C(O)C(OC(=O)c2cc(O)c(O)c(O)c2)C1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)c(O)c1)C
MOL013207	0.9278	0.0722	0.9021	Polygoni Avicularis Herba	isotachioside	15098566	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)c1c(cc(cc1)O)OC
MOL013207	0.9278	0.0722	0.9021	Polygoni Cuspidati Rhizoma Et Radix	isotachioside	15098566	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)c1c(cc(cc1)O)OC
MOL013210	0.9637	0.0363	0.8195	Caryophylliflos	Eugenin	10189	FALSE	o1c2c(c(O)cc(OC)c2)c(=O)cc1C
MOL013211	0.9672	0.0328	0.8403	Caryophylliflos	Eugenitin	3083581	FALSE	c1(cc(=O)c2c(o1)cc(c(c2O)C)OC)C
MOL013212	0.1358	0.8642	0.7397	Caryophylliflos	Euglobal-Ia1	Not Available	FALSE	c1(c(c(c2c(c1C=O)OC1(C(C2CC(C)C)(CC(C=C1)C(C)C)C)C)O)C=O)O

MOL013213	0.7448	0.2552	0.8233	Smilacis Glabrae Rhixoma	Isoeruboside_B	Not Available	FALSE	C1(C(C(OC(C1O)CO)OC1C(C(OC(C1O)CO)OC1C(C(C(OC1CO)OC1CC2C(CC1)(C1C(CC2O)C2C(CC1)(C1C(C2)OC2(C1C)CCC(C)CO2)C)C)O)O)OC1OC(C(C(C1O)O)O)CO)O)O
MOL013213	0.7448	0.2552	0.8233	Caryophylliflos	Isoeruboside_B	Not Available	FALSE	C1(C(C(OC(C1O)CO)OC1C(C(OC(C1O)CO)OC1C(C(C(OC1CO)OC1CC2C(CC1)(C1C(CC2O)C2C(CC1)(C1C(C2)OC2(C1C)CCC(C)CO2)C)C)O)O)OC1OC(C(C(C1O)O)O)CO)O)O
MOL013214	0.3431	0.6569	0.7584	Caryophylliflos	Isoeruboside_B_qt	Not Available	FALSE	OC1CC2C(CC1)(C1C(CC2O)C2C(CC1)(C1C(C2)OC2(C1C)CCC(C)CO2)C)C
MOL013214	0.3431	0.6569	0.7584	Smilacis Glabrae Rhixoma	Isoeruboside_B_qt	Not Available	FALSE	OC1CC2C(CC1)(C1C(CC2O)C2C(CC1)(C1C(C2)OC2(C1C)CCC(C)CO2)C)C
MOL013215	0.9426	0.0574	0.9696	Caryophylliflos	Lilac alcohol A	Not Available	FALSE	O1C(CCC1(C)C=C)C(CO)C
MOL013216	0.9263	0.0737	0.9396	Caryophylliflos	Butyrone	31246	FALSE	C(=O)(CCC)CCC
MOL013217	0.9222	0.0778	0.9605	Caryophylliflos	m-Anisaldehyde	11569	FALSE	c1c(cccc1OC)C=O
MOL013219	0.7568	0.2432	0.8489	Caryophylliflos	Strictosamide_qt	Not Available	FALSE	c1cccc2c1c1c([nH]2)C2N(CC1)C(=O)C1=COC(C(C1C2)C=C)O
MOL013220	0.9158	0.0842	0.8895	Caryophylliflos	trans-3,5-dimethyl-1,6-octadien	Not Available	FALSE	C=CC(CC(/C=C/C)C)C
MOL013221	0.9069	0.0931	0.7258	Caryophylliflos	(2S,4aS,8aR)-2,5,5,8a-tetramethyl-3,4,4a,6-tetrahydro-2H-chromene	11116929	FALSE	C1(CCC2C(O1)(C=CCC2(C)C)C)C
MOL013222	0.9434	0.0566	0.9422	Caryophylliflos	m-Acetoxyanisole	138507	FALSE	c1c(cc(cc1)OC(=O)C)OC
MOL013223	0.9207	0.0793	0.9445	Caryophylliflos	Lutidine, beta-	10823	FALSE	c1(cccnc1)CC
MOL013225	0.9497	0.0503	0.8160	Caryophylliflos	6,6-dimethyl-Bicyclo[3.1.1]hept-2-ene-2-carboxaldehyd	Not Available	FALSE	C12C(=C)C(=O)C(CC1(C)C)C2
MOL013227	0.9591	0.0409	0.8774	Caryophylliflos	Acetisoeugenol	876160	FALSE	c1(c(cc(cc1)/C=C/C)OC)OC(=O)C
MOL013228	0.8450	0.1550	0.6560	Caryophylliflos	caryophyllene alcohol	Not Available	FALSE	C12C3(CC(CCC1C(C2)(C)C)(CCC3)C)O
MOL013229	0.8450	0.1550	0.6560	Caryophylliflos	caryophyllenol	Not Available	FALSE	OC12C3C(C(C3)(C)C)CCC(C1)(CCC2)C

MOL013230	0.8305	0.1695	0.7441	Caryophylliflos	Casuariin	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OC(C1C(c3c(c(c(c2c3C(=O)O1)O)O)O)O)C1C(O)COC(=O)c2cc(c(c(c2c2c(C(=O)O1)cc(c(c2O)O)O)O)O)O)O)O
MOL013231	0.8342	0.1658	0.7254	Caryophylliflos	Chebulagic acid	Not Available	FALSE	c1(c(c2c(cc1O)C(=O)OCC1OC(C3C(C1OC(=O)C(Cc1c(C(=O)O3)cc(c(c1O)O)O)C(O)C(=O)O)CC(=O)O)OC(=O)c1c2c(c(c(c1)O)O)O)OC(=O)c1cc(c(c(c1)O)O)O)O)O
MOL013232	0.8406	0.1594	0.7115	Caryophylliflos	Cubenol	12304222	FALSE	OC12C(C(CCC1C)C(C)C)C=C(CC2)C
MOL013233	0.2056	0.7944	0.7254	Dioscoreae Septemlo Bae Rhizoma	EINECS 213-897-0	Not Available	FALSE	C12C3(C(CC1OC1(C2C)CCC(CO1)C)C1C(CC3)C2(C(=CC1)CC(CC2)OC(=O)C)C)C
MOL013233	0.2056	0.7944	0.7254	Dioscoreae Hypoglaucae Rhizoma	EINECS 213-897-0	Not Available	FALSE	C12C3(C(CC1OC1(C2C)CCC(CO1)C)C1C(CC3)C2(C(=CC1)CC(CC2)OC(=O)C)C)C
MOL013234	0.7554	0.2446	0.7994	Dioscoreae Septemlo Bae Rhizoma	protogracillin	Not Available	FALSE	C12(C(C3C(C4(C(=CC3)CC(OC3C(C(OC5C(C(C(C(O5)CO)O)O)O)C(C(O3)CO)O)OC3C(C(C(C(O3)C)O)O)O)CC4)C)CC2)CC2C1C(C(O2)(CCC(COC1C(C(C(C(O1)CO)O)O)O)C)O)C)C
MOL013234	0.7554	0.2446	0.7994	Dioscoreae Hypoglaucae Rhizoma	protogracillin	Not Available	FALSE	C12(C(C3C(C4(C(=CC3)CC(OC3C(C(OC5C(C(C(C(O5)CO)O)O)O)C(C(O3)CO)O)OC3C(C(C(C(O3)C)O)O)O)CC4)C)CC2)CC2C1C(C(O2)(CCC(COC1C(C(C(C(O1)CO)O)O)O)C)O)C)C
MOL013235	0.3408	0.6592	0.7742	Dioscoreae Septemlo Bae Rhizoma	protogracillin_qt	Not Available	FALSE	C12(C(C3C(C4(C(=CC3)CC(O)CC4)C)CC2)CC2C1C(C(O2)(CCC(CO)C)O)C)C
MOL013235	0.3408	0.6592	0.7742	Dioscoreae Hypoglaucae Rhizoma	protogracillin_qt	Not Available	FALSE	C12(C(C3C(C4(C(=CC3)CC(O)CC4)C)CC2)CC2C1C(C(O2)(CCC(CO)C)O)C)C
MOL013236	0.2056	0.7944	0.7254	Dioscoreae Septemlo Bae Rhizoma	yamogenin acetate	Not Available	FALSE	O1C2C(C3(C(C4C(CC3)C3(C(=CC4)CC(OC(=O)C)CC3)C)C2)C)C(C21OCC(CC2)C)C
MOL013236	0.2056	0.7944	0.7254	Dioscoreae Hypoglaucae Rhizoma	yamogenin acetate	Not Available	FALSE	O1C2C(C3(C(C4C(CC3)C3(C(=CC4)CC(OC(=O)C)CC3)C)C2)C)C(C21OCC(CC2)C)C
MOL013237	0.8537	0.1463	0.6679	Citri Sarcodactylis Fructus	CH3COSH	10484	FALSE	SC(=O)C
MOL013239	0.9061	0.0939	0.9499	Citri Sarcodactylis Fructus	Lupetazine	7818	FALSE	N1(CCN(CC1)C)C
MOL013240	0.9296	0.0704	0.9661	Citri Sarcodactylis Fructus	(3R)-3-methylpentanal	12477208	FALSE	C(=O)CC(CC)C
MOL013241	0.9550	0.0450	0.9428	Citri Sarcodactylis Fructus	[(2S,3S)-3-methyl-3-(4-methylpent-3-enyl)oxiran-2-yl]methyl acetate	23255879	FALSE	O1C(C1(CCC=C(C)C)C)COC(=O)C
MOL013242	0.9554	0.0446	0.9502	Citri Sarcodactylis Fructus	delta-Terpinene	Not Available	FALSE	C1(CC=C(C(C)C)C=C1)C
MOL013243	0.9360	0.0640	0.9544	Citri Sarcodactylis Fructus	Cyclohexanone,2-pentyl	Not Available	FALSE	C1(=O)C(CCCC1)CCCCC

