

Supporting Information

Development and Validation of Decision Forest Model for Estrogen Receptor Binding Prediction of Chemicals Using Large Data Sets

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Table S1. Binding data for the 3308 training set chemicals from EADB. Activity (Act) =1 indicates that the compound is active while activity =0 indicates that the compound is inactive; total number of data points (#D); total number of data point(s) indicating the chemical as active (# Act); total number of data point(s) indicating the chemical as inactive (# Inact).

CAS #	Chemical Name	Act	# D	# Act	# Inact	SMILES
50-28-2	estradiol	1	126	126	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O</chem>
446-72-0	genistein	1	31	31	0	<chem>Oc1ccc(cc1)C2=COc3cc(O)cc(O)c3C2=O</chem>
84449-90-1	2-(4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	29	29	0	<chem>Oc1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>
10540-29-1	tamoxifen	1	27	27	0	<chem>CC\C/C(=C/c1ccccc1)\c2ccc(OCCN(C)C)cc2\c3ccccc3</chem>
56-53-1	diethylstilbestrol	1	19	19	0	<chem>CC\C/C(=C(\CC)/c1ccc(O)cc1)\c2ccc(O)cc2</chem>
72732-26-4	4-hydroxytamoxifen	1	16	16	0	<chem>CC\C/C(=C/c1ccc(O)cc1)\c2ccc(OCCN(C)C)cc2\c3ccccc3</chem>
53-16-7	estrone	1	14	14	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CCC2=O</chem>
50-27-1	estriol	1	13	13	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1C[C@@H](O)[C@@H]2O</chem>
479-13-0	5,14-dihydroxy-8,17-dioxatetracyclo[8.7.0.0.0{2,7}.0{11,16}]heptadeca-1(10),2,4,6,11(16),12,14-heptaen-9-one	1	11	11	0	<chem>Oc1ccc2c(OC(=O)c3c2oc4cc(O)ccc34)c1</chem>

486-66-8	daidzein	1	10	10	0	<chem>Oc1ccc(cc1)C2=COc3cc(O)ccc3C2=O</chem>
	(1S,9R,10R,11S,14S,15S)-15-methyl-9-[9-(4,4,5,5,5-pentafluoropentanesulfinyl)nonyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	10	10	0	<chem>C[C@]12CC[C@H]3[C@@H]([C@H](CCCCCCCC[S+])([O-])CCCC(F)(F)C(F)(F)F)Cc4cc(O)ccc34)[C@@H]1CC[C@@H]2O</chem>
17924-92-4	(-)-zearalenone	1	10	10	0	<chem>C[C@H]1CCCC(=O)CCC\C=C\C2cc(O)cc(O)c2C(=O)O1</chem>
77538-56-8	ethinyl estradiol	1	9	9	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)C#C</chem>
	dihydrodiethylstilbestrol	1	9	9	0	<chem>CCC(C(CC)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	(2S,3R)-3-(4-hydroxyphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1,4-benzoxathiin-6-ol	1	9	9	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5CCCC5)cc4</chem>
27100-33-0	Bisphenol A	1	8	8	0	<chem>CC(C)(c1ccc(O)cc1)c2ccc(O)cc2</chem>
461015-54-3	chamomile	1	8	8	0	<chem>Oc1ccc(cc1)C2=CC(=O)c3c(O)cc(O)cc3O2</chem>
98007-99-9	N-butyl-11-[(1S,9R,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-9-yl]-N-methylundecanamide	1	8	8	0	<chem>CCCCN(C)C(=O)CCCCCCCC[C@@H]1Cc2cc(O)ccc2[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4[C@H]13</chem>

257630-50-5	progesterone	1	7	6	1	<chem>CC(=O)[C@H]1CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>
58-22-0	testosterone	1	7	6	1	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
140-66-9	p-tert-octylphenol	1	7	7	0	<chem>CC(C)(C)CC(C)(C)c1ccc(O)cc1</chem>
	naringenin	1	7	7	0	<chem>Oc1ccc(cc1)[C@@H]2CC(=O)c3c(O)cc(O)cc3O2</chem>
12040-51-6	dihydrotestosterone	1	7	7	0	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
434-22-0	nandrolone	1	7	7	0	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@H]34)[C@@H]1CC[C@@H]2O</chem>
104-40-5	4-nonylphenol	1	6	5	1	<chem>CCCCCCCCCc1ccc(O)cc1</chem>
57-91-0	estradiol 17 α	1	6	6	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@H]2O</chem>
	kepone	1	6	6	0	<chem>ClC1(Cl)C2(Cl)C3(Cl)C4(Cl)C(=O)C5(Cl)C(Cl)(C1(Cl)C35Cl)C24Cl</chem>
491-80-5	biochanin	1	6	6	0	<chem>COc1ccc(cc1)C2=COc3cc(O)cc(O)c3C2=O</chem>
520-18-3	kaempferol	1	6	6	0	<chem>OC1=C(Oc2cc(O)cc(O)c2C1=O)c3ccc(O)cc3</chem>
	(5R,11S)-5,11-dimethyl-5,6,11,12-tetrahydrochrysene-2,8-diol	1	6	6	0	<chem>C[C@@H]1Cc2cc(O)ccc2C3=C1c4ccc(O)cc4C[C@@H]3C</chem>
72-43-5	moxie	1	5	5	0	<chem>COc1ccc(cc1)C(c2ccc(OC)cc2)C(Cl)(Cl)Cl</chem>

180916-16-9	lasofoxifene	1	5	5	0	<chem>Oc1ccc2[C@H]([C@H](CCc2c1)c3ccccc3)c4ccc(OCCN5CCCC5)cc4</chem>
	2,3-bis(4-hydroxyphenyl)propanenitrile	1	5	5	0	<chem>Oc1ccc(CC(C#N)c2ccc(O)cc2)cc1</chem>
73123-10-1	quercetin	1	5	5	0	<chem>OC1=C(Oc2cc(O)cc(O)c2C1=O)c3ccc(O)c(O)c3</chem>
92-88-6	DOD	1	5	5	0	<chem>Oc1ccc(cc1)c2ccc(O)cc2</chem>
485-72-3	formononetin	1	5	5	0	<chem>COc1ccc(cc1)C2=COc3cc(O)ccc3C2=O</chem>
	(1S,10S,11S,14S,15S,17S)-17-ethyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	5	5	0	<chem>CC[C@H]1C[C@]2(C)[C@@H](O)CC[C@H]2[C@@H]3CCc4c(O)ccc4[C@@H]13</chem>
	4-[3,5-bis(4-hydroxyphenyl)-4-propylpyrazol-1-yl]phenol	1	5	5	0	<chem>CCCC1c(nn(c2ccc(O)cc2)c1c3ccc(O)cc3)c4ccc(O)cc4</chem>
525-82-6	flavone	1	5	4	1	<chem>O=C1C=C(Oc2ccccc12)c3ccccc3</chem>
480-40-0	chrysin	1	5	4	1	<chem>Oc1cc(O)c2C(=O)C=C(Oc2c1)c3ccccc3</chem>
	(5R,11R)-5,11-diethyl-5,6,11,12-tetrahydrochrysene-2,8-diol	1	5	5	0	<chem>CC[C@@H]1Cc2cc(O)ccc2C3=C1c4ccc(O)cc4C[C@H]3CC</chem>
	(2S)-3-{4-[(2,2-dimethylpropanoyl)oxy]phenyl}-4-methyl-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2H-chromen-7-yl	1	5	5	0	<chem>CC1=C([C@@H](Oc2cc(OC(=O)C(C)(C)C)ccc12)c3ccc(OCCN4CCCC4)cc3)c5ccc(OC(=O)C(C)(C)C)cc5</chem>

	2,2-dimethylpropanoate					
	1-chloro-2-[2,2,2-trichloro-1-(4-chlorophenyl)ethyl]benzene	1	4	4	0	<chem>Clc1ccc(cc1)C(c2ccccc2Cl)C(Cl)(Cl)Cl</chem>
1322-20-9	phenylphenol	1	4	4	0	<chem>Oc1ccc(cc1)c2ccccc2</chem>
521-17-5	5-androstenediol	1	4	4	0	<chem>C[C@]12CC[C@H]3[C@@H](CC=C4C[C@@H](O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
71765-94-1	(1S,10R,11S,13R,14R,15S)-13-iodo-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	4	4	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1C[C@@H](I)[C@@H]2O</chem>
124042-17-7	hydroxychlor	1	4	4	0	<chem>Oc1ccc(cc1)C(c2ccc(O)cc2)C(Cl)(Cl)Cl</chem>
31477-60-8	ormeloxifene	1	4	4	0	<chem>COc1ccc2[C@H]([C@H](c3ccccc3)C(C)(C)Oc2c1)c4ccc(OCCN5CCCC5)cc4</chem>
	(1S,10S,11S,14R,15S)-14-ethynyl-17-methoxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	4	4	0	<chem>COC1C[C@@]2(C)[C@@H](CC[C@@]2(O)C#C)[C@@H]3CCc4cc(O)ccc4[C@@H]13</chem>
155701-61-4	(2E)-3-{4-[(1Z)-1,2-diphenylbut-1-en-1-yl]phenyl}prop-2-enoic acid	1	4	4	0	<chem>CC\C/C(=C/c1ccccc1)\c2ccc(\C=C\C(=O)O)cc2)\c3ccccc3</chem>

1852-53-5	3 α ,17 β -dihydroxy-5 α -androstane	1	4	4	0	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@H]4C[C@H](O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
35212-22-7	osten	1	4	4	0	<chem>CC(C)Oc1ccc2C(=O)C(=COc2c1)c3ccccc3</chem>
362-05-0	ECS	1	4	4	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)c(O)cc34)[C@@H]1CC[C@@H]2O</chem>
98094-87-2	5,7,14-trihydroxy-2,17-dioxatetracyclo[8.7.0.0{3,8}.0{11,16}]heptadeca-1(10),3,5,7,11(16),12,14-heptaen-9-one	1	4	4	0	<chem>Oc1ccc2c3C(=O)c4c(O)cc(O)cc4Oc3oc2c1</chem>
5976-61-4	4-hydroxyestradiol	1	4	4	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4c(O)c(O)ccc34)[C@@H]1CC[C@@H]2O</chem>
491-54-3	kaempferide	1	4	3	1	<chem>COc1ccc(cc1)C2=C(O)C(=O)c3c(O)cc(O)cc3O2</chem>
182167-04-0	(2S)-3-(4-hydroxyphenyl)-4-methyl-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2H-chromen-7-ol	1	4	4	0	<chem>CC1=C([C@@H](Oc2cc(O)ccc12)c3ccc(OCCN4CCCCC4)cc3)c5ccc(O)cc5</chem>
	(1R,10S,11S,14S,15S,17S)-17-[(E)-2-iodoethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	4	4	0	<chem>C[C@]12C[C@H](\\C=C\\I)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O</chem>
67651-34-7	OH-pcb-61	1	3	3	0	<chem>Oc1ccc(cc1)c2cc(Cl)c(Cl)c(Cl)c2Cl</chem>

5189-40-2	4-[cyclohexylidene(4-hydroxyphenyl)methyl]phenol	1	3	3	0	<chem>Oc1ccc(cc1)C(=C2CCCCC2)c3ccc(O)cc3</chem>
	2-(4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol hydrochloride	1	3	3	0	<chem>Cl.Oc1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>
71902-25-5	4-octylphenol	1	3	2	1	<chem>CCCCCCCCc1ccc(O)cc1</chem>
1845-11-0	NFX	1	3	3	0	<chem>COc1ccc2C(=C(CCc2c1)c3cccc3)c4ccc(OCCN5CCCC5)cc4</chem>
13029-44-2	dienestrol	1	3	3	0	<chem>C\C=C(\C(=C\C)\c1ccc(O)cc1)/c2ccc(O)cc2</chem>
	3-(4-hydroxyphenyl)-2-methyl-2H-1,4-benzoxazine-5,7-diol	1	3	3	0	<chem>CC1Oc2cc(O)cc(O)c2N=C1c3ccc(O)cc3</chem>
98-54-4	4-tert-butylphenol	1	3	3	0	<chem>CC(C)(C)c1ccc(O)cc1</chem>
53-43-0	3-β-hydroxy-5-androsten-17-one	1	3	3	0	<chem>C[C@]12CC[C@H]3[C@@H](CC=C4C[C@@H](O)CC[C@]34C)[C@@H]1CCC2=O</chem>
	6-[(1E)-(hydroxyimino)methyl]-2,3-diphenylphenol	1	3	3	0	<chem>O\N=C\c1ccc(c2cccc2)c(c1O)c3cccc3</chem>
	(2S,3R)-3-(4-hydroxyphenyl)-2-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1,4-benzoxathiin-6-ol	1	3	3	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5CCCC5)cc4</chem>
	prinaberel	1	3	3	0	<chem>Oc1cc(C=C)c2oc(nc2c1)c3ccc(O)c(F)c3</chem>
60-82-2	dihydronaringenin	1	3	3	0	<chem>Oc1ccc(CCC(=O)c2c(O)cc(O)cc2O)cc1</chem>

91221-46-4	4-[1-(4-hydroxyphenyl)-2-phenylbut-1-en-1-yl]phenol	1	3	3	0	<chem>CCC(=C(c1ccc(O)cc1)c2ccc(O)cc2)c3ccccc3</chem>
68-23-5	norethynodrel	1	3	3	0	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=C3CCC(=O)C4)[C@@H]1CC[C@@]2(O)C#C</chem>
42422-68-4	taleranol	1	3	3	0	<chem>C[C@H]1CCC[C@@H](O)CCCCc2cc(O)cc(O)c2C(=O)O1</chem>
36455-72-8	α -zearalenol	1	3	3	0	<chem>C[C@H]1CCC[C@H](O)CCC\C=C\c2cc(O)cc(O)c2C(=O)O1</chem>
71030-11-0	β -zearalenol	1	3	3	0	<chem>C[C@H]1CCC[C@@H](O)CCC\C=C\c2cc(O)cc(O)c2C(=O)O1</chem>
	2-(4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	3	3	0	<chem>Oc1ccc(cc1)c2oc3ccc(O)cc3n2</chem>
	7-bromo-2-(4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	3	3	0	<chem>Oc1ccc(cc1)c2oc3c(Br)cc(O)cc3n2</chem>
	7-bromo-2-(3-fluoro-4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	3	3	0	<chem>Oc1cc(Br)c2oc(nc2c1)c3ccc(O)c(F)c3</chem>
72-54-8	DDD	1	3	2	1	<chem>ClC(Cl)C(c1ccc(Cl)cc1)c2ccc(Cl)cc2</chem>
566-75-6	16-ketoestradiol	1	3	3	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC(=O)[C@@H]2O</chem>
	3-(4-hydroxyphenyl)-1,2-benzoxazol-6-ol	1	3	3	0	<chem>Oc1ccc(cc1)c2noc3cc(O)ccc23</chem>
	5-hydroxy-2-(4-hydroxyphenyl)-1,3-	1	3	3	0	<chem>Oc1ccc(cc1)c2oc3c(cc(O)cc3n2)C#N</chem>

	benzoxazole-7-carbonitrile					
	5-hydroxy-2-(4-hydroxyphenyl)-1,3-benzoxazole-7-carbaldehyde	1	3	3	0	<chem>Oc1ccc(cc1)c2oc3c(C=O)cc(O)cc3n2</chem>
	2-(4-hydroxyphenyl)-1,3-benzoxazol-6-ol	1	3	3	0	<chem>Oc1ccc(cc1)c2oc3cc(O)ccc3n2</chem>
	5,6,11,12-tetrahydrochrysene-2,8-diol	1	3	3	0	<chem>Oc1ccc2C3=C(Cc2c1)c4ccc(O)cc4CC3</chem>
	4-{bicyclo[3.3.1]nonan-9-ylidene(4-hydroxyphenyl)methyl}phenol	1	3	3	0	<chem>Oc1ccc(cc1)C(=C2C3CCCC2CCC3)c4ccc(O)cc4</chem>
68-22-4	norethindrone	1	3	3	0	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@H]34)[C@@H]1CC[C@@]2(O)C#C</chem>
	(1S,11S,14R,15S)-14-ethynyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6,9-tetraene-5,14-diol	1	3	3	0	<chem>C[C@]12CC[C@H]3C(=CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)C#C</chem>
54982-79-5	16 α -(77br)-bromoestradiol-17 β	1	3	3	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1C[C@@H](Br)[C@@H]2O</chem>
	(1S,10S,11S,14S,15S,17R)-17-ethenyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	3	3	0	<chem>C[C@]12C[C@H](C=C)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O</chem>

	(1R,10S,11R,14R,15R)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	3	3	0	<chem>C[C@@]12CC[C@@H]3[C@H](CCc4cc(O)ccc34)[C@H]1CC[C@H]2O</chem>
	(1S,10S,11S,14R,15S,17S)-14-[(E)-2-iodoethenyl]-5,17-dimethoxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-ol	1	3	3	0	<chem>CO[C@H]1C[C@@]2(C)[C@@H](CC[C@@]2(O)\C=C\I)[C@@H]2CCc3cc(OC)ccc3[C@@H]12</chem>
	(1S,10S,11S,14R,15S,17S)-14-[(Z)-2-iodoethenyl]-5,17-dimethoxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-ol	1	3	3	0	<chem>CO[C@H]1C[C@@]2(C)[C@@H](CC[C@@]2(O)\C=C/I)[C@@H]2CCc3cc(OC)ccc3[C@@H]12</chem>
	(1S,10R,11R,14R,15R)-14-hydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-5-yl benzoate	1	3	3	0	<chem>C[C@@]12CC[C@H]3[C@@H](CCc4cc(OC(=O)c5ccccc5)ccc34)[C@H]1CC[C@H]2O</chem>
	4-(2-methylphenyl)phenol	1	3	3	0	<chem>Cc1ccccc1-c1ccc(O)cc1</chem>
	4-(3-methylphenyl)phenol	1	3	3	0	<chem>Cc1cccc(c1)-c1ccc(O)cc1</chem>
26191-64-0	4-(4-methylphenyl)phenol	1	3	3	0	<chem>Cc1ccc(cc1)-c1ccc(O)cc1</chem>
1228-72-4	17-epiestriol	1	3	3	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1C[C@@H](O)[C@H]2O</chem>

	(1S,10S,11S,14S,15S,17R)-17-(2-hydroxyethyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	3	3	0	<chem>C[C@]12C[C@H](CCO)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O</chem>
	(1S,10R,11S,14R,15S)-14-[(Z)-2-chloroethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	3	3	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)\C=C/Cl</chem>
129000-35-7	(1S,10S,11S,14S,15S,17R)-17-(2-fluoroethyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	3	3	0	<chem>C[C@]12C[C@H](CCF)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O</chem>
	(1S,10R,11S,14R,15S)-14-[(E)-2-chloroethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	3	3	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)\C=C\Cl</chem>
63676-25-5	2-(4-hydroxyphenyl)-3-{4-[2-(pyrrolidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	3	3	0	<chem>Oc1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCC5)cc4</chem>
	9-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-8,17-	1	3	3	0	<chem>Oc1ccc2c(OC(c3ccc(OCCN4CCCC4)cc3)c5c2oc6cc(O)ccc56)c1</chem>

	dioxatetracyclo[8.7.0.0{2,7}.0{11,16}]heptadeca-1(10),2,4,6,11(16),12,14-heptaene-5,14-diol					
	4-[4-(4-hydroxyphenyl)-1-iodohexan-3-yl]phenol	1	3	3	0	<chem>CCC(C(CCl)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	(1S,10R,11S,14R,15S)-15-methyl-14-[(E)-2-phenylethenyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	3	3	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)\C=C\c5ccccc5</chem>
	(1S,10R,11S,14R,15S)-15-methyl-14-[(E)-2-[4-(trifluoromethyl)phenyl]ethenyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	3	3	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)\C=C\c5ccc(cc5)C(F)(F)F</chem>
	(1S,10R,11S,14S,15S)-15-methyl-14-phenyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	3	3	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)c5ccccc5</chem>
	(10S,11S,14S,15R,17R)-17-[4-(dimethylamino)phenyl]-14-hydroxy-15-methyl-14-(prop-1-yn-1-	1	2	2	0	<chem>CC#C[C@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CCC4=C3[C@H](C[C@@]12C)c5ccc(cc5)N(C)C</chem>

	yl)tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-1,6-dien-5-one					
50-29-3	detox	1	2	2	0	<chem>Clc1ccc(cc1)C(c2ccc(Cl)cc2)C(Cl)(Cl)Cl</chem>
14962-28-8	2,4,6-trichloro-4'-biphenylol	1	2	2	0	<chem>Oc1ccc(cc1)c2c(Cl)cc(Cl)cc2Cl</chem>
92497-66-0	(2Z)-2,3-bis(4-hydroxyphenyl)prop-2-enenitrile	1	2	2	0	<chem>Oc1ccc(\C=C(/C#N)\c2ccc(O)cc2)cc1</chem>
	(2R,3S)-3-(4-hydroxyphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1,4-benzoxathiin-6-ol	1	2	2	0	<chem>Oc1ccc(cc1)[C@@H]2Sc3cc(O)ccc3O[C@@H]2c4ccc(OCCN5CCCCC5)cc4</chem>
	2-phenyl-1-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-3,4-dihydro-1H-isoquinolin-6-ol	1	2	2	0	<chem>Oc1ccc2C(N(CCc2c1)c3cccc3)c4ccc(OCCN5CCCCC5)cc4</chem>
	2,3-bis(4-hydroxyphenyl)butanedinitrile	1	2	2	0	<chem>Oc1ccc(cc1)C(C#N)C(C#N)c2ccc(O)cc2</chem>
	4-[1-(4-hydroxyphenyl)propan-2-yl]phenol	1	2	2	0	<chem>CC(Cc1ccc(O)cc1)c2ccc(O)cc2</chem>
53905-28-5	2,5-dichloro-4'-biphenylol	1	2	2	0	<chem>Oc1ccc(cc1)-c1cc(Cl)ccc1Cl</chem>
3424-82-6	1-chloro-2-[2,2-dichloro-1-(4-chlorophenyl)ethenyl]benzene	1	2	2	0	<chem>ClC(=C(c1ccc(Cl)cc1)c2ccccc2Cl)Cl</chem>
	2-chloro-6-[(1E)-(hydroxyimino)methyl]-3-(4-	1	2	2	0	<chem>O\N=C\c1ccc(c(Cl)c1O)c2ccc(O)cc2</chem>

	hydroxyphenyl)phenol					
28034-99-3	4-chloro-4'-biphenylol	1	2	2	0	<chem>Oc1ccc(cc1)-c1ccc(Cl)cc1</chem>
63-05-8	4-androstenedione	0	2	1	1	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CCC2=O</chem>
72-55-9	P,P'-dde	0	2	1	1	<chem>ClC(=C(c1ccc(Cl)cc1)c2ccc(Cl)cc2)Cl</chem>
	@compound 4-D	1	2	2	0	<chem>Oc1ccc(cc1)C2Sc3cc(O)ccc3OC2c4ccc(OCCN5CCCCC5)cc4</chem>
474-86-2	equilin	1	2	2	0	<chem>C[C@]12CC[C@H]3C(=CCc4cc(O)ccc34)[C@@H]1CCC2=O</chem>
	1-(4-fluorophenyl)-2-phenyl-3,4-dihydro-1H-isoquinolin-6-ol	1	2	2	0	<chem>Oc1ccc2C(N(CCc2c1)c3ccccc3)c4ccc(F)cc4</chem>
	4-[(1Z)-1-(4-hydroxyphenyl)-2-phenylbut-1-en-1-yl]phenoxyacetic acid	1	2	2	0	<chem>CC\C/C(=C/c1ccc(O)cc1)\c2ccc(OCC(=O)O)cc2)\c3ccccc3</chem>
	(2R,3S)-2,3-bis(4-hydroxyphenyl)pentanenitrile	1	2	2	0	<chem>CC[C@@H]([C@@H](C#N)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	(2R,3S)-2,3-bis(4-hydroxyphenyl)butanenitrile	1	2	2	0	<chem>C[C@@H]([C@@H](C#N)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	3-(4-hydroxy-2-methylphenyl)-2-(4-hydroxyphenyl)propanenitrile	1	2	2	0	<chem>Cc1cc(O)ccc1CC(C#N)c2ccc(O)cc2</chem>
80-46-6	ptap	1	2	2	0	<chem>CCC(C)(C)c1ccc(O)cc1</chem>
	1-chloro-2-[2,2-dichloro-1-(4-	1	2	2	0	<chem>ClC(Cl)C(c1ccc(Cl)cc1)c2ccccc2Cl</chem>

	chlorophenyl)ethyl]benzene					
	citro; clomifene	1	2	2	0	<chem>CCN(CC)CCOc1ccc(cc1)\C=C(\Cl)/c2ccccc2)\c3ccccc3.O C(=O)CC(O)(CC(=O)O)C(=O)O</chem>
85-68-7	BBP	1	2	2	0	<chem>CCCCOC(=O)c1ccccc1C(=O)OCc2ccccc2</chem>
150304-08-8	C12H6cl4O	1	2	2	0	<chem>Oc1ccc(c(Cl)c1)-c1c(Cl)cc(Cl)cc1Cl</chem>
192190-09-3	C12H5cl5O	1	2	2	0	<chem>Oc1ccc(cc1Cl)-c1cc(Cl)c(Cl)c(Cl)c1Cl</chem>
	(2S,3R)-3-(4-hydroxyphenyl)-2-(4-{2-[(3R)-3-methylpyrrolidin-1-yl]ethoxy}phenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	2	2	0	<chem>C[C@@H]1CCN(CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5)C1</chem>
	(2S,3R)-3-(4-hydroxyphenyl)-2-(4-[(2S)-2-(pyrrolidin-1-yl)propoxy]phenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	2	2	0	<chem>C[C@@H](COc1ccc(cc1)[C@@H]2Oc3ccc(O)cc3S[C@@H]2c4ccc(O)cc4)N5CCCC5</chem>
	6-(3-hydroxyphenyl)naphthalen-2-ol	1	2	2	0	<chem>Oc1cccc(c1)c2ccc3cc(O)ccc3c2</chem>
	(1S,10R,11S,14R,15S)-14-[(Z)-2-iodoethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	2	2	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)\C=C/I</chem>

	(1S,10R,11S,14R,15S)-14-[(E)-2-iodoethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	2	2	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)\C=C\I</chem>
	hexestrol	1	2	2	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(O)cc2</chem>
571-20-0	5 α -androstane-3 β ,17 β -diol	1	2	2	0	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@H]4C[C@@H](O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
	4-{3-[(1E)-1-(4-hydroxyphenyl)-4-phenylbut-1-en-1-yl]phenoxy}butanoic acid	1	2	2	0	<chem>OC(=O)CCCOc1ccc(c1)\C(=C\CCc2ccccc2)\c3ccc(O)cc3</chem>
	4-{3-[(1E)-1-(3-hydroxyphenyl)-4-phenylbut-1-en-1-yl]phenoxy}butanoic acid	1	2	2	0	<chem>OC(=O)CCCOc1ccc(c1)\C(=C\CCc2ccccc2)\c3ccc(O)c3</chem>
	4-[(1E)-1-(3-hydroxyphenyl)-2-phenylbut-1-en-1-yl]phenoxyacetic acid	1	2	2	0	<chem>CC\C(=C\c1ccc(OCC(=O)O)cc1)/c2ccc(O)c2)\c3ccccc3</chem>
29471-88-3	ethylphenol	0	2	1	1	<chem>CCc1ccc(O)cc1</chem>
88-18-6	2-tert-butylphenol	0	2	1	1	<chem>CC(C)(C)c1ccccc1O</chem>
	2,3-bis(4-hydroxyphenyl)pyrazolo[1,5-a]pyrimidin-6-ol	1	2	2	0	<chem>Oc1ccc(cc1)c2nn3cc(O)cnc3c2c4ccc(O)cc4</chem>

	C12H5Cl5O	1	2	2	0	<chem>Oc1ccc(c(Cl)c1)-c1cc(Cl)c(Cl)c(Cl)c1Cl</chem>
150304-10-2	C12H5Cl5O	1	2	2	0	<chem>Oc1ccc(c(Cl)c1)-c1c(Cl)cc(Cl)c(Cl)c1Cl</chem>
150304-11-3	C12H5Cl5O	1	2	2	0	<chem>Oc1ccc(c(Cl)c1)-c1c(Cl)c(Cl)cc(Cl)c1Cl</chem>
189578-02-7	C12H5Cl5O	1	2	2	0	<chem>Oc1ccc(cc1Cl)-c1c(Cl)c(Cl)cc(Cl)c1Cl</chem>
	4-{3-[(1S,2S)-1-(4-hydroxyphenyl)-2-methyl-2-phenylbutyl]phenoxy}butanoic acid	1	2	2	0	<chem>CC[C@@](C)([C@@H](c1ccc(O)cc1)c2cccc(OCCCC(=O)O)c2)c3cccc3</chem>
50-22-6	corticosterone	0	2	1	1	<chem>C[C@]12C[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2C(=O)CO</chem>
	(2S,3R)-3-(4-hydroxyphenyl)-2-{4-[(2R)-2-(pyrrolidin-1-yl)propoxy]phenyl}-2,3-dihydro-1,4-benzoxathiin-6-ol	1	2	2	0	<chem>C[C@H](COc1ccc(cc1)[C@@H]2Oc3ccc(O)cc3S[C@@H]2c4ccc(O)cc4)N5CCCC5</chem>
	(2S,3R)-3-(4-hydroxyphenyl)-2-(4-{2-[(3S)-3-methylpyrrolidin-1-yl]ethoxy}phenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	2	2	0	<chem>C[C@H]1CCN(CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5)C1</chem>
	2-(4-hydroxyphenyl)-1-benzofuran-5-ol	1	2	2	0	<chem>Oc1ccc(cc1)c2oc3ccc(O)cc3c2</chem>

	4-[1-(4-hydroxyphenyl)-2-{1-methyl-1-ferraspiro[pentacyclo[2.2.0.0{1,3}.0{1,5}.0{2,6}]]hexane-1,1'-tetracyclo[2.2.0.0{1,3}.0{2,6}]]hexane]-6'-yl}but-1-en-1-yl]phenol	1	2	2	0	CCC(=C(c1ccc(O)cc1)c2ccc(O)cc2)C34CC5C6C3[Fe]456789%10(C)C%11C7C8C9C%10%11
1156-92-9	4-androstenediol	1	2	2	0	C[C@]12CC[C@H]3[C@@H](CCC4=C[C@@H](O)CC[C@]34C)[C@@H]1CC[C@@H]2O
585-34-2	3-tert-butylphenol	0	2	1	1	CC(C)(C)c1ccc(O)c1
571-92-6	(1S,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-8-one	1	2	2	0	C[C@]12CC[C@H]3[C@@H](CC(=O)c4cc(O)ccc34)[C@@H]1CC[C@@H]2O
	7-(cyclopentyloxy)-3-(4-hydroxyphenyl)chromen-4-one	1	2	2	0	Oc1ccc(cc1)C2=COc3cc(OC4CCCC4)ccc3C2=O
	(1S,10R,11S,14S,15S)-4-(hydroxymethyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	2	2	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)c(CO)cc34)[C@@H]1CC[C@@H]2O
	(1S,10S,11S,14R,15S,17S)-14-[(E)-2-iodoethenyl]-17-methoxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-	1	2	2	0	CO[C@H]1C[C@@]2(C)[C@@H](CC[C@@]2(O)\C=C\I)[C@@H]3CCc4cc(O)ccc4[C@@H]13

	diol					
	(1S,10S,11S,14R,15S,17S)-14-[(Z)-2-iodoethenyl]-17-methoxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	CO[C@H]1C[C@@]2(C)[C@@H](CC[C@@]2(O)\C=C/I)[C@@H]3CCc4cc(O)ccc4[C@H]13
192190-10-6	C12H5Cl5O	1	2	2	0	Oc1ccc(cc1Cl)-c1c(Cl)cc(Cl)c(Cl)c1Cl
152969-11-4	C12H5Cl5O	1	2	2	0	Oc1c(Cl)cc(-c2ccc(Cl)c(Cl)c2)c(Cl)c1Cl
	5,11-diethyl-5,6,11,12-tetrahydrochrysene-2,8-diol	1	2	2	0	CCC1Cc2cc(O)ccc2C3=C1c4ccc(O)cc4CC3CC
1336-35-2	phenol	0	2	1	1	Oc1ccccc1
	(1S,10S)-17-ethyltetracyclo[8.7.0.0{2,7}.0{11,16}]heptadeca-2,4,6,11(16),12,14-hexaene-5,14-diol	1	2	2	0	CCC1[C@H]2[C@H](CCc3cc(O)ccc23)c4ccc(O)cc14
	(2S,3S)-7-hydroxy-3-(4-hydroxyphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1-benzopyran-4-one	1	2	2	0	Oc1ccc(cc1)[C@H]2[C@H](Oc3cc(O)ccc3C2=O)c4ccc(OCCN5CCCCC5)cc4
	(2S,3S)-3-(4-hydroxyphenyl)-2-{4-	1	2	2	0	Oc1ccc(cc1)[C@@H]2Cc3ccc(O)cc3O[C@@H]2c4ccc(OCCN

	[2-(piperidin-1-yl)ethoxy]phenyl)-3,4-dihydro-2H-1-benzopyran-7-ol					5CCCCC5)cc4
	4-[9-(4-hydroxyphenyl)bicyclo[3.3.1]nonan-9-yl]phenol	1	2	2	0	Oc1ccc(cc1)C2(C3CCCC2CCC3)c4ccc(O)cc4
	1-[4-(6-hydroxy-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-2-yl)phenyl]ethanone	1	2	2	0	CC(=O)c1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4
	4-(6-hydroxy-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-2-yl)-N,N-dimethylbenzamide	1	2	2	0	CN(C)C(=O)c1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4
	ethyl 4-(6-hydroxy-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-2-yl)benzoate	1	2	2	0	CCOC(=O)c1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4
	1-[2-(4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-yl]ethanone	1	2	2	0	CC(=O)c1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(O)cc5
	2-(4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophene-6-carboxamide	1	2	2	0	NC(=O)c1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(O)cc5
	2-(4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-	0	2	0	2	OC(=O)c1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5c

	benzothiophene-6-carboxylic acid					<chem>cc(O)cc5</chem>
	diethyl 2-(4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ylphosphonate	1	2	2	0	<chem>CCOP(=O)(OCC)c1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(O)cc5</chem>
	diethyl 4-(6-hydroxy-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-2-yl)phenylphosphonate	1	2	2	0	<chem>CCOP(=O)(OCC)c1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCN5CCCCC5)cc4</chem>
	2-(4-ethenylphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	2	2	0	<chem>Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(C=C)cc5</chem>
	2-(4-ethynylphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	2	2	0	<chem>Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(cc5)C#C</chem>
	4-(6-hydroxy-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-2-yl)benzamide	1	2	2	0	<chem>NC(=O)c1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>
	4-(6-hydroxy-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-2-yl)benzoic acid	1	2	2	0	<chem>OC(=O)c1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>
	methyl 4-(6-hydroxy-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-2-yl)benzoate	1	2	2	0	<chem>COC(=O)c1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>

	4-(6-ethynyl-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-2-yl)phenol	1	2	2	0	<chem>Oc1ccc(cc1)c2sc3cc(ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4)C#C</chem>
90-43-7	o-phenylphenol	0	2	1	1	<chem>Oc1ccccc1c2ccccc2</chem>
580-51-8	m-hydroxydiphenyl	0	2	1	1	<chem>Oc1cccc(c1)c2ccccc2</chem>
	4-[3,5-bis(4-hydroxyphenyl)-4-(2-methylpropyl)pyrazol-1-yl]phenol	1	2	2	0	<chem>CC(C)Cc1c(nn(c2ccc(O)cc2)c1c3ccc(O)cc3)c4ccc(O)cc4</chem>
965-93-5	metribolona	1	2	2	0	<chem>C[C@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CCC4=C3C=C[C@]12C</chem>
	6-(4-phenylhexan-3-yl)pyridin-3-ol	1	2	2	0	<chem>CCC(C(CC)c1ccc(O)cn1)c2ccccc2</chem>
	6-(4-hydroxyphenyl)naphthalen-2-ol	1	2	2	0	<chem>Oc1ccc(cc1)c2ccc3cc(O)ccc3c2</chem>
	(2R)-2,3-bis(4-hydroxyphenyl)propanenitrile	1	2	2	0	<chem>Oc1ccc(C[C@@H](C#N)c2ccc(O)cc2)cc1</chem>
	4-chloro-2-(4-hydroxyphenyl)quinolin-6-ol	1	2	2	0	<chem>Oc1ccc(cc1)c2cc(Cl)c3cc(O)ccc3n2</chem>
	4-bromo-2-(4-hydroxyphenyl)quinolin-6-ol	1	2	2	0	<chem>Oc1ccc(cc1)c2cc(Br)c3cc(O)ccc3n2</chem>
	4-ethenyl-2-(4-hydroxyphenyl)quinolin-6-ol	1	2	2	0	<chem>Oc1ccc(cc1)c2cc(C=C)c3cc(O)ccc3n2</chem>
	4-ethyl-2-(4-	1	2	2	0	<chem>CCc1cc(nc2ccc(O)cc12)c3ccc(O)cc3</chem>

	hydroxyphenyl)quinolin-6-ol					
	4-ethynyl-2-(4-hydroxyphenyl)quinolin-6-ol	1	2	2	0	<chem>Oc1ccc(cc1)c2cc(C#C)c3cc(O)ccc3n2</chem>
	6-hydroxy-2-(4-hydroxyphenyl)quinoline-4-carbonitrile	1	2	2	0	<chem>Oc1ccc(cc1)c2cc(C#N)c3cc(O)ccc3n2</chem>
	4-bromo-9a-butyl-7-hydroxy-2,9-dihydro-1H-fluoren-3-one	1	2	2	0	<chem>CCCCC12CCC(=O)C(=C1c3ccc(O)cc3C2)Br</chem>
	4-hydroxyphenyl (2S)-5,6-diphenyl-7-oxabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	2	2	0	<chem>Oc1ccc(OS(=O)(=O)[C@H]2CC3OC2C(=C3c4ccccc4)c5ccccc5)cc1</chem>
	phenyl (2S)-5,6-bis(4-hydroxyphenyl)-7-oxabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	2	2	0	<chem>Oc1ccc(cc1)C2=C(C3OC2C[C@@H]3S(=O)(=O)Oc4ccccc4)c5ccc(O)cc5</chem>
	(1S,2S,5S,10R,11S,14S,15S)-2-ethenyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-7-ene-5,14-diol	1	2	2	0	<chem>C[C@]12CC[C@H]3[C@@H](CC=C4C[C@@H](O)CC[C@]34C=C)[C@@H]1CC[C@@H]2O</chem>
	(1S,2S,10R,11S,14S,15S)-2-ethenyl-14-hydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-5-one	1	2	2	0	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C=C)[C@@H]1CC[C@@H]2O</chem>

	2-[(1E)-(hydroxyimino)methyl]-5-(4-hydroxyphenyl)phenol	1	2	2	0	<chem>O\\N=C\\c1ccc(cc1O)c2ccc(O)cc2</chem>
	4-[1-(4-hydroxyphenyl)butan-2-yl]phenol	1	2	2	0	<chem>CCC(Cc1ccc(O)cc1)c2ccc(O)cc2</chem>
1229-24-9	(1S,8S,10R,11S,14S,15S)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,8,14-triol	1	2	2	0	<chem>C[C@]12CC[C@H]3[C@@H](C[C@H](O)c4cc(O)ccc34)[C@@H]1CC[C@@H]2O</chem>
81-90-3	phenolphthalin	0	2	1	1	<chem>OC(=O)c1cccc1C(c2ccc(O)cc2)c3ccc(O)cc3</chem>
	dithane	1	2	2	0	<chem>SC(=S)NCCNC(=S)S</chem>
362-06-1	2-hydroxyestrone	1	2	2	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)c(O)cc34)[C@@H]1CCC2=O</chem>
	(1S,10S,11S,14R,15S,17S)-14-ethynyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14,17-triol	1	2	2	0	<chem>C[C@]12C[C@H](O)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)C#C</chem>
	(1S,9R,10R,11S,14R,15S)-14-ethynyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,9,14-triol	1	2	2	0	<chem>C[C@]12CC[C@H]3[C@@H]([C@H](O)Cc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)C#C</chem>
	(1S,10S,11S,14S,15R)-14-ethyl-15-	1	2	2	0	<chem>CC[C@H]1CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@H]3CC[C</chem>

	methylnetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-5-ol					@]12C
34816-55-2	moxestrel	1	2	2	0	CO[C@H]1C[C@@]2(C)[C@@H](CC[C@@]2(O)C#C)[C@@H]3CCc4cc(O)ccc4[C@@H]13
	androstane-3,17-diol	1	2	2	0	C[C@]12CC[C@H]3[C@@H](CCC4CC(O)CC[C@]34C)[C@@H]1CCC2O
846-46-8	androstanedione	0	2	1	1	C[C@]12CC[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CCC2=O
189578-00-5	C12H6cl4O	1	2	2	0	Oc1ccc(cc1Cl)-c1c(Cl)cc(Cl)cc1Cl
145413-90-7	C12H4cl6O	1	2	2	0	Oc1c(Cl)cc(c(Cl)c1Cl)-c1cc(Cl)c(Cl)cc1Cl
158076-69-8	C12H3cl7O	1	2	2	0	Oc1c(Cl)c(Cl)cc(c1Cl)-c1cc(Cl)c(Cl)c(Cl)c1Cl
149589-55-9	C12H5cl5O	1	2	2	0	Oc1c(Cl)cc(cc1Cl)-c1ccc(Cl)c(Cl)c1Cl
158076-62-1	C12H4cl6O	1	2	2	0	Oc1c(Cl)cc(c(Cl)c1Cl)-c1ccc(Cl)c(Cl)c1Cl
158076-64-3	C12H3cl7O	1	2	2	0	Oc1c(Cl)cc(c(Cl)c1Cl)-c1cc(Cl)c(Cl)c(Cl)c1Cl
158076-68-	C12H3cl7O	1	2	2	0	Oc1c(Cl)c(Cl)c(c(Cl)c1Cl)-c1cc(Cl)c(Cl)cc1Cl

7						
	4-[5-(4-hydroxyphenyl)-3,6-dipropylpyrazin-2-yl]phenol	1	2	2	0	<chem>CCCC1nc(c(CCC)nc1-c1ccc(O)cc1)-c1ccc(O)cc1</chem>
	2-fluoro-4-phenylphenol	1	2	2	0	<chem>Oc1ccc(cc1F)-c1ccccc1</chem>
	4-(3-chlorophenyl)phenol	1	2	2	0	<chem>Oc1ccc(cc1)-c1cccc(Cl)c1</chem>
	4-(3-chlorophenyl)-2-fluorophenol	1	2	2	0	<chem>Oc1ccc(cc1F)-c1cccc(Cl)c1</chem>
4291-32-1	4-(3,5-dichlorophenyl)phenol	1	2	2	0	<chem>Oc1ccc(cc1)-c1cc(Cl)cc(Cl)c1</chem>
	2,6-dichloro-4-(4-hydroxyphenyl)benzaldehyde	1	2	2	0	<chem>Oc1ccc(cc1)-c1cc(Cl)c(C=O)c(Cl)c1</chem>
	4-(3,5-dichloro-4-methylphenyl)phenol	1	2	2	0	<chem>Cc1c(Cl)cc(cc1Cl)-c1ccc(O)cc1</chem>
	4-(3,5-dichlorophenyl)-2-fluorophenol	1	2	2	0	<chem>Oc1ccc(cc1F)-c1cc(Cl)cc(Cl)c1</chem>
	2,6-dichloro-4-(3-fluoro-4-hydroxyphenyl)benzaldehyde	1	2	2	0	<chem>Oc1ccc(cc1F)-c1cc(Cl)c(C=O)c(Cl)c1</chem>
	4-(3,5-dichloro-4-methylphenyl)-2-fluorophenol	1	2	2	0	<chem>Cc1c(Cl)cc(cc1Cl)-c1ccc(O)c(F)c1</chem>
	2,3-dichloro-4-(3-fluoro-4-hydroxyphenyl)benzaldehyde	1	2	2	0	<chem>Oc1ccc(cc1F)-c1ccc(C=O)c(Cl)c1Cl</chem>
	2-cyclohexyl-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-	1	2	2	0	<chem>Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)C5CCCCC5</chem>

	benzothiophen-6-ol					5
	2-methyl-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	2	2	0	<chem>Cc1sc2cc(O)ccc2c1C(=O)c3ccc(OCCN4CCCCC4)cc3</chem>
	2-isopropyl-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	2	2	0	<chem>CC(C)c1sc2cc(O)ccc2c1C(=O)c3ccc(OCCN4CCCCC4)cc3</chem>
	2-cyclopentyl-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	2	2	0	<chem>Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)C5CCCC5</chem>
	2-ethyl-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	2	2	0	<chem>CCc1sc2cc(O)ccc2c1C(=O)c3ccc(OCCN4CCCCC4)cc3</chem>
	3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-2-[(1r,4r)-4-hydroxycyclohexyl]-1-benzothiophen-6-ol	1	2	2	0	<chem>O[C@@H]1CC[C@H](CC1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCN5CCCCC5)cc4</chem>
	(5R,11R)-5,11-dipropyl-5,6,11,12-tetrahydrochrysene-2,8-diol	1	2	2	0	<chem>CCC[C@@H]1Cc2cc(O)ccc2C3=C1c4ccc(O)cc4C[C@H]3CCC</chem>
	(5S,11S)-5,11-diethyl-5,6,11,12-tetrahydrochrysene-2,8-diol	1	2	2	0	<chem>CC[C@H]1Cc2cc(O)ccc2C3=C1c4ccc(O)cc4C[C@@H]3CCC</chem>
	5,11-dipropyl-5,6,11,12-tetrahydrochrysene-2,8-diol	1	2	2	0	<chem>CCCC1Cc2cc(O)ccc2C3=C1c4ccc(O)cc4CC3CCC</chem>

(5S,11S)-5,11-dipropyl-5,6,11,12-tetrahydrochrysene-2,8-diol	1	2	2	0	<chem>CCC[C@H]1Cc2cc(O)ccc2C3=C1c4ccc(O)cc4C[C@@H]3CCC</chem>
3-[(1E)-1-(4-hydroxyphenyl)-2-phenylbut-1-en-1-yl]phenoxyacetic acid	1	2	2	0	<chem>CC\C/C(=C(\c1ccc(O)cc1)/c2cccc(OCC(=O)O)c2)\c3ccccc3</chem>
4-[4-ethyl-3,5-bis(4-hydroxyphenyl)furan-2-yl]phenol	1	2	2	0	<chem>CCc1c(oc(c2ccc(O)cc2)c1c3ccc(O)cc3)c4ccc(O)cc4</chem>
4-[3,5-bis(4-hydroxyphenyl)-4-methylfuran-2-yl]phenol	1	2	2	0	<chem>Cc1c(oc(c2ccc(O)cc2)c1c3ccc(O)cc3)c4ccc(O)cc4</chem>
4-(4-ethyl-3,5-diphenylfuran-2-yl)phenol	1	2	2	0	<chem>CCc1c(oc(c2ccc(O)cc2)c1c3ccccc3)c4ccccc4</chem>
4-[4-ethyl-5-(4-hydroxyphenyl)-2-phenylfuran-3-yl]phenol	1	2	2	0	<chem>CCc1c(oc(c2cccc2)c1c3ccc(O)cc3)c4ccc(O)cc4</chem>
4-[4-ethyl-5-(4-hydroxyphenyl)-3-phenylfuran-2-yl]phenol	1	2	2	0	<chem>CCc1c(oc(c2ccc(O)cc2)c1c3ccccc3)c4ccc(O)cc4</chem>
4-(3-ethyl-4,5-diphenylfuran-2-yl)phenol	1	2	2	0	<chem>CCc1c(oc(c2cccc2)c1c3ccccc3)c4ccc(O)cc4</chem>
4-[4-ethyl-3-(4-hydroxyphenyl)-5-phenylfuran-2-yl]phenol	1	2	2	0	<chem>CCc1c(oc(c2ccc(O)cc2)c1c3ccc(O)cc3)c4ccccc4</chem>
4-(4-ethyl-2,5-diphenylfuran-3-yl)phenol	1	2	2	0	<chem>CCc1c(oc(c2cccc2)c1c3ccc(O)cc3)c4ccccc4</chem>

4-[5-(4-hydroxyphenyl)-2-phenyl-4-propylfuran-3-yl]phenol	1	2	2	0	<chem>CCCC1c(oc(c2ccccc2)c1c3ccc(O)cc3)c4ccc(O)cc4</chem>
4-[tris(4-hydroxyphenyl)furan-3-yl]phenol	1	2	2	0	<chem>Oc1ccc(cc1)c2oc(c3ccc(O)cc3)c(c4ccc(O)cc4)c2c5ccc(O)cc5</chem>
4-[3,5-bis(4-hydroxyphenyl)-4-propylfuran-2-yl]phenol	1	2	2	0	<chem>CCCC1c(oc(c2ccc(O)cc2)c1c3ccc(O)cc3)c4ccc(O)cc4</chem>
4-[4-butyl-3,5-bis(4-hydroxyphenyl)furan-2-yl]phenol	1	2	2	0	<chem>CCCCC1c(oc(c2ccc(O)cc2)c1c3ccc(O)cc3)c4ccc(O)cc4</chem>
(14S,15S,17S)-17-methoxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	<chem>CO[C@H]1C[C@]2(C)[C@@H](O)CCC2C3CCc4cc(O)ccc4C13</chem>
2-hydroxy-3,4-diphenylbenzaldehyde	1	2	2	0	<chem>Oc1c(C=O)ccc(c2ccccc2)c1c3ccccc3</chem>
5,6-diphenylnaphthalen-2-ol	1	2	2	0	<chem>Oc1ccc2c(c3ccccc3)c(ccc2c1)c4ccccc4</chem>
6-[(1E)-(methoxyimino)methyl]-2,3-diphenylphenol	1	2	2	0	<chem>CO\\N=C\\c1ccc(c2ccccc2)c(c1O)c3ccccc3</chem>
4-[(3S,4R)-4-phenylhexan-3-yl]phenol	1	2	2	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccccc2</chem>
4-[(1E)-2-(4-hydroxyphenyl)-1-{1-methyl-1-ferraspiro[pentacyclo[2.2.0.0{1,3}.0{1,5}.0{2,6}]]hexane-1,1'-	1	2	2	0	<chem>CC\\C(=C(\\C1C2C3C4C1[Fe]2345678(C)C9C5C6C7C89)/c%10ccc(O)cc%10)\\c%11ccc(O)cc%11</chem>

	tetracyclo[2.2.0.0{1,3}.0{2,6}]hexane-5'-yl}but-1-en-1-yl]phenol					
	9a-benzyl-7-hydroxy-4-methyl-2,9-dihydro-1H-fluoren-3-one	1	2	2	0	<chem>CC1=C2c3ccc(O)cc3CC2(Cc4ccccc4)CCC1=O</chem>
	(1S,10R,11S,14S,15S)-15-methyl-14-(prop-1-yn-1-yl)tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	<chem>CC#C[C@]1(O)CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@H]3CC[C@]12C</chem>
302-76-1	methylestradiol	1	2	2	0	<chem>C[C@]1(O)CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@H]3CC[C@]12C</chem>
	N-(5-({3-({6-[(1S,9R,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-9-yl}hexyl}carbamoylethyl)propyl}carbamoyl)-1-methylpyrrol-3-yl)-4-(3-methanesulfonylpropanamido)-1-methylpyrrole-2-carboxamide	1	2	2	0	<chem>Cn1cc(NC(=O)c2cc(NC(=O)CCS(=O)(=O)C)cn2C)cc1C(=O)NCCCCC(=O)NCCCCC[C@@H]3Cc4cc(O)ccc4[C@H]5CC[C@]6(C)[C@@H](O)CC[C@H]6[C@H]35</chem>
53890-77-0	4-(3,4-dichlorophenyl)phenol	1	2	2	0	<chem>Oc1ccc(cc1)-c1ccc(Cl)c(Cl)c1</chem>
	(14R,15S)-15-methyl-14-[(E)-2-phenylethenyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	2	2	0	<chem>C[C@]12CCC3C(CCc4cc(O)ccc34)C1CC[C@@]2(O)\C=C\c1ccccc1</chem>

4-[4-(4-hydroxyphenyl)hexan-3-yl]-2-iodophenol	1	2	2	0	<chem>CCC(C(CC)c1ccc(O)c(I)c1)c2ccc(O)cc2</chem>
4-[1-bromo-4-(4-hydroxyphenyl)hexan-3-yl]phenol	1	2	2	0	<chem>CCC(C(CBr)c1ccc(O)cc1)c2ccc(O)cc2</chem>
4-[1-fluoro-4-(4-hydroxyphenyl)hexan-3-yl]phenol	1	2	2	0	<chem>CCC(C(CF)c1ccc(O)cc1)c2ccc(O)cc2</chem>
pentyl 2,3-bis(4-hydroxyphenyl)pentanoate	1	2	2	0	<chem>CCCCCOC(=O)C(C(CC)c1ccc(O)cc1)c2ccc(O)cc2</chem>
methyl 2,3-bis(4-hydroxyphenyl)pentanoate	1	2	2	0	<chem>CCC(C(C(=O)OC)c1ccc(O)cc1)c2ccc(O)cc2</chem>
4-[6-hydroxy-4-(4-hydroxyphenyl)hexan-3-yl]phenol	1	2	2	0	<chem>CCC(C(CCO)c1ccc(O)cc1)c2ccc(O)cc2</chem>
pentyl 3,4-bis(4-hydroxyphenyl)hexanoate	1	2	2	0	<chem>CCCCCOC(=O)CC(C(CC)c1ccc(O)cc1)c2ccc(O)cc2</chem>
4-[2,6-dibromo-4-(hydroxymethyl)phenyl]phenol	1	2	2	0	<chem>OCc1cc(Br)c(c(Br)c1)c2ccc(O)cc2</chem>
4-[4-(hydroxymethyl)-2,6-dinitrophenyl]phenol	1	2	2	0	<chem>OCc1cc(c(c2ccc(O)cc2)c(c1)[N+](=O)[O-])[N+](=O)[O-]</chem>
4-[2,6-dichloro-4-(hydroxymethyl)phenyl]phenol	1	2	2	0	<chem>OCc1cc(Cl)c(c(Cl)c1)c2ccc(O)cc2</chem>
4-[4-(hydroxymethyl)-2-	1	2	2	0	<chem>OCc1ccc(c2ccc(O)cc2)c(c1)C(F)(F)F</chem>

	(trifluoromethyl)phenyl]phenol					
	(2R)-3-(4-hydroxyphenyl)-4-methyl-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2H-chromen-7-ol	1	2	2	0	<chem>CC1=C([C@H](Oc2cc(O)ccc12)c3ccc(OCCN4CCCC4)cc3)c5cc(O)cc5</chem>
	4-{2-ethyl-11-azatricyclo[5.3.1.0{4,11}]undeca-1,3,5,7,9-pentaen-3-yl}phenol	1	2	2	0	<chem>CCc1c(c2ccc(O)cc2)c3C=Cc4cccc1n34</chem>
	(13R,14R,15S,17S)-6-fluoro-13-iodo-17-methoxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6,8-tetraene-5,14-diol	1	2	2	0	<chem>CO[C@H]1C[C@]2(C)[C@@H](O)[C@H](I)CC2C3C=Cc4c(F)c(O)ccc4C13</chem>
	(13R,14R,15S,17S)-4-fluoro-13-iodo-17-methoxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6,8-tetraene-5,14-diol	1	2	2	0	<chem>CO[C@H]1C[C@]2(C)[C@@H](O)[C@H](I)CC2C3C=Cc4cc(O)c(F)cc4C13</chem>
	3-{3-methyl-4-[2-(piperidin-1-yl)ethoxy]phenyl}-2',3'-dihydro-1,1'-spirobi[indene]-5,5'-diol	1	2	2	0	<chem>Cc1cc(ccc1OCCN2CCCCC2)C3=CC4(CCC5cc(O)ccc45)c6ccc(O)cc36</chem>
	6-phenyl-5-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-7,8-dihydronaphthalen-2-ol	1	2	2	0	<chem>Oc1ccc2C(=C(CCc2c1)c3ccccc3)C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>

	11-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-5H,6H,11H-benzo[a]fluoren-3-ol	1	2	2	0	<chem>Oc1ccc2C3=C(Cc2c1)c4cccc4C3c5ccc(OCCN6CCCCC6)cc5</chem>
	11-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-5H,6H,11H-benzo[a]fluorene-3,9-diol	1	2	2	0	<chem>Oc1ccc2C3=C(Cc2c1)c4ccc(O)cc4C3c5ccc(OCCN6CCCCC6)cc5</chem>
	6-(4-hydroxyphenyl)-5-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-7,8-dihydronaphthalen-2-ol	1	2	2	0	<chem>Oc1ccc(cc1)C2=C(C(=O)c3ccc(OCCN4CCCCC4)cc3)c5ccc(O)c5CC2</chem>
	ruthenium(1+) ion 14-hydroxytetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3-dien-5-one pentamethylcyclopentadiene tetrafluoroborate	1	2	2	0	<chem>[Ru+].CC1C(=C(C)C(=C1C)C)C.OC2CCC3C2CCC4C3CCC5=C4C=CC(=O)C5.F[B-](F)(F)F</chem>
362-08-3	2-methoxyestrone	1	2	2	0	<chem>COc1cc2[C@H]3CC[C@@]4(C)[C@@H](CCC4=O)[C@@H]3CCc2cc1O</chem>
107256-99-5	(2-{4-[(1Z)-1,2-diphenylbut-1-en-1-yl]phenoxy}ethyl)trimethylazanium iodide	1	2	2	0	<chem>[I-].CC\C=C(/c1ccccc1)\c2ccc(OCC[N+](C)(C)C)cc2\c3ccccc3</chem>
	(2-{4-[(1Z)-1,2-diphenylbut-1-en-1-yl]phenoxy}ethyl)(ethyl)dimethylazanium bromide	1	2	2	0	<chem>[Br-].CC\C=C(/c1ccccc1)\c2ccc(OCC[N+](C)(C)CC)cc2\c3ccccc3</chem>
	(2-{4-[(1Z)-1,2-diphenylbut-1-en-1-yl]phenoxy}ethyl)(isopropyl)dimeth	1	2	2	0	<chem>[Br-].CC\C=C(/c1ccccc1)\c2ccc(OCC[N+](C)(C)C(C)C)cc2\c3</chem>

	ylazanium bromide					cccc3
	butyl(2-{4-[(1Z)-1,2-diphenylbut-1-en-1-yl]phenoxy}ethyl)dimethylazanium bromide	1	2	2	0	[Br-].CCCC[N+](C)(C)CCOc1ccc(cc1)\C(=C(\CC)/c2ccccc2)\c3ccccc3
1624-62-0	(1S,10R,11S,15S)-5-methoxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-one	1	2	2	0	COc1ccc2[C@H]3CC[C@@]4(C)[C@@H](CCC4=O)[C@@H]3CCc2c1
	(1R,10S,11S,14S,15S,17S)-17-ethynyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	C[C@]12C[C@H](C#C)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O
	(1R,10S,11S,14S,15S,17S)-15-methyl-17-(prop-1-yn-1-yl)tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	CC#C[C@H]1C[C@]2(C)[C@@H](O)CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@@H]13
	4-[(1S,10S,11S,14S,15S,17S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-17-yl]butanenitrile	1	2	2	0	C[C@]12C[C@H](CCCC#N)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O
	(1S,10R,11S,14R,15S)-14-[(E)-2-(4-fluorophenyl)ethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,	1	2	2	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)\C=C\c5ccc(F)cc5

	15]]heptadeca-2(7),3,5-triene-5,14-diol					
	4-[(E)-2-[(1S,10R,11S,14R,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]]heptadeca-2(7),3,5-trien-14-yl]ethenyl]benzonitrile	1	2	2	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)\C=C\c5ccc(cc5)C#N
	1-{4-[(E)-2-[(1S,10R,11S,14R,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]]heptadeca-2(7),3,5-trien-14-yl]ethenyl]phenyl}ethanone	1	2	2	0	CC(=O)c1ccc(\C=C\[C@]2(O)CC[C@H]3[C@@H]4CCc5cc(O)ccc5[C@H]4CC[C@]23C)cc1
	(1S,10S,11S,14S,15S,17S)-17-methoxy-15-methyl-14-(prop-1-yn-1-yl)tetracyclo[8.7.0.0{2,7}.0{11,15}]]heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	CO[C@H]1C[C@@]2(C)[C@@H](CC[C@@]2(O)C#CC)[C@@H]3CCc4cc(O)ccc4[C@@H]13
	(1S,10S,11S,13R,14S,15S,17S)-17-methoxy-15-methyl-14-(prop-1-yn-1-yl)tetracyclo[8.7.0.0{2,7}.0{11,15}]]heptadeca-2,4,6-triene-5,13,14-triol	1	2	2	0	CO[C@H]1C[C@@]2(C)[C@@H](C[C@@H](O)[C@@]2(O)C#CC)[C@@H]3CCc4cc(O)ccc4[C@@H]13
	(1S,10S,11S,13R,14R,15S,17S)-14-ethynyl-17-methoxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,	1	2	2	0	CO[C@H]1C[C@@]2(C)[C@@H](C[C@@H](O)[C@@]2(O)C#C)[C@@H]3CCc4cc(O)ccc4[C@@H]13

	15]]heptadeca-2,4,6-triene-5,13,14-triol					
	(1S,10S,11S,13R,14R,15S,17S)-17-methoxy-14,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-2,4,6-triene-5,13,14-triol	1	2	2	0	CO[C@H]1C[C@@]2(C)[C@@H](C[C@@H](O)[C@]2(C)O)[C@@H]3CCc4cc(O)ccc4[C@@H]13
	(1S,10S,11S,13R,14R,15S,17S)-17-methoxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-2,4,6-triene-5,13,14-triol	1	2	2	0	CO[C@H]1C[C@]2(C)[C@@H](O)[C@H](O)C[C@H]2[C@@H]3CCc4cc(O)ccc4[C@@H]13
	(1S,10R,11S,14R,15S)-15-methyl-14-[(1E)-prop-1-en-1-yl]tetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	C\\C=C\\[C@]1(O)CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@H]3CC[C@]12C
	(1S,10S,11S,14S,15S,17S)-17-methoxy-15-methyl-14-phenyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	CO[C@H]1C[C@@]2(C)[C@@H](CC[C@@]2(O)c3ccccc3)[C@@H]4CCc5cc(O)ccc5[C@@H]14
	(1S,10R,11S,13R,14R,15S)-14,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-2,4,6-triene-5,13,14-triol	1	2	2	0	C[C@]1(O)[C@H](O)C[C@H]2[C@@H]3CCc4cc(O)ccc4[C@H]3CC[C@]12C

	(1S,10R,11S,13R,14R,15S)-14-ethynyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,13,14-triol	1	2	2	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1C[C@@H](O)[C@@]2(O)C#C
	(1S,10R,11S,13R,14S,15S)-15-methyl-14-phenyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,13,14-triol	1	2	2	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1C[C@@H](O)[C@@]2(O)c5ccccc5
	(1S,10S,11S,13R,14R,15S,17S)-17-ethyl-14-ethynyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,13,14-triol	1	2	2	0	CC[C@H]1C[C@@]2(C)[C@@H](C[C@@H](O)[C@@]2(O)C#C)[C@@H]3CCc4cc(O)ccc4[C@@H]13
39845-47-1	(1S,10S,11S,14R,15S,17S)-17-ethyl-14-ethynyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	CC[C@H]1C[C@@]2(C)[C@@H](CC[C@@]2(O)C#C)[C@@H]3CCc4cc(O)ccc4[C@@H]13
	(1S,10S,11S,14S,15S,17S)-17-ethyl-14,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	CC[C@H]1C[C@@]2(C)[C@@H](CC[C@]2(C)O)[C@@H]3CCc4cc(O)ccc4[C@@H]13

	(1S,10R,11S,13R,14S,15S)-15-methyl-14-(prop-1-yn-1-yl)tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,13,14-triol	1	2	2	0	CC#C[C@]1(O)[C@H](O)C[C@H]2[C@@H]3CCc4cc(O)ccc4[C@H]3CC[C@]12C
	(1S,10S,11S,14S,15S,17S)-17-ethyl-15-methyl-14-(prop-1-yn-1-yl)tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	CC[C@H]1C[C@@]2(C)[C@@H](CC[C@@]2(O)C#CC)[C@@H]3CCc4cc(O)ccc4[C@@H]13
	(1S,10S,11S,14R,15S,17S)-17-methoxy-15-methyl-14-[(1E)-prop-1-en-1-yl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	CO[C@H]1C[C@@]2(C)[C@@H](CC[C@@]2(O)\C=C\)[C@@H]3CCc4cc(O)ccc4[C@@H]13
	(1S,10S,11S,13R,14S,15S,17S)-17-methoxy-15-methyl-14-phenyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,13,14-triol	1	2	2	0	CO[C@H]1C[C@@]2(C)[C@@H](C[C@@H](O)[C@@]2(O)c3ccccc3)[C@@H]4CCc5cc(O)ccc5[C@@H]14
	(1S,10S,11S,14R,15S,17R)-17-ethenyl-14-[(E)-2-iodoethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	C[C@]12C[C@H](C=C)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)\C=C\I
	(1S,10S,11S,14R,15S,17S)-14-[(Z)-2-chloroethenyl]-17-methoxy-15-	1	2	2	0	CO[C@H]1C[C@@]2(C)[C@@H](CC[C@@]2(O)\C=C/Cl)[C@@H]3CCc4cc(O)ccc4[C@@H]13

	methylnonacyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol					
	(1S,10S,11S,14R,15S,17R)-17-ethenyl-14-[(Z)-2-iodoethenyl]-15-methylnonacyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	C[C@]12C[C@H](C=C)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)\C=C/I
	(1S,10S,11S,14R,15S,17R)-14-[(E)-2-chloroethenyl]-17-ethenyl-15-methylnonacyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	C[C@]12C[C@H](C=C)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)\C=C\Cl
	(1S,10S,11S,14R,15S,17S)-14-[(E)-2-chloroethenyl]-17-methoxy-15-methylnonacyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	CO[C@H]1C[C@@]2(C)[C@@H](CC[C@@]2(O)\C=C\Cl)[C@@H]3CCc4cc(O)ccc4[C@@H]13
	(1R,10S,11S,13R,14R,15S,17S)-15-methyl-17-(prop-1-yn-1-yl)nonacyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,13,14-triol	1	2	2	0	CC#C[C@H]1C[C@]2(C)[C@@H](O)[C@H](O)C[C@H]2[C@@H]3CCc4cc(O)ccc4[C@@H]13
	(1S,10R,11S,14R,15S)-14-[(E)-2-(4-methoxyphenyl)ethenyl]-15-methylnonacyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	COc1ccc(\C=C\[C@]2(O)CC[C@H]3[C@@H]4CCc5cc(O)ccc5[C@H]4CC[C@]23C)cc1

	15]]heptadeca-2(7),3,5-triene-5,14-diol					
	(1S,10R,11S,14R,15S)-15-methyl-14-[(E)-2-(4-methylphenyl)ethenyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	2	2	0	<chem>Cc1ccc(\C=C\[C@]2(O)CC[C@H]3[C@@H]4CCc5cc(O)ccc5[C@H]4CC[C@]23C)cc1</chem>
	4-[(E)-2-[(1S,10R,11S,14R,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-14-yl]ethenyl]benzoic acid	1	2	2	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)\C=C\c5ccc(cc5)C(=O)O</chem>
	3-[(1S,10S,11S,14S,15S,17S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-17-yl]propanenitrile	1	2	2	0	<chem>C[C@]12C[C@H](CCC#N)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O</chem>
	(1R,10S,11S,13R,14R,15S,17S)-17-ethynyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,13,14-triol	1	2	2	0	<chem>C[C@]12C[C@H](C#C)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1C[C@@H](O)[C@@H]2O</chem>
	methyl 4-[(E)-2-[(1S,10R,11S,14R,15S)-5,14-dihydroxy-15-	1	2	2	0	<chem>COC(=O)c1ccc(\C=C\[C@]2(O)CC[C@H]3[C@@H]4CCc5cc(O)ccc5[C@H]4CC[C@]23C)cc1</chem>

	methylnitratetetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-14-yl]ethenyl]benzoate					
	(1S,10S,11S,13R,14R,15S,17S)-17-ethyl-14,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,13,14-triol	1	2	2	0	<chem>CC[C@H]1C[C@@]2(C)[C@@H](C[C@@H](O)[C@]2(C)O)[C@@H]3CCc4cc(O)ccc4[C@@H]13</chem>
	(1S,10S,11S,14S,15S,17S)-17-methoxy-14,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	<chem>CO[C@H]1C[C@@]2(C)[C@@H](CC[C@]2(C)O)[C@@H]3CCc4cc(O)ccc4[C@@H]13</chem>
	(1S,10S,11S,13R,14R,15S,17S)-17-ethyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,13,14-triol	1	2	2	0	<chem>CC[C@H]1C[C@]2(C)[C@@H](O)[C@H](O)C[C@H]2[C@@H]3CCc4cc(O)ccc4[C@@H]13</chem>
	(1S,10R,11S,14R,15S)-14-[(E)-2-(4-hydroxyphenyl)ethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	2	2	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)\C=C\c5ccc(O)cc5</chem>
	ruthenium(1+) ion estradiol pentamethylcyclopentadiene	0	2	1	1	<chem>[Ru+].CC1C(=C(C)C(=C1C)C)C.C[C@]23CC[C@H]4[C@@H](CCc5cc(O)ccc45)[C@@H]2CC[C@@H]3O.[O-</chem>

	triflate					<chem>]S(=O)(=O)C(F)(F)F</chem>
	[(1S,10R,11S,14S,15S)-14-hydroxy-5-(3-hydroxypropoxy)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-6-yl]chromiumtricarbaldehyde	1	2	2	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4c3ccc(OCCCCO)c4[Cr](C=O)(C=O)C=O)[C@@H]1CC[C@H]2O</chem>
	(1S,10S,11S,14S,15S,17S)-17-(3-fluoropropyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	<chem>C[C@]12C[C@H](CCCF)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@H]2O</chem>
	(1S,10S,11S,14R,15S,17R)-14-[(Z)-2-chloroethenyl]-17-ethenyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	<chem>C[C@]12C[C@H](C=C)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)\C=C/Cl</chem>
	(1S,10S,11S,14S,15S,17S)-17-(4-fluorobutyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	2	2	0	<chem>C[C@]12C[C@H](CCCCF)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@H]2O</chem>
	(1S,10S,11S,13R,14S,15S,17S)-17-ethyl-15-methyl-14-(prop-1-yn-1-yl)tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,13,14-triol	1	2	2	0	<chem>CC[C@H]1C[C@@]2(C)[C@@H](C[C@@H](O)[C@@]2(O)C#CC)[C@@H]3CCc4cc(O)ccc4[C@@H]13</chem>