MOL013244	0.9569	0.0431	0.9671	Citri Sarcodactylis Fructus	Cyclohexanone,2-butyl	12330567	FALSE	C1(=O)C(CCCC1)CCCC
MOL013245	0.9318	0.0682	0.9849	Citri Sarcodactylis Fructus	Cyclohexanol, 4-methoxy	140332	FALSE	C1(CCC(CC1)OC)O
MOL013246	0.9646	0.0354	0.8202	Citri Sarcodactylis Fructus	3,4,7-trimethoxycoumarin	606454	FALSE	o1c(=O)c(c(c2ccc(cc12)OC)OC)OC
MOL013247	0.9020	0.0980	0.9598	Citri Sarcodactylis Fructus	Hydroxybutyric acid-	10413	FALSE	OCCCC(=O)O
MOL013248	0.8193	0.1807	0.6101	Citri Sarcodactylis Fructus	Bicyclo[7,2,0]undec-4-ene,4,11,11-trimethyl-8-methyl	Not Available	FALSE	C12CC/C(=C\CCC(C1CC2(C)C)C)/C
MOL013249	0.9155	0.0845	0.8425	Citri Sarcodactylis Fructus	Bicyclo[6.3.0]undeca-1,7-dien-3-one, 5,5-dimethyl-	5372011	FALSE	O=C1CC(CC=C2C(=C1)CCC2)(C)C
MOL013250	0.8409	0.1591	0.6193	Citri Sarcodactylis Fructus	Bicyclo[5,2,0]nonane,2-methylene-4,8,8-trimethyl-4-vinyl	Not Available	FALSE	C12C(=C)CC(CCC1C(C2)(C)C)(C=C)C
MOL013251	0.9332	0.0668	0.7778	Citri Sarcodactylis Fructus	Bicyclo[3,1,1]hept-2-en-6-ol,2,7,7-trimethyl-,acetate	Not Available	FALSE	C12C(=CCC(C1OC(=O)C)C2(C)C)C
MOL013252	0.9334	0.0666	0.9518	Citri Sarcodactylis Fructus	(2E,6S)-2,6-dimethylocta-2,7-diene-1,6-diol	11206026	FALSE	C(/C(=C/CCC(C=C)(O)C)/C)O
MOL013253	0.8658	0.1342	0.7370	Citri Sarcodactylis Fructus	5,2',5'-Trihydroxy-6,7,8-trimethoxyflavone	5322092	FALSE	COc1c(OC)c2c(c(c1OC)O)c(=O)c(c(o2)c1cc(ccc1O)O)O
MOL013254	0.9453	0.0547	0.9565	Citri Sarcodactylis Fructus	2-Oxepanone,7-butyl	Not Available	FALSE	O1C(=O)CCCCC1CCCC

MOL013255	0.9324	0.0676	0.9396	Citri Sarcodactylis Fructus	6,7-Dihydrogeraniol	5365836	FALSE	C(/C=C(/CCCC(C)C)\C)O
MOL013256	0.9356	0.0644	0.9480	Citri Sarcodactylis Fructus	linalool oxide, trans-pyranoid	6427788	FALSE	C1(C(CCC(O1)(C)C=C)O)(C)C
MOL013257	0.9596	0.0404	0.9673	Citri Sarcodactylis Fructus	cis-2,8-Menthadien-1-ol	111274	FALSE	C1(C=CC(CC1)C(=C)C)(O)C
MOL013258	0.9353	0.0647	0.9542	Citri Sarcodactylis Fructus	trans,trans-2,6-Dimethyl-2,6-octadiene-1,8-diol	5363397	FALSE	C(/C(=C/CC/C(=C/CO)/C)/C)O
MOL013259	0.9200	0.0800	0.9157	Citri Sarcodactylis Fructus	2,4,4-Trimethyl-3-(3-oxobutyl)cyclohex-2-enone	596567	FALSE	C1(=O)C(=C(C(CC1)(C)C)CCC(=O)C)C
MOL013260	0.9720	0.0280	0.8671	Citri Sarcodactylis Fructus	2,3-dehydro-1,8-cineole	11564505	FALSE	C12(OC(C(C=C1)CC2)(C)C)C
MOL013261	0.9308	0.0692	0.9353	Citri Sarcodactylis Fructus	1,7-Octadien-3-ol,3,7-dimethyl	Not Available	FALSE	C=CC(CCCC(=C)C)(O)C
MOL013262	0.8833	0.1167	0.8118	Citri Sarcodactylis Fructus	4-Methoxydibenzyl	139728	FALSE	C(Cc1ccccc1)c1ccc(cc1)OC
MOL013263	0.9138	0.0862	0.9108	Citri Sarcodactylis Fructus	.alpha.-Myrcene	519324	FALSE	C(CC(=C)C)CC(=C)C=C
MOL013264	0.9329	0.0671	0.9370	Citri Sarcodactylis Fructus	α-Citronellal	Not Available	FALSE	O=CCC(CCCC(=C)C)C
MOL013265	0.9464	0.0536	0.9644	Citri Sarcodactylis Fructus	1,2-Cyclohexanediol,1-methyl-4-(1-methylethyl)	24862667	FALSE	C1(C(CC(CC1)C(C)C)O)(O)C
MOL013266	0.9279	0.0721	0.9578	Zanthoxyli Pericarpium	(2S)-3-methoxypropane-1,2-diol	156179	FALSE	O(CC(O)CO)C
MOL013267	0.9102	0.0898	0.8703	Zanthoxyli Pericarpium	(E)-4-[(1R)-2,2-dimethyl-6-methylenecyclohexyl]but-3-en-2-one	11389922	FALSE	O=C(/C=C/C1C(CCCC1=C)(C)C)C

MOL013268	0.9597	0.0403	0.8096	Zanthoxyli Pericarpium	cis-Pinene hydrate	1268143	FALSE	OC1(C2C(C(C2)CC1)(C)C)C
MOL013270	0.8481	0.1519	0.7759	Zanthoxyli Pericarpium	Haplopine	165368	FALSE	o1c2[nH]c3c(c(OC)c2cc1)ccc(=O)c3OC
MOL013271	0.8691	0.1309	0.8625	Zanthoxyli Pericarpium	Kokusaginin	10227	FALSE	o1c2nc3c(c(OC)c2cc1)cc(OC)c(OC)c3
MOL013272	0.7344	0.2656	0.7235	Zanthoxyli Pericarpium	nerohdyl acetate	Not Available	FALSE	O(C(CC/C=C(/CCC=C(C)C)\C)(C)C=C)C(=O)C
MOL013273	0.8486	0.1514	0.6614	Zanthoxyli Pericarpium	Dymel A	8254	FALSE	O(C)C
MOL013274	0.6998	0.3002	0.6818	Zanthoxyli Pericarpium	sanshool	Not Available	FALSE	C(=O)(/C=C/CC/C=C/C=C\C=C\C)NCC(C)C
MOL013275	0.6751	0.3249	0.8428	Zanthoxyli Pericarpium	Schinifoline	133504	FALSE	O=c1cc(n(c2c1cccc2)C)CCCCCCC
MOL013276	0.7903	0.2097	0.8319	Citri Exocarpium Rubrum	poncirin	45359875	FALSE	c12c(C(=O)CC(O1)c1ccc(cc1)OC)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL013276	0.7903	0.2097	0.8319	Citri Grandis Exocarpium	poncirin	45359875	FALSE	c12c(C(=O)CC(O1)c1ccc(cc1)OC)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL013276	0.7903	0.2097	0.8319	Aurantii Fructus Immaturus	poncirin	45359875	FALSE	c12c(C(=O)CC(O1)c1ccc(cc1)OC)c(cc(c2)OC1C(OC2C(C(C(C(O2)C)O)O)O)C(C(C(O1)CO)O)O)O
MOL013277	0.6681	0.3319	0.9391	Citri Grandis Exocarpium	Isosinensetin	632135	FALSE	c1(cc(=O)c2c(o1)c(c(cc2OC)OC)OC)c1cc(c(cc1)OC)OC
MOL013277	0.6681	0.3319	0.9391	Aurantii Fructus Immaturus	Isosinensetin	632135	FALSE	c1(cc(=O)c2c(o1)c(c(cc2OC)OC)OC)c1cc(c(cc1)OC)OC
MOL013278	0.6530	0.3470	0.9362	Aurantii Fructus Immaturus	4',5,7,8-Tetramethoxy flavone	629964	FALSE	c12c(c(cc(c1OC)OC)OC)c(=O)cc(o2)c1ccc(cc1)OC
MOL013278	0.6530	0.3470	0.9362	Citri Grandis Exocarpium	4',5,7,8-Tetramethoxy flavone	629964	FALSE	c12c(c(cc(c1OC)OC)OC)c(=O)cc(o2)c1ccc(cc1)OC
MOL013279	0.7412	0.2588	0.9596	Aurantii Fructus Immaturus	5,7,4'-Trimethylapigenin	79730	TRUE	c12c(c(cc(c2)OC)OC)c(=O)cc(o1)c1ccc(cc1)OC
MOL013279	0.7412	0.2588	0.9596	Citri Grandis Exocarpium	5,7,4'-Trimethylapigenin	79730	TRUE	c12c(c(cc(c2)OC)OC)c(=O)cc(o1)c1ccc(cc1)OC
MOL013280	0.8449	0.1551	0.7126	Polygoni Cuspidati Rhizoma Et Radix	(-)-3-Hydroxy-4-methoxy-8-9-methylenedioxy pterocarpan	Not Available	FALSE	c1(ccc2c(c1OC)OCC1C2Oc2c1cc1c(c2)OCO1)O
MOL013281	0.8495	0.1505	0.8375	Polygoni Cuspidati Rhizoma Et Radix	6,8-Dihydroxy-7-methoxyxanthone	5316798	FALSE	c1cccc2c1c(=O)c1c(o2)cc(c(c1O)OC)O
MOL013282	0.9627	0.0373	0.8156	Polygoni Cuspidati Rhizoma Et Radix	7-hydroxy-2,5-dimethyl-chromone	5316891	FALSE	c1(cc(=O)c2c(o1)cc(cc2C)O)C