	(2S)-7-hydroxy-8-[(1Z)-3-hydroxy-3-methylbut-1-en-1-yl]-5-methoxy-2-phenyl-2,3-dihydro-1-benzopyran-4-one	1	2	2	0	<chem>COc1cc(O)c(\C=C/C(C)(C)O)c2O[C@@H](CC(=O)c12)c3ccc</chem> <chem>cc3</chem>
	7-hydroxy-8-[(1Z)-3-hydroxy-3-methylbut-1-en-1-yl]-2-(4-hydroxyphenyl)-5-methoxy-2,3-dihydro-1-benzopyran-4-one	1	2	2	0	<chem>COc1cc(O)c(\C=C/C(C)(C)O)c2OC(CC(=O)c12)c3ccc(O)cc3</chem>
	(2E)-1-[2,4-dihydroxy-3-[(1Z)-3-hydroxy-3-methylbut-1-en-1-yl]-6-methoxyphenyl]-3-(4-hydroxyphenyl)prop-2-en-1-one	1	2	2	0	<chem>COc1cc(O)c(\C=C/C(C)(C)O)c(O)c1C(=O)\C=C\c2ccc(O)cc</chem> <chem>2</chem>
	(1R,2R,4aR,5R,8aS)-2-isopropyl-4a-methyl-8-methylidene-hexahydro-1H-naphthalene-1,2,5-triol	1	2	2	0	<chem>CC(C)[C@]1(O)CC[C@@]2(C)[C@H](O)CCC(=C)[C@@H]2[C</chem> <chem>@H]1O</chem>
469-01-2	pisatin	1	2	2	0	<chem>COc1ccc2[C@H]3Oc4cc5OCOc5cc4[C@@]3(O)COc2c1</chem>
29799-07-3	4-(adamantan-1-yl)phenol	1	2	2	0	<chem>Oc1ccc(cc1)C12CC3CC(CC(C3)C1)C2</chem>
57103-57-8	glyceollin	1	1	1	0	<chem>CC1(C)Oc2ccc3[C@@H]4Oc5cc(O)ccc5[C@]4(O)COc3c2C=</chem> <chem>C1</chem>
116057-75-1	idoxifene	1	1	1	0	<chem>CC\C/C(=C/c1ccc(I)cc1)\c2ccc(OCCN3CCCC3)cc2)\c4cccc</chem> <chem>4</chem>
	(14S,15S)-17-[4-(dimethylamino)phenyl]-14-	1	1	1	0	<chem>CN(C)c1ccc(cc1)C2C[C@@]3(C)C(CC[C@]3(O)CCCC)C4CCC</chem> <chem>5=CC(=O)CCC5=C24</chem>

	hydroxy-14-(3-hydroxypropyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-1,6-dien-5-one					
97-77-8	disulfiram	1	1	1	0	<chem>CCN(CC)C(=S)SSC(=S)N(CC)CC</chem>
	6-(3-methylbutyl)-2-N,4-N-bis(2-methylpropyl)pyrimidine-2,4-diamine	1	1	1	0	<chem>CC(C)CCc1cc(NCC(C)C)nc(NCC(C)C)n1</chem>
84-74-2	dibutyl-phthalate	0	1	0	1	<chem>CCCCOC(=O)c1cccc1C(=O)OCCCC</chem>
	6-(3-hydroxyphenyl)-1-phenylnaphthalen-2-ol	1	1	1	0	<chem>Oc1cccc(c1)c2ccc3c(c(O)ccc3c2)c4cccc4</chem>
	6-(3-hydroxyphenyl)-1-(pyridin-3-yl)naphthalen-2-ol	1	1	1	0	<chem>Oc1cccc(c1)c2ccc3c(c(O)ccc3c2)c4ccnnc4</chem>
	6-(3-hydroxyphenyl)-1-(6-methoxypyridin-3-yl)naphthalen-2-ol	1	1	1	0	<chem>COc1ccc(cn1)c2c(O)ccc3cc(ccc23)c4cccc(O)c4</chem>
	1,6-bis(3-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1cccc(c1)c2ccc3c(c(O)ccc3c2)c4cccc(O)c4</chem>
	N-{3-[2-hydroxy-6-(3-hydroxyphenyl)naphthalen-1-yl]phenyl}methanesulfonamide	1	1	1	0	<chem>CS(=O)(=O)Nc1cccc(c1)c2c(O)ccc3cc(ccc23)c4cccc(O)c4</chem>
	3-acetyl-7-(4-methoxyphenyl)chromen-2-one	0	1	0	1	<chem>COc1ccc(cc1)c2ccc3C=C(C(=O)C)C(=O)Oc3c2</chem>

	3-acetyl-7-(4-hydroxyphenyl)chromen-2-one	0	1	0	1	<chem>CC(=O)C1=Cc2ccc(cc2OC1=O)c3ccc(O)cc3</chem>
	1,2-bis(4-hydroxyphenyl)-3H-inden-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(c3ccc(O)cc3)c4ccc(O)cc4C2</chem>
362-07-2	2-methoxyestradiol	1	1	1	0	<chem>COc1cc2[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4[C@@H]3CCc2cc1O</chem>
	1-ethyl-2-(4-hydroxyphenyl)-3H-inden-5-ol	1	1	1	0	<chem>CCC1=C(Cc2cc(O)ccc12)c3ccc(O)cc3</chem>
	2-phenyl-1-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}-3,4-dihydro-1H-isoquinolin-6-ol	1	1	1	0	<chem>Oc1ccc2C(N(CCc2c1)c3cccc3)c4ccc(OCCN5CCCC5)cc4</chem>
	6-[(1E)-(hydroxyimino)methyl]-2,3-diphenylaniline	1	1	1	0	<chem>Nc1c(\C=N\O)ccc(c2cccc2)c1c3cccc3</chem>
	(E)-N-[(3,4-diphenylphenyl)methylidene]hydroxylamine	1	1	1	0	<chem>O\N=C\c1ccc(c2cccc2)c(c1)c3cccc3</chem>
	6-[(1E)-(hydroxyimino)methyl]-N-methyl-2,3-diphenylaniline	1	1	1	0	<chem>CNc1c(\C=N\O)ccc(c2cccc2)c1c3cccc3</chem>
	N-ethyl-6-[(1E)-(hydroxyimino)methyl]-2,3-diphenylaniline	1	1	1	0	<chem>CCNc1c(\C=N\O)ccc(c2cccc2)c1c3cccc3</chem>
	6-butyl-2-N,4-N-	1	1	1	0	<chem>CCCCc1cc(NCCC)nc(NCCC)n1</chem>

	dipropylpyrimidine-2,4-diamine					
	α -endosulfan	1	1	1	0	<chem>ClC1=C(Cl)C2(Cl)C3COS(=O)OCC3C1(Cl)C2(Cl)Cl</chem>
	3-acetyl-2-oxochromen-7-yl trifluoromethanesulfonate	0	1	0	1	<chem>CC(=O)C1=Cc2ccc(OS(=O)(=O)C(F)(F)F)cc2OC1=O</chem>
	1-(furan-3-yl)-6-(3- hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1cccc(c1)c2ccc3c(c(O)ccc3c2)c4cocc4</chem>
	6-(3-hydroxyphenyl)-1-(pyridin-4- yl)naphthalen-2-ol	1	1	1	0	<chem>Oc1cccc(c1)c2ccc3c(c(O)ccc3c2)c4ccncc4</chem>
	1-(3-aminophenyl)-6-(3- hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Nc1cccc(c1)c2c(O)ccc3cc(ccc23)c4cccc(O)c4</chem>
552-80-7	dimethylstilbestrol	1	1	1	0	<chem>C\C=C(\C)/c1ccc(O)cc1)\c2ccc(O)cc2</chem>
	@estriol	1	1	1	0	<chem>CC12CCC3C(CCc4cc(O)ccc34)C1CC(O)C2O</chem>
	2-(4-hydroxyphenyl)-1- benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2cc3ccc(O)cc3s2</chem>
	2-(4-hydroxyphenyl)-1-phenyl-3H- inden-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(c3ccccc3)c4ccc(O)cc4C2</chem>
	1,3-diethyl-2-(4-hydroxyphenyl)- 3H-inden-5-ol	1	1	1	0	<chem>CCC1C(=C(CC)c2ccc(O)cc12)c3ccc(O)cc3</chem>
	(2S,3R)-3-(3-hydroxyphenyl)-2-{4- [2-(pyrrolidin-1-yl)ethoxy]phenyl}- 2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>Oc1ccc2O[C@H]([C@H](Sc2c1)c3cccc(O)c3)c4ccc(OCCN5CCCC5)cc4</chem>

	(2S,3R)-3-(3-hydroxyphenyl)-2-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>Oc1cccc(c1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5CCCCC5)cc4</chem>
	2-(3-fluorophenyl)-1-[4-(1-methylpiperidin-4-yl)phenyl]-3,4-dihydro-1H-isoquinolin-6-ol	1	1	1	0	<chem>CN1CCC(CC1)c2ccc(cc2)C3N(CCc4cc(O)ccc34)c5cccc(F)c5</chem>
	2-(3-hydroxyphenyl)-1-[4-[4-(2-methylpropyl)piperazin-1-yl]phenyl]-3,4-dihydro-1H-isoquinolin-6-ol	1	1	1	0	<chem>CC(C)CN1CCN(CC1)c2ccc(cc2)C3N(CCc4cc(O)ccc34)c5cccc(O)c5</chem>
	1-[4-(1-methylpiperidin-4-yl)phenyl]-2-phenyl-3,4-dihydro-1H-isoquinolin-6-ol	1	1	1	0	<chem>CN1CCC(CC1)c2ccc(cc2)C3N(CCc4cc(O)ccc34)c5cccc5</chem>
2529-64-8	3-deoxy-17 β -estradiol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cccc34)[C@@H]1CC[C@@H]2O</chem>
	1-(4-fluorophenyl)-2-(4-hydroxyphenyl)-3H-inden-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(c3ccc(F)cc3)c4ccc(O)cc4C2</chem>
6052-84-2	4,4'-dihydroxybibenzyl	1	1	1	0	<chem>Oc1ccc(CCc2ccc(O)cc2)cc1</chem>
43085-54-7	mestranol	1	1	1	0	<chem>COc1ccc2[C@H]3CC[C@@]4(C)[C@@H](CC[C@@]4(O)C#C)[C@@H]3CCc2c1</chem>
	3-chloro-2-[(1E)-(hydroxyimino)methyl]-4-(4-hydroxyphenyl)phenol	1	1	1	0	<chem>O\N=C\c1c(O)ccc(c1Cl)c2ccc(O)cc2</chem>

	3-chloro-4-(3-fluoro-4-hydroxyphenyl)-2-[(1E)-(hydroxyimino)methyl]phenol	1	1	1	0	<chem>O\\N=C\\c1c(O)ccc(c1Cl)c2ccc(O)c(F)c2</chem>
5300-03-8	tretinoin	0	1	0	1	<chem>C\\C(=C/C=C/C(=C/C(=O)O)/C)\\C=C\\C1=C(C)CCCC1(C)C</chem>
	(2-{4-[2,2-dichloro-1-(4-methoxyphenyl)-3-phenylcyclopropyl]phenoxy}ethyl)dimethylamine	1	1	1	0	<chem>COc1ccc(cc1)C2(C(c3cccc3)C2(Cl)Cl)c4ccc(OCCN(C)C)cc4</chem>
	1-(2,2-dichloro-1,3-diphenylcyclopropyl)-4-methoxybenzene	1	1	1	0	<chem>COc1ccc(cc1)C2(C(c3cccc3)C2(Cl)Cl)c4cccc4</chem>
	1-(benzyloxy)-4-[2,2-dichloro-1,3-bis(4-methoxyphenyl)cyclopropyl]benzene	1	1	1	0	<chem>COc1ccc(cc1)C2C(Cl)(Cl)C2(c3ccc(OC)cc3)c4ccc(OCc5cccc5)cc4</chem>
	1-(benzyloxy)-4-[2,2-dichloro-1-(4-methoxyphenyl)-3-phenylcyclopropyl]benzene	1	1	1	0	<chem>COc1ccc(cc1)C2(C(c3cccc3)C2(Cl)Cl)c4ccc(OCc5cccc5)cc4</chem>
	(2,2-dichloro-3-phenylcyclopropyl)benzene	1	1	1	0	<chem>ClC1(Cl)C(C1c2cccc2)c3cccc3</chem>
	{2-[4-(2,2-dichloro-1,3-diphenylcyclopropyl)phenoxy]ethyl}dimethylamine	1	1	1	0	<chem>CN(C)CCOc1ccc(cc1)C2(C(c3cccc3)C2(Cl)Cl)c4cccc4</chem>

(1R,10S,11R,14R,15R)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	<chem>C[C@@]12CC[C@@H]3[C@H](CCc4cc(O)ccc34)[C@H]1CC[C@H]2O</chem>
5-amino-2-(4-aminophenyl)chromen-4-one	1	1	1	0	<chem>Nc1ccc(cc1)C2=CC(=O)c3c(N)cccc3O2</chem>
(2R,3S)-3-(4-hydroxyphenyl)-2-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-2,3-dihydro-1,4-benzoxathiin-7-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@@H]2Sc3ccc(O)cc3O[C@@H]2c4ccc(OCCN5CCCCC5)cc4</chem>
2-(4-chlorophenyl)-1-methyl-1-[4-[2-(pyrrolidin-1-yl)ethoxy]phenyl]-3,4-dihydroisoquinolin-6-ol	1	1	1	0	<chem>CC1(N(CCc2cc(O)ccc12)c3ccc(Cl)cc3)c4ccc(OCCN5CCCC5)cc4</chem>
2-(4-fluorophenyl)-1-methyl-1-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-3,4-dihydroisoquinolin-6-ol	1	1	1	0	<chem>CC1(N(CCc2cc(O)ccc12)c3ccc(F)cc3)c4ccc(OCCN5CCCCC5)cc4</chem>
2-(4-fluorophenyl)-1-methyl-1-[4-[2-(pyrrolidin-1-yl)ethoxy]phenyl]-3,4-dihydroisoquinolin-6-ol	1	1	1	0	<chem>CC1(N(CCc2cc(O)ccc12)c3ccc(F)cc3)c4ccc(OCCN5CCCC5)cc4</chem>
1-[4-[2-(azepan-1-yl)ethoxy]phenyl]-1-methyl-2-phenyl-3,4-dihydroisoquinolin-6-ol	1	1	1	0	<chem>CC1(N(CCc2cc(O)ccc12)c3ccccc3)c4ccc(OCCN5CCCCC5)cc4</chem>
1-methyl-2-phenyl-1-[4-[2-(piperidin-1-yl)ethoxy]phenyl]-3,4-	1	1	1	0	<chem>CC1(N(CCc2cc(O)ccc12)c3ccccc3)c4ccc(OCCN5CCCCC5)cc4</chem>

	dihydroisoquinolin-6-ol					
	2-[3-(dimethylamino)phenyl]-1-methyl-1-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-3,4-dihydroisoquinolin-6-ol	1	1	1	0	<chem>CN(C)c1cccc(c1)N2CCc3cc(O)ccc3C2(C)c4ccc(OCCN5CCCCC5)cc4</chem>
	1-methyl-2-(4-methylphenyl)-1-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}-3,4-dihydroisoquinolin-6-ol	1	1	1	0	<chem>Cc1ccc(cc1)N2CCc3cc(O)ccc3C2(C)c4ccc(OCCN5CCCC5)cc4</chem>
	2-(4-isopropylphenyl)-1-methyl-1-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}-3,4-dihydroisoquinolin-6-ol	1	1	1	0	<chem>CC(C)c1ccc(cc1)N2CCc3cc(O)ccc3C2(C)c4ccc(OCCN5CCCC5)cc4</chem>
	2-(3-fluorophenyl)-1-methyl-1-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}-3,4-dihydroisoquinolin-6-ol	1	1	1	0	<chem>CC1(N(CCC2cc(O)ccc12)c3cccc(F)c3)c4ccc(OCCN5CCCC5)cc4</chem>
	2-(3-hydroxyphenyl)-1-methyl-1-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-3,4-dihydroisoquinolin-6-ol	1	1	1	0	<chem>CC1(N(CCC2cc(O)ccc12)c3cccc(O)c3)c4ccc(OCCN5CCCCC5)cc4</chem>
	2-(4-chlorophenyl)-1-methyl-1-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-3,4-dihydroisoquinolin-6-ol	1	1	1	0	<chem>CC1(N(CCC2cc(O)ccc12)c3ccc(Cl)cc3)c4ccc(OCCN5CCCCC5)cc4</chem>
	2-(3-hydroxyphenyl)-1-methyl-1-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}-	1	1	1	0	<chem>CC1(N(CCC2cc(O)ccc12)c3cccc(O)c3)c4ccc(OCCN5CCCC5)cc4</chem>

	3,4-dihydroisoquinolin-6-ol					
	2-(4-isopropylphenyl)-1-methyl-1-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-3,4-dihydroisoquinolin-6-ol	1	1	1	0	<chem>CC(C)c1ccc(cc1)N2CCc3cc(O)ccc3C2(C)c4ccc(OCCN5CCCCC5)cc4</chem>
	2-[3-(dimethylamino)phenyl]-1-methyl-1-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}-3,4-dihydroisoquinolin-6-ol	1	1	1	0	<chem>CN(C)c1cccc(c1)N2CCc3cc(O)ccc3C2(C)c4ccc(OCCN5CCCCC5)cc4</chem>
	2-(3-isopropylphenyl)-1-methyl-1-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-3,4-dihydroisoquinolin-6-ol	1	1	1	0	<chem>CC(C)c1cccc(c1)N2CCc3cc(O)ccc3C2(C)c4ccc(OCCN5CCCCC5)cc4</chem>
	2-(3-chlorophenyl)-1-methyl-1-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-3,4-dihydroisoquinolin-6-ol	1	1	1	0	<chem>CC1(N(Cc2cc(O)ccc12)c3cccc(Cl)c3)c4ccc(OCCN5CCCCC5)cc4</chem>
	2-(3-chlorophenyl)-1-methyl-1-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}-3,4-dihydroisoquinolin-6-ol	1	1	1	0	<chem>CC1(N(Cc2cc(O)ccc12)c3cccc(Cl)c3)c4ccc(OCCN5CCCCC5)cc4</chem>
	2,3-bis(4-hydroxyphenyl)-2-methylpropanenitrile	1	1	1	0	<chem>CC(Cc1ccc(O)cc1)(C#N)c2ccc(O)cc2</chem>
	(3S)-3,4-bis(4-hydroxyphenyl)butanenitrile	1	1	1	0	<chem>Oc1ccc(C[C@@H](C#N)c2ccc(O)cc2)cc1</chem>

2-(4-hydroxy-2-methylphenyl)-3-(4-hydroxyphenyl)propanenitrile	1	1	1	0	<chem>Cc1cc(O)ccc1C(Cc2ccc(O)cc2)C#N</chem>
methyl 2,3-bis(4-hydroxyphenyl)propanoate	1	1	1	0	<chem>COC(=O)C(Cc1ccc(O)cc1)c2ccc(O)cc2</chem>
3,4-bis(4-hydroxyphenyl)butan-2-one	1	1	1	0	<chem>CC(=O)C(Cc1ccc(O)cc1)c2ccc(O)cc2</chem>
2-(3-hydroxyphenyl)-3-(4-hydroxyphenyl)butanedinitrile	1	1	1	0	<chem>Oc1ccc(cc1)C(C#N)C(C#N)c2cccc(O)c2</chem>
1,1,1-trifluoro-3,4-bis(4-hydroxyphenyl)butan-2-one	1	1	1	0	<chem>Oc1ccc(CC(C(=O)C(F)(F)F)c2ccc(O)cc2)cc1</chem>
4-[1-(4-hydroxyphenyl)pent-3-yn-2-yl]phenol	1	1	1	0	<chem>CC#CC(Cc1ccc(O)cc1)c2ccc(O)cc2</chem>
4-[1-(4-hydroxyphenyl)but-3-yn-2-yl]phenol	1	1	1	0	<chem>Oc1ccc(CC(C#C)c2ccc(O)cc2)cc1</chem>
2-(4-hydroxyphenyl)-2-[(4-hydroxyphenyl)methyl]propanedinitrile	1	1	1	0	<chem>Oc1ccc(CC(C#N)(C#N)c2ccc(O)cc2)cc1</chem>
4-[3,3,4,4,4-pentafluoro-1-(4-hydroxyphenyl)butan-2-yl]phenol	1	1	1	0	<chem>Oc1ccc(CC(c2ccc(O)cc2)C(F)(F)C(F)(F)F)cc1</chem>
4-[1,1,1-trifluoro-3-(4-hydroxyphenyl)propan-2-yl]phenol	1	1	1	0	<chem>Oc1ccc(CC(c2ccc(O)cc2)C(F)(F)F)cc1</chem>

	4-[4-(4-hydroxyphenyl)hexa-1,5-diyn-3-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)C(C#C)C(C#C)c2ccc(O)cc2</chem>
	1-methyl-2-(4-methylphenyl)-1-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-3,4-dihydroisoquinolin-6-ol	1	1	1	0	<chem>Cc1ccc(cc1)N2CCc3cc(O)ccc3C2(C)c4ccc(OCCN5CCCCC5)cc4</chem>
	7-bromo-2-(4-hydroxyphenyl)indazol-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)n2cc3ccc(O)c(Br)c3n2</chem>
	2-(4-hydroxyphenyl)indazol-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)n2cc3cc(O)ccc3n2</chem>
	3-bromo-2-(4-hydroxyphenyl)indazol-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)n2nc3ccc(O)cc3c2Br</chem>
	3-ethyl-2-(4-hydroxyphenyl)indazol-5-ol	1	1	1	0	<chem>CCc1c2cc(O)ccc2nn1c3ccc(O)cc3</chem>
	3-chloro-2-(4-hydroxyphenyl)indazol-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)n2nc3ccc(O)cc3c2Cl</chem>
	2-(4-hydroxyphenyl)-3-(trifluoromethyl)indazol-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)n2nc3ccc(O)cc3c2C(F)(F)F</chem>
	2-(4-hydroxyphenyl)-3-methylindazol-5-ol	1	1	1	0	<chem>Cc1c2cc(O)ccc2nn1c3ccc(O)cc3</chem>
	2-(4-hydroxyphenyl)-3-iodoindazol-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)n2nc3ccc(O)cc3c2I</chem>
	2-(4-hydroxyphenyl)indazol-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)n2cc3ccc(O)cc3n2</chem>

	2-(4-hydroxyphenyl)-3-phenylindazol-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)n2nc3ccc(O)cc3c2c4ccccc4</chem>
	5-hydroxy-2-(4-hydroxyphenyl)indazole-3-carbonitrile	1	1	1	0	<chem>Oc1ccc(cc1)n2nc3ccc(O)cc3c2C#N</chem>
	4-[3-phenyl-5,7-bis(trifluoromethyl)pyrazolo[1,5-a]pyrimidin-2-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2nn3c(cc(nc3c2c4ccccc4)C(F)(F)F)C(F)(F)F</chem>
	4-[2-(4-hydroxyphenyl)-5,7-bis(trifluoromethyl)pyrazolo[1,5-a]pyrimidin-3-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2nn3c(cc(nc3c2c4ccc(O)cc4)C(F)(F)F)C(F)(F)F</chem>
	4-[2-phenyl-5,7-bis(trifluoromethyl)pyrazolo[1,5-a]pyrimidin-3-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2c(nn3c(cc(nc23)C(F)(F)F)C(F)(F)F)c4ccccc4</chem>
	1-[4-(4-ethyl-3-methylpiperazin-1-yl)phenyl]-2-phenyl-3,4-dihydro-1H-isoquinolin-6-ol	1	1	1	0	<chem>CCN1CCN(CC1C)c2ccc(cc2)C3N(CCc4cc(O)ccc34)c5ccccc5</chem>
	1-[4-(4-methylpiperazin-1-yl)phenyl]-2-phenyl-3,4-dihydro-1H-isoquinolin-6-ol	1	1	1	0	<chem>CN1CCN(CC1)c2ccc(cc2)C3N(CCc4cc(O)ccc34)c5ccccc5</chem>
	2-(4-fluorophenyl)-1-[4-(1-methylpiperidin-4-yl)phenyl]-3,4-dihydro-1H-isoquinolin-6-ol	1	1	1	0	<chem>CN1CCC(CC1)c2ccc(cc2)C3N(CCc4cc(O)ccc34)c5ccc(F)cc5</chem>

	2-(3-hydroxyphenyl)-1-[4-(4-methylpiperazin-1-yl)phenyl]-3,4-dihydro-1H-isoquinolin-6-ol	1	1	1	0	CN1CCN(CC1)c2ccc(cc2)C3N(CCc4cc(O)ccc34)c5cccc(O)c5
	1-[4-(4-cyclohexylpiperazin-1-yl)phenyl]-2-(3-hydroxyphenyl)-3,4-dihydro-1H-isoquinolin-6-ol	1	1	1	0	Oc1cccc(c1)N2CCc3cc(O)ccc3C2c4ccc(cc4)N5CCN(CC5)C6CCCC6
	1-[4-(3-ethyl-4-methylpiperazin-1-yl)phenyl]-2-phenyl-3,4-dihydro-1H-isoquinolin-6-ol	1	1	1	0	CCC1CN(CCN1C)c2ccc(cc2)C3N(CCc4cc(O)ccc34)c5ccccc5
	2-(3-hydroxyphenyl)-1-[4-(1-methylpiperidin-4-yl)phenyl]-3,4-dihydro-1H-isoquinolin-6-ol	1	1	1	0	CN1CCC(CC1)c2ccc(cc2)C3N(CCc4cc(O)ccc34)c5cccc(O)c5
	2-(3-hydroxyphenyl)-1-[4-(4-isopropylpiperazin-1-yl)phenyl]-3,4-dihydro-1H-isoquinolin-6-ol	1	1	1	0	CC(C)N1CCN(CC1)c2ccc(cc2)C3N(CCc4cc(O)ccc34)c5cccc(O)c5
	1-[4-(4-cyclopentylpiperazin-1-yl)phenyl]-2-(3-hydroxyphenyl)-3,4-dihydro-1H-isoquinolin-6-ol	1	1	1	0	Oc1cccc(c1)N2CCc3cc(O)ccc3C2c4ccc(cc4)N5CCN(CC5)C6CCCC6
	1-(4-{octahydropyrido[1,2-a]piperazin-2-yl}phenyl)-2-phenyl-3,4-dihydro-1H-isoquinolin-6-ol	1	1	1	0	Oc1ccc2C(N(CCc2c1)c3ccccc3)c4ccc(cc4)N5CCN6CCCCC6C5
	1-[4-(3,4-dimethylpiperazin-1-yl)phenyl]-2-phenyl-3,4-dihydro-	1	1	1	0	CC1CN(CCN1C)c2ccc(cc2)C3N(CCc4cc(O)ccc34)c5ccccc5

	1H-isoquinolin-6-ol					
	1-benzyl-2-(4-hydroxyphenyl)-3H-inden-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(Cc3ccccc3)c4ccc(O)cc4C2</chem>
	3-ethyl-6-hydroxy-2-(4-hydroxyphenyl)-1H-indene-1-carboxylic acid	1	1	1	0	<chem>CCC1=C(C(C(=O)O)c2cc(O)ccc12)c3ccc(O)cc3</chem>
	3-ethyl-6-hydroxy-2-(4-hydroxyphenyl)-N-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-1H-indene-1-carboxamide	1	1	1	0	<chem>CCC1=C(C(C(=O)Nc2ccc(OCCN3CCCCC3)cc2)c4cc(O)ccc14)c5ccc(O)cc5</chem>
	N-{4-[2-(dimethylamino)ethoxy]phenyl}-3-ethyl-6-hydroxy-2-(4-hydroxyphenyl)-1H-indene-1-carboxamide	1	1	1	0	<chem>CCC1=C(C(C(=O)Nc2ccc(OCCN(C)C)cc2)c3cc(O)ccc13)c4ccc(O)cc4</chem>
	1-(4-chlorophenyl)-2-(4-hydroxyphenyl)-3H-inden-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(c3ccc(Cl)cc3)c4ccc(O)cc4C2</chem>
	2-(4-hydroxyphenyl)-1-[4-(trifluoromethyl)phenyl]-3H-inden-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(c3ccc(cc3)C(F)(F)F)c4ccc(O)cc4C2</chem>
	1-(4-aminophenyl)-2-(4-hydroxyphenyl)-3H-inden-5-ol	1	1	1	0	<chem>Nc1ccc(cc1)C2=C(Cc3cc(O)ccc23)c4ccc(O)cc4</chem>
	1-[4-(bromomethyl)phenyl]-2-(4-	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(c3ccc(CBr)cc3)c4ccc(O)cc4C2</chem>

	hydroxyphenyl)-3H-inden-5-ol					
	9-{4-[2-(dimethylamino)ethoxy]phenyl}-8,17-dioxatetracyclo[8.8.0.0{2,7}.0{11,16}]octadeca-1(10),2,4,6,11(16),12,14-heptaene-5,14-diol	1	1	1	0	CN(C)CCOc1ccc(cc1)C2Oc3cc(O)ccc3C4=C2c5ccc(O)cc5OC4
	9-{4-[2-(morpholin-4-yl)ethoxy]phenyl}-8,17-dioxatetracyclo[8.8.0.0{2,7}.0{11,16}]octadeca-1(10),2,4,6,11(16),12,14-heptaene-5,14-diol	1	1	1	0	Oc1ccc2C3=C(COc2c1)c4ccc(O)cc4OC3c5ccc(OCCN6CCOCC6)cc5
	9-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}-8,17-dioxatetracyclo[8.8.0.0{2,7}.0{11,16}]octadeca-1(10),2,4,6,11(16),12,14-heptaene-5,14-diol	1	1	1	0	Oc1ccc2C3=C(COc2c1)c4ccc(O)cc4OC3c5ccc(OCCN6CCCC6)cc5
	9-{4-[2-(azepan-1-yl)ethoxy]phenyl}-8,17-dioxatetracyclo[8.8.0.0{2,7}.0{11,16}]octadeca-1(10),2,4,6,11(16),12,14-heptaene-	1	1	1	0	Oc1ccc2C3=C(COc2c1)c4ccc(O)cc4OC3c5ccc(OCCN6CCCCC6)cc5

	5,14-diol					
	9-phenyl-8,17-dioxatetracyclo[8.8.0.0{2,7}.0{11,16}]octadeca-1(10),2,4,6,11(16),12,14-heptaene-5,14-diol	1	1	1	0	<chem>Oc1ccc2C3=C(COc2c1)c4ccc(O)cc4OC3c5ccccc5</chem>
	9-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-8,17-dioxatetracyclo[8.8.0.0{2,7}.0{11,16}]octadeca-1(10),2,4,6,11(16),12,14-heptaene-5,14-diol	1	1	1	0	<chem>Oc1ccc2C3=C(COc2c1)c4ccc(O)cc4OC3c5ccc(OCCN6CCCC6)cc5</chem>
	2-(4-methanesulfonylphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]phenoxy}-1-benzothiophen-6-ol	1	1	1	0	<chem>CS(=O)(=O)c1ccc(cc1)c2sc3cc(O)ccc3c2Oc4ccc(OCCN5CCCC5)cc4</chem>
	2-N,4-N-bis(2-methylpropyl)-6-(2-phenylethyl)pyrimidine-2,4-diamine	1	1	1	0	<chem>CC(C)CNc1cc(CCc2ccccc2)nc(NCC(C)C)n1</chem>
	4-N-benzyl-2-N,6-N-bis(2-methylpropyl)pyrimidine-2,4,6-triamine	1	1	1	0	<chem>CC(C)CNc1cc(NCc2ccccc2)nc(NCC(C)C)n1</chem>
	(6S)-6-phenyl-5-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}-5,6,7,8-tetrahydronaphthalen-2-ol	1	1	1	0	<chem>Cl.Oc1ccc2C([C@H])(CCc2c1)c3ccccc3)c4ccc(OCCN5CCCC5)cc4</chem>

	hydrochloride					
	6-[2-(4-hydroxyphenyl)pentan-3-yl]pyridin-3-ol	1	1	1	0	<chem>CC[C@@H]([C@H](C)c1ccc(O)cc1)c2ccc(O)cn2</chem>
	6-[4-(4-hydroxyphenyl)hexan-3-yl]pyridin-3-ol	1	1	1	0	<chem>CC[C@@H]([C@H](CC)c1ccc(O)cn1)c2ccc(O)cc2</chem>
	6-[1-(4-hydroxyphenyl)butan-2-yl]pyridin-3-ol	1	1	1	0	<chem>CCC(Cc1ccc(O)cc1)c2ccc(O)cn2</chem>
	6-[4-(4-hydroxyphenyl)hexan-3-yl]pyridin-3-ol	1	1	1	0	<chem>CC[C@@H]([C@H](CC)c1ccc(O)cn1)c2ccc(O)cc2</chem>
	6-[1-(4-hydroxyphenyl)propan-2-yl]pyridin-3-ol	1	1	1	0	<chem>CC(Cc1ccc(O)cc1)c2ccc(O)cn2</chem>
	6-[2-(4-hydroxyphenyl)propyl]pyridin-3-ol	1	1	1	0	<chem>CC(Cc1ccc(O)cn1)c2ccc(O)cc2</chem>
72108-22-6	4-[(1E)-1-(4-hydroxyphenyl)prop-1-en-2-yl]phenol	1	1	1	0	<chem>C\C=C/c1ccc(O)cc1)\c2ccc(O)cc2</chem>
3691-71-2	4-[(1E)-1-(4-hydroxyphenyl)but-1-en-2-yl]phenol	1	1	1	0	<chem>CC\C=C/c1ccc(O)cc1)\c2ccc(O)cc2</chem>
	4-[2-(4-hydroxyphenyl)-2-methylpropyl]phenol	1	1	1	0	<chem>CC(C)(Cc1ccc(O)cc1)c2ccc(O)cc2</chem>
	4-[2-(4-hydroxyphenyl)-2-methylbutyl]phenol	1	1	1	0	<chem>CCC(C)(Cc1ccc(O)cc1)c2ccc(O)cc2</chem>

	4-[2-(4-hydroxyphenyl)-2-methylpentyl]phenol	1	1	1	0	<chem>CCCC(C)(Cc1ccc(O)cc1)c2ccc(O)cc2</chem>
	4-[1-(4-hydroxyphenyl)pentan-2-yl]phenol	1	1	1	0	<chem>CCCC(Cc1ccc(O)cc1)c2ccc(O)cc2</chem>
	2,2-diethyl 5-[(1S,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-14-yl]-1,3-dihydroindene-2,2-dicarboxylate	1	1	1	0	<chem>CCOC(=O)C1(Cc2ccc(cc2C1)[C@]3(O)CC[C@H]4[C@@H]5Cc6cc(O)ccc6[C@H]5CC[C@]34C)C(=O)OCC</chem>
	1-{2-acetyl-5-[(1S,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-14-yl]-1,3-dihydroinden-2-yl}ethanone	1	1	1	0	<chem>CC(=O)C1(Cc2ccc(cc2C1)[C@]3(O)CC[C@H]4[C@@H]5CCc6cc(O)ccc6[C@H]5CC[C@]34C)C(=O)C</chem>
	ethyl 2-acetyl-5-[(1S,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-14-yl]-1,3-dihydroindene-2-carboxylate	1	1	1	0	<chem>CCOC(=O)C1(Cc2ccc(cc2C1)[C@]3(O)CC[C@H]4[C@@H]5Cc6cc(O)ccc6[C@H]5CC[C@]34C)C(=O)C</chem>
	ethyl 2-cyano-5-[(1S,10R,11S,14S,15S)-5,14-dihydroxy-15-	1	1	1	0	<chem>CCOC(=O)C1(Cc2ccc(cc2C1)[C@]3(O)CC[C@H]4[C@@H]5Cc6cc(O)ccc6[C@H]5CC[C@]34C)C#N</chem>

	methylnonacyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-14-yl]-1,3-dihydroindene-2-carboxylate					
	(1S,10R,11S,14S,15S)-15-methyl-14-[2-(4-methylbenzenesulfonyl)-1,3-dihydroisoindol-5-yl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	<chem>Cc1ccc(cc1)S(=O)(=O)N2Cc3ccc(cc3C2)[C@]4(O)CC[C@H]5[C@@H]6CCc7cc(O)ccc7[C@H]6CC[C@]45C</chem>
	(1S,10R,11S,14S,15S)-14-(1,3-dihydro-2-benzofuran-5-yl)-15-methylnonacyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)c5ccc6COCc6c5</chem>
	(1S,10R,11S,13R,14R,15S)-13-fluoro-15-methylnonacyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1C[C@@H](F)[C@@H]2O</chem>
	2-[(1E)-(hydroxyimino)methyl]-3,4-bis(4-hydroxyphenyl)phenol	1	1	1	0	<chem>O\\N=C\\c1c(O)ccc(c2ccc(O)cc2)c1c3ccc(O)cc3</chem>
	(1S,9R,10R,11S,14S,15S)-15-methyl-9-{9-[(S)-4,4,5,5,5-pentafluoropentanesulfinyl]nonyl}tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@H]([C@@H]1CC[C@@H]2O)[C@H](CCCCCCCC[S@](=O)CCCC(F)(F)C(F)(F)F)Cc1cc(O)ccc31</chem>

	(3R)-3-(4-hydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-7-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@@H]1COc2cc(O)ccc2C1</chem>
	4-[(1Z)-1-{4-[2-(dimethylamino)ethoxy]phenyl}hept-1-en-1-yl]phenol	1	1	1	0	<chem>CCCCC\C=C(\c1ccc(O)cc1)/c2ccc(OCCN(C)C)cc2</chem>
	4-[cyclohexylidene({4-[2-(diisopropylamino)ethoxy]phenyl})methyl]phenol	1	1	1	0	<chem>CC(C)N(CCOc1ccc(cc1)C(=C2CCCCC2)c3ccc(O)cc3)C(C)C</chem>
	4-[(1E)-1-{4-[2-(diethylamino)ethoxy]phenyl}-3-methylbut-1-en-1-yl]phenol	1	1	1	0	<chem>CCN(CC)CCOc1ccc(cc1)\C(=C\C(C)C)\c2ccc(O)cc2</chem>
	4-[(1Z)-1-{4-[2-(diethylamino)ethoxy]phenyl}-3-methylbut-1-en-1-yl]phenol	1	1	1	0	<chem>CCN(CC)CCOc1ccc(cc1)\C(=C/C(C)C)\c2ccc(O)cc2</chem>
	4-[(1E)-1-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}hept-1-en-1-yl]phenol	1	1	1	0	<chem>CCCCC\C=C(/c1ccc(O)cc1)\c2ccc(OCCN3CCCC3)cc2</chem>
	4-[(1Z)-1-{4-[2-(diethylamino)ethoxy]phenyl}hexadec-1-en-1-yl]phenol	1	1	1	0	<chem>CCCCCCCCCCCCC\C=C(\c1ccc(O)cc1)/c2ccc(OCCN(CC)CC)cc2</chem>
	4-[(1Z)-1-{4-[2-(diethylamino)ethoxy]phenyl}dec-1-en-1-yl]phenol	1	1	1	0	<chem>CCCCCCCCC\C=C(\c1ccc(O)cc1)/c2ccc(OCCN(CC)CC)cc2</chem>

4-[(1E)-1-{4-[2-(diethylamino)ethoxy]phenyl}hept-1-en-1-yl]phenol	1	1	1	0	CCCCC\C=C(/c1ccc(O)cc1)\c2ccc(OCCN(CC)CC)cc2
{2-[4-(1-{4-[2-(diethylamino)ethoxy]phenyl}hept-1-en-1-yl)phenoxy]ethyl}diethylamine	1	1	1	0	CCCCC=C(c1ccc(OCCN(CC)CC)cc1)c2ccc(OCCN(CC)CC)cc2
4-[(1E)-1-{4-[2-(diethylamino)ethoxy]phenyl}hexadec-1-en-1-yl]phenol	1	1	1	0	CCCCCCCCCCCCC\C=C(/c1ccc(O)cc1)\c2ccc(OCCN(CC)CC)cc2
(2-{4-[cyclohexylidene({4-[2-(diisopropylamino)ethoxy]phenyl})methyl]phenoxy}ethyl)diisopropylamine	1	1	1	0	CC(C)N(CCOc1ccc(cc1)C(=C2CCCCC2)c3ccc(OCCN(C(C)C)C(C)C)cc3)C(C)C
4-[(1Z)-1-{4-[2-(diethylamino)ethoxy]phenyl}-3-phenylprop-1-en-1-yl]phenol	1	1	1	0	CCN(CC)CCOc1ccc(cc1)\C(=C/Cc2ccccc2)\c3ccc(O)cc3
4-[(1E)-1-{4-[2-(diethylamino)ethoxy]phenyl}-3-phenylprop-1-en-1-yl]phenol	1	1	1	0	CCN(CC)CCOc1ccc(cc1)\C(=C\Cc2ccccc2)\c3ccc(O)cc3
4-[(1E)-1-{4-[2-(diethylamino)ethoxy]phenyl}hex-1-en-1-yl]phenol	1	1	1	0	CCCC\C=C(/c1ccc(O)cc1)\c2ccc(OCCN(CC)CC)cc2

	{2-[4-(1-{4-[2-(diisopropylamino)ethoxy]phenyl}-3-methylbut-1-en-1-yl)phenoxy]ethyl}diisopropylamine	1	1	1	0	<chem>CC(C)C=C(c1ccc(OCCN(C(C)C)C(C)C)cc1)c2ccc(OCCN(C(C)C)C(C)C)cc2</chem>
	4-[(1Z)-1-{4-[2-(diethylamino)ethoxy]phenyl}hex-1-en-1-yl]phenol	1	1	1	0	<chem>CCCC\C=C(\c1ccc(O)cc1)/c2ccc(OCCN(CC)CC)cc2</chem>
	4-[(1E)-1-{4-[2-(dimethylamino)ethoxy]phenyl}hept-1-en-1-yl]phenol	1	1	1	0	<chem>CCCCC\C=C(/c1ccc(O)cc1)\c2ccc(OCCN(C)C)cc2</chem>
	4-[(1Z)-1-{4-[2-(diethylamino)ethoxy]phenyl}hept-1-en-1-yl]phenol	1	1	1	0	<chem>CCCCC\C=C(\c1ccc(O)cc1)/c2ccc(OCCN(CC)CC)cc2</chem>
	4-[(1E)-1-{4-[2-(diethylamino)ethoxy]phenyl}dec-1-en-1-yl]phenol	1	1	1	0	<chem>CCCCCCCC\C=C(/c1ccc(O)cc1)\c2ccc(OCCN(CC)CC)cc2</chem>
	4-[(1E)-1-{4-[2-(diethylamino)ethoxy]phenyl}oct-1-en-1-yl]phenol	1	1	1	0	<chem>CCCCCC\C=C(/c1ccc(O)cc1)\c2ccc(OCCN(CC)CC)cc2</chem>
	4-[(1Z)-1-{4-[2-(diethylamino)ethoxy]phenyl}oct-1-en-1-yl]phenol	1	1	1	0	<chem>CCCCCC\C=C(\c1ccc(O)cc1)/c2ccc(OCCN(CC)CC)cc2</chem>
	atrazine	0	1	0	1	<chem>CCNc1nc(Cl)nc(NC(C)C)n1</chem>

	(1R,2R,3S,4R,5S,6S)-1,2,3,4,5,6-hexachlorocyclohexane	0	1	0	1	Cl[C@@H]1[C@@H](Cl)[C@H](Cl)[C@H](Cl)[C@@H](Cl)[C@@H]1Cl
50356-19-9	ional	1	1	1	0	Cc1cc(c(O)c(c1)C(C)(C)C(C)(C)C
	2-(4-hydroxy-2-methylphenyl)-1-benzothiophen-6-ol	1	1	1	0	Cc1cc(O)ccc1c2cc3ccc(O)cc3s2
	2-(4-hydroxy-3-propylphenyl)-1-benzothiophen-6-ol	1	1	1	0	CCCc1cc(ccc1O)c2cc3ccc(O)cc3s2
	2-phenyl-1-benzothiophen-6-ol	1	1	1	0	Oc1ccc2cc(sc2c1)c3ccccc3
	2-(3-fluoro-4-hydroxyphenyl)-1-benzothiophen-6-ol	1	1	1	0	Oc1ccc2cc(sc2c1)c3ccc(O)c(F)c3
	2-(4-methylphenyl)-1-benzothiophen-6-ol	1	1	1	0	Cc1ccc(cc1)c2cc3ccc(O)cc3s2
	{4-[(1Z)-1-{4-[2-(dimethylamino)ethoxy]phenyl}-2-phenylbut-1-en-1-yl]phenyl}methanol	1	1	1	0	CC\C=C(/c1ccc(CO)cc1)\c2ccc(OCCN(C)C)cc2)\c3ccccc3
	5-amino-2-[4-(ethylamino)phenyl]chromen-4-one	1	1	1	0	CCNc1ccc(cc1)C2=CC(=O)c3c(N)cccc3O2
	5-amino-2-[4-(methylamino)phenyl]chromen-4-one	1	1	1	0	CNc1ccc(cc1)C2=CC(=O)c3c(N)cccc3O2

	7-ethenyl-2-(2-fluoro-4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1ccc(c(F)c1)c2oc3c(C=C)cc(O)cc3n2</chem>
496916-40-6	spironolactone	0	1	0	1	<chem>CC(=O)S[C@@H]1CC2=CC(=O)CC[C@]2(C)[C@H]3CC[C@@]4(C)[C@@H](CC[C@@]45CCC(=O)O5)[C@H]13</chem>
	2-(4-hydroxyphenyl)-1-(4-methylphenyl)-3H-inden-5-ol	1	1	1	0	<chem>Cc1ccc(cc1)C2=C(Cc3cc(O)ccc23)c4ccc(O)cc4</chem>
	9-[4-(dimethylamino)phenyl]-8,17-dioxatetracyclo[8.8.0.0{2,7}.0{11,16}]octadeca-1(10),2,4,6,11(16),12,14-heptaene-5,14-diol	1	1	1	0	<chem>CN(C)c1ccc(cc1)C2Oc3cc(O)ccc3C4=C2c5ccc(O)cc5OC4</chem>
	vinclozolin	0	1	0	1	<chem>CC1(OC(=O)N(C1=O)c2cc(Cl)cc(Cl)c2)C=C</chem>
	2-N,4-N-bis(2-methylpropyl)-6-[(E)-2-phenylethenyl]pyrimidine-2,4-diamine	1	1	1	0	<chem>CC(C)CNc1cc(\C=C\c2ccccc2)nc(NCC(C)C)n1</chem>
	tert-butyl N-benzyl-N-{2-[(2-methylpropyl)amino]-6-[(E)-2-phenylethenyl]pyrimidin-4-yl}carbamate	1	1	1	0	<chem>CC(C)CNc1nc(\C=C\c2ccccc2)cc(n1)N(Cc3ccccc3)C(=O)OC(C)(C)C</chem>
	2-N-benzyl-4-N-(2-methylpropyl)-6-(2-phenylethyl)pyrimidine-2,4-diamine	1	1	1	0	<chem>CC(C)CNc1cc(CCc2ccccc2)nc(NCc3ccccc3)n1</chem>

	2-N,4-N-dibenzyl-6-(3-methylbutyl)pyrimidine-2,4-diamine	1	1	1	0	<chem>CC(C)CCc1cc(NCc2cccc2)nc(NCc3cccc3)n1</chem>
	2-N-benzyl-6-(3-methylbutyl)-4-N-(2-methylpropyl)pyrimidine-2,4-diamine	1	1	1	0	<chem>CC(C)CCc1cc(NCC(C)C)nc(NCc2cccc2)n1</chem>
	6-ethyl-2-N,4-N-bis(2-methylpropyl)pyrimidine-2,4-diamine	1	1	1	0	<chem>CCc1cc(NCC(C)C)nc(NCC(C)C)n1</chem>
	6-(3-methylbutyl)-4-N-(2-methylpropyl)-2-N-(naphthalen-1-ylmethyl)pyrimidine-2,4-diamine	1	1	1	0	<chem>CC(C)CCc1cc(NCC(C)C)nc(NCc2cccc3cccc23)n1</chem>
	2-N,4-N,6-N-tris(2-methylpropyl)pyrimidine-2,4,6-triamine	1	1	1	0	<chem>CC(C)CNc1cc(NCC(C)C)nc(NCC(C)C)n1</chem>
	4-N-methyl-2-N,4-N-bis(2-methylpropyl)-6-[2-(naphthalen-1-yl)ethyl]pyrimidine-2,4-diamine	1	1	1	0	<chem>CC(C)CNc1nc(CCc2cccc3cccc23)cc(n1)N(C)CC(C)C</chem>
	2-N,4-N-dibenzyl-6-[(E)-2-phenylethenyl]pyrimidine-2,4-diamine	1	1	1	0	<chem>C(Nc1cc(\C=C\c2cccc2)nc(NCc3cccc3)n1)c4cccc4</chem>
	2-N-benzyl-4-N-(2-methylpropyl)-6-[(E)-2-phenylethenyl]pyrimidine-	1	1	1	0	<chem>CC(C)CNc1cc(\C=C\c2cccc2)nc(NCc3cccc3)n1</chem>

	2,4-diamine					
	4-N-benzyl-2-N-(2-methylpropyl)-6-[(E)-2-phenylethenyl]pyrimidine-2,4-diamine	1	1	1	0	<chem>CC(C)CNc1nc(NCc2ccccc2)cc(\C=C\c3ccccc3)n1</chem>
	4-N-benzyl-2-N-(2-methylpropyl)-6-(2-phenylethyl)pyrimidine-2,4-diamine	1	1	1	0	<chem>CC(C)CNc1nc(CCc2ccccc2)cc(NCc3ccccc3)n1</chem>
	2-N,4-N-bis(2-methylpropyl)-6-[2-(naphthalen-1-yl)ethyl]pyrimidine-2,4-diamine	1	1	1	0	<chem>CC(C)CNc1cc(CCc2cccc3ccccc23)nc(NCC(C)C)n1</chem>
	tert-butyl N-(2-methylpropyl)-N-{2-[(2-methylpropyl)amino]-6-[2-(naphthalen-1-yl)ethyl]pyrimidin-4-yl}carbamate	1	1	1	0	<chem>CC(C)CNc1nc(CCc2cccc3ccccc23)cc(n1)N(CC(C)C)C(=O)OC(C)(C)C</chem>
	4-N-benzyl-6-(3-methylbutyl)-2-N-(2-methylpropyl)pyrimidine-2,4-diamine	1	1	1	0	<chem>CC(C)CCc1cc(NCc2ccccc2)nc(NCC(C)C)n1</chem>
	6-(3-methylbutyl)-2-N-(2-methylpropyl)-4-N-(naphthalen-1-ylmethyl)pyrimidine-2,4-diamine	1	1	1	0	<chem>CC(C)CCc1cc(NCc2cccc3ccccc23)nc(NCC(C)C)n1</chem>
	2,4,6-tris[(2-methylpropyl)sulfanyl]pyrimidine	1	1	1	0	<chem>CC(C)CSc1cc(SCC(C)C)nc(SCC(C)C)n1</chem>

	2-N-methyl-6-(3-methylbutyl)-2-N,4-N-bis(2-methylpropyl)pyrimidine-2,4-diamine	1	1	1	0	<chem>CC(C)CCc1cc(NCC(C)C)nc(n1)N(C)CC(C)C</chem>
	4-N-methyl-2-N,4-N-bis(2-methylpropyl)-6-(2-phenylethyl)pyrimidine-2,4-diamine	1	1	1	0	<chem>CC(C)CNc1nc(CCc2ccccc2)cc(n1)N(C)CC(C)C</chem>
	2-chloro-3-(3-fluoro-4-hydroxyphenyl)-6-[(1E)-(hydroxyimino)methyl]phenol	1	1	1	0	<chem>O\\N=C\\c1ccc(c(Cl)c1O)c2ccc(O)c(F)c2</chem>
	2-[(1E)-(hydroxyimino)methyl]-4-(4-hydroxyphenyl)phenol	1	1	1	0	<chem>O\\N=C\\c1cc(ccc1O)c2ccc(O)cc2</chem>
	3,4-bis(4-hydroxyphenyl)-6-phenylpyran-2-one	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(C(=O)OC(=C2)c3ccccc3)c4ccc(O)cc4</chem>
	3-(4-hydroxyphenyl)-6-(4-methoxyphenyl)-4-phenylpyran-2-one	1	1	1	0	<chem>COc1ccc(cc1)C2=CC(=C(C(=O)O2)c3ccc(O)cc3)c4ccccc4</chem>
	4,6-bis(4-hydroxyphenyl)-3-phenylpyran-2-one	1	1	1	0	<chem>Oc1ccc(cc1)C2=CC(=C(C(=O)O2)c3ccccc3)c4ccc(O)cc4</chem>
59-50-7	baktol	0	1	0	1	<chem>Cc1cc(O)ccc1Cl</chem>
	4-[(1E)-1-{4-[2-(diethylamino)ethoxy]phenyl}-2-	1	1	1	0	<chem>CCCC\\C(=C\\c1ccc(O)cc1)/c2ccc(OCCN(CC)CC)cc2\\\\CC.C CCC\\C(=C/c3ccc(O)cc3)\\c4ccc(OCCN(CC)CC)cc4\\\\CC</chem>

	ethylhex-1-en-1-yl]phenol; 4-[(1Z)-1-{4-[2-(diethylamino)ethoxy]phenyl}-2-ethylhex-1-en-1-yl]phenol					
	(1R,2S,5R,8R,9S)-1,9,10,11,12,12-hexachloro-4,6-dioxo-5,8-thiatricyclo[7.2.1.0{2,8}]dodec-10-en-5-one	0	1	0	1	<chem>ClC1=C(Cl)[C@]2(Cl)[C@@H]3CO[S@@](=O)OC[C@@H]3[C@@]1(Cl)C2(Cl)Cl</chem>
	(1R,2S,4R,5R,6S)-1,2,4,5,6,7,7-heptachloro-2-(chloromethyl)-3,3-dimethylbicyclo[2.2.1]heptane	1	1	1	0	<chem>CC1(C)[C@](Cl)(CCl)[C@]2(Cl)[C@@H](Cl)[C@@H](Cl)[C@@]1(Cl)C2(Cl)Cl</chem>
58-72-0	triphenylethene	1	1	1	0	<chem>C(=C(c1ccccc1)c1ccccc1)c1ccccc1</chem>
	4-[2,4-bis(4-hydroxyphenyl)-3-methylpyrrol-1-yl]phenol	1	1	1	0	<chem>Cc1c(cnc(c1-c1ccc(O)cc1)-c1ccc(O)cc1)-c1ccc(O)cc1</chem>
	4-[3-ethyl-2,4-bis(4-hydroxyphenyl)pyrrol-1-yl]phenol	1	1	1	0	<chem>CCc1c(cnc(c1-c1ccc(O)cc1)-c1ccc(O)cc1)-c1ccc(O)cc1</chem>
	[1,2,4-tris(4-hydroxyphenyl)pyrrol-3-yl]praseodymium	1	1	1	0	<chem>Oc1ccc(cc1)-c1cn(c(c1[Pr]))-c1ccc(O)cc1)-c1ccc(O)cc1</chem>
120-47-8	ethylparaben	0	1	0	1	<chem>CCOC(=O)c1ccc(O)cc1</chem>
	2-hydroxy-N-[[[3-hydroxy-2-methyl-6-[[[(1S,3S)-3,5,12-trihydroxy-3-(2-hydroxyacetyl)-10-methoxy-6,11-dioxo-2,4-dihydro-	1	1	1	0	<chem>CC\ C(=C(\ c1ccc(O)cc1)/c2ccc(OCCN(C)CCOCCO\ N=C\ c3ccc(O)c(c3)C(=O)NCNC4CC(O[C@H]5C[C@@](O)(Cc6c(O)c7C(=O)c8cccc(OC)c8C(=O)c7c(O)c56)C(=O)CO)OC(C)C4O)cc2)\ c9cccc9</chem>

	1H-tetracen-1-yl]oxy}oxan-4-yl)amino]methyl}-5-[(11E)-1-{4-[(1E)-1-(4-hydroxyphenyl)-2-phenylbut-1-en-1-yl]phenyl}-4-methyl-1,7,10-trioxa-4,11-diazadodec-11-en-12-yl]benzamide					
	2-hydroxy-N-{[(3-hydroxy-2-methyl-6-[(1S,3S)-3,5,12-trihydroxy-3-(2-hydroxyacetyl)-10-methoxy-6,11-dioxo-2,4-dihydro-1H-tetracen-1-yl]oxy}oxan-4-yl)amino]methyl}-5-[(14E)-1-{4-[(1E)-1-(4-hydroxyphenyl)-2-phenylbut-1-en-1-yl]phenyl}-4-methyl-1,7,10,13-tetraoxa-4,14-diazapentadec-14-en-15-yl]benzamide	1	1	1	0	CC\\C(=C(\\c1ccc(O)cc1)/c2ccc(OCCN(C)CCOCCOCCO\\N=C\\c3ccc(O)c(c3)C(=O)NCNC4CC(O[C@H]5C[C@@](O)(Cc6c(O)c7C(=O)c8cccc(OC)c8C(=O)c7c(O)c56)C(=O)CO)OC(C)C4O)cc2)\\c9cccc9
	2-hydroxy-N-{[(3-hydroxy-2-methyl-6-[(1S,3S)-3,5,12-trihydroxy-3-(2-hydroxyacetyl)-10-methoxy-6,11-dioxo-2,4-dihydro-1H-tetracen-1-yl]oxy}oxan-4-yl)amino]methyl}-5-[(8E)-1-{4-[(1E)-1-(4-hydroxyphenyl)-2-phenylbut-1-en-1-yl]phenyl}-4-methyl-1,7-dioxa-4,8-diazanon-8-en-9-yl]benzamide	1	1	1	0	CC\\C(=C(\\c1ccc(O)cc1)/c2ccc(OCCN(C)CCO\\N=C\\c3ccc(O)c(c3)C(=O)NCNC4CC(O[C@H]5C[C@@](O)(Cc6c(O)c7C(=O)c8cccc(OC)c8C(=O)c7c(O)c56)C(=O)CO)OC(C)C4O)cc2)\\c9cccc9

	4-[(1E)-1-{4-[(dimethylamino)methoxy]phenyl}-2-phenylbut-1-en-1-yl]phenol	1	1	1	0	<chem>CC\C=C(\c1ccc(O)cc1)/c2ccc(OCN(C)C)cc2)\c3ccccc3</chem>
	4-sec-butylphenol	1	1	1	0	<chem>CCC(C)c1ccc(O)cc1</chem>
	2-(3-fluoro-4-hydroxyphenyl)-1-benzothiophene-4,6-diol	1	1	1	0	<chem>Oc1cc(O)c2cc(sc2c1)c3ccc(O)c(F)c3</chem>
	4-(6-hydroxy-1-benzothiophen-2-yl)benzene-1,2-diol	1	1	1	0	<chem>Oc1ccc2cc(sc2c1)c3ccc(O)c(O)c3</chem>
	1-[2-hydroxy-5-(6-hydroxy-1-benzothiophen-2-yl)phenyl]ethanone	1	1	1	0	<chem>CC(=O)c1cc(ccc1O)c2cc3ccc(O)cc3s2</chem>
	2-(3-hydroxyphenyl)-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1cccc(c1)c2cc3ccc(O)cc3s2</chem>
	2-(3-ethyl-4-hydroxyphenyl)-1-benzothiophen-6-ol	1	1	1	0	<chem>CCc1cc(ccc1O)c2cc3ccc(O)cc3s2</chem>
	2-(4-hydroxy-3-methylphenyl)-1-benzothiophene-4,6-diol	1	1	1	0	<chem>Cc1cc(ccc1O)c2cc3c(O)cc(O)cc3s2</chem>
	2-(4-hydroxy-3-methylphenyl)-1-benzothiophen-6-ol	1	1	1	0	<chem>Cc1cc(ccc1O)c2cc3ccc(O)cc3s2</chem>
5959-71-7	3-[(3E)-4-(3-hydroxyphenyl)hex-3-en-3-yl]phenol	1	1	1	0	<chem>CC\C=C(\CC)/c1cccc(O)c1)\c2cccc(O)c2</chem>

	2-(4-butylphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>CCCCc1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>
	MER25	1	1	1	0	<chem>CCN(CC)CCOc1ccc(cc1)C(O)(Cc2ccc(OC)cc2)c3ccccc3</chem>
	4-[(1Z)-1,2-diphenylbut-1-en-1-yl]phenol	1	1	1	0	<chem>CC\C/C(=C/c1ccccc1)\c2ccc(O)cc2)\c3ccccc3</chem>
	2-(4-hydroxyphenyl)quinolin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2ccc3cc(O)ccc3n2</chem>
467-29-8	purga	1	1	1	0	<chem>Oc1ccc(cc1)C2(OC(=O)c3ccccc23)c4ccc(O)cc4</chem>
1801-42-9	2,3-diphenyl-1-indenone	1	1	1	0	<chem>O=C1C(=C(c2ccccc2)c3ccccc13)c4ccccc4</chem>
	3-(4-hydroxyphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(Oc3ccc(O)cc3S2)c4ccc(OCCN5CCCCC5)cc4</chem>
	3-(3-bromo-4-hydroxyphenyl)-2-ethyl-5-methyl-2H-1,4-benzoxazin-7-ol	1	1	1	0	<chem>CCC1Oc2cc(O)cc(C)c2N=C1c3ccc(O)c(Br)c3</chem>
	3-(3-bromo-4-hydroxyphenyl)-2,5-dimethyl-2H-1,4-benzoxazin-7-ol	1	1	1	0	<chem>CC1Oc2cc(O)cc(C)c2N=C1c3ccc(O)c(Br)c3</chem>
	3-(3-bromo-4-hydroxyphenyl)-2,2-dimethyl-1,4-benzoxazine-5,7-diol	1	1	1	0	<chem>CC1(C)Oc2cc(O)cc(O)c2N=C1c3ccc(O)c(Br)c3</chem>
	2-oxa-9-azatetracyclo[8.7.0.0{3,8}.0{11,16}]heptadeca-3,5,7,9,11(16),12,14-	1	1	1	0	<chem>Oc1ccc2C3=Nc4ccc(O)cc4OC3Cc2c1</chem>

	heptaene-5,14-diol					
	3-(4-hydroxyphenyl)-2-methyl-2H-1,4-benzoxazin-7-ol	1	1	1	0	<chem>CC1Oc2cc(O)ccc2N=C1c3ccc(O)cc3</chem>
	2-ethyl-3-(4-hydroxyphenyl)-2H-1,4-benzoxazin-7-ol	1	1	1	0	<chem>CCC1Oc2cc(O)ccc2N=C1c3ccc(O)cc3</chem>
	3-(4-hydroxyphenyl)-2H-1,4-benzoxazine-5,7-diol	1	1	1	0	<chem>Oc1ccc(cc1)C2=Nc3c(O)cc(O)cc3OC2</chem>
	11,12-dihydro-10aH-10-oxa-5-azatetraphene-2,8-diol	1	1	1	0	<chem>Oc1ccc2C3=Nc4ccc(O)cc4OC3CCc2c1</chem>
	3-(4-hydroxyphenyl)-2H-1,4-benzoxazin-7-ol	1	1	1	0	<chem>Oc1ccc(cc1)C2=Nc3ccc(O)cc3OC2</chem>
	3-(4-hydroxyphenyl)-2,2-dimethyl-1,4-benzoxazin-7-ol	1	1	1	0	<chem>CC1(C)Oc2cc(O)ccc2N=C1c3ccc(O)cc3</chem>
	3-(4-hydroxyphenyl)-2-propyl-2H-1,4-benzoxazin-7-ol	1	1	1	0	<chem>CCCC1Oc2cc(O)ccc2N=C1c3ccc(O)cc3</chem>
	2-ethyl-3-(4-hydroxyphenyl)-2H-1,4-benzoxazine-5,7-diol	1	1	1	0	<chem>CCC1Oc2cc(O)cc(O)c2N=C1c3ccc(O)cc3</chem>
	3-(3-bromo-4-hydroxyphenyl)-2-ethyl-2H-1,4-benzoxazine-5,7-diol	1	1	1	0	<chem>CCC1Oc2cc(O)cc(O)c2N=C1c3ccc(O)c(Br)c3</chem>
	2-(3-bromobenzoyl)-3-(naphthalen-1-yl)-1-benzofuran-6-ol	1	1	1	0	<chem>Oc1ccc2c(c(oc2c1)C(=O)c3cccc(Br)c3)c4cccc5ccccc45</chem>

	2-(2-chlorobenzoyl)-3-(naphthalen-1-yl)-1-benzofuran-6-ol	1	1	1	0	<chem>Oc1ccc2c(c(oc2c1)C(=O)c3ccccc3Cl)c4cccc5ccccc45</chem>
	2-(4-fluorobenzoyl)-3-(naphthalen-1-yl)-1-benzofuran-6-ol	1	1	1	0	<chem>Oc1ccc2c(c(oc2c1)C(=O)c3ccc(F)cc3)c4cccc5ccccc45</chem>
	2-(3-fluorobenzoyl)-3-(naphthalen-1-yl)-1-benzofuran-6-ol	1	1	1	0	<chem>Oc1ccc2c(c(oc2c1)C(=O)c3cccc(F)c3)c4cccc5ccccc45</chem>
	2-benzoyl-3-(naphthalen-1-yl)-1-benzofuran-6-ol	1	1	1	0	<chem>Oc1ccc2c(c(oc2c1)C(=O)c3ccccc3)c4cccc5ccccc45</chem>
	1-methyl-2-phenyl-1-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}-3,4-dihydroisoquinolin-6-ol	1	1	1	0	<chem>CC1(N(Cc2cc(O)ccc12)c3ccccc3)c4ccc(OCCN5CCCC5)cc4</chem>
	3-(4-hydroxyphenyl)-7-isopropoxychromen-4-one	1	1	1	0	<chem>CC(C)Oc1ccc2C(=O)C(=COc2c1)c3ccc(O)cc3</chem>
148672-09-7	(1S,10R,11S,15S)-15-methyl-14-oxotetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-5-yl sulfamate	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(OS(=O)(=O)N)ccc34)[C@@H]1CCC2=O</chem>
620-92-8	HDM	1	1	1	0	<chem>Oc1ccc(Cc2ccc(O)cc2)cc1</chem>
2624-43-3	cyclofenil	1	1	1	0	<chem>CC(=O)Oc1ccc(cc1)C(=C2CCCC2)c3ccc(OC(=O)C)cc3</chem>
911-45-5	clomifene	1	1	1	0	<chem>CCN(CC)CCOc1ccc(cc1)\C(=C(/Cl)\c2ccccc2)\c3ccccc3</chem>
	(2S,3R)-3-(4-hydroxyphenyl)-2-{4-[(2S)-2-[(3R)-3-methylpyrrolidin-1-	1	1	1	0	<chem>C[C@@H](COc1ccc(cc1)[C@@H]2Oc3ccc(O)cc3S[C@@H]2</chem>

	yl]propoxy]phenyl}-2,3-dihydro-1,4-benzoxathiin-6-ol					<chem>c4ccc(O)cc4)N5CC[C@@H](C)C5</chem>
	4-{2-phenylpyrazolo[1,5-a]pyrimidin-3-yl}phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2c(nn3cccnc23)c4ccccc4</chem>
	4-[2-(4-hydroxyphenyl)pyrazolo[1,5-a]pyrimidin-3-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2nn3cccnc3c2c4ccc(O)cc4</chem>
	4-{3-phenylpyrazolo[1,5-a]pyrimidin-2-yl}phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2nn3cccnc3c2c4ccccc4</chem>
79-94-7	tetrabromobisphenol A	0	1	0	1	<chem>CC(C)(c1cc(Br)c(O)c(Br)c1)c2cc(Br)c(O)c(Br)c2</chem>
	2-(5-hydroxynaphthalen-1-yl)-1,3-benzoxazol-6-ol	1	1	1	0	<chem>Oc1ccc2nc(oc2c1)c3cccc4c(O)cccc34</chem>
	2-(2,3-difluoro-4-hydroxyphenyl)-7-ethenyl-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1cc(C=C)c2oc(nc2c1)c3ccc(O)c(F)c3F</chem>
	2-(3-fluoro-4-hydroxyphenyl)-7-(prop-2-en-1-yl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1cc(CC=C)c2oc(nc2c1)c3ccc(O)c(F)c3</chem>
	2-(4-hydroxyphenyl)-7-methoxy-1,3-benzoxazol-5-ol	1	1	1	0	<chem>COc1cc(O)cc2nc(oc12)c3ccc(O)cc3</chem>
	ethyl 5-hydroxy-2-(4-hydroxyphenyl)-1,3-benzoxazole-7-carboxylate	1	1	1	0	<chem>CCOC(=O)c1cc(O)cc2nc(oc12)c3ccc(O)cc3</chem>