MOL013283	0.8992	0.1008	0.7965	Polygoni Cuspidati Rhizoma Et Radix	3,4,3',5'-Tetrahydroxystilbene-3-glucoside	Not Available	FALSE	c1c(c(cc(c1)/C=C\c1cc(cc(c1)O)O)OC1C(C(C(C(O1)CO)O)O)O)O
MOL013285	0.9363	0.0637	0.7375	Polygoni Cuspidati Rhizoma Et Radix	Citreorosein	361512	FALSE	Oc1c2c(C(=O)c3c(C2=O)c(O)cc(O)c3)cc(c1)CO
MOL013286	0.9052	0.0948	0.7534	Polygoni Cuspidati Rhizoma Et Radix	Fallacinol	3083633	FALSE	Oc1c2c(C(=O)c3c(C2=O)c(O)cc(OC)c3)cc(c1)CO
MOL013287	0.9074	0.0926	0.6393	Polygoni Cuspidati Rhizoma Et Radix	Physovenine	442113	FALSE	c1(ccc2c(c1)C1(C(N2C)OCC1)C)OC(=O)NC
MOL013288	0.6476	0.3524	0.7001	Polygoni Cuspidati Rhizoma Et Radix	Picralinal	Not Available	FALSE	c1ccc2c(c1)C13C4(N2)C2N(C(C1)O4)C/C(=C\C)/C(C3(C=O)C(=O)OC)C2
MOL013289	0.8521	0.1479	0.7960	Polygoni Cuspidati Rhizoma Et Radix	polydatin	5281718	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc(cc(O)c1)/C=C/c1ccc(O)cc1)CO
MOL013290	0.7437	0.2563	0.7406	Polygoni Cuspidati Rhizoma Et Radix	Polygalacic acid	Not Available	FALSE	C1(C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(C(C2)O)(CCC(C1)(C)C)C(=O)O)C)C)(C)CO)O)O
MOL013291	0.8820	0.1180	0.8079	Polygoni Cuspidati Rhizoma Et Radix	Quercetin-3-rhamnoside-7-glucoside	Not Available	FALSE	c1c(cc(c2c1oc(c(c2=O)OC1OC(C(C(C1O)O)O)C)c1ccc(c(c1)O)O)O)OC1OC(C(C(C1O)O)O)CO
MOL013292	0.8844	0.1156	0.7943	Polygoni Cuspidati Rhizoma Et Radix	Quercetin-5,3-di-D-galactoside	Not Available	FALSE	c1(cc(ccc1O)c1c(OC2OC(C(C(C2O)O)O)CO)c(=O)c2c(o1)cc(cc2OC1OC(C(C(C1O)O)O)CO)O)O
MOL013293	0.9027	0.0973	0.7411	Polygoni Cuspidati Rhizoma Et Radix	Questinol	147621	FALSE	c1(cc(cc2c1C(=O)c1c(C2=O)cc(cc1O)CO)O)OC
MOL013294	0.7347	0.2653	0.7870	Polygoni Cuspidati Rhizoma Et Radix	Quillaic acid	Not Available	FALSE	C1(CCC2(C(C1(C=O)C)CCC1(C)C3(C)CC(C4(C(=O)O)CCC(C)(C)CC4C3=CCC21)O)C)O
MOL013295	0.8936	0.1064	0.8235	Polygoni Cuspidati Rhizoma Et Radix	Torachrysone-8-O-beta-D-glucoside	11972479	FALSE	C(=O)(C)c1c(c2c(cc1C)cc(cc2OC1C(O)C(O)C(O)C(O1)CO)OC)O
MOL013296	0.9189	0.0811	0.8670	Capsellae Herba	Fustin	5317435	FALSE	c1c(ccc2c1OC(C(C2=O)O)c1cc(c(cc1)O)O)O
MOL013296	0.9189	0.0811	0.8670	Gleditsiae Spina	Fustin	5317435	FALSE	c1c(ccc2c1OC(C(C2=O)O)c1cc(c(cc1)O)O)O
MOL013297	0.9304	0.0696	0.9371	Capsellae Herba	2-propoxypropane	12304	FALSE	O(C(C)C)CCC
MOL013298	0.9213	0.0787	0.9567	Capsellae Herba	4,4-DIMETHYL HEXANAL	22218	FALSE	O=CCCC(CC)(C)C
MOL013299	0.8556	0.1444	0.9201	Capsellae Herba	8-azabicyclo[5.1.0]octane	39429422	FALSE	C12CCCCCC1N2

MOL013300	0.9189	0.0811	0.8670	Capsellae Herba	Flavanone, 3,3',4',7-tetrahydroxy-(VAN) (8CI)	72282	FALSE	O1C(C(O)C(=O)c2c1cc(O)cc2)c1cc(O)c(O)cc1
MOL013303	0.1061	0.8939	0.9658	Capsellae Herba	ergocristine	Not Available	FALSE	C12(N(C(C(=O)N3C1CCC3)Cc1ccccc1)C(=O)C(O2)(NC(=O)C1C=C2c3c4c(CC2N(C1)C)c[nH]c4ccc3)C(C)C)O
MOL013304	0.4913	0.5087	0.7927	Capsellae Herba	Fumaricine	442236	FALSE	COc1c(OC)cc2c(c1)CCN(C12C(c2c(C1)ccc1c2OCO1)O)C
MOL013305	0.8950	0.1050	0.8580	Capsellae Herba	Garbanzol	442410	FALSE	O1C(C(O)C(=O)c2c1cc(O)cc2)c1ccc(O)cc1
MOL013306	0.6793	0.3207	0.8573	Capsellae Herba	Gossypetin hexamethyl ether	146093	FALSE	o1c2c(c(=O)c(OC)c1c1cc(OC)c(OC)cc1)c(OC)cc(OC)c2OC
MOL013307	0.9299	0.0701	0.8948	Capsellae Herba	Gossypetin-7-methylether	5317830	FALSE	c1c(c(c2c(c1O)c(=O)c(c(o2)c1ccc(c(c1)O)O)O)O)OC
MOL013308	0.9233	0.0767	0.9569	Capsellae Herba	Paracetat	7915	FALSE	O(C(C)C)C(=O)C
MOL013309	0.5889	0.4111	0.7130	Capsellae Herba	Luteone	5281797	FALSE	C(=C(C)C)CC1c(O)cc2c(c1O)c(=O)c(c1c(O)cc(cc1)O)co2
MOL013310	0.7578	0.2422	0.7812	Capsellae Herba	Robinetinidol-(4alpha->8)-catechin-(6->4alpha)-robinetinidol	442689	FALSE	c1(c(cc(cc1O)C1Oc2c(C(C1O)c1c(O)c3c(c(c1O)C1C(O)C(Oc4c1ccc(c4)O)c1cc(c(c(c1)O)O)O)OC(C(C3)O)c1cc(c(cc1)O)O)ccc(c2)O)O)O
MOL013311	0.9298	0.0702	0.8987	Capsellae Herba	2,6-dimethoxy-4-prop-1-enylphenol	5352905	FALSE	C/C=C/c1cc(OC)c(O)c(OC)c1
MOL013312	0.8286	0.1714	0.7204	Capsellae Herba	sinigrin	Not Available	FALSE	S(C1OC(C(O)C(O)C1O)CO)/C(=N/OS(=O)(=O)O)/CC=C
MOL013313	0.8381	0.1619	0.8865	Capsellae Herba	Sulfanilsaeure	5232424	FALSE	S(=O)(=O)(c1ccc(cc1)N)O
MOL013314	0.8902	0.1098	0.9254	Abri Herba	CHALCONE, 2',4'-DIHYDROXY-	5376979	FALSE	c1(c(cc(cc1)O)O)C(=O)/C=C/c1ccccc1
MOL013315	0.4158	0.5842	0.7795	Abri Herba	Abrisapogenol A	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(CC(C1)(CO)C)O)C)C)C)C)(C)C)O
MOL013316	0.4605	0.5395	0.7456	Abri Herba	Abrisapogenol B	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(CC(C1)(C)CO)O)C)C)C)C)(CO)C)O
MOL013317	0.3772	0.6228	0.7662	Abri Herba	Abrisapogenol F	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(=O)CC(C1)(C)C)C)C)C)C)(C)C)O
MOL013318	0.3964	0.6036	0.7743	Abri Herba	Abrisapogenol G	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=C3C(CC2)(C(CC(C3)(C)C)O)C)CC1)C)C)C)(C)C)O
MOL013319	0.9130	0.0870	0.9453	Abri Herba	alpha-D-glucuronic acid	444791	FALSE	OC1C(O)C(O)C(O)C(O1)C(=O)O

MOL013320	0.6409	0.3591	0.7875	Abri Herba	Abrusoside A	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C(CC2)C(C)C1(CC=C(C(=O)O1)C)C)C)C)C3)(C(=O)O)C)OC1OC(C(C(C1O)O)O)CO
MOL013321	0.6411	0.3589	0.7440	Abri Herba	Abrusoside A_qt	Not Available	FALSE	C1C(C(C2C3(C1)C1(C(CC2)C2(C(CC1)(C(CC2)C(C)C1(CC=C(C(=O)O1)C)C)C)C)C3)(C(=O)O)C)O
MOL013322	0.9343	0.0657	0.8905	Abri Herba	Biflorin	441959	FALSE	O1C(C(O)C(O)C(O)C1CO)c1c(O)c2c(oc(cc2=O)C)cc1O
MOL013323	0.9261	0.0739	0.8728	Abri Herba	5,7-dihydroxy-2-methyl-8-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-4-one	10090524	FALSE	c1(c2c(c(cc1O)O)c(=O)cc(o2)C)OC1OC(C(C(C1O)O)O)CO
MOL013324	0.9465	0.0535	0.8155	Abri Herba	5,7,8-trihydroxy-2-methyl-chromone	5488208	FALSE	c1(c2c(c(cc1O)O)c(=O)cc(o2)C)O
MOL013325	0.7070	0.2930	0.7061	Abri Herba	kaikasaponin III_qt	Not Available	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(O)CC(C3)(C)C)C)C)(CC2)C)(CC1)C)(C)C)C1OC(C(O)C(O)C1O)C(=O)O
MOL013326	0.9492	0.0508	0.8985	Abri Herba	kainic acid	44338126	FALSE	C1(CNC(C1CC(=O)O)C(=O)O)C(=C)C

MOL013327	0.7201	0.2799	0.7672	Abri Herba	(2S,3S,4S,5R,6R)-6-[[(3S,4S,4aR,6aR,6bS,8aR,9R,12aS,14aR,14bR)-9-hydroxy-4-(hydroxymethyl)-4,6a,6b,8a,11,11,14b-heptamethyl-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydropicen-3-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	13632905	FALSE	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(C(O)CC(C3)(C)C)C)C)(CC2)C)(CC1)C)(CO)C)C1OC(C(O)C(O)C1O)C(=O)O
MOL013328	0.7776	0.2224	0.8286	Abri Herba	Soyasaponin V	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(CC(C1)(C)C)O)C)C)C)(CO)C)OC1OC(C(C(C1OC1OC(C(C(C1OC1OC(C(C(C1O)O)O)O)CO)O)O)C(=O)O
MOL013329	0.7201	0.2799	0.7672	Abri Herba	Soyasaponin V_qt	Not Available	FALSE	C1C(C(C2C(C1)(C1C(CC2)(C2(C(=CC1)C1C(CC2)(C(CC(C1)(C)C)O)C)C)C)(CO)C)OC1OC(C(C(C1O)O)O)C(=O)O
MOL013330	0.6209	0.3791	0.7509	Aurantii Fructus Immaturus	deacetylnomilin	Not Available	FALSE	C123C4(C(C5(C(CC4=O)C(OC(=O)CC5O)(C)C)C)CCC2(C(OC(=O)C1O3)c1ccoc1)C)C
MOL013330	0.6209	0.3791	0.7509	Citri Exocarpium Rubrum	deacetylnomilin	Not Available	FALSE	C123C4(C(C5(C(CC4=O)C(OC(=O)CC5O)(C)C)C)CCC2(C(OC(=O)C1O3)c1ccoc1)C)C
MOL013331	0.9161	0.0839	0.9183	Citri Exocarpium Rubrum	Isomeranzin	473252	FALSE	o1c2c(CC(=O)C(C)C)c(OC)ccc2ccc1=O
MOL013332	0.7912	0.2088	0.7428	Citri Exocarpium Rubrum	Pranferol	159751	FALSE	O(CC(O)C(C)C)c1c2c(occ2)cc2oc(=O)ccc12
MOL013333	0.8611	0.1389	0.7772	Glechomae Herba	Clerodendrin	5488004	FALSE	O(C1C(O)C(O)C(OC1Oc1cc2oc(cc(=O)c2c(O)c1)c1ccc(O)cc1)C(=O)O)C1OC(C(O)C(O)C1O)C(=O)O
MOL013334	0.7894	0.2106	0.6271	Glechomae Herba	glechomafuran	Not Available	FALSE	O1C2(C1Cc1c(occ1C)CC1(OC1CC2)C)C
MOL013335	0.7991	0.2009	0.7536	Glechomae Herba	glechomanolide	44593362	FALSE	O1C2C(=C(C1=O)C)C/C=C(/CC/C=C(/C2)\C)\C
MOL013336	0.8656	0.1344	0.8817	Fortunes Bossfern Rhizome	Narirutin	442431	FALSE	c12c(C(=O)CC(O1)c1ccc(cc1)O)c(cc(c2)OC1OC(COC2C(C(C(C(O2)C)O)O)O)C(C(C1O)O)O)O

MOL013336	0.8656	0.1344	0.8817	Aurantii Fructus Immaturus	Narirutin	442431	FALSE	c12c(C(=O)CC(O1)c1ccc(cc1)O)c(cc(c2)OC1OC(COC2C(C(C(O2)C)O)O)O)C(C(C1O)O)O)O
MOL013336	0.8656	0.1344	0.8817	Drynariae Rhizoma	Narirutin	442431	FALSE	c12c(C(=O)CC(O1)c1ccc(cc1)O)c(cc(c2)OC1OC(COC2C(C(C(O2)C)O)O)O)C(C(C1O)O)O)O
MOL013336	0.8656	0.1344	0.8817	Citri Reticulatae Pericarpium Viride	Narirutin	442431	FALSE	c12c(C(=O)CC(O1)c1ccc(cc1)O)c(cc(c2)OC1OC(COC2C(C(C(O2)C)O)O)O)C(C(C1O)O)O)O
MOL013337	0.9300	0.0700	0.7868	Kaempferiae Rhizoma	5-phenylthiazole	595209	FALSE	n1csc(c1)c1ccccc1
MOL013338	0.5674	0.4326	0.6337	Kaempferiae Rhizoma	9,12-octadecadienal	5283383	FALSE	C(=O)CCCCCCC/C=C/C/C=C/CCCCC
MOL013339	0.9499	0.0501	0.9459	Kaempferiae Rhizoma	p-Vinylguaiacol	12507	FALSE	c1(ccc(cc1)OC)C=C
MOL013340	0.7092	0.2908	0.8534	Hemerocallis Radix	2-Methoxy-obtusifolin	5319478	FALSE	O(c1c2c(C(=O)c3c(C2=O)c(O)ccc3)cc(c1OC)C)C
MOL013341	0.8010	0.1990	0.7750	Hemerocallis Radix	3'-Methoxypuerarin	5319485	FALSE	c1c(c(=O)c2c(o1)c(c(cc2)O)C1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)O)OC
MOL013342	0.4122	0.5878	0.6279	Hemerocallis Radix	Stypandrol	188516	FALSE	Oc1c(c2c(O)c3c(cc2)cc(c(c3O)C(=O)C)C)ccc2c1c(O)c(c(c2)C)C(=O)C
MOL013343	0.6241	0.3759	0.7833	Hemerocallis Radix	Hemerocallone	5318001	FALSE	o1c2c(c(OC)c3OCOc3c2)c(=O)c(c2c(OC)ccc(OC)c2)c1
MOL013344	0.9425	0.0575	0.9302	Hemerocallis Radix	p-Methylcinnamic acid	731767	FALSE	OC(=O)/C=C/c1ccc(cc1)C
MOL013346	0.6855	0.3145	0.6136	Hemerocallis Radix	picraquassioside C_qt	Not Available	FALSE	Oc1c(cc(cc1OC)C(C(CO)Oc1c(cc(cc1OC)/C=C/CO)OC)O)OC
MOL013347	0.9488	0.0512	0.9348	Foeniculi Fructus	Butyrophenone	10315	FALSE	c1(C(=O)CCC)ccccc1
MOL013348	0.2780	0.7220	0.6009	Citri Fructus	cryptoflavin	Not Available	FALSE	O1C2(C(=CC1/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C1=C(CC(O)CC1(C)C)C)\C)\C)/C)/C)C(CCC2)(C)C)C
MOL013352	0.3918	0.6082	0.7565	Dictamni Cortex	Obacunone	Not Available	FALSE	O1C23C4(C(C5(C(CC4=O)C(OC(=O)C=C5)(C)C)C)CCC2(C(OC(=O)C13)c1ccoc1)C)C
MOL013352	0.3918	0.6082	0.7565	Coptidis Rhizoma	Obacunone	Not Available	FALSE	O1C23C4(C(C5(C(CC4=O)C(OC(=O)C=C5)(C)C)C)CCC2(C(OC(=O)C13)c1ccoc1)C)C
MOL013352	0.3918	0.6082	0.7565	Citri Exocarpium Rubrum	Obacunone	Not Available	FALSE	O1C23C4(C(C5(C(CC4=O)C(OC(=O)C=C5)(C)C)C)CCC2(C(OC(=O)C13)c1ccoc1)C)C
MOL013352	0.3918	0.6082	0.7565	Evodiae Fructus	Obacunone	Not Available	FALSE	O1C23C4(C(C5(C(CC4=O)C(OC(=O)C=C5)(C)C)C)CCC2(C(OC(=O)C13)c1ccoc1)C)C
MOL013352	0.3918	0.6082	0.7565	Phellodendri Chinrnsis Cortex	Obacunone	Not Available	FALSE	O1C23C4(C(C5(C(CC4=O)C(OC(=O)C=C5)(C)C)C)CCC2(C(OC(=O)C13)c1ccoc1)C)C
MOL013352	0.3918	0.6082	0.7565	Aurantii Fructus Immaturus	Obacunone	Not Available	FALSE	O1C23C4(C(C5(C(CC4=O)C(OC(=O)C=C5)(C)C)C)CCC2(C(OC(=O)C13)c1ccoc1)C)C

MOL013352	0.3918	0.6082	0.7565	Citri Fructus	Obacunone	Not Available	FALSE	O1C23C4(C(C5(C(CC4=O)C(OC(=O)C=C5)(C)C)C)CCC2(C(OC(=O)C13)c1ccoc1)C)C
MOL013353	0.9306	0.0694	0.9817	Citri Fructus	D-synephrine	854067	FALSE	OC(CNC)c1ccc(O)cc1
MOL013353	0.9306	0.0694	0.9817	Aurantii Fructus	D-synephrine	854067	FALSE	OC(CNC)c1ccc(O)cc1
MOL013356	0.2160	0.7840	0.6553	Maydis Seigma	stigmasta-4,22-diene-3beta,6beta-diol	Not Available	FALSE	C1(CCC2(C(=C1)C(CC1C3CCC(C(/C=C/C(CC)C(C)C)C)C3(C)CCC21)O)C)O
MOL013357	0.2389	0.7611	0.6482	Maydis Seigma	(3S,6R,8S,9S,10R,13R,14S,17R)-17-[(1R,4R)-4-ethyl-1,5-dimethylhexyl]-10,13-dimethyl-2,3,6,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,6-diol	10550610	FALSE	C1(CCC2(C(=C1)C(CC1C3CCC(C(CCC(CC)C(C)C)C)C3(C)CCC21)O)C)O
MOL013358	0.2141	0.7859	0.6801	Maydis Seigma	(3S,7S,8S,9S,10R,13R,14S,17R)-17-[(E,2R,5S)-5-ethyl-6-methylhept-3-en-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,7-diol	21769896	FALSE	C1(CCC2(C(=CC(C3C4CCC(C(/C=C/C(CC)C(C)C)C)C4(C)CCC23)O)C1)C)O
MOL013359	0.2400	0.7600	0.6133	Maydis Seigma	stigmasta-7-en-3-ol	Not Available	FALSE	C1(CCC2(C(C1)CC=C1C3CCC(C(CCC(CC)C(C)C)C)C3(C)CCC21)C)O