	3-(6-hydroxynaphthalen-2-yl)-1,2-benzoxazol-6-ol	1	1	1	0	<chem>Oc1ccc2c(noc2c1)c3ccc4cc(O)ccc4c3</chem>
	2-(4-hydroxyphenyl)-7-propyl-1,3-benzoxazol-5-ol	1	1	1	0	<chem>CCCc1cc(O)cc2nc(oc12)c3ccc(O)cc3</chem>
	7-ethynyl-2-(4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2oc3c(cc(O)cc3n2)C#C</chem>
	2-(3-fluoro-4-hydroxyphenyl)-5-hydroxy-1,3-benzoxazole-7-carbonitrile	1	1	1	0	<chem>Oc1cc(C#N)c2oc(nc2c1)c3ccc(O)c(F)c3</chem>
	2-(2-fluoro-4-hydroxyphenyl)-5-hydroxy-1,3-benzoxazole-7-carbonitrile	1	1	1	0	<chem>Oc1ccc(c(F)c1)c2oc3c(cc(O)cc3n2)C#N</chem>
	7-ethenyl-2-(4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2oc3c(C=C)cc(O)cc3n2</chem>
	7-ethyl-2-(4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>CCC1cc(O)cc2nc(oc12)c3ccc(O)cc3</chem>
	1-{4-[4-(cyclopropylmethyl)piperazin-1-yl]phenyl}-2-(3-hydroxyphenyl)-3,4-dihydro-1H-isoquinolin-6-ol	1	1	1	0	<chem>Oc1cccc(c1)N2CCc3cc(O)ccc3C2c4ccc(cc4)N5CCN(CC6CC6)CC5</chem>
94-13-3	propylparaben	1	1	1	0	<chem>CCCOC(=O)c1ccc(O)cc1</chem>
77-40-7	bisphenol B	1	1	1	0	<chem>CCC(C)(c1ccc(O)cc1)c2ccc(O)cc2</chem>

611-99-4	4-(4-hydroxybenzoyl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)C(=O)c2ccc(O)cc2</chem>
659-22-3	trans-stilbene-4,4'-diol	1	1	1	0	<chem>Oc1ccc(\C=C\c2ccc(O)cc2)cc1</chem>
	3-ethyl-6-hydroxy-N,2-bis(4-hydroxyphenyl)-1H-indene-1-carboxamide	0	1	0	1	<chem>CCC1=C(C(C(=O)Nc2ccc(O)cc2)c3cc(O)ccc13)c4ccc(O)cc4</chem>
	2-(4-hydroxyphenyl)-1-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-3H-inden-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(c3ccc(OCCN4CCCCC4)cc3)c5ccc(O)cc5C2</chem>
	4-[5-hydroxy-2-(4-hydroxyphenyl)-3H-inden-1-yl]benzamide	1	1	1	0	<chem>NC(=O)c1ccc(cc1)C2=C(Cc3cc(O)ccc23)c4ccc(O)cc4</chem>
	1-{4-[5-hydroxy-2-(4-hydroxyphenyl)-3H-inden-1-yl]phenyl}ethanone	1	1	1	0	<chem>CC(=O)c1ccc(cc1)C2=C(Cc3cc(O)ccc23)c4ccc(O)cc4</chem>
	3,8-dihydroxy-4,7-dimethylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1c(O)ccc2c1OC(=O)c3c(C)c(O)ccc23</chem>
	10-ethenyl-3-hydroxy-4,8-dimethylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1cc(C=C)c2c(c1)C(=O)Oc3c(C)c(O)ccc23</chem>
	5-hydroxy-3-(4-hydroxyphenyl)-7-methoxyquinazolin-4-one	1	1	1	0	<chem>COc1cc(O)c2C(=O)N(C=Nc2c1)c3ccc(O)cc3</chem>
	(9aS)-9a-butyl-7-hydroxy-4-methyl-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>CCCC[C@@]12CCC(=O)C(=C1c3ccc(O)cc3C2)C</chem>

137098-19-2	dexamethasone	0	1	0	1	<chem>C[C@@H]1C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@]2(C)[C@@]1(O)C(=O)CO</chem>
	4-(3-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-5,7-bis(trifluoromethyl)pyrazolo[1,5-a]pyrimidin-2-yl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2nn3c(cc(nc3c2c4ccc(OCCN5CCCCC5)cc4)C(F)(F)F)C(F)(F)F</chem>
	4-(3-{4-[2-(dimethylamino)ethoxy]phenyl}-5,7-bis(trifluoromethyl)pyrazolo[1,5-a]pyrimidin-2-yl)phenol	1	1	1	0	<chem>CN(C)CCOc1ccc(cc1)c2c(nn3c(cc(nc23)C(F)(F)F)C(F)(F)F)c4ccc(O)cc4</chem>
	4-(2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-5,7-bis(trifluoromethyl)pyrazolo[1,5-a]pyrimidin-3-yl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2c(nn3c(cc(nc23)C(F)(F)F)C(F)(F)F)c4ccc(OCCN5CCCCC5)cc4</chem>
	4-(2-{4-[2-(dimethylamino)ethoxy]phenyl}-5,7-bis(trifluoromethyl)pyrazolo[1,5-a]pyrimidin-3-yl)phenol	1	1	1	0	<chem>CN(C)CCOc1ccc(cc1)c2nn3c(cc(nc3c2c4ccc(O)cc4)C(F)(F)F)C(F)(F)F</chem>
83-46-5	stigmast-5-EN-3-ol, (3β)-	1	1	1	0	<chem>CC[C@H](CC[C@H](C)[C@@H]1CC[C@H]2[C@H]3CC=C4C[C@@H](O)CC[C@@]4(C)[C@H]3CC[C@@]12C)C(C)C</chem>
98388-00-2	4-(4-hydroxybenzenesulfonyl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)S(=O)(=O)c2ccc(O)cc2</chem>

50-23-7	hydrocortisone	0	1	0	1	<chem>C[C@]12CCC(=O)C=C1CC[C@H]3[C@@H]4CC[C@](O)(C(=O)CO)[C@@]4(C)C[C@H](O)[C@H]23</chem>
182133-25-1	arzoxifene	1	1	1	0	<chem>COc1ccc(cc1)c2sc3cc(O)ccc3c2Oc4ccc(OCCN5CCCCC5)cc4</chem>
	2-(4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]phenoxy}-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2sc3cc(O)ccc3c2Oc4ccc(OCCN5CCCCC5)cc4</chem>
	2-(4-fluorophenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]phenoxy}-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc2c(Oc3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(F)cc5</chem>
	2-(4-bromophenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]phenoxy}-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc2c(Oc3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(Br)cc5</chem>
	2-phenyl-3-{4-[2-(piperidin-1-yl)ethoxy]phenoxy}-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc2c(Oc3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccccc5</chem>
	2-(4-aminophenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]phenoxy}-1-benzothiophen-6-ol	1	1	1	0	<chem>Nc1ccc(cc1)c2sc3cc(O)ccc3c2Oc4ccc(OCCN5CCCCC5)cc4</chem>
	2-chloro-N-[4-(6-hydroxy-3-{4-[2-(piperidin-1-yl)ethoxy]phenoxy}-1-benzothiophen-2-yl)phenyl]acetamide	1	1	1	0	<chem>Oc1ccc2c(Oc3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(NC(=O)CCl)cc5</chem>

	2-{4-[(2-chloroethyl)amino]phenyl}-3-{4-[2-(piperidin-1-yl)ethoxy]phenoxy}-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc2c(Oc3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(NCCCCI)cc5</chem>
	(2R)-2-(4-hydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-7-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2CCc3ccc(O)cc3O2</chem>
5975-78-0	zanone	1	1	1	0	<chem>C[C@H]1CCCC(=O)CCCCC2cc(O)cc(O)c2C(=O)O1</chem>
94-18-8	benzylparaben	1	1	1	0	<chem>Oc1ccc(cc1)C(=O)OCc2ccccc2</chem>
	2-[3-(4-hydroxyphenyl)propyl]-5-methoxyphenol	1	1	1	0	<chem>COc1ccc(CCCc2ccc(O)cc2)c(O)c1</chem>
	(1R,2S,3S,6R,7R,8S,9S,11S)-3,4,5,6,13,13-hexachloro-10-oxapentacyclo[6.3.1.1{3,6}.0{2,7}.0{9,11}]tridec-4-ene	1	1	1	0	<chem>ClC1=C(Cl)[C@@]2(Cl)[C@H]3[C@H]4C[C@H]([C@@H]5O[C@@H]45)[C@H]3[C@]1(Cl)C2(Cl)Cl</chem>
	4-N-benzyl-2-N-(naphthalen-1-ylmethyl)-6-[(E)-2-phenylethenyl]pyrimidine-2,4-diamine	1	1	1	0	<chem>C(Nc1cc(\C=C\c2ccccc2)nc(NCc3cccc4cccc34)n1)c5ccccc5</chem>
94-26-8	butylparaben	1	1	1	0	<chem>CCCCOC(=O)c1ccc(O)cc1</chem>
	(1S,3aS,5S,7aS)-5-(4-hydroxyphenyl)-7a-methyloctahydroinden-1-ol	1	1	1	0	<chem>C[C@]12CC[C@@H](C[C@@H]1CC[C@@H]2O)c3ccc(O)cc3</chem>

(1S,3aS,5S,7aS)-5-(3-fluoro-4-hydroxyphenyl)-7a-methyl-octahydroinden-1-ol	1	1	1	0	<chem>C[C@]12CC[C@@H](C[C@@H]1CC[C@@H]2O)c3ccc(O)c(F)c3</chem>
(1S,3aS,5S,7aS)-5-(4-hydroxy-2-methylphenyl)-7a-methyl-octahydroinden-1-ol	1	1	1	0	<chem>Cc1cc(O)ccc1[C@H]2CC[C@]3(C)[C@@H](O)CC[C@H]3C2</chem>
(1S,3aS,5S,7aS)-5-(2-fluoro-4-hydroxyphenyl)-7a-methyl-octahydroinden-1-ol	1	1	1	0	<chem>C[C@]12CC[C@@H](C[C@@H]1CC[C@@H]2O)c3ccc(O)cc3F</chem>
4-[(2R)-7-hydroxy-3,4-dihydro-2H-1-benzopyran-2-yl]-3-(3-methylbut-2-en-1-yl)benzene-1,2-diol	1	1	1	0	<chem>CC(=CCc1c(O)c(O)ccc1[C@H]2CCc3ccc(O)cc3O2)C</chem>
5-[(2R)-7-hydroxy-3,4-dihydro-2H-1-benzopyran-2-yl]-3,4-bis(3-methylbut-2-en-1-yl)benzene-1,2-diol	1	1	1	0	<chem>CC(=CCc1c(O)c(O)cc([C@H]2CCc3ccc(O)cc3O2)c1CC=C(C)C</chem>
3-(4-hydroxyphenyl)-8,8-dimethylpyrano[2,3-h]chromen-4-one	1	1	1	0	<chem>CC1(C)Oc2ccc3C(=O)C(=COc3c2C=C1)c4ccc(O)cc4</chem>
3-(4-hydroxyphenyl)-7-(2-methylpropoxy)chromen-4-one	1	1	1	0	<chem>CC(C)COc1ccc2C(=O)C(=COc2c1)c3ccc(O)cc3</chem>
N-butyl-N-methyl-11-[[[(1S,8R,9S,10R,11S,14S,15S)-5,8,14-trihydroxy-15-	1	1	1	0	<chem>CCCCN(C)C(=O)CCCCCCCCCS[C@@H]1[C@H](O)c2cc(O)cc2[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4[C@H]13</chem>

	methylnonacyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-9-yl)sulfanyl}undecanamide					
	(1S,9S,10R,11S,14S,15S)-9-[(4-bromophenyl)sulfanyl]-15-methylnonacyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,8,14-triol	1	1	1	0	C[C@]12CC[C@H]3[C@@H]([C@H](Sc4ccc(Br)cc4)C(O)c5cc(O)ccc35)[C@@H]1CC[C@@H]2O
	N-butyl-11-[[[(1S,9R,10R,11S,14S,15S)-5,14-dihydroxy-15-methylnonacyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-9-yl)sulfanyl]-N-methylundecanamide	1	1	1	0	CCCCN(C)C(=O)CCCCCCCCCS[C@@H]1Cc2cc(O)ccc2[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4[C@H]13
	(1S,9S,10R,11S,14S,15S)-9-[(4-bromophenyl)sulfanyl]-5-hydroxy-15-methyl-8-oxononacyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-yl acetate	0	1	0	1	CC(=O)O[C@H]1CC[C@H]2[C@H]3[C@H](CC[C@]12C)c4cc(O)cc4C(=O)[C@H]3Sc5ccc(Br)cc5
	(2E)-3-(4-[[[(1S,9R,10R,11S,14S,15S)-5,14-dihydroxy-15-methylnonacyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-9-yl)sulfanyl]phenyl)-N,N-	1	1	1	0	CN(C)C(=O)\C=C\c1ccc(S[C@@H]2Cc3cc(O)ccc3[C@H]4C[C@]5(C)[C@@H](O)CC[C@H]5[C@H]24)cc1

	dimethylprop-2-enamide					
	(1S,9R,10R,11S,14S,15S)-5-methoxy-15-methyl-9-({4-[2-(piperidin-1-yl)ethoxy]phenyl}sulfanyl)tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-ol	0	1	0	1	<chem>COc1ccc2[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4[C@@H]3[C@@H](Cc2c1)Sc5ccc(OCCN6CCCCC6)cc5</chem>
1090-04-6	(1S,10S,11S,13R,15R)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,13-diol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1C[C@@H](O)C2</chem>
53-45-2	estratrien-17-one	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4ccccc34)[C@@H]1CCC2=O</chem>
	(1R,10S,11S,15S,17S)-17-(methoxymethyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	<chem>COC[C@H]1C[C@]2(C)C(O)CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@@H]13</chem>
	(2E)-3-(4-(((1S,9R,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-9-yl)sulfanyl)phenyl)prop-2-enoic	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H]([C@@H](Cc4cc(O)ccc34)Sc5ccc(\C=C\C(=O)O)cc5)[C@@H]1CC[C@@H]2O</chem>

	acid					
	N-butyl-11- {[(1S,9S,10R,11S,14S,15S)-5,14- dihydroxy-15-methyl-8- oxotetracyclo[8.7.0.0{2,7}.0{11,15}] heptadeca-2,4,6-trien-9- yl)sulfanyl}-N- methylundecanamide	1	1	1	0	CCCCN(C)C(=O)CCCCCCCCCS[C@H]1[C@@H]2[C@H](CC[C@]3(C)[C@@H](O)CC[C@@H]23)c4ccc(O)cc4C1=O
	(1S,3aR,5S,7aS)-5-(4- hydroxyphenyl)-7a-methyl- octahydroinden-1-ol	1	1	1	0	C[C@]12CC[C@@H](C[C@H]1CC[C@@H]2O)c3ccc(O)cc3
	(1S,3aR,5S,7aS)-5-(3-fluoro-4- hydroxyphenyl)-7a-methyl- octahydroinden-1-ol	1	1	1	0	C[C@]12CC[C@@H](C[C@H]1CC[C@@H]2O)c3ccc(O)c(F)c3
	(1S,3aR,5S,7aS)-5-(2-fluoro-4- hydroxyphenyl)-7a-methyl- octahydroinden-1-ol	1	1	1	0	C[C@]12CC[C@@H](C[C@H]1CC[C@@H]2O)c3ccc(O)cc3F
	(1S,3aR,5S,7aS)-5-(2-chloro-4- hydroxyphenyl)-7a-methyl- octahydroinden-1-ol	1	1	1	0	C[C@]12CC[C@@H](C[C@H]1CC[C@@H]2O)c3ccc(O)cc3Cl
	(1S,3aR,5S,7aS)-5-(4-hydroxy-2- methylphenyl)-7a-methyl- octahydroinden-1-ol	1	1	1	0	Cc1cc(O)ccc1[C@H]2CC[C@]3(C)[C@@H](O)CC[C@@H]3C2

	(1S,3aR,5S,7aS)-5-(3,5-dichloro-4-hydroxyphenyl)-7a-methyl-octahydroinden-1-ol	1	1	1	0	<chem>C[C@]12CC[C@@H](C[C@H]1CC[C@@H]2O)c3cc(Cl)c(O)c(Cl)c3</chem>
	(1S,3aR,5S,7aS)-5-(2,3-difluoro-4-hydroxyphenyl)-7a-methyl-octahydroinden-1-ol	1	1	1	0	<chem>C[C@]12CC[C@@H](C[C@H]1CC[C@@H]2O)c3ccc(O)c(F)c3F</chem>
	(1S,3aR,5S,7aS)-7a-methyl-5-(2,3,5-trifluoro-4-hydroxyphenyl)-octahydroinden-1-ol	1	1	1	0	<chem>C[C@]12CC[C@@H](C[C@H]1CC[C@@H]2O)c3cc(F)c(O)c(F)c3F</chem>
	(1R,3aR,5S,7aS)-1-ethynyl-5-(4-hydroxyphenyl)-7a-methyl-hexahydro-2H-inden-1-ol	1	1	1	0	<chem>C[C@]12CC[C@@H](C[C@H]1CC[C@@]2(O)C#C)c3ccc(O)c3</chem>
	(1S,3aR,7aS)-5-(2-chloro-4-hydroxyphenyl)-7a-methyl-1,2,3,3a,6,7-hexahydroinden-1-ol	1	1	1	0	<chem>C[C@]12CCC(=C[C@H]1CC[C@@H]2O)c3ccc(O)cc3Cl</chem>
	(1S,3aR,7aS)-5-(2-chloro-4-hydroxyphenyl)-7a-methyl-1,2,3,3a,4,7-hexahydroinden-1-ol	1	1	1	0	<chem>C[C@]12CC=C(C[C@H]1CC[C@@H]2O)c3ccc(O)cc3Cl</chem>
	(1R,2S,5S,8R,9S)-1,9,10,11,12,12-hexachloro-4,6-dioxo-5H[4]-thiatricyclo[7.2.1.0{2,8}]dodec-10-en-5-one	0	1	0	1	<chem>ClC1=C(Cl)[C@]2(Cl)[C@@H]3CO[S@](=O)OC[C@@H]3[C@@]1(Cl)C2(Cl)Cl</chem>
79881-33-7	2,6-dichloro-4'-biphenylol	1	1	1	0	<chem>Oc1ccc(cc1)-c1c(Cl)cccc1Cl</chem>

23719-22-4	2-chloro-4-biphenylol	1	1	1	0	<chem>Oc1ccc(c(Cl)c1)-c1ccccc1</chem>
	endosulfan	1	1	1	0	<chem>ClC1=C(Cl)[C@]2(Cl)[C@H]3CO[S@@](=O)OC[C@@H]3[C@@]1(Cl)C2(Cl)Cl</chem>
	2'-chloro-4-biphenylol	1	1	1	0	<chem>Oc1ccc(cc1)-c1ccccc1Cl</chem>
	(2S)-2-ethylhexyl 4-hydroxybenzoate	1	1	1	0	<chem>CCCC[C@H](CC)COC(=O)c1ccc(O)cc1</chem>
56558-16-8	1,3,5-trichloro-2-(2,6-dichlorophenyl)benzene	1	1	1	0	<chem>Clc1cc(Cl)c(c(Cl)c1)-c1c(Cl)cccc1Cl</chem>
	4-[3-(trifluoromethyl)phenyl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1cccc(c1)C(F)(F)F</chem>
	4-[2,4-bis(4-hydroxyphenyl)pyrrol-1-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1cc(-c2ccc(O)cc2)n(c1)-c1ccc(O)cc1</chem>
	4-[3-ethyl-2,4-bis(4-hydroxyphenyl)-5-propylpyrrol-1-yl]phenol	1	1	1	0	<chem>CCCC1c(c(CC)c(-c2ccc(O)cc2)n1-c1ccc(O)cc1)-c1ccc(O)cc1</chem>
	[1,2,4-tris(4-hydroxyphenyl)-5-propylpyrrol-3-yl]praseodymium	1	1	1	0	<chem>CCCC1c(c([Pr])c(-c2ccc(O)cc2)n1-c1ccc(O)cc1)-c1ccc(O)cc1</chem>
	2-fluoro-4-[4-(3-fluoro-4-hydroxyphenyl)hexan-3-yl]phenol	1	1	1	0	<chem>CCC(C(CC)c1ccc(O)c(F)c1)c2ccc(O)c(F)c2</chem>
	4-[4-(4-hydroxy-3-iodophenyl)hexan-3-yl]-2-	1	1	1	0	<chem>CCC(C(CC)c1ccc(O)c(I)c1)c2ccc(O)c(I)c2</chem>

	iodophenol					
	2-bromo-4-[4-(3-bromo-4-hydroxyphenyl)hexan-3-yl]phenol	1	1	1	0	<chem>CCC(C(CC)c1ccc(O)c(Br)c1)c2ccc(O)c(Br)c2</chem>
	nordihydroguaiaretic acid	1	1	1	0	<chem>CC(Cc1ccc(O)c(O)c1)C(C)Cc2ccc(O)c(O)c2</chem>
135-19-3	β naphthol	1	1	1	0	<chem>Oc1ccc2ccccc2c1</chem>
	9-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-8-oxatetracyclo[8.8.0.0{2,7}.0{11,16}]octadeca-1(10),2,4,6,11(16),12,14,17-octaene-5,14-diol	1	1	1	0	<chem>Oc1ccc2c(OC(c3ccc(OCCN4CCCC4)cc3)c5c2ccc6cc(O)ccc56)c1</chem>
	2-(4-hydroxyphenyl)-1-[(4-hydroxyphenyl)methyl]-3-methylindol-5-ol	1	1	1	0	<chem>Cc1c(c2ccc(O)cc2)n(Cc3ccc(O)cc3)c4ccc(O)cc14</chem>
6699-27-0	benzo(A)pyrene	0	1	0	1	<chem>c1ccc2c(c1)cc3ccc4cccc5ccc2c3c45</chem>
645-56-7	p-propylphenol	0	1	0	1	<chem>CCCc1ccc(O)cc1</chem>
	carbofuran	0	1	0	1	<chem>CNC(=O)Oc1cccc2CC(C)(C)Oc12</chem>
	carbaryl	0	1	0	1	<chem>CNC(=O)Oc1cccc2ccccc12</chem>
620-17-7	3-ethylphenol	0	1	0	1	<chem>CCc1cccc(O)c1</chem>
117095-65-5	4-[(E)-1-chloro-2-{4-[2-(diethylamino)ethoxy]phenyl}-2-	1	1	1	0	<chem>CCN(CC)CCOc1ccc(cc1)\C=C(\Cl)/c2ccc(O)c(OC)c2\c3ccccc3</chem>

	phenylethenyl]-2-methoxyphenol					
117095-59-7	4-[(Z)-2-chloro-1-{4-[2-(diethylamino)ethoxy]phenyl}-2-phenylethenyl]-2-methoxyphenol	1	1	1	0	<chem>CCN(CC)CCOc1ccc(cc1)\C(=C(\Cl)/c2ccccc2)\c3ccc(O)c(OC)c3</chem>
501-36-0	resveratrol	1	1	1	0	<chem>Oc1ccc(\C=C\c2cc(O)cc(O)c2)cc1</chem>
	2,2-dichloro-3-[11,12,12-tris(4-methoxyphenyl)dodec-11-en-1-yl]-1,3-diaza-2-platinacyclopentane-1,3-diium	1	1	1	0	<chem>COc1ccc(cc1)C(=C(c2ccc(OC)cc2)c3ccc(OC)cc3)CCCCCCCCC[NH+]4CC[NH2+][Pt]4(Cl)Cl</chem>
	3-[12,12-bis(4-methoxyphenyl)-11-phenyldodec-11-en-1-yl]-2,2-dichloro-1,3-diaza-2-platinacyclopentane-1,3-diium	1	1	1	0	<chem>COc1ccc(cc1)C(=C(CCCCCCCCC[NH+]2CC[NH2+][Pt]2(Cl)Cl)c3ccccc3)c4ccc(OC)cc4</chem>
	3-[10,10-bis(4-methoxyphenyl)-9-phenyldec-9-en-1-yl]-2,2-dichloro-1,3-diaza-2-platinacyclopentane-1,3-diium	1	1	1	0	<chem>COc1ccc(cc1)C(=C(CCCCCCCC[NH+]2CC[NH2+][Pt]2(Cl)Cl)c3ccccc3)c4ccc(OC)cc4</chem>
	3-[8,8-bis(4-methoxyphenyl)-7-phenyloct-7-en-1-yl]-2,2-dichloro-1,3-diaza-2-platinacyclopentane-1,3-diium	1	1	1	0	<chem>COc1ccc(cc1)C(=C(CCCCCC[NH+]2CC[NH2+][Pt]2(Cl)Cl)c3ccccc3)c4ccc(OC)cc4</chem>
101802-54-4	permite	0	1	0	1	<chem>Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl</chem>

218-01-9	chrysene	0	1	0	1	<chem>c1ccc2c(c1)ccc3c4ccccc4ccc23</chem>
	2-(4-hydroxybenzoyl)-3-(naphthalen-1-yl)-1-benzofuran-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)C(=O)c2oc3cc(O)ccc3c2c4cccc5ccccc45</chem>
131-11-3	dimethyl phthalate	0	1	0	1	<chem>COC(=O)c1ccccc1C(=O)OC</chem>
103-30-0	trans-stilbene	0	1	0	1	<chem>C(=C)\c1ccccc1)/c2ccccc2</chem>
	7-ethoxy-3-(4-hydroxyphenyl)chromen-4-one	1	1	1	0	<chem>CCOc1ccc2C(=O)C(=COc2c1)c3ccc(O)cc3</chem>
	4-(5-amino-4-oxochromen-2-yl)benzonitrile	1	1	1	0	<chem>Nc1cccc2OC(=CC(=O)c12)c3ccc(cc3)C#N</chem>
	N-[4-(5-amino-4-oxochromen-2-yl)phenyl]acetamide	1	1	1	0	<chem>CC(=O)Nc1ccc(cc1)C2=CC(=O)c3c(N)cccc3O2</chem>
	5-amino-2-[4-(dimethylamino)phenyl]chromen-4-one	1	1	1	0	<chem>CN(C)c1ccc(cc1)C2=CC(=O)c3c(N)cccc3O2</chem>
	5-amino-2-[4-(benzylamino)phenyl]chromen-4-one	1	1	1	0	<chem>Nc1cccc2OC(=CC(=O)c12)c3ccc(NCc4ccccc4)cc3</chem>
	5-amino-2-(4-hydroxyphenyl)chromen-4-one	1	1	1	0	<chem>Nc1cccc2OC(=CC(=O)c12)c3ccc(O)cc3</chem>
	5-amino-2-phenylchromen-4-one	1	1	1	0	<chem>Nc1cccc2OC(=CC(=O)c12)c3ccccc3</chem>

	5-amino-2-(4-bromophenyl)chromen-4-one	1	1	1	0	<chem>Nc1cccc2OC(=CC(=O)c12)c3ccc(Br)cc3</chem>
	5-amino-2-[4-(butylamino)phenyl]chromen-4-one	1	1	1	0	<chem>CCCCNc1ccc(cc1)C2=CC(=O)c3c(N)cccc3O2</chem>
	5-amino-2-[4-(propylamino)phenyl]chromen-4-one	1	1	1	0	<chem>CCCNc1ccc(cc1)C2=CC(=O)c3c(N)cccc3O2</chem>
	5-amino-2-(4-methoxyphenyl)chromen-4-one	1	1	1	0	<chem>COc1ccc(cc1)C2=CC(=O)c3c(N)cccc3O2</chem>
	(2S,3R)-3-(4-hydroxyphenyl)-2-[3-(piperidin-1-yl)propyl]-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2CCCN4CCCC4</chem>
	(2S,3R)-3-(4-hydroxyphenyl)-2-[4-(1,2,3,6-tetrahydropyridin-4-yl)phenyl]-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(cc4)C5=CCNCC5</chem>
	(2S,3R)-3-(4-hydroxyphenyl)-2-[4-(piperazin-1-yl)phenyl]-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(cc4)N5CCNCC5</chem>
	(2S,3R)-2-[4-(4-ethylpiperazin-1-yl)phenyl]-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>CCN1CCN(CC1)c2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5</chem>

(2S,3R)-2-{3-bromo-4-[2-(piperidin-1-yl)ethoxy]phenyl}-3-(3-hydroxyphenyl)-2,3-dihydro-1,4-benzodithiin-6-ol	1	1	1	0	<chem>Oc1cccc(c1)[C@H]2Sc3cc(O)ccc3S[C@H]2c4ccc(OCCN5CCC(CC5)c(Br)c4</chem>
(2S,3R)-2-{3-bromo-4-[2-(piperidin-1-yl)ethoxy]phenyl}-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzodithiin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3S[C@H]2c4ccc(OCCN5CCC(CC5)c(Br)c4</chem>
(2S,3R)-3-(4-hydroxyphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1,4-benzodithiin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3S[C@H]2c4ccc(OCCN5CCC(CC5)cc4</chem>
(2S,3R)-3-(4-hydroxyphenyl)-2-[4-(4-methyl-1,4-diazepan-1-yl)phenyl]-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>CN1CCCN(CC1)c2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5</chem>
(2S,3R)-2-{3-bromo-4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzodithiin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3S[C@H]2c4ccc(OCCN5CCC(C5)c(Br)c4</chem>
(2S,3R)-2-[4-(1,4-diazepan-1-yl)phenyl]-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(cc4)N5CCCNCC5</chem>
(2S,3R)-3-(3-hydroxyphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-	1	1	1	0	<chem>Oc1cccc(c1)[C@H]2Sc3cc(O)ccc3S[C@H]2c4ccc(OCCN5CCC(CC5)cc4</chem>

	2,3-dihydro-1,4-benzodithiin-6-ol					
	(2S,3R)-3-(4-hydroxyphenyl)-2-[4-[3-(piperidin-1-yl)propyl]phenyl]-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(CCCN5CCC5)cc4</chem>
	(2S,3R)-3-(4-hydroxyphenyl)-2-[4-(piperidin-4-yl)phenyl]-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(cc4)C5CCNCC5</chem>
	(2S,3R)-3-(4-hydroxyphenyl)-2-[4-(4-methylpiperazin-1-yl)phenyl]-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>CN1CCN(CC1)c2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5</chem>
	(2S,3R)-3-(4-hydroxyphenyl)-2-[4-{{2-(piperidin-1-yl)ethoxy}methyl}phenyl]-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(COCCN5CCCC5)cc4</chem>
	(2S,3R)-3-(4-hydroxyphenyl)-2-[4-[2-(pyrrolidin-1-yl)ethoxy]phenyl]-2,3-dihydro-1,4-benzodithiin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3S[C@H]2c4ccc(OCCN5CCCC5)cc4</chem>
94-25-7	butamben	1	1	1	0	<chem>CCCCOC(=O)c1ccc(N)cc1</chem>
	4-[4-ethyl-3,5-bis(4-hydroxyphenyl)pyrazol-1-yl]phenol	1	1	1	0	<chem>CCc1c(nn(c2ccc(O)cc2)c1c3ccc(O)cc3)c4ccc(O)cc4</chem>
	4-[4-ethyl-5-(4-hydroxyphenyl)-2-phenylpyrazol-3-yl]phenol	1	1	1	0	<chem>CCc1c(nn(c2ccccc2)c1c3ccc(O)cc3)c4ccc(O)cc4</chem>

6093-71-6	ethyl 7-hydroxy-2-oxochromene-3-carboxylate	0	1	0	1	<chem>CCOC(=O)C1=Cc2ccc(O)cc2OC1=O</chem>
72624-02-3	4-n-heptylphenol	1	1	1	0	<chem>CCCCCCCc1ccc(O)cc1</chem>
	4-[3-(4-hydroxyphenyl)butan-2-yl]phenol	1	1	1	0	<chem>CC(C(C)c1ccc(O)cc1)c2ccc(O)cc2</chem>
94-75-7	2,4-dichlorophenoxyacetic acid	0	1	0	1	<chem>OC(=O)COc1ccc(Cl)cc1Cl</chem>
	2-phenylindazol-5-ol	1	1	1	0	<chem>Oc1ccc2nn(cc2c1)c3ccccc3</chem>
	4-(3-chloroindazol-2-yl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)n2nc3ccccc3c2Cl</chem>
	(2R,3R,4S)-3-(4-hydroxyphenyl)-4-methyl-2-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}-3,4-dihydro-2H-1-benzopyran-6-ol	1	1	1	0	<chem>C[C@@H]1[C@@H]([C@@H](Oc2ccc(O)cc12)c3ccc(OCCN4CCCC4)cc3)c5ccc(O)cc5</chem>
	(2R,3R,4S)-3-(4-hydroxyphenyl)-4-methyl-2-(4-{[(2S)-1-(pyrrolidin-1-yl)propan-2-yl]oxy}phenyl)-3,4-dihydro-2H-1-benzopyran-6-ol	1	1	1	0	<chem>C[C@@@H](CN1CCCC1)Oc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4[C@@H](C)[C@@H]3c5ccc(O)cc5</chem>
	(2R,3R,4S)-3-(4-hydroxyphenyl)-4-methyl-2-{4-[(2S)-2-(pyrrolidin-1-yl)propoxy]phenyl}-3,4-dihydro-2H-1-benzopyran-6-ol	1	1	1	0	<chem>C[C@@@H](COc1ccc(cc1)[C@@H]2Oc3ccc(O)cc3[C@@H](C)[C@@H]2c4ccc(O)cc4)N5CCCC5</chem>
	(2R,3R,4S)-2-{4-[2-(azepan-1-yl)ethoxy]phenyl}-5-fluoro-3-(4-hydroxyphenyl)-4-methyl-3,4-	1	1	1	0	<chem>C[C@@H]1[C@@H]([C@@H](Oc2ccc(O)c(F)c12)c3ccc(OCCN4CCCCC4)cc3)c5ccc(O)cc5</chem>

	dihydro-2H-1-benzopyran-6-ol					
	(2R,3R,4S)-5-fluoro-3-(4-hydroxyphenyl)-4-methyl-2-{4-[(2S)-2-(pyrrolidin-1-yl)propoxy]phenyl}-3,4-dihydro-2H-1-benzopyran-6-ol	1	1	1	0	<chem>C[C@@H](COc1ccc(cc1)[C@@H]2Oc3ccc(O)c(F)c3[C@@H](C)[C@@H]2c4ccc(O)cc4)N5CCCC5</chem>
	(2R,3R,4S)-5-fluoro-3-(4-hydroxyphenyl)-4-methyl-2-{4-[(2S)-2-[(2R)-2-methylpyrrolidin-1-yl]propoxy]phenyl}-3,4-dihydro-2H-1-benzopyran-6-ol	1	1	1	0	<chem>C[C@@H](COc1ccc(cc1)[C@@H]2Oc3ccc(O)c(F)c3[C@@H](C)[C@@H]2c4ccc(O)cc4)N5CCC[C@H]5C</chem>
	(2R,3R,4S)-3-(4-hydroxyphenyl)-4-methyl-2-{4-[(2S)-2-[(3R)-3-methylpyrrolidin-1-yl]propoxy]phenyl}-3,4-dihydro-2H-1-benzopyran-6-ol	1	1	1	0	<chem>C[C@@H](COc1ccc(cc1)[C@@H]2Oc3ccc(O)cc3[C@@H](C)[C@@H]2c4ccc(O)cc4)N5CC[C@@H](C)C5</chem>
	(2R,3R,4S)-5-fluoro-3-(4-hydroxyphenyl)-4-methyl-2-{4-[(2S)-2-[(3R)-3-methylpyrrolidin-1-yl]propoxy]phenyl}-3,4-dihydro-2H-1-benzopyran-6-ol	1	1	1	0	<chem>C[C@@H](COc1ccc(cc1)[C@@H]2Oc3ccc(O)c(F)c3[C@@H](C)[C@@H]2c4ccc(O)cc4)N5CC[C@@H](C)C5</chem>
	(2R,3R,4S)-3-(4-hydroxyphenyl)-4-methyl-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-3,4-dihydro-2H-1-benzopyran-6-ol	1	1	1	0	<chem>C[C@H]1[C@@H]([C@@H](Oc2ccc(O)cc12)c3ccc(OCCN4CCCC4)cc3)c5ccc(O)cc5</chem>

(2R,3R,4S)-3-(4-hydroxyphenyl)-4-methyl-2-(4-{2-[(3R)-3-methylpyrrolidin-1-yl]ethoxy}phenyl)-3,4-dihydro-2H-1-benzopyran-6-ol	1	1	1	0	<chem>C[C@@H]1CCN(CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4[C@@H](C)[C@@H]3c5ccc(O)cc5)C1</chem>
(2R,3R,4S)-5-fluoro-3-(4-hydroxyphenyl)-4-methyl-2-{4-[(2S)-2-[(3S)-3-methylpyrrolidin-1-yl]propoxy]phenyl}-3,4-dihydro-2H-1-benzopyran-6-ol	1	1	1	0	<chem>C[C@@H](COc1ccc(cc1)[C@@H]2Oc3ccc(O)c(F)c3[C@@H](C)[C@@H]2c4ccc(O)cc4)N5CC[C@H](C)C5</chem>
(2R,3R,4S)-5-fluoro-3-(4-hydroxyphenyl)-4-methyl-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-3,4-dihydro-2H-1-benzopyran-6-ol	1	1	1	0	<chem>C[C@H]1[C@@H]([C@@H](Oc2ccc(O)c(F)c12)c3ccc(OCCN4CCCCC4)cc3)c5ccc(O)cc5</chem>
(2R,3R,4S)-5-fluoro-3-(4-hydroxyphenyl)-4-methyl-2-(4-{2-[(3R)-3-methylpyrrolidin-1-yl]ethoxy}phenyl)-3,4-dihydro-2H-1-benzopyran-6-ol	1	1	1	0	<chem>C[C@@H]1CCN(CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)c(F)c4[C@@H](C)[C@@H]3c5ccc(O)cc5)C1</chem>
(2R,3R,4S)-3-(4-hydroxyphenyl)-4-methyl-2-(4-{2-[(3S)-3-methylpyrrolidin-1-yl]ethoxy}phenyl)-3,4-dihydro-2H-1-benzopyran-6-ol	1	1	1	0	<chem>C[C@H]1CCN(CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4[C@@H](C)[C@@H]3c5ccc(O)cc5)C1</chem>

	(2R,3R,4S)-5-fluoro-3-(4-hydroxyphenyl)-4-methyl-2-(4-{2-[(3S)-3-methylpyrrolidin-1-yl]ethoxy}phenyl)-3,4-dihydro-2H-1-benzopyran-6-ol	1	1	1	0	<chem>C[C@H]1CCN(CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)c(F)c4[C@@H](C)[C@@H]3c5ccc(O)cc5)C1</chem>
	1-(2-{4-[(3S,4R)-7-methoxy-3-phenyl-3,4-dihydro-1H-2-benzopyran-4-yl]phenoxy}ethyl)pyrrolidine	1	1	1	0	<chem>COc1ccc2[C@H]([C@H](OCc2c1)c3ccccc3)c4ccc(OCCN5CCC5)cc4</chem>
	1-(2-{4-[(3S,4R)-7-methoxy-3-phenyl-3,4-dihydro-1H-2-benzothiopyran-4-yl]phenoxy}ethyl)pyrrolidine	1	1	1	0	<chem>COc1ccc2[C@H]([C@H](SCc2c1)c3ccccc3)c4ccc(OCCN5CCC5)cc4</chem>
	(3S,4R)-3-phenyl-4-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}-3,4-dihydro-1H-2-benzopyran-7-ol	1	1	1	0	<chem>Oc1ccc2[C@H]([C@H](OCc2c1)c3ccccc3)c4ccc(OCCN5CCCC5)cc4</chem>
	(3S,4R)-3-phenyl-4-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}-3,4-dihydro-1H-2-benzothiopyran-7-ol	1	1	1	0	<chem>Oc1ccc2[C@H]([C@H](SCc2c1)c3ccccc3)c4ccc(OCCN5CCCC5)cc4</chem>
	(2S,3R)-3-(4-hydroxyphenyl)-2-(4-{2-[(3R)-3-isopropylpyrrolidin-1-yl]ethoxy}phenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>CC(C)[C@H]1CCN(CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5)C1</chem>
	(2S,3R)-3-(4-hydroxyphenyl)-2-(4-{[(2R)-1-(pyrrolidin-1-yl)propan-2-	1	1	1	0	<chem>C[C@H](CN1CCCC1)Oc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C</chem>

	yl]oxy}phenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol					@@H]3c5ccc(O)cc5
	(2S,3R)-2-{4-[2-(3,3-dimethylpyrrolidin-1-yl)ethoxy]phenyl}-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	CC1(C)CCN(CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5)C1
	(2S,3R)-2-{4-[2-(3-ethylpyrrolidin-1-yl)ethoxy]phenyl}-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	CCC1CCN(CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5)C1
	(2S,3R)-3-(4-hydroxyphenyl)-2-{4-[2-methyl-2-(pyrrolidin-1-yl)propoxy]phenyl}-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	CC(C)(COc1ccc(cc1)[C@@H]2Oc3ccc(O)cc3S[C@@H]2c4ccc(O)cc4)N5CCCC5
	(2S,3R)-3-(4-hydroxyphenyl)-2-(4-{2-[(3S)-3-isopropylpyrrolidin-1-yl]ethoxy}phenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	CC(C)[C@@H]1CCN(CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5)C1
	(2S,3R)-3-(4-hydroxyphenyl)-2-(4-{[(2S)-1-(pyrrolidin-1-yl)propan-2-yl]oxy}phenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	C[C@@H](CN1CCCC1)Oc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5
	(2S,3R)-3-(4-hydroxyphenyl)-2-(4-{2-[(2S)-2-methylpyrrolidin-1-	1	1	1	0	C[C@H]1CCCN1CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C

	yl]ethoxy}phenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol					@@H]3c5ccc(O)cc5
	(2S,3R)-3-(4-hydroxyphenyl)-2-{4-[(2R)-3-methyl-2-(pyrrolidin-1-yl)butoxy]phenyl}-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	CC(C)[C@H](COc1ccc(cc1)[C@@H]2Oc3ccc(O)cc3S[C@@H]2c4ccc(O)cc4)N5CCCC5
	(2S,3R)-2-(4-{2-[(3R)-3-ethylpyrrolidin-1-yl]ethoxy}phenyl)-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	CC[C@@H]1CCN(CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5)C1
	(2S,3R)-3-(4-hydroxyphenyl)-2-{4-[3-(pyrrolidin-1-yl)propoxy]phenyl}-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCCN5CCCC5)cc4
	(2S,3R)-3-(4-hydroxyphenyl)-2-{4-[(2S)-3-methyl-2-(pyrrolidin-1-yl)butoxy]phenyl}-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	CC(C)[C@@H](COc1ccc(cc1)[C@@H]2Oc3ccc(O)cc3S[C@@H]2c4ccc(O)cc4)N5CCCC5
	(2S,3R)-3-(4-hydroxyphenyl)-2-(4-{[(2R)-1-(pyrrolidin-1-yl)butan-2-yl]oxy}phenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	CC[C@H](CN1CCCC1)Oc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5
	(2S,3R)-2-{4-[2-(2,2-dimethylpyrrolidin-1-yl)ethoxy]phenyl}-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-	1	1	1	0	CC1(C)CCCN1CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5

	benzoxathiin-6-ol					
	(2S,3R)-3-(4-hydroxyphenyl)-2-(4- {[(2S)-1-(pyrrolidin-1-yl)butan-2- yl]oxy}phenyl)-2,3-dihydro-1,4- benzoxathiin-6-ol	1	1	1	0	<chem>CC[C@@H](CN1CCCC1)Oc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5</chem>
	(2S,3R)-3-(4-hydroxyphenyl)-2-(4- {2-[(2R)-2-methylpyrrolidin-1- yl]ethoxy}phenyl)-2,3-dihydro-1,4- benzoxathiin-6-ol	1	1	1	0	<chem>C[C@@H]1CCCN1CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5</chem>
	(2S,3R)-2-(4-{2-[(3R,4S)-3,4- dimethylpyrrolidin-1- yl]ethoxy}phenyl)-3-(4- hydroxyphenyl)-2,3-dihydro-1,4- benzoxathiin-6-ol	1	1	1	0	<chem>C[C@@H]1CN(CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5)C[C@@H]1C</chem>
	(2S,3R)-3-(4-hydroxyphenyl)-2-(4- [(2R)-2-(pyrrolidin-1- yl)butoxy]phenyl)-2,3-dihydro-1,4- benzoxathiin-6-ol	1	1	1	0	<chem>CC[C@H](COc1ccc(cc1)[C@@H]2Oc3ccc(O)cc3S[C@@H]2c4ccc(O)cc4)N5CCCC5</chem>
	(2S,3R)-2-[4-(2- {bicyclo[3.1.0]hexan-3- yl}ethoxy)phenyl]-3-(4- hydroxyphenyl)-2,3-dihydro-1,4- benzoxathiin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCC5CC6CC6C5)cc4</chem>
	(2S,3R)-2-(4-{2-[(3R,4R)-3,4- dimethylpyrrolidin-1-	1	1	1	0	<chem>C[C@H]1CN(CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@</chem>

	yl]ethoxy}phenyl)-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol					H]3c5ccc(O)cc5)C[C@@H]1C
	(2S,3R)-3-(4-hydroxyphenyl)-2-{4-[(2S)-2-(pyrrolidin-1-yl)butoxy]phenyl}-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	CC[C@@H](COc1ccc(cc1)[C@@H]2Oc3ccc(O)cc3S[C@@H]2c4ccc(O)cc4)N5CCCC5
4225-26-7	2,2'-biphenol	0	1	0	1	Oc1ccccc1c2ccccc2O
	4-bromo-2-(4-hydroxyphenyl)-7-methoxy-1-benzofuran-5-ol	1	1	1	0	COc1cc(O)c(Br)c2cc(oc12)c3ccc(O)cc3
	4-bromo-2-(3-fluoro-4-hydroxyphenyl)-7-methoxy-1-benzofuran-5-ol	1	1	1	0	COc1cc(O)c(Br)c2cc(oc12)c3ccc(O)c(F)c3
	(2S,3R)-2-[4-(2-{8-azaspiro[4.5]decan-8-yl}ethoxy)phenyl]-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5CC6(CCCC6)CC5)cc4
	(2S,3R)-2-(4-{2-[(2R)-2-(hydroxymethyl)pyrrolidin-1-yl]ethoxy}phenyl)-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	OC[C@H]1CCCN1CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5

(2S,3R)-2-[4-(2-{3-azabicyclo[3.2.0]heptan-3-yl}ethoxy)phenyl]-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5CC6CCC6C5)cc4</chem>
(2S,3R)-2-(4-{2-[(3aR,7aS)-octahydroisoidol-2-yl]ethoxy}phenyl)-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5C[C@H]6CCCC[C@H]6C5)cc4</chem>
(3R)-1-(2-{4-[(2S,3R)-6-hydroxy-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-2-yl]phenoxy}ethyl)pyrrolidin-3-ol	1	1	1	0	<chem>O[C@@H]1CCN(CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5)C1</chem>
(2S,3R)-2-[4-(2-{3-azabicyclo[3.1.0]hexan-3-yl}ethoxy)phenyl]-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5CC6CC6C5)cc4</chem>
1-(2-{4-[(2S,3R)-6-hydroxy-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-2-yl]phenoxy}ethyl)piperidine-4-carboxamide	1	1	1	0	<chem>NC(=O)C1CCN(CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5)CC1</chem>

(2S,3R)-2-(4-{2-[(3aR,6aS)-hexahydro-1H-cyclopenta[c]pyrrol-2-yl]ethoxy}phenyl)-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5C[C@H]6CCC[C@H]6C5)cc4
(2S,3R)-2-(4-{2-[(3R)-3-fluoropyrrolidin-1-yl]ethoxy}phenyl)-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5CC[C@@H](F)C5)cc4
(2S,3R)-2-[4-(2-{7-azabicyclo[2.2.1]heptan-7-yl}ethoxy)phenyl]-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5C6CCC5CC6)cc4
(2S,3R)-2-[4-(2-{9-azabicyclo[3.3.1]nonan-9-yl}ethoxy)phenyl]-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5C6CCCC5CCC6)cc4
4-(2-{4-[(2S,3R)-6-hydroxy-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-2-yl]phenoxy}ethyl)-1 <i>H</i> -4-thiomorpholine-1,1-dione	1	1	1	0	Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5CCS(=O)(=O)CC5)cc4
(2S,3R)-2-[4-(2-{8-	1	1	1	0	Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5C6

	azabicyclo[3.2.1]octan-8-yl}ethoxy)phenyl]-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol					CCCC5CC6)cc4
	(2S,3R)-3-(4-hydroxyphenyl)-2-{4-[2-(thiomorpholin-4-yl)ethoxy]phenyl}-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5CCS5)cc4
	(2S,3R)-2-[4-(2-{2-azaspiro[3.3]heptan-2-yl}ethoxy)phenyl]-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5CC6(CCC6)C5)cc4
	(2S,3R)-2-(4-{2-[(2S)-2-(hydroxymethyl)pyrrolidin-1-yl]ethoxy}phenyl)-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	OC[C@@H]1CCCN1CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5
	(2S,3R)-2-(4-{2-[(1R,5S)-2-azabicyclo[3.1.0]hexan-2-yl]ethoxy}phenyl)-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5CC[C@H]6C[C@@H]56)cc4
	(2S,3R)-2-(4-{2-[4-(hydroxymethyl)piperidin-1-	1	1	1	0	OCC1CCN(CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5)CC1

	yl]ethoxy}phenyl)-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol					
	(2S,3R)-2-[4-(2-{4-azatricyclo[4.3.1.1{3,8}}]undecan-4-yl)ethoxy}phenyl]-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5CC6CC7CC(C6)CC5C7)cc4
	1-(2-{4-[(2S,3R)-6-hydroxy-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-2-yl]phenoxy}ethyl)piperidin-4-ol	1	1	1	0	OC1CCN(CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5)CC1
	(2S,3R)-2-[4-(2-{2-azabicyclo[2.2.2]octan-2-yl}ethoxy}phenyl)-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5CC6CCC5CC6)cc4
	(2S,3R)-2-[4-(2-{1,4-dioxa-8-azaspiro[4.5]decan-8-yl}ethoxy}phenyl)-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5CC6(CC5)OCCO6)cc4
	(2S,3R)-2-[4-{2-[(1S,5R)-2-azabicyclo[3.1.0]hexan-2-yl]ethoxy}phenyl)-3-(4-	1	1	1	0	Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5CC[C@@H]6C[C@H]56)cc4

	hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol					
	(2S,3R)-2-(4-{2-[4-(2-hydroxyethyl)piperidin-1-yl]ethoxy}phenyl)-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>OCCCC1CCN(CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5)CC1</chem>
	(2S,3R)-3-(4-hydroxyphenyl)-2-[4-(2-{2-oxa-5-azabicyclo[2.2.1]heptan-5-yl}ethoxy)phenyl]-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5CC6CC5CO6)cc4</chem>
	(2S,3R)-2-(4-[2-(4,4-difluoropiperidin-1-yl)ethoxy]phenyl)-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5CC(F)(F)CC5)cc4</chem>
	4,6-dibromo-7-ethenyl-2-(3-fluoro-4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1ccc(cc1F)c2oc3c(C=C)c(Br)c(O)c(Br)c3n2</chem>
	4-bromo-2-(3-fluoro-4-hydroxyphenyl)-7-methoxy-1,3-benzoxazol-5-ol	1	1	1	0	<chem>COc1cc(O)c(Br)c2nc(oc12)c3ccc(O)c(F)c3</chem>
	4,6-dibromo-2-(3-fluoro-4-hydroxyphenyl)-7-methoxy-1,3-	1	1	1	0	<chem>COc1c(Br)c(O)c(Br)c2nc(oc12)c3ccc(O)c(F)c3</chem>

	benzoxazol-5-ol					
	2-(3-fluoro-4-hydroxyphenyl)-7-methyl-1-benzofuran-5-ol	1	1	1	0	<chem>Cc1cc(O)cc2cc(oc12)c3ccc(O)c(F)c3</chem>
	2-[5-hydroxy-2-(4-hydroxyphenyl)-1-benzofuran-7-yl]acetonitrile	1	1	1	0	<chem>Oc1ccc(cc1)c2oc3c(CC#N)cc(O)cc3c2</chem>
	1-[5-hydroxy-2-(4-hydroxyphenyl)-1-benzofuran-7-yl]propan-1-one	1	1	1	0	<chem>CCC(=O)c1cc(O)cc2cc(oc12)c3ccc(O)cc3</chem>
	5-hydroxy-2-(4-hydroxyphenyl)-1-benzofuran-7-carbaldehyde	1	1	1	0	<chem>Oc1ccc(cc1)c2oc3c(C=O)cc(O)cc3c2</chem>
	2-[4-chloro-5-hydroxy-2-(4-hydroxyphenyl)-1-benzofuran-7-yl]acetonitrile	1	1	1	0	<chem>Oc1ccc(cc1)c2oc3c(CC#N)cc(O)c(Cl)c3c2</chem>
	1-[5-hydroxy-2-(4-hydroxyphenyl)-1-benzofuran-7-yl]ethanone	1	1	1	0	<chem>CC(=O)c1cc(O)cc2cc(oc12)c3ccc(O)cc3</chem>
	2-[2-(3-fluoro-4-hydroxyphenyl)-5-hydroxy-1-benzofuran-7-yl]acetonitrile	1	1	1	0	<chem>Oc1cc(CC#N)c2oc(cc2c1)c3ccc(O)c(F)c3</chem>
	2-[4-bromo-5-hydroxy-2-(4-hydroxyphenyl)-1-benzofuran-7-yl]acetonitrile	1	1	1	0	<chem>Oc1ccc(cc1)c2oc3c(CC#N)cc(O)c(Br)c3c2</chem>
	5-hydroxy-2-(4-hydroxyphenyl)-1-benzofuran-7-carbonitrile	1	1	1	0	<chem>Oc1ccc(cc1)c2oc3c(cc(O)cc3c2)C#N</chem>

	2-(3-fluoro-4-hydroxyphenyl)-5-hydroxy-1-benzofuran-7-carbonitrile	1	1	1	0	<chem>Oc1cc(C#N)c2oc(cc2c1)c3ccc(O)c(F)c3</chem>
	4-bromo-6-(6-hydroxy-1,2-benzoxazol-3-yl)benzene-1,3-diol	1	1	1	0	<chem>Oc1ccc2c(noc2c1)c3cc(Br)c(O)cc3O</chem>
	4-chloro-6-(6-hydroxy-1,2-benzoxazol-3-yl)benzene-1,3-diol	1	1	1	0	<chem>Oc1ccc2c(noc2c1)c3cc(Cl)c(O)cc3O</chem>
	3-(4-hydroxy-2-methylphenyl)-1,2-benzoxazol-6-ol	1	1	1	0	<chem>Cc1cc(O)ccc1c2noc3cc(O)ccc23</chem>
	3-(4-hydroxy-2-propylphenyl)-1,2-benzoxazol-6-ol	1	1	1	0	<chem>CCCc1cc(O)ccc1c2noc3cc(O)ccc23</chem>
	3-(4-hydroxy-2,5-dipropylphenyl)-1,2-benzoxazol-6-ol	1	1	1	0	<chem>CCCc1cc(c(CCC)cc1O)c2noc3cc(O)ccc23</chem>
	4-(1,2-benzoxazol-3-yl)benzene-1,3-diol	1	1	1	0	<chem>Oc1ccc(c(O)c1)c2noc3ccccc23</chem>
	3-(3-chloro-4-hydroxyphenyl)-1,2-benzoxazol-6-ol	1	1	1	0	<chem>Oc1ccc2c(noc2c1)c3ccc(O)c(Cl)c3</chem>
	5-hydroxy-2-(6-hydroxy-1,2-benzoxazol-3-yl)benzonitrile	1	1	1	0	<chem>Oc1ccc(c(c1)C#N)c2noc3cc(O)ccc23</chem>
	2-[5-hydroxy-2-(6-hydroxy-1,2-benzoxazol-3-yl)phenyl]acetonitrile	1	1	1	0	<chem>Oc1ccc(c(CC#N)c1)c2noc3cc(O)ccc23</chem>

3-{4-hydroxy-2-[(1E)-(hydroxyimino)methyl]phenyl}-1,2-benzoxazol-6-ol	1	1	1	0	<chem>O\\N=C\\c1cc(O)ccc1c2noc3cc(O)ccc23</chem>
4-(5-hydroxy-1,2-benzoxazol-3-yl)benzene-1,3-diol	1	1	1	0	<chem>Oc1ccc(c(O)c1)c2noc3ccc(O)cc23</chem>
3-(4-hydroxyphenyl)-1,2-benzoxazol-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2noc3ccc(O)cc23</chem>
3-(4-hydroxy-3-methylphenyl)-1,2-benzoxazol-6-ol	1	1	1	0	<chem>Cc1cc(ccc1O)c2noc3cc(O)ccc23</chem>
4-(6-hydroxy-1,2-benzoxazol-3-yl)-6-methylbenzene-1,3-diol	1	1	1	0	<chem>Cc1cc(c(O)cc1O)c2noc3cc(O)ccc23</chem>
3-(2-ethyl-4-hydroxy-5-propylphenyl)-1,2-benzoxazol-6-ol	1	1	1	0	<chem>CCCC1cc(c(CC)cc1O)c2noc3cc(O)ccc23</chem>
3-(2-hydroxyphenyl)-1,2-benzoxazol-6-ol	1	1	1	0	<chem>Oc1ccc2c(noc2c1)c3cccc3O</chem>
3-(4-hydroxy-3-propylphenyl)-1,2-benzoxazol-6-ol	1	1	1	0	<chem>CCCC1cc(ccc1O)c2noc3cc(O)ccc23</chem>
4-(6-hydroxy-1,2-benzoxazol-3-yl)-2-methylbenzene-1,3-diol	1	1	1	0	<chem>Cc1c(O)ccc(c1O)c2noc3cc(O)ccc23</chem>
3-(3-bromo-4-hydroxyphenyl)-1,2-benzoxazol-6-ol	1	1	1	0	<chem>Oc1ccc2c(noc2c1)c3ccc(O)c(Br)c3</chem>

3-(3-fluoro-4-hydroxyphenyl)-1,2-benzoxazol-6-ol	1	1	1	0	<chem>Oc1ccc2c(noc2c1)c3ccc(O)c(F)c3</chem>
2-(3-fluoro-4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1ccc2oc(nc2c1)c3ccc(O)c(F)c3</chem>
7-butyl-2-(4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>CCCCc1cc(O)cc2nc(oc12)c3ccc(O)cc3</chem>
2-(6-hydroxynaphthalen-1-yl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1ccc2c(cccc2c1)c3oc4ccc(O)cc4n3</chem>
2-(5-hydroxy-7-methylnaphthalen-1-yl)-1,3-benzoxazol-6-ol	1	1	1	0	<chem>Cc1cc(O)c2cccc(c3oc4cc(O)ccc4n3)c2c1</chem>
3-(5-bromo-6-hydroxynaphthalen-2-yl)-1,2-benzoxazol-6-ol	1	1	1	0	<chem>Oc1ccc2c(noc2c1)c3ccc4c(Br)c(O)ccc4c3</chem>
3-(6-hydroxynaphthalen-2-yl)-1,2-benzoxazol-5-ol	1	1	1	0	<chem>Oc1ccc2cc(ccc2c1)c3noc4ccc(O)cc34</chem>
4-(5-hydroxy-1,3-benzoxazol-2-yl)benzene-1,3-diol	1	1	1	0	<chem>Oc1ccc(c(O)c1)c2oc3ccc(O)cc3n2</chem>
7-bromo-2-(4-hydroxy-2-methylphenyl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Cc1cc(O)ccc1c2oc3c(Br)cc(O)cc3n2</chem>
6-chloro-2-(4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2oc3cc(Cl)c(O)cc3n2</chem>
2-(2-fluoro-4-hydroxyphenyl)-7-(prop-2-en-1-yl)-1,3-benzoxazol-5-	1	1	1	0	<chem>Oc1ccc(c(F)c1)c2oc3c(CC=C)cc(O)cc3n2</chem>

	ol					
	2-(6-hydroxynaphthalen-1-yl)-1,3-benzoxazol-6-ol	1	1	1	0	Oc1ccc2nc(oc2c1)c3cccc4cc(O)ccc34
	2-(2,6-difluoro-4-hydroxyphenyl)-7-ethenyl-1,3-benzoxazol-5-ol	1	1	1	0	Oc1cc(F)c(c(F)c1)c2oc3c(C=C)cc(O)cc3n2
	2-(3-fluoro-4-hydroxyphenyl)-1,3-benzoxazol-6-ol	1	1	1	0	Oc1ccc2nc(oc2c1)c3ccc(O)c(F)c3
	2-(3-chloro-4-hydroxyphenyl)-1,3-benzoxazol-6-ol	1	1	1	0	Oc1ccc2nc(oc2c1)c3ccc(O)c(Cl)c3
	5-hydroxy-2-(4-hydroxyphenyl)-1,3-benzoxazole-7-carboxamide	1	1	1	0	NC(=O)c1cc(O)cc2nc(oc12)c3ccc(O)cc3
	2-(4-hydroxyphenyl)-7-(1,3-thiazol-2-yl)-1,3-benzoxazol-5-ol	1	1	1	0	Oc1ccc(cc1)c2oc3c(cc(O)cc3n2)c4nccs4
	7-(bromomethyl)-2-(4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	1	1	0	Oc1ccc(cc1)c2oc3c(CBr)cc(O)cc3n2
	7-cyclopentyl-2-(4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	1	1	0	Oc1ccc(cc1)c2oc3c(cc(O)cc3n2)C4CCCC4
	2-[5-hydroxy-2-(4-hydroxyphenyl)-1,3-benzoxazol-7-yl]acetonitrile	1	1	1	0	Oc1ccc(cc1)c2oc3c(CC#N)cc(O)cc3n2
	7-ethenyl-2-(4-hydroxy-2-	1	1	1	0	Cc1cc(O)ccc1c2oc3c(C=C)cc(O)cc3n2

	methylphenyl)-1,3-benzoxazol-5-ol					
	2-(4-hydroxyphenyl)-7-phenyl-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2oc3c(cc(O)cc3n2)c4ccccc4</chem>
	3-(7-hydroxynaphthalen-1-yl)-1,2-benzoxazol-6-ol	1	1	1	0	<chem>Oc1ccc2c(noc2c1)c3cccc4ccc(O)cc34</chem>
	2-(5-bromo-6-hydroxynaphthalen-1-yl)-1,3-benzoxazol-6-ol	1	1	1	0	<chem>Oc1ccc2nc(oc2c1)c3cccc4c(Br)c(O)ccc34</chem>
	5-fluoro-2-(6-hydroxynaphthalen-1-yl)-1,3-benzoxazol-6-ol	1	1	1	0	<chem>Oc1ccc2c(cccc2c1)c3oc4cc(O)c(F)cc4n3</chem>
	3-(5-hydroxynaphthalen-2-yl)-1,2-benzoxazol-6-ol	1	1	1	0	<chem>Oc1ccc2c(noc2c1)c3ccc4c(O)cccc4c3</chem>
	3-(5-hydroxy-1,3-benzoxazol-2-yl)benzene-1,2-diol	1	1	1	0	<chem>Oc1ccc2oc(nc2c1)c3ccc(O)c3O</chem>
	2-(3-fluoro-4-hydroxyphenyl)-7-[(Z)-2-fluoroethenyl]-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1cc(\C=C/F)c2oc(nc2c1)c3ccc(O)c(F)c3</chem>
	7-bromo-2-(2-fluoro-4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1ccc(c(F)c1)c2oc3c(Br)cc(O)cc3n2</chem>
	2-(2-fluoro-4-hydroxyphenyl)-7-[(1Z)-prop-1-en-1-yl]-1,3-benzoxazol-5-ol	1	1	1	0	<chem>C\C=C/c1cc(O)cc2nc(oc12)c3ccc(O)cc3F</chem>

2-(3-butoxy-4-hydroxyphenyl)-1,3-benzoxazol-6-ol	1	1	1	0	<chem>CCCCOc1cc(ccc1O)c2oc3cc(O)ccc3n2</chem>
2-(3-chloro-4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1ccc2oc(nc2c1)c3ccc(O)c(Cl)c3</chem>
2-(2-chloro-4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1ccc(c(Cl)c1)c2oc3ccc(O)cc3n2</chem>
3-(6-hydroxy-1,3-benzoxazol-2-yl)benzene-1,2-diol	1	1	1	0	<chem>Oc1ccc2nc(oc2c1)c3ccc(O)c3O</chem>
4-(6-hydroxy-1,3-benzoxazol-2-yl)benzene-1,2-diol	1	1	1	0	<chem>Oc1ccc2nc(oc2c1)c3ccc(O)c(O)c3</chem>
2-(4-hydroxyphenyl)-7-isopropyl-1,3-benzoxazol-5-ol	1	1	1	0	<chem>CC(C)c1cc(O)cc2nc(oc12)c3ccc(O)cc3</chem>
2-(4-hydroxyphenyl)-7-(prop-2-en-1-yl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2oc3c(CC=C)cc(O)cc3n2</chem>
methyl 5-hydroxy-2-(4-hydroxyphenyl)-1,3-benzoxazole-7-carboxylate	1	1	1	0	<chem>COC(=O)c1cc(O)cc2nc(oc12)c3ccc(O)cc3</chem>
2-(4-hydroxyphenyl)-7-(thiophen-2-yl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2oc3c(cc(O)cc3n2)c4cccs4</chem>
2-(6-hydroxynaphthalen-2-yl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1ccc2cc(ccc2c1)c3oc4ccc(O)cc4n3</chem>

	2-(6-hydroxynaphthalen-2-yl)-1,3-benzoxazol-6-ol	1	1	1	0	Oc1ccc2nc(oc2c1)c3ccc4cc(O)ccc4c3
	3-(6-hydroxynaphthalen-1-yl)-1,2-benzoxazol-6-ol	1	1	1	0	Oc1ccc2c(noc2c1)c3cccc4cc(O)ccc34
	3-(5-hydroxynaphthalen-1-yl)-1,2-benzoxazol-6-ol	1	1	1	0	Oc1ccc2c(noc2c1)c3cccc4c(O)cccc34
	6-chloro-2-(3-fluoro-4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	1	1	0	Oc1ccc(cc1F)c2oc3cc(Cl)c(O)cc3n2
	2-(2,5-difluoro-4-hydroxyphenyl)-7-ethenyl-1,3-benzoxazol-5-ol	1	1	1	0	Oc1cc(C=C)c2oc(nc2c1)c3cc(F)c(O)cc3F
	6-bromo-2-(3-fluoro-4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	1	1	0	Oc1ccc(cc1F)c2oc3cc(Br)c(O)cc3n2
	2-(4-hydroxynaphthalen-1-yl)-1,3-benzoxazol-6-ol	1	1	1	0	Oc1ccc2nc(oc2c1)c3ccc(O)c4cccc34
	2-(naphthalen-1-yl)-1,3-benzoxazol-6-ol	1	1	1	0	Oc1ccc2nc(oc2c1)c3cccc4cccc34
	2-(3,5-difluoro-4-hydroxyphenyl)-7-ethenyl-1,3-benzoxazol-5-ol	1	1	1	0	Oc1cc(C=C)c2oc(nc2c1)c3cc(F)c(O)c(F)c3
	5-chloro-2-(4-hydroxyphenyl)-1,3-benzoxazol-6-ol	1	1	1	0	Oc1ccc(cc1)c2oc3cc(O)c(Cl)cc3n2

	2-(3-tert-butyl-4-hydroxyphenyl)-1,3-benzoxazol-6-ol	1	1	1	0	<chem>CC(C)(C)c1cc(ccc1O)c2oc3cc(O)ccc3n2</chem>
	5-hydroxy-2-(4-hydroxyphenyl)-1,3-benzoxazole-7-carboxylic acid	1	1	1	0	<chem>OC(=O)c1cc(O)cc2nc(oc12)c3ccc(O)cc3</chem>
	4-(6-hydroxy-1,3-benzoxazol-2-yl)benzene-1,3-diol	1	1	1	0	<chem>Oc1ccc(c(O)c1)c2oc3cc(O)ccc3n2</chem>
	4-bromo-7-ethenyl-2-(3-fluoro-4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1ccc(cc1F)c2oc3c(C=C)cc(O)c(Br)c3n2</chem>
	7-(furan-2-yl)-2-(4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2oc3c(cc(O)cc3n2)c4occc4</chem>
74296-32-5	butylbenzene	0	1	0	1	<chem>CCCCc1ccccc1</chem>
	6-(2-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc2cc(ccc2c1)c3ccccc3O</chem>
106-46-7	PARA	0	1	0	1	<chem>Clc1ccc(Cl)cc1</chem>
1341-82-8	3-tert-butyl-4-hydroxyanisole	0	1	0	1	<chem>COc1ccc(O)c(c1)C(C)(C)C</chem>
1570-64-5	4-chloro-2-methylphenol	0	1	0	1	<chem>Cc1cc(Cl)ccc1O</chem>
103-16-2	monobenzene	1	1	1	0	<chem>Oc1ccc(OCc2ccccc2)cc1</chem>
121714-72-5	norgestrel	1	1	1	0	<chem>CC[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@H]34)[C@@H]1CC[C@@]2(O)C#C</chem>