MOL013361	0.9107	0.0893	0.9264	Maydis Seigma	Hexa-2,4-diene	638071	FALSE	C/C=C/C=C/C
MOL013362	0.8997	0.1003	0.9618	Maydis Seigma	Hystl	62695	FALSE	C(=C\C)/C
MOL013363	0.5700	0.4300	0.6011	Maydis Seigma	5,14-di-Butyloctacosane	Not Available	FALSE	CCCCC(CCCCCCCCC(CCCCCCCCCCCCCC)CCCC)CCCC
MOL013366	0.8199	0.1801	0.8048	Maydis Seigma	Apimaysin	Not Available	FALSE	O(C1C(OC(C(=O)C1O)C)c1c(O)c2c(oc(cc2=O)c2ccc(O)cc2)cc1O)C1OC(C(O)C(O)C1O)C
MOL013367	0.9339	0.0661	0.9490	Maydis Seigma	Butyl propionate	11529	FALSE	C(=O)(OCCCC)CC
MOL013368	0.1941	0.8059	0.7153	Maydis Seigma	Insularine	Not Available	FALSE	c1c(c2c3c4c1CCN(C)C4Cc1ccc(cc1)Oc1c4c(cc(c1OC)OC)CCN(C4Cc1ccc(c(c1)CO2)O3)C)OC
MOL013369	0.8676	0.1324	0.8159	Maydis Seigma	Maysin	Not Available	FALSE	O(C1C(OC(C(=O)C1O)C)c1c(O)c2c(oc(cc2=O)c2cc(O)c(O)cc2)cc1O)C1OC(C(O)C(O)C1O)C
MOL013370	0.8544	0.1456	0.8252	Maydis Seigma	Maysin_qt	Not Available	FALSE	OC1C(OC(C(=O)C1O)C)c1c(O)c2c(oc(cc2=O)c2cc(O)c(O)cc2)cc1O
MOL013371	0.9350	0.0650	0.9690	Maydis Seigma	(-)-Methyl 2-methylbutyrate	644216	FALSE	C(C(=O)OC)(CC)C
MOL013372	0.9228	0.0772	0.9718	Maydis Seigma	Methyl butyrate	12180	FALSE	C(=O)(CCC)OC
MOL013374	0.9450	0.0550	0.9005	Hoveniae Dulcis Semen	ampelopsin	161557	FALSE	O1C(C(O)C(=O)c2c1cc(O)cc2O)c1cc(O)c(O)c(O)c1
MOL013374	0.9450	0.0550	0.9005	Gleditsiae Spina	ampelopsin	161557	FALSE	O1C(C(O)C(=O)c2c1cc(O)cc2O)c1cc(O)c(O)c(O)c1
MOL013376	0.3975	0.6025	0.7953	Hoveniae Dulcis Semen	jujubogenin	Not Available	FALSE	C1(CCC2(C(C1(C)C)CCC1(C)C34COC5(C3)C(C(CC(C=C(C)C)O5)(C)O)C4CCC21)C)O
MOL013378	0.9349	0.0651	0.9680	Hoveniae Dulcis Semen	METHYL VALERATE	12206	FALSE	C(=O)(CCCC)OC
MOL013379	0.9229	0.0771	0.9530	Hoveniae Dulcis Semen	mono-Methyl suberate	554191	FALSE	O(C(=O)CCCCCCC(=O)O)C
MOL013381	0.5927	0.4073	0.7374	Aurantii Fructus	Marmin	6450230	FALSE	OC(C(O)CC/C(=C/COc1cc2oc(=O)ccc2cc1)/C)(C)C
MOL013382	0.9219	0.0781	0.9414	Aurantii Fructus	8-[[(2S)-3,3-dimethyloxiran-2-yl]methyl]-7-methoxy-coumarin	1803558	FALSE	c1(=O)ccc2c(o1)c(c(cc2)OC)CC1OC1(C)C
MOL013383	0.8504	0.1496	0.8704	Aurantii Fructus	Neohesperidin	442439	FALSE	O(C1C(O)C(O)C(OC1Oc1cc2OC(CC(=O)c2c(O)c1)c1cc(O)c(OC)cc1)CO)C1OC(C(O)C(O)C1O)C
MOL013384	0.9560	0.0440	0.9613	Euphorbiae Helioscopiae Herba	MELILOTATE	873	FALSE	c1cccc(c1O)CCC(=O)O

MOL013385	0.9305	0.0695	0.9184	Euphorbiae Helioscopiae Herba	3,4-Dihydroxybenzyl alcohol-4-glucoside	11972338	FALSE	C1(C(C(C(OC1CO)Oc1c(cc(cc1)CO)O)O)O)O
MOL013386	0.7064	0.2936	0.7465	Euphorbiae Helioscopiae Herba	carpinusin	Not Available	FALSE	O1C2C3OC(=O)C4=CC(=O)C5(Oc6c(C4C5(O)O)c(C(=O)OC(C3OC(=O)c3cc(O)c(O)c(O)c3)C1OC(=O)c1c(c3c(C(OC2)O)cc(O)c(O)c3O)c(O)c(O)c(O)c1)cc(O)c6O)O
MOL013389	0.0439	0.9561	0.7290	Euphorbiae Helioscopiae Herba	epieuphoscopin B	Not Available	FALSE	C12C(C(C(/C=C/C(C(=O)CC(/C(=C/1)/C)OC(=O)C)(C)C)C)OC(=O)C)(CC(C2OC(=O)c1ccccc1)C)OC(=O)C
MOL013390	0.0713	0.9287	0.6064	Euphorbiae Helioscopiae Herba	epieuphoscopin F	Not Available	FALSE	C12(C(/C=C(/C(CC(=O)C(/C=C/C(C1=O)C)(C)C)OC(=O)C)\C)C(C(C2)C)OC(=O)c1ccccc1)OC(=O)C
MOL013391	0.9353	0.0647	0.8698	Euphorbiae Helioscopiae Herba	euphohelin B	Not Available	FALSE	CC(CC(C)OC(=O)C)(C)OC(=O)C
MOL013392	0.0794	0.9206	0.7735	Euphorbiae Helioscopiae Herba	euphohelin C	Not Available	FALSE	O1C2(C1C1C3(C(C(C(C(C(C(CC2OC(=O)C)OC(=O)C)(C)C)OC(=O)c2ccccc2)O3)C)OC(=O)C)CC(C1OC(=O)c1ccccc1)C)C
MOL013393	0.0657	0.9343	0.7036	Euphorbiae Helioscopiae Herba	euphohelin D	Not Available	FALSE	O1C2(C1C1C3(C(=O)C(C(C(=O)C(C(CC2OC(=O)C)OC(=O)C)(C)C)O3)C)CC(C1OC(=O)c1ccccc1)C)C
MOL013394	0.0769	0.9231	0.6952	Euphorbiae Helioscopiae Herba	euphohelin E	Not Available	FALSE	O1C2(C1C1C3(C(=O)C(C(C(C(C(CC2OC(=O)C)OC(=O)C)(C)C)O)O3)C)CC(C1OC(=O)c1ccccc1)C)C
MOL013395	0.1150	0.8850	0.7331	Euphorbiae Helioscopiae Herba	euphoheliono ne	Not Available	FALSE	C12C3(C(C(C(C4C(CC(/C(=C\1)/C)OC(=O)c1ccccc1)C4(C)C)O3)C)OC(=O)c1ccccc1)CC(C2OC(=O)c1ccccc1)C
MOL013396	0.0338	0.9662	0.7339	Euphorbiae Helioscopiae Herba	euphornin A	Not Available	FALSE	OC12C(C(OC(=O)c3ccccc3)C(C1)C)/C=C(/C(OC(=O)C)CC(OC(=O)C)C(/C=C\C(C2OC(=O)C)C)(C)C)\C
MOL013397	0.0636	0.9364	0.6315	Euphorbiae Helioscopiae Herba	[(1R,2S,3S,4E,7R,9R,10E,12S,13S,14S)-2,9-diacetoxy-1,7-dihydroxy-3,6,6,10,14-pentamethyl-13-bicyclo[10.3.0]pentadeca-4,10-dienyl] benzoate	21771753	FALSE	OC12C(C(OC(=O)c3ccccc3)C(C1)C)/C=C(/C(OC(=O)C)CC(O)C(/C=C/C(C2OC(=O)C)C)(C)C)\C
MOL013398	0.0627	0.9373	0.6082	Euphorbiae Helioscopiae Herba	euphornin C	Not Available	FALSE	C12C(C(C(/C=C\C(C(CC(=O)/C(=C\1)/C)OC(=O)C)(C)C)C)OC(=O)C)(CC(C2OC(=O)c1ccccc1)C)O
MOL013399	0.0329	0.9671	0.7433	Euphorbiae Helioscopiae Herba	euphornin D	Not Available	FALSE	C12(C(/C=C(/C(CC(C(/C=C/C(C1OC(=O)C)C)(C)C)OC(=O)C)OC(=O)C)\C)C(C(C2)C)OC(=O)c1ccccc1)OC(=O)C