481-30-1	epitestosterone	0	1	0	1	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@H]2O</chem>
599-64-4	p-cumylphenol	1	1	1	0	<chem>CC(C)(c1ccccc1)c2ccc(O)cc2</chem>
92092-63-2	benzophenone-1	1	1	1	0	<chem>Oc1ccc(C(=O)c2ccccc2)c(O)c1</chem>
93-76-5	fortex	0	1	0	1	<chem>OC(=O)COc1cc(Cl)c(Cl)cc1Cl</chem>
3839-46-1	trans-4-hydroxystilbene	1	1	1	0	<chem>Oc1ccc(\C=C\c2ccccc2)cc1</chem>
	4-[5-hydroxy-2-(4-hydroxyphenyl)-3H-inden-1-yl]benzoic acid	1	1	1	0	<chem>OC(=O)c1ccc(cc1)C2=C(Cc3cc(O)ccc23)c4ccc(O)cc4</chem>
	7-hydroxy-3-(4-hydroxyphenyl)-5-methylquinazoline-4-thione	1	1	1	0	<chem>Cc1cc(O)cc2N=CN(C(=S)c12)c3ccc(O)cc3</chem>
603-45-2	aurin	1	1	1	0	<chem>Oc1ccc(cc1)C(=C2C=CC(=O)C=C2)c3ccc(O)cc3</chem>
68988-18-1	DEP	0	1	0	1	<chem>CCOC(=O)c1ccccc1C(=O)OCC</chem>
	2-(2-phenyl-1H-indol-3-yl)-N-(4-phenylbutan-2-yl)acetamide	1	1	1	0	<chem>CC(CCC1ccccc1)NC(=O)Cc2c([nH]c3ccccc23)c4ccccc4</chem>
	N-[4-(4-hydroxyphenyl)butan-2-yl]-2-(2-phenyl-1H-indol-3-yl)acetamide	1	1	1	0	<chem>CC(CCC1ccc(O)cc1)NC(=O)Cc2c([nH]c3ccccc23)c4ccccc4</chem>
	N-[(2S)-4-(4-hydroxyphenyl)butan-2-yl]-2-(2-phenyl-1H-indol-3-yl)acetamide	1	1	1	0	<chem>C[C@@H](CCc1ccc(O)cc1)NC(=O)Cc2c([nH]c3ccccc23)c4ccccc4</chem>

N-[(2R)-4-(4-hydroxyphenyl)butan-2-yl]-2-(2-phenyl-1H-indol-3-yl)acetamide	1	1	1	0	<chem>C[C@H](CCc1ccc(O)cc1)NC(=O)Cc2c([nH]c3ccccc23)c4ccccc4</chem>
N-[(2R)-4-(4-hydroxyphenyl)butan-2-yl]-2-{2-phenyl-5-[4-(piperidin-1-yl)butoxy]-1H-indol-3-yl}acetamide	1	1	1	0	<chem>C[C@H](CCc1ccc(O)cc1)NC(=O)Cc2c([nH]c3ccc(OCCCCN4CCCC4)cc23)c5ccccc5</chem>
N-[(2R)-4-(4-hydroxyphenyl)butan-2-yl]-2-(2-phenyl-5-{[5-(piperidin-1-yl)pentyl]oxy}-1H-indol-3-yl)acetamide	1	1	1	0	<chem>C[C@H](CCc1ccc(O)cc1)NC(=O)Cc2c([nH]c3ccc(OCCCCCN4CCCC4)cc23)c5ccccc5</chem>
N-[(2R)-4-(4-hydroxyphenyl)butan-2-yl]-2-{2-phenyl-6-[2-(piperidin-1-yl)ethoxy]-1H-indol-3-yl}acetamide	1	1	1	0	<chem>C[C@H](CCc1ccc(O)cc1)NC(=O)Cc2c([nH]c3cc(OCCN4CCCC4)ccc23)c5ccccc5</chem>
N-[(2R)-4-(4-hydroxyphenyl)butan-2-yl]-2-{2-phenyl-6-[3-(piperidin-1-yl)propoxy]-1H-indol-3-yl}acetamide	1	1	1	0	<chem>C[C@H](CCc1ccc(O)cc1)NC(=O)Cc2c([nH]c3cc(OCCCN4CCCC4)ccc23)c5ccccc5</chem>
N-[(2R)-4-(4-hydroxyphenyl)butan-2-yl]-2-{2-phenyl-6-[4-(piperidin-1-yl)butoxy]-1H-indol-3-yl}acetamide	1	1	1	0	<chem>C[C@H](CCc1ccc(O)cc1)NC(=O)Cc2c([nH]c3cc(OCCCCN4CCCC4)ccc23)c5ccccc5</chem>
N-[(2R)-4-(4-hydroxyphenyl)butan-2-yl]-2-{2-phenyl-6-[2-(pyrrolidin-1-yl)ethoxy]-1H-indol-3-yl}acetamide	1	1	1	0	<chem>C[C@H](CCc1ccc(O)cc1)NC(=O)Cc2c([nH]c3cc(OCCN4CCCC4)ccc23)c5ccccc5</chem>

N-[(2R)-4-(4-hydroxyphenyl)butan-2-yl]-2-[2-phenyl-6-[3-(pyrrolidin-1-yl)propoxy]-1H-indol-3-yl]acetamide	1	1	1	0	<chem>C[C@H](CCc1ccc(O)cc1)NC(=O)Cc2c([nH])c3cc(OCCCN4CCC4)ccc23)c5ccccc5</chem>
N-[(2R)-4-(4-hydroxyphenyl)butan-2-yl]-2-[2-phenyl-1-({4-[2-(piperidin-1-yl)ethoxy]phenyl}methyl)indol-3-yl]acetamide	1	1	1	0	<chem>C[C@H](CCc1ccc(O)cc1)NC(=O)Cc2c(c3ccccc3)n(Cc4ccc(OCN5CCCCC5)cc4)c6ccccc26</chem>
N-[(2R)-4-(4-hydroxyphenyl)butan-2-yl]-2-(2-phenyl-1-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}indol-3-yl)acetamide	1	1	1	0	<chem>C[C@H](CCc1ccc(O)cc1)NC(=O)Cc2c(c3ccccc3)n(C(=O)c4ccc(OCN5CCCCC5)cc4)c6ccccc26</chem>
N-[(2R)-4-(4-hydroxyphenyl)butan-2-yl]-2-[2-phenyl-1-({4-[3-(piperidin-1-yl)propoxy]phenyl}methyl)indol-3-yl]acetamide	1	1	1	0	<chem>C[C@H](CCc1ccc(O)cc1)NC(=O)Cc2c(c3ccccc3)n(Cc4ccc(OCN5CCCCC5)cc4)c6ccccc26</chem>
N-[(2R)-4-(4-hydroxyphenyl)butan-2-yl]-2-[2-phenyl-1-({4-[4-(piperidin-1-yl)butoxy]phenyl}methyl)indol-3-yl]acetamide	1	1	1	0	<chem>C[C@H](CCc1ccc(O)cc1)NC(=O)Cc2c(c3ccccc3)n(Cc4ccc(OCN5CCCCC5)cc4)c6ccccc26</chem>
N-[(1S)-1-{5-hydroxy-3-methyl-1-[(4-{2-[(3S)-3-methylpyrrolidin-1-	1	1	1	0	<chem>C[C@H](NC(=O)Cc1c([nH])c2ccccc12)c3ccccc3)c4c(C)c5cc(O)ccc5n4Cc6ccc(OCCN7CC[C@H](C)C7)cc6</chem>

	yl]ethoxy}phenyl)methyl]indol-2-yl}ethyl]-2-(2-phenyl-1H-indol-3-yl)acetamide					
	N-[(1S)-1-[5-hydroxy-3-methyl-1-({4-[2-(piperidin-1-yl)ethoxy]phenyl)methyl]indol-2-yl}ethyl]-2-(2-phenyl-1H-indol-3-yl)acetamide	1	1	1	0	<chem>C[C@H](NC(=O)Cc1c([nH]c2cccc12)c3cccc3)c4c(C)c5cc(O)ccc5n4Cc6ccc(OCCN7CCCCC7)cc6</chem>
53-63-4	(1S,10S,11S,15S)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-5-ol	1	1	1	0	<chem>C[C@@]12CCC[C@H]1[C@@H]3CCc4cc(O)ccc4[C@H]3CC2</chem>
2877-88-5	phenol red	0	1	0	1	<chem>Oc1ccc(cc1)C2(OS(=O)(=O)c3ccccc23)c4ccc(O)cc4</chem>
	4-(3-chlorophenyl)-2-methylphenol	1	1	1	0	<chem>Cc1cc(ccc1O)c2cccc(Cl)c2</chem>
	1-(2R)-2-ethylhexyl 2-(2S)-2-ethylhexyl phthalate	1	1	1	0	<chem>CCCC[C@@H](CC)COC(=O)c1ccccc1C(=O)OC[C@@H](CC)C</chem>
40957-83-3	glycitein	1	1	1	0	<chem>COc1cc2C(=O)C(=COc2cc1O)c3ccc(O)cc3</chem>
	@isoformononetin	1	1	1	0	<chem>COc1ccc2C(=O)C(=COc2c1)c3ccc(O)cc3</chem>
	2-(2,4-dihydroxyphenyl)-4-hydroxy-6-methoxy-1-benzofuran-3-carbaldehyde	1	1	1	0	<chem>COc1cc(O)c2c(C=O)c(oc2c1)c3ccc(O)cc3O</chem>
1752-24-5	phenol, 4,4'-iminobis-	1	1	1	0	<chem>Oc1ccc(Nc2ccc(O)cc2)cc1</chem>

4-[(4-hydroxyphenyl)(methyl)amino]phenol	1	1	1	0	<chem>CN(c1ccc(O)cc1)c2ccc(O)cc2</chem>
4-[(4-hydroxyphenyl)(isopropyl)amino]phenol	1	1	1	0	<chem>CC(C)N(c1ccc(O)cc1)c2ccc(O)cc2</chem>
4-[(4-hydroxyphenyl)(3-methylbutyl)amino]phenol	1	1	1	0	<chem>CC(C)CCN(c1ccc(O)cc1)c2ccc(O)cc2</chem>
4-[hexyl(4-hydroxyphenyl)amino]phenol	1	1	1	0	<chem>CCCCCCN(c1ccc(O)cc1)c2ccc(O)cc2</chem>
4-[(cyclohexylmethyl)(4-hydroxyphenyl)amino]phenol	1	1	1	0	<chem>Oc1ccc(cc1)N(CC2CCCCC2)c3ccc(O)cc3</chem>
4-[(2-cyclohexylethyl)(4-hydroxyphenyl)amino]phenol	1	1	1	0	<chem>Oc1ccc(cc1)N(CCC2CCCCC2)c3ccc(O)cc3</chem>
4-[[3-bromoadamantan-1-yl)methyl](4-hydroxyphenyl)amino]phenol	1	1	1	0	<chem>Oc1ccc(cc1)N(CC23CC4CC(CC(Br)(C4)C2)C3)c5ccc(O)cc5</chem>
4-[benzyl(4-hydroxyphenyl)amino]phenol	1	1	1	0	<chem>Oc1ccc(cc1)N(Cc2ccccc2)c3ccc(O)cc3</chem>
4-[(4-hydroxyphenyl)[(4-hydroxyphenyl)methyl]amino]phenol	1	1	1	0	<chem>Oc1ccc(CN(c2ccc(O)cc2)c3ccc(O)cc3)cc1</chem>

4-[cyclohexyl(4-hydroxyphenyl)amino]phenol	1	1	1	0	<chem>Oc1ccc(cc1)N(C2CCCCC2)c3ccc(O)cc3</chem>
4-[(4-hydroxyphenyl)(phenyl)amino]phenol	1	1	1	0	<chem>Oc1ccc(cc1)N(c2ccccc2)c3ccc(O)cc3</chem>
N,N-bis(4-hydroxyphenyl)acetamide	1	1	1	0	<chem>CC(=O)N(c1ccc(O)cc1)c2ccc(O)cc2</chem>
N,N-bis(4-hydroxyphenyl)benzamide	1	1	1	0	<chem>Oc1ccc(cc1)N(C(=O)c2ccccc2)c3ccc(O)cc3</chem>
4-hydroxy-N,N-bis(4-hydroxyphenyl)benzamide	1	1	1	0	<chem>Oc1ccc(cc1)N(C(=O)c2ccc(O)cc2)c3ccc(O)cc3</chem>
N,N-bis(4-hydroxyphenyl)methanesulfonamide	1	1	1	0	<chem>CS(=O)(=O)N(c1ccc(O)cc1)c2ccc(O)cc2</chem>
N,N-bis(4-hydroxyphenyl)benzenesulfonamide	1	1	1	0	<chem>Oc1ccc(cc1)N(c2ccc(O)cc2)S(=O)(=O)c3ccccc3</chem>
4-hydroxy-N,N-bis(4-hydroxyphenyl)benzenesulfonamide	1	1	1	0	<chem>Oc1ccc(cc1)N(c2ccc(O)cc2)S(=O)(=O)c3ccc(O)cc3</chem>
4-(4-hydroxyphenyl)-3,6-diphenylpyran-2-one	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(C(=O)OC(=C2)c3ccccc3)c4ccccc4</chem>

	6-(4-hydroxyphenyl)-3,4-diphenylpyran-2-one	1	1	1	0	<chem>Oc1ccc(cc1)C2=CC(=C(C(=O)O2)c3ccccc3)c4ccccc4</chem>
	3-(4-hydroxyphenyl)-4,6-diphenylpyran-2-one	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(C(=C(OC2=O)c3ccccc3)c4ccccc4</chem>
	3-(4-hydroxyphenyl)-4-(4-methoxyphenyl)-6-phenylpyran-2-one	1	1	1	0	<chem>COc1ccc(cc1)C2=C(C(=O)OC(=C2)c3ccccc3)c4ccc(O)cc4</chem>
	3,6-bis(4-hydroxyphenyl)-4-phenylpyran-2-one	1	1	1	0	<chem>Oc1ccc(cc1)C2=CC(=C(C(=O)O2)c3ccc(O)cc3)c4ccccc4</chem>
	3,6-diphenyl-4-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}pyran-2-one	1	1	1	0	<chem>O=C1OC(=CC(=C1c2ccccc2)c3ccc(OCCN4CCCC4)cc3)c5ccccc5</chem>
	3,6-diphenyl-4-{4-[2-(piperidin-1-yl)ethoxy]phenyl}pyran-2-one	1	1	1	0	<chem>O=C1OC(=CC(=C1c2ccccc2)c3ccc(OCCN4CCCCC4)cc3)c5cccc5</chem>
	3,4-diphenyl-6-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}pyran-2-one	1	1	1	0	<chem>O=C1OC(=CC(=C1c2ccccc2)c3ccccc3)c4ccc(OCCN5CCCC5)cc4</chem>
	3,4-diphenyl-6-{4-[2-(piperidin-1-yl)ethoxy]phenyl}pyran-2-one	1	1	1	0	<chem>O=C1OC(=CC(=C1c2ccccc2)c3ccccc3)c4ccc(OCCN5CCCCC5)cc4</chem>
	4,6-diphenyl-3-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}pyran-2-one	1	1	1	0	<chem>O=C1OC(=CC(=C1c2ccc(OCCN3CCCC3)cc2)c4ccccc4)c5ccccc5</chem>
	4,6-diphenyl-3-{4-[2-(piperidin-1-yl)ethoxy]phenyl}pyran-2-one	1	1	1	0	<chem>O=C1OC(=CC(=C1c2ccc(OCCN3CCCCC3)cc2)c4ccccc4)c5cccc5</chem>

	4-(4-methoxyphenyl)-6-phenyl-3-{4-[2-(piperidin-1-yl)ethoxy]phenyl}pyran-2-one	1	1	1	0	<chem>COc1ccc(cc1)C2=C(C(=O)OC(=C2)c3ccccc3)c4ccc(OCCN5CCCC5)cc4</chem>
569-57-3	1-[2-chloro-1,2-bis(4-methoxyphenyl)ethenyl]-4-methoxybenzene	1	1	1	0	<chem>COc1ccc(cc1)C(=C(c2ccc(OC)cc2)c3ccc(OC)cc3)Cl</chem>
	3-(4-hydroxyphenyl)-7-propoxychromen-4-one	1	1	1	0	<chem>CCCOc1ccc2C(=O)C(=COc2c1)c3ccc(O)cc3</chem>
	7-butoxy-3-(4-hydroxyphenyl)chromen-4-one	1	1	1	0	<chem>CCCCOc1ccc2C(=O)C(=COc2c1)c3ccc(O)cc3</chem>
126-00-1	diphenolic acid	1	1	1	0	<chem>CC(CCC(=O)O)(c1ccc(O)cc1)c2ccc(O)cc2</chem>
118-55-8	salol	0	1	0	1	<chem>Oc1ccccc1C(=O)Oc2ccccc2</chem>
84-69-5	diisobutyl phthalate	1	1	1	0	<chem>CC(C)COC(=O)c1ccccc1C(=O)OCC(C)C</chem>
192-97-2	benzo(E)pyrene	0	1	0	1	<chem>c1ccc2c(c1)c3cccc4ccc5cccc2c5c34</chem>
15972-60-8	LAZO	0	1	0	1	<chem>CCc1cccc(CC)c1N(COC)C(=O)CCl</chem>
131-16-8	dipropyl phthalate	0	1	0	1	<chem>CCCOC(=O)c1ccccc1C(=O)OCCC</chem>
	CDT	0	1	0	1	<chem>CCNc1nc(Cl)nc(NCC)n1</chem>
	2,2-difluoroethyl (1S,10S,11S,13R)-5,14-dihydroxytetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-13-	1	1	1	0	<chem>OC1C2CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]2C[C@H]1C(=O)OCC(F)F</chem>

	carboxylate					
	2-fluoroethyl (1S,10S,11S,13R,14R)-5,14-dihydroxytetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-13-carboxylate	1	1	1	0	<chem>O[C@@H]1C2CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]2C[C@H]1C(=O)OCCF</chem>
	flavan ethyl (1S,10R,12S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-12-carboxylate	1	1	1	0	<chem>C.CCOC(=O)[C@H]1C[C@H](O)[C@@]2(C)CC[C@H]3[C@@H](CCc4cc(O)ccc34)C12</chem>
	(1S,10S,11S,14S)-tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	<chem>O[C@H]1CC[C@@H]2C1CC[C@H]3[C@H]2CCc4cc(O)ccc34</chem>
	(1S,10R,11S,14S,15S)-4-(3-hydroxypropyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)c(CCCO)cc34)[C@@H]1CC[C@@H]2O</chem>
	ethyl 3-[(1S,10S,11S,14S,15S,17S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-17-yl]propanoate	1	1	1	0	<chem>CCOC(=O)CC[C@H]1C[C@]2(C)[C@@H](O)CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@@H]13</chem>

	(1S,10R,11S,14R,15S)-14-[(Z)-2-bromoethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)\C=C/Br
5444-22-4	(1S,10S,11S,14S,15S,17S)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14,17-triol	1	1	1	0	C[C@]12C[C@H](O)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O
	(1S,10R,11S,14S,15S)-6-(2-hydroxyethyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4c(CCO)c(O)ccc34)[C@@H]1CC[C@@H]2O
6301-88-8	(1S,10R,11S,14S,15S)-6-amino-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4c(N)c(O)ccc34)[C@@H]1CC[C@@H]2O
6298-51-7	2-nitroestradiol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)c(cc34)[N+](=O)[O-])[C@@H]1CC[C@@H]2O
	(1S,10R,11S,14S,15S)-6-(hydroxymethyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4c(CO)c(O)ccc34)[C@@H]1CC[C@@H]2O

(1R,10S,11S,14S,15S,17S)-15-methyl-17-(propoxymethyl)tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	CCOC[C@H]1C[C@]2(C)[C@@H](O)CC[C@H]2[C@@H]3Cc4cc(O)ccc4[C@@H]13
(1S,10S,11S,14S,15S,17R)-17-[2-(2-fluoroethoxy)ethyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	C[C@]12C[C@H](CCOCCF)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O
(1R,10S,11S,14S,15S,17S)-17-(ethoxymethyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	CCOC[C@H]1C[C@]2(C)[C@@H](O)CC[C@H]2[C@@H]3Cc4cc(O)ccc4[C@@H]13
(1S,10S,11S,14S,15S,17R)-17-(2-methoxyethyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	COCC[C@H]1C[C@]2(C)[C@@H](O)CC[C@H]2[C@@H]3Cc4cc(O)ccc4[C@@H]13
(1S,10S,11S,14S,15S,17S)-17-[3-(tert-butoxy)propyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	CC(C)(C)OCCC[C@H]1C[C@]2(C)[C@@H](O)CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@@H]13

(1S,10S,11S,14S,15S,17S)-17-(3-ethoxypropyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	CCOCCC[C@H]1C[C@]2(C)[C@@H](O)CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@@H]13
(1S,10S,11S,14S,15S,17R)-15-methyl-17-(2-propoxyethyl)tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	CCCOCC[C@H]1C[C@]2(C)[C@@H](O)CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@@H]13
(1S,10S,11S,14S,15S,17S)-17-(3-methoxypropyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	COCCC[C@H]1C[C@]2(C)[C@@H](O)CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@@H]13
(1S,10S,11S,14S,15S,17R)-17-(2-isopropoxyethyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	CC(C)OCC[C@H]1C[C@]2(C)[C@@H](O)CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@@H]13
(1S,10S,11S,14S,15S,17S)-17-[3-(2-fluoroethoxy)propyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	C[C@]12C[C@H](CCCOCCF)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O

(1S,10S,11S,14S,15S,17S)-17-butoxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	CCCCO[C@H]1C[C@]2(C)[C@@H](O)CC[C@H]2[C@@H]3Cc4cc(O)ccc4[C@@H]13
(1S,10S,11S,14S,15S,17R)-17-(2-ethoxyethyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	CCOCC[C@H]1C[C@]2(C)[C@@H](O)CC[C@H]2[C@@H]3Cc4cc(O)ccc4[C@@H]13
(1S,10S,11S,14S,15S,17R)-17-[2-(tert-butoxy)ethyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	CC(C)(C)OCC[C@H]1C[C@]2(C)[C@@H](O)CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@@H]13
ethyl (1S,10R,11S,13R,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-13-carboxylate	1	1	1	0	CCOC(=O)[C@@H]1C[C@H]2[C@@H]3CCc4cc(O)ccc4[C@H]3CC[C@]2(C)[C@H]1O
ethyl (1S,9R,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-9-carboxylate	1	1	1	0	CCOC(=O)[C@@H]1Cc2cc(O)ccc2[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4[C@H]13

	ethyl (1S,10S,11S,13R,14R)-5,14-dihydroxytetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-13-carboxylate	1	1	1	0	CCOC(=O)[C@@H]1C[C@@H]2C(CC[C@H]3[C@H]2CCc4cc(O)ccc34)[C@H]1O
	ethyl 2-[(1S,10S,11S,14S,15S,17R)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-17-yl]acetate	1	1	1	0	CCOC(=O)C[C@H]1C[C@]2(C)[C@@H](O)CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@@H]13
	(1S,10R,11S,14S,15S)-6-(3-hydroxypropyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4c(CCCO)c(O)ccc34)[C@@H]1CC[C@@H]2O
6936-94-3	(1S,10R,11S,14S,15S)-15-methyl-6-nitrotetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4c3ccc(O)c4[N+](=O)[O-])[C@@H]1CC[C@@H]2O
2259-89-4	2-hydroxy-3-deoxyestradiol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4ccc(O)cc34)[C@@H]1CC[C@@H]2O
6301-87-7	2-aminoestradiol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)c(N)cc34)[C@@H]1CC[C@@H]2O
	(1R,10S,11S,14S,15S,17S)-17-[(2-fluoroethoxy)methyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-	1	1	1	0	C[C@]12C[C@H](COCCF)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O

	diol					
	(1S,10S,11S,14S,15S,17S)-17-(3-isopropoxypropyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	CC(C)OCCC[C@H]1C[C@]2(C)[C@@H](O)CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@@H]13
	(1R,10S,11S,14S,15S,17S)-17-(butoxymethyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	CCCCOC[C@H]1C[C@]2(C)[C@@H](O)CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@@H]13
	methyl (1S,10S,11S,13R,14R)-5,14-dihydroxytetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-13-carboxylate	1	1	1	0	COC(=O)[C@@H]1C[C@@H]2C(CC[C@H]3[C@H]2CCc4cc(O)ccc34)[C@H]1O
	(1S,10R,11S,14R,15S)-14-[(E)-2-bromoethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)\C=C\Br
	(1S,10R,11S,14S,15S)-4-(2-hydroxyethyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)c(CCO)cc34)[C@@H]1CC[C@@H]2O

	diol					
56-55-3	benz[a]anthracene	1	1	1	0	<chem>c1ccc2cc3c(ccc4ccccc34)cc2c1</chem>
28553-12-0	diisononyl phthalate	1	1	1	0	<chem>CC(C)CCCCCOC(=O)c1ccccc1C(=O)OCCCCC(C)C</chem>
	(3R)-5,7-dihydroxy-3-(4-hydroxyphenyl)-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>Oc1ccc(cc1)[C@@H]1COc2cc(O)cc(O)c2C1=O</chem>
33935-87-4	bisphenol C	1	1	1	0	<chem>Cc1cc(ccc1O)C(C)(C)c1ccc(O)c(C)c1</chem>
	2-[(2R)-butan-2-yl]phenol	0	1	0	1	<chem>CC[C@@H](C)c1ccccc1O</chem>
	4-[(2R)-butan-2-yl]phenol	1	1	1	0	<chem>CC[C@@H](C)c1ccc(O)cc1</chem>
6640-27-3	2-chloro-4-methylphenol	0	1	0	1	<chem>Cc1ccc(O)c(Cl)c1</chem>
74472-48-3	1,2,3,5-tetrachloro-4-(2,4,6-trichlorophenyl)benzene	1	1	1	0	<chem>Clc1cc(Cl)c(c(Cl)c1)-c1c(Cl)cc(Cl)c(Cl)c1Cl</chem>
74487-85-7	1,2,4,5-tetrachloro-3-(2,4,6-trichlorophenyl)benzene	1	1	1	0	<chem>Clc1cc(Cl)c(c(Cl)c1)-c1c(Cl)c(Cl)cc(Cl)c1Cl</chem>
	4-[2,4-bis(4-hydroxyphenyl)-3-methyl-5-propylpyrrol-1-yl]phenol	1	1	1	0	<chem>CCCc1c(c(C)c(-c2ccc(O)cc2)n1-c1ccc(O)cc1)-c1ccc(O)cc1</chem>
	2-fluoro-4-[4-(4-hydroxyphenyl)hexan-3-yl]phenol	1	1	1	0	<chem>CCC(C(CC)c1ccc(O)c(F)c1)c2ccc(O)cc2</chem>
	4-[(2E)-1,1,1,4,4,4-hexafluoro-3-(4-hydroxyphenyl)but-2-en-2-	1	1	1	0	<chem>Oc1ccc(cc1)\C=C(\c2ccc(O)cc2)/C(F)(F)F\C(F)(F)F</chem>

	yl]phenol					
20426-12-4	4-hydroxychalcone	1	1	1	0	<chem>Oc1ccc(\C=C\C(=O)c2ccccc2)cc1</chem>
38239-52-0	4'-hydroxychalcone	1	1	1	0	<chem>Oc1ccc(cc1)C(=O)\C=C\c2ccccc2</chem>
92-86-4	4,4'-dibromobiphenyl	0	1	0	1	<chem>BrC1ccc(cc1)c2ccc(Br)cc2</chem>
491-67-8	baicalein	1	1	1	0	<chem>Oc1cc2OC(=CC(=O)c2c(O)c1O)c3ccccc3</chem>
68-12-2	dimethylformamide	0	1	0	1	<chem>CN(C)C=O</chem>
591-27-5	m-aminophenol	0	1	0	1	<chem>Nc1cccc(O)c1</chem>
	5-hydroxy-2-phenylisoindole-1,3-dione	1	1	1	0	<chem>Oc1ccc2C(=O)N(C(=O)c2c1)c3ccccc3</chem>
	ETU	0	1	0	1	<chem>SC1=NCCN1</chem>
485-63-2	3',4',7-trihydroxyisoflavone	1	1	1	0	<chem>Oc1ccc2C(=O)C(=COc2c1)c3ccc(O)c(O)c3</chem>
57534-13-1	α -hydroquinone	0	1	0	1	<chem>Oc1ccc(O)cc1</chem>
2051-62-9	4-chlorobiphenyl	1	1	1	0	<chem>Clc1ccc(cc1)c2ccccc2</chem>
99-96-7	@P-hydroxybenzoic acid	0	1	0	1	<chem>OC(=O)c1ccc(O)cc1</chem>
81846-81-3	diphenyl	0	1	0	1	<chem>c1ccc(cc1)c2ccccc2</chem>
	colchicine	0	1	0	1	<chem>COC1=CC=C2C(=CC1=O)[C@H](CCc3cc(OC)c(OC)c(OC)c23)NC(=O)C</chem>
	(2S,3R)-2-(4-hydroxyphenyl)-3-{4-	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3[C@@H]2C(=O)c4ccc(OCC</chem>

	[2-(piperidin-1-yl)ethoxy]benzoyl}- 2,3-dihydro-1-benzothiophen-6-ol					N5CCCCC5)cc4
71701-02-5	caffeine	0	1	0	1	CN1C(=O)N(C)c2ncn(C)c2C1=O
68411-45-0	chlorobenzene	0	1	0	1	Clc1ccccc1
98-95-3	nitro-benzene	0	1	0	1	[O-][N+](=O)c1ccccc1
72269-62-6	P-cresol	0	1	0	1	Cc1ccc(O)cc1
	(9R,14R)-14-hydroxy-14-[(E)-2- iodoethenyl]-9,15- dimethyltetracyclo[8.7.0.0{2,7}.0{1 1,15}]heptadec-6-en-5-one	1	1	1	0	C[C@@H]1CC2=CC(=O)CCC2C3CCC4(C)C(CC[C@@]4(O))\C =C\)C13
	(7R,9R)-14-hydroxy-9-iodo-2,15- dimethyltetracyclo[8.7.0.0{2,7}.0{1 1,15}]heptadecan-5-one	1	1	1	0	CC12CCC3C([C@H](I)C[C@H]4CC(=O)CCC34C)C1CCC2O
	(4bR,10bR)-4b,5,6,10b,11,12- hexahydrochrysene-2,8-diol	1	1	1	0	Oc1ccc2[C@@H]3CCc4cc(O)ccc4[C@@H]3CCc2c1
	9-{4-[2- (diethylamino)ethoxy]phenyl}-8- oxa-17- thiatetracyclo[8.7.0.0{2,7}.0{11,16}]heptadeca- 1(10),2,4,6,11(16),12,14-heptaene- 5,14-diol	1	1	1	0	CCN(CC)CCOc1ccc(cc1)C2Oc3cc(O)ccc3c4sc5cc(O)ccc5c24

9-{4-[2-(dimethylamino)ethoxy]phenyl}-8-oxa-17-thiatetracyclo[8.7.0.0{2,7}.0{11,16}]heptadeca-1(10),2,4,6,11(16),12,14-heptaene-5,14-diol	1	1	1	0	CN(C)CCOc1ccc(cc1)C2Oc3cc(O)ccc3c4sc5cc(O)ccc5c24
1-[2-(4-{5,14-dimethoxy-8-oxa-17-thiatetracyclo[8.7.0.0{2,7}.0{11,16}]heptadeca-1(10),2,4,6,11(16),12,14-heptaen-9-yl}phenoxy)ethyl]piperidine	1	1	1	0	COc1ccc2c(OC(c3ccc(OCCN4CCCCC4)cc3)c5c2sc6cc(OC)ccc56)c1
1-[2-(4-{8-oxa-17-thiatetracyclo[8.7.0.0{2,7}.0{11,16}]heptadeca-1(10),2,4,6,11(16),12,14-heptaen-9-yl}phenoxy)ethyl]piperidine	1	1	1	0	C(CN1CCCCC1)Oc2ccc(cc2)C3Oc4cccc4c5sc6cccc6c35
(1R,10S,17S)-17-{4-[2-(piperidin-1-yl)ethoxy]phenyl}tetracyclo[8.7.0.0{2,7}.0{11,16}]heptadeca-2,4,6,11(16),12,14-hexaene-5,14-diol	1	1	1	0	Oc1ccc2[C@@H]3[C@H](CCc2c1)c4ccc(O)cc4[C@@H]3c5ccc(OCCN6CCCCC6)cc5
9-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-8-oxa-17-thiatetracyclo[8.7.0.0{2,7}.0{11,16}]heptadeca-	1	1	1	0	Oc1ccc2c3C(Oc4cccc4c3sc2c1)c5ccc(OCCN6CCCCC6)cc5

	1(10),2,4,6,11(16),12,14-heptaen-14-ol					
	(4bS,5S,10bS)-5-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-4b,5,6,10b,11,12-hexahydrochrysene-2,8-diol	1	1	1	0	Oc1ccc2[C@@H]3[C@H](CCc2c1)c4ccc(O)cc4C[C@@H]3c5ccc(OCCN6CCCCC6)cc5
	5,11-diethyl-4b,5,6,10b,11,12-hexahydrochrysene-2,8-diol	1	1	1	0	CCC1Cc2cc(O)ccc2C3C(CC)Cc4cc(O)ccc4C13
	(6aS,11aS)-3,9-dihydroxy-5H,6H,6aH,11aH-benzo[a]fluoren-11-one	1	1	1	0	Oc1ccc2[C@@H]3[C@H](CCc2c1)c4ccc(O)cc4C3=O
	(6aS,11aS)-5H,6H,6aH,11H,11aH-benzo[a]fluorene-3,9-diol	1	1	1	0	Oc1ccc2[C@H]3Cc4cc(O)ccc4[C@H]3CCc2c1
	(4bS,10bS)-4b,5,6,10b,11,12-hexahydrochrysene-2,8-diol	1	1	1	0	Oc1ccc2[C@H]3CCc4cc(O)ccc4[C@H]3CCc2c1
	9-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}-8-oxa-17-thiatetracyclo[8.7.0.0{2,7}.0{11,16}]heptadeca-1(10),2,4,6,11(16),12,14-heptaene-5,14-diol	1	1	1	0	Oc1ccc2c(OC(c3ccc(OCCN4CCCC4)cc3)c5c2sc6cc(O)ccc56)c1
	9-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-8-oxa-17-thiatetracyclo[8.7.0.0{2,7}.0{11,16}]heptadeca-1(10),2,4,6,11(16),12,14-heptaene-5,14-diol	1	1	1	0	Oc1ccc2c(OC(c3ccc(OCCN4CCCC4)cc3)c5c2sc6cc(O)ccc56)c1

	]heptadeca-1(10),2,4,6,11(16),12,14-heptaene-5,14-diol					
	9-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-8-oxa-17-thiatetracyclo[8.7.0.0{2,7}.0{11,16}]heptadeca-1(10),2,4,6,11(16),12,14-heptaen-5-ol	1	1	1	0	<chem>Oc1ccc2c(OC(c3ccc(OCCN4CCCC4)cc3)c5c2sc6cccc56)c1</chem>
	1-[2-(4-{5,14-dihydroxy-8-oxa-17-thiatetracyclo[8.7.0.0{2,7}.0{11,16}]heptadeca-1(10),2,4,6,11(16),12,14-heptaen-9-yl}phenoxy)ethyl]pyrrolidin-2-one	1	1	1	0	<chem>Oc1ccc2c(OC(c3ccc(OCCN4CCCC4=O)cc3)c5c2sc6cc(O)ccc56)c1</chem>
	9-{4-[2-(morpholin-4-yl)ethoxy]phenyl}-8-oxa-17-thiatetracyclo[8.7.0.0{2,7}.0{11,16}]heptadeca-1(10),2,4,6,11(16),12,14-heptaene-5,14-diol	1	1	1	0	<chem>Oc1ccc2c(OC(c3ccc(OCCN4CCOCC4)cc3)c5c2sc6cc(O)ccc56)c1</chem>
	8-acetyl-3-hydroxy-2-methoxybenzo[c]chromen-6-one	1	1	1	0	<chem>COc1cc2c(OC(=O)c3cc(ccc23)C(=O)C)cc1O</chem>
	8-acetyl-3-methoxybenzo[c]chromen-6-one	1	1	1	0	<chem>COc1ccc2c(OC(=O)c3cc(ccc23)C(=O)C)c1</chem>

	4-[(2R,3S)-3-(4-hydroxyphenyl)pentan-2-yl]phenol	1	1	1	0	<chem>CC[C@@H]([C@@H](C)c1ccc(O)cc1)c2ccc(O)cc2</chem>
37349-32-9	1,2-dihydroxybenzene	0	1	0	1	<chem>Oc1ccccc1O</chem>
50356-26-8	2,4-di-T-butylphenol	1	1	1	0	<chem>CC(C)(C)c1ccc(O)c(c1)C(C)(C)C</chem>
	2-sec-butylphenol	1	1	1	0	<chem>CCC(C)c1ccccc1O</chem>
89-83-8	thymol	0	1	0	1	<chem>CC(C)c1ccc(C)cc1O</chem>
499-75-2	karvakrol	0	1	0	1	<chem>CC(C)c1ccc(C)c(O)c1</chem>
	pronamide	0	1	0	1	<chem>CC(C)(NC(=O)c1cc(Cl)cc(Cl)c1)C#C</chem>
1582-09-8	tristar	0	1	0	1	<chem>CCCN(CCC)c1c(cc(cc1[N+](=O)[O-])C(F)(F)F)[N+](=O)[O-]</chem>
11128-85-1	bois d,arc	1	1	1	0	<chem>OC1=C(Oc2cc(O)cc(O)c2C1=O)c3ccc(O)cc3O</chem>
108-93-0	cyclohexanol	0	1	0	1	<chem>OC1CCCCC1</chem>
528-48-3	viset	1	1	1	0	<chem>OC1=C(Oc2cc(O)ccc2C1=O)c3ccc(O)c(O)c3</chem>
	(2S,3S)-7-hydroxy-3-(4-hydroxyphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-5-propyl-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>CCCC1cc(O)cc2O[C@@H]([C@@H](C(=O)c12)c3ccc(O)cc3)c4ccc(OCCN5CCCCC5)cc4</chem>
	(2S,3S)-7-hydroxy-3-(4-hydroxyphenyl)-5-methyl-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>Cc1cc(O)cc2O[C@@H]([C@@H](C(=O)c12)c3ccc(O)cc3)c4cc(OCCN5CCCCC5)cc4</chem>

(2S,3S)-7-hydroxy-2,3-bis(4-hydroxyphenyl)-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2Oc3cc(O)ccc3C(=O)[C@H]2c4ccc(O)cc4</chem>
(2S,3S)-7-hydroxy-3-isopropyl-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>CC(C)[C@H]1[C@H](Oc2cc(O)ccc2C1=O)c3ccc(OCCN4CCCC4)cc3</chem>
(2S,3R,4Z)-4-(hydroxyimino)-3-(4-hydroxyphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1-benzopyran-7-ol	1	1	1	0	<chem>O\\N=C/1\\[C@H]([C@H](Oc2cc(O)ccc12)c3ccc(OCCN4CCCC4)cc3)c5ccc(O)cc5</chem>
(2S,3R)-7-hydroxy-3-(4-hydroxyphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>Oc1ccc(cc1)[C@@H]2[C@H](Oc3cc(O)ccc3C2=O)c4ccc(OCN5CCCCC5)cc4</chem>
(2S,3S)-7-hydroxy-3-phenyl-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>Oc1ccc2C(=O)[C@H]([C@H](Oc2c1)c3ccc(OCCN4CCCCC4)c3)c5ccccc5</chem>
(2S,3R)-7-hydroxy-3-isopropyl-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>CC(C)[C@@H]1[C@H](Oc2cc(O)ccc2C1=O)c3ccc(OCCN4CCCCC4)cc3</chem>
(2S,3R)-7-hydroxy-3-methyl-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>C[C@@H]1[C@H](Oc2cc(O)ccc2C1=O)c3ccc(OCCN4CCCCC4)cc3</chem>

(2S,3S)-7-hydroxy-3-methyl-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>C[C@H]1[C@H](Oc2cc(O)ccc2C1=O)c3ccc(OCCN4CCCCC4)cc3</chem>
(2S,3S)-7-hydroxy-3-(4-hydroxy-3,5-dimethylphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>Cc1cc(cc(C)c1O)[C@H]2[C@H](Oc3cc(O)ccc3C2=O)c4ccc(OCCN5CCCCC5)cc4</chem>
(2S,3S)-5,7-dihydroxy-3-methyl-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>C[C@H]1[C@H](Oc2cc(O)cc(O)c2C1=O)c3ccc(OCCN4CCCCC4)cc3</chem>
(2S,3S)-3-(4-hydroxyphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2[C@H](Oc3cccc3C2=O)c4ccc(OCCN5CCCCC5)cc4</chem>
(2S,3S)-5-ethyl-7-hydroxy-3-(4-hydroxyphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>CCc1cc(O)cc2O[C@@H]([C@@H](C(=O)c12)c3ccc(O)cc3)c4ccc(OCCN5CCCCC5)cc4</chem>
(2S,3R,4R)-3-(4-hydroxyphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-3,4-dihydro-2H-1-benzopyran-4,7-diol	1	1	1	0	<chem>O[C@@H]1[C@H]([C@H](Oc2cc(O)ccc12)c3ccc(OCCN4CCCCC4)cc3)c5ccc(O)cc5</chem>
(2S,3S)-7-hydroxy-3-(4-hydroxy-3-methoxyphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1-	1	1	1	0	<chem>COc1cc(ccc1O)[C@H]2[C@H](Oc3cc(O)ccc3C2=O)c4ccc(OCCN5CCCCC5)cc4</chem>

	benzopyran-4-one					
	(2S,3S)-7-hydroxy-3-(4-hydroxyphenyl)-5-pentyl-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>CCCCCc1cc(O)cc2O[C@@H]([C@@H](C(=O)c12)c3ccc(O)cc3)c4ccc(OCCN5CCCCC5)cc4</chem>
	(2S,3S)-7-hydroxy-3-(4-hydroxy-2-methoxyphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>COc1cc(O)ccc1[C@H]2[C@H](Oc3cc(O)ccc3C2=O)c4ccc(OCN5CCCCC5)cc4</chem>
	(2S,3S)-5-chloro-7-hydroxy-3-(4-hydroxyphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2[C@H](Oc3cc(O)cc(Cl)c3C2=O)c4ccc(OCN5CCCCC5)cc4</chem>
	(2S,3S)-5-fluoro-7-hydroxy-3-(4-hydroxyphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2[C@H](Oc3cc(O)cc(F)c3C2=O)c4ccc(OCN5CCCCC5)cc4</chem>
537-98-4	ferulic acid	0	1	0	1	<chem>COc1cc(\C=C\C(=O)O)ccc1O</chem>
	7-hydroxy-3-(4-hydroxyphenyl)-2-[(4-hydroxyphenyl)sulfanyl]chromen-4-one	1	1	1	0	<chem>Oc1ccc(SC2=C(C(=O)c3ccc(O)cc3O2)c4ccc(O)cc4)cc1</chem>
	7-hydroxy-2-(4-hydroxyphenoxy)-3-	1	1	1	0	<chem>Oc1ccc(OC2=C(C(=O)c3ccc(O)cc3O2)c4ccc(O)cc4)cc1</chem>

	(4-hydroxyphenyl)chromen-4-one					
	7-hydroxy-3-(4-hydroxyphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenoxy}chromen-4-one	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(Oc3ccc(OCCN4CCCC4)cc3)Oc5cc(O)ccc5C2=O</chem>
	7-hydroxy-3-(4-hydroxyphenyl)-2-({4-[2-(piperidin-1-yl)ethoxy]phenyl}sulfanyl)chromen-4-one	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(Oc3cc(O)ccc3C2=O)Sc4ccc(OCCN5CCCC5)cc4</chem>
122-39-4	diphenylamine	0	1	0	1	<chem>N(c1ccccc1)c2ccccc2</chem>
56-49-5	16-methylpentacyclo[11.6.1.0{2,11}.0{5,10}.0{17,20}]icosa-1(20),2(11),3,5(10),6,8,12,14,16-nonaene	0	1	0	1	<chem>Cc1ccc2cc3c(ccc4cccc34)c5CCc1c25</chem>
	4-[(4-hydroxyphenyl)({1,3,3-trimethylbicyclo[2.2.1]heptan-2-ylidene})methyl]phenol	1	1	1	0	<chem>CC12CCC(C1)C(C)(C)C2=C(c3ccc(O)cc3)c4ccc(O)cc4</chem>
	4-{bicyclo[3.3.1]nonan-9-yl(4-hydroxyphenyl)methyl}phenol	1	1	1	0	<chem>Oc1ccc(cc1)C(C2C3CCCC2CCC3)c4ccc(O)cc4</chem>
	3-{bicyclo[3.3.1]nonan-9-ylidene(4-hydroxyphenyl)methyl}phenol	1	1	1	0	<chem>Oc1ccc(cc1)C(=C2C3CCCC2CCC3)c4cccc(O)c4</chem>
	4-{bicyclo[3.3.1]nonan-9-ylidene(phenyl)methyl}phenol	1	1	1	0	<chem>Oc1ccc(cc1)C(=C2C3CCCC2CCC3)c4ccccc4</chem>

	4-[(4-hydroxyphenyl)({1,7,7-trimethylbicyclo[2.2.1]heptan-2-ylidene})methyl]phenol	1	1	1	0	<chem>CC1(C)C2CCC1(C)C(=C(c3ccc(O)cc3)c4ccc(O)cc4)C2</chem>
	4-{bicyclo[3.3.1]nonan-9-ylidene(4-hydroxyphenyl)methyl}benzene-1,2-diol	1	1	1	0	<chem>Oc1ccc(cc1)C(=C2C3CCCC2CCC3)c4ccc(O)c(O)c4</chem>
	4-{bicyclo[3.3.1]nonan-9-ylidene(4-fluorophenyl)methyl}phenol	1	1	1	0	<chem>Oc1ccc(cc1)C(=C2C3CCCC2CCC3)c4ccc(F)cc4</chem>
	4-[cyclohexyl(4-hydroxyphenyl)methyl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)C(C2CCCCC2)c3ccc(O)cc3</chem>
	4-[(4-hydroxyphenyl)[(1R,6R,8S)-2,2,6,7,7-pentamethyltricyclo[6.2.1.0{1,6}]undecan-4-ylidene]methyl]phenol	1	1	1	0	<chem>CC1(C)CC(=C(c2ccc(O)cc2)c3ccc(O)cc3)C[C@]4(C)C(C)(C)[C@H]5CC[C@@]14C5</chem>
	4-[(4-hydroxyphenyl)(tricyclo[5.2.1.0{2,6}]decan-8-ylidene)methyl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)C(=C2CC3CC2C4CCCC34)c5ccc(O)cc5</chem>
	4-{bicyclo[2.2.1]heptan-2-ylidene(4-hydroxyphenyl)methyl}phenol	1	1	1	0	<chem>Oc1ccc(cc1)C(=C2CC3CCC2C3)c4ccc(O)cc4</chem>
	4-[adamantan-2-ylidene(4-hydroxyphenyl)methyl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)C(=C2C3CC4CC(CC2C4)C3)c5ccc(O)cc5</chem>
	2-[(4-hydroxyphenyl)methyl]-3-{4-	1	1	1	0	<chem>Oc1ccc(Cc2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4)c</chem>

	[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol					c1
	[4-(6-methoxy-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-2-yl)phenyl]methanol	1	1	1	0	COc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(CO)cc5
	2-{4-[(ethylsulfanyl)methyl]phenyl}-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	CCSCc1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4
	3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-2-(pyridin-4-yl)-1-benzothiophen-6-ol	1	1	1	0	Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccncc5
	4-(6-hydroxy-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-2-yl)pyridin-1-ium-1-olate	1	1	1	0	Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5cc[n+](O-)]cc5
	3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-2-[4-(trifluoromethyl)phenyl]-1-benzothiophen-6-ol	1	1	1	0	Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(cc5)C(F)(F)F
	2-(4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophene-5,6-diol	1	1	1	0	Oc1ccc(cc1)c2sc3cc(O)c(O)cc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4

	2-(4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-7-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2sc3c(O)cccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>
	2-(4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-4-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2sc3cccc(O)c3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>
63697-18-7	1,2, 4-trichlorobenzene	0	1	0	1	<chem>Clc1ccc(Cl)c(Cl)c1</chem>
	1-(2-{4-[2-(2H-1,3-benzodioxol-5-yl)-6-methoxy-1-benzothiophene-3-carbonyl]phenoxy}ethyl)piperidine	1	1	1	0	<chem>COc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc6OCOc6c5</chem>
	2-(4-nitrophenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(cc5)[N+](=O)[O-]</chem>
	3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-2-(thiophen-3-yl)-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccsc5</chem>
	3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-2-(thiophen-2-yl)-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5cccs5</chem>
	4-(6-hydroxy-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-2-yl)-N-methylbenzamide; trifluoroacetic	1	1	1	0	<chem>CNC(=O)c1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4.OC(=O)C(F)(F)F</chem>

	acid					
	2-(4-phenylphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(cc5)c6ccccc6</chem>
	5-fluoro-2-(4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2sc3cc(O)c(F)cc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>
	2-(4-hydroxyphenyl)-5,7-dimethyl-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>Cc1cc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c(C)c1O)c5cc(O)c5</chem>
	2-(4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophene-4,6-diol	1	1	1	0	<chem>Oc1ccc(cc1)c2sc3cc(O)cc(O)c3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>
	2-(4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2sc3ccc(O)cc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>
	2-(3-fluorophenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5cccc(F)c5</chem>
	2-(2-methylphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>Cc1ccccc1c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>

	2-(3-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1cccc(c1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>
	2-(4-ethylphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>CCc1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>
	2-(2-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5cccc5O</chem>
	1-{2-[4-(6-methoxy-2-phenyl-1-benzothiophene-3-carbonyl)phenoxy]ethyl}piperidine	1	1	1	0	<chem>COc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5cccc5</chem>
	2-(4-hydroxyphenyl)-1-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}naphtho[2,1-b]thiophen-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2sc3cc(O)c4ccccc4c3c2C(=O)c5ccc(OCCN6CCCCC6)cc5</chem>
	2-(4-isopropylphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>CC(C)c1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>
95-50-1	o-dichlorobenzene	0	1	0	1	<chem>Clc1ccccc1Cl</chem>
	2-(4-hydroxy-3,5-dimethylphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-	1	1	1	0	<chem>Cc1cc(cc(C)c1O)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>

	benzothiophen-6-ol					
	2-(4-hydroxyphenyl)-4,7-dimethyl-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>Cc1cc(O)c(C)c2sc(c3ccc(O)cc3)c(C(=O)c4ccc(OCCN5CCCCC5)cc4)c12</chem>
	2-(4-hydroxy-2-methylphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>Cc1cc(O)ccc1c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>
	2-(3-fluoro-4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(O)c(F)c5</chem>
	2-(3-chloro-4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(O)c(Cl)c5</chem>
	2-(4-methoxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>COc1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>
	2-(4-hydroxy-2-methoxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>COc1cc(O)ccc1c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>
	2-(naphthalen-2-yl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-	1	1	1	0	<chem>Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc6ccccc6c5</chem>

	benzothiophen-6-ol					
	2-(naphthalen-1-yl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc2c(C(=O)c3ccc(OCCN4CCCC4)cc3)c(sc2c1)c5cccc6cccc56</chem>
	2-(4-hydroxy-3-methylphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>Cc1cc(ccc1O)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCC5)c4</chem>
	2-(4-hydroxynaphthalen-1-yl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc2c(C(=O)c3ccc(OCCN4CCCC4)cc3)c(sc2c1)c5ccc(O)c6cccc56</chem>
	4-(6-methoxy-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-2-yl)phenol	1	1	1	0	<chem>COc1ccc2c(C(=O)c3ccc(OCCN4CCCC4)cc3)c(sc2c1)c5ccc(O)cc5</chem>
	1-(4-chlorophenyl)-3-(2,6-difluorobenzoyl)urea	0	1	0	1	<chem>Fc1cccc(F)c1C(=O)NC(=O)Nc2ccc(Cl)cc2</chem>
109640-20-2	(2-{4-[(1R,2R)-1,2-diphenylbutyl]phenoxy}ethyl)dimethylamine	1	1	1	0	<chem>CC[C@H]([C@H](c1cccc1)c2ccc(OCCN(C)C)cc2)c3cccc3</chem>
68684-63-9	4-[(1E)-1,2-diphenylbut-1-en-1-yl]phenol	1	1	1	0	<chem>CC\C/C(=C(\c1cccc1)/c2ccc(O)cc2)\c3cccc3</chem>
	(2-{4-[(1S,2S)-1,2-diphenylbutyl]phenoxy}ethyl)dimethylamine	1	1	1	0	<chem>CC[C@@H]([C@@H](c1cccc1)c2ccc(OCCN(C)C)cc2)c3cccc3</chem>

	1-nitro-4-[(4,6,6-trimethyl-2-methylidenecyclohex-3-en-1-yl)methyl]benzene	1	1	1	0	<chem>CC1=CC(=C)C(Cc2ccc(cc2)[N+](=O)[O-])C(C)(C)C1</chem>
	5-bromo-2-[[[(1R)-2,2-dimethyl-6-methylidenecyclohexyl)methyl]-4-methoxyphenol	1	1	1	0	<chem>COc1cc(C[C@H]2C(=C)CCCC2(C)C)c(O)cc1Br</chem>
	4-[(1R,5R)-5-(hydroxymethyl)-8-methyl-3-oxabicyclo[3.3.1]non-7-en-2-yl]phenol	1	1	1	0	<chem>CC1=CC[C@@]2(CO)COC([C@@H]1C2)c3ccc(O)cc3</chem>
	4-[(1R,2R,5S)-5-(hydroxymethyl)bicyclo[3.3.1]non-7-en-2-yl]phenol	1	1	1	0	<chem>OC[C@]12CC[C@H]([C@H](C1)C=CC2)c3ccc(O)cc3</chem>
106-41-2	4-bromophenol	0	1	0	1	<chem>Oc1ccc(Br)cc1</chem>
100-00-5	p-chloronitrobenzene	0	1	0	1	<chem>[O-][N+](=O)c1ccc(Cl)cc1</chem>
	4-{6-[methyl(2-phenylethyl)amino]-4-phenylpyridin-2-yl}phenol	1	1	1	0	<chem>CN(CCC1CCCCC1)c2cc(cc(n2)c3ccc(O)cc3)c4CCCCC4</chem>
	2-methyl-4-{6-[methyl(2-phenylethyl)amino]-4-phenylpyridin-2-yl}phenol	1	1	1	0	<chem>CN(CCC1CCCCC1)c2cc(cc(n2)c3ccc(O)c(C)c3)c4CCCCC4</chem>
	4-[6-(4-benzylpiperidin-1-yl)-4-phenylpyridin-2-yl]-2-methylphenol	1	1	1	0	<chem>Cc1cc(ccc1O)c2cc(cc(n2)N3CCC(Cc4CCCCC4)CC3)c5CCCCC5</chem>
	4-{6-[bis(2-ethoxyethyl)amino]-4-	1	1	1	0	<chem>CCOCCN(CCOCC)c1cc(cc(n1)c2ccc(O)c(C)c2)c3CCCCC3</chem>

	phenylpyridin-2-yl}-2-methylphenol					
	4-{4-phenyl-6-[propyl(pyridin-2-ylmethyl)amino]pyridin-2-yl}phenol	1	1	1	0	CCCN(Cc1cccn1)c2cc(cc(n2)c3ccc(O)cc3)c4cccc4
	2-methyl-4-[4-phenyl-6-(pyrrolidin-1-yl)pyridin-2-yl]phenol	0	1	0	1	Cc1cc(ccc1O)c2cc(cc(n2)N3CCCC3)c4cccc4
	2-methyl-4-{6-[methyl(2-methylpropyl)amino]-4-phenylpyridin-2-yl}phenol	1	1	1	0	CC(C)CN(C)c1cc(cc(n1)c2ccc(O)c(C)c2)c3cccc3
	2-methyl-4-{6-[methyl(naphthalen-1-ylmethyl)amino]-4-phenylpyridin-2-yl}phenol	1	1	1	0	CN(Cc1cccc2cccc12)c3cc(cc(n3)c4ccc(O)c(C)c4)c5cccc5
	4-{6-[methyl(2-phenylethyl)amino]-4-(2-methylphenyl)pyridin-2-yl}phenol	1	1	1	0	CN(CCc1cccc1)c2cc(cc(n2)c3ccc(O)cc3)c4cccc4C
	4-[4-(4-hydroxyphenyl)-6-[methyl(2-phenylethyl)amino]pyridin-2-yl]phenol	1	1	1	0	CN(CCc1cccc1)c2cc(cc(n2)c3ccc(O)cc3)c4ccc(O)cc4
	4-{6-[benzyl(2-phenylethyl)amino]-4-phenylpyridin-2-yl}-2-methylphenol	1	1	1	0	Cc1cc(ccc1O)c2cc(cc(n2)N(CCc3cccc3)Cc4cccc4)c5cccc5
	4-{6-[ethyl(pyridin-4-ylmethyl)amino]-4-phenylpyridin-2-	1	1	1	0	CCN(Cc1ccncc1)c2cc(cc(n2)c3ccc(O)c(C)c3)c4cccc4

	yl}-2-methylphenol					
	3-methyl-4-{4-phenyl-6-[propyl(pyridin-2-ylmethyl)amino]pyridin-2-yl}phenol	0	1	0	1	<chem>CCCN(Cc1cccn1)c2cc(cc(n2)c3ccc(O)cc3C)c4ccccc4</chem>
	4-{6-[butyl(methyl)amino]-4-phenylpyridin-2-yl}-2-methylphenol	1	1	1	0	<chem>CCCCN(C)c1cc(cc(n1)c2ccc(O)c(C)c2)c3ccccc3</chem>
	4-(6-{[2-(dimethylamino)ethyl](methyl)amino}-4-phenylpyridin-2-yl)-2-methylphenol	0	1	0	1	<chem>CN(C)CCN(C)c1cc(cc(n1)c2ccc(O)c(C)c2)c3ccccc3</chem>
	4-{6-[benzyl(methyl)amino]-4-phenylpyridin-2-yl}-2-methylphenol	1	1	1	0	<chem>CN(Cc1ccccc1)c2cc(cc(n2)c3ccc(O)c(C)c3)c4ccccc4</chem>
	4-{6-[methyl(2-methylpropyl)amino]-4-phenylpyridin-2-yl}phenol	1	1	1	0	<chem>CC(C)CN(C)c1cc(cc(n1)c2ccc(O)cc2)c3ccccc3</chem>
	2-methyl-4-{4-phenyl-6-[propyl(pyridin-2-ylmethyl)amino]pyridin-2-yl}phenol	1	1	1	0	<chem>CCCN(Cc1cccn1)c2cc(cc(n2)c3ccc(O)c(C)c3)c4ccccc4</chem>
	2-methyl-4-(6-{methyl[2-(pyridin-2-yl)ethyl]amino}-4-phenylpyridin-2-yl)phenol	1	1	1	0	<chem>CN(CCc1cccn1)c2cc(cc(n2)c3ccc(O)c(C)c3)c4ccccc4</chem>
529-44-2	myricetin	1	1	1	0	<chem>OC1=C(Oc2cc(O)cc(O)c2C1=O)c3cc(O)c(O)c(O)c3</chem>

7400-08-0	para-coumaric acid	0	1	0	1	<chem>OC(=O)\C=C\c1ccc(O)cc1</chem>
	(2R,3S)-6-hydroxy-3-(4-hydroxyphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1,4-benzoxathiine-4,4-dione	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2[C@H](Oc3ccc(O)cc3S2(=O)=O)c4ccc(OCCN5CCCCC5)cc4</chem>
	4-[(2R,3S)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1,4-benzoxathiin-3-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)[C@@H]2Sc3cccc3O[C@@H]2c4ccc(OCCN5CCCCC5)cc4</chem>
	(2R,3S)-6-hydroxy-3-(4-hydroxyphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1,4-benzoxathiin-4-ium-4-olate	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2[C@H](Oc3ccc(O)cc3[S+](O-))c4ccc(OCCN5CCCCC5)cc4</chem>
	(2R,3S)-3-phenyl-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>Oc1ccc2O[C@@H]([C@@H](Sc2c1)c3cccc3)c4ccc(OCCN5CCCCC5)cc4</chem>
	carbendazim	0	1	0	1	<chem>COC(=O)Nc1nc2cccc2[nH]1</chem>
70-70-2	POP	0	1	0	1	<chem>CCC(=O)c1ccc(O)cc1</chem>
	(2R,5S,14S,15S)-2,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-7-ene-5,14-diol	1	1	1	0	<chem>C[C@]12CCC3C(CC=C4C[C@@H](O)CC[C@]34C)C1CC[C@@H]2O</chem>
88-06-2	2,4,6-trichlorophenol	0	1	0	1	<chem>Oc1c(Cl)cc(Cl)cc1Cl</chem>

15-bromo-6,13-dihydroxy-9,17-dioxatetracyclo[8.7.0.0{3,8}.0{11,16}]heptadeca-1(10),3(8),4,6,11(16),12,14-heptaen-2-one	1	1	1	0	<chem>Oc1ccc2C(=O)c3oc4c(Br)cc(O)cc4c3Oc2c1</chem>
6-hydroxy-9-oxa-17-thiatetracyclo[8.7.0.0{3,8}.0{11,16}]heptadeca-1(10),3(8),4,6,11(16),12,14-heptaen-2-one	1	1	1	0	<chem>Oc1ccc2C(=O)c3sc4cccc4c3Oc2c1</chem>
4,6-dihydroxy-9-oxa-17-thiatetracyclo[8.7.0.0{3,8}.0{11,16}]heptadeca-1(10),3(8),4,6,11(16),12,14-heptaen-2-one	1	1	1	0	<chem>Oc1cc(O)c2C(=O)c3sc4cccc4c3Oc2c1</chem>
4,6,13-trihydroxy-9,17-dioxatetracyclo[8.7.0.0{3,8}.0{11,16}]heptadeca-1(10),3,5,7,11(16),12,14-heptaen-2-one	1	1	1	0	<chem>Oc1ccc2oc3C(=O)c4c(O)cc(O)cc4Oc3c2c1</chem>
7,14-dihydroxy-5-methoxy-2,17-dioxatetracyclo[8.7.0.0{3,8}.0{11,16}]heptadeca-1(10),3,5,7,11(16),12,14-heptaen-9-one	1	1	1	0	<chem>COc1cc(O)c2C(=O)c3c(Oc2c1)oc4cc(O)ccc34</chem>

15-bromo-4,6,13-trihydroxy-9,17-dioxatetracyclo[8.7.0.0{3,8}.0{11,16}]heptadeca-1(10),3(8),4,6,11(16),12,14-heptaen-2-one	1	1	1	0	<chem>Oc1cc(O)c2C(=O)c3oc4c(Br)cc(O)cc4c3Oc2c1</chem>
5,13-dihydroxy-9,17-dioxatetracyclo[8.7.0.0{3,8}.0{11,16}]heptadeca-1(10),3(8),4,6,11(16),12,14-heptaen-2-one	1	1	1	0	<chem>Oc1ccc2Oc3c(oc4ccc(O)cc34)C(=O)c2c1</chem>
14-hydroxy-9,17-dioxatetracyclo[8.7.0.0{3,8}.0{11,16}]heptadeca-1(10),3(8),4,6,11(16),12,14-heptaen-2-one	1	1	1	0	<chem>Oc1ccc2c3Oc4cccc4C(=O)c3oc2c1</chem>
6-hydroxy-9,17-dioxatetracyclo[8.7.0.0{3,8}.0{11,16}]heptadeca-1(10),3(8),4,6,11(16),12,14-heptaen-2-one	1	1	1	0	<chem>Oc1ccc2C(=O)c3oc4cccc4c3Oc2c1</chem>
4,6,13-trihydroxy-2-oxo-9,17-dioxatetracyclo[8.7.0.0{3,8}.0{11,16}]heptadeca-1(10),3(8),4,6,11(16),12,14-heptaene-15-carbonitrile	1	1	1	0	<chem>Oc1cc(O)c2C(=O)c3oc4c(cc(O)cc4c3Oc2c1)C#N</chem>

6,13-dihydroxy-2-oxo-9,17-dioxatetracyclo[8.7.0.0{3,8}.0{11,16}]heptadeca-1(10),3(8),4,6,11(16),12,14-heptaene-15-carbonitrile	1	1	1	0	<chem>Oc1ccc2C(=O)c3oc4c(cc(O)cc4c3Oc2c1)C#N</chem>
4,6-dihydroxy-9,17-dioxatetracyclo[8.7.0.0{3,8}.0{11,16}]heptadeca-1(10),3(8),4,6,11(16),12,14-heptaen-2-one	1	1	1	0	<chem>Oc1cc(O)c2C(=O)c3oc4cccc4c3Oc2c1</chem>
4,6,14-trihydroxy-9,17-dioxatetracyclo[8.7.0.0{3,8}.0{11,16}]heptadeca-1(10),3(8),4,6,11(16),12,14-heptaen-2-one	1	1	1	0	<chem>Oc1ccc2c3Oc4cc(O)cc(O)c4C(=O)c3oc2c1</chem>
6,13-dihydroxy-9,17-dioxatetracyclo[8.7.0.0{3,8}.0{11,16}]heptadeca-1(10),3(8),4,6,11(16),12,14-heptaen-2-one	1	1	1	0	<chem>Oc1ccc2C(=O)c3oc4ccc(O)cc4c3Oc2c1</chem>
6,14-dihydroxy-9,17-dioxatetracyclo[8.7.0.0{3,8}.0{11,16}]heptadeca-1(10),3(8),4,6,11(16),12,14-heptaen-2-one	1	1	1	0	<chem>Oc1ccc2C(=O)c3oc4cc(O)ccc4c3Oc2c1</chem>

	5,14-dihydroxy-9,17-dioxatetracyclo[8.7.0.0{3,8}.0{11,16}]heptadeca-1(10),3(8),4,6,11(16),12,14-heptaen-2-one	1	1	1	0	<chem>Oc1ccc2Oc3c(oc4cc(O)ccc34)C(=O)c2c1</chem>
	temik 10 G	0	1	0	1	<chem>CNC(=O)O\N=C\C(C)(C)SC</chem>
119-61-9	benzophenone	0	1	0	1	<chem>O=C(c1ccccc1)c2ccccc2</chem>
	2-benzoyl-3-phenyl-1-benzofuran-6-ol	1	1	1	0	<chem>Oc1ccc2c(c3ccccc3)c(oc2c1)C(=O)c4ccccc4</chem>
	2-(2-chlorobenzoyl)-3-phenyl-1-benzofuran-6-ol	1	1	1	0	<chem>Oc1ccc2c(c3ccccc3)c(oc2c1)C(=O)c4ccccc4Cl</chem>
	3-(naphthalen-1-yl)-2-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzofuran-6-ol	1	1	1	0	<chem>Oc1ccc2c(c(oc2c1)C(=O)c3ccc(OCCN4CCCC4)cc3)c5cccc6ccccc56</chem>
	2-(2,4-dimethylbenzoyl)-3-phenyl-1-benzofuran-6-ol	1	1	1	0	<chem>Cc1ccc(C(=O)c2oc3cc(O)ccc3c2c4ccccc4)c(C)c1</chem>
	2-(2,4-dimethylbenzoyl)-3-(naphthalen-1-yl)-1-benzofuran-6-ol	1	1	1	0	<chem>Cc1ccc(C(=O)c2oc3cc(O)ccc3c2c4cccc5ccccc45)c(C)c1</chem>
	3-(naphthalen-1-yl)-2-{3-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzofuran-6-ol	1	1	1	0	<chem>Oc1ccc2c(c(oc2c1)C(=O)c3cccc(OCCN4CCCC4)c3)c5cccc6ccccc56</chem>

	2-(2-chlorobenzoyl)-3-pentyl-1-benzofuran-6-ol	1	1	1	0	CCCCCc1c(oc2cc(O)ccc12)C(=O)c3cccc3Cl
	3-(naphthalen-1-yl)-2-(4-phenylbenzoyl)-1-benzofuran-6-ol	1	1	1	0	Oc1ccc2c(c(oc2c1)C(=O)c3ccc(cc3)c4cccc4)c5cccc6cccc56
	2-(3,4-dihydro-2H-1,5-benzodioxepine-7-carbonyl)-3-(naphthalen-1-yl)-1-benzofuran-6-ol	1	1	1	0	Oc1ccc2c(c(oc2c1)C(=O)c3ccc4OCCCOc4c3)c5cccc6cccc56
	2-(4-bromobenzoyl)-3-(naphthalen-1-yl)-1-benzofuran-6-ol	1	1	1	0	Oc1ccc2c(c(oc2c1)C(=O)c3ccc(Br)cc3)c4cccc5cccc45
	2-(2,4-dimethylbenzoyl)-3-[(2-methoxyphenyl)methyl]-1-benzofuran-6-ol	1	1	1	0	COc1cccc1Cc2c(oc3cc(O)ccc23)C(=O)c4ccc(C)cc4C
	2-[4-(difluoromethoxy)benzoyl]-3-(naphthalen-1-yl)-1-benzofuran-6-ol	1	1	1	0	Oc1ccc2c(c(oc2c1)C(=O)c3ccc(OC(F)F)cc3)c4cccc5cccc45
	2-(2,3-dihydro-1,4-benzodioxine-6-carbonyl)-3-(naphthalen-1-yl)-1-benzofuran-6-ol	1	1	1	0	Oc1ccc2c(c(oc2c1)C(=O)c3ccc4OCCOc4c3)c5cccc6cccc56
	2-(2-chlorobenzoyl)-3-[(2-methoxyphenyl)methyl]-1-benzofuran-6-ol	1	1	1	0	COc1cccc1Cc2c(oc3cc(O)ccc23)C(=O)c4cccc4Cl
90-00-6	2-ethylphenol	0	1	0	1	CCc1cccc1O

119-36-8	methyl salicylate	0	1	0	1	<chem>COC(=O)c1ccccc1O</chem>
25167-80-0	2-chlorophenol	0	1	0	1	<chem>Oc1ccccc1Cl</chem>
95-95-4	2,4,5-trichlorophenol	0	1	0	1	<chem>Oc1cc(Cl)c(Cl)cc1Cl</chem>
120-83-2	2,4-dichlorophenol	0	1	0	1	<chem>Oc1ccc(Cl)cc1Cl</chem>
39660-70-3	dibenzyl	0	1	0	1	<chem>C(Cc1ccccc1)c2ccccc2</chem>
	rokon	1	1	1	0	<chem>Sc1nc2ccccc2s1</chem>
	7-hydroxy-3-phenyl-4-{3-[4-(piperidin-1-yl)butoxy]phenyl}chromen-2-one	1	1	1	0	<chem>Oc1ccc2C(=C(C(=O)Oc2c1)c3ccccc3)c4ccc(OCCCCN5CCCCC5)cc4</chem>
	7-hydroxy-3-phenyl-4-(4-{[5-(piperidin-1-yl)pentyl]oxy}phenyl)chromen-2-one	1	1	1	0	<chem>Oc1ccc2C(=C(C(=O)Oc2c1)c3ccccc3)c4ccc(OCCCCCN5CCCCC5)cc4</chem>
	7-hydroxy-3-phenyl-4-{4-[2-(piperidin-1-yl)ethoxy]phenyl}chromen-2-one	1	1	1	0	<chem>Oc1ccc2C(=C(C(=O)Oc2c1)c3ccccc3)c4ccc(OCCN5CCCCC5)cc4</chem>
	7-hydroxy-3-phenyl-4-{4-[4-(piperidin-1-yl)butoxy]phenyl}chromen-2-one	1	1	1	0	<chem>Oc1ccc2C(=C(C(=O)Oc2c1)c3ccccc3)c4ccc(OCCCCN5CCCCC5)cc4</chem>
	7-hydroxy-3-phenyl-4-(4-{[6-(piperidin-1-	1	1	1	0	<chem>Oc1ccc2C(=C(C(=O)Oc2c1)c3ccccc3)c4ccc(OCCCCCN5CCCCC5)cc4</chem>

	yl)hexyl]oxy}phenyl)chromen-2-one					
	7-hydroxy-3-phenyl-4-{4-[3-(piperidin-1-yl)propoxy]phenyl}chromen-2-one	1	1	1	0	<chem>Oc1ccc2C(=C(C(=O)Oc2c1)c3ccccc3)c4ccc(OCCCN5CCCCC5)cc4</chem>
	7-hydroxy-3-phenyl-4-(3-{[5-(piperidin-1-yl)pentyl]oxy}phenyl)chromen-2-one	1	1	1	0	<chem>Oc1ccc2C(=C(C(=O)Oc2c1)c3ccccc3)c4ccc(OCCCCN5CCCCC5)c4</chem>
	7-hydroxy-3-phenyl-4-{3-[2-(piperidin-1-yl)ethoxy]phenyl}chromen-2-one	1	1	1	0	<chem>Oc1ccc2C(=C(C(=O)Oc2c1)c3ccccc3)c4ccc(OCCN5CCCCC5)c4</chem>
	7-hydroxy-3-phenyl-4-({4-[4-(piperidin-1-yl)butoxy]phenyl}methyl)chromen-2-one	1	1	1	0	<chem>Oc1ccc2C(=C(C(=O)Oc2c1)c3ccccc3)Cc4ccc(OCCCN5CCCCC5)cc4</chem>
	7-hydroxy-3-phenyl-4-({4-[2-(piperidin-1-yl)ethoxy]phenyl}methyl)chromen-2-one	1	1	1	0	<chem>Oc1ccc2C(=C(C(=O)Oc2c1)c3ccccc3)Cc4ccc(OCCN5CCCCC5)cc4</chem>
	7-hydroxy-3-phenyl-4-({4-[3-(piperidin-1-yl)propoxy]phenyl}methyl)chromen-2-one	1	1	1	0	<chem>Oc1ccc2C(=C(C(=O)Oc2c1)c3ccccc3)Cc4ccc(OCCCN5CCCCC5)cc4</chem>

15797-52-1	4-[3,5-bis(4-hydroxyphenyl)phenyl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2cc(cc(c2)c3ccc(O)cc3)c4ccc(O)cc4</chem>
	7-hydroxy-3-phenyl-4-{3-[3-(piperidin-1-yl)propoxy]phenyl}chromen-2-one	1	1	1	0	<chem>Oc1ccc2C(=C(C(=O)Oc2c1)c3ccccc3)c4cccc(OCCCN5CCCCC5)c4</chem>
57-85-2	testosterone propionate	0	1	0	1	<chem>CCC(=O)O[C@H]1CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>
127-18-4	PERK	0	1	0	1	<chem>ClC(=C(Cl)Cl)Cl</chem>
137-26-8	tulisan	1	1	1	0	<chem>CN(C)C(=S)SSC(=S)N(C)C</chem>
1423-97-8	(11S,14S,15S)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-1(10),2,4,6,8-pentaene-5,14-diol	1	1	1	0	<chem>C[C@]12CCc3c(ccc4cc(O)ccc34)[C@@H]1CC[C@@H]2O</chem>
	β-dihydroequilin	1	1	1	0	<chem>C[C@]12CC[C@H]3C(=CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O</chem>
	(1S,10S,11S,14S,15S)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6,8-tetraene-5,14-diol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@H](C=Cc4cc(O)ccc34)[C@@H]1CC[C@@H]2O</chem>
	(1S,2S,5S,7S,10S,11S,14S,15S)-2,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadecane-5,14-diol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@H](CC[C@H]4C[C@@H](O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>

	(1S,2R,5S,10S,11S,14S,15S)-2,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-7-ene-5,14-diol	1	1	1	0	C[C@]12CC[C@H]3[C@H](CC=C4C[C@@H](O)CC[C@]34C)[C@@H]1CC[C@@H]2O
	(1S,2S,5R,7S,10S,11S,14S,15S)-2,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadecane-5,14-diol	1	1	1	0	C[C@]12CC[C@H]3[C@H](CC[C@H]4C[C@H](O)CC[C@]34C)[C@@H]1CC[C@@H]2O
	(10R,11S,14S,15S)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-1(17),2,4,6-tetraene-5,14-diol	1	1	1	0	C[C@]12CC=C3[C@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O
90-15-3	naphthol	0	1	0	1	Oc1cccc2ccccc12
	(2S,3R)-3-(4-hydroxyphenyl)-2-[4-(piperidin-1-ylmethyl)phenyl]-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(CN5CCCCC5)cc4
835-11-0	2-(2-hydroxybenzoyl)phenol	0	1	0	1	Oc1ccccc1C(=O)c2ccccc2O
961-29-5	isoliquiritigenin	1	1	1	0	Oc1ccc(\C=C\C(=O)c2ccc(O)cc2O)cc1
	2-(4-hydroxyphenyl)-3-phenylpropanenitrile	1	1	1	0	Oc1ccc(cc1)C(Cc2ccccc2)C#N
	2,3-bis(3-hydroxyphenyl)propanenitrile	1	1	1	0	Oc1cccc(CC(C#N)c2cccc(O)c2)c1
	2-(3-hydroxyphenyl)-3-(4-	1	1	1	0	Oc1ccc(CC(C#N)c2cccc(O)c2)cc1

	hydroxyphenyl)propanenitrile					
	3-(3-hydroxyphenyl)-2-(4-hydroxyphenyl)propanenitrile	1	1	1	0	<chem>Oc1ccc(cc1)C(Cc2cccc(O)c2)C#N</chem>
	N,N-diethyl-2,3-bis(4-hydroxyphenyl)propanamide	1	1	1	0	<chem>CCN(CC)C(=O)C(Cc1ccc(O)cc1)c2ccc(O)cc2</chem>
	2,3-bis(4-hydroxyphenyl)-N-propylpropanamide	1	1	1	0	<chem>CCCNC(=O)C(Cc1ccc(O)cc1)c2ccc(O)cc2</chem>
	3-(4-hydroxyphenyl)-2-phenylpropanenitrile	1	1	1	0	<chem>Oc1ccc(CC(C#N)c2ccccc2)cc1</chem>
	4-[1-hydroxy-3-(4-hydroxyphenyl)propan-2-yl]phenol	1	1	1	0	<chem>OCC(Cc1ccc(O)cc1)c2ccc(O)cc2</chem>
	2,3-bis(4-hydroxyphenyl)propanoic acid	1	1	1	0	<chem>OC(=O)C(Cc1ccc(O)cc1)c2ccc(O)cc2</chem>
	2,3-bis(3-hydroxyphenyl)butanedinitrile	1	1	1	0	<chem>Oc1cccc(c1)C(C#N)C(C#N)c2cccc(O)c2</chem>
	2-(adamantan-1-yl)-4-oxo-2,3-dihydro-1-benzopyran-6-yl sulfamate	1	1	1	0	<chem>NS(=O)(=O)Oc1ccc2OC(CC(=O)c2c1)C34CC5CC(CC(C5)C3)C4</chem>
	2-(2-methyldecan-2-yl)-4-oxochromen-6-yl sulfamate	1	1	1	0	<chem>CCCCCCCCC(C)(C)C1=CC(=O)c2cc(OS(=O)(=O)N)ccc2O1</chem>
	2-nonyl-4-oxochromen-6-yl	1	1	1	0	<chem>CCCCCCCCCCC1=CC(=O)c2cc(OS(=O)(=O)N)ccc2O1</chem>

	sulfamate					
	4-oxo-2-(2-phenylethyl)chromen-6-yl sulfamate	1	1	1	0	<chem>NS(=O)(=O)Oc1ccc2OC(=CC(=O)c2c1)CCc3ccccc3</chem>
	2-(adamantan-1-yl)-4-oxothiochromen-6-yl sulfamate	1	1	1	0	<chem>NS(=O)(=O)Oc1ccc2SC(=CC(=O)c2c1)C34CC5CC(CC(C5)C3)C4</chem>
	2-cyclododecyl-4-oxochromen-6-yl sulfamate	1	1	1	0	<chem>NS(=O)(=O)Oc1ccc2OC(=CC(=O)c2c1)C3CCCCCCCCCCC3</chem>
	4-oxo-2-(2,2,3,3-tetramethylcyclopropyl)chromen-6-yl sulfamate	1	1	1	0	<chem>CC1(C)C(C2=CC(=O)c3cc(OS(=O)(=O)N)ccc3O2)C1(C)C</chem>
	2-tert-butyl-4-oxochromen-6-yl sulfamate	1	1	1	0	<chem>CC(C)(C)C1=CC(=O)c2cc(OS(=O)(=O)N)ccc2O1</chem>
6665-83-4	6-hydroxyflavone	1	1	1	0	<chem>Oc1ccc2OC(=CC(=O)c2c1)c3ccccc3</chem>
	2-chloro-1-{4-[(3R,4S)-4-(4-hydroxyphenyl)hexan-3-yl]phenyl}ethanone	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(cc2)C(=O)CCl</chem>
	4-[(3S,4R)-4-[4-(bromomethyl)phenyl]hexan-3-yl]phenol	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(CBr)cc2</chem>
	4-[(3S,4R)-4-[4-(chloromethyl)phenyl]hexan-3-yl]phenol	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(CCl)cc2</chem>

4-[(3R,4S)-4-(4-hydroxyphenyl)hexan-3-yl]benzenesulfonyl fluoride	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(cc2)S(=O)(=O)F</chem>
1-bromo-3-{4-[(3R,4S)-4-(4-hydroxyphenyl)hexan-3-yl]phenoxy}propan-2-one	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(OCC(=O)CBr)cc2</chem>
4-[(3S,4R)-4-[4-(3-chloro-2-hydroxypropoxy)phenyl]hexan-3-yl]phenol	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(OCC(O)CCl)cc2</chem>
4-[(3S,4R)-4-[4-(3-bromo-2-hydroxypropoxy)phenyl]hexan-3-yl]phenol	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(OCC(O)CBr)cc2</chem>
1,9-diazatetracyclo[7.7.1.0{2,7}.0{10,15}]heptadeca-2,4,6,10(15),11,13-hexaene-5,13-diol	1	1	1	0	<chem>Oc1ccc2N3CN(Cc2c1)c4ccc(O)cc4C3</chem>
4-{bicyclo[3.3.1]nonan-9-yl}phenol	1	1	1	0	<chem>Oc1ccc(cc1)C2C3CCCC2CCC3</chem>
4-{bicyclo[3.3.1]non-2-en-2-yl}phenol	1	1	1	0	<chem>Oc1ccc(cc1)C2=CCC3CCCC2C3</chem>
2-bromo-1-{4-[(3R,4S)-4-(4-hydroxyphenyl)hexan-3-yl]phenyl}ethanone	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(cc2)C(=O)CBr</chem>
4-(1-{bicyclo[3.3.1]nonan-9-	1	1	1	0	<chem>CC(=C1C2CCCC1CCC2)c3ccc(O)cc3</chem>

	ylidene}ethyl)phenol					
	4-{9-methylbicyclo[3.3.1]nonan-9-yl}phenol	1	1	1	0	CC1(C2CCCC1CCC2)c3ccc(O)cc3
	1-chloro-3-{4-[(3R,4S)-4-(4-hydroxyphenyl)hexan-3-yl]phenoxy}propan-2-one	1	1	1	0	CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(OCC(=O)CCl)cc2
	4-[(3S,4R)-4-[4-(oxiran-2-ylmethoxy)phenyl]hexan-3-yl]phenol	1	1	1	0	CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(OCC3CO3)cc2
	tetracyclo[7.7.1.0{2,7}.0{10,15}]heptadeca-2,4,6,10(15),11,13-hexaene-5,13-diol	1	1	1	0	Oc1ccc2C3CC(Cc2c1)c4ccc(O)cc4C3
	(8S,16S)-8,16-dimethyltetracyclo[7.7.1.0{2,7}.0{10,15}]heptadeca-2,4,6,10(15),11,13-hexaene-4,12-diol	1	1	1	0	C[C@H]1C2CC([C@H](C)c3ccc(O)cc23)c4cc(O)ccc14
	4,12-dihydroxytetracyclo[7.7.1.0{2,7}.0{10,15}]heptadeca-2,4,6,10(15),11,13-hexaene-8,16-dione	1	1	1	0	Oc1ccc2C(=O)C3CC(C(=O)c4ccc(O)cc34)c2c1
	4-[6-(4-hydroxyphenyl)bicyclo[3.3.1]nonan	1	1	1	0	Oc1ccc(cc1)C2CCC3CC2CCC3c4ccc(O)cc4

	-2-yl]phenol					
	tetracyclo[7.7.1.0{2,7}.0{10,15}]heptadeca-2,4,6,10(15),11,13-hexaene-4,12-diol	1	1	1	0	Oc1ccc2CC3CC(Cc4ccc(O)cc34)c2c1
	5,13-dihydroxytetracyclo[7.7.1.0{2,7}.0{10,15}]heptadeca-2,4,6,10(15),11,13-hexaene-8,16-dione	1	1	1	0	Oc1ccc2C3CC(C(=O)c2c1)c4ccc(O)cc4C3=O
	(8S,16S)-8,16-dimethyltetracyclo[7.7.1.0{2,7}.0{10,15}]heptadeca-2,4,6,10(15),11,13-hexaene-5,13-diol	1	1	1	0	C[C@H]1C2CC([C@H](C)c3cc(O)ccc23)c4ccc(O)cc14
	4-(4-ethyl-3,5-diphenylpyrazol-1-yl)phenol	1	1	1	0	CCc1c(nn(c2ccc(O)cc2)c1c3ccccc3)c4ccccc4
	4-[4-butyl-3,5-bis(4-hydroxyphenyl)pyrazol-1-yl]phenol	1	1	1	0	CCCCc1c(nn(c2ccc(O)cc2)c1c3ccc(O)cc3)c4ccc(O)cc4
	4-[5-(4-hydroxyphenyl)-2-phenyl-4-propylpyrazol-3-yl]phenol	1	1	1	0	CCCc1c(nn(c2ccccc2)c1c3ccc(O)cc3)c4ccc(O)cc4
	4-[5-(4-hydroxyphenyl)-4-(2-methylpropyl)-2-phenylpyrazol-3-yl]phenol	1	1	1	0	CC(C)Cc1c(nn(c2ccccc2)c1c3ccc(O)cc3)c4ccc(O)cc4

4-[5-(4-hydroxyphenyl)-4-isopropyl-2-phenylpyrazol-3-yl]phenol	1	1	1	0	<chem>CC(C)c1c(nn(c2cccc2)c1c3ccc(O)cc3)c4ccc(O)cc4</chem>
4-[4-ethyl-3-(4-hydroxyphenyl)-5-phenylpyrazol-1-yl]phenol	1	1	1	0	<chem>CCc1c(nn(c2ccc(O)cc2)c1c3cccc3)c4ccc(O)cc4</chem>
4-[5-(4-hydroxyphenyl)-4-methyl-2-phenylpyrazol-3-yl]phenol	1	1	1	0	<chem>Cc1c(nn(c2cccc2)c1c3ccc(O)cc3)c4ccc(O)cc4</chem>
4-(4-ethyl-2,5-diphenylpyrazol-3-yl)phenol	1	1	1	0	<chem>CCc1c(nn(c2cccc2)c1c3ccc(O)cc3)c4cccc4</chem>
4-[4-butyl-5-(4-hydroxyphenyl)-2-phenylpyrazol-3-yl]phenol	1	1	1	0	<chem>CCCCc1c(nn(c2cccc2)c1c3ccc(O)cc3)c4ccc(O)cc4</chem>
4-(4-ethyl-1,5-diphenylpyrazol-3-yl)phenol	1	1	1	0	<chem>CCc1c(nn(c2cccc2)c1c3cccc3)c4ccc(O)cc4</chem>
4-[4-ethyl-5-(4-hydroxyphenyl)-3-phenylpyrazol-1-yl]phenol	1	1	1	0	<chem>CCc1c(nn(c2ccc(O)cc2)c1c3ccc(O)cc3)c4cccc4</chem>
4-oxo-2-{4-pentylbicyclo[2.2.2]octan-2-yl}chromen-6-yl sulfamate	1	1	1	0	<chem>CCCCC12CCC(CC1)C(C2)C3=CC(=O)c4cc(OS(=O)(=O)N)ccc4O3</chem>
2-(adamantan-1-yl)-6-hydroxythiochromen-4-one	1	1	1	0	<chem>Oc1ccc2SC(=CC(=O)c2c1)C34CC5CC(CC(C5)C3)C4</chem>
2-(adamantan-1-yl)-6-hydroxychromen-4-one	1	1	1	0	<chem>Oc1ccc2OC(=CC(=O)c2c1)C34CC5CC(CC(C5)C3)C4</chem>

2-(adamantan-1-yl)-6-hydroxy-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>Oc1ccc2OC(CC(=O)c2c1)C34CC5CC(CC(C5)C3)C4</chem>
2-(adamantan-1-yl)-4-oxochromen-6-yl sulfamate	1	1	1	0	<chem>NS(=O)(=O)Oc1ccc2OC(=CC(=O)c2c1)C34CC5CC(CC(C5)C3)C4</chem>
6-hydroxy-2-nonylchromen-4-one	1	1	1	0	<chem>CCCCCCCCC1=CC(=O)c2cc(O)ccc2O1</chem>
6-hydroxy-2-(2-phenylethyl)chromen-4-one	1	1	1	0	<chem>Oc1ccc2OC(=CC(=O)c2c1)CCc3ccccc3</chem>
6-hydroxy-2-{4-pentylbicyclo[2.2.2]octan-2-yl}chromen-4-one	1	1	1	0	<chem>CCCCC12CCC(CC1)C(C2)C3=CC(=O)c4cc(O)ccc4O3</chem>
2-tert-butyl-6-hydroxychromen-4-one	1	1	1	0	<chem>CC(C)(C)C1=CC(=O)c2cc(O)ccc2O1</chem>
2-cyclododecyl-6-hydroxychromen-4-one	1	1	1	0	<chem>Oc1ccc2OC(=CC(=O)c2c1)C3CCCCCCCCCCC3</chem>
6-hydroxy-2-(2,2,3,3-tetramethylcyclopropyl)chromen-4-one	1	1	1	0	<chem>CC1(C)C(C2=CC(=O)c3cc(O)ccc3O2)C1(C)C</chem>
6-hydroxy-2-(2-methyldecan-2-yl)chromen-4-one	1	1	1	0	<chem>CCCCCCCCC(C)(C)C1=CC(=O)c2cc(O)ccc2O1</chem>
2-(4-hydroxyphenyl)-3-{4-[3-(piperidin-1-yl)propyl]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(CCCN5CCCCC5)cc4</chem>

	2-(4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethanesulfonyl]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(cc4)S(=O)(=O)CCN5CCCCC5</chem>
	2-(4-hydroxyphenyl)-3-(4-{[2-(piperidin-1-yl)ethyl]amino}benzoyl)-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(NCCN5CCCCC5)cc4</chem>
	1-(3-{4-[6-methoxy-2-(4-methoxyphenyl)-1-benzothiophene-3-carbonyl]phenyl}propyl)piperidine	1	1	1	0	<chem>COc1ccc(cc1)c2sc3cc(OC)ccc3c2C(=O)c4ccc(CCCN5CCCCC5)cc4</chem>
	1-(2-{4-[6-methoxy-2-(4-methoxyphenyl)-1-benzothiophene-3-carbonyl]benzenesulfonyl}ethyl)piperidine	1	1	1	0	<chem>COc1ccc(cc1)c2sc3cc(OC)ccc3c2C(=O)c4ccc(cc4)S(=O)(=O)CCN5CCCCC5</chem>
	2-(4-hydroxyphenyl)-3-(4-{[2-(piperidin-1-yl)ethyl]sulfanyl}benzoyl)-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(SCCN5CCCCC5)cc4</chem>
	2-(4-hydroxyphenyl)-3-(4-{methyl[2-(piperidin-1-yl)ethyl]amino}benzoyl)-1-benzothiophen-6-ol	1	1	1	0	<chem>CN(CCN1CCCCC1)c2ccc(cc2)C(=O)c3c(sc4cc(O)ccc34)c5ccc(O)cc5</chem>

1638-22-8	4-n-butylphenol	1	1	1	0	<chem>CCCCc1ccc(O)cc1</chem>
65916-15-6	4-n-pentylphenol	1	1	1	0	<chem>CCCCCc1ccc(O)cc1</chem>
99-99-0	P-nitrotoluene	0	1	0	1	<chem>Cc1ccc(cc1)[N+](=O)[O-]</chem>
122-14-5	fenitrothion	0	1	0	1	<chem>COP(=S)(OC)Oc1ccc(c(C)c1)[N+](=O)[O-]</chem>
97-02-9	2,4-dinitraniline	0	1	0	1	<chem>Nc1ccc(cc1[N+](=O)[O-])[N+](=O)[O-]</chem>
528-29-0	o-dinitrobenzene	0	1	0	1	<chem>[O-][N+](=O)c1ccccc1[N+](=O)[O-]</chem>
95828-55-0	dichlorvos	0	1	0	1	<chem>COP(=O)(OC)OC=C(Cl)Cl</chem>
	4-[(3S,4R)-4-(4-hydroxyphenyl)-8-(piperazin-1-yl)octan-3-yl]phenol	1	1	1	0	<chem>CC[C@@H]([C@@H](CCCCN1CCNCC1)c2ccc(O)cc2)c3ccc(O)cc3</chem>
	methyl 2-phenyl-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophene-6-carboxylate	1	1	1	0	<chem>COC(=O)c1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccccc5</chem>
	methyl 4-(3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-2-yl)benzoate	0	1	0	1	<chem>COC(=O)c1ccc(cc1)c2sc3ccccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>
	methyl 2-[4-(methoxycarbonyl)phenyl]-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophene-6-carboxylate	1	1	1	0	<chem>COC(=O)c1ccc(cc1)c2sc3cc(ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4)C(=O)OC</chem>
	4-(6-hydroxy-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-	1	1	1	0	<chem>Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(cc5)C#N</chem>

	benzothiophen-2-yl)benzonitrile					
	methyl 2-(4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophene-6-carboxylate	1	1	1	0	<chem>COC(=O)c1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(O)cc5</chem>
	2-methylpropyl 2-(4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophene-6-carboxylate	1	1	1	0	<chem>CC(C)COC(=O)c1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(O)cc5</chem>
	4-(6-hydroxy-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-2-yl)-N-methylbenzamide	1	1	1	0	<chem>CNC(=O)c1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCC5)cc4</chem>
	butyl 2-(4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophene-6-carboxylate	1	1	1	0	<chem>CCCCOC(=O)c1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(O)cc5</chem>
	4-[2-cyclohexyl-5-(4-hydroxyphenyl)-4-propylpyrazol-3-yl]phenol	1	1	1	0	<chem>CCCc1c(nn(C2CCCCC2)c1c3ccc(O)cc3)c4ccc(O)cc4</chem>
	4-[3-(4-hydroxyphenyl)-4,5,6,7-tetrahydroindazol-1-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2nn(c3CCCCc23)c4ccc(O)cc4</chem>
	4-[5-cyclopentyl-3-(4-hydroxyphenyl)-4-propylpyrazol-1-yl]phenol	1	1	1	0	<chem>CCCc1c(nn(c2ccc(O)cc2)c1C3CCCC3)c4ccc(O)cc4</chem>

4-[3-(4-hydroxyphenyl)-4H,5H,6H,7H,8H-cyclohepta[c]pyrazol-1-yl]phenol	1	1	1	0	Oc1ccc(cc1)c2nn(c3CCCCCc23)c4ccc(O)cc4
4-[2-cyclopentyl-5-(4-hydroxyphenyl)-4-propylpyrazol-3-yl]phenol	1	1	1	0	CCCc1c(nn(C2CCCC2)c1c3ccc(O)cc3)c4ccc(O)cc4
4-[5-cyclopentyl-4-ethyl-3-(4-hydroxyphenyl)pyrazol-1-yl]phenol	1	1	1	0	CCc1c(nn(c2ccc(O)cc2)c1C3CCCC3)c4ccc(O)cc4
4-[5-cyclohexyl-3-(4-hydroxyphenyl)-4-propylpyrazol-1-yl]phenol	1	1	1	0	CCCc1c(nn(c2ccc(O)cc2)c1C3CCCCC3)c4ccc(O)cc4
4-[5-cyclohexyl-4-ethyl-3-(4-hydroxyphenyl)pyrazol-1-yl]phenol	1	1	1	0	CCc1c(nn(c2ccc(O)cc2)c1C3CCCCC3)c4ccc(O)cc4
2-(3-chloro-4-hydroxyphenyl)indazol-5-ol	1	1	1	0	Oc1ccc2nn(cc2c1)c3ccc(O)c(Cl)c3
2-(4-hydroxyphenyl)-3-(prop-2-en-1-yl)indazol-5-ol	1	1	1	0	Oc1ccc(cc1)n2nc3ccc(O)cc3c2CC=C
3-chloro-2-(4-hydroxyphenyl)indazol-6-ol	1	1	1	0	Oc1ccc(cc1)n2nc3cc(O)ccc3c2Cl
3-chloro-2-phenylindazol-5-ol	1	1	1	0	Oc1ccc2nn(c(Cl)c2c1)c3ccccc3
3-chloro-2-(3-chloro-4-hydroxyphenyl)indazol-5-ol	1	1	1	0	Oc1ccc2nn(c(Cl)c2c1)c3ccc(O)c(Cl)c3

	2-(4-hydroxyphenyl)-3-propylindazol-5-ol	1	1	1	0	<chem>CCCc1c2cc(O)ccc2nn1c3ccc(O)cc3</chem>
	2-(4-hydroxyphenyl)-3-isopropylindazol-5-ol	1	1	1	0	<chem>CC(C)c1c2cc(O)ccc2nn1c3ccc(O)cc3</chem>
	4-(indazol-2-yl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)n2cc3ccccc3n2</chem>
	3,7-dichloro-2-(4-hydroxyphenyl)indazol-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)n2nc3c(Cl)c(O)ccc3c2Cl</chem>
	(2R,3R,4R)-3-(4-hydroxyphenyl)-4-methyl-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-3,4-dihydro-2H-1-benzopyran-6-ol	1	1	1	0	<chem>C[C@@H]1[C@@H]([C@@H](Oc2ccc(O)cc12)c3ccc(OCCN4CCCC4)cc3)c5ccc(O)cc5</chem>
	(2R,3R,4S)-5-fluoro-3-(4-hydroxyphenyl)-4-methyl-2-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}-3,4-dihydro-2H-1-benzopyran-6-ol	1	1	1	0	<chem>C[C@H]1[C@@H]([C@@H](Oc2ccc(O)c(F)c12)c3ccc(OCCN4CCCC4)cc3)c5ccc(O)cc5</chem>
	(2R,3R,4S)-3-(4-hydroxyphenyl)-4-methyl-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-3,4-dihydro-2H-1-benzopyran-7-ol	1	1	1	0	<chem>C[C@H]1[C@@H]([C@@H](Oc2cc(O)ccc12)c3ccc(OCCN4CCCC4)cc3)c5ccc(O)cc5</chem>
	(2R,3R,4S)-4-ethyl-3-(4-hydroxyphenyl)-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-3,4-dihydro-2H-1-benzopyran-6-ol	1	1	1	0	<chem>CC[C@H]1[C@@H]([C@@H](Oc2ccc(O)cc12)c3ccc(OCCN4CCCC4)cc3)c5ccc(O)cc5</chem>

(2R,3R,4R)-3-(4-hydroxyphenyl)-4-methyl-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-3,4-dihydro-2H-1-benzopyran-7-ol	1	1	1	0	<chem>C[C@@H]1[C@@H]([C@@H](Oc2cc(O)ccc12)c3ccc(OCCN4CCCC4)cc3)c5ccc(O)cc5</chem>
(2S,3R)-3-(4-hydroxyphenyl)-2-{4-[(2R)-2-[(3S)-3-methylpyrrolidin-1-yl]propoxy]phenyl}-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>C[C@H](COc1ccc(cc1)[C@@H]2Oc3ccc(O)cc3S[C@@H]2c4ccc(O)cc4)N5CC[C@H](C)C5</chem>
(2S,3R)-2-(4-{2-[(3S,4S)-3,4-dimethylpyrrolidin-1-yl]ethoxy}phenyl)-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>C[C@@H]1CN(CCOc2ccc(cc2)[C@@H]3Oc4ccc(O)cc4S[C@@H]3c5ccc(O)cc5)C[C@H]1C</chem>
(2S,3R)-3-(3-hydroxyphenyl)-2-{4-[(2S)-2-[(3R)-3-methylpyrrolidin-1-yl]propoxy]phenyl}-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>C[C@@H](COc1ccc(cc1)[C@@H]2Oc3ccc(O)cc3S[C@@H]2c4cccc(O)c4)N5CC[C@@H](C)C5</chem>
(2S,3R)-3-(4-hydroxyphenyl)-2-{4-[(2R)-2-[(3R)-3-methylpyrrolidin-1-yl]propoxy]phenyl}-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>C[C@H](COc1ccc(cc1)[C@@H]2Oc3ccc(O)cc3S[C@@H]2c4ccc(O)cc4)N5CC[C@@H](C)C5</chem>
(2S,3R)-5-fluoro-3-(4-hydroxyphenyl)-2-{4-[(2S)-2-[(3R)-3-methylpyrrolidin-1-yl]propoxy]phenyl}-2,3-dihydro-	1	1	1	0	<chem>C[C@@H](COc1ccc(cc1)[C@@H]2Oc3ccc(O)c(F)c3S[C@@H]2c4ccc(O)cc4)N5CC[C@@H](C)C5</chem>

	1,4-benzoxathiin-6-ol					
	(2S,3R)-3-(4-hydroxyphenyl)-2-{4-[(2S)-2-[(3S)-3-methylpyrrolidin-1-yl]propoxy]phenyl}-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>C[C@@H](COc1ccc(cc1)[C@@H]2Oc3ccc(O)cc3S[C@@H]2c4ccc(O)cc4)N5CC[C@H](C)C5</chem>
	(2S,3R)-5-fluoro-3-(3-hydroxyphenyl)-2-{4-[(2S)-2-[(3R)-3-methylpyrrolidin-1-yl]propoxy]phenyl}-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>C[C@@H](COc1ccc(cc1)[C@@H]2Oc3ccc(O)c(F)c3S[C@@H]2c4cccc(O)c4)N5CC[C@H](C)C5</chem>
	2-(4-hydroxyphenyl)-7-methoxy-1-benzofuran-5-ol	1	1	1	0	<chem>COc1cc(O)cc2cc(oc12)c3ccc(O)cc3</chem>
	2-(3-fluoro-4-hydroxyphenyl)-7-methoxy-1-benzofuran-5-ol	1	1	1	0	<chem>COc1cc(O)cc2cc(oc12)c3ccc(O)c(F)c3</chem>
	7-bromo-2-(4-hydroxyphenyl)-1-benzofuran-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2oc3c(Br)cc(O)cc3c2</chem>
	7-bromo-2-(3-fluoro-4-hydroxyphenyl)-1-benzofuran-5-ol	1	1	1	0	<chem>Oc1cc(Br)c2oc(cc2c1)c3ccc(O)c(F)c3</chem>
	(2S,3R)-2-{4-[2-(4-fluoropiperidin-1-yl)ethoxy]phenyl}-3-(4-hydroxyphenyl)-2,3-dihydro-1,4-benzoxathiin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)[C@H]2Sc3cc(O)ccc3O[C@H]2c4ccc(OCCN5CC(F)CC5)cc4</chem>

	7-chloro-2-(4-hydroxyphenyl)-1-benzofuran-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2oc3c(Cl)cc(O)cc3c2</chem>
	2-(4-hydroxyphenyl)-7-methyl-1-benzofuran-5-ol	1	1	1	0	<chem>Cc1cc(O)cc2cc(oc12)c3ccc(O)cc3</chem>
	4-chloro-2-(4-hydroxyphenyl)-7-methoxy-1-benzofuran-5-ol	1	1	1	0	<chem>COc1cc(O)c(Cl)c2cc(oc12)c3ccc(O)cc3</chem>
	5-hydroxy-2-(4-hydroxyphenyl)-7-methoxy-1-benzofuran-4-carbonitrile	1	1	1	0	<chem>COc1cc(O)c(C#N)c2cc(oc12)c3ccc(O)cc3</chem>
	2-(4-hydroxyphenyl)-3-phenylpyrazolo[1,5-a]pyrimidin-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2nn3cc(O)cnc3c2c4ccccc4</chem>
	2-[ethyl(1-phenylpropyl)amino]pyrimidin-5-ol	1	1	1	0	<chem>CCC(N(CC)c1ncc(O)cn1)c2ccccc2</chem>
	6-[benzyl(ethyl)amino]pyridin-3-ol	1	1	1	0	<chem>CCN(Cc1ccccc1)c2ccc(O)cn2</chem>
	6-[ethyl(1-phenylpropyl)amino]pyridin-3-ol	1	1	1	0	<chem>CCC(N(CC)c1ccc(O)cn1)c2ccccc2</chem>
	2-[benzyl(ethyl)amino]pyrimidin-5-ol	1	1	1	0	<chem>CCN(Cc1ccccc1)c2ncc(O)cn2</chem>
615-58-7	2,4-dibromophenol	0	1	0	1	<chem>Oc1ccc(Br)cc1Br</chem>
	4-(6-hydroxy-1,2-benzoxazol-3-	1	1	1	0	<chem>Oc1ccc(c(O)c1)c2noc3cc(O)ccc23</chem>

	yl)benzene-1,3-diol					
	2-(3-fluoro-4-hydroxyphenyl)-7-(furan-2-yl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1cc(c2occc2)c3oc(nc3c1)c4ccc(O)c(F)c4</chem>
	7-[(Z)-2-bromoethenyl]-2-(4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2oc3c(\C=C/Br)cc(O)cc3n2</chem>
	7-[(Z)-2-bromoethenyl]-2-(2-fluoro-4-hydroxyphenyl)-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1ccc(c(F)c1)c2oc3c(\C=C/Br)cc(O)cc3n2</chem>
	7-bromo-2-[4-hydroxy-3-(trifluoromethyl)phenyl]-1,3-benzoxazol-5-ol	1	1	1	0	<chem>Oc1cc(Br)c2oc(nc2c1)c3ccc(O)c(c3)C(F)(F)F</chem>
	2-(4-hydroxyphenyl)-7-[(1Z)-prop-1-en-1-yl]-1,3-benzoxazol-5-ol	1	1	1	0	<chem>C\C=C/c1cc(O)cc2nc(oc12)c3ccc(O)cc3</chem>
	3-(ethylsulfanyl)-5-hydroxy-2-(4-hydroxyphenyl)inden-1-one	1	1	1	0	<chem>CCSC1=C(C(=O)c2ccc(O)cc12)c3ccc(O)cc3</chem>
	5-hydroxy-2-(4-hydroxyphenyl)-3-phenylinden-1-one	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(c3ccccc3)c4cc(O)ccc4C2=O</chem>
	3-bromo-4,6-dihydroxy-2-(4-hydroxyphenyl)inden-1-one	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(Br)c3c(O)cc(O)cc3C2=O</chem>
	4,6-dihydroxy-2-(4-hydroxyphenyl)-3-(methylsulfanyl)inden-1-one	1	1	1	0	<chem>CSC1=C(C(=O)c2cc(O)cc(O)c12)c3ccc(O)cc3</chem>

5-hydroxy-2-(4-hydroxyphenyl)-3-methylinden-1-one	1	1	1	0	<chem>CC1=C(C(=O)c2ccc(O)cc12)c3ccc(O)cc3</chem>
5-hydroxy-2-(4-hydroxyphenyl)-3-(methylsulfanyl)inden-1-one	1	1	1	0	<chem>CSC1=C(C(=O)c2ccc(O)cc12)c3ccc(O)cc3</chem>
3-amino-6-hydroxy-2-(4-hydroxyphenyl)inden-1-one	1	1	1	0	<chem>NC1=C(C(=O)c2cc(O)ccc12)c3ccc(O)cc3</chem>
(3E)-3-(ethylimino)-2-(4-hydroxyphenyl)indene-1,4,6-triol	1	1	1	0	<chem>CC\\N=C/1\\C(=C(O)c2cc(O)cc(O)c12)c3ccc(O)cc3</chem>
4,6-dihydroxy-2-(4-hydroxyphenyl)-3-phenylinden-1-one	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(c3ccccc3)c4c(O)cc(O)cc4C2=O</chem>
3-bromo-6-hydroxy-2-(4-hydroxyphenyl)inden-1-one	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(Br)c3ccc(O)cc3C2=O</chem>
3,6-dihydroxy-2-(4-hydroxyphenyl)inden-1-one	1	1	1	0	<chem>OC1=C(C(=O)c2cc(O)ccc12)c3ccc(O)cc3</chem>
3,5,7-trihydroxy-2-(4-hydroxyphenyl)inden-1-one	1	1	1	0	<chem>OC1=C(C(=O)c2c(O)cc(O)cc12)c3ccc(O)cc3</chem>
5,7-dihydroxy-2-(4-hydroxyphenyl)-3-methylinden-1-one	1	1	1	0	<chem>CC1=C(C(=O)c2c(O)cc(O)cc12)c3ccc(O)cc3</chem>
5,7-dihydroxy-2-(4-hydroxyphenyl)-3-phenylinden-1-one	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(c3ccccc3)c4cc(O)cc(O)c4C2=O</chem>
3-bromo-5-hydroxy-2-(4-	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(Br)c3cc(O)ccc3C2=O</chem>

	hydroxyphenyl)inden-1-one					
	3-bromo-2-(4-hydroxyphenyl)-5-methoxyinden-1-one	1	1	1	0	<chem>COc1ccc2C(=O)C(=C(Br)c2c1)c3ccc(O)cc3</chem>
	3-(ethylsulfanyl)-4,6-dihydroxy-2-(4-hydroxyphenyl)inden-1-one	1	1	1	0	<chem>CCSC1=C(C(=O)c2cc(O)cc(O)c12)c3ccc(O)cc3</chem>
	6-hydroxy-2-(4-hydroxyphenyl)-3-phenylinden-1-one	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(c3ccccc3)c4ccc(O)cc4C2=O</chem>
	3-bromo-6-hydroxy-2-(4-hydroxyphenyl)-4-methoxyinden-1-one	1	1	1	0	<chem>COc1cc(O)cc2C(=O)C(=C(Br)c12)c3ccc(O)cc3</chem>
	3-(ethylsulfanyl)-6-hydroxy-2-(4-hydroxyphenyl)inden-1-one	1	1	1	0	<chem>CCSC1=C(C(=O)c2cc(O)ccc12)c3ccc(O)cc3</chem>
	6-hydroxy-2-(4-hydroxyphenyl)-3-methylinden-1-one	1	1	1	0	<chem>CC1=C(C(=O)c2cc(O)ccc12)c3ccc(O)cc3</chem>
	6-hydroxy-2-(4-hydroxyphenyl)-3-(methylsulfanyl)inden-1-one	1	1	1	0	<chem>CSC1=C(C(=O)c2cc(O)ccc12)c3ccc(O)cc3</chem>
	cyclopenta-2,4-dien-1-yl({3-[(1Z)-1-{4-[3-(dimethylamino)propoxy]phenyl}-1-(4-hydroxyphenyl)but-1-en-2-yl]cyclopenta-2,4-dien-1-yl})ruthenium	1	1	1	0	<chem>CC\C=C(/c1ccc(O)cc1)\c2ccc(OCCCN(C)C)cc2)\C3=CC([Ru]C4C=CC=C4)C=C3</chem>

	cyclopenta-2,4-dien-1-yl({3-[(1Z)-1-{4-[4-(dimethylamino)butoxy]phenyl}-1-(4-hydroxyphenyl)but-1-en-2-yl]cyclopenta-2,4-dien-1-yl})ruthenium	1	1	1	0	<chem>CC\C(=C(/c1ccc(O)cc1)\c2ccc(OCCCCN(C)C)cc2)\C3=CC([Ru]C4C=CC=C4)C=C3</chem>
	cyclopenta-2,4-dien-1-yl({3-[(1Z)-1-{4-[2-(dimethylamino)ethoxy]phenyl}-1-(4-hydroxyphenyl)but-1-en-2-yl]cyclopenta-2,4-dien-1-yl})ruthenium	1	1	1	0	<chem>CC\C(=C(/c1ccc(O)cc1)\c2ccc(OCCN(C)C)cc2)\C3=CC([Ru]C4C=CC=C4)C=C3</chem>
	cyclopenta-2,4-dien-1-yl({3-[(1Z)-1-(4-{[5-(dimethylamino)pentyl]oxy}phenyl)-1-(4-hydroxyphenyl)but-1-en-2-yl]cyclopenta-2,4-dien-1-yl})ruthenium	1	1	1	0	<chem>CC\C(=C(/c1ccc(O)cc1)\c2ccc(OCCCCCN(C)C)cc2)\C3=CC([Ru]C4C=CC=C4)C=C3</chem>
95-53-4	toluidine	0	1	0	1	<chem>Cc1ccccc1N</chem>
70955-17-8	ethylbenzene	0	1	0	1	<chem>CCc1ccccc1</chem>
27323-18-8	aroclor 1232	0	1	0	1	<chem>Clc1ccccc1c2ccccc2</chem>
	1-chloro-6-(4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2ccc3c(Cl)c(O)ccc3c2</chem>

1-bromo-6-(4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2ccc3c(Br)c(O)ccc3c2</chem>
1-chloro-8-fluoro-6-(3-fluoro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc(cc1F)c2cc(F)c3c(Cl)c(O)ccc3c2</chem>
1-chloro-6-(2-chloro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc(c(Cl)c1)c2ccc3c(Cl)c(O)ccc3c2</chem>
6-phenylnaphthalen-2-ol	1	1	1	0	<chem>Oc1ccc2cc(ccc2c1)c3ccccc3</chem>
7-(4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2ccc3ccc(O)cc3c2</chem>
6-(3,5-difluoro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc2cc(ccc2c1)c3cc(F)c(O)c(F)c3</chem>
8-chloro-6-(4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2cc(Cl)c3cc(O)ccc3c2</chem>
4-ethenyl-6-(3-fluoro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1cc(C=C)c2cc(ccc2c1)c3ccc(O)c(F)c3</chem>
4-ethyl-6-(3-fluoro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>CCc1cc(O)cc2ccc(cc12)c3ccc(O)c(F)c3</chem>
6-(4-hydroxy-2-methoxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>COc1cc(O)ccc1c2ccc3cc(O)ccc3c2</chem>
3-(2,5-difluoro-4-hydroxyphenyl)-7-hydroxynaphthalene-1-carbonitrile	1	1	1	0	<chem>Oc1ccc2cc(cc(C#N)c2c1)c3cc(F)c(O)cc3F</chem>

	3-(2,6-difluoro-4-hydroxyphenyl)-7-hydroxynaphthalene-1-carbonitrile	1	1	1	0	<chem>Oc1ccc2cc(cc(C#N)c2c1)c3c(F)cc(O)cc3F</chem>
	1-chloro-6-(3,5-difluoro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc2cc(ccc2c1Cl)c3cc(F)c(O)c(F)c3</chem>
	7-(3-fluoro-4-hydroxyphenyl)-3-hydroxy-4-methylnaphthalene-1-carbonitrile	1	1	1	0	<chem>Cc1c(O)cc(C#N)c2cc(ccc12)c3ccc(O)c(F)c3</chem>
	4-chloro-3-hydroxy-7-(4-hydroxyphenyl)naphthalene-1-carbonitrile	1	1	1	0	<chem>Oc1ccc(cc1)c2ccc3c(Cl)c(O)cc(C#N)c3c2</chem>
	6-(4-hydroxyphenyl)-1-phenylnaphthalen-2-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2ccc3c(c(O)ccc3c2)c4ccccc4</chem>
	6-(4-hydroxyphenyl)-1-methylnaphthalen-2-ol	1	1	1	0	<chem>Cc1c(O)ccc2cc(ccc12)c3ccc(O)cc3</chem>
	3-(3-fluoro-4-hydroxyphenyl)-7-hydroxynaphthalene-1-carbonitrile	1	1	1	0	<chem>Oc1ccc2cc(cc(C#N)c2c1)c3ccc(O)c(F)c3</chem>
	1-chloro-6-(2-fluoro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc(c(F)c1)c2ccc3c(Cl)c(O)ccc3c2</chem>
	6-(2,5-difluoro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc2cc(ccc2c1)c3cc(F)c(O)cc3F</chem>
	8-ethenyl-6-(3-fluoro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc2cc(cc(C=C)c2c1)c3ccc(O)c(F)c3</chem>

	1-chloro-6-(4-hydroxy-2-methylphenyl)naphthalen-2-ol	1	1	1	0	<chem>Cc1cc(O)ccc1c2ccc3c(Cl)c(O)ccc3c2</chem>
	7-(3-fluoro-4-hydroxyphenyl)-3-hydroxynaphthalene-1-carbonitrile	1	1	1	0	<chem>Oc1cc(C#N)c2cc(ccc2c1)c3ccc(O)c(F)c3</chem>
	7-phenylnaphthalen-2-ol	1	1	1	0	<chem>Oc1ccc2ccc(cc2c1)c3ccccc3</chem>
6336-82-9	4-(naphthalen-2-yl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2ccc3ccccc3c2</chem>
	8-bromo-7-hydroxy-3-(4-hydroxyphenyl)naphthalene-1-carbonitrile	1	1	1	0	<chem>Oc1ccc(cc1)c2cc(C#N)c3c(Br)c(O)ccc3c2</chem>
	1-chloro-8-fluoro-6-(4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2cc(F)c3c(Cl)c(O)ccc3c2</chem>
	6-(3-fluoro-4-hydroxyphenyl)-4-(prop-1-yn-1-yl)naphthalen-2-ol	1	1	1	0	<chem>CC#Cc1cc(O)cc2ccc(cc12)c3ccc(O)c(F)c3</chem>
	7-(3-fluoro-4-hydroxyphenyl)-3-hydroxynaphthalene-1-carbaldehyde	1	1	1	0	<chem>Oc1cc(C=O)c2cc(ccc2c1)c3ccc(O)c(F)c3</chem>
	1-chloro-6-(2,6-difluoro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1cc(F)c(c(F)c1)c2ccc3c(Cl)c(O)ccc3c2</chem>
	6-(2-chloro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc(c(Cl)c1)c2ccc3cc(O)ccc3c2</chem>
	6-(3-fluoro-4-hydroxyphenyl)-8-	1	1	1	0	<chem>CC#Cc1cc(cc2ccc(O)cc12)c3ccc(O)c(F)c3</chem>

	(prop-1-yn-1-yl)naphthalen-2-ol					
	3-(2-fluoro-4-hydroxyphenyl)-7-hydroxynaphthalene-1-carbonitrile	1	1	1	0	<chem>Oc1ccc(c(F)c1)c2cc(C#N)c3cc(O)ccc3c2</chem>
	6-(3-chloro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc2cc(ccc2c1)c3ccc(O)c(Cl)c3</chem>
	1-chloro-6-(3-chloro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc(cc1Cl)c2ccc3c(Cl)c(O)ccc3c2</chem>
	6-(2-fluoro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc(c(F)c1)c2ccc3cc(O)ccc3c2</chem>
	4-bromo-7-(3-fluoro-4-hydroxyphenyl)-3-hydroxynaphthalene-1-carbonitrile	1	1	1	0	<chem>Oc1ccc(cc1F)c2ccc3c(Br)c(O)cc(C#N)c3c2</chem>
	6-(3-fluoro-4-hydroxyphenyl)-2-hydroxynaphthalene-1,4-dicarbonitrile	1	1	1	0	<chem>Oc1ccc(cc1F)c2ccc3c(C#N)c(O)cc(C#N)c3c2</chem>
	8-fluoro-3-(3-fluoro-4-hydroxyphenyl)-7-hydroxynaphthalene-1-carbonitrile	1	1	1	0	<chem>Oc1ccc(cc1F)c2cc(C#N)c3c(F)c(O)ccc3c2</chem>
	3-(3-fluoro-4-hydroxyphenyl)-7-hydroxynaphthalene-1-carbaldehyde	1	1	1	0	<chem>Oc1ccc2cc(cc(C=O)c2c1)c3ccc(O)c(F)c3</chem>
	6-(4-hydroxy-2-	1	1	1	0	<chem>Cc1cc(O)ccc1c2ccc3cc(O)ccc3c2</chem>

	methylphenyl)naphthalen-2-ol					
	3-(3,5-difluoro-4-hydroxyphenyl)-7-hydroxynaphthalene-1-carbonitrile	1	1	1	0	<chem>Oc1ccc2cc(cc(C#N)c2c1)c3cc(F)c(O)c(F)c3</chem>
	3-hydroxy-7-(4-hydroxyphenyl)naphthalene-1-carbonitrile	1	1	1	0	<chem>Oc1ccc(cc1)c2ccc3cc(O)cc(C#N)c3c2</chem>
	1-fluoro-6-(4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2ccc3c(F)c(O)ccc3c2</chem>
	2-hydroxy-6-(4-hydroxyphenyl)naphthalene-1-carbonitrile	1	1	1	0	<chem>Oc1ccc(cc1)c2ccc3c(C#N)c(O)ccc3c2</chem>
	1,8-dichloro-6-(4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2cc(Cl)c3c(Cl)c(O)ccc3c2</chem>
	7-(3-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1cccc(c1)c2ccc3ccc(O)cc3c2</chem>
	7-hydroxy-3-(4-hydroxyphenyl)naphthalene-1-carbonitrile	1	1	1	0	<chem>Oc1ccc(cc1)c2cc(C#N)c3cc(O)ccc3c2</chem>
	8-fluoro-6-(4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2cc(F)c3cc(O)ccc3c2</chem>
	8-fluoro-6-(3-fluoro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc2cc(cc(F)c2c1)c3ccc(O)c(F)c3</chem>

	4-chloro-7-(3-fluoro-4-hydroxyphenyl)-3-hydroxynaphthalene-1-carbonitrile	1	1	1	0	<chem>Oc1ccc(cc1F)c2ccc3c(Cl)c(O)cc(C#N)c3c2</chem>
	1-chloro-6-(2,5-difluoro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc2cc(ccc2c1Cl)c3cc(F)c(O)cc3F</chem>
	4-ethynyl-6-(3-fluoro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1cc(C#C)c2cc(ccc2c1)c3ccc(O)c(F)c3</chem>
	6-(4-hydroxyphenyl)-1-methoxynaphthalen-2-ol	1	1	1	0	<chem>COc1c(O)ccc2cc(ccc12)c3ccc(O)cc3</chem>
	6-(4-hydroxyphenyl)-1-nitronaphthalen-2-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2ccc3c(c(O)ccc3c2)[N+](=O)[O-]</chem>
	6-(2,6-difluoro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc2cc(ccc2c1)c3c(F)cc(O)cc3F</chem>
	8-ethyl-6-(3-fluoro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>CCc1cc(cc2ccc(O)cc12)c3ccc(O)c(F)c3</chem>
	8-ethynyl-6-(3-fluoro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc2cc(cc(C#C)c2c1)c3ccc(O)c(F)c3</chem>
	6-(3-hydroxyphenyl)naphthalen-1-ol	1	1	1	0	<chem>Oc1cccc(c1)c2ccc3c(O)cccc3c2</chem>
	6-(4-hydroxyphenyl)naphthalen-1-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2ccc3c(O)cccc3c2</chem>

6-(3-fluoro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc2cc(ccc2c1)c3ccc(O)c(F)c3</chem>
8-chloro-7-hydroxy-3-(4-hydroxyphenyl)naphthalene-1-carbonitrile	1	1	1	0	<chem>Oc1ccc(cc1)c2cc(C#N)c3c(Cl)c(O)ccc3c2</chem>
8-chloro-3-(3-fluoro-4-hydroxyphenyl)-7-hydroxynaphthalene-1-carbonitrile	1	1	1	0	<chem>Oc1ccc(cc1F)c2cc(C#N)c3c(Cl)c(O)ccc3c2</chem>
1-chloro-6-(3-fluoro-4-hydroxyphenyl)naphthalen-2-ol	1	1	1	0	<chem>Oc1ccc(cc1F)c2ccc3c(Cl)c(O)ccc3c2</chem>
(2E)-3-{4-[(2-ethyl-7-hydroxy-3-phenylquinolin-4-yl)oxy]phenyl}-N-isopropylprop-2-enamide	1	1	1	0	<chem>CCc1nc2cc(O)ccc2c(Oc3ccc(\C=C\C(=O)NC(C)C)cc3)c1c4cccc4</chem>
(2E)-3-{3-[(2-ethyl-7-hydroxy-3-phenylquinolin-4-yl)oxy]phenyl}prop-2-enoic acid	1	1	1	0	<chem>CCc1nc2cc(O)ccc2c(Oc3cccc(\C=C\C(=O)O)c3)c1c4cccc4</chem>
(2E)-3-{4-[(2-ethyl-7-hydroxy-3-phenylquinolin-4-yl)oxy]phenyl}-1-(piperidin-1-yl)prop-2-en-1-one	1	1	1	0	<chem>CCc1nc2cc(O)ccc2c(Oc3ccc(\C=C\C(=O)N4CCCCC4)cc3)c1c5cccc5</chem>
(2E)-3-[4-{(2-ethyl-7-hydroxy-3-[3-(trifluoromethyl)phenyl]quinolin-4-yl)oxy}phenyl]prop-2-enoic acid	1	1	1	0	<chem>CCc1nc2cc(O)ccc2c(Oc3ccc(\C=C\C(=O)O)cc3)c1c4cccc(c4)C(F)(F)F</chem>
(2E)-3-{4-[(2-ethyl-7-hydroxy-3-	1	1	1	0	<chem>CCc1nc2cc(O)ccc2c(Oc3ccc(\C=C\C(=O)N)cc3)c1c4cccc4</chem>

	phenylquinolin-4-yl)oxy]phenyl}prop-2-enamide					
	4-{4-[2-(dimethylamino)ethoxy]phenoxy}-2-ethyl-3-phenylquinolin-7-ol	1	1	1	0	<chem>CCc1nc2cc(O)ccc2c(Oc3ccc(OCCN(C)C)cc3)c1c4ccccc4</chem>
	(2E)-3-{4-[(2-ethyl-7-hydroxy-3-phenylquinolin-4-yl)oxy]phenyl}-N,N-dimethylprop-2-enamide	1	1	1	0	<chem>CCc1nc2cc(O)ccc2c(Oc3ccc(\C=C\C(=O)N(C)C)cc3)c1c4cccc4</chem>
	(2E)-3-{4-[(7-hydroxy-2,3-diphenylquinolin-4-yl)oxy]phenyl}prop-2-enoic acid	1	1	1	0	<chem>OC(=O)\C=C\c1ccc(Oc2c(c3ccccc3)c(nc4cc(O)ccc24)c5ccccc5)cc1</chem>
	(2E)-3-{4-[(1E)-1-(4-hydroxyphenyl)-2-phenylbut-1-en-1-yl]phenyl}prop-2-enoic acid	1	1	1	0	<chem>CC\C=C(/c1ccc(O)cc1)\c2ccc(\C=C\C(=O)O)cc2)\c3ccccc3</chem>
	(2E)-3-{4-[(2-ethyl-7-hydroxy-3-phenylquinolin-4-yl)oxy]phenyl}prop-2-enoic acid	1	1	1	0	<chem>CCc1nc2cc(O)ccc2c(Oc3ccc(\C=C\C(=O)O)cc3)c1c4ccccc4</chem>
13037-86-0	4-heptyloxyphenol	0	1	0	1	<chem>CCCCCCCCOc1ccc(O)cc1</chem>
104-43-8	dodecylphenol	1	1	1	0	<chem>CCCCCCCCCCCCc1ccc(O)cc1</chem>
571-22-2	5β-dihydrotestosterone	0	1	0	1	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
1300-17-0	dianabol	0	1	0	1	<chem>C[C@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C</chem>

						@H]3CC[C@]12C
	(2R,3S)-2,3-bis(4-hydroxyphenyl)butanedinitrile	1	1	1	0	Oc1ccc(cc1)[C@H](C#N)[C@H](C#N)c2ccc(O)cc2
	(2S,3R)-5-fluoro-2,3-bis(4-hydroxyphenyl)pentanenitrile	1	1	1	0	Oc1ccc(cc1)[C@H](CCF)[C@H](C#N)c2ccc(O)cc2
	4-chloro-2-(3-fluoro-4-hydroxyphenyl)quinolin-6-ol	1	1	1	0	Oc1ccc2nc(cc(Cl)c2c1)c3ccc(O)c(F)c3
	4-bromo-2-(3-fluoro-4-hydroxyphenyl)quinolin-6-ol	1	1	1	0	Oc1ccc2nc(cc(Br)c2c1)c3ccc(O)c(F)c3
	5-chloro-2-(4-hydroxyphenyl)quinolin-6-ol	1	1	1	0	Oc1ccc(cc1)c2ccc3c(Cl)c(O)ccc3n2
	5-bromo-2-(4-hydroxyphenyl)quinolin-6-ol	1	1	1	0	Oc1ccc(cc1)c2ccc3c(Br)c(O)ccc3n2
	4-bromo-2-(3,5-difluoro-4-hydroxyphenyl)quinolin-6-ol	1	1	1	0	Oc1ccc2nc(cc(Br)c2c1)c3cc(F)c(O)c(F)c3
	4-ethenyl-2-(3-fluoro-4-hydroxyphenyl)quinolin-6-ol	1	1	1	0	Oc1ccc2nc(cc(C=C)c2c1)c3ccc(O)c(F)c3
	4-ethyl-2-(3-fluoro-4-hydroxyphenyl)quinolin-6-ol	1	1	1	0	CCc1cc(nc2ccc(O)cc12)c3ccc(O)c(F)c3
	4-ethynyl-2-(3-fluoro-4-hydroxyphenyl)quinolin-6-ol	1	1	1	0	Oc1ccc2nc(cc(C#C)c2c1)c3ccc(O)c(F)c3

	2-(3,5-difluoro-4-hydroxyphenyl)-4-ethynylquinolin-6-ol	1	1	1	0	<chem>Oc1ccc2nc(cc(C#C)c2c1)c3cc(F)c(O)c(F)c3</chem>
	2-(3-fluoro-4-hydroxyphenyl)-6-hydroxyquinoline-4-carbonitrile	1	1	1	0	<chem>Oc1ccc2nc(cc(C#N)c2c1)c3ccc(O)c(F)c3</chem>
	1-[6-hydroxy-2-(4-hydroxyphenyl)quinolin-4-yl]ethanone	1	1	1	0	<chem>CC(=O)c1cc(nc2ccc(O)cc12)c3ccc(O)cc3</chem>
	1-[2-(3-fluoro-4-hydroxyphenyl)-6-hydroxyquinolin-4-yl]ethanone	1	1	1	0	<chem>CC(=O)c1cc(nc2ccc(O)cc12)c3ccc(O)c(F)c3</chem>
	2-(3-fluoro-4-hydroxyphenyl)-4-phenylquinolin-6-ol	1	1	1	0	<chem>Oc1ccc2nc(cc(c3ccccc3)c2c1)c4ccc(O)c(F)c4</chem>
	2-(4-hydroxyphenyl)-4-methoxyquinolin-6-ol	1	1	1	0	<chem>COc1cc(nc2ccc(O)cc12)c3ccc(O)cc3</chem>
	2-(3-fluoro-4-hydroxyphenyl)-4-(1-hydroxyethyl)quinolin-6-ol	1	1	1	0	<chem>CC(O)c1cc(nc2ccc(O)cc12)c3ccc(O)c(F)c3</chem>
5890-93-7	4-[3-(4-hydroxyphenyl)-1H-indol-2-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2[nH]c3ccccc3c2c4ccc(O)cc4</chem>
	4-(2-phenyl-1H-indol-3-yl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2c([nH]c3ccccc23)c4ccccc4</chem>
	4-(3-phenyl-1H-indol-2-yl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2[nH]c3ccccc3c2c4ccccc4</chem>
	4-(2-phenyl-1,3-benzodiazol-1-yl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)n2c(nc3ccccc23)c4ccccc4</chem>

	4-[2-(thiophen-2-yl)-1,3-benzodiazol-1-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)n2c(nc3ccccc23)c4cccs4</chem>
	4-[2-(1-methylpyrrol-2-yl)-1,3-benzodiazol-1-yl]phenol	1	1	1	0	<chem>Cn1cccc1c2nc3ccccc3n2c4ccc(O)cc4</chem>
	4-[2-(3-methyl-1,2-oxazol-4-yl)-1,3-benzodiazol-1-yl]phenol	1	1	1	0	<chem>Cc1nocc1c2nc3ccccc3n2c4ccc(O)cc4</chem>
	4-[2-(2-chlorophenyl)-1,3-benzodiazol-1-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)n2c(nc3ccccc23)c4ccccc4Cl</chem>
	4-[4-phenyl-5-(trifluoromethyl)-1,2-oxazol-3-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2noc(c2c3ccccc3)C(F)(F)F</chem>
	4-[5-phenyl-2-(trifluoromethyl)-3H-imidazol-4-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2[nH]c(nc2c3ccccc3)C(F)(F)F</chem>
3469-20-3	2,3-diphenyl-1H-indole	1	1	1	0	<chem>c1ccc(cc1)c2[nH]c3ccccc3c2c4ccccc4</chem>
	(2R,5S,14S,15S)-2-[(E)-2-chloroethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-7-ene-5,14-diol	1	1	1	0	<chem>C[C@]12CCC3C(CC=C4C[C@@H](O)CC[C@]34\\C=C\\Cl)C1CC[C@@H]2O</chem>
	(2S,5S,14S,15S)-2-ethenyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-7-ene-5,14-diol	1	1	1	0	<chem>C[C@]12CCC3C(CC=C4C[C@@H](O)CC[C@]34C=C)C1CC[C@@H]2O</chem>
	(2R,5S,14S,15S)-2-[(E)-2-fluoroethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,	1	1	1	0	<chem>C[C@]12CCC3C(CC=C4C[C@@H](O)CC[C@]34\\C=C\\F)C1CC[C@@H]2O</chem>

	15}}heptadec-7-ene-5,14-diol					
	(2R,5S,14S,15S)-2-[(Z)-2-chloroethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-7-ene-5,14-diol	1	1	1	0	C[C@]12CCC3C(CC=C4C[C@@H](O)CC[C@]34\C=C/Cl)C1C[C@@H]2O
	(2R,5S,14S,15S)-2-[(Z)-2-fluoroethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-7-ene-5,14-diol	1	1	1	0	C[C@]12CCC3C(CC=C4C[C@@H](O)CC[C@]34\C=C/F)C1C[C@@H]2O
	(2S,5S,14S,15S)-15-methyl-2-[(1E)-prop-1-en-1-yl]tetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-7-ene-5,14-diol	1	1	1	0	C\C=C\[C@]12CC[C@H](O)CC1=CCC3C4CC[C@H](O)[C@]4(C)CCC23
	(2S,5S,14S,15S)-2-[(1Z)-but-1-en-1-yl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-7-ene-5,14-diol	1	1	1	0	CC\C=C/[C@]12CC[C@H](O)CC1=CCC3C4CC[C@H](O)[C@]4(C)CCC23
	(2R,5S,14S,15S)-2-ethynyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-7-ene-5,14-diol	1	1	1	0	C[C@]12CCC3C(CC=C4C[C@@H](O)CC[C@]34C#C)C1CC[C@@H]2O
	(2S,5S,14S,15S)-15-methyl-2-(prop-1-yn-1-yl)tetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-7-ene-5,14-diol	1	1	1	0	CC#C[C@]12CC[C@H](O)CC1=CCC3C4CC[C@H](O)[C@@]4(C)CCC23

2-[(2S,5S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-7-en-2-yl]acetaldehyde	1	1	1	0	<chem>C[C@]12CCC3C(CC=C4C[C@@H](O)CC[C@]34CC=O)C1CC[C@@H]2O</chem>
(2S,5S,14S,15S)-15-methyl-2-(prop-2-en-1-yl)tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-7-ene-5,14-diol	1	1	1	0	<chem>C[C@]12CCC3C(CC=C4C[C@@H](O)CC[C@]34CC=C)C1CC[C@@H]2O</chem>
(2R,5S,14S,15S)-2-ethyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-7-ene-5,14-diol	1	1	1	0	<chem>CC[C@]12CC[C@H](O)CC1=CCC3C4CC[C@H](O)[C@@]4(C)CCC23</chem>
(2R,5S,14S,15S)-15-methyl-2-propyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-7-ene-5,14-diol	1	1	1	0	<chem>CCC[C@]12CC[C@H](O)CC1=CCC3C4CC[C@H](O)[C@@]4(C)CCC23</chem>
(2R,5S,14S,15S)-2-[(Z)-2-methoxyethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-7-ene-5,14-diol	1	1	1	0	<chem>CO\C=C/[C@]12CC[C@H](O)CC1=CCC3C4CC[C@H](O)[C@@]4(C)CCC23</chem>
(2R,5S,14S,15S)-2-[(E)-2-methoxyethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-7-ene-5,14-diol	1	1	1	0	<chem>CO\C=C/[C@]12CC[C@H](O)CC1=CCC3C4CC[C@H](O)[C@@]4(C)CCC23</chem>
(2S,5S,14S,15S)-15-methyl-2-[(1Z)-prop-1-en-1-	1	1	1	0	<chem>C\C=C/[C@]12CC[C@H](O)CC1=CCC3C4CC[C@H](O)[C@</chem>

	yl]tetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-7-ene-5,14-diol					@]4(C)CCC23
	(2S,5S,14S,15S)-2-(hydroxymethyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-7-ene-5,14-diol	1	1	1	0	C[C@]12CCC3C(CC=C4C[C@@H](O)CC[C@]34CO)C1CC[C@@H]2O
	(2S,5S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-7-ene-2-carbaldehyde	1	1	1	0	C[C@]12CCC3C(CC=C4C[C@@H](O)CC[C@]34C=O)C1CC[C@@H]2O
	(2S,5S,14S,15S)-2-ethenyl-14,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-7-ene-5,14-diol	1	1	1	0	C[C@]1(O)CCC2C3CC=C4C[C@@H](O)CC[C@]4(C=C)C3CC[C@]12C
	(2S,5S,14R,15S)-2-ethenyl-14-ethynyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-7-ene-5,14-diol	1	1	1	0	C[C@]12CCC3C(CC=C4C[C@@H](O)CC[C@]34C=C)C1CC[C@@]2(O)C#C
	(2R,5S,14S,15S)-2-[(Z)-2-bromoethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-7-ene-5,14-diol	1	1	1	0	C[C@]12CCC3C(CC=C4C[C@@H](O)CC[C@]34\C=C/Br)C1CC[C@@H]2O
	(2R,5S,14S,15S)-2-[(E)-2-bromoethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-7-ene-5,14-diol	1	1	1	0	C[C@]12CCC3C(CC=C4C[C@@H](O)CC[C@]34\C=C\Br)C1CC[C@@H]2O