MOL013400	0.0650	0.9350	0.6871	Euphorbiae Helioscopiae Herba	euphornin E	Not Available	FALSE	C\1/2=C(\C(/C=C/C(C(CC(/C(=C/C1C(C(C2)C)OC(=O)c1ccccc1)/C)OC(=O)C)OC(=O)C)(C)C)C)/OC(=O)C
MOL013402	0.0560	0.9440	0.6320	Euphorbiae Helioscopiae Herba	euphornin G	Not Available	FALSE	C12C(C(C(/C=C/C(C(=O)CC(/C(=C/1)/C)OC(=O)C)(C)C)C)OC(=O)C)(CC(C2OC(=O)c1ccccc1)C)O
MOL013403	0.0750	0.9250	0.6191	Euphorbiae Helioscopiae Herba	euphornin K	Not Available	FALSE	C12C(C(C(/C=C/C(C(=O)CC(/C(=C/1)/C)O)(C)C)C)OC(=O)C)(CC(C2OC(=O)c1ccccc1)C)OC(=O)C
MOL013404	0.0439	0.9561	0.7290	Euphorbiae Helioscopiae Herba	euphoscopin B	Not Available	FALSE	C12C(C(C(/C=C\C(C(=O)CC(/C(=C\1)/C)OC(=O)C)(C)C)C)OC(=O)C)(CC(C2OC(=O)c1ccccc1)C)OC(=O)C
MOL013405	0.0632	0.9368	0.7052	Euphorbiae Helioscopiae Herba	euphoscopin C	Not Available	FALSE	C12C(C(C(/C=C\C(C(=O)CC(/C(=C\1)/C)OC(=O)c1ccccc1)(C)C)C)OC(=O)C)(CC(C2OC(=O)c1ccccc1)C)OC(=O)C
MOL013406	0.0823	0.9177	0.6250	Euphorbiae Helioscopiae Herba	euphoscopin D	Not Available	FALSE	C12C(C(C(/C=C\C(C(=O)CC(=O)/C(=C\1)/C)(C)C)C)OC(=O)C)(CC(C2OC(=O)c1ccccc1)C)OC(=O)C
MOL013408	0.0713	0.9287	0.6064	Euphorbiae Helioscopiae Herba	euphoscopin F	Not Available	FALSE	C12(C(/C=C(/C(CC(=O)C(/C=C/C(C1=O)C)(C)C)OC(=O)C)\C)C(C(C2)C)OC(=O)c1ccccc1)OC(=O)C
MOL013410	0.0560	0.9440	0.6320	Euphorbiae Helioscopiae Herba	euphoscopin H	Not Available	FALSE	C12C(C(C(/C=C/C(C(=O)CC(/C(=C/1)/C)OC(=O)C)(C)C)C)OC(=O)C)(CC(C2OC(=O)c1ccccc1)C)O
MOL013414	0.4085	0.5915	0.8652	Euphorbiae Helioscopiae Herba	helioscopinolide A	10245246	FALSE	OC1C(C2C(C3C(=CC4=C(C(=O)OC4C3)C)CC2)(CC1)C)(C)C
MOL013415	0.4085	0.5915	0.8652	Euphorbiae Helioscopiae Herba	helioscopinolide B	10335933	FALSE	OC1C(C2C(C3C(=CC4=C(C(=O)OC4C3)C)CC2)(CC1)C)(C)C
MOL013416	0.5716	0.4284	0.8566	Euphorbiae Helioscopiae Herba	helioscopinolide C	Not Available	FALSE	O1C2C(=C(C1=O)C)C=C1C(C2)C2(CC(=O)C(C(C2CC1)(C)C)O)C
MOL013417	0.8130	0.1870	0.6473	Euphorbiae Helioscopiae Herba	7-Angelyl-9-echimidinylheliotridine	5281732	FALSE	C1(CCN2C1C(=CC2)COC(=O)C(O)(C(C)(O)C)C(C)O)OC(=O)/C(=C\C)/C
MOL013418	0.0587	0.9413	0.7338	Euphorbiae Helioscopiae Herba	Mauritine A	Not Available	FALSE	c12ccc(cc1)/C=C\NC(=O)C(NC(=O)C1N(CCC1O2)C(=O)C(NC(=O)C(N(C)C)C)C(C)C)Cc1ccccc1
MOL013419	0.7145	0.2855	0.7373	Euphorbiae Helioscopiae Herba	persicogenin-3'glucoside	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1cc(C2Oc3c(C(=O)C2)c(O)cc(OC)c3)ccc1OC)CO
MOL013420	0.8422	0.1578	0.8609	Euphorbiae Helioscopiae Herba	Purine	1044	FALSE	n1cnc2c(c1)[nH]cn2
MOL013421	0.8648	0.1352	0.7325	Euphorbiae Helioscopiae Herba	quercetin-3-digalactoside	Not Available	FALSE	O(CC(O)/C(=C(\O)/C(O)COCC(O)/C(=C(\O)/C(O)CO)/O)/O)c1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)cc1
MOL013422	0.8986	0.1014	0.8189	Euphorbiae Helioscopiae Herba	Quercetin-3-diglucoside	Not Available	FALSE	c1(c(ccc(c1)c1c(OC2OC(C(C(C2O)O)O)COC2OC(C(C(C2O)O)O)CO)c(=O)c2c(o1)cc(cc2O)O)O)O
MOL013423	0.8884	0.1116	0.9637	Euphorbiae Helioscopiae Herba	RCO	5054	FALSE	Oc1cc(O)ccc1
MOL013424	0.8015	0.1985	0.7909	Euphorbiae Helioscopiae Herba	sakuranin	Not Available	FALSE	O1C(C(O)C(O)C(O)C1Oc1c2c(OC(CC2=O)c2ccc(O)cc2)cc(OC)c1)CO

MOL013425	0.9047	0.0953	0.7852	Euphorbiae Helioscopiae Herba	(2R)-5-hydroxy-2-(4-hydroxyphenyl)-7-methoxychroman-4-one	821416	FALSE	Oc1c2c(OC(CC2=O)c2ccc(O)cc2)cc(OC)c1
MOL013426	0.8487	0.1513	0.7728	Euphorbiae Helioscopiae Herba	terchebin	Not Available	FALSE	O1C2(O)C3c4c1c(O)c(O)cc4C(=O)OC1C(OC(=O)c4cc(O)c(O)c(O)c4)C(OC(=O)C3=CC(=O)C2(O)O)C(OC1OC(=O)c1cc(O)c(O)c(O)c1)COC(=O)c1cc(O)c(O)c(O)c1
MOL013428	0.7870	0.2130	0.8147	Aurantii Fructus Immaturus	isosakuranetin-7-rutinoside	Not Available	FALSE	c12c(OC(CC1=O)c1ccc(cc1)OC)cc(cc2O)OC1OC(C(C(C1O)O)O)COC1C(C(C(C(O1)C)O)O)O
MOL013429	0.9279	0.0721	0.8302	Aurantii Fructus Immaturus	beta-D-Glucopyranoside, 2-methoxy-4-(2-propenyl)phenyl	3084296	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)c1c(OC)cc(CC=C)cc1
MOL013430	0.7550	0.2450	0.8045	Aurantii Fructus Immaturus	Prangenin	17897	FALSE	c1(c2c(cc3c1occ3)ccc(=O)o2)OCC1C(O1)(C)C
MOL013431	0.8736	0.1264	0.7975	Aurantii Fructus Immaturus	3,8-di-C-glucosylapigenin	Not Available	FALSE	c1(c(c(=O)c2c(o1)c(c(cc2O)O)C1C(O)C(O)C(O)C(O1)CO)C1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)OC)O
MOL013432	0.8736	0.1264	0.7975	Aurantii Fructus Immaturus	3,8-di-C-glucosyldiosmetin	Not Available	FALSE	c1(c(c(=O)c2c(o1)c(c(cc2O)O)C1C(O)C(O)C(O)C(O1)CO)C1C(O)C(O)C(O)C(O1)CO)c1cc(c(cc1)OC)O
MOL013433	0.8763	0.1237	0.7489	Aurantii Fructus Immaturus	prangenin hydrate	40429858	FALSE	c1(c2c(cc3c1occ3)ccc(=O)o2)OCC(C(C)(C)O)O
MOL013434	0.4430	0.5570	0.8226	Aurantii Fructus Immaturus	Auraptene	1550607	FALSE	c12c(cc(cc1)OC/C=C(/CCC=C(C)C)\C)oc(=O)cc2
MOL013435	0.4358	0.5642	0.7707	Aurantii Fructus Immaturus	poncimarin	Not Available	FALSE	c1(=O)ccc2c(o1)c(c(cc2)OCC1OC1(C)C)CC1OC1(C)C
MOL013436	0.4688	0.5312	0.7626	Aurantii Fructus Immaturus	isoponcimarin	Not Available	FALSE	c1(=O)ccc2c(o1)c(c(cc2)OCC1OC1(C)C)CC(=O)C(C)C
MOL013437	0.3037	0.6963	0.8263	Aurantii Fructus Immaturus	6-Methoxy aurapten	5319406	FALSE	c12c(ccc(=O)o1)cc(c(c2)OC/C=C(/CCC=C(C)C)\C)OC
MOL013438	0.6030	0.3970	0.6298	Aurantii Fructus Immaturus	citrusin A	Not Available	FALSE	O(C1C(O)C(O)C(O)C(O1)CO)c1c(cc(cc1)C(C(CO)Oc1c(cc(cc1)/C=C/CO)OC)O)OC
MOL013439	0.7110	0.2890	0.7133	Aurantii Fructus Immaturus	citrusin A_qt	Not Available	FALSE	Oc1c(cc(cc1)C(C(CO)Oc1c(cc(cc1)/C=C\CO)OC)O)OC
MOL013441	0.6882	0.3118	0.6759	Aurantii Fructus Immaturus	citrusin B_qt	Not Available	FALSE	Oc1c(cc(cc1)C(C(CO)Oc1c(cc(cc1OC)/C=C\CO)OC)O)OC

MOL013442	0.5541	0.4459	0.6888	Aurantii Fructus Immaturus	dehydrodiconiferylalcohol-4-β-D-glucoside	Not Available	FALSE	c12c(cc(cc1OC)/C=C/CO)C(C(O2)c1cc(c(cc1)OC1OC(C(C(C1O)O)O)CO)OC)CO
MOL013444	0.8465	0.1535	0.7856	Aurantii Fructus Immaturus	naringenin-4'-glucoside-7-rutinoside	Not Available	FALSE	C1(CC(=O)c2c(O1)cc(cc2O)OC1C(O)C(O)C(O)C(O1)COC1C(O)C(O)C(O)C(O1)C)c1ccc(cc1)OC1C(O)C(O)C(O)C(O1)CO
MOL013445	0.9305	0.0695	0.7892	Aurantii Fructus Immaturus	naringenin-4'-glucoside-7-rutinoside_qt	Not Available	FALSE	C1(CC(=O)c2c(O1)cc(cc2O)O)/C(=C/C=C/O)/C