	15]]heptadec-7-ene-5,14-diol					
	(2S,14S,15S)-2-ethenyl-14-hydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15]]heptadec-6-en-5-one	1	1	1	0	<chem>C[C@]12CCC3C(CCC4=CC(=O)CC[C@]34C=C)C1CC[C@@H]2O</chem>
	(2S,5S,14S,15S)-15-methyl-2-(prop-2-yn-1-yl)tetracyclo[8.7.0.0{2,7}.0{11,15]]heptadec-7-ene-5,14-diol	1	1	1	0	<chem>C[C@]12CCC3C(CC=C4C[C@@H](O)CC[C@]34CC#C)C1CC[C@@H]2O</chem>
	3-hydroxy-4-methylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1c(O)ccc2c1OC(=O)c3ccccc23</chem>
	3-hydroxy-4,7-dimethylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1cccc2c3ccc(O)c(C)c3OC(=O)c12</chem>
	3-hydroxy-8-methoxy-4-methylbenzo[c]chromen-6-one	1	1	1	0	<chem>COc1ccc2c(c1)C(=O)Oc3c(C)c(O)ccc23</chem>
	8-bromo-3-hydroxy-4-methylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1c(O)ccc2c1OC(=O)c3cc(Br)ccc23</chem>
	N-{3-hydroxy-4,7-dimethyl-6-oxobenzo[c]chromen-8-yl}methanesulfonamide	1	1	1	0	<chem>Cc1c(O)ccc2c1OC(=O)c3c(C)c(NS(=O)(=O)C)ccc23</chem>
	3-hydroxy-4,10-dimethylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1cccc2C(=O)Oc3c(C)c(O)ccc3c12</chem>

10-ethenyl-3-hydroxy-4-methylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1c(O)ccc2c1OC(=O)c3cccc(C=C)c23</chem>
4,6,7,10-tetramethyl-6H-benzo[c]chromene-3,8-diol	1	1	1	0	<chem>CC1Oc2c(C)c(O)ccc2c3c(C)cc(O)c(C)c13</chem>
6-ethyl-4,7,10-trimethyl-6H-benzo[c]chromene-3,8-diol	1	1	1	0	<chem>CCC1Oc2c(C)c(O)ccc2c3c(C)cc(O)c(C)c13</chem>
4,10-dimethyl-6-(2-methylpropyl)-6H-benzo[c]chromene-3,8-diol	1	1	1	0	<chem>CC(C)CC1Oc2c(C)c(O)ccc2c3c(C)cc(O)cc13</chem>
4,6,6,7-tetramethylbenzo[c]chromene-3,8-diol	1	1	1	0	<chem>Cc1c(O)ccc2c1OC(C)(C)c3c(C)c(O)ccc23</chem>
4,6,7,10-tetramethyl-6-(prop-2-en-1-yl)benzo[c]chromene-3,8-diol	1	1	1	0	<chem>Cc1cc(O)c(C)c2c1c3ccc(O)c(C)c3OC2(C)CC=C</chem>
3-hydroxy-8,10-dimethylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1cc(C)c2c(c1)C(=O)Oc3cc(O)ccc23</chem>
8-bromo-4-ethyl-3-hydroxybenzo[c]chromen-6-one	1	1	1	0	<chem>CCc1c(O)ccc2c1OC(=O)c3cc(Br)ccc23</chem>
4,10-dimethyl-6-propyl-6H-benzo[c]chromene-3,8-diol	1	1	1	0	<chem>CCCC1Oc2c(C)c(O)ccc2c3c(C)cc(O)cc13</chem>
7-ethyl-4-fluoro-3,8-dihydroxybenzo[c]chromen-6-one	1	1	1	0	<chem>CCc1c(O)ccc2c3ccc(O)c(F)c3OC(=O)c12</chem>

	4-bromo-3,8-dihydroxy-7-methylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1c(O)ccc2c3ccc(O)c(Br)c3OC(=O)c12</chem>
	10-ethyl-3,8-dihydroxy-4-methylbenzo[c]chromen-6-one	1	1	1	0	<chem>CCc1cc(O)cc2C(=O)Oc3c(C)c(O)ccc3c12</chem>
	3,8-dihydroxy-4,10-dimethylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1cc(O)cc2C(=O)Oc3c(C)c(O)ccc3c12</chem>
	8-ethenyl-3-hydroxy-4-methylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1c(O)ccc2c1OC(=O)c3cc(C=C)ccc23</chem>
	4,7-dimethyl-6H-benzo[c]chromene-3,8-diol	1	1	1	0	<chem>Cc1c(O)ccc2c1COc3c(C)c(O)ccc23</chem>
	3,8-dihydroxy-1,4,7-trimethylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1cc(O)c(C)c2OC(=O)c3c(C)c(O)ccc3c12</chem>
	3,8-dihydroxy-4,7,10-trimethylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1cc(O)c(C)c2C(=O)Oc3c(C)c(O)ccc3c12</chem>
	4,7-dichloro-9-fluoro-3,8-dihydroxybenzo[c]chromen-6-one	1	1	1	0	<chem>Oc1ccc2c(OC(=O)c3c(Cl)c(O)c(F)cc23)c1Cl</chem>
	4,9-dichloro-3,8-dihydroxy-7-methylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1c(O)c(Cl)cc2c3ccc(O)c(Cl)c3OC(=O)c12</chem>
	4,9-dichloro-3,8-dihydroxy-7,10-dimethylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1c(O)c(Cl)c(C)c2c3ccc(O)c(Cl)c3OC(=O)c12</chem>
	3-hydroxy-4-methyl-10-[(1E)-prop-	1	1	1	0	<chem>C\\C=C\\c1cccc2C(=O)Oc3c(C)c(O)ccc3c12</chem>

	1-en-1-yl]benzo[c]chromen-6-one					
73166-28-6	5-ethenyl-1-methyl-9,10-dihydrophenanthrene-2,7-diol	1	1	1	0	<chem>Cc1c(O)ccc2c1CCc3cc(O)cc(C=C)c23</chem>
	3,8-dihydroxy-4-methylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1c(O)ccc2c1OC(=O)c3cc(O)ccc23</chem>
	3-hydroxy-8-methoxy-4,7-dimethylbenzo[c]chromen-6-one	1	1	1	0	<chem>COc1ccc2c3ccc(O)c(C)c3OC(=O)c2c1C</chem>
	3,8-dihydroxy-7-methylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1c(O)ccc2c3ccc(O)cc3OC(=O)c12</chem>
	3,8-dihydroxy-1,4-dimethylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1cc(O)c(C)c2OC(=O)c3cc(O)ccc3c12</chem>
	8-amino-3-hydroxy-4,7-dimethylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1c(O)ccc2c1OC(=O)c3c(C)c(N)ccc23</chem>
	4,7-dichloro-3,8-dihydroxy-10-methylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1cc(O)c(Cl)c2C(=O)Oc3c(Cl)c(O)ccc3c12</chem>
	3,7,8-trihydroxy-4-methylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1c(O)ccc2c1OC(=O)c3c(O)c(O)ccc23</chem>
	7-ethyl-3,8-dihydroxy-4-methylbenzo[c]chromen-6-one	1	1	1	0	<chem>CCc1c(O)ccc2c3ccc(O)c(C)c3OC(=O)c12</chem>
	4-ethyl-3,8-dihydroxy-7-methylbenzo[c]chromen-6-one	1	1	1	0	<chem>CCc1c(O)ccc2c1OC(=O)c3c(C)c(O)ccc23</chem>

	4-fluoro-3,8-dihydroxy-7-methylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1c(O)ccc2c3ccc(O)c(F)c3OC(=O)c12</chem>
	6-ethyl-4,7-dimethyl-6H-benzo[c]chromene-3,8-diol	1	1	1	0	<chem>CCC1Oc2c(C)c(O)ccc2c3ccc(O)c(C)c13</chem>
	6-ethyl-4,10-dimethyl-6H-benzo[c]chromene-3,8-diol	1	1	1	0	<chem>CCC1Oc2c(C)c(O)ccc2c3c(C)cc(O)cc13</chem>
	3,8-dihydroxy-1,7-dimethylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1cc(O)cc2OC(=O)c3c(C)c(O)ccc3c12</chem>
	4,10-dimethyl-6H-benzo[c]chromene-3,8-diol	1	1	1	0	<chem>Cc1cc(O)cc2COc3c(C)c(O)ccc3c12</chem>
	4,6,10-trimethyl-6H-benzo[c]chromene-3,8-diol	1	1	1	0	<chem>CC1Oc2c(C)c(O)ccc2c3c(C)cc(O)cc13</chem>
	4,6,7-trimethyl-6H-benzo[c]chromene-3,8-diol	1	1	1	0	<chem>CC1Oc2c(C)c(O)ccc2c3ccc(O)c(C)c13</chem>
	8-bromo-3-hydroxy-4,9-dimethylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1cc2c(cc1Br)C(=O)Oc3c(C)c(O)ccc23</chem>
	9-bromo-3-hydroxy-8-methoxy-4-methylbenzo[c]chromen-6-one	1	1	1	0	<chem>COc1cc2C(=O)Oc3c(C)c(O)ccc3c2cc1Br</chem>
	8-bromo-9-[(1E)-but-1-en-1-yl]-3-hydroxy-4-methylbenzo[c]chromen-6-one	1	1	1	0	<chem>CC\C=C\c1cc2c(cc1Br)C(=O)Oc3c(C)c(O)ccc23</chem>

3-hydroxy-4,8,10-trimethylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1cc(C)c2c(c1)C(=O)Oc3c(C)c(O)ccc23</chem>
7,9-dibromo-3-hydroxy-4-methylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1c(O)ccc2c1OC(=O)c3c(Br)cc(Br)cc23</chem>
10-bromo-3-hydroxy-4,8-dimethylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1cc(Br)c2c(c1)C(=O)Oc3c(C)c(O)ccc23</chem>
3-hydroxy-4,8-dimethyl-10-(prop-2-en-1-yl)benzo[c]chromen-6-one	1	1	1	0	<chem>Cc1cc(CC=C)c2c(c1)C(=O)Oc3c(C)c(O)ccc23</chem>
10-ethyl-3-hydroxy-8-methoxy-4-methylbenzo[c]chromen-6-one	1	1	1	0	<chem>CCc1cc(OC)cc2C(=O)Oc3c(C)c(O)ccc3c12</chem>
3-hydroxy-4,7,10-trimethylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1ccc(C)c2c3ccc(O)c(C)c3OC(=O)c12</chem>
N-{3-hydroxy-4,7-dimethyl-6-oxobenzo[c]chromen-8-yl}formamide	1	1	1	0	<chem>Cc1c(O)ccc2c1OC(=O)c3c(C)c(NC=O)ccc23</chem>
10-ethenyl-3-hydroxy-8-methoxy-4-methylbenzo[c]chromen-6-one	1	1	1	0	<chem>COc1cc(C=C)c2c(c1)C(=O)Oc3c(C)c(O)ccc23</chem>
9-bromo-3-hydroxy-4,8,10-trimethylbenzo[c]chromen-6-one	1	1	1	0	<chem>Cc1cc2C(=O)Oc3c(C)c(O)ccc3c2c(C)c1Br</chem>
3-hydroxy-9-methoxy-4,8,10-trimethylbenzo[c]chromen-6-one	1	1	1	0	<chem>COc1c(C)cc2C(=O)Oc3c(C)c(O)ccc3c2c1C</chem>

7-bromo-3-hydroxy-9-methoxy-4,8,10-trimethylbenzo[c]chromen-6-one	1	1	1	0	<chem>COc1c(C)c(Br)c2C(=O)Oc3c(C)c(O)ccc3c2c1C</chem>
5,7-dihydroxy-3-(4-hydroxyphenyl)-8-methylquinazolin-4-one	1	1	1	0	<chem>Cc1c(O)cc(O)c2C(=O)N(C=Nc12)c3ccc(O)cc3</chem>
5,7-dihydroxy-3-(4-hydroxyphenyl)-6-propylquinazolin-4-one	1	1	1	0	<chem>CCCC1c(O)cc2N=CN(C(=O)c2c1O)c3ccc(O)cc3</chem>
7-hydroxy-3-(4-hydroxyphenyl)quinazolin-4-one	1	1	1	0	<chem>Oc1ccc(cc1)N2C=Nc3cc(O)ccc3C2=O</chem>
5-ethyl-7-hydroxy-3-(4-hydroxyphenyl)quinazolin-4-one	1	1	1	0	<chem>CCc1cc(O)cc2N=CN(C(=O)c12)c3ccc(O)cc3</chem>
5,7-dihydroxy-3-(4-hydroxyphenyl)chromene-4-thione	1	1	1	0	<chem>Oc1ccc(cc1)C2=COc3cc(O)cc(O)c3C2=S</chem>
5,7-dihydroxy-3-(3-hydroxyphenyl)quinazolin-4-one	1	1	1	0	<chem>Oc1cccc(c1)N2C=Nc3cc(O)cc(O)c3C2=O</chem>
5,7-dihydroxy-3-phenylquinazolin-4-one	1	1	1	0	<chem>Oc1cc(O)c2C(=O)N(C=Nc2c1)c3ccccc3</chem>
5,7-dihydroxy-3-(4-hydroxyphenyl)-2-methylquinazolin-4-one	1	1	1	0	<chem>CC1=Nc2cc(O)cc(O)c2C(=O)N1c3ccc(O)cc3</chem>
5,7-dihydroxy-3-(4-hydroxy-2-methylphenyl)quinazolin-4-one	1	1	1	0	<chem>Cc1cc(O)ccc1N2C=Nc3cc(O)cc(O)c3C2=O</chem>

3-(3-chloro-4-hydroxyphenyl)-5,7-dihydroxyquinazolin-4-one	1	1	1	0	<chem>Oc1cc(O)c2C(=O)N(C=Nc2c1)c3ccc(O)c(Cl)c3</chem>
5,7-dihydroxy-3-(4-hydroxyphenyl)quinazolin-4-one	1	1	1	0	<chem>Oc1ccc(cc1)N2C=Nc3cc(O)cc(O)c3C2=O</chem>
3-(2-fluoro-4-hydroxyphenyl)-5,7-dihydroxyquinazolin-4-one	1	1	1	0	<chem>Oc1ccc(N2C=Nc3cc(O)cc(O)c3C2=O)c(F)c1</chem>
3-(2-chloro-4-hydroxyphenyl)-5,7-dihydroxyquinazolin-4-one	1	1	1	0	<chem>Oc1ccc(N2C=Nc3cc(O)cc(O)c3C2=O)c(Cl)c1</chem>
5,7-dihydroxy-3-(4-hydroxy-3-methylphenyl)quinazolin-4-one	1	1	1	0	<chem>Cc1cc(ccc1O)N2C=Nc3cc(O)cc(O)c3C2=O</chem>
5,7-dihydroxy-3-(5-hydroxypyridin-2-yl)quinazolin-4-one	1	1	1	0	<chem>Oc1ccc(nc1)N2C=Nc3cc(O)cc(O)c3C2=O</chem>
2-ethyl-5,7-dihydroxy-3-(4-hydroxyphenyl)quinazolin-4-one	1	1	1	0	<chem>CCC1=Nc2cc(O)cc(O)c2C(=O)N1c3ccc(O)cc3</chem>
5,7-dihydroxy-3-(4-hydroxyphenyl)-2-propylquinazolin-4-one	1	1	1	0	<chem>CCCC1=Nc2cc(O)cc(O)c2C(=O)N1c3ccc(O)cc3</chem>
2-butyl-5,7-dihydroxy-3-(4-hydroxyphenyl)quinazolin-4-one	1	1	1	0	<chem>CCCCC1=Nc2cc(O)cc(O)c2C(=O)N1c3ccc(O)cc3</chem>
5,7-dihydroxy-3-(4-hydroxyphenyl)-2-isopropylquinazolin-4-one	1	1	1	0	<chem>CC(C)C1=Nc2cc(O)cc(O)c2C(=O)N1c3ccc(O)cc3</chem>
methyl 7-hydroxy-3-(4-hydroxyphenyl)-4-oxoquinazoline-	1	1	1	0	<chem>COC(=O)c1cc(O)cc2N=CN(C(=O)c12)c3ccc(O)cc3</chem>

	5-carboxylate					
	7-hydroxy-3-(4-hydroxyphenyl)-5-phenylquinazolin-4-one	1	1	1	0	<chem>Oc1ccc(cc1)N2C=Nc3cc(O)cc(c4ccccc4)c3C2=O</chem>
	7-hydroxy-5-(hydroxymethyl)-3-(4-hydroxyphenyl)quinazolin-4-one	1	1	1	0	<chem>OCc1cc(O)cc2N=CN(C(=O)c12)c3ccc(O)cc3</chem>
	7-hydroxy-3-(4-hydroxyphenyl)-5-(prop-1-en-2-yl)quinazolin-4-one	1	1	1	0	<chem>CC(=C)c1cc(O)cc2N=CN(C(=O)c12)c3ccc(O)cc3</chem>
	5,7-dihydroxy-3-(4-hydroxyphenyl)-2-sulfanylidene-1H-quinazolin-4-one	1	1	1	0	<chem>Oc1ccc(cc1)N2C(=S)Nc3cc(O)cc(O)c3C2=O</chem>
	5,7-dihydroxy-3-(4-hydroxyphenyl)-1H-quinazoline-2,4-dione	1	1	1	0	<chem>Oc1ccc(cc1)N2C(=O)Nc3cc(O)cc(O)c3C2=O</chem>
	5,7-dihydroxy-3-(4-hydroxyphenyl)quinazoline-4-thione	1	1	1	0	<chem>Oc1ccc(cc1)N2C=Nc3cc(O)cc(O)c3C2=S</chem>
	3-(3-fluoro-4-hydroxyphenyl)-5,7-dihydroxyquinazoline-4-thione	1	1	1	0	<chem>Oc1cc(O)c2C(=S)N(C=Nc2c1)c3ccc(O)c(F)c3</chem>
	5,7-dihydroxy-3-(4-hydroxy-3-methylphenyl)quinazoline-4-thione	1	1	1	0	<chem>Cc1cc(ccc1O)N2C=Nc3cc(O)cc(O)c3C2=S</chem>
	5,7-dihydroxy-3-(6-hydroxypyridin-3-yl)quinazolin-4-one	1	1	1	0	<chem>Oc1cc(O)c2C(=O)N(C=Nc2c1)c3ccc(O)nc3</chem>

	3-(3-fluoro-4-hydroxyphenyl)-5,7-dihydroxyquinazolin-4-one	1	1	1	0	<chem>Oc1cc(O)c2C(=O)N(C=Nc2c1)c3ccc(O)c(F)c3</chem>
	5-ethyl-7-hydroxy-3-(4-hydroxyphenyl)quinazoline-4-thione	1	1	1	0	<chem>CCc1cc(O)cc2N=CN(C(=S)c12)c3ccc(O)cc3</chem>
	7-hydroxy-2,3-bis(4-hydroxyphenyl)quinazolin-4-one	1	1	1	0	<chem>Oc1ccc(cc1)N2C(=O)c3ccc(O)cc3N=C2c4ccc(O)cc4</chem>
	5-amino-7-hydroxy-3-(4-hydroxyphenyl)quinazolin-4-one	1	1	1	0	<chem>Nc1cc(O)cc2N=CN(C(=O)c12)c3ccc(O)cc3</chem>
	7-hydroxy-3-(4-hydroxyphenyl)-5-methylquinazolin-4-one	1	1	1	0	<chem>Cc1cc(O)cc2N=CN(C(=O)c12)c3ccc(O)cc3</chem>
	5,7-dihydroxy-3-(5-hydroxypyridin-2-yl)quinazoline-4-thione	1	1	1	0	<chem>Oc1ccc(nc1)N2C=Nc3cc(O)cc(O)c3C2=S</chem>
	9a-benzyl-7-hydroxy-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>Oc1ccc2C3=CC(=O)CCC3(Cc4ccccc4)Cc2c1</chem>
	7-hydroxy-4,9a-dimethyl-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>CC1=C2c3ccc(O)cc3CC2(C)CCC1=O</chem>
	9a-ethyl-7-hydroxy-4-methyl-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>CCC12CCC(=O)C(=C1c3ccc(O)cc3C2)C</chem>
	7-hydroxy-4-methyl-9a-propyl-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>CCCC12CCC(=O)C(=C1c3ccc(O)cc3C2)C</chem>

7-hydroxy-9a-isopropyl-4-methyl-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>CC(C)C12CCC(=O)C(=C1c3ccc(O)cc3C2)C</chem>
7-hydroxy-3-oxo-9a-phenyl-2,9-dihydro-1H-fluorene-4-carbonitrile	1	1	1	0	<chem>Oc1ccc2C3=C(C#N)C(=O)CCC3(Cc2c1)c4ccccc4</chem>
9a-butyl-7-hydroxy-4-methyl-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>CCCCC12CCC(=O)C(=C1c3ccc(O)cc3C2)C</chem>
7-hydroxy-4-methyl-9a-(2-methylpropyl)-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>CC(C)CC12CCC(=O)C(=C1c3ccc(O)cc3C2)C</chem>
7-hydroxy-9a-pentyl-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>CCCCCC12CCC(=O)C(=C1c3ccc(O)cc3C2</chem>
7-hydroxy-9a-(2-hydroxyethyl)-4-methyl-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>CC1=C2c3ccc(O)cc3CC2(CCO)CCC1=O</chem>
7-hydroxy-4-methyl-9a-phenyl-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>CC1=C2c3ccc(O)cc3CC2(CCC1=O)c4ccccc4</chem>
9a-butyl-7-hydroxy-4-phenyl-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>CCCCC12CCC(=O)C(=C1c3ccc(O)cc3C2)c4ccccc4</chem>
9a-butyl-7-hydroxy-3-oxo-2,9-dihydro-1H-fluorene-4-carbonitrile	1	1	1	0	<chem>CCCCC12CCC(=O)C(=C1c3ccc(O)cc3C2)C#N</chem>
9a-butyl-7-hydroxy-4-(trifluoromethyl)-2,9-dihydro-1H-	1	1	1	0	<chem>CCCCC12CCC(=O)C(=C1c3ccc(O)cc3C2)C(F)(F)F</chem>

	fluoren-3-one					
	9a-butyl-4-chloro-7-hydroxy-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>CCCC12CCC(=O)C(=C1c3ccc(O)cc3C2)Cl</chem>
	9a-butyl-7-hydroxy-4-iodo-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>CCCC12CCC(=O)C(=C1c3ccc(O)cc3C2)I</chem>
	4-bromo-7-hydroxy-9a-phenyl-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>Oc1ccc2C3=C(Br)C(=O)CCC3(Cc2c1)c4ccccc4</chem>
	4-(furan-2-yl)-7-hydroxy-9a-phenyl-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>Oc1ccc2C3=C(C(=O)CCC3(Cc2c1)c4ccccc4)c5occc5</chem>
	7-hydroxy-1,2,9,9a-tetrahydrofluoren-3-one	1	1	1	0	<chem>Oc1ccc2C3=CC(=O)CCC3Cc2c1</chem>
	7-hydroxy-9a-methyl-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>CC12CCC(=O)C=C1c3ccc(O)cc3C2</chem>
	9a-ethyl-7-hydroxy-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>CCC12CCC(=O)C=C1c3ccc(O)cc3C2</chem>
	4-bromo-7-hydroxy-9a-methyl-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>CC12CCC(=O)C(=C1c3ccc(O)cc3C2)Br</chem>
	4-bromo-9a-ethyl-7-hydroxy-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>CCC12CCC(=O)C(=C1c3ccc(O)cc3C2)Br</chem>
	7-hydroxy-9a-propyl-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>CCCC12CCC(=O)C=C1c3ccc(O)cc3C2</chem>

9a-butyl-7-hydroxy-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	CCCCC12CCC(=O)C=C1c3ccc(O)cc3C2
4-bromo-7-hydroxy-9a-propyl-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	CCCC12CCC(=O)C(=C1c3ccc(O)cc3C2)Br
9a-butyl-4-ethyl-7-hydroxy-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	CCCCC12CCC(=O)C(=C1c3ccc(O)cc3C2)CC
9a-butyl-7-hydroxy-4-propyl-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	CCCCC12CCC(=O)C(=C1c3ccc(O)cc3C2)CCC
4,9a-dibutyl-7-hydroxy-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	CCCCC1=C2c3ccc(O)cc3CC2(CCCC)CCC1=O
9a-butyl-4-(furan-2-yl)-7-hydroxy-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	CCCCC12CCC(=O)C(=C1c3ccc(O)cc3C2)c4occc4
9a-butyl-7-hydroxy-4-(thiophen-2-yl)-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	CCCCC12CCC(=O)C(=C1c3ccc(O)cc3C2)c4cccs4
(9aR)-9a-butyl-7-hydroxy-4-methyl-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	CCCC[C@]12CCC(=O)C(=C1c3ccc(O)cc3C2)C
(9aS)-4-bromo-9a-butyl-7-hydroxy-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	CCCC[C@@]12CCC(=O)C(=C1c3ccc(O)cc3C2)Br
(9aR)-4-bromo-9a-butyl-7-hydroxy-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	CCCC[C@]12CCC(=O)C(=C1c3ccc(O)cc3C2)Br
(9aS)-9a-ethyl-6-phenyl-3H,8H,9H,10H-indeno[2,1-	1	1	1	0	CC[C@@]12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2)c5ccccc5

	e]indazol-7-one					
	6-bromo-9a-ethyl-1-fluoro-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	CCC12CCC(=O)C(=C1c3ccc4[nH]nc(F)c4c3C2)Br
	6,9a-diethyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	CCC1=C2c3ccc4[nH]ncc4c3CC2(CC)CCC1=O
	(9aS)-9a-butyl-6-ethyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	CCCC[C@@]12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2)CC
	methyl 9a-ethyl-7-oxo-3H,8H,9H,10H-indeno[2,1-e]indazole-6-carboxylate	1	1	1	0	CCC12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2)C(=O)OC
	(9aS)-6-chloro-9a-ethyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	CC[C@@]12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2)Cl
	6-bromo-9a-methyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	CC12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2)Br
	(9aS)-6-bromo-9a-(2-cyclopropylethyl)-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	BrC1=C2c3ccc4[nH]ncc4c3C[C@]2(CCC5CC5)CCC1=O
	(9aS)-9a-methyl-6-(trifluoromethyl)-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	C[C@@]12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2)C(F)(F)F

	methyl (9aS)-9a-butyl-7-oxo-3H,8H,9H,10H-indeno[2,1-e]indazole-6-carboxylate	1	1	1	0	<chem>CCCC[C@@]12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2)C(=O)OC</chem>
	9a-ethyl-6-methyl-3H,8H,9H-indeno[2,1-e]indazole-7,10-dione	1	1	1	0	<chem>CCC12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2=O)C</chem>
	9a-ethyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CCC12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2</chem>
	(9aS)-9a-ethyl-6-(trifluoromethyl)-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CC[C@@]12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2)C(F)(F)F</chem>
	9a-butyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CCCCC12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2</chem>
	6,9a-dimethyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CC1=C2c3ccc4[nH]ncc4c3CC2(C)CCC1=O</chem>
	(9aS)-9a-butyl-6-(trifluoromethyl)-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CCCC[C@@]12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2)C(F)(F)F</chem>
	(9aS)-6-cyclopropyl-9a-ethyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CC[C@@]12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2)C5CC5</chem>
	(9aS)-9a-ethyl-6-methyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CC[C@@]12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2)C</chem>

(9aS)-6-bromo-9a-ethyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CC[C@@]12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2)Br</chem>
6-bromo-9a-propyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CCCC12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2)Br</chem>
(9aR)-6-bromo-9a-(cyclopropylmethyl)-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>BrC1=C2c3ccc4[nH]ncc4c3C[C@]2(CC5CC5)CCC1=O</chem>
(9aS)-9a-ethyl-1-fluoro-6-(trifluoromethyl)-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CC[C@@]12CCC(=O)C(=C1c3ccc4[nH]nc(F)c4c3C2)C(F)(F)F</chem>
(9aS)-9a-butyl-6-ethyl-1-fluoro-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CCCC[C@@]12CCC(=O)C(=C1c3ccc4[nH]nc(F)c4c3C2)CC</chem>
(9aS)-9a-butyl-1-fluoro-6-(trifluoromethyl)-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CCCC[C@@]12CCC(=O)C(=C1c3ccc4[nH]nc(F)c4c3C2)C(F)(F)F</chem>
(9aR)-6-chloro-9a-ethyl-3H,8H,9H-indeno[2,1-e]indazole-7,10-dione	1	1	1	0	<chem>CC[C@@]12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2=O)Cl</chem>
6-bromo-9a-ethyl-3H,8H,9H-indeno[2,1-e]indazole-7,10-dione	1	1	1	0	<chem>CCC12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2=O)Br</chem>
(9aR)-9a-ethyl-6-(trifluoromethyl)-3H,8H,9H-indeno[2,1-e]indazole-	1	1	1	0	<chem>CC[C@@]12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2=O)C(F)(F)F</chem>

	7,10-dione					
	(9aR)-9a-butyl-6-(trifluoromethyl)-3H,8H,9H-indeno[2,1-e]indazole-7,10-dione	1	1	1	0	<chem>CCCC[C@@]12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2=O)C(F)(F)F</chem>
	(9aR)-9a-ethyl-6-methyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CC[C@]12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2)C</chem>
	9a-butyl-6-cyclopropyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CCCCC12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2)C5CC5</chem>
	1-chloro-9a-ethyl-6-methyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CCC12CCC(=O)C(=C1c3ccc4[nH]nc(Cl)c4c3C2)C</chem>
	1-bromo-9a-ethyl-6-methyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CCC12CCC(=O)C(=C1c3ccc4[nH]nc(Br)c4c3C2)C</chem>
	(9aS)-6-chloro-9a-ethyl-1-fluoro-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CC[C@@]12CCC(=O)C(=C1c3ccc4[nH]nc(F)c4c3C2)Cl</chem>
	6-methyl-9a-propyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CCCC12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2)C</chem>
	9a-butyl-6-methyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CCCCC12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2)C</chem>

6-[(1E)-(hydroxyimino)methyl]-2,3-bis(4-methoxyphenyl)-N-methylaniline	1	1	1	0	CNc1c(\C=N\O)ccc(c2ccc(OC)cc2)c1c3ccc(OC)cc3
4-{4-[(1E)-(hydroxyimino)methyl]-3-(methylamino)-2-phenylphenyl}phenol	1	1	1	0	CNc1c(\C=N\O)ccc(c2ccc(O)cc2)c1c3cccc3
6-bromo-9a-butyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	CCCCC12CCC(=O)C(=C1c3ccc4[nH]ncc4c3C2)Br
4-{3-[(1E)-(hydroxyimino)methyl]-2-(methylamino)-6-phenylphenyl}phenol	1	1	1	0	CNc1c(\C=N\O)ccc(c2cccc2)c1c3ccc(O)cc3
6-[(1E)-(hydroxyimino)methyl]-2,3-bis(3-methoxyphenyl)-N-methylaniline	1	1	1	0	CNc1c(\C=N\O)ccc(c2ccc(OC)c2)c1c3ccc(OC)c3
4-{3-[(1E)-(hydroxyimino)methyl]-6-(4-hydroxyphenyl)-2-(methylamino)phenyl}phenol	1	1	1	0	CNc1c(\C=N\O)ccc(c2ccc(O)cc2)c1c3ccc(O)cc3
6-[(1E)-(hydroxyimino)methyl]-N-methyl-2,3-bis(4-methylphenyl)aniline	1	1	1	0	CNc1c(\C=N\O)ccc(c2ccc(C)cc2)c1c3ccc(C)cc3
6-[(1E)-(hydroxyimino)methyl]-N-methyl-2,3-bis(3-methylphenyl)aniline	1	1	1	0	CNc1c(\C=N\O)ccc(c2ccc(C)c2)c1c3ccc(C)c3

3-{3-[(1E)-(hydroxyimino)methyl]-6-(3-hydroxyphenyl)-2-(methylamino)phenyl}phenol	1	1	1	0	CNc1c(\C=N\O)ccc(c2cccc(O)c2)c1c3cccc(O)c3
9a-benzyl-7-hydroxy-4-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	Oc1ccc2C3=C(C(=O)CCC3(Cc4cccc4)Cc2c1)c5ccc(OCCN6CCCC6)cc5
9a-benzyl-4-butyl-7-hydroxy-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	CCCCC1=C2c3ccc(O)cc3CC2(Cc4cccc4)CCC1=O
9a-benzyl-7-hydroxy-4-(4-hydroxyphenyl)-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	Oc1ccc(cc1)C2=C3c4ccc(O)cc4CC3(Cc5cccc5)CCC2=O
9a-benzyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	O=C1CCC2(Cc3cccc3)Cc4c(ccc5[nH]ncc45)C2=C1
9a-benzyl-6-methyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	CC1=C2c3ccc4[nH]ncc4c3CC2(Cc5cccc5)CCC1=O
9a-benzyl-7-hydroxy-4-{4-[2-(morpholin-4-yl)ethoxy]phenyl}-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	Oc1ccc2C3=C(C(=O)CCC3(Cc4cccc4)Cc2c1)c5ccc(OCCN6COC6)cc5
9a-benzyl-4-{4-[2-(dimethylamino)ethoxy]phenyl}-7-hydroxy-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	CN(C)CCOc1ccc(cc1)C2=C3c4ccc(O)cc4CC3(Cc5cccc5)CCC2=O
9a-[(4-fluorophenyl)methyl]-6-	1	1	1	0	CC1=C2c3ccc4[nH]ncc4c3CC2(Cc5ccc(F)cc5)CCC1=O

	methyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one					
	9a-[(3-fluorophenyl)methyl]-6-methyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CC1=C2c3ccc4[nH]ncc4c3CC2(Cc5cccc(F)c5)CCC1=O</chem>
	9a-[(2-fluorophenyl)methyl]-6-methyl-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>CC1=C2c3ccc4[nH]ncc4c3CC2(Cc5ccccc5F)CCC1=O</chem>
	9a-benzyl-6-methyl-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	<chem>CC1=C2c3ccc4[nH]nnc4c3CC2(Cc5ccccc5)CCC1=O</chem>
	9a-[(4-chlorophenyl)methyl]-7-hydroxy-4-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>Oc1ccc2C3=C(C(=O)CCC3(Cc4ccc(Cl)cc4)Cc2c1)c5ccc(OCCN6CCCCC6)cc5</chem>
	9a-[(4-fluorophenyl)methyl]-6-methyl-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	<chem>CC1=C2c3ccc4[nH]nnc4c3CC2(Cc5ccc(F)cc5)CCC1=O</chem>
	9a-benzyl-6-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-3H,8H,9H,10H-indeno[2,1-e]indazol-7-one	1	1	1	0	<chem>O=C1CCC2(Cc3ccccc3)Cc4c(ccc5[nH]ncc45)C2=C1c6ccc(OCN7CCCCC7)cc6</chem>
	(9aS)-9a-butyl-6-(trifluoromethyl)-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	<chem>CCCC[C@@]12CCC(=O)C(=C1c3ccc4[nH]nnc4c3C2)C(F)(F)F</chem>

9a-butyl-6-(furan-2-yl)-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	CCCCC12CCC(=O)C(=C1c3ccc4[nH]nnc4c3C2)c5occc5
(9aS)-9a-butyl-6-(thiophen-2-yl)-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	CCCC[C@@]12CCC(=O)C(=C1c3ccc4[nH]nnc4c3C2)c5cccs5
6-bromo-9a-butyl-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	CCCCC12CCC(=O)C(=C1c3ccc4[nH]nnc4c3C2)Br
(9aS)-9a-ethyl-6-(trifluoromethyl)-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	CC[C@@]12CCC(=O)C(=C1c3ccc4[nH]nnc4c3C2)C(F)(F)F
6-methyl-9a-propyl-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	CCCC12CCC(=O)C(=C1c3ccc4[nH]nnc4c3C2)C
6-ethyl-9a-propyl-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	CCCC12CCC(=O)C(=C1c3ccc4[nH]nnc4c3C2)CC
6,9a-dipropyl-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	CCCC1=C2c3ccc4[nH]nnc4c3CC2(CCC)CCC1=O
6-bromo-9a-propyl-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	CCCC12CCC(=O)C(=C1c3ccc4[nH]nnc4c3C2)Br
9a-butyl-6-methyl-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	CCCCC12CCC(=O)C(=C1c3ccc4[nH]nnc4c3C2)C
(9aR)-9a-butyl-6-ethyl-3H,8H,9H,10H-fluoreno[1,2-	1	1	1	0	CCCC[C@]12CCC(=O)C(=C1c3ccc4[nH]nnc4c3C2)CC

	d][1,2,3]triazol-7-one					
	(9aS)-9a-butyl-6-ethyl-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	CCCC[C@@]12CCC(=O)C(=C1c3ccc4[nH]nnc4c3C2)CC
	9a-butyl-6-propyl-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	CCCCC12CCC(=O)C(=C1c3ccc4[nH]nnc4c3C2)CCC
	9a-ethyl-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	CCC12CCC(=O)C(=C1c3ccc4[nH]nnc4c3C2
	9a-ethyl-6-methyl-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	CCC12CCC(=O)C(=C1c3ccc4[nH]nnc4c3C2)C
	6,9a-diethyl-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	CCC1=C2c3ccc4[nH]nnc4c3CC2(CC)CCC1=O
	(9aR)-6,9a-diethyl-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	CCC1=C2c3ccc4[nH]nnc4c3C[C@@]2(CC)CCC1=O
	(9aS)-6,9a-diethyl-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	CCC1=C2c3ccc4[nH]nnc4c3C[C@]2(CC)CCC1=O
	9a-ethyl-6-propyl-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	CCCC1=C2c3ccc4[nH]nnc4c3CC2(CC)CCC1=O
	6-butyl-9a-ethyl-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	CCCCC1=C2c3ccc4[nH]nnc4c3CC2(CC)CCC1=O
	9a-ethyl-6-(4-hydroxyphenyl)-3H,8H,9H,10H-fluoreno[1,2-	1	1	1	0	CCC12CCC(=O)C(=C1c3ccc4[nH]nnc4c3C2)c5ccc(O)cc5

	d][1,2,3]triazol-7-one					
	6-bromo-9a-ethyl-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	<chem>CCC12CCC(=O)C(=C1c3ccc4[nH]nnc4c3C2)Br</chem>
	(9aS)-6-bromo-9a-butyl-3H,8H,9H,10H-fluoreno[1,2-d][1,2,3]triazol-7-one	1	1	1	0	<chem>CCCC[C@@]12CCC(=O)C(=C1c3ccc4[nH]nnc4c3C2)Br</chem>
	(2S)-5,7-dihydroxy-2-(4-hydroxyphenyl)-8-methyl-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>Cc1c(O)cc(O)c2C(=O)C[C@H](Oc12)c3ccc(O)cc3</chem>
	(2S)-5,7-dihydroxy-2-(4-hydroxyphenyl)-8-propyl-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>CCCc1c(O)cc(O)c2C(=O)C[C@H](Oc12)c3ccc(O)cc3</chem>
	(2S)-5,7-dihydroxy-2-(4-hydroxyphenyl)-8-pentyl-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>CCCCCc1c(O)cc(O)c2C(=O)C[C@H](Oc12)c3ccc(O)cc3</chem>
	(2S)-8-heptyl-5,7-dihydroxy-2-(4-hydroxyphenyl)-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>CCCCCCCc1c(O)cc(O)c2C(=O)C[C@H](Oc12)c3ccc(O)cc3</chem>
	(2S)-5,7-dihydroxy-2-(4-hydroxyphenyl)-8-nonyl-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>CCCCCCCCCc1c(O)cc(O)c2C(=O)C[C@H](Oc12)c3ccc(O)cc3</chem>
	(2S)-5,7-dihydroxy-2-(4-hydroxyphenyl)-8-undecyl-2,3-	1	1	1	0	<chem>CCCCCCCCCCCc1c(O)cc(O)c2C(=O)C[C@H](Oc12)c3ccc(O)cc3</chem>

	dihydro-1-benzopyran-4-one					
	(2S)-5,7-dihydroxy-2-(4-hydroxyphenyl)-8-(3-methylbutyl)-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>CC(C)CCc1c(O)cc(O)c2C(=O)C[C@H](Oc12)c3ccc(O)cc3</chem>
	(2S)-5,7-dihydroxy-2-(4-hydroxyphenyl)-8-(2-methylpropyl)-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>CC(C)Cc1c(O)cc(O)c2C(=O)C[C@H](Oc12)c3ccc(O)cc3</chem>
	(2S)-8-(2,2-dimethylpropyl)-5,7-dihydroxy-2-(4-hydroxyphenyl)-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>CC(C)(C)Cc1c(O)cc(O)c2C(=O)C[C@H](Oc12)c3ccc(O)cc3</chem>
	(2S)-8-benzyl-5,7-dihydroxy-2-(4-hydroxyphenyl)-2,3-dihydro-1-benzopyran-4-one	1	1	1	0	<chem>Oc1ccc(cc1)[C@@H]2CC(=O)c3c(O)cc(O)c(Cc4ccccc4)c3O2</chem>
118-79-6	2,4,6-tribromophenol	0	1	0	1	<chem>Oc1c(Br)cc(Br)cc1Br</chem>
	2,3-dimethyl 5,6-bis(4-hydroxyphenyl)-7-oxabicyclo[2.2.1]hepta-2,5-diene-2,3-dicarboxylate	1	1	1	0	<chem>COC(=O)C1=C(C2OC1C(=C2c3ccc(O)cc3)c4ccc(O)cc4)C(=O)OC</chem>
	8,9-bis(4-hydroxyphenyl)-4-methyl-10-oxa-4-azatricyclo[5.2.1.0{2,6}]dec-8-ene-3,5-dione	1	1	1	0	<chem>CN1C(=O)C2C3OC(C2C1=O)C(=C3c4ccc(O)cc4)c5ccc(O)cc5</chem>

8,9-bis(4-hydroxyphenyl)-4-phenyl-10-oxa-4-azatricyclo[5.2.1.0{2,6}]dec-8-ene-3,5-dione	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(C3OC2C4C3C(=O)N(C4=O)c5ccccc5)c6ccc(O)cc6</chem>
phenyl 6-(3-hydroxyphenyl)-5-(4-hydroxyphenyl)-7-oxabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(C3OC2CC3S(=O)(=O)Oc4ccccc4)c5cccc(O)c5</chem>
3-[6-(benzenesulfonyl)-3-(4-hydroxyphenyl)-7-oxabicyclo[2.2.1]hept-2-en-2-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(C3OC2CC3S(=O)(=O)c4ccccc4)c5cccc(O)c5</chem>
phenyl 5-(4-hydroxyphenyl)-6-(4-methoxyphenyl)-7-oxabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>COc1ccc(cc1)C2=C(C3CC(C2O3)S(=O)(=O)Oc4ccccc4)c5ccc(O)cc5</chem>
4-[5-(benzenesulfonyl)-3-(4-methoxyphenyl)-7-oxabicyclo[2.2.1]hept-2-en-2-yl]phenol	1	1	1	0	<chem>COc1ccc(cc1)C2=C(C3CC(C2O3)S(=O)(=O)c4ccccc4)c5ccc(O)cc5</chem>
phenyl 5,6-diphenyl-7-oxabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>O=S(=O)(Oc1ccccc1)C2CC3OC2C(=C3c4ccccc4)c5ccccc5</chem>
5-(benzenesulfonyl)-2,3-diphenyl-	1	1	1	0	<chem>O=S(=O)(C1CC2OC1C(=C2c3ccccc3)c4ccccc4)c5ccccc5</chem>

	7-oxabicyclo[2.2.1]hept-2-ene					
	8,9-diphenyl-4,10-dioxatricyclo[5.2.1.0{2,6}]dec-8-ene-3,5-dione	1	1	1	0	<chem>O=C1OC(=O)C2C3OC(C12)C(=C3c4ccccc4)c5ccccc5</chem>
	4-methoxyphenyl 5,6-bis(4-hydroxyphenyl)-7-oxabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>COc1ccc(OS(=O)(=O)C2CC3OC2C(=C3c4ccc(O)cc4)c5ccc(O)cc5)cc1</chem>
	4-[6-(benzenesulfonyl)-3-(4-hydroxyphenyl)-7-oxabicyclo[2.2.1]hept-2-en-2-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(C3OC2CC3S(=O)(=O)c4ccccc4)c5ccc(O)cc5</chem>
	4-[6-(ethanesulfonyl)-3-(4-hydroxyphenyl)-7-oxabicyclo[2.2.1]hept-2-en-2-yl]phenol	1	1	1	0	<chem>CCS(=O)(=O)C1CC2OC1C(=C2c3ccc(O)cc3)c4ccc(O)cc4</chem>
	2,3-diethyl 5,6-bis(4-hydroxyphenyl)-7-oxabicyclo[2.2.1]hept-5-ene-2,3-dicarboxylate	1	1	1	0	<chem>CCOC(=O)C1C2OC(C1C(=O)OCC)C(=C2c3ccc(O)cc3)c4ccc(O)cc4</chem>
	4-hydroxyphenyl 5,6-bis(4-hydroxyphenyl)-7-oxabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>Oc1ccc(OS(=O)(=O)C2CC3OC2C(=C3c4ccc(O)cc4)c5ccc(O)cc5)cc1</chem>

	methyl 3,5,6-triphenyl-7-oxabicyclo[2.2.1]hepta-2,5-diene-2-carboxylate	1	1	1	0	<chem>COC(=O)C1=C(C2OC1C(=C2c3ccccc3)c4ccccc4)c5ccccc5</chem>
	methyl 3-(4-hydroxyphenyl)-5,6-diphenyl-7-oxabicyclo[2.2.1]hepta-2,5-diene-2-carboxylate	1	1	1	0	<chem>COC(=O)C1=C(C2OC1C(=C2c3ccccc3)c4ccccc4)c5ccc(O)cc5</chem>
122-94-1	4-butoxyphenol	0	1	0	1	<chem>CCCCOc1ccc(O)cc1</chem>
18979-55-0	4-hexyloxyphenol	0	1	0	1	<chem>CCCCCCOc1ccc(O)cc1</chem>
	6β-hydroxy-17β-estradiol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](C[C@@H](O)c4cc(O)ccc34)[C@@H]1CC[C@@H]2O</chem>
115-32-2	dicofol	1	1	1	0	<chem>OC(c1ccc(Cl)cc1)(c2ccc(Cl)cc2)C(Cl)(Cl)Cl</chem>
	lindane	0	1	0	1	<chem>Cl[C@@H]1[C@@H](Cl)[C@H](Cl)[C@@H](Cl)[C@H](Cl)[C@H]1Cl</chem>
2385-85-5	mirex	0	1	0	1	<chem>ClC1(Cl)C2(Cl)C3(Cl)C4(Cl)C(Cl)(Cl)C5(Cl)C(Cl)(C1(Cl)C35Cl)C24Cl</chem>
30583-38-1	diazinon	0	1	0	1	<chem>CCOP(=S)(OCC)Oc1cc(C)nc(n1)C(C)C</chem>
	5-hydroxy-2-(4-hydroxyphenyl)isoindole-1,3-dione	1	1	1	0	<chem>Oc1ccc(cc1)N2C(=O)c3ccc(O)cc3C2=O</chem>
	5-hydroxy-2-(3-hydroxyphenyl)isoindole-1,3-dione	1	1	1	0	<chem>Oc1cccc(c1)N2C(=O)c3ccc(O)cc3C2=O</chem>
7154-85-0	2-(4-hydroxyphenyl)isoindole-1,3-	1	1	1	0	<chem>Oc1ccc(cc1)N2C(=O)c3ccccc3C2=O</chem>

	dione					
	5-hydroxy-2-(4-methoxyphenyl)isoindole-1,3-dione	1	1	1	0	<chem>COc1ccc(cc1)N2C(=O)c3ccc(O)cc3C2=O</chem>
	2-(2,4-dimethoxyphenyl)-5-hydroxyisoindole-1,3-dione	1	1	1	0	<chem>COc1ccc(N2C(=O)c3ccc(O)cc3C2=O)c(OC)c1</chem>
	2-(3,5-dihydroxyphenyl)-5-hydroxyisoindole-1,3-dione	1	1	1	0	<chem>Oc1ccc2C(=O)N(C(=O)c2c1)c3cc(O)cc(O)c3</chem>
	5-hydroxy-2-[(1r,4r)-4-hydroxycyclohexyl]isoindole-1,3-dione	1	1	1	0	<chem>O[C@@H]1CC[C@H](CC1)N2C(=O)c3ccc(O)cc3C2=O</chem>
	5-hydroxy-2-(5-hydroxynaphthalen-1-yl)isoindole-1,3-dione	1	1	1	0	<chem>Oc1ccc2C(=O)N(C(=O)c2c1)c3cccc4c(O)cccc34</chem>
	5-hydroxy-2-(4-hydroxynaphthalen-1-yl)isoindole-1,3-dione	1	1	1	0	<chem>Oc1ccc2C(=O)N(C(=O)c2c1)c3ccc(O)c4cccc34</chem>
	5-hydroxy-2-(4-methoxy-2-nitrophenyl)isoindole-1,3-dione	1	1	1	0	<chem>COc1ccc(N2C(=O)c3ccc(O)cc3C2=O)c(c1)[N+](=O)[O-]</chem>
	5-hydroxy-2-(4-hydroxy-2-nitrophenyl)isoindole-1,3-dione	1	1	1	0	<chem>Oc1ccc2C(=O)N(C(=O)c2c1)c3ccc(O)cc3[N+](=O)[O-]</chem>
	5-hydroxy-2-(4-hydroxy-2-methylphenyl)isoindole-1,3-dione	1	1	1	0	<chem>Cc1cc(O)ccc1N2C(=O)c3ccc(O)cc3C2=O</chem>
	2-(2-fluoro-4-hydroxyphenyl)-5-	1	1	1	0	<chem>Oc1ccc(N2C(=O)c3ccc(O)cc3C2=O)c(F)c1</chem>

	hydroxyisoindole-1,3-dione					
	4-bromo-2-(4-hydroxyphenyl)-6-methoxyisoindole-1,3-dione	1	1	1	0	<chem>COc1cc(Br)c2C(=O)N(C(=O)c2c1)c3ccc(O)cc3</chem>
	4-bromo-6-hydroxy-2-(4-hydroxyphenyl)isoindole-1,3-dione	1	1	1	0	<chem>Oc1ccc(cc1)N2C(=O)c3cc(O)cc(Br)c3C2=O</chem>
	4-{4-[(1E)-(hydroxyimino)methyl]naphthalen-1-yl}phenol	1	1	1	0	<chem>O\\N=C\\c1ccc(c2ccc(O)cc2)c3ccccc13</chem>
	2-fluoro-4-{4-[(1E)-(hydroxyimino)methyl]naphthalen-1-yl}phenol	1	1	1	0	<chem>O\\N=C\\c1ccc(c2ccc(O)c(F)c2)c3ccccc13</chem>
	4-{7-[(1E)-(hydroxyimino)methyl]-1-benzothiophen-4-yl}phenol	1	1	1	0	<chem>O\\N=C\\c1ccc(c2ccc(O)cc2)c3ccsc13</chem>
	4-{4-[(1E)-(hydroxyimino)methyl]-1-benzothiophen-7-yl}phenol	1	1	1	0	<chem>O\\N=C\\c1ccc(c2ccc(O)cc2)c3sccc13</chem>
	4-{7-[(1E)-(hydroxyimino)methyl]-1-benzofuran-4-yl}phenol	1	1	1	0	<chem>O\\N=C\\c1ccc(c2ccc(O)cc2)c3ccoc13</chem>
	4-{4-[(1E)-(hydroxyimino)methyl]-1-benzofuran-7-yl}phenol	1	1	1	0	<chem>O\\N=C\\c1ccc(c2ccc(O)cc2)c3occc13</chem>
	4-{3-[(1E)-(hydroxyimino)methyl]indol-1-yl}phenol	1	1	1	0	<chem>O\\N=C\\c1cn(c2ccc(O)cc2)c3ccccc13</chem>

	4-{3-[(1E)-(hydroxyimino)methyl]-2-methylindol-1-yl}phenol	1	1	1	0	<chem>Cc1c(\C=N\O)c2ccccc2n1c3ccc(O)cc3</chem>
	2-fluoro-4-{3-[(1E)-(hydroxyimino)methyl]-2-methylindol-1-yl}phenol	1	1	1	0	<chem>Cc1c(\C=N\O)c2ccccc2n1c3ccc(O)c(F)c3</chem>
	4-{3,5-dichloro-4-[(1E)-(hydroxyimino)methyl]phenyl}-2-fluorophenol	1	1	1	0	<chem>O\N=C\c1c(Cl)cc(cc1Cl)c2ccc(O)c(F)c2</chem>
	ATA	0	1	0	1	<chem>Nc1nc[nH]n1</chem>
86-77-1	2-hydroxydibenzofuran	0	1	0	1	<chem>Oc1ccc2oc3ccccc3c2c1</chem>
51225-30-0	wighteone	1	1	1	0	<chem>CC(=CCc1c(O)cc2OC=C(C(=O)c2c1O)c3ccc(O)cc3)C</chem>
34086-50-5	alpinumisoflavone	1	1	1	0	<chem>CC1(C)Oc2cc3OC=C(C(=O)c3c(O)c2C=C1)c4ccc(O)cc4</chem>
	N-[(2R)-4-(4-hydroxyphenyl)butan-2-yl]-2-{2-phenyl-4-[2-(piperidin-1-yl)ethoxy]-1H-indol-3-yl}acetamide	1	1	1	0	<chem>C[C@H](CCc1ccc(O)cc1)NC(=O)Cc2c([nH])c3cccc(OCCN4CCC(CC4)c23)c5ccccc5</chem>
	N-[(2R)-4-(4-hydroxyphenyl)butan-2-yl]-2-{2-phenyl-5-[2-(piperidin-1-yl)ethoxy]-1H-indol-3-yl}acetamide	1	1	1	0	<chem>C[C@H](CCc1ccc(O)cc1)NC(=O)Cc2c([nH])c3ccc(OCCN4CCC(CC4)cc23)c5ccccc5</chem>
	N-[(2R)-4-(4-hydroxyphenyl)butan-2-yl]-2-{2-phenyl-5-[3-(piperidin-1-yl)propoxy]-1H-indol-3-yl}acetamide	1	1	1	0	<chem>C[C@H](CCc1ccc(O)cc1)NC(=O)Cc2c([nH])c3ccc(OCCCN4CCC(CC4)cc23)c5ccccc5</chem>

N-[(2R)-4-(4-hydroxyphenyl)butan-2-yl]-2-{2-phenyl-7-[2-(piperidin-1-yl)ethoxy]-1H-indol-3-yl}acetamide	1	1	1	0	C[C@H](CCc1ccc(O)cc1)NC(=O)Cc2c([nH])c3c(OCCCN4CCCC4)cccc23)c5cccc5
N-[(2R)-4-(4-hydroxyphenyl)butan-2-yl]-2-{2-phenyl-7-[3-(piperidin-1-yl)propoxy]-1H-indol-3-yl}acetamide	1	1	1	0	C[C@H](CCc1ccc(O)cc1)NC(=O)Cc2c([nH])c3c(OCCCN4CCCC4)cccc23)c5cccc5
N-[(2R)-4-(4-hydroxyphenyl)butan-2-yl]-2-{2-phenyl-7-[4-(piperidin-1-yl)butoxy]-1H-indol-3-yl}acetamide	1	1	1	0	C[C@H](CCc1ccc(O)cc1)NC(=O)Cc2c([nH])c3c(OCCCCN4CCCC4)cccc23)c5cccc5
N-[(2R)-4-(4-hydroxyphenyl)butan-2-yl]-2-(2-phenyl-7-{[5-(piperidin-1-yl)pentyl]oxy}-1H-indol-3-yl)acetamide	1	1	1	0	C[C@H](CCc1ccc(O)cc1)NC(=O)Cc2c([nH])c3c(OCCCCCN4CCCC4)cccc23)c5cccc5
(1S,2R,5S,10R,11S,14S,15S)-2-ethyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-7-ene-5,14-diol	1	1	1	0	CC[C@]12CC[C@H](O)CC1=CC[C@H]3[C@@H]4CC[C@H](O)[C@@]4(C)CC[C@H]23
(1S,2S,5S,10R,11S,14S,15S)-15-methyl-2-[(1Z)-prop-1-en-1-yl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-7-ene-5,14-diol	1	1	1	0	C\C=C/[C@]12CC[C@H](O)CC1=CC[C@H]3[C@@H]4CC[C@H](O)[C@@]4(C)CC[C@H]23
(1S,2S,5S,6R,10R,11S,14S,15S)-2-ethenyl-15-methyl-6-(prop-2-en-1-yl)tetracyclo[8.7.0.0{2,7}.0{11,15}]h	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CC=C4[C@@H](CC=C)[C@@H](O)CC[C@]34C=C)[C@@H]1CC[C@@H]2O

	eptadec-7-ene-5,14-diol					
	(1S,2S,5S,6S,9S,10R,14R,15S)-5-methylpentacyclo[12.3.3.0{1,13}.0{2,10}.0{5,9}]icosa-12,18-diene-6,15-diol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CC=C4[C@H]5CC=C[C@@]34CC[C@@H]5O)[C@@H]1CC[C@@H]2O
	(1R,2S,5S,6S,9S,10R,13S,14R,15S)-5-methylpentacyclo[12.3.3.0{1,13}.0{2,10}.0{5,9}]icosane-6,15-diol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CC[C@H]4[C@H]5CCC[C@@]34CC[C@@H]5O)[C@@H]1CC[C@@H]2O
	(1R,2S,5S,6S,9S,10R,14R,15S)-5-methylpentacyclo[12.3.2.0{1,13}.0{2,10}.0{5,9}]nonadec-12-ene-6,15-diol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CC=C4[C@H]5CC[C@@]34CC[C@@H]5O)[C@@H]1CC[C@@H]2O
	(1R,2S,5S,6S,9S,10R,14R,15R)-5-methylpentacyclo[12.3.2.0{1,13}.0{2,10}.0{5,9}]nonadec-12-ene-6,15-diol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CC=C4[C@H]5CC[C@@]34CC[C@@H]5O)[C@@H]1CC[C@@H]2O
	(1S,2S,5S,6S,9S,10R,15S)-5-methyl-16-oxapentacyclo[13.3.2.0{1,13}.0{2,10}.0{5,9}]icos-12-en-6-ol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CC=C4C[C@@H]5CC[C@]34CCO5)[C@@H]1CC[C@@H]2O
	(1S,2S,5S,6S,9S,10R,14S,19R)-6,19-dihydroxy-5-methylpentacyclo[12.3.2.0{1,13}.0{	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CC=C4[C@H]5[C@H](O)C[C@@]34CCC5=O)[C@@H]1CC[C@@H]2O

	2,10}.0{5,9}]nonadec-12-en-15-one					
	(1S,2S,5S,6S,9S,10R,14S,19S)-6,19-dihydroxy-5-methylpentacyclo[12.3.2.0{1,13}.0{2,10}.0{5,9}]nonadec-12-en-15-one	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CC=C4[C@H]5[C@@H](O)C[C@@]34CCC5=O)[C@@H]1CC[C@@H]2O
	(1S,2S,5S,6S,9S,10R,19R)-6,19-dihydroxy-5-methylpentacyclo[10.5.2.0{1,13}.0{2,10}.0{5,9}]nonadec-13-en-15-one	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CC4[C@H](O)C[C@@]35CCC(=O)C=C45)[C@@H]1CC[C@@H]2O
	(1S,2S,5S,6S,9S,10R,15S)-6-hydroxy-5-methyl-16-oxapentacyclo[13.3.2.0{1,13}.0{2,10}.0{5,9}]icos-12-en-17-one	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CC=C4C[C@@H]5CC[C@]34CC(=O)O5)[C@@H]1CC[C@@H]2O
	(1R,2S,5S,6S,9S,10R,14R)-6-hydroxy-5-methylpentacyclo[12.3.2.0{1,13}.0{2,10}.0{5,9}]nonadec-12-en-15-one	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CC=C4[C@H]5CC[C@@]34CCC5=O)[C@@H]1CC[C@@H]2O
	12-chloro-11H-10-oxa-5-azatetraphene-2,8-diol	1	1	1	0	Oc1ccc2c(OCc3c(Cl)c4cc(O)ccc4nc23)c1
	12-bromo-11H-10-oxa-5-azatetraphene-2,8-diol	1	1	1	0	Oc1ccc2c(OCc3c(Br)c4cc(O)ccc4nc23)c1
	2,8-dihydroxy-11H-10-oxa-5-	1	1	1	0	Oc1ccc2c(OCc3c2nc4ccc(O)cc4c3C#N)c1

	azatetraphene-12-carbonitrile					
	12-ethenyl-11H-10-oxa-5-azatetraphene-2,8-diol	1	1	1	0	<chem>Oc1ccc2c(OCc3c(C=C)c4cc(O)ccc4nc23)c1</chem>
	12-ethynyl-11H-10-oxa-5-azatetraphene-2,8-diol	1	1	1	0	<chem>Oc1ccc2c(OCc3c2nc4ccc(O)cc4c3C#C)c1</chem>
	12-ethyl-11H-10-oxa-5-azatetraphene-2,8-diol	1	1	1	0	<chem>CCc1c2COc3cc(O)ccc3c2nc4ccc(O)cc14</chem>
	12-(4-chlorophenyl)-11H-10-oxa-5-azatetraphene-2,8-diol	1	1	1	0	<chem>Oc1ccc2c(OCc3c2nc4ccc(O)cc4c3c5ccc(Cl)cc5)c1</chem>
	4-(2,8-dihydroxy-11H-10-oxa-5-azatetraphen-12-yl)benzonitrile	1	1	1	0	<chem>Oc1ccc2c(OCc3c2nc4ccc(O)cc4c3c5ccc(cc5)C#N)c1</chem>
	12-[4-(trifluoromethyl)phenyl]-11H-10-oxa-5-azatetraphene-2,8-diol	1	1	1	0	<chem>Oc1ccc2c(OCc3c2nc4ccc(O)cc4c3c5ccc(cc5)C(F)(F)F)c1</chem>
	12-(4-methoxyphenyl)-11H-10-oxa-5-azatetraphene-2,8-diol	1	1	1	0	<chem>COc1ccc(cc1)c2c3COc4cc(O)ccc4c3nc5ccc(O)cc25</chem>
	12-(3-chlorophenyl)-11H-10-oxa-5-azatetraphene-2,8-diol	1	1	1	0	<chem>Oc1ccc2c(OCc3c2nc4ccc(O)cc4c3c5cccc(Cl)c5)c1</chem>
	3-(2,8-dihydroxy-11H-10-oxa-5-azatetraphen-12-yl)benzonitrile	1	1	1	0	<chem>Oc1ccc2c(OCc3c2nc4ccc(O)cc4c3c5cccc(c5)C#N)c1</chem>
	12-(3-methoxyphenyl)-11H-10-oxa-	1	1	1	0	<chem>COc1cccc(c1)c2c3COc4cc(O)ccc4c3nc5ccc(O)cc25</chem>

	5-azatetraphene-2,8-diol					
	(1S,2S,5S,10R,11S,14S,15S)-2-ethenyl-5,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-7-ene-5,14-diol	1	1	1	0	<chem>C[C@]1(O)CC[C@]2(C=C)[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4[C@@H]3CC=C2C1</chem>
	(1S,2S,5R,10R,11S,14S,15S)-2-ethenyl-5,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-7-ene-5,14-diol	1	1	1	0	<chem>C[C@@]1(O)CC[C@]2(C=C)[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4[C@@H]3CC=C2C1</chem>
	(1S,2S,10R,11S,14S,15S)-2-ethenyl-5,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-5,7-dien-14-ol	1	1	1	0	<chem>CC1=CC2=CC[C@H]3[C@@H]4CC[C@H](O)[C@@]4(C)CC[C@@H]3[C@]2(CC1)C=C</chem>
	(1S,2S,10R,11S,14S,15S)-2-ethenyl-5-ethyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-5,7-dien-14-ol	1	1	1	0	<chem>CCC1=CC2=CC[C@H]3[C@@H]4CC[C@H](O)[C@@]4(C)CC[C@@H]3[C@]2(CC1)C=C</chem>
	(1S,2S,10R,11S,14S,15S)-2-ethenyl-15-methyl-5-phenyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-5,7-dien-14-ol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CC=C4C=C(CC[C@]34C=C)c5ccc5)[C@@H]1CC[C@@H]2O</chem>
	(1S,2S,10R,11S,14S,15S)-5-chloro-2-ethenyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-5,7-dien-14-ol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CC=C4C=C(Cl)CC[C@]34C=C)[C@@H]1CC[C@@H]2O</chem>

	15}}heptadeca-5,7-dien-14-ol					
	(1S,2S,10R,11S,14S,15S)-2-ethenyl-5,14,15-trimethyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-5,7-dien-14-ol	1	1	1	0	CC1=CC2=CC[C@H]3[C@@H]4CC[C@](C)(O)[C@@]4(C)CC[C@@H]3[C@]2(CC1)C=C
	(1S,2S,10R,11S,14R,15S)-2-ethenyl-14-ethynyl-5,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-5,7-dien-14-ol	1	1	1	0	CC1=CC2=CC[C@H]3[C@@H]4CC[C@](O)(C#C)[C@@]4(C)CC[C@@H]3[C@]2(CC1)C=C
	(1S,2S,5S,10R,11S,14S,15S)-2-ethenyl-14,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-7-ene-5,14-diol	1	1	1	0	C[C@]1(O)CC[C@H]2[C@@H]3CC=C4C[C@@H](O)CC[C@]4(C=C)[C@H]3CC[C@]12C
	(1S,2S,5S,10R,11S,14R,15S)-2-ethenyl-14-ethynyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-7-ene-5,14-diol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CC=C4C[C@@H](O)CC[C@]34C=C)[C@@H]1CC[C@@]2(O)C#C
	(1S,2S,10R,11S,14S,15S)-2-ethenyl-15-methyl-5-methylidenetetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-6-en-14-ol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCC4=CC(=C)CC[C@]34C=C)[C@@H]1CC[C@@H]2O
21952-93-2	(1S,2R,10R,11S,14S,15S)-2,15-dimethyl-5-methylidenetetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-6-en-14-ol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCC4=CC(=C)CC[C@]34C)[C@@H]1CC[C@@H]2O

	0{11,15}}heptadec-6-en-14-ol					
60397-35-5	(1S,2R,10R,11S,14S,15S)-2,5,15-trimethyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-5,7-dien-14-ol	1	1	1	0	<chem>CC1=CC2=CC[C@H]3[C@@H]4CC[C@H](O)[C@@]4(C)CC[C@@H]3[C@@]2(C)CC1</chem>
88-04-0	dettol	0	1	0	1	<chem>Cc1cc(O)cc(C)c1Cl</chem>
	permethrin	0	1	0	1	<chem>CC1(C)C(C=C(Cl)Cl)C1C(=O)OCc2cccc(Oc3cccc3)c2</chem>
1143-72-2	4-benzoylbenzene-1,2,3-triol	1	1	1	0	<chem>Oc1ccc(C(=O)c2ccccc2)c(O)c1O</chem>
24381-12-2	(1S,10R,11S,14S,15S)-4-iodo-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)c(I)cc34)[C@@H]1CC[C@@H]2O</chem>
	4-(4-methoxyphenyl)phenol	1	1	1	0	<chem>COc1ccc(cc1)c2ccc(O)cc2</chem>
	2-hydroxy-3-[(1E)-(hydroxyimino)methyl]-6-(4-hydroxyphenyl)benzonitrile	1	1	1	0	<chem>O\\N=C\\c1ccc(c2ccc(O)cc2)c(C#N)c1O</chem>
	6-[(1E)-(hydroxyimino)methyl]-3-(4-hydroxyphenyl)-2-methylphenol	1	1	1	0	<chem>Cc1c(O)c(\\C=N\\O)ccc1c2ccc(O)cc2</chem>
	6-[(1E)-(hydroxyimino)methyl]-3-(4-methoxyphenyl)-2-methylphenol	1	1	1	0	<chem>COc1ccc(cc1)c2ccc(\\C=N\\O)c(O)c2C</chem>
	2-[(1E)-(hydroxyimino)methyl]-5-(4-methoxyphenyl)phenol	1	1	1	0	<chem>COc1ccc(cc1)c2ccc(\\C=N\\O)c(O)c2</chem>

	2-[(1E)-(hydroxyimino)methyl]-5-phenylphenol	1	1	1	0	<chem>O\\N=C\\c1ccc(cc1O)c2ccccc2</chem>
	typhon	0	1	0	1	<chem>CC(C)(C)C(=O)C(Oc1ccc(Cl)cc1)n2cncn2</chem>
82-68-8	pentachloronitrobenzene	0	1	0	1	<chem>[O-][N+](=O)c1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl</chem>
	zyban	0	1	0	1	<chem>COC(=O)NC(=S)Nc1ccccc1NC(=S)NC(=O)OC</chem>
	triforine	0	1	0	1	<chem>ClC(Cl)(Cl)C(NC=O)N1CCN(CC1)C(NC=O)C(Cl)(Cl)Cl</chem>
	rhoden	0	1	0	1	<chem>CNC(=O)Oc1ccccc1OC(C)C</chem>
	sophoraflavanone B	1	1	1	0	<chem>CC(=CCc1c(O)cc(O)c2C(=O)CC(Oc12)c3ccc(O)cc3)C</chem>
	5,7-dihydroxy-3-[4-hydroxy-3-(3-methylbut-2-en-1-yl)phenyl]-8-(3-methylbut-2-en-1-yl)chromen-4-one	1	1	1	0	<chem>CC(=CCc1cc(ccc1O)C2=COc3c(CC=C(C)C)c(O)cc(O)c3C2=O)C</chem>
74515-47-2	(1S,10S)-14-methoxy-15-(3-methylbut-2-en-1-yl)-8,17-dioxatetracyclo[8.7.0.0{2,7}.0{11,16}]heptadeca-2,4,6,11(16),12,14-hexaene-5,10-diol	1	1	1	0	<chem>COc1ccc2c(O[C@H]3c4ccc(O)cc4OC[C@@]23O)c1CC=C(C)C</chem>
	linuron	0	1	0	1	<chem>CON(C)C(=O)Nc1ccc(Cl)c(Cl)c1</chem>
	phenylhydrazine	0	1	0	1	<chem>NNc1ccccc1</chem>
	double strength	0	1	0	1	<chem>CC(Oc1cc(Cl)c(Cl)cc1Cl)C(=O)O</chem>

27955-94-8	4-[1,1-bis(4-hydroxyphenyl)ethyl]phenol	1	1	1	0	<chem>CC(c1ccc(O)cc1)(c2ccc(O)cc2)c3ccc(O)cc3</chem>
	isowighteone	1	1	1	0	<chem>CC(=CCc1cc(ccc1O)C2=COc3cc(O)cc(O)c3C2=O)C</chem>
37221-95-7	ethylene glycol	0	1	0	1	<chem>OCCO</chem>
	triadimenol	0	1	0	1	<chem>CC(C)(C)C(O)C(Oc1ccc(Cl)cc1)n2cncn2</chem>
	tirade	0	1	0	1	<chem>CC(C)C(C(=O)OC(C#N)c1cccc(Oc2cccc2)c1)c3ccc(Cl)cc3</chem>
	4-[1-(4-hydroxyphenyl)-4-methyl-5-{4-[2-(piperidin-1-yl)ethoxy]phenyl}pyrazol-3-yl]phenol	1	1	1	0	<chem>Cc1c(nn(c2ccc(O)cc2)c1c3ccc(OCCN4CCCC4)cc3)c5ccc(O)cc5</chem>
	4-[1-(4-hydroxyphenyl)-4-methyl-5-{4-[3-(piperidin-1-yl)propyl]phenyl}pyrazol-3-yl]phenol	1	1	1	0	<chem>Cc1c(nn(c2ccc(O)cc2)c1c3ccc(CCCN4CCCC4)cc3)c5ccc(O)cc5</chem>
	4-[1,5-bis(4-hydroxyphenyl)-4-methylpyrazol-3-yl]phenol	1	1	1	0	<chem>Cc1c(nn(c2ccc(O)cc2)c1c3ccc(O)cc3)c4ccc(O)cc4</chem>
	(2E)-3-{4-[2,5-bis(4-hydroxyphenyl)-4-methylpyrazol-3-yl]phenyl}-1-(piperidin-1-yl)prop-2-en-1-one	1	1	1	0	<chem>Cc1c(nn(c2ccc(O)cc2)c1c3ccc(\C=C\C(=O)N4CCCC4)cc3)c5ccc(O)cc5</chem>
	2-chloro-3-(3-fluoro-4-methoxyphenyl)-6-[(1E)-	1	1	1	0	<chem>COc1ccc(cc1F)c2ccc(\C=N\O)c(O)c2Cl</chem>

	(hydroxyimino)methyl]phenol					
	2-[(1E)-(hydroxyimino)methyl]-4-(4-methoxyphenyl)phenol	1	1	1	0	<chem>COc1ccc(cc1)c2ccc(O)c(\C=N\O)c2</chem>
	4-(3-fluoro-4-hydroxyphenyl)-2-[(1E)-(hydroxyimino)methyl]phenol	1	1	1	0	<chem>O\N=C\c1cc(ccc1O)c2ccc(O)c(F)c2</chem>
	4-(3-fluoro-4-methoxyphenyl)-2-[(1E)-(hydroxyimino)methyl]phenol	1	1	1	0	<chem>COc1ccc(cc1F)c2ccc(O)c(\C=N\O)c2</chem>
	2-chloro-6-[(1E)-1-(hydroxyimino)ethyl]-3-(4-hydroxyphenyl)phenol	1	1	1	0	<chem>C\C(=N/O)\c1ccc(c(Cl)c1O)c2ccc(O)cc2</chem>
	2-chloro-6-[(1E)-1-(hydroxyimino)ethyl]-3-(4-methoxyphenyl)phenol	1	1	1	0	<chem>COc1ccc(cc1)c2ccc(\C(=N\O)\C)c(O)c2Cl</chem>
	2-chloro-3-(3-fluoro-4-hydroxyphenyl)-6-[(1E)-1-(hydroxyimino)ethyl]phenol	1	1	1	0	<chem>C\C(=N/O)\c1ccc(c(Cl)c1O)c2ccc(O)c(F)c2</chem>
	2-chloro-3-(3-fluoro-4-methoxyphenyl)-6-[(1E)-1-(hydroxyimino)ethyl]phenol	1	1	1	0	<chem>COc1ccc(cc1F)c2ccc(\C(=N\O)\C)c(O)c2Cl</chem>
	2,6-dihydroxy-3-(4-[[[1S,10R,11S,14S,15S)-5-hydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2OC(=O)CCC(=O)Nc5ccc(O)c(C(=O)O)c5O</chem>

	15]]heptadeca-2,4,6-trien-14-yl]oxy}-4-oxobutanamido)benzoic acid					
	2,3-bis(4-hydroxyphenyl)butanenitrile	1	1	1	0	<chem>CC(C#N)c1ccc(O)cc1c2ccc(O)cc2</chem>
	2,3-bis(4-hydroxyphenyl)pentanenitrile	1	1	1	0	<chem>CCC(C#N)c1ccc(O)cc1c2ccc(O)cc2</chem>
	4-fluoro-2,3-bis(4-hydroxyphenyl)butanenitrile	1	1	1	0	<chem>Oc1ccc(cc1)C(CF)C(C#N)c2ccc(O)cc2</chem>
	3-(4-hydroxy-3-methylphenyl)-2-(4-hydroxyphenyl)propanenitrile	1	1	1	0	<chem>Cc1cc(CC(C#N)c2ccc(O)cc2)ccc1O</chem>
	3-(3,4-dihydroxyphenyl)-2-(4-hydroxyphenyl)propanenitrile	1	1	1	0	<chem>Oc1ccc(cc1)C(Cc2ccc(O)c(O)c2)C#N</chem>
	3-(3-fluoro-4-hydroxyphenyl)-2-(4-hydroxyphenyl)propanenitrile	1	1	1	0	<chem>Oc1ccc(cc1)C(Cc2ccc(O)c(F)c2)C#N</chem>
	3-(3-chloro-4-hydroxyphenyl)-2-(4-hydroxyphenyl)propanenitrile	1	1	1	0	<chem>Oc1ccc(cc1)C(Cc2ccc(O)c(Cl)c2)C#N</chem>
	3-(3-bromo-4-hydroxyphenyl)-2-(4-hydroxyphenyl)propanenitrile	1	1	1	0	<chem>Oc1ccc(cc1)C(Cc2ccc(O)c(Br)c2)C#N</chem>
	3-(4-hydroxy-3-iodophenyl)-2-(4-hydroxyphenyl)propanenitrile	1	1	1	0	<chem>Oc1ccc(cc1)C(Cc2ccc(O)c(I)c2)C#N</chem>

	3-[3-(2-fluoroethyl)-4-hydroxyphenyl]-2-(4-hydroxyphenyl)propanenitrile	1	1	1	0	<chem>Oc1ccc(cc1)C(Cc2ccc(O)c(CCF)c2)C#N</chem>
	3-[3-(3-fluoropropyl)-4-hydroxyphenyl]-2-(4-hydroxyphenyl)propanenitrile	1	1	1	0	<chem>Oc1ccc(cc1)C(Cc2ccc(O)c(CCCF)c2)C#N</chem>
	3-[4-hydroxy-3-(hydroxymethyl)phenyl]-2-(4-hydroxyphenyl)propanenitrile	1	1	1	0	<chem>OCc1cc(CC(C#N)c2ccc(O)cc2)ccc1O</chem>
	estrone sulfate	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(OS(=O)(=O)O)ccc34)[C@@H]1CCC2=O</chem>
	procymidone	0	1	0	1	<chem>CC12CC1(C)C(=O)N(C2=O)c3cc(Cl)cc(Cl)c3</chem>
	(2E)-3-{4-[(3-cyclopropyl-6-hydroxy-2-phenylnaphthalen-1-yl)oxy]phenyl}prop-2-enoic acid	1	1	1	0	<chem>OC(=O)\C=C\c1ccc(Oc2c(c3ccccc3)c(cc4cc(O)ccc24)C5CC5)cc1</chem>
	(2E)-3-{4-[(3-butyl-6-hydroxy-2-phenylnaphthalen-1-yl)oxy]phenyl}prop-2-enoic acid	1	1	1	0	<chem>CCCCc1cc2cc(O)ccc2c(Oc3ccc(\C=C\C(=O)O)cc3)c1c4cccc4</chem>
	(2E)-3-{4-[(6-hydroxy-3-(2-methylpropyl)-2-phenylnaphthalen-1-yl)oxy]phenyl}prop-2-enoic acid	1	1	1	0	<chem>CC(C)Cc1cc2cc(O)ccc2c(Oc3ccc(\C=C\C(=O)O)cc3)c1c4cccc4</chem>
	(2E)-3-{4-[(6-hydroxy-3-pentyl-2-	1	1	1	0	<chem>CCCCCc1cc2cc(O)ccc2c(Oc3ccc(\C=C\C(=O)O)cc3)c1c4ccc</chem>

	phenylnaphthalen-1-yl)oxy]phenyl}prop-2-enoic acid					cc4
	(2E)-3-{4-[(6-hydroxy-3-octyl-2-phenylnaphthalen-1-yl)oxy]phenyl}prop-2-enoic acid	1	1	1	0	CCCCCCCCc1cc2cc(O)ccc2c(Oc3ccc(\C=C\C(=O)O)cc3)c1c4cccc4
	(2E)-3-(4-{[3-(methoxymethyl)-2-phenylnaphthalen-1-yl]oxy}phenyl)prop-2-enoic acid	1	1	1	0	COCc1cc2cccc2c(Oc3ccc(\C=C\C(=O)O)cc3)c1c4cccc4
	(2E)-3-{4-[(3-butyl-2-phenylnaphthalen-1-yl)oxy]phenyl}prop-2-enoic acid	1	1	1	0	CCCCc1cc2cccc2c(Oc3ccc(\C=C\C(=O)O)cc3)c1c4cccc4
	(2E)-3-(4-{[3-butyl-2-(4-fluorophenyl)naphthalen-1-yl]oxy}phenyl)prop-2-enoic acid	1	1	1	0	CCCCc1cc2cccc2c(Oc3ccc(\C=C\C(=O)O)cc3)c1c4ccc(F)cc4
	(2E)-3-(4-{[3-butyl-2-(4-methoxyphenyl)naphthalen-1-yl]oxy}phenyl)prop-2-enoic acid	1	1	1	0	CCCCc1cc2cccc2c(Oc3ccc(\C=C\C(=O)O)cc3)c1c4ccc(OC)cc4
	(2E)-3-(4-{[3-butyl-2-(4-hydroxyphenyl)naphthalen-1-yl]oxy}phenyl)prop-2-enoic acid	1	1	1	0	CCCCc1cc2cccc2c(Oc3ccc(\C=C\C(=O)O)cc3)c1c4ccc(O)cc4
	4-[(cyclopropylmethyl)(4-hydroxyphenyl)amino]phenol	1	1	1	0	Oc1ccc(cc1)N(CC2CC2)c3ccc(O)cc3
	2-(4-hydroxyphenyl)-1-[(4-	1	1	1	0	COc1ccc(Cn2c(c(C)c3cc(O)ccc23)c4ccc(O)cc4)cc1

	methoxyphenyl)methyl]-3-methylindol-5-ol					
	1-[(4-butoxyphenyl)methyl]-2-(4-hydroxyphenyl)-3-methylindol-5-ol	1	1	1	0	CCCCOc1ccc(Cn2c(c(C)c3cc(O)ccc23)c4ccc(O)cc4)cc1
	2-(4-hydroxyphenyl)-1-(6-methoxyhexyl)-3-methylindol-5-ol	1	1	1	0	COCCCCCn1c(c(C)c2cc(O)ccc12)c3ccc(O)cc3
	1-(6-butoxyhexyl)-2-(4-hydroxyphenyl)-3-methylindol-5-ol	1	1	1	0	CCCCOCCCCCn1c(c(C)c2cc(O)ccc12)c3ccc(O)cc3
	1-(6-hydroxyhexyl)-2-(4-hydroxyphenyl)-3-methylindol-5-ol	1	1	1	0	Cc1c(c2ccc(O)cc2)n(CCCCCO)c3ccc(O)cc13
	1-(3-{4-[bis(ethylsulfanyl)methyl]phenoxy}propyl)-2-(4-hydroxyphenyl)-3-methylindol-5-ol	1	1	1	0	CCSC(SCC)c1ccc(OCCn2c(c(C)c3cc(O)ccc23)c4ccc(O)cc4)cc1
	N-(2-[[[4-{3-[5-hydroxy-2-(4-hydroxyphenyl)-3-methylindol-1-yl]propoxy}phenyl)methyl]amino}ethyl)acetamide	1	1	1	0	CC(=O)NCCNCc1ccc(OCCn2c(c(C)c3cc(O)ccc23)c4ccc(O)cc4)cc1
	1-(4-aminobutyl)-2-(4-hydroxyphenyl)-3-methylindol-5-ol	1	1	1	0	Cc1c(c2ccc(O)cc2)n(CCCCN)c3ccc(O)cc13
	N-{4-[5-hydroxy-2-(4-hydroxyphenyl)-3-methylindol-1-yl]butyl}-4-methylbenzamide	1	1	1	0	Cc1ccc(cc1)C(=O)NCCCCn2c(c(C)c3cc(O)ccc23)c4ccc(O)cc4

	4-[[2-(acetamidoethyl)amino]methyl]-N-{4-[5-hydroxy-2-(4-hydroxyphenyl)-3-methylindol-1-yl]butyl}benzamide	1	1	1	0	<chem>CC(=O)NCCNCc1ccc(cc1)C(=O)NCCCCn2c(c(C)c3cc(O)ccc23)c4ccc(O)cc4</chem>
402955-02-6	triphenyl phosphate	0	1	0	1	<chem>O=P(Oc1ccccc1)(Oc2ccccc2)Oc3ccccc3</chem>
	(1S,3aS,5S,7aS)-5-(2-chloro-4-hydroxyphenyl)-7a-methyloctahydroinden-1-ol	1	1	1	0	<chem>C[C@]12CC[C@@H](C[C@@H]1CC[C@@H]2O)c3ccc(O)cc3Cl</chem>
	(1S,3aS,5S,7aS)-5-(2,3-difluoro-4-hydroxyphenyl)-7a-methyloctahydroinden-1-ol	1	1	1	0	<chem>C[C@]12CC[C@@H](C[C@@H]1CC[C@@H]2O)c3ccc(O)c(F)c3F</chem>
	(1S,3aS,5S,7aS)-5-(2,5-difluoro-4-hydroxyphenyl)-7a-methyloctahydroinden-1-ol	1	1	1	0	<chem>C[C@]12CC[C@@H](C[C@@H]1CC[C@@H]2O)c3cc(F)c(O)cc3F</chem>
	(1S,3aS,5S,7aS)-7a-methyl-5-(2,3,5-trifluoro-4-hydroxyphenyl)-octahydroinden-1-ol	1	1	1	0	<chem>C[C@]12CC[C@@H](C[C@@H]1CC[C@@H]2O)c3cc(F)c(O)c(F)c3F</chem>
	(1S,3aS,5S,7aS)-5-(3,5-difluoro-4-hydroxyphenyl)-7a-methyloctahydroinden-1-ol	1	1	1	0	<chem>C[C@]12CC[C@@H](C[C@@H]1CC[C@@H]2O)c3cc(F)c(O)c(F)c3</chem>
	(1S,3aS,5R,7aS)-5-(4-hydroxyphenyl)-7a-methyl-	1	1	1	0	<chem>C[C@]12CC[C@H](C[C@@H]1CC[C@@H]2O)c3ccc(O)cc3</chem>

	octahydroinden-1-ol					
	4-(6-methyl-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-2-yl)phenol hydrochloride	0	1	0	1	Cl.Cc1ccc2c(C(=O)c3ccc(OCCN4CCCC4)cc3)c(sc2c1)c5ccc(O)cc5
	2-(4-methylphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol hydrochloride	1	1	1	0	Cl.Cc1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCC5)cc4
	1-(2-{4-[5,6,7-trimethoxy-2-(4-methoxyphenyl)-1-benzothiophene-3-carbonyl]phenoxy}ethyl)piperidine hydrochloride	1	1	1	0	Cl.COc1ccc(cc1)c2sc3c(OC)c(OC)c(OC)cc3c2C(=O)c4ccc(OCN5CCCC5)cc4
	1-(2-{4-[2-(4-chlorophenyl)-1-benzothiophene-3-carbonyl]phenoxy}ethyl)piperidine hydrochloride	1	1	1	0	Cl.Clc1ccc(cc1)c2sc3cccc3c2C(=O)c4ccc(OCCN5CCCC5)cc4
	methyl 2-(4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophene-6-carboxylate hydrochloride	1	1	1	0	Cl.COC(=O)c1ccc2c(C(=O)c3ccc(OCCN4CCCC4)cc3)c(sc2c1)c5ccc(O)cc5
	1-(2-{4-[6-methoxy-2-(4-methoxyphenyl)-1-benzothiophene-3-carbonyl]phenoxy}ethyl)piperidine	1	1	1	0	Cl.COc1ccc(cc1)c2sc3cc(OC)ccc3c2C(=O)c4ccc(OCCN5CCCC5)cc4

	hydrochloride					
	4-(6-chloro-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-2-yl)phenol hydrochloride	1	1	1	0	Cl.Oc1ccc(cc1)c2sc3cc(Cl)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4
	2-(4-chlorophenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol hydrochloride	1	1	1	0	Cl.Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(Cl)cc5
	2-phenyl-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol hydrochloride	1	1	1	0	Cl.Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5cccc5
	2-(4-hydroxyphenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]phenoxy}-1-benzothiophen-6-ol hydrochloride	1	1	1	0	Cl.Oc1ccc(cc1)c2sc3cc(O)ccc3c2Oc4ccc(OCCN5CCCCC5)cc4
	1-{2-[4-(2-phenyl-1-benzothiophene-3-carbonyl)phenoxy]ethyl}piperidine hydrochloride	1	1	1	0	Cl.O=C(c1ccc(OCCN2CCCCC2)cc1)c3c(sc4ccccc34)c5ccccc5
	4-(3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-2-yl)phenol hydrochloride	1	1	1	0	Cl.Oc1ccc(cc1)c2sc3ccccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4
	2-(4-fluorophenyl)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-	1	1	1	0	Cl.Oc1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(

	yl}oxy)phenyl]ethynyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol					
	6-[1-(4-hydroxyphenyl)pentan-2-yl]pyridin-3-ol	1	1	1	0	CCCC(Cc1ccc(O)cc1)c2ccc(O)cn2
	14-(2-{4-[4-(4-{4-[4-(2-{5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-yl}ethynyl)phenoxy]butoxy]butoxy]butoxy}phenyl)ethynyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	C[C@@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@H]1CC[C@]2(O)C#Cc5ccc(OCCCCOCCCCOCCCCO)c6ccc(cc6)C#C[C@@]7(O)CC[C@H]8[C@H]9CCc%10cc(O)ccc%10[C@H]9CC[C@@]78C)cc5
	6-(4-phenylhexan-3-yl)pyridin-3-ol	1	1	1	0	CC[C@H]([C@H](CC)c1ccc(O)cn1)c2ccccc2
	14-{2-[4-({1-[4-(2-{5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-yl}ethynyl)phenyl]-1,6,11,16-tetraoxaicosan-20-yl}oxy)phenyl]ethynyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-	1	1	1	0	C[C@]12CC[C@H]3[C@H](CCc4cc(O)ccc34)[C@@H]1CC[C@]2(O)C#Cc5ccc(OCCCCOCCCCOCCCCOCCCCO)c6ccc(cc6)C#C[C@@]7(O)CC[C@@H]8[C@@H]9CCc%10cc(O)ccc%10[C@H]9CC[C@@]78C)cc5

	6-[2-(4-hydroxyphenyl)butyl]pyridin-3-ol	1	1	1	0	<chem>CCC(Cc1ccc(O)cn1)c2ccc(O)cc2</chem>
	14-{2-[4-(3-{3-[4-(2-{5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]]heptadeca-2,4,6-trien-14-yl}ethynyl)phenoxy]propoxy)propoxy)phenyl}ethynyl}-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	<chem>C[C@@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@H]1CC[C@]2(O)C#Cc5ccc(OCCCCOCCOc6ccc(cc6)C#C[C@@]7(O)CC[C@@H]8[C@H]9CCc%10cc(O)ccc%10[C@H]9CC[C@@]78C)cc5</chem>
	14-{2-[4-({1-[4-(2-{5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]]heptadeca-2,4,6-trien-14-yl}ethynyl)phenyl]-1,5,9,13,17,21-hexaoxatetracosan-24-yl}oxy)phenyl}ethynyl}-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	<chem>C[C@@]12CC[C@@H]3[C@H](CCc4cc(O)ccc34)[C@H]1CC[C@]2(O)C#Cc5ccc(OCCCCOCCCOCCCOCCCOCCCOCCCOc6ccc(cc6)C#C[C@@]7(O)CC[C@H]8[C@H]9CCc%10cc(O)ccc%10[C@H]9CC[C@@]78C)cc5</chem>
	6-(4-phenylhexan-3-yl)pyridin-3-ol	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cn1)c2ccccc2</chem>
	14-(2-{4-[3-(3-{3-[4-(2-{5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]]heptadeca-2,4,6-trien-14-	1	1	1	0	<chem>C[C@@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@H]1CC[C@]2(O)C#Cc5ccc(OCCCCOCCCOCCCOc6ccc(cc6)C#C[C@@]7(O)CC[C@H]8[C@H]9CCc%10cc(O)ccc%10[C@H]9CC[C@</chem>

	yl}ethynyl)phenoxy]propoxy}propoxy)propoxy]phenyl}ethynyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol					@]78C)cc5
	14-{2-[4-({1-[4-(2-{5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-yl}ethynyl)phenyl]-1,5,9,13-tetraoxahexadecan-16-yl}oxy)phenyl}ethynyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	C[C@@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@H]1CC[C@]2(O)C#Cc5ccc(OCCCCOCCCCOCCCCOc6ccc(cc6)C#C[C@@]7(O)CC[C@H]8[C@H]9CCc%10cc(O)ccc%10[C@H]9CC[C@@]78C)cc5
	14-{2-[4-(4-{4-[4-(2-{5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-yl}ethynyl)phenoxy]butoxy}butoxy)phenyl}ethynyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	C[C@@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@H]1CC[C@]2(O)C#Cc5ccc(OCCCCOCCCCOc6ccc(cc6)C#C[C@@]7(O)CC[C@H]8[C@H]9CCc%10cc(O)ccc%10[C@H]9CC[C@@]78C)cc5
	4-[1-(4-hydroxyphenyl)hexan-2-yl]phenol	1	1	1	0	CCCCC(Cc1ccc(O)cc1)c2ccc(O)cc2

4-[(1E)-1-(4-hydroxyphenyl)pent-1-en-2-yl]phenol	1	1	1	0	<chem>CCC\C(=C/c1ccc(O)cc1)\c2ccc(O)cc2</chem>
4-[2-(4-hydroxyphenyl)-2-propylpentyl]phenol	1	1	1	0	<chem>CCCC(CCC)(Cc1ccc(O)cc1)c2ccc(O)cc2</chem>
4-{1-[(4-hydroxyphenyl)methyl]cyclopentyl}phenol	1	1	1	0	<chem>Oc1ccc(CC2(CCCC2)c3ccc(O)cc3)cc1</chem>
4-{1-[(4-hydroxyphenyl)methyl]cyclohexyl}phenol	1	1	1	0	<chem>Oc1ccc(CC2(CCCCC2)c3ccc(O)cc3)cc1</chem>
1,2-bis(4-hydroxyphenyl)propan-1-one	1	1	1	0	<chem>CC(C(=O)c1ccc(O)cc1)c2ccc(O)cc2</chem>
1,2-bis(4-hydroxyphenyl)butan-1-one	1	1	1	0	<chem>CCC(C(=O)c1ccc(O)cc1)c2ccc(O)cc2</chem>
1,2-bis(4-hydroxyphenyl)-2-methylpropan-1-one	1	1	1	0	<chem>CC(C)(C(=O)c1ccc(O)cc1)c2ccc(O)cc2</chem>
4-[1-(4-hydroxyphenyl)-3-methylbutan-2-yl]phenol	1	1	1	0	<chem>CC(C)C(Cc1ccc(O)cc1)c2ccc(O)cc2</chem>
3-[2,4-dihydroxy-5-(3-methylbut-2-en-1-yl)phenyl]-5-hydroxy-7-methoxychromen-4-one	1	1	1	0	<chem>COc1cc(O)c2C(=O)C(=COc2c1)c3cc(CC=C(C)C)c(O)cc3O</chem>
5-hydroxy-3-[4-hydroxy-3-(2-hydroxy-3-methylbut-2-en-1-	1	1	1	0	<chem>COc1cc(O)c2C(=O)C(=COc2c1)c3ccc(O)c(CC(=C(C)C)O)c3</chem>

	yl)phenyl]-7-methoxychromen-4-one					
	3-(3,7-dihydroxy-2,2-dimethyl-3,4-dihydro-1-benzopyran-6-yl)-5-hydroxy-7-methoxychromen-4-one	1	1	1	0	<chem>COc1cc(O)c2C(=O)C(=COc2c1)c3cc4CC(O)C(C)(C)Oc4cc3O</chem>
	(2E)-3-{4-[1-(4-hydroxyphenyl)-2-phenylbut-1-en-1-yl]phenyl}prop-2-enoic acid	1	1	1	0	<chem>CC\C=C(/c1ccc(O)cc1)\c2ccc(\C=C\C(=O)O)cc2)\c3ccc</chem> <chem>cc3</chem>
	(2E)-3-{4-[cyclohexylidene(4-hydroxyphenyl)methyl]phenyl}prop-2-enoic acid	1	1	1	0	<chem>OC(=O)\C=C\c1ccc(cc1)C(=C2CCCCC2)c3ccc(O)cc3</chem>
	(2E)-3-{4-[bicyclo[3.3.1]nonan-9-ylidene(4-hydroxyphenyl)methyl]phenyl}prop-2-enoic acid	1	1	1	0	<chem>OC(=O)\C=C\c1ccc(cc1)C(=C2C3CCCC2CCC3)c4ccc(O)cc4</chem>
	4-[cyclohexylidene(4-hydroxyphenyl)methyl]phenoxyacetic acid	1	1	1	0	<chem>OC(=O)COc1ccc(cc1)C(=C2CCCCC2)c3ccc(O)cc3</chem>
	4-{bicyclo[3.3.1]nonan-9-ylidene(4-hydroxyphenyl)methyl}phenoxyacetic acid	1	1	1	0	<chem>OC(=O)COc1ccc(cc1)C(=C2C3CCCC2CCC3)c4ccc(O)cc4</chem>
	6-{4-[cyclohexylidene(4-hydroxyphenyl)methyl]phenoxy}he	1	1	1	0	<chem>OC(=O)CCCCCOc1ccc(cc1)C(=C2CCCCC2)c3ccc(O)cc3</chem>

	xanoic acid					
	6-(4-{bicyclo[3.3.1]nonan-9-ylidene(4-hydroxyphenyl)methyl}phenoxy)hexanoic acid	1	1	1	0	<chem>OC(=O)CCCCCOC1CCC(CC1)C(=C2C3CCCC2CCC3)C4CCC(O)CC4</chem>
	6-(4-{bicyclo[3.3.1]nonan-9-ylidene(phenyl)methyl}phenoxy)hexanoic acid	1	1	1	0	<chem>OC(=O)CCCCCOC1CCC(CC1)C(=C2C3CCCC2CCC3)C4CCCCC4</chem>
	4-{bicyclo[3.3.1]nonan-9-ylidene[4-(carboxymethoxy)phenyl]methyl}phenoxyacetic acid	1	1	1	0	<chem>OC(=O)COC1CCC(CC1)C(=C2C3CCCC2CCC3)C4CCC(OCC(=O)O)CC4</chem>
	ethyl 6-(4-{bicyclo[3.3.1]nonan-9-ylidene(4-hydroxyphenyl)methyl}phenoxy)hexanoate	1	1	1	0	<chem>CCOC(=O)CCCCCOC1CCC(CC1)C(=C2C3CCCC2CCC3)C4CCC(O)CC4</chem>
	(E)-2-(4-{bicyclo[3.3.1]nonan-9-ylidene(4-hydroxyphenyl)methyl}phenyl)ethyl(methoxy)phosphinic acid	1	1	1	0	<chem>COP(=O)(O)\C=C\c1ccc(cc1)C(=C2C3CCCC2CCC3)C4CCC(O)CC4</chem>
	4-{bicyclo[3.3.1]nonan-9-ylidene(4-hydroxyphenyl)methyl}phenyl trifluoromethanesulfonate	1	1	1	0	<chem>Oc1ccc(cc1)C(=C2C3CCCC2CCC3)C4CCC(OS(=O)(=O)C(F)(F)F)CC4</chem>
	(3E)-4-(4-{bicyclo[3.3.1]nonan-9-ylidene(4-	1	1	1	0	<chem>OC(=O)C\C=C\c1ccc(cc1)C(=C2C3CCCC2CCC3)C4CCC(O)CC4</chem>

	hydroxyphenyl)methyl}phenyl)but-3-enoic acid					
	(4E)-5-(4-{bicyclo[3.3.1]nonan-9-ylidene(4-hydroxyphenyl)methyl}phenyl)pent-4-enoic acid	1	1	1	0	<chem>OC(=O)CC\C=C\c1ccc(cc1)C(=C2C3CCCC2CCC3)c4ccc(O)cc4</chem>
	(5E)-6-(4-{bicyclo[3.3.1]nonan-9-ylidene(4-hydroxyphenyl)methyl}phenyl)hex-5-enoic acid	1	1	1	0	<chem>OC(=O)CCC\C=C\c1ccc(cc1)C(=C2C3CCCC2CCC3)c4ccc(O)cc4</chem>
	(6E)-7-(4-{bicyclo[3.3.1]nonan-9-ylidene(4-hydroxyphenyl)methyl}phenyl)hept-6-enoic acid	1	1	1	0	<chem>OC(=O)CCCC\C=C\c1ccc(cc1)C(=C2C3CCCC2CCC3)c4ccc(O)cc4</chem>
	4-(4-{bicyclo[3.3.1]nonan-9-ylidene(4-hydroxyphenyl)methyl}phenoxy)butanoic acid	1	1	1	0	<chem>OC(=O)CCCCOc1ccc(cc1)C(=C2C3CCCC2CCC3)c4ccc(O)cc4</chem>
	5-(4-{bicyclo[3.3.1]nonan-9-ylidene(4-hydroxyphenyl)methyl}phenoxy)pentanoic acid	1	1	1	0	<chem>OC(=O)CCCCOc1ccc(cc1)C(=C2C3CCCC2CCC3)c4ccc(O)cc4</chem>
	7-(4-{bicyclo[3.3.1]nonan-9-ylidene(4-hydroxyphenyl)methyl}phenoxy)heptanoic acid	1	1	1	0	<chem>OC(=O)CCCCCOc1ccc(cc1)C(=C2C3CCCC2CCC3)c4ccc(O)cc4</chem>

	ptanoic acid					
	11-(4-{bicyclo[3.3.1]nonan-9-ylidene(4-hydroxyphenyl)methyl}phenoxy)undecanoic acid	1	1	1	0	<chem>OC(=O)CCCCCCCCCOc1ccc(cc1)C(=C2C3CCCC2CCC3)c4ccc(O)cc4</chem>
	(2E)-3-{4-[(1Z)-1-(4-hydroxyphenyl)-2-phenylbut-1-en-1-yl]phenyl}prop-2-enoic acid	1	1	1	0	<chem>CC\C=C(\c1ccc(O)cc1)/c2ccc(\C=C\C(=O)O)cc2)\c3ccc3</chem>
	3-[4-(6-methoxypyridin-3-yl)phenyl]phenol	1	1	1	0	<chem>COc1ccc(cn1)c2ccc(cc2)c3cccc(O)c3</chem>
	3-[4-(5-chlorothiophen-2-yl)phenyl]phenol	1	1	1	0	<chem>Oc1cccc(c1)c2ccc(cc2)c3ccc(Cl)s3</chem>
	3-[3-(5-chlorothiophen-2-yl)phenyl]phenol	1	1	1	0	<chem>Oc1cccc(c1)c2cccc(c2)c3ccc(Cl)s3</chem>
	3-[3-(1-benzothiophen-2-yl)phenyl]phenol	1	1	1	0	<chem>Oc1cccc(c1)c2cccc(c2)c3cc4ccccc4s3</chem>
	3-[2-(5-chlorothiophen-2-yl)pyridin-4-yl]phenol	1	1	1	0	<chem>Oc1cccc(c1)c2ccnc(c2)c3ccc(Cl)s3</chem>
	3-[6-(5-chlorothiophen-2-yl)pyridin-2-yl]phenol	1	1	1	0	<chem>Oc1cccc(c1)c2cccc(n2)c3ccc(Cl)s3</chem>
	3-[4-(5-chlorothiophen-2-yl)pyridin-2-yl]phenol	1	1	1	0	<chem>Oc1cccc(c1)c2cc(ccn2)c3ccc(Cl)s3</chem>

	1-(2-{4-[2-(4-methoxyphenyl)-1-benzothiophene-3-carbonyl]phenoxy}ethyl)piperidine; citro	1	1	1	0	<chem>COc1ccc(cc1)c2sc3ccccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4.OC(=O)CC(O)(CC(=O)O)C(=O)O</chem>
	cyano(3-phenoxyphenyl)methyl (2S)-2-{{2-chloro-4-(trifluoromethyl)phenyl}amino}-3-methylbutanoate	0	1	0	1	<chem>CC(C)[C@H](Nc1ccc(cc1Cl)C(F)(F)F)C(=O)OC(C#N)c2cccc(OC3ccccc3)c2</chem>
	malathion	0	1	0	1	<chem>CCOC(=O)CC(SP(=S)(OC)OC)C(=O)OCC</chem>
79-45-8	dimethyl[sulfanyl(carbonothioyl)]amine	1	1	1	0	<chem>CN(C)C(=S)S</chem>
	4-{{bis(2,4,6-trimethylphenyl)boranyl}(2,2,2-trifluoroethyl)amino}phenol	1	1	1	0	<chem>Cc1cc(C)c(B(N(CC(F)(F)F)c2ccc(O)cc2)c3c(C)cc(C)cc3C)c(C)c1</chem>
1229-12-5	5β-androstane-3,17-dione	1	1	1	0	<chem>C[C@]12CCC(=O)C[C@H]1CC[C@@H]3[C@@H]2CC[C@@]4(C)[C@H]3CCC4=O</chem>
	2-phenyl-1-({4-[2-(piperidin-1-yl)ethoxy]phenyl}methyl)-1,3-benzodiazol-5-ol	1	1	1	0	<chem>Oc1ccc2c(c1)nc(c3ccccc3)n2Cc4ccc(OCCN5CCCCC5)cc4</chem>
39336-60-2	way up	0	1	0	1	<chem>CCC(CC)Nc1c(cc(C)c(C)c1[N+](=O)[O-])[N+](=O)[O-]</chem>
131-53-3	2-(2-hydroxybenzoyl)-5-methoxyphenol	0	1	0	1	<chem>COc1ccc(C(=O)c2ccccc2O)c(O)c1</chem>

66746-42-7	DFFD	1	1	1	0	<chem>N(c1ccccc1)c2ccc(Nc3ccccc3)cc2</chem>
80094-39-9	tributyl phosphate	0	1	0	1	<chem>CCCCOP(=O)(OCCCC)OCCCC</chem>
68411-66-5	tris(2-chloroethyl)phosphate	0	1	0	1	<chem>ClCCOP(=O)(OCCCl)OCCCl</chem>
	(1S,10R,11R,13R,14S,15R)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,13,14-triol	1	1	1	0	<chem>C[C@@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@H]1C[C@@H](O)[C@H]2O</chem>
	rabon	0	1	0	1	<chem>COP(=O)(OC)O\C=C/Cl\c1cc(Cl)c(Cl)cc1Cl</chem>
	4-[1-(4-hydroxyphenyl)ethenyl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)C(=C)c2ccc(O)cc2</chem>
131-18-0	DPP	1	1	1	0	<chem>CCCCCOC(=O)c1ccccc1C(=O)OCCCCC</chem>
95-77-2	3,4-dichlorophenol	0	1	0	1	<chem>Oc1ccc(Cl)c(Cl)c1</chem>
583-78-8	2,5-dichlorophenol	0	1	0	1	<chem>Oc1cc(Cl)ccc1Cl</chem>
	dimethoate	0	1	0	1	<chem>CNC(=O)CSP(=S)(OC)OC</chem>
73250-68-7	mefenacet	0	1	0	1	<chem>CN(C(=O)COc1nc2ccccc2s1)c3ccccc3</chem>
55-38-9	fenthion	0	1	0	1	<chem>COP(=S)(OC)Oc1ccc(SC)c(C)c1</chem>
	(1S,10R,11S,13R,14R,15S)-13-chloro-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1C[C@@H](Cl)[C@@H]2O</chem>

	diol					
	(1S,11S,14S,15S)-6-bromo-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol; flavan	1	1	1	0	C.C[C@]12CC[C@H]3C(CCc4c(Br)c(O)ccc34)[C@@H]1CC[C@@H]2O
	(1S,10R,11S,15S)-4-methoxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	COc1cc2[C@H]3CC[C@]4(C)C(O)CC[C@H]4[C@@H]3CCc2cc1O
	(1S,10S,11S,15S)-15-methyl-14-methylidenetetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-5-ol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CCC2=C
	(1S,10S,11S,14S,15R,17S)-14-ethyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,17-diol	1	1	1	0	CC[C@H]1CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@H]3[C@@H](O)C[C@]12C
	(1S,10R,11S,14S,15S)-15-methyl-5-nitrotetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-ol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(ccc34)[N+](=O)[O-])[C@@H]1CC[C@@H]2O
	(1S,10R,11S,14S,15S)-15-methyl-4-nitrotetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-ol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4ccc(cc34)[N+](=O)[O-])[C@@H]1CC[C@@H]2O

	(1S,10S,11S,14S,15S)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-3,14-diol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cccc(O)c34)[C@@H]1CC[C@@H]2O</chem>
	(1S,10R,11S,14S,15S)-15-methyl-6-nitrotetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-ol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4c3cccc4[N+](=O)[O-])[C@@H]1CC[C@@H]2O</chem>
	(1S,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-9-one	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@H]([C@@H]1CC[C@@H]2O)C(=O)Cc4cc(O)ccc34</chem>
	(1S,10R,11S,14S,15S)-6-iodo-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-ol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4c(I)cccc34)[C@@H]1CC[C@@H]2O</chem>
3398-11-6	(1S,9R,10R,11S,14S,15S)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,9,14-triol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H]([C@H](O)Cc4cc(O)ccc34)[C@@H]1CC[C@@H]2O</chem>
	(1S,10R,11S,14S,15S)-4-amino-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-ol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4ccc(N)cc34)[C@@H]1CC[C@@H]2O</chem>
	(1S,10R,11S,14S,15S)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-6,14-	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4c(O)cccc34)[C@@H]1CC[C@@H]2O</chem>

	diol					
	2-bromo-N-{2- [(1S,10R,11S,14R,15S)-5,14- dihydroxy-15- methyltetracyclo[8.7.0.0{2,7}.0{11, 15}]heptadeca-2,4,6-trien-14- yl]ethyl}acetamide	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)CCNC(=O)CBr
	2-bromo-N-{3- [(1S,10R,11S,14R,15S)-5,14- dihydroxy-15- methyltetracyclo[8.7.0.0{2,7}.0{11, 15}]heptadeca-2,4,6-trien-14- yl]propyl}acetamide	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)CCCNC(=O)CBr
	(1S,10R,11S,14S,15S)-3-amino-15- methyltetracyclo[8.7.0.0{2,7}.0{11, 15}]heptadeca-2,4,6-trien-14-ol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cccc(N)c34)[C@@H]1CC[C@@H]2O
	(1S,9S,10R,11S,14S,15S)-15- methyltetracyclo[8.7.0.0{2,7}.0{11, 15}]heptadeca-2,4,6-triene-5,9,14- triol	1	1	1	0	C[C@]12CC[C@H]3[C@@H]([C@@H](O)Cc4cc(O)ccc34)[C@@H]1CC[C@@H]2O
	(1S,10S,11S,14S,15S,17R)-15- methyltetracyclo[8.7.0.0{2,7}.0{11, 15}]heptadeca-2,4,6-triene- 5,14,17-triol	1	1	1	0	C[C@]12C[C@@H](O)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O

10427-24-4	(1S,10R,11S,14S,15S)-5-amino-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-ol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(N)ccc34)[C@@H]1CC[C@@H]2O
1217-09-0	(1S,10S,11S,15S)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene	1	1	1	0	C[C@@]12CCC[C@H]1[C@@H]3CCc4ccccc4[C@H]3CC2
	(1S,10R,11S,14S,15S)-5-iodo-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-ol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(I)ccc34)[C@@H]1CC[C@@H]2O
	(1S,10R,11S,15S)-15-methyl-14-oxotetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-5-yl acetate	1	1	1	0	CC(=O)Oc1ccc2[C@H]3CC[C@@]4(C)[C@@H](CCC4=O)[C@@H]3CCc2c1
	(1S,9R,10R,11S,14S,15S)-15-methyl-9-[(4R,8R)-4,8,12-trimethyltridecyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	CC(C)CCC[C@@H](C)CCC[C@@H](C)CCC[C@@H]1Cc2cc(O)ccc2[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4[C@H]13
	(1S,10S,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-17-one	1	1	1	0	C[C@]12CC(=O)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O
	(1S,10R,11S,14S,15S)-4-bromo-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)c(Br)cc34)[C@@H]1CC[C@@H]2O

	diol					
	N-{3-[(1S,10R,11S,14R,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-yl]propyl}-2-iodoacetamide	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)CCNC(=O)CI</chem>
	2-bromo-N-{[(1S,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-yl)methyl}acetamide	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)CNC(=O)CBr</chem>
	(1S,10R,11S,14S,15S)-15-methyl-3-nitrotetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-ol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cccc(c34)[N+](=O)[O-])[C@@H]1CC[C@@H]2O</chem>
	(1S,10R,11S,14S,15S)-4-iodo-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-ol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4ccc(I)cc34)[C@@H]1CC[C@@H]2O</chem>
	(1S,10R,11S,14S,15S)-6-amino-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-ol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4c(N)ccc34)[C@@H]1CC[C@@H]2O</chem>
68-22-4	norethindrone	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@H]34)[C@@H]1CC[C@@]2(O)C#C</chem>

(1S,3aR,5S,7aS)-5-[4-hydroxy-2-(trifluoromethyl)phenyl]-7a-methyl-octahydroinden-1-ol	1	1	1	0	<chem>C[C@]12CC[C@@H](C[C@H]1CC[C@@H]2O)c3ccc(O)cc3C(F)(F)F</chem>
(1S,3aR,5S,7aS)-5-(3,5-difluoro-4-hydroxyphenyl)-7a-methyl-octahydroinden-1-ol	1	1	1	0	<chem>C[C@]12CC[C@@H](C[C@H]1CC[C@@H]2O)c3cc(F)c(O)c(F)c3</chem>
(1S,3aR,5S,7aS)-5-(2,5-difluoro-4-hydroxyphenyl)-7a-methyl-octahydroinden-1-ol	1	1	1	0	<chem>C[C@]12CC[C@@H](C[C@H]1CC[C@@H]2O)c3cc(F)c(O)cc3F</chem>
(1S,3aR,5S,7aS)-5-(2-fluoro-4-hydroxy-3-methylphenyl)-7a-methyl-octahydroinden-1-ol	1	1	1	0	<chem>Cc1c(O)ccc([C@H]2CC[C@]3(C)[C@@H](O)CC[C@@H]3C2)c1F</chem>
(1S,3aR,5S,7aS)-5-(4-hydroxy-2,3-dimethylphenyl)-7a-methyl-octahydroinden-1-ol	1	1	1	0	<chem>Cc1c(C)c(ccc1O)[C@H]2CC[C@]3(C)[C@@H](O)CC[C@@H]3C2</chem>
(3aR,5S,7aS)-5-(4-hydroxyphenyl)-7a-methyl-hexahydro-2H-inden-1-one	1	1	1	0	<chem>C[C@]12CC[C@@H](C[C@H]1CCC2=O)c3ccc(O)cc3</chem>
6-[(1E)-(hydroxyimino)methyl]-2,3-bis(4-hydroxyphenyl)phenol	1	1	1	0	<chem>O\\N=C\\c1ccc(c2ccc(O)cc2)c(c1O)c3ccc(O)cc3</chem>
3-chloro-2-[(1E)-(hydroxyimino)methyl]-4-(4-hydroxyphenyl)-6-methylphenol	1	1	1	0	<chem>Cc1cc(c(Cl)c(\\C=N\\O)c1O)c2ccc(O)cc2</chem>

	6-chloro-2-[(1E)-(hydroxyimino)methyl]-4-(4-hydroxyphenyl)-3-methylphenol	1	1	1	0	<chem>Cc1c(\C=N\O)c(O)c(Cl)cc1c2ccc(O)cc2</chem>
	6-chloro-4-(3-fluoro-4-hydroxyphenyl)-2-[(1E)-(hydroxyimino)methyl]-3-methylphenol	1	1	1	0	<chem>Cc1c(\C=N\O)c(O)c(Cl)cc1c2ccc(O)c(F)c2</chem>
101-81-5	diphenylmethane	0	1	0	1	<chem>C(c1ccccc1)c2ccccc2</chem>
30777-18-5	benzo(A)fluorene	0	1	0	1	<chem>C1c2ccccc2c3ccc4ccccc4c13</chem>
	4-[[bis(2,4,6-trimethylphenyl)boranyl]amino]phenol	1	1	1	0	<chem>Cc1cc(C)c(B(Nc2ccc(O)cc2)c3c(C)cc(C)cc3C)c(C)c1</chem>
	4-[[bis(2,4,6-trimethylphenyl)boranyl](methyl)amino]phenol	1	1	1	0	<chem>CN(B(c1c(C)cc(C)cc1C)c2c(C)cc(C)cc2C)c3ccc(O)cc3</chem>
	4-[[bis(2,4,6-trimethylphenyl)boranyl](ethyl)amino]phenol	1	1	1	0	<chem>CCN(B(c1c(C)cc(C)cc1C)c2c(C)cc(C)cc2C)c3ccc(O)cc3</chem>
	4-[[bis(2,4,6-trimethylphenyl)boranyl](pentyl)amino]phenol	1	1	1	0	<chem>CCCCCN(B(c1c(C)cc(C)cc1C)c2c(C)cc(C)cc2C)c3ccc(O)cc3</chem>
	4-[[bis(2,6-dimethylphenyl)boranyl](methyl)amino]phenol	1	1	1	0	<chem>CN(B(c1c(C)cccc1C)c2c(C)cccc2C)c3ccc(O)cc3</chem>

	mino}phenol					
	4-[[bis(2,6-dimethylphenyl)boranyl](2,2,2-trifluoroethyl)amino}phenol	1	1	1	0	<chem>Cc1cccc(C)c1B(N(CC(F)(F)F)c2ccc(O)cc2)c3c(C)cccc3C</chem>
	iprodione	0	1	0	1	<chem>CC(C)NC(=O)N1CC(=O)N(C1=O)c2cc(Cl)cc(Cl)c2</chem>
2212-67-1	jalan	0	1	0	1	<chem>CCSC(=O)N1CCCCC1</chem>
744-45-6	1,3-diphenyl benzene-1,3-dicarboxylate	0	1	0	1	<chem>O=C(Oc1ccccc1)c2cccc(c2)C(=O)Oc3ccccc3</chem>
	cyanazine	0	1	0	1	<chem>CCNc1nc(Cl)nc(NC(C)(C)C#N)n1</chem>
	simetryn	0	1	0	1	<chem>CCNc1nc(NCC)nc(SC)n1</chem>
	(3Z)-hex-3-en-1-yl 2-hydroxybenzoate	0	1	0	1	<chem>CC\C=C/CCOC(=O)c1ccccc1O</chem>
110444-90-1	bisphenol AF	1	1	1	0	<chem>Oc1ccc(cc1)C(c2ccc(O)cc2)(C(F)(F)F)C(F)(F)F</chem>
21087-64-9	sencor	0	1	0	1	<chem>CSC1=NN=C(C(=O)N1N)C(C)(C)C</chem>
21664-09-5	tetralol	1	1	1	0	<chem>Oc1ccc2CCCCc2c1</chem>
15231-91-1	6-bromo-2-naphthol	1	1	1	0	<chem>Oc1ccc2cc(Br)ccc2c1</chem>
145667-72-7	(2R)-1,2-dibromo-3-chloropropane	0	1	0	1	<chem>ClC[C@@H](Br)CBr</chem>

	N-[(R)-methoxy(methylsulfanyl)phosphoryl]acetamide	0	1	0	1	<chem>CO[P@](=O)(NC(C)=O)SC</chem>
	(3aR,7aR)-2-[(trichloromethyl)sulfanyl]-3a,4,7,7a-tetrahydroisoindole-1,3-dione	1	1	1	0	<chem>ClC(Cl)(Cl)SN1C(=O)[C@@H]2CC=CC[C@H]2C1=O</chem>
61432-55-1	dimepiperate	0	1	0	1	<chem>CC(C)(SC(=O)N1CCCCC1)c1cccc1</chem>
	butyl (2R)-2-(4-{[4-(trifluoromethyl)pyridin-2-yl]oxy}phenoxy)propanoate	0	1	0	1	<chem>CCCCOC(=O)[C@@H](C)Oc1ccc(Oc2cc(ccn2)C(F)(F)F)cc1</chem>
5315-79-7	1-hydroxypyrene	0	1	0	1	<chem>Oc1ccc2ccc3cccc4ccc1c2c34</chem>
2443-58-5	2-hydroxyfluorene	1	1	1	0	<chem>Oc1ccc-2c(Cc3cccc-23)c1</chem>
3228-02-2	o-cymen-5-ol	0	1	0	1	<chem>CC(C)c1ccc(O)cc1C</chem>
2446-69-7	4-n-hexylphenol	1	1	1	0	<chem>CCCCCCc1ccc(O)cc1</chem>
29155-33-7	tetrachlorobisphenol A	0	1	0	1	<chem>CC(C)(c1cc(Cl)c(O)c(Cl)c1)c1cc(Cl)c(O)c(Cl)c1</chem>
169741-16-6	dicyclohexyl phthalate	1	1	1	0	<chem>O=C(OC1CCCCC1)c1cccc1C(=O)OC1CCCCC1</chem>
275818-86-5	DHPP	1	1	1	0	<chem>CCCCCCCCOC(=O)c1cccc1C(=O)OCCCCCCC</chem>
105009-98-	diisodecyl phthalate	1	1	1	0	<chem>CC(C)CCCCCCCCOC(=O)c1cccc1C(=O)OCCCCCCCC(C)C</chem>

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25103-50-8	diop	1	1	1	0	<chem>CC(C)CCCCCOC(=O)c1ccccc1C(=O)OCCCCC(C)C</chem>
605-45-8	diisopropyl phthalate	0	1	0	1	<chem>CC(C)OC(=O)c1ccccc1C(=O)OC(C)C</chem>
84-75-3	di-n-hexyl phthalate	1	1	1	0	<chem>CCCCCOC(=O)c1ccccc1C(=O)OCCCCC</chem>
	(1R,2R,6S,7S)- tricyclo[5.2.1.0{2,6}]deca-3,8-diene	0	1	0	1	<chem>C1C=C[C@@H]2[C@@H]3C[C@@H](C=C3)[C@H]12</chem>
22717-94-8	tetracyclo[8.8.0.0{2,7}.0{13,18}]oct adeca-1(18),2,4,6,8,10,12,14,16- nonaen-4-ol	1	1	1	0	<chem>Oc1ccc2ccc3ccc4ccccc4c3c2c1</chem>
65945-06-4	chrysen-2-ol	1	1	1	0	<chem>Oc1ccc2c(ccc3c4ccccc4ccc23)c1</chem>
3010-80-8	tris(4-chlorophenyl)methanol	0	1	0	1	<chem>OC(c1ccc(Cl)cc1)(c1ccc(Cl)cc1)c1ccc(Cl)cc1</chem>
	(2R)-6-hydroxy-2-phenyl-2,3- dihydro-1-benzopyran-4-one	1	1	1	0	<chem>Oc1ccc2O[C@H](CC(=O)c2c1)c1ccccc1</chem>
	(1S,10R,11S,13R,14R,15S)-5- methoxy-15- methyltetracyclo[8.7.0.0{2,7}.0{11, 15}]heptadeca-2(7),3,5-triene- 13,14-diol	1	1	1	0	<chem>COc1ccc2[C@H]3CC[C@]4(C)[C@@H](O)[C@H](O)C[C@H]4[C@@H]3CCc2c1</chem>
	4-[5-ethyl-4-(4-hydroxyphenyl)-6- phenylpyrimidin-2-yl]phenol	1	1	1	0	<chem>CCc1c(nc(nc1-c1ccc(O)cc1)-c1ccc(O)cc1)-c1ccccc1</chem>
	4-[2-(4-hydroxyphenyl)-6-phenyl-5-	1	1	1	0	<chem>CCc1c(nc(nc1-c1ccc(O)cc1)-c1ccc(O)cc1)-c1ccccc1</chem>

	propylpyrimidin-4-yl]phenol					
	4-[5-ethyl-2,6-bis(4-hydroxyphenyl)pyrimidin-4-yl]phenol; ethan	1	1	1	0	CC.CCc1c(nc(nc1-c1ccc(O)cc1)-c1ccc(O)cc1)-c1ccc(O)cc1
	4-[2,6-bis(4-hydroxyphenyl)-5-propylpyrimidin-4-yl]phenol	1	1	1	0	CCCc1c(nc(nc1-c1ccc(O)cc1)-c1ccc(O)cc1)-c1ccc(O)cc1
	4-[6-ethyl-2-(4-hydroxyphenyl)-5-phenylpyrimidin-4-yl]phenol	1	1	1	0	CCc1nc(nc(-c2ccc(O)cc2)c1-c1ccccc1)-c1ccc(O)cc1
	4-[2-(4-hydroxyphenyl)-5-phenyl-6-propylpyrimidin-4-yl]phenol	1	1	1	0	CCCc1nc(nc(-c2ccc(O)cc2)c1-c1ccccc1)-c1ccc(O)cc1
	4-[4-ethyl-2,6-bis(4-hydroxyphenyl)pyrimidin-5-yl]phenol	1	1	1	0	CCc1nc(nc(-c2ccc(O)cc2)c1-c1ccc(O)cc1)-c1ccc(O)cc1
	4-[2,5-bis(4-hydroxyphenyl)-6-propylpyrimidin-4-yl]phenol	1	1	1	0	CCCc1nc(nc(-c2ccc(O)cc2)c1-c1ccc(O)cc1)-c1ccc(O)cc1
	4-[5-ethyl-2-(4-hydroxyphenyl)-6-methylpyrimidin-4-yl]phenol	1	1	1	0	CCc1c(C)nc(nc1-c1ccc(O)cc1)-c1ccc(O)cc1
	4-[2-(4-hydroxyphenyl)-6-methyl-5-propylpyrimidin-4-yl]phenol	1	1	1	0	CCCc1c(C)nc(nc1-c1ccc(O)cc1)-c1ccc(O)cc1
	4-[6-benzyl-2-(4-hydroxyphenyl)-5-methylpyrimidin-4-yl]phenol	1	1	1	0	Cc1c(Cc2ccccc2)nc(nc1-c1ccc(O)cc1)-c1ccc(O)cc1

	4-[6-benzyl-5-ethyl-2-(4-hydroxyphenyl)pyrimidin-4-yl]phenol	1	1	1	0	<chem>CCc1c(Cc2ccccc2)nc(nc1-c1ccc(O)cc1)-c1ccc(O)cc1</chem>
	4-[2-(4-hydroxyphenyl)-6-[(4-hydroxyphenyl)methyl]-5-methylpyrimidin-4-yl]phenol	1	1	1	0	<chem>Cc1c(Cc2ccc(O)cc2)nc(nc1-c1ccc(O)cc1)-c1ccc(O)cc1</chem>
	4-[4-ethyl-2-(4-hydroxyphenyl)-6-methylpyrimidin-5-yl]phenol	1	1	1	0	<chem>CCc1nc(nc(C)c1-c1ccc(O)cc1)-c1ccc(O)cc1</chem>
	4-[2-(4-hydroxyphenyl)-4,6-dimethylpyrimidin-5-yl]phenol	1	1	1	0	<chem>Cc1nc(nc(C)c1-c1ccc(O)cc1)-c1ccc(O)cc1</chem>
	4-[2-(4-hydroxyphenyl)-4-methyl-6-propylpyrimidin-5-yl]phenol	1	1	1	0	<chem>CCCc1nc(nc(C)c1-c1ccc(O)cc1)-c1ccc(O)cc1</chem>
	4-[4,6-diethyl-2-(4-hydroxyphenyl)pyrimidin-5-yl]phenol	1	1	1	0	<chem>CCc1nc(nc(CC)c1-c1ccc(O)cc1)-c1ccc(O)cc1</chem>
	4-[4-ethyl-2-(4-hydroxyphenyl)-6-propylpyrimidin-5-yl]phenol	1	1	1	0	<chem>CCCc1nc(nc(CC)c1-c1ccc(O)cc1)-c1ccc(O)cc1</chem>
	4-[5-ethyl-3,6-bis(4-hydroxyphenyl)pyrazin-2-yl]phenol	1	1	1	0	<chem>CCc1nc(-c2ccc(O)cc2)c(nc1-c1ccc(O)cc1)-c1ccc(O)cc1</chem>
	4-[3,5-bis(4-hydroxyphenyl)-6-propylpyrazin-2-yl]phenol	1	1	1	0	<chem>CCCc1nc(-c2ccc(O)cc2)c(nc1-c1ccc(O)cc1)-c1ccc(O)cc1</chem>
	4-[tris(4-hydroxyphenyl)pyrazin-2-	1	1	1	0	<chem>Oc1ccc(cc1)-c1nc(-c2ccc(O)cc2)c(nc1-c1ccc(O)cc1)-</chem>

	yl]phenol					c1ccc(O)cc1
	4-[5,6-diethyl-3-(4-hydroxyphenyl)pyrazin-2-yl]phenol	1	1	1	0	CCc1nc(-c2ccc(O)cc2)c(nc1CC)-c1ccc(O)cc1
	4-[3-(4-hydroxyphenyl)-5,6-dipropylpyrazin-2-yl]phenol	1	1	1	0	CCCc1nc(-c2ccc(O)cc2)c(nc1CCC)-c1ccc(O)cc1
	4-[3,6-diethyl-5-(4-hydroxyphenyl)pyrazin-2-yl]phenol	1	1	1	0	CCc1nc(c(CC)nc1-c1ccc(O)cc1)-c1ccc(O)cc1
	4-[5-(4-hydroxyphenyl)-6-isopropyl-3-(sec-butyl)pyrazin-2-yl]phenol	1	1	1	0	CCC(C)c1nc(-c2ccc(O)cc2)c(nc1-c1ccc(O)cc1)C(C)C
	4-[5-(4-hydroxyphenyl)-3,6-dimethylpyrazin-2-yl]phenol	1	1	1	0	Cc1nc(c(C)nc1-c1ccc(O)cc1)-c1ccc(O)cc1
	6-[(1E)-(hydroxyimino)methyl]-2,3-diphenylphenol	1	1	1	0	O\\N=C\\c1ccc(-c2ccccc2)c(-c2ccccc2)c1O
	2-hydroxy-3,4-diphenylbenzaldehyde	1	1	1	0	Oc1c(C=O)ccc(-c2ccccc2)c1-c1ccccc1
	2-hydroxy-3-(4-methoxyphenyl)-4-phenylbenzaldehyde	1	1	1	0	COc1ccc(cc1)-c1c(O)c(C=O)ccc1-c1ccccc1
	6-[(1E)-(hydroxyimino)methyl]-2-(4-methoxyphenyl)-3-phenylphenol	1	1	1	0	COc1ccc(cc1)-c1c(O)c(\C=N\O)ccc1-c1ccccc1
	6-[(1E)-(hydroxyimino)methyl]-2-(4-hydroxyphenyl)-3-phenylphenol	1	1	1	0	O\\N=C\\c1ccc(-c2ccccc2)c(-c2ccc(O)cc2)c1O

	2-hydroxy-3-(4-hydroxyphenyl)-4-phenylbenzaldehyde	1	1	1	0	<chem>Oc1ccc(cc1)-c1c(O)c(C=O)ccc1-c1ccccc1</chem>
	2-hydroxy-4-(4-methoxyphenyl)-3-phenylbenzaldehyde	1	1	1	0	<chem>COc1ccc(cc1)-c1ccc(C=O)c(O)c1-c1ccccc1</chem>
	6-[(1E)-(hydroxyimino)methyl]-3-(4-methoxyphenyl)-2-phenylphenol	1	1	1	0	<chem>COc1ccc(cc1)-c1ccc(\C=N\O)c(O)c1-c1ccccc1</chem>
	6-[(1E)-(hydroxyimino)methyl]-3-(4-hydroxyphenyl)-2-phenylphenol	1	1	1	0	<chem>O\N=C\c1ccc(-c2ccc(O)cc2)c(-c2ccccc2)c1O</chem>
	2-hydroxy-4-(4-hydroxyphenyl)-3-phenylbenzaldehyde	1	1	1	0	<chem>Oc1ccc(cc1)-c1ccc(C=O)c(O)c1-c1ccccc1</chem>
	2-hydroxy-3,4-bis(4-methoxyphenyl)benzaldehyde	1	1	1	0	<chem>COc1ccc(cc1)-c1ccc(C=O)c(O)c1-c1ccc(OC)cc1</chem>
	6-[(1E)-(hydroxyimino)methyl]-2,3-bis(4-methoxyphenyl)phenol	0	1	0	1	<chem>COc1ccc(cc1)-c1ccc(\C=N\O)c(O)c1-c1ccc(OC)cc1</chem>
	6-[(1E)-(hydroxyimino)methyl]-2,3-bis(4-hydroxyphenyl)phenol	1	1	1	0	<chem>O\N=C\c1ccc(-c2ccc(O)cc2)c(-c2ccc(O)cc2)c1O</chem>
	2-hydroxy-3,4-bis(4-hydroxyphenyl)benzaldehyde	1	1	1	0	<chem>Oc1ccc(cc1)-c1ccc(C=O)c(O)c1-c1ccc(O)cc1</chem>
92-04-6	4-phenyl-2-chlorophenol	1	1	1	0	<chem>Oc1ccc(cc1Cl)-c1ccccc1</chem>
	2-methyl-4-phenylphenol	0	1	0	1	<chem>Cc1cc(ccc1O)-c1ccccc1</chem>
	3-fluoro-4-phenylphenol	1	1	1	0	<chem>Oc1ccc(c(F)c1)-c1ccccc1</chem>

	3-methyl-4-phenylphenol	1	1	1	0	<chem>Cc1cc(O)ccc1-c1ccccc1</chem>
321-62-0	4-(2-fluorophenyl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1ccccc1F</chem>
	4-(3-fluorophenyl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1cccc(F)c1</chem>
324-94-7	4-(4-fluorophenyl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1ccc(F)cc1</chem>
611-62-1	2-(4-hydroxyphenyl)phenol	0	1	0	1	<chem>Oc1ccc(cc1)-c1ccccc1O</chem>
18855-13-5	3-(4-hydroxyphenyl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1cccc(O)c1</chem>
	4-(2-phenylphenyl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1ccccc1-c1ccccc1</chem>
	4-(3-phenylphenyl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1cccc(c1)-c1ccccc1</chem>
	4-(4-phenylphenyl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1ccc(cc1)-c1ccccc1</chem>
	4-[2-(trifluoromethyl)phenyl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1ccccc1C(F)(F)F</chem>
	4-[4-(trifluoromethyl)phenyl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1ccc(cc1)C(F)(F)F</chem>
	2-(4-hydroxyphenyl)benzonitrile	1	1	1	0	<chem>Oc1ccc(cc1)-c1ccccc1C#N</chem>
154848-44-9	3-(4-hydroxyphenyl)benzonitrile	1	1	1	0	<chem>Oc1ccc(cc1)-c1cccc(c1)C#N</chem>
19812-93-2	4-(4-hydroxyphenyl)benzonitrile	1	1	1	0	<chem>Oc1ccc(cc1)-c1ccc(cc1)C#N</chem>
	4-(2-ethylphenyl)phenol	1	1	1	0	<chem>CCc1ccccc1-c1ccc(O)cc1</chem>

	4-(3-ethylphenyl)phenol	1	1	1	0	<chem>CCc1cccc(c1)-c1ccc(O)cc1</chem>
	4-(4-ethylphenyl)phenol	1	1	1	0	<chem>CCc1ccc(cc1)-c1ccc(O)cc1</chem>
	4-(4-chloro-3-ethylphenyl)phenol	1	1	1	0	<chem>CCc1cc(ccc1Cl)-c1ccc(O)cc1</chem>
53890-76-9	4-(2,4-dichlorophenyl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1ccc(Cl)cc1Cl</chem>
	4-[2-fluoro-5-(trifluoromethyl)phenyl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1cc(ccc1F)C(F)(F)F</chem>
	4-(3-chlorophenyl)-2-methylphenol	1	1	1	0	<chem>Cc1cc(ccc1O)-c1cccc(Cl)c1</chem>
	4-(3-chlorophenyl)-3-fluorophenol	1	1	1	0	<chem>Oc1ccc(c(F)c1)-c1cccc(Cl)c1</chem>
	3-chloro-4-(3-chlorophenyl)phenol	1	1	1	0	<chem>Oc1ccc(c(Cl)c1)-c1cccc(Cl)c1</chem>
	4-(3-chlorophenyl)-3-methylphenol	1	1	1	0	<chem>Cc1cc(O)ccc1-c1cccc(Cl)c1</chem>
53714-66-2	4-(2,3-dichlorophenyl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1cccc(Cl)c1Cl</chem>
	4-(3-chloro-4-fluorophenyl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1ccc(F)c(Cl)c1</chem>
	4-(3-chloro-4-methylphenyl)phenol	1	1	1	0	<chem>Cc1ccc(cc1Cl)-c1ccc(O)cc1</chem>
	2-chloro-4-(4-hydroxyphenyl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1ccc(O)c(Cl)c1</chem>
	4-(4-amino-3-chlorophenyl)phenol	1	1	1	0	<chem>Nc1ccc(cc1Cl)-c1ccc(O)cc1</chem>
	2-chloro-4-(4-hydroxyphenyl)benzonitrile	1	1	1	0	<chem>Oc1ccc(cc1)-c1ccc(C#N)c(Cl)c1</chem>

	2,6-dichloro-4-(4-hydroxyphenyl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1cc(Cl)c(O)c(Cl)c1</chem>
	2,6-dichloro-4-(3-fluoro-4-hydroxyphenyl)phenol	1	1	1	0	<chem>Oc1ccc(cc1F)-c1cc(Cl)c(O)c(Cl)c1</chem>
	4-[2-fluoro-3-(trifluoromethyl)phenyl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1cccc(c1F)C(F)(F)F</chem>
	4-[2-chloro-3-(trifluoromethyl)phenyl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1cccc(c1Cl)C(F)(F)F</chem>
	4-[4-fluoro-3-(trifluoromethyl)phenyl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1ccc(F)c(c1)C(F)(F)F</chem>
	4-[4-chloro-3-(trifluoromethyl)phenyl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1ccc(Cl)c(c1)C(F)(F)F</chem>
	4-[4-amino-3-(trifluoromethyl)phenyl]phenol	1	1	1	0	<chem>Nc1ccc(cc1C(F)(F)F)-c1ccc(O)cc1</chem>
	4-[4-(dimethylamino)-3-(trifluoromethyl)phenyl]phenol	1	1	1	0	<chem>CN(C)c1ccc(cc1C(F)(F)F)-c1ccc(O)cc1</chem>
	4-[3,5-bis(trifluoromethyl)phenyl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1cc(cc(c1)C(F)(F)F)C(F)(F)F</chem>
	4-[2-chloro-5-(trifluoromethyl)phenyl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1cc(ccc1Cl)C(F)(F)F</chem>
1844-00-4	4,4'-isobutylidenediphenol	1	1	1	0	<chem>CC(C)C(c1ccc(O)cc1)c1ccc(O)cc1</chem>

24887-75-0	5 α -androstane	0	1	0	1	<chem>C[C@@]12CCC[C@H]1[C@@H]1CC[C@H]3CCCC[C@]3(C)[C@H]1CC2</chem>
	4-{4-[(1E)-(hydroxyimino)methyl]phenyl}phenol	1	1	1	0	<chem>O\\N=C\\c1ccc(cc1)-c1ccc(O)cc1</chem>
	2-fluoro-4-{4-[(1E)-(hydroxyimino)methyl]phenyl}phenol	1	1	1	0	<chem>O\\N=C\\c1ccc(cc1)-c1ccc(O)c(F)c1</chem>
	4-{3-chloro-4-[(1E)-(hydroxyimino)methyl]phenyl}phenol	1	1	1	0	<chem>O\\N=C\\c1ccc(cc1Cl)-c1ccc(O)cc1</chem>
	4-{2-chloro-4-[(1E)-(hydroxyimino)methyl]phenyl}phenol	1	1	1	0	<chem>O\\N=C\\c1ccc(c(Cl)c1)-c1ccc(O)cc1</chem>
	4-{3-fluoro-4-[(1E)-(hydroxyimino)methyl]phenyl}phenol	1	1	1	0	<chem>O\\N=C\\c1ccc(cc1F)-c1ccc(O)cc1</chem>
	4-{2-fluoro-4-[(1E)-(hydroxyimino)methyl]phenyl}phenol	1	1	1	0	<chem>O\\N=C\\c1ccc(c(F)c1)-c1ccc(O)cc1</chem>
	4-{4-[(1E)-(hydroxyimino)methyl]-3-methoxyphenyl}phenol	1	1	1	0	<chem>COc1cc(ccc1\\C=N\\O)-c1ccc(O)cc1</chem>
	4-{2,6-dichloro-4-[(1E)-	1	1	1	0	<chem>O\\N=C\\c1cc(Cl)c(c(Cl)c1)-c1ccc(O)cc1</chem>