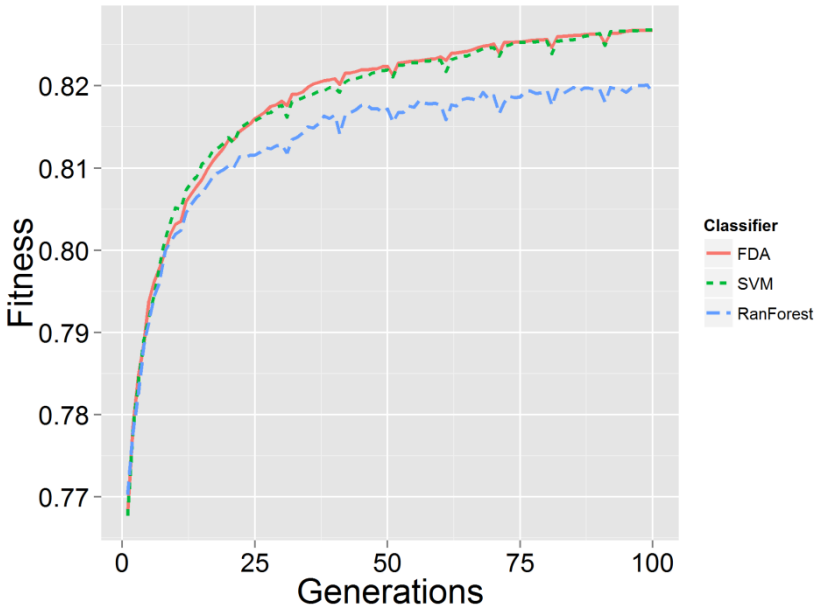


Figure S1. Fitness evolution in different classifiers

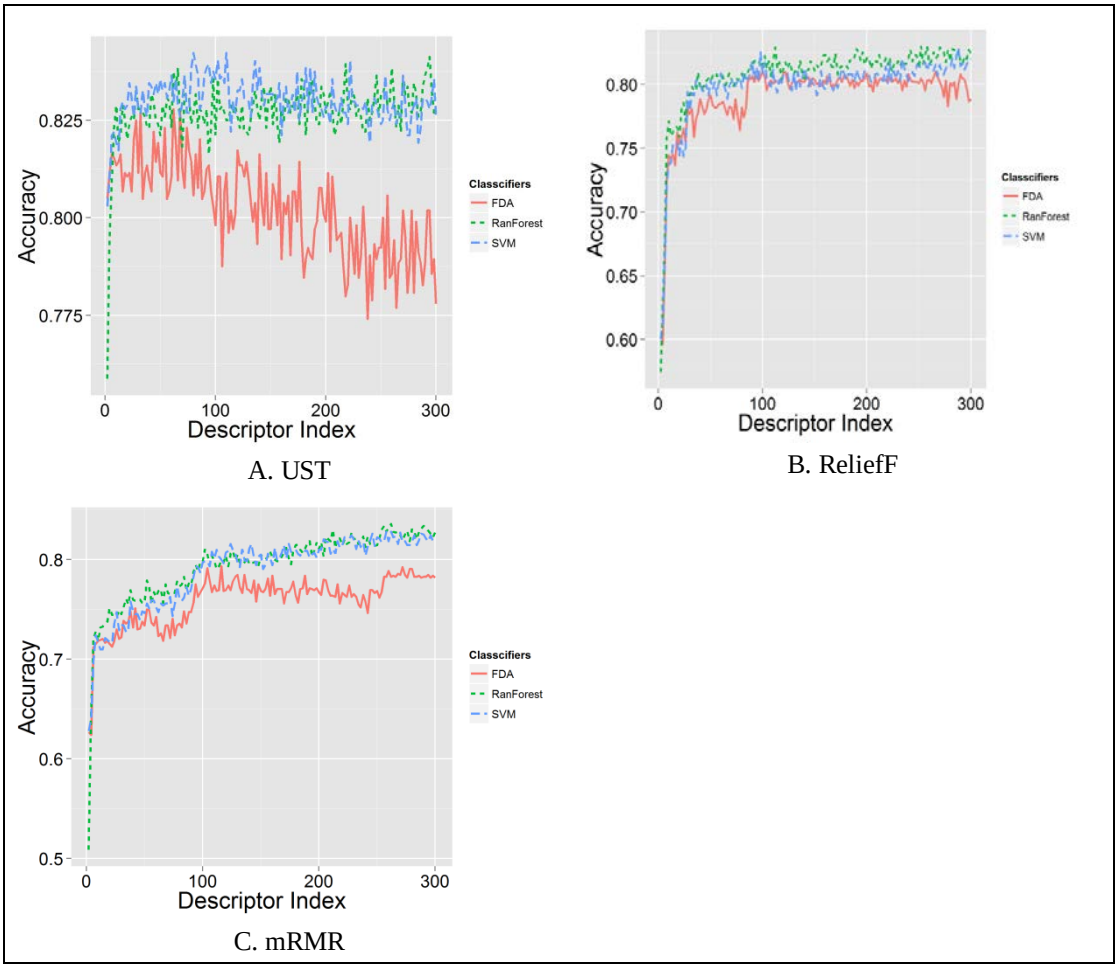
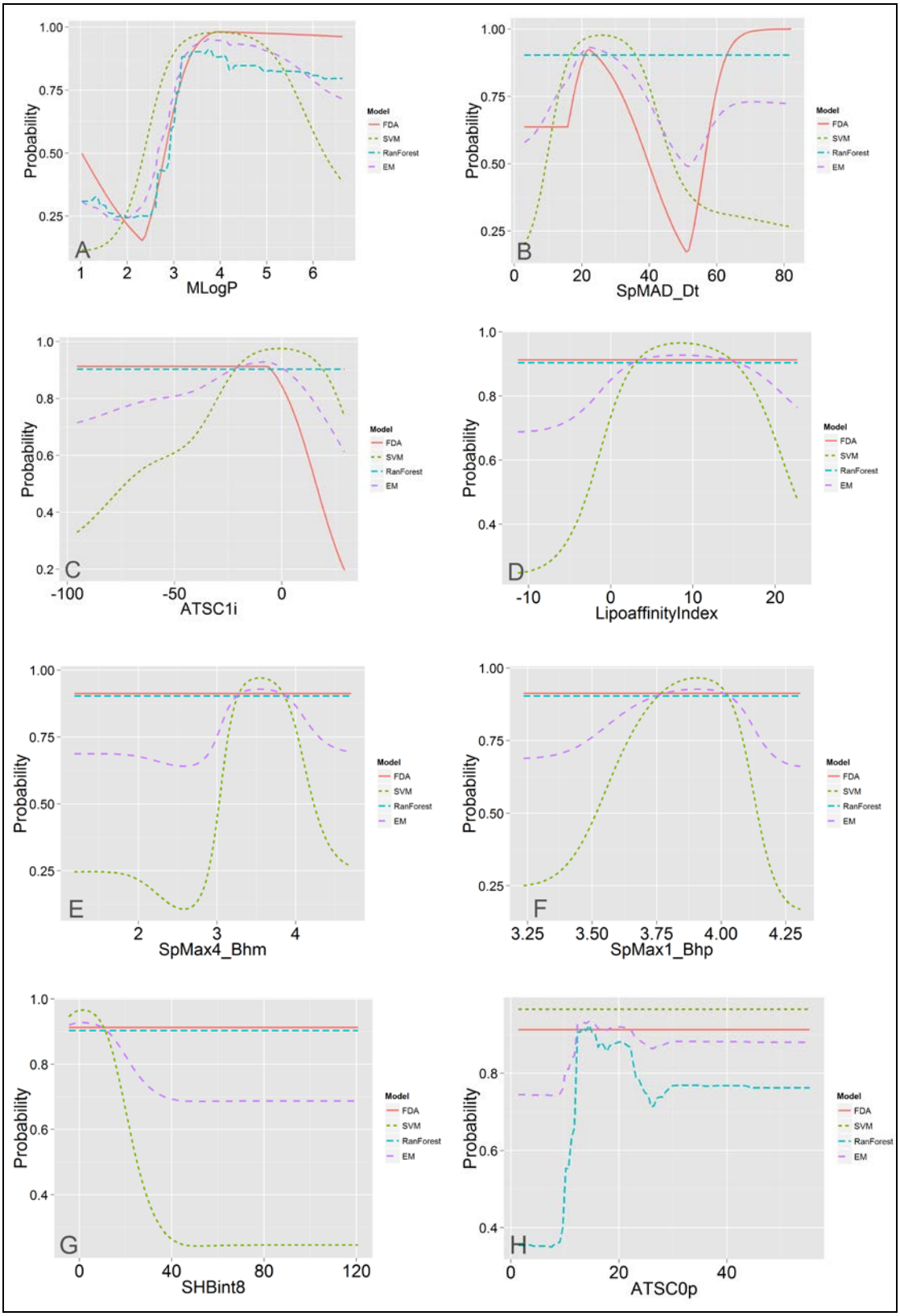


Figure S2. Accuracy curves of different rank-based feature selection methods for each classifier. (A) UST, (B) ReliefF, and (C) mRMR. UST, univariate statistical test.