	(hydroxyimino)methyl]phenyl}phenol					
	2-fluoro-4-{3-fluoro-4-[(1E)-(hydroxyimino)methyl]phenyl}phenol	1	1	1	0	<chem>O\\N=C\\c1ccc(cc1F)-c1ccc(O)c(F)c1</chem>
	4-{3-chloro-4-[(1E)-(hydroxyimino)methyl]phenyl}-3-methylphenol	1	1	1	0	<chem>Cc1cc(O)ccc1-c1ccc(\\C=N\\O)c(Cl)c1</chem>
	4-{3-chloro-4-[(1E)-(hydroxyimino)methyl]phenyl}-2,6-difluorophenol	1	1	1	0	<chem>O\\N=C\\c1ccc(cc1Cl)-c1cc(F)c(O)c(F)c1</chem>
	4-{2,6-dichloro-4-[(1E)-(hydroxyimino)methyl]phenyl}-2-fluorophenol	1	1	1	0	<chem>O\\N=C\\c1cc(Cl)c(c(Cl)c1)-c1ccc(O)c(F)c1</chem>
	4-{4-[(1E)-(hydroxyimino)methyl]-2-methylphenyl}phenol	1	1	1	0	<chem>Cc1cc(\\C=N\\O)ccc1-c1ccc(O)cc1</chem>
	4-{4-[(1E)-(hydroxyimino)methyl]-3-methylphenyl}phenol	1	1	1	0	<chem>Cc1cc(ccc1\\C=N\\O)-c1ccc(O)cc1</chem>
	2-fluoro-4-{4-[(1E)-(hydroxyimino)methyl]-3-methylphenyl}phenol	1	1	1	0	<chem>Cc1cc(ccc1\\C=N\\O)-c1ccc(O)c(F)c1</chem>
	4-{2,3-dichloro-4-[(1E)-(hydroxyimino)methyl]phenyl}phenol	1	1	1	0	<chem>O\\N=C\\c1ccc(c(Cl)c1Cl)-c1ccc(O)cc1</chem>

	ol					
	4-{2,3-dichloro-4-[(1E)-(hydroxyimino)methyl]phenyl}-2-fluorophenol	1	1	1	0	<chem>O\\N=C\\c1ccc(c(Cl)c1Cl)-c1ccc(O)c(F)c1</chem>
	4-{3,5-dichloro-4-[(1E)-(hydroxyimino)methyl]phenyl}phenol	1	1	1	0	<chem>O\\N=C\\c1c(Cl)cc(cc1Cl)-c1ccc(O)cc1</chem>
	4-{3,5-dichloro-4-[(1E)-(hydroxyimino)methyl]phenyl}-2-fluorophenol	1	1	1	0	<chem>O\\N=C\\c1c(Cl)cc(cc1Cl)-c1ccc(O)c(F)c1</chem>
	2-chloro-1-methyl-4-phenylbenzene	1	1	1	0	<chem>Cc1ccc(cc1Cl)-c1ccccc1</chem>
	2-chloro-4-(3-fluorophenyl)-1-methylbenzene	1	1	1	0	<chem>Cc1ccc(cc1Cl)-c1cccc(F)c1</chem>
	4-(2,3-dichloro-4-methylphenyl)phenol	1	1	1	0	<chem>Cc1ccc(c(Cl)c1Cl)-c1ccc(O)cc1</chem>
	4-(2,3-dichloro-4-methylphenyl)-2-fluorophenol	1	1	1	0	<chem>Cc1ccc(c(Cl)c1Cl)-c1ccc(O)c(F)c1</chem>
	(14R,15S)-15-methyl-14-[(E)-2-(pyridin-2-yl)ethenyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	<chem>C[C@]12CCC3C(CCC4cc(O)ccc34)C1CC[C@@]2(O)\\C=C\\c1ccccc1</chem>

(14R,15S)-15-methyl-14-[(E)-2-(pyridin-3-yl)ethenyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	<chem>C[C@]12CCC3C(CCc4cc(O)ccc34)C1CC[C@@]2(O)\C=C\c1cccnc1</chem>
(14R,15S)-15-methyl-14-[(E)-2-(pyridin-4-yl)ethenyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	<chem>C[C@]12CCC3C(CCc4cc(O)ccc34)C1CC[C@@]2(O)\C=C\c1ccncc1</chem>
(14R,15S)-15-methyl-14-[(E)-2-(pyrimidin-5-yl)ethenyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	<chem>C[C@]12CCC3C(CCc4cc(O)ccc34)C1CC[C@@]2(O)\C=C\c1cncnc1</chem>
(14R,15S)-15-methyl-14-[(E)-2-(thiophen-2-yl)ethenyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	<chem>C[C@]12CCC3C(CCc4cc(O)ccc34)C1CC[C@@]2(O)\C=C\c1cccs1</chem>
(14R,15S)-15-methyl-14-[(E)-2-(thiophen-3-yl)ethenyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	<chem>C[C@]12CCC3C(CCc4cc(O)ccc34)C1CC[C@@]2(O)\C=C\c1ccsc1</chem>

(2S)-2,3-bis(4-hydroxyphenyl)propanenitrile	1	1	1	0	<chem>Oc1ccc(C[C@H](C#N)c2ccc(O)cc2)cc1</chem>
phenyl 5,6-bis(4-hydroxyphenyl)-7-oxo-7 <i>S</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>Oc1ccc(cc1)C1=C(C2C(CC1S2=O)S(=O)(=O)Oc1ccccc1)c1ccc(O)cc1</chem>
4-methoxyphenyl 5,6-bis(4-hydroxyphenyl)-7-oxo-7 <i>S</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>COc1ccc(OS(=O)(=O)C2CC3C(=C(C2S3=O)c2ccc(O)cc2)c2ccc(O)cc2)cc1</chem>
4-hydroxyphenyl 5,6-bis(4-hydroxyphenyl)-7-oxo-7 <i>S</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>Oc1ccc(OS(=O)(=O)C2CC3C(=C(C2S3=O)c2ccc(O)cc2)c2ccc(O)cc2)cc1</chem>
8,9-bis(4-hydroxyphenyl)-4-phenyl-10 <i>S</i> {4}-thia-4-azatricyclo[5.2.1.0{2,6}]dec-8-ene-3,5,10-trione	1	1	1	0	<chem>Oc1ccc(cc1)C1=C(C2C3C(C1S2=O)C(=O)N(C3=O)c1ccccc1)c1ccc(O)cc1</chem>
2,3-diethyl 5,6-bis(4-hydroxyphenyl)-7-oxo-7 <i>S</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2,3-dicarboxylate	1	1	1	0	<chem>CCOC(=O)C1C(C2C(=C(C1S2=O)c1ccc(O)cc1)c1ccc(O)cc1)C(=O)OCC</chem>
phenyl 5,6-bis(4-hydroxy-2-methylphenyl)-7-oxo-7 <i>S</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-	1	1	1	0	<chem>Cc1cc(O)ccc1C1=C(C2C(CC1S2=O)S(=O)(=O)Oc1ccccc1)c1ccc(O)cc1C</chem>

	sulfonate					
	4-methoxyphenyl 5,6-bis(4-hydroxy-2-methylphenyl)-7-oxo-7 <i>l</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>COc1ccc(OS(=O)(=O)C2CC3C(=C(C2S3=O)c2ccc(O)cc2C)c2ccc(O)cc2C)cc1</chem>
	2-fluorophenyl 5,6-bis(4-hydroxy-2-methylphenyl)-7-oxo-7 <i>l</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>Cc1cc(O)ccc1C1=C(C2C(CC1S2=O)S(=O)(=O)Oc1ccccc1F)c1ccc(O)cc1C</chem>
	2-chlorophenyl 5,6-bis(4-hydroxy-2-methylphenyl)-7-oxo-7 <i>l</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>Cc1cc(O)ccc1C1=C(C2C(CC1S2=O)S(=O)(=O)Oc1ccccc1Cl)c1ccc(O)cc1C</chem>
	2-bromophenyl 5,6-bis(4-hydroxy-2-methylphenyl)-7-oxo-7 <i>l</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>Cc1cc(O)ccc1C1=C(C2C(CC1S2=O)S(=O)(=O)Oc1ccccc1Br)c1ccc(O)cc1C</chem>
	4-fluorophenyl 5,6-bis(4-hydroxy-2-methylphenyl)-7-oxo-7 <i>l</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>Cc1cc(O)ccc1C1=C(C2C(CC1S2=O)S(=O)(=O)Oc1ccc(F)cc1)c1ccc(O)cc1C</chem>
	4-chlorophenyl 5,6-bis(4-hydroxy-2-methylphenyl)-7-oxo-7 <i>l</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-	1	1	1	0	<chem>Cc1cc(O)ccc1C1=C(C2C(CC1S2=O)S(=O)(=O)Oc1ccc(Cl)cc1)c1ccc(O)cc1C</chem>

	sulfonate					
	4-bromophenyl 5,6-bis(4-hydroxy-2-methylphenyl)-7-oxo-7 <i>S</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>Cc1cc(O)ccc1C1=C(C2C(CC1S2=O)S(=O)(=O)Oc1ccc(Br)cc1)c1ccc(O)cc1C</chem>
	3-chlorophenyl 5,6-bis(4-hydroxy-2-methylphenyl)-7-oxo-7 <i>S</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>Cc1cc(O)ccc1C1=C(C2C(CC1S2=O)S(=O)(=O)Oc1cccc(Cl)c1)c1ccc(O)cc1C</chem>
	naphthalen-1-yl 5,6-bis(4-hydroxy-2-methylphenyl)-7-oxo-7 <i>S</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>Cc1cc(O)ccc1C1=C(C2C(CC1S2=O)S(=O)(=O)Oc1cccc2cccc12)c1ccc(O)cc1C</chem>
	4-hydroxyphenyl 5,6-bis(4-hydroxy-2-methylphenyl)-7-oxo-7 <i>S</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>Cc1cc(O)ccc1C1=C(C2C(CC1S2=O)S(=O)(=O)Oc1ccc(O)cc1)c1ccc(O)cc1C</chem>
	8,9-bis(4-hydroxy-2-methylphenyl)-4-phenyl-10 <i>S</i> {4}-thia-4-azatricyclo[5.2.1.0{2,6}]dec-8-ene-3,5,10-trione	1	1	1	0	<chem>Cc1cc(O)ccc1C1=C(C2C3C(C1S2=O)C(=O)N(C3=O)c1cccc1)c1ccc(O)cc1C</chem>
	phenyl 5,6-bis(4-hydroxy-3-methylphenyl)-7-oxo-7 <i>S</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-	1	1	1	0	<chem>Cc1cc(ccc1O)C1=C(C2C(CC1S2=O)S(=O)(=O)Oc1cccc1)c1cc(O)c(C)c1</chem>

	sulfonate					
	4-methoxyphenyl 5,6-bis(4-hydroxy-3-methylphenyl)-7-oxo-7 <i>S</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>COc1ccc(OS(=O)(=O)C2CC3C(=C(C2S3=O)c2ccc(O)c(C)c2)c2ccc(O)c(C)c2)cc1</chem>
	2-fluorophenyl 5,6-bis(4-hydroxy-3-methylphenyl)-7-oxo-7 <i>S</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>Cc1cc(ccc1O)C1=C(C2C(CC1S2=O)S(=O)(=O)Oc1ccccc1F)c1ccc(O)c(C)c1</chem>
	2-chlorophenyl 5,6-bis(4-hydroxy-3-methylphenyl)-7-oxo-7 <i>S</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>Cc1cc(ccc1O)C1=C(C2C(CC1S2=O)S(=O)(=O)Oc1ccccc1Cl)c1ccc(O)c(C)c1</chem>
	2-bromophenyl 5,6-bis(4-hydroxy-3-methylphenyl)-7-oxo-7 <i>S</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>Cc1cc(ccc1O)C1=C(C2C(CC1S2=O)S(=O)(=O)Oc1ccccc1Br)c1ccc(O)c(C)c1</chem>
	naphthalen-1-yl 5,6-bis(4-hydroxy-3-methylphenyl)-7-oxo-7 <i>S</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>Cc1cc(ccc1O)C1=C(C2C(CC1S2=O)S(=O)(=O)Oc1cccc2ccccc12)c1ccc(O)c(C)c1</chem>
	4-hydroxyphenyl 5,6-bis(4-hydroxy-3-methylphenyl)-7-oxo-7 <i>S</i> {4}-thiabicyclo[2.2.1]hept-5-ene-2-	1	1	1	0	<chem>Cc1cc(ccc1O)C1=C(C2C(CC1S2=O)S(=O)(=O)Oc1ccc(O)cc1)c1ccc(O)c(C)c1</chem>

	sulfonate					
	8,9-bis(4-hydroxy-3-methylphenyl)-4-phenyl-10 <i>S</i> l{4}-thia-4-azatricyclo[5.2.1.0{2,6}]dec-8-ene-3,5,10-trione	1	1	1	0	<chem>Cc1cc(ccc1O)C1=C(C2C3C(C1S2=O)C(=O)N(C3=O)c1ccccc1)c1ccc(O)c(C)c1</chem>
	2,3-diethyl 5,6-bis(4-hydroxy-3-methylphenyl)-7-oxo-7 <i>S</i> l{4}-thiabicyclo[2.2.1]hept-5-ene-2,3-dicarboxylate	1	1	1	0	<chem>CCOC(=O)C1C(C2C(=C(C1S2=O)c1ccc(O)c(C)c1)c1ccc(O)c(C)c1)C(=O)OCC</chem>
	4-hydroxyphenyl 7-oxo-5,6-diphenyl-7 <i>S</i> l{4}-thiabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>Oc1ccc(OS(=O)(=O)C2CC3C(=C(C2S3=O)c2ccccc2)c2ccccc2)cc1</chem>
	4-hydroxyphenyl 5,6-bis(4-methylphenyl)-7-oxo-7 <i>S</i> l{4}-thiabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>Cc1ccc(cc1)C1=C(C2C(CC1S2=O)S(=O)(=O)Oc1ccc(O)cc1)c1ccc(C)cc1</chem>
	4-hydroxyphenyl 5-(4-hydroxy-3-methylphenyl)-7-oxo-6-phenyl-7 <i>S</i> l{4}-thiabicyclo[2.2.1]hept-5-ene-2-sulfonate	1	1	1	0	<chem>Cc1cc(ccc1O)C1=C(C2C(CC1S2=O)S(=O)(=O)Oc1ccc(O)cc1)c1ccccc1</chem>
	4-[4-(4-hydroxyphenyl)thiophen-3-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1cscc1-c1ccc(O)cc1</chem>

	4-[4-(4-hydroxy-2-methylphenyl)thiophen-3-yl]-3-methylphenol	1	1	1	0	<chem>Cc1cc(O)ccc1-c1cscc1-c1ccc(O)cc1C</chem>
	4-[4-(4-hydroxy-3-methylphenyl)thiophen-3-yl]-2-methylphenol	1	1	1	0	<chem>Cc1cc(ccc1O)-c1cscc1-c1ccc(O)c(C)c1</chem>
54-11-5	(S)-nicotine	0	1	0	1	<chem>CN1CCC[C@H]1c2cccnc2</chem>
70458-96-7	norfloxacin	0	1	0	1	<chem>CCN1C=C(C(=O)O)C(=O)c2cc(F)c(cc12)N3CCNCC3</chem>
	2,6-dibromo-4-[4-(3,5-dibromo-4-hydroxyphenyl)hexan-3-yl]phenol	1	1	1	0	<chem>CCC(C(CC)c1cc(Br)c(O)c(Br)c1)c2cc(Br)c(O)c(Br)c2</chem>
	2,6-dibromo-4-[4-(3-bromo-4-hydroxyphenyl)hexan-3-yl]phenol	1	1	1	0	<chem>CCC(C(CC)c1cc(Br)c(O)c(Br)c1)c2ccc(O)c(Br)c2</chem>
	4-[4-(4-hydroxy-3-iodophenyl)hexan-3-yl]-2,6-diiodophenol	1	1	1	0	<chem>CCC(C(CC)c1cc(I)c(O)c(I)c1)c2ccc(O)c(I)c2</chem>
	4-[4-(4-hydroxy-3,5-diiodophenyl)hexan-3-yl]-2,6-diiodophenol	1	1	1	0	<chem>CCC(C(CC)c1cc(I)c(O)c(I)c1)c2cc(I)c(O)c(I)c2</chem>
	4-[4-(4-hydroxyphenyl)hexan-3-yl]-2,6-diiodophenol	1	1	1	0	<chem>CCC(C(CC)c1cc(I)c(O)c(I)c1)c2ccc(O)cc2</chem>
	2-bromo-4-[4-(4-hydroxyphenyl)hexan-3-yl]phenol	1	1	1	0	<chem>CCC(C(CC)c1ccc(O)c(Br)c1)c2ccc(O)cc2</chem>

	4-[3,3,3-trifluoro-1-phenyl-2-(trifluoromethyl)prop-1-en-1-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)C(=C(C(F)(F)F)C(F)(F)F)c2ccccc2</chem>
	4-[(2E)-1,1,1,4,4,4-hexafluoro-3-phenylbut-2-en-2-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)\C(=C(\c2ccccc2)/C(F)(F)F)\C(F)(F)F</chem>
	4-[1-chloro-4-(4-hydroxyphenyl)hexan-3-yl]phenol	1	1	1	0	<chem>CCC(C(CCl)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	phenobarbital	0	1	0	1	<chem>CCC1(C(=O)NC(=O)NC1=O)c2ccccc2</chem>
83-79-4	cube root	0	1	0	1	<chem>COc1cc2OC[C@H]3Oc4c5C[C@@H](Oc5ccc4C(=O)[C@H]3c2cc1OC)C(=C)C</chem>
56274-95-4	propyl gallate	0	1	0	1	<chem>CCOC(=O)c1cc(O)c(O)c(O)c1</chem>
52-86-8	haloperidol	0	1	0	1	<chem>OC1(CCN(CCCC(=O)c2ccc(F)cc2)CC1)c3ccc(Cl)cc3</chem>
6640-24-0	m-chlorophenylpiperazine	0	1	0	1	<chem>Clc1cccc(c1)N2CCNCC2</chem>
	(2R,4S)-ketoconazole	0	1	0	1	<chem>CC(=O)N1CCN(CC1)c2ccc(OC[C@H]3CO[C@@](Cn4ccnc4)(O3)c5ccc(Cl)cc5Cl)cc2</chem>
	[6-methoxy-2-(4-methoxyphenyl)-1-benzothiophen-3-yl](3,4,5-trimethoxyphenyl)methanone	1	1	1	0	<chem>COc1ccc(cc1)c2sc3cc(OC)ccc3c2C(=O)c4cc(OC)c(OC)c(OC)c4</chem>
	physostigmine	0	1	0	1	<chem>CNC(=O)Oc1ccc2N(C)[C@H]3N(C)CC[C@@]3(C)c2c1</chem>
	caprolactam	0	1	0	1	<chem>O=C1CCCCCN1</chem>

90-33-5	4-methylumbelliferone	0	1	0	1	<chem>CC1=CC(=O)Oc2cc(O)ccc12</chem>
22395-24-0	2-(3,4-dimethoxyphenyl)-7-methoxychromen-4-one	0	1	0	1	<chem>COc1ccc2C(=O)C=C(Oc2c1)c3ccc(OC)c(OC)c3</chem>
1157-39-7	7,4'-di-O-methyldaidzein	0	1	0	1	<chem>COc1ccc(cc1)C2=COc3cc(OC)ccc3C2=O</chem>
120-44-5	1,2-bis(4-methoxyphenyl)ethanone	0	1	0	1	<chem>COc1ccc(CC(=O)c2ccc(OC)cc2)cc1</chem>
97950-17-9	isotretinoin	0	1	0	1	<chem>C\\C(=C\\C(=O)O)\\C=C\\C=C(/C)\\C=C\\C1=C(C)CCCC1(C)C</chem>
	1-(2-{4-[(2S,3R)-6-methoxy-2-(4-methoxyphenyl)-2,3-dihydro-1-benzothiophene-3-carbonyl]phenoxy}ethyl)piperidine	1	1	1	0	<chem>COc1ccc(cc1)[C@H]2Sc3cc(OC)ccc3[C@@H]2C(=O)c4ccc(OCCN5CCCCC5)cc4</chem>
779-51-1	[(1E)-1-phenylprop-1-en-2-yl]benzene	0	1	0	1	<chem>C\\C(=C/c1ccccc1)\\c2ccccc2</chem>
51-49-0	D-thyroxine	0	1	0	1	<chem>N[C@H](Cc1cc(I)c(Oc2cc(I)c(O)c(I)c2)c(I)c1)C(=O)O</chem>
	fenoxycarb	0	1	0	1	<chem>CCOC(=O)NCCOc1ccc(Oc2ccccc2)cc1</chem>
58-39-9	perphenazine	0	1	0	1	<chem>OCCN1CCN(CCCN2c3ccccc3Sc4ccc(Cl)cc24)CC1</chem>
	dynex	0	1	0	1	<chem>CN(C)C(=O)Nc1ccc(Cl)c(Cl)c1</chem>
108-86-1	bromobenzene	0	1	0	1	<chem>Brc1ccccc1</chem>
1034-01-1	octyl gallate	1	1	1	0	<chem>CCCCCCCCOC(=O)c1cc(O)c(O)c(O)c1</chem>
21785-09-1	7-methoxy-2-phenylchromen-4-	0	1	0	1	<chem>COc1ccc2C(=O)C=C(Oc2c1)c3ccccc3</chem>

	one					
	(14R)-14-ethynyl-14-hydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-1,6-dien-5-one	1	1	1	0	CC12CCC3=C4CCC(=O)C=C4CCC3C1CC[C@@]2(O)C#C
6665-86-7	7-hydroxyflavone	0	1	0	1	Oc1ccc2C(=O)C=C(Oc2c1)c3ccccc3
491-78-1	5-hydroxyflavone	0	1	0	1	Oc1cccc2OC(=CC(=O)c12)c3ccccc3
	(14S)-14-acetyl-14,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-1,6-dien-5-one	1	1	1	0	CC(=O)[C@@]1(C)CCC2C3CCC4=CC(=O)CCC4=C3CCC12C
	(2R)-15'-methylspiro[1,5]l[4]-oxathiolane-2,14'-tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadecan]-6'-ene-5,5'-dione	1	1	1	0	CC12CCC3C(CCC4=CC(=O)CCC34)C1CC[C@@]25CCS(=O)O5
3843-74-1	methyl caffeate	1	1	1	0	COC(=O)\C=C\c1ccc(O)c(O)c1
88025-82-5	clofentezine	0	1	0	1	Clc1ccccc1c2nnc(nn2)c3ccccc3Cl
	2-hydroxy-5-[(8E)-1-{4-[1-(4-hydroxyphenyl)-2-phenylbutyl]phenyl}-4-methyl-1,7-dioxa-4,8-diazanon-8-en-9-yl]benzamide	1	1	1	0	CCC(C(c1ccc(O)cc1)c2ccc(OCCN(C)CCO\N=C\c3ccc(O)c(c3)C(=O)N)cc2)c4ccccc4
	2-hydroxy-5-[(11E)-1-{4-[1-(4-hydroxyphenyl)-2-phenylbutyl]phenyl}-4-methyl-	1	1	1	0	CCC(C(c1ccc(O)cc1)c2ccc(OCCN(C)CCOCCO\N=C\c3ccc(O)c(c3)C(=O)N)cc2)c4ccccc4

	1,7,10-trioxa-4,11-diazadodec-11-en-12-yl]benzamide					
	2-hydroxy-5-[(14E)-1-{4-[1-(4-hydroxyphenyl)-2-phenylbutyl]phenyl}-4-methyl-1,7,10,13-tetraoxa-4,14-diazapentadec-14-en-15-yl]benzamide	1	1	1	0	<chem>CCC(C(c1ccc(O)cc1)c2ccc(OCCN(C)CCOCCOCCO\\N=C\\c3ccc(O)c(c3)C(=O)N)cc2)c4ccccc4</chem>
51-44-5	3,4-dichlorobenzoic acid	0	1	0	1	<chem>OC(=O)c1ccc(Cl)c(Cl)c1</chem>
	M-phenoxybenzoic acid	0	1	0	1	<chem>OC(=O)c1cccc(Oc2ccccc2)c1</chem>
49562-28-9	isopropyl 2-[4-(4-chlorobenzoyl)phenoxy]-2-methylpropanoate	0	1	0	1	<chem>CC(C)OC(=O)C(C)(C)Oc1ccc(cc1)C(=O)c2ccc(Cl)cc2</chem>
	tripotassium 24-(4-{4-[(14R,15R)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-yl]phenyl}buta-1,3-diyn-1-yl)-2 <i>S</i> {5},11,20,29,38,39 <i>S</i> {5},40,41-octaaza-1-zincadodecacyclo[19.17.1.1{1,12}.1{3,37}.0{2,10}.0{4,9}.0{13,18}.0{22,27}.0{28,39}.0{30,38}.0{31,36}.0{19,41}]hentetraconta-2,4(9),5,7,10,12,14,16,18,20,22(27)	1	1	1	0	<chem>[Na+].[Na+].[Na+].C[C@@]12CCC3C(Cc4cc(O)ccc34)C1CC[C@]2(O)c5ccc(cc5)C#CC#Cc6ccc7C8=[N+]9C(=Nc%10c%11c%12N=C%13c%14ccc(cc%14C%15=[N+])%13[Zn]9(N%16C(=N%15)c%17ccc(cc%17C%16=N8)S(=O)(=O)[O-])n%10%12)S(=O)(=O)[O-])S(=O)(=O)[O-])c7c6</chem>

	,23,25,28(39),29,31(36),32,34,37(40)-nonadecaene-2,39-bis(ylum)-6,15,33-trisulfonate					
	6,15,33-tributyl-24-(4-{3-[(14R,15R)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-yl]phenyl}buta-1,3-diyn-1-yl)-2\$I{5},11,20,29,38,39\$I{5},40,41-octaaza-1-zincadodecacyclo[19.17.1.1{1,12}.1{3,37}.0{2,10}.0{4,9}.0{13,18}.0{22,27}.0{28,39}.0{30,38}.0{31,36}.0{19,41}]hentetraconta-2,4(9),5,7,10,12,14,16,18,20,22(27),23,25,28(39),29,31(36),32,34,37(40)-nonadecaene-2,39-bis(ylum)	1	1	1	0	CCCCc1ccc2C3=NC4=[N+]5C(=Nc6c7cc(CCCC)ccc7c8N=C9c%10cc(ccc%10C%11=[N+]9[Zn]5(N3C(=N%11)c2c1)n68)C#CC#Cc%12cccc(c%12)[C@@]%13(O)CCC%14C%15CCc%16cc(O)ccc%16C%15CC[C@@]%13%14C)c%17ccc(CCCC)cc4%17
	8,21,34-tributyl-45-{2-[(14R,15R)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-yl]ethynyl}-2,15,28,41,50\$I{5},51\$I{5},52,53-octaaza-1-	1	1	1	0	CCCCc1ccc2cc3C4=NC5=[N+]6C(=Nc7c8cc9cc(CCCC)ccc9cc8c%10N=C%11c%12cc(ccc%12C%13=[N+]%11[Zn]6(N4C(=N%13)c3cc2c1)n7%10)C#C[C@@]%14(O)CCC%15C%16CCc%17cc(O)ccc%17C%16CC[C@@]%14%15C)c%18cc%19ccc(CCCC)cc%19cc5%18

zincapentadecacyclo[25.23.1.1{1,2 9}.1{3,49}.0{2,14}.0{4,13}.0{6,11}.0{ 16,51}.0{17,26}.0{19,24}.0{30,39}.0{ 32,37}.0{42,50}.0{43,48}.0{40,53}]t ripentaconta- 3(52),4(13),5,7,9,11,14,16(51),17(2 6),18,20,22,24,27,29,31,33,35,37,3 9,41,43(48),44,46,49- pentacosae-50,51-bis(ylum)					
tripotassium 24-{2-[(14R,15R)-5,14- dihydroxy-15- methylnetracyclo[8.7.0.0{2,7}.0{11, 15}]heptadeca-2,4,6-trien-14- yl]ethynyl}- 2\$I{5},11,20,29,38,39\$I{5},40,41- octaaza-1- zincadodecacyclo[19.17.1.1{1,12}.1 {3,37}.0{2,10}.0{4,9}.0{13,18}.0{22, 27}.0{28,39}.0{30,38}.0{31,36}.0{19 ,41}]hentetraconta- 2,4(9),5,7,10,12,14,16,18,20,22(27) ,23,25,28(39),29,31(36),32,34,37(4 0)-nonadecaene-2,39-bis(ylum)- 6,15,34-trisulfonate	1	1	1	0	[Na+].[Na+].[Na+].C[C@@]12CCC3C(CCc4cc(O)ccc34)C1CC[C@]2(O)C#Cc5ccc6C7=[N+]8C(=Nc9c%10ccc(cc%10c%11N=C%12c%13ccc(cc%13C%14=[N+]%12[Zn]8(N%15C(=N7)c%16ccc(cc%16C%15=N%14)S(=O)(=O)[O-])n9%11)S(=O)(=O)[O-])S(=O)(=O)[O-])c6c5

tripotassium 6-{8-[(14R,15R)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-yl]octa-1,3-diyn-1-yl}-2 <i>I</i> {5},11,20,29,38,39 <i>I</i> {5},40,41-octaaza-1-zincadodecacyclo[19.17.1.1{1,12}.1{3,37}.0{2,10}.0{4,9}.0{13,18}.0{22,27}.0{28,39}.0{30,38}.0{31,36}.0{19,41}]hentetraconta-2(10),3(40),4(9),5,7,11,13(18),14,16,19,21(39),22(27),23,25,28,30,32,34,36-nonadecaene-2,39-bis(ylium)-15,24,33-trisulfonate	1	1	1	0	[Na+].[Na+].[Na+].C[C@@]12CCC3C(CCc4cc(O)ccc34)C1CC[C@]2(O)CCCCC#CC#Cc5ccc6C7=[N+]8C(=Nc9c%10ccc(cc%10c%11N=C%12c%13ccc(cc%13C%14=[N+]%12[Zn]8(N%15C(=N%14)c%16ccc(cc%16C%15=N7)S(=O)(=O)[O-])n9%11)S(=O)(=O)[O-])S(=O)(=O)[O-])c6c5
16,25,34-tributyl-8-{2-[(14R,15R)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-yl]ethynyl}-2 <i>I</i> {5},11,20,29,38,39 <i>I</i> {5},40,41-octaaza-1-zincadodecacyclo[19.17.1.1{1,12}.1{3,37}.0{2,10}.0{4,9}.0{13,18}.0{22,27}.0{28,39}.0{30,38}.0{31,36}.0{19,41}]hentetraconta-2,4(9),5,7,10,12,14,16,18,20,22(27),23,25,28(39),29,31(36),32,34,37(4	1	1	1	0	CCCCc1ccc2C3=NC4=[N+]5C(=Nc6c7cc(CCCC)ccc7c8N=C9c%10c(cccc%10C%11=[N+]9[Zn]5(N3C(=N%11)c2c1)n68)C#C[C@@]%12(O)CCC%13C%14CCc%15cc(O)ccc%15C%14CC[C@@]%12%13C)c%16ccc(CCCC)cc4%16

	0)-nonadecaene-2,39-bis(ylum)					
	16,25,34-tributyl-7-{8-[(14R,15R)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-yl]octa-1,3-diyn-1-yl}-2\$I{5},11,20,29,38,39\$I{5},40,41-octaaza-1-zincadodecacyclo[19.17.1.1{1,12}.1{3,37}.0{2,10}.0{4,9}.0{13,18}.0{22,27}.0{28,39}.0{30,38}.0{31,36}.0{19,41}]hentetraconta-2,4(9),5,7,10,12,14,16,18,20,22(27),23,25,28(39),29,31(36),32,34,37(40)-nonadecaene-2,39-bis(ylum)	1	1	1	0	CCCCc1ccc2C3=NC4=[N+]5C(=Nc6c7cc(CCCC)ccc7c8N=C9c%10cc(ccc%10C%11=[N+]9[Zn]5(N3C(=N%11)c2c1)n68)C#CC#CCCC[C@@]%12(O)CCC%13C%14CCc%15cc(O)ccc%15C%14CC[C@@]%12%13C)c%16ccc(CCCC)cc4%16
	tripotassium 24-(4-{3-[(14R,15R)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-yl]phenyl}buta-1,3-diyn-1-yl)-2\$I{5},11,20,29,38,39\$I{5},40,41-octaaza-1-zincadodecacyclo[19.17.1.1{1,12}.1	1	1	1	0	[Na+].[Na+].[Na+].C[C@@]12CCC3C(CCc4cc(O)ccc34)C1CC[C@]2(O)c5cccc(c5)C#CC#Cc6ccc7C8=[N+]9C(=Nc%10c%11c cc(cc%11c%12N=C%13c%14ccc(cc%14C%15=[N+]%13[Zn]9(N%16C(=N%15)c%17ccc(cc%17C%16=N8)S(=O)(=O)[O-])n%10%12)S(=O)(=O)[O-])S(=O)(=O)[O-])c7c6

	{3,37}.0{2,10}.0{4,9}.0{13,18}.0{22,27}.0{28,39}.0{30,38}.0{31,36}.0{19,41}}hentetraconta-2,4(9),5,7,10,12,14,16,18,20,22(27),23,25,28(39),29,31(36),32,34,37(40)-nonadecaene-2,39-bis(ylum)-6,15,33-trisulfonate					
	tripotassium 5-{8-[(14R,15R)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]]heptadeca-2,4,6-trien-14-yl]octa-1,3-diyn-1-yl}-2\$I{5},11,20,29,38,39\$I{5},40,41-octaaza-1-zincadodecacyclo[19.17.1.1{1,12}.1{3,37}.0{2,10}.0{4,9}.0{13,18}.0{22,27}.0{28,39}.0{30,38}.0{31,36}.0{19,41}}hentetraconta-2(10),3(40),4(9),5,7,11,13(18),14,16,19,21(39),22(27),23,25,28,30,32,34,36-nonadecaene-2,39-bis(ylum)-15,24,33-trisulfonate	1	1	1	0	[Na+].[Na+].[Na+].C[C@@]12CCC3C(CCc4cc(O)ccc34)C1CC[C@]2(O)CCCCC#CC#Cc5cccc6C7=[N+]8C(=Nc9c%10ccc(cc%10c%11N=C%12c%13ccc(cc%13C%14=[N+]%12[Zn]8(N%15C(=N%14)c%16ccc(cc%16C%15=N7)S(=O)(=O)[O-]))n9%11)S(=O)(=O)[O-])S(=O)(=O)[O-])c56

tripotassium 7-{2-[(15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]]heptadeca-2,4,6-trien-14-yl]ethynyl}-2\$I{5},15,24,33,42,43,44,45\$I{5}-octaaza-1-zincatridecacyclo[21.19.1.1{1,25}.1{3,41}.0{2,14}.0{4,13}.0{6,11}.0{16,43}.0{17,22}.0{26,31}.0{34,42}.0{35,40}.0{32,45}]]pentatetraconta-2(14),3(44),4(13),5,7,9,11,15,17(22),18,20,23,25(45),26(31),27,29,32,34,36,38,40-henicosane-2,45-bis(ylum)-20,28,37-trisulfonate	1	1	1	0	[Na+].[Na+].[Na+].C[C@]12CCC3C(CCc4cc(O)ccc34)C1CC[C@@]2(O)C#Cc5cccc6cc7C8=[N+]9C(=Nc%10c%11ccc(cc%11c%12N=C%13c%14ccc(cc%14C%15=[N+]%13[Zn]9(N%16C(=N8)c%17ccc(cc%17C%16=N%15)S(=O)(=O)[O-])n%10%12)S(=O)(=O)[O-])S(=O)(=O)[O-])c7cc56
6,15,33-tributyl-24-{2-[(14R,15R)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]]heptadeca-2,4,6-trien-14-yl]ethynyl}-2\$I{5},11,20,29,38,39\$I{5},40,41-octaaza-1-zincadodecacyclo[19.17.1.1{1,12}.1{3,37}.0{2,10}.0{4,9}.0{13,18}.0{22,27}.0{28,39}.0{30,38}.0{31,36}.0{19,41}]]hentetraconta-2,4(9),5,7,10,12,14,16,18,20,22(27),23,25,28(39),29,31(36),32,34,37(4	1	1	1	0	CCCCc1ccc2C3=NC4=[N+]5C(=Nc6c7cc(CCCC)ccc7c8N=C9c%10cc(ccc%10C%11=[N+]9[Zn]5(N3C(=N%11)c2c1)n68)C#C[C@@]%12(O)CCC%13C%14CCc%15cc(O)ccc%15C%14CC[C@@]%12%13C)c%16ccc(CCCC)cc4%16

	0)-nonadecaene-2,39-bis(ylum)					
1022-46-4	2-phenyl-3,1-benzoxazin-4-one	0	1	0	1	<chem>O=C1OC(=Nc2ccccc12)c3ccccc3</chem>
	(4R,5S)-4,5-bis(4-hydroxyphenyl)heptan-2-one	1	1	1	0	<chem>CC[C@@H]([C@@H](CC(=O)C)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	(7R,8S)-7,8-bis(4-hydroxyphenyl)decan-5-one	1	1	1	0	<chem>CCCCC(=O)C[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	(2R,3S)-2,3-bis(4-hydroxyphenyl)pentanamide	1	1	1	0	<chem>CC[C@@H]([C@@H](C(=O)N)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	4-[(3S)-4-(4-hydroxyphenyl)hexan-3-yl]phenol	1	1	1	0	<chem>CC[C@@H](C(CC)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	(2R,3S)-2,3-bis(4-hydroxyphenyl)-N-pentylpentanamide	1	1	1	0	<chem>CCCCCNC(=O)[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	4-[(2R,3S)-1-bromo-2-(4-hydroxyphenyl)pentan-3-yl]phenol	1	1	1	0	<chem>CC[C@@H]([C@@H](CBr)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	(4R,5S)-4,5-bis(4-hydroxyphenyl)-2-oxoheptane-1-diazonium	1	1	1	0	<chem>CC[C@@H]([C@@H](CC(=O)C[N+]#N)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	4-[(2R,3S)-1-hydroxy-2-(4-	1	1	1	0	<chem>CC[C@@H]([C@@H](CO)c1ccc(O)cc1)c2ccc(O)cc2</chem>

	hydroxyphenyl)pentan-3-yl]phenol					
	(3R,4S)-3,4-bis(4-hydroxyphenyl)hexan-2-one	1	1	1	0	<chem>CC[C@@H]([C@@H](C(=O)C)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	(3S,4R)-3,4-bis(4-hydroxyphenyl)nonan-5-one	1	1	1	0	<chem>CCCCC(=O)[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	methyl (3R,4S)-3,4-bis(4-hydroxyphenyl)hexanoate	1	1	1	0	<chem>CC[C@@H]([C@@H](CC(=O)OC)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	4-[(2R,3S)-2-(4-hydroxyphenyl)-1-iodopentan-3-yl]phenol	1	1	1	0	<chem>CC[C@@H]([C@@H](Cl)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	(3R,4S)-3,4-bis(4-hydroxyphenyl)-N-pentylhexanamide	1	1	1	0	<chem>CCCCCNC(=O)C[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	(3R,4S)-3,4-bis(4-hydroxyphenyl)hexanamide	1	1	1	0	<chem>CC[C@@H]([C@@H](CC(=O)N)c1ccc(O)cc1)c2ccc(O)cc2</chem>
83303-93-9	4-[(2R,3S)-1-fluoro-2-(4-hydroxyphenyl)pentan-3-yl]phenol	1	1	1	0	<chem>CC[C@@H]([C@@H](CF)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	(3R,4S)-3,4-bis(4-hydroxyphenyl)-2-oxohexane-1-diazonium	1	1	1	0	<chem>CC[C@@H]([C@@H](C(=O)C[N+]#N)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	alitretinoin	0	1	0	1	<chem>C\\C(=C\\C=C\\C(=C\\C(=O)O)\\C)\\C=C\\C1=C(C)CCCC1(C)C</chem>
117-99-7	O-hydroxybenzophenone	0	1	0	1	<chem>Oc1ccccc1C(=O)c2ccccc2</chem>
95-55-6	2-aminophenol	0	1	0	1	<chem>Nc1ccccc1O</chem>

87-65-0	2,6-dichlorophenol	0	1	0	1	<chem>Oc1c(Cl)cccc1Cl</chem>
6051-87-2	β -naphthoflavone	0	1	0	1	<chem>O=C1C=C(Oc2ccc3ccccc3c12)c4ccccc4</chem>
604-59-1	α -naphthoflavone	0	1	0	1	<chem>O=C1C=C(Oc2c1ccc3ccccc23)c4ccccc4</chem>
99-89-8	P-isopropylphenol	1	1	1	0	<chem>CC(C)c1ccc(O)cc1</chem>
15485-76-4	ethyl 5,7-dihydroxy-3-(4-methoxyphenyl)-4-oxochromene-2-carboxylate	1	1	1	0	<chem>CCOC(=O)C1=C(C(=O)c2c(O)cc(O)cc2O1)c3ccc(OC)cc3</chem>
516-15-4	11-ketoprogesterone	0	1	0	1	<chem>CC(=O)[C@H]1CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3C(=O)C[C@]12C</chem>
1407-38-1	methyl (1R,15S,17R,18R,19S,20S)-6,18-dimethoxy-17-(3,4,5-trimethoxybenzoyloxy)-3,13-diazapentacyclo[11.8.0.0{2,10}.0{4,9}.0{15,20}]henicosa-2(10),4,6,8-tetraene-19-carboxylate	0	1	0	1	<chem>CO[C@H]1[C@@H](C[C@@H]2CN3CCc4c([nH]c5cc(OC)ccc45)[C@H]3C[C@@H]2[C@@H]1C(=O)OC)OC(=O)c6cc(OC)c(OC)c(OC)c6</chem>
501-24-6	phenol, 3-pentadecyl-	0	1	0	1	<chem>CCCCCCCCCCCCCCCCc1ccc(O)c1</chem>
	3-{3-[3-(acetyloxy)phenyl]-2,3-dimethyloxiran-2-yl}phenyl acetate	1	1	1	0	<chem>CC(=O)Oc1cccc(c1)C2(C)OC2(C)c3cccc(OC(=O)C)c3</chem>
	3-{3-[3-(acetyloxy)phenyl]-2,3-dipropyloxiran-2-yl}phenyl acetate	1	1	1	0	<chem>CCCC1(OC1(CCC)c2cccc(OC(=O)C)c2)c3cccc(OC(=O)C)c3</chem>
97-23-4	trivex	0	1	0	1	<chem>Oc1ccc(Cl)cc1Cc2cc(Cl)ccc2O</chem>

86111-26-4	zindoxifene	1	1	1	0	<chem>CCn1c(c(C)c2cc(OC(=O)C)ccc12)c3ccc(OC(=O)C)cc3</chem>
	3-[(2E)-3-[3-(acetyloxy)phenyl]but-2-en-2-yl]phenyl acetate	1	1	1	0	<chem>CC(=O)Oc1cccc(c1)\C=C(/C)\c2cccc(OC(=O)C)c2)\C</chem>
	ethyl (2S)-3-(4-hydroxyphenyl)-2-(phenylformamido)propanoate	0	1	0	1	<chem>CCOC(=O)[C@H](Cc1ccc(O)cc1)NC(=O)c2ccccc2</chem>
	3-[2,3-diethyl-3-(3-hydroxyphenyl)oxiran-2-yl]phenol	1	1	1	0	<chem>CCC1(OC1(CC)c2cccc(O)c2)c3cccc(O)c3</chem>
	3-{3-[3-(acetyloxy)phenyl]-2,3-dibutyloxiran-2-yl}phenyl acetate	1	1	1	0	<chem>CCCCC1(OC1(CCCC)c2cccc(OC(=O)C)c2)c3cccc(OC(=O)C)c3</chem>
	3-{3-[3-(acetyloxy)phenyl]-2,3-diethyloxiran-2-yl}phenyl acetate	1	1	1	0	<chem>CCC1(OC1(CC)c2cccc(OC(=O)C)c2)c3cccc(OC(=O)C)c3</chem>
491-70-3	luteolin	1	1	1	0	<chem>Oc1cc(O)c2C(=O)C=C(Oc2c1)c3ccc(O)c(O)c3</chem>
	3-[(3E)-4-[3-(acetyloxy)phenyl]hex-3-en-3-yl]phenyl acetate	1	1	1	0	<chem>CC\C=C(\CC)/c1cccc(OC(=O)C)c1)\c2cccc(OC(=O)C)c2</chem>
	3-[(4E)-5-[3-(acetyloxy)phenyl]oct-4-en-4-yl]phenyl acetate	1	1	1	0	<chem>CCC\C=C(\CCC)/c1cccc(OC(=O)C)c1)\c2cccc(OC(=O)C)c2</chem>
	3-[(5E)-6-[3-(acetyloxy)phenyl]dec-5-en-5-yl]phenyl acetate	1	1	1	0	<chem>CCCC\C=C(\CCCC)/c1cccc(OC(=O)C)c1)\c2cccc(OC(=O)C)c2</chem>
	flutamide	0	1	0	1	<chem>CC(C)C(=O)Nc1ccc(c(c1)C(F)(F)F)[N+](=O)[O-]</chem>
	brompheniramine	0	1	0	1	<chem>CN(C)CCC(c1ccc(Br)cc1)c2cccn2</chem>

108-43-0	3-chlorophenol	0	1	0	1	<chem>Oc1cccc(Cl)c1</chem>
	bifenthrin	0	1	0	1	<chem>Cc1c(COC(=O)[C@H]2[C@@H](\C=C(/Cl)\C(F)(F)F)C2(C)C)cccc1c3cccc3</chem>
	triac	1	1	1	0	<chem>OC(=O)Cc1cc(I)c(Oc2ccc(O)c(I)c2)c(I)c1</chem>
51-26-3	thyropropic acid	1	1	1	0	<chem>OC(=O)CCc1cc(I)c(Oc2ccc(O)c(I)c2)c(I)c1</chem>
	4-[4-(4-hydroxyphenyl)hexan-3-yl]-2-(prop-2-en-1-yl)phenol	1	1	1	0	<chem>CCC(C(CC)c1ccc(O)c(CC=C)c1)c2ccc(O)cc2</chem>
	N-(7-([2,3-bis(4-hydroxyphenyl)pentyl]sulfanyl)heptyl)-5-(dimethylamino)naphthalene-1-sulfonamide	1	1	1	0	<chem>CCC(C(CSCCCCCCNS(=O)(=O)c1ccc2c(cccc12)N(C)C)c3ccc(O)cc3)c4ccc(O)cc4</chem>
	4-{6-[2-(2-chloroethoxy)ethoxy]-4-(4-hydroxyphenyl)hexan-3-yl}phenol	1	1	1	0	<chem>CCC(C(CCOCCOCCCl)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	methyl 3,4-bis(4-hydroxyphenyl)hexanoate	1	1	1	0	<chem>CCC(C(CC(=O)OC)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	4-[6-(butylsulfanyl)-4-(4-hydroxyphenyl)hexan-3-yl]phenol	1	1	1	0	<chem>CCCCSCCC(C(CC)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	2-(4-([2,3-bis(4-hydroxyphenyl)pentyl]sulfanyl)butyl)isoindole-1,3-dione	1	1	1	0	<chem>CCC(C(CSCCCCN1C(=O)c2ccccc2C1=O)c3ccc(O)cc3)c4ccc(O)cc4</chem>

2-(7-{[2,3-bis(4-hydroxyphenyl)pentyl]sulfanyl}heptyl)isoindole-1,3-dione	1	1	1	0	<chem>CCC(C(CSCCCCCCN1C(=O)c2ccccc2C1=O)c3ccc(O)cc3)c4ccc(O)cc4</chem>
4-{1-[2-(2-chloroethoxy)ethoxy]-2-(4-hydroxyphenyl)pentan-3-yl}phenol	1	1	1	0	<chem>CCC(C(COCCOCCCl)c1ccc(O)cc1)c2ccc(O)cc2</chem>
4-[4-(4-hydroxyphenyl)hexan-3-yl]-2-(3-hydroxypropyl)phenol	1	1	1	0	<chem>CCC(C(CC)c1ccc(O)c(CCCO)c1)c2ccc(O)cc2</chem>
2-azido-4-[4-(4-hydroxyphenyl)hexan-3-yl]phenol	1	1	1	0	<chem>CCC(C(CC)c1ccc(O)c(c1)N=[N+]=[N-])c2ccc(O)cc2</chem>
4-[3-(4-hydroxyphenyl)pentan-2-yl]phenol	1	1	1	0	<chem>CCC(C(C)c1ccc(O)cc1)c2ccc(O)cc2</chem>
4-amino-2-(3-{2-hydroxy-5-[4-(4-hydroxyphenyl)hexan-3-yl]phenyl}propyl)isoindole-1,3-dione	1	1	1	0	<chem>CCC(C(CC)c1ccc(O)c(CCCN2C(=O)c3ccccc(N)c3C2=O)c1)c4ccc(O)cc4</chem>
5-(dimethylamino)-N-(3-{2-hydroxy-5-[4-(4-hydroxyphenyl)hexan-3-yl]phenyl}propyl)naphthalene-1-sulfonamide	1	1	1	0	<chem>CCC(C(CC)c1ccc(O)c(CCCNS(=O)(=O)c2cccc3c(cccc23)N(C)C)c1)c4ccc(O)cc4</chem>
4-[2-(4-hydroxyphenyl)-1-{5-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]pentyl}sulfanyl]pentan-3-	1	1	1	0	<chem>CCC(C(CSCCCCCNc1ccc(c2nonc12)[N+](=O)[O-])c3ccc(O)cc3)c4ccc(O)cc4</chem>

	yl]phenol					
	4-[2-(4-hydroxyphenyl)-1-({4-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]butyl}sulfanyl)pentan-3-yl]phenol	1	1	1	0	CCC(C(CSCCCCNc1ccc(c2nonc12)[N+](=O)[O-])c3ccc(O)cc3)c4ccc(O)cc4
	4-[2-(4-hydroxyphenyl)-1-({2-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]ethyl}sulfanyl)pentan-3-yl]phenol	1	1	1	0	CCC(C(CSCCNc1ccc(c2nonc12)[N+](=O)[O-])c3ccc(O)cc3)c4ccc(O)cc4
	4-[1-(butylsulfanyl)-2-(4-hydroxyphenyl)pentan-3-yl]phenol	1	1	1	0	CCCCSCC(C(CC)c1ccc(O)cc1)c2ccc(O)cc2
	4-[2-(4-hydroxyphenyl)-1-({3-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]propyl}sulfanyl)pentan-3-yl]phenol	1	1	1	0	CCC(C(CSCCCCNc1ccc(c2nonc12)[N+](=O)[O-])c3ccc(O)cc3)c4ccc(O)cc4
	4-[2-(4-hydroxyphenyl)-1-({7-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]heptyl}sulfanyl)pentan-3-yl]phenol	1	1	1	0	CCC(C(CSCCCCCCNc1ccc(c2nonc12)[N+](=O)[O-])c3ccc(O)cc3)c4ccc(O)cc4
	4-[2-(4-hydroxyphenyl)-1-({6-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]hexyl}sulfanyl)pentan-3-yl]phenol	1	1	1	0	CCC(C(CSCCCCCCNc1ccc(c2nonc12)[N+](=O)[O-])c3ccc(O)cc3)c4ccc(O)cc4

2-[3-(benzyloxy)propyl]-4-[4-(4-hydroxyphenyl)hexan-3-yl]phenol	1	1	1	0	<chem>CCC(C(CC)c1ccc(O)c(CCCOCc2ccccc2)c1)c3ccc(O)cc3</chem>
4-[4-(4-hydroxyphenyl)hexan-3-yl]-2-(3-methoxypropyl)phenol	1	1	1	0	<chem>CCC(C(CC)c1ccc(O)c(CCCOC)c1)c2ccc(O)cc2</chem>
2-[3-(butylsulfanyl)propyl]-4-[4-(4-hydroxyphenyl)hexan-3-yl]phenol	1	1	1	0	<chem>CCCCSCCCc1cc(ccc1O)C(CC)C(CC)c2ccc(O)cc2</chem>
2-[3-(2,4-dinitrophenoxy)propyl]-4-[4-(4-hydroxyphenyl)hexan-3-yl]phenol	1	1	1	0	<chem>CCC(C(CC)c1ccc(O)c(CCCOc2ccc(cc2[N+](=O)[O-]))[N+](=O)[O-])c1)c3ccc(O)cc3</chem>
4-[2-(4-hydroxyphenyl)-1-iodopentan-3-yl]phenol	1	1	1	0	<chem>CCC(C(Cl)c1ccc(O)cc1)c2ccc(O)cc2</chem>
4-[1-hydroxy-2-(4-hydroxyphenyl)pentan-3-yl]phenol	1	1	1	0	<chem>CCC(C(CO)c1ccc(O)cc1)c2ccc(O)cc2</chem>
2-(3-{2-hydroxy-5-[4-(4-hydroxyphenyl)hexan-3-yl]phenyl}propyl)-4-nitroisindole-1,3-dione	1	1	1	0	<chem>CCC(C(CC)c1ccc(O)c(CCCN2C(=O)c3cccc(c3C2=O)[N+](=O)[O-])c1)c4ccc(O)cc4</chem>
2-{3-[(2,4-dinitrophenyl)amino]propyl}-4-[4-(4-hydroxyphenyl)hexan-3-yl]phenol	1	1	1	0	<chem>CCC(C(CC)c1ccc(O)c(CCCNc2ccc(cc2[N+](=O)[O-]))[N+](=O)[O-])c1)c3ccc(O)cc3</chem>
2-(3-{2-hydroxy-5-[4-(4-hydroxyphenyl)hexan-3-	1	1	1	0	<chem>CCC(C(CC)c1ccc(O)c(CCCN2C(=O)c3ccccc3C2=O)c1)c4ccc(O)cc4</chem>

	yl]phenyl}propyl)isoindole-1,3-dione					
	4-[4-(4-hydroxyphenyl)hexan-3-yl]-2-{3-[(7-nitro-2,1,3-benzoxadiazol-4-yl)amino]propyl}phenol	1	1	1	0	CCC(C(CC)c1ccc(O)c(CCCNc2ccc(c3nonc23)[N+](=O)[O-])c1)c4ccc(O)cc4
108-39-4	M-cresol	0	1	0	1	Cc1ccc(O)c1
63697-20-1	1,2,3,4-tetrachlorobenzene	1	1	1	0	Clc1ccc(Cl)c(Cl)c1Cl
88-72-2	mononitrotoluene	0	1	0	1	Cc1ccccc1[N+](=O)[O-]
12408-10-5	1,2,4,5-tetrachlorobenzene	0	1	0	1	Clc1cc(Cl)c(Cl)cc1Cl
608-93-5	pentachlorobenzene	0	1	0	1	Clc1cc(Cl)c(Cl)c(Cl)c1Cl
634-90-2	1,2,3,5-tetrachlorobenzene	0	1	0	1	Clc1cc(Cl)c(Cl)c(Cl)c1
108-70-3	1,3,5-trichloro-benzene	0	1	0	1	Clc1cc(Cl)cc(Cl)c1
	2-[4-(methylsulfonyl)phenyl]-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	CSc1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(OCCN5CCCCC5)cc4
	4-[6-(dimethylamino)-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-2-yl]phenol	1	1	1	0	CN(C)c1ccc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2c1)c5ccc(O)cc5
	2-(4-hydroxyphenyl)-5-methyl-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-6-ol	1	1	1	0	Cc1cc2c(C(=O)c3ccc(OCCN4CCCCC4)cc3)c(sc2cc1O)c5ccc(O)cc5

541-73-1	3-dichlorobenzene	0	1	0	1	Clc1cccc(Cl)c1
	1-{4-[(2-aminoethyl)amino]butyl}- 2-(4-hydroxyphenyl)-3-methylindol- 5-ol	1	1	1	0	Cc1c(c2ccc(O)cc2)n(CCCCNCCN)c3ccc(O)cc13
	1-{5-[(2-aminoethyl)amino]pentyl}- 2-(4-hydroxyphenyl)-3-methylindol- 5-ol	1	1	1	0	Cc1c(c2ccc(O)cc2)n(CCCCCNCCN)c3ccc(O)cc13
	1-{6-[(2-aminoethyl)amino]hexyl}- 2-(4-hydroxyphenyl)indol-6-ol	1	1	1	0	NCCNCCCCCn1c(cc2ccc(O)cc12)c3ccc(O)cc3
	1-{4-[(2-aminoethyl)amino]butyl}- 2-(4-hydroxyphenyl)indol-5-ol	1	1	1	0	NCCNCCCCn1c(cc2cc(O)ccc12)c3ccc(O)cc3
	1-{4-[(2-aminoethyl)amino]butyl}- 2-(4-hydroxyphenyl)-3-methylindol- 5-ol; platinum(II) chloride	1	1	1	0	Cc1c(c2ccc(O)cc2)n(CCCCNCCN)c3ccc(O)cc13.Cl[Pt]Cl
	1-{6-[(2-aminoethyl)amino]hexyl}- 2-(4-hydroxyphenyl)indol-5-ol	1	1	1	0	NCCNCCCCCn1c(cc2cc(O)ccc12)c3ccc(O)cc3
	1-{4-[(2-aminoethyl)amino]butyl}- 2-(4-hydroxyphenyl)indol-5-ol; platinum(II) chloride	1	1	1	0	NCCNCCCCn1c(cc2cc(O)ccc12)c3ccc(O)cc3.Cl[Pt]Cl
	1-{4-[(2-aminoethyl)amino]butyl}- 2-(4-hydroxyphenyl)indol-6-ol	1	1	1	0	NCCNCCCCn1c(cc2ccc(O)cc12)c3ccc(O)cc3
	1-{6-[(2-aminoethyl)amino]hexyl}- 2-(4-hydroxyphenyl)-3-methylindol-	1	1	1	0	Cc1c(c2ccc(O)cc2)n(CCCCCNCCN)c3ccc(O)cc13

	5-ol					
	1-{4-[(2-aminoethyl)amino]butyl}-2-(4-hydroxyphenyl)indol-6-ol; platinum(II) chloride	1	1	1	0	NCCNCCCCn1c(cc2ccc(O)cc12)c3ccc(O)cc3.Cl[Pt]Cl
	1-[(4-{[(2-aminoethyl)amino]methyl}phenyl)methyl]-2-(4-hydroxyphenyl)-3-methylindol-5-ol	1	1	1	0	Cc1c(c2ccc(O)cc2)n(Cc3ccc(CNCCN)cc3)c4ccc(O)cc14
	1-{6-[(2-aminoethyl)amino]hexyl}-2-(4-hydroxyphenyl)-3-methylindol-5-ol; platinum(II) chloride	1	1	1	0	Cc1c(c2ccc(O)cc2)n(CCCCCCNCCN)c3ccc(O)cc13.Cl[Pt]Cl
	1-{5-[(2-aminoethyl)amino]pentyl}-2-(4-hydroxyphenyl)-3-methylindol-5-ol; platinum(II) chloride	1	1	1	0	Cc1c(c2ccc(O)cc2)n(CCCCCNCCN)c3ccc(O)cc13.Cl[Pt]Cl
	1-{6-[(2-aminoethyl)amino]hexyl}-2-(4-hydroxyphenyl)indol-6-ol; platinum(II) chloride	1	1	1	0	NCCNCCCCCn1c(cc2ccc(O)cc12)c3ccc(O)cc3.Cl[Pt]Cl
	1-{6-[(2-aminoethyl)amino]hexyl}-2-(4-hydroxyphenyl)indol-5-ol; platinum(II) chloride	1	1	1	0	NCCNCCCCCn1c(cc2cc(O)ccc12)c3ccc(O)cc3.Cl[Pt]Cl
	1-[(4-{[(2-aminoethyl)amino]methyl}phenyl)methyl]-2-(4-hydroxyphenyl)-3-methylindol-5-ol; platinum(II)	1	1	1	0	Cc1c(c2ccc(O)cc2)n(Cc3ccc(CNCCN)cc3)c4ccc(O)cc14.Cl[Pt]Cl

	chloride					
	4-[2,6-difluoro-4-(hydroxymethyl)phenyl]phenol	1	1	1	0	<chem>OCc1cc(F)c(c(F)c1)c2ccc(O)cc2</chem>
	4-[2-chloro-4-(hydroxymethyl)-6-methoxyphenyl]phenol	1	1	1	0	<chem>COc1cc(CO)cc(Cl)c1c2ccc(O)cc2</chem>
	4-[2-bromo-4-(hydroxymethyl)-6-(pyrrol-1-yl)phenyl]phenol	1	1	1	0	<chem>OCc1cc(Br)c(c2ccc(O)cc2)c(c1)n3cccc3</chem>
	4-[2-amino-6-bromo-4-(hydroxymethyl)phenyl]phenol	1	1	1	0	<chem>Nc1cc(CO)cc(Br)c1c2ccc(O)cc2</chem>
	3,5-dichloro-4-[4-(hydroxymethyl)phenyl]phenol	1	1	1	0	<chem>OCc1ccc(cc1)c2c(Cl)cc(O)cc2Cl</chem>
	2,3,5,6-tetrachloro-4-[4-(hydroxymethyl)phenyl]phenol	0	1	0	1	<chem>OCc1ccc(cc1)c2c(Cl)c(Cl)c(O)c(Cl)c2Cl</chem>
	4-[2,3,5,6-tetrachloro-4-(hydroxymethyl)phenyl]phenol	1	1	1	0	<chem>OCc1c(Cl)c(Cl)c(c(Cl)c1Cl)c2ccc(O)cc2</chem>
	4-[2-chloro-4-(hydroxymethyl)phenyl]phenol	1	1	1	0	<chem>OCc1ccc(c(Cl)c1)c2ccc(O)cc2</chem>
	4-[2-chloro-4-(hydroxymethyl)-6-(trifluoromethyl)phenyl]phenol	1	1	1	0	<chem>OCc1cc(Cl)c(c2ccc(O)cc2)c(c1)C(F)(F)F</chem>
	4-[3-chloro-5-(hydroxymethyl)-2-(4-hydroxyphenyl)phenyl]phenol	1	1	1	0	<chem>OCc1cc(Cl)c(c2ccc(O)cc2)c(c1)c3ccc(O)cc3</chem>

	4-[2-bromo-4-(hydroxymethyl)-6-nitrophenyl]phenol	1	1	1	0	<chem>OCc1cc(Br)c(c2ccc(O)cc2)c(c1)[N+](=O)[O-]</chem>
	4-[4-(hydroxymethyl)-2,6-dimethylphenyl]phenol	1	1	1	0	<chem>Cc1cc(CO)cc(C)c1c2ccc(O)cc2</chem>
	4-[4-(hydroxymethyl)-2,6-dimethoxyphenyl]phenol	1	1	1	0	<chem>COc1cc(CO)cc(OC)c1c2ccc(O)cc2</chem>
	4-[2-bromo-4-(hydroxymethyl)-6-(methylsulfanyl)phenyl]phenol	1	1	1	0	<chem>CSc1cc(CO)cc(Br)c1c2ccc(O)cc2</chem>
	4-[4-(hydroxymethyl)phenyl]-3,5-dimethylphenol	1	1	1	0	<chem>Cc1cc(O)cc(C)c1c2ccc(CO)cc2</chem>
	4-[4-(hydroxymethyl)phenyl]-2,6-dimethylphenol	0	1	0	1	<chem>Cc1cc(cc(C)c1O)c2ccc(CO)cc2</chem>
	2,6-dibromo-4-[4-(hydroxymethyl)phenyl]phenol	0	1	0	1	<chem>OCc1ccc(cc1)c2cc(Br)c(O)c(Br)c2</chem>
	4-[2-amino-4-(hydroxymethyl)-6-nitrophenyl]phenol	1	1	1	0	<chem>Nc1cc(CO)cc(c1c2ccc(O)cc2)[N+](=O)[O-]</chem>
	4-{2-bromo-6-[2-(dimethylamino)ethynyl]-4-(hydroxymethyl)phenyl}phenol	1	1	1	0	<chem>CN(C)C#Cc1cc(CO)cc(Br)c1c2ccc(O)cc2</chem>
	2-benzyl-4-[2,6-dichloro-4-(hydroxymethyl)phenyl]phenol	1	1	1	0	<chem>OCc1cc(Cl)c(c(Cl)c1)c2ccc(O)c(Cc3ccccc3)c2</chem>

	3-chloro-4-[4-(hydroxymethyl)phenyl]phenol	1	1	1	0	<chem>OCc1ccc(cc1)c2ccc(O)cc2Cl</chem>
	3-chloro-4-[2,6-dichloro-4-(hydroxymethyl)phenyl]phenol	1	1	1	0	<chem>OCc1cc(Cl)c(c(Cl)c1)c2ccc(O)cc2Cl</chem>
	4-[5-(hydroxymethyl)-2-(4-hydroxyphenyl)phenyl]phenol	1	1	1	0	<chem>OCc1ccc(c2ccc(O)cc2)c(c1)c3ccc(O)cc3</chem>
	4-[2-chloro-4-(hydroxymethyl)-6-isopropylphenyl]phenol	1	1	1	0	<chem>CC(C)c1cc(CO)cc(Cl)c1c2ccc(O)cc2</chem>
	4-[2-bromo-4-(hydroxymethyl)-6-iodophenyl]phenol	1	1	1	0	<chem>OCc1cc(Br)c(c(I)c1)c2ccc(O)cc2</chem>
22494-42-4	diflunisal	0	1	0	1	<chem>OC(=O)c1cc(ccc1O)c2ccc(F)cc2F</chem>
40112-23-0	gossypol	0	1	0	1	<chem>CC(C)c1c(O)c(O)c(C=O)c2c(O)c(c(C)cc12)c3c(C)cc4c(C(C)C)(O)c(O)c(C=O)c4c3O</chem>
29550-13-8	negletein	1	1	1	0	<chem>COc1cc2OC(=CC(=O)c2c(O)c1O)c3ccccc3</chem>
	(1S,12aS)-3,3,12a-trimethyl-1,2,4,4a,4b,5,6,10b,11,12-decahydrochrysene-1,8-diol	1	1	1	0	<chem>CC1(C)C[C@H](O)[C@@]2(C)CCC3C(CC4cc(O)ccc34)C2C1</chem>
	(2S,4S,6S,13R,14S)-4,13-diethynyl-14-methyltetracyclo[7.7.0.0{2,6}.0{10,14}]hexadecane-4,13-diol	1	1	1	0	<chem>C[C@]12CCC3[C@H]4C[C@@](O)(C[C@@H]4CCC3C1CC[C@@]2(O)C#C)C#C</chem>

	(1S,12aS)-12a-methyl-2,3,4,4a,4b,5,6,10b,11,12-decahydro-1H-chrysene-1,8-diol	1	1	1	0	<chem>C[C@]12CCC3C(CCc4cc(O)ccc34)C1CCC[C@@H]2O</chem>
	(1S,12aS)-4,4,12a-trimethyl-1,2,3,4a,4b,5,6,10b,11,12-decahydrochrysene-1,8-diol	1	1	1	0	<chem>CC1(C)CC[C@H](O)[C@@]2(C)CCC3C(CCc4cc(O)ccc34)C12</chem>
19044-88-3	oryzalin	0	1	0	1	<chem>CCCN(CCC)c1c(cc(cc1[N+](=O)[O-])S(=O)(=O)N)[N+](=O)[O-]</chem>
	(3S,4R)-3-phenyl-4-(4-{[2-(piperidin-1-yl)ethyl]sulfanyl}phenyl)-3,4-dihydro-2H-1-benzopyran-7-ol	1	1	1	0	<chem>Oc1ccc2[C@H]([C@H](COc2c1)c3ccccc3)c4ccc(SCCN5CCCCC5)cc4</chem>
	(3S,4R)-3-phenyl-4-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-3,4-dihydro-2H-1-benzopyran-7-ol	1	1	1	0	<chem>Oc1ccc2[C@H]([C@H](COc2c1)c3ccccc3)c4ccc(OCCN5CCCCC5)cc4</chem>
	(3S,4R)-3-phenyl-4-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}-3,4-dihydro-2H-1-benzopyran-7-ol	1	1	1	0	<chem>Oc1ccc2[C@H]([C@H](COc2c1)c3ccccc3)c4ccc(OCCN5CCCC5)cc4</chem>
577-85-5	flavonol	0	1	0	1	<chem>OC1=C(Oc2ccccc2C1=O)c3ccccc3</chem>
10420-73-2	6-chloroflavone	0	1	0	1	<chem>Clc1ccc2OC(=CC(=O)c2c1)c3ccccc3</chem>
	4-methyl-2(1H)-quinolinone	0	1	0	1	<chem>CC1=CC(=O)Nc2ccccc12</chem>
77-08-7	3,3,3',3'-tetramethyl-2H,2'H-1,1'-	1	1	1	0	<chem>CC1(C)CC2(CC(C)(C)c3cc(O)c(O)cc23)c4cc