A
Probability
MLogP
B
SpMAD_Dt
C
ATSC1i
D
LipoaffinityIndex
E
SpMax4_Bhm
F
SpMax1_Bhp
G
SHBint8
H
ATSC0p
Model
FDA
SVM
RanForest
EM

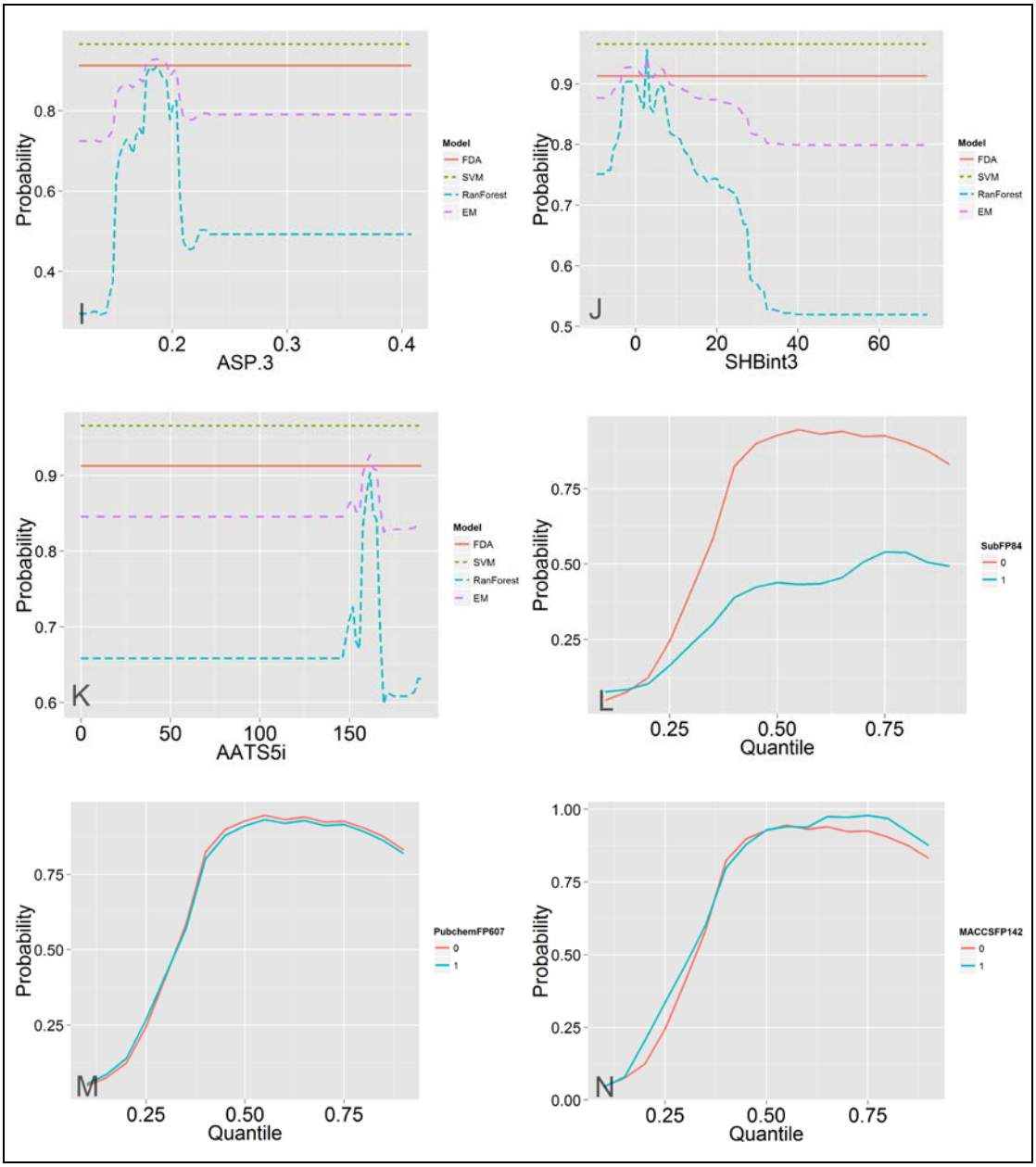
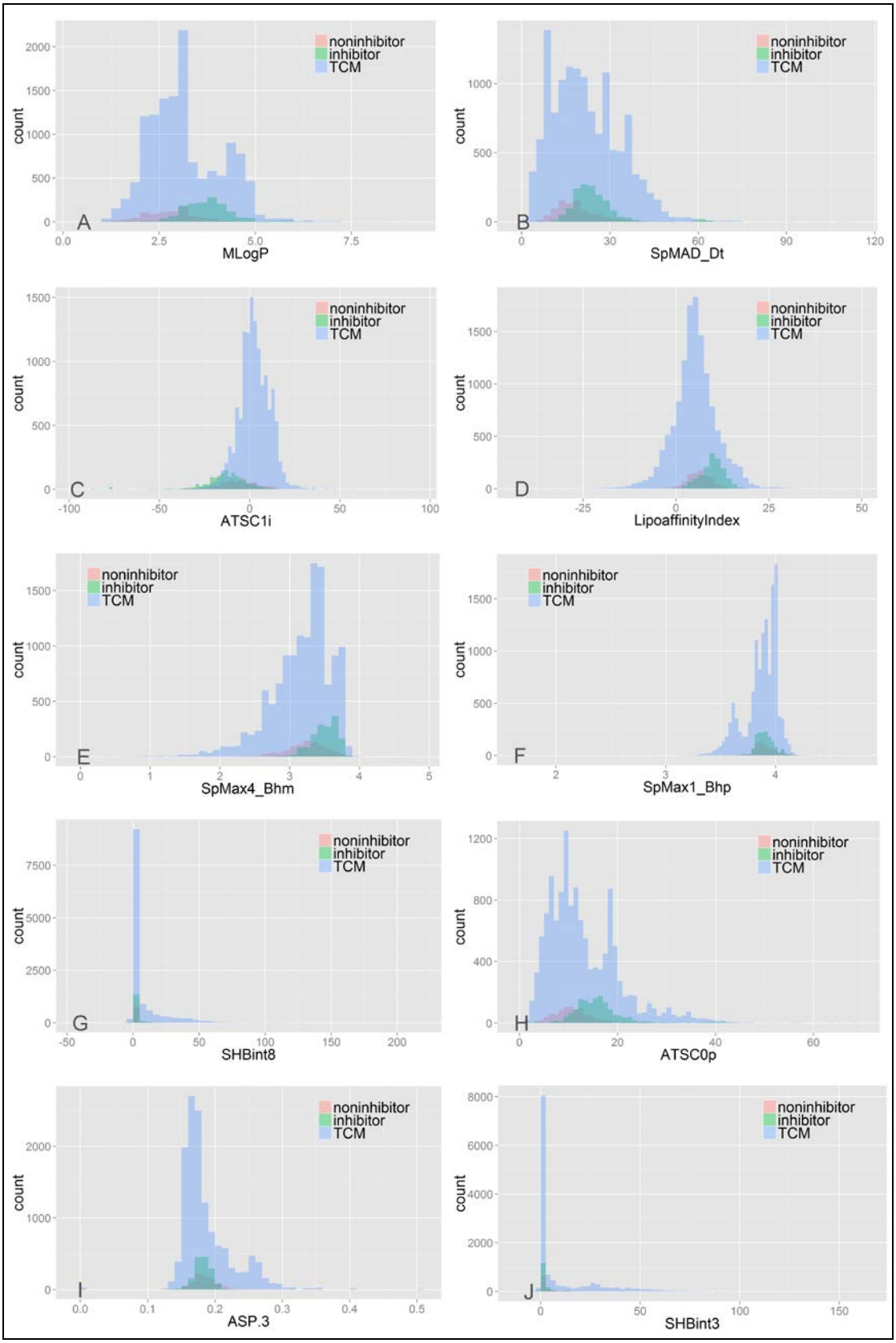


Figure S3. Probability response curves for the optimal descriptors. (A) MLogP, (B) SpMAD_Dt, (C) ATSC1i, (D) LipoaffinityIndex, (E) SpMax4_Bhm, (F) SpMax1_Bhp, (G) SHBint8, (H) ATSC0p, (I) ASP.3, (J) SHBint3, (K) AATS5i, (L) SubFP84, (M) PubchemFP607, and (N) MACCSFP142. For the continuous descriptors (A-K), probability response curves were obtained by varying one specific descriptor from its minimum to maximum. For the binary fingerprint descriptors (L-N), probability response curves were obtained on the different quantile values of the continuous descriptors.


noninhibitor
inhibitor
TCM
count
A
MLogP
B
SpMAD_Dt
C
ATSC1i
D
LipoaffinityIndex
E
SpMax4_Bhm
F
SpMax1_Bhp
G
SHBint8
H
ATSC0p
I
ASP.3
J
SHBint3

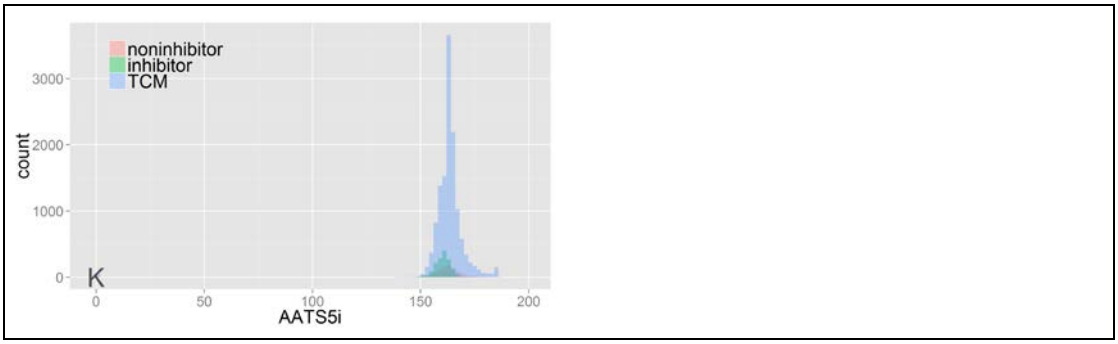


Figure S4. Distributions of continuous optimal descriptors for the combination of TCMSP database and modeling dataset. (A) MLogP, (B) SpMAD_Dt, (C) ATSC1i, (D) LipoaffinityIndex, (E) SpMax4_Bhm, (F) SpMax1_Bhp, (G) SHBint8, (H) ATSC0p, (I) ASP.3, (J) SHBint3, and (K) AATS5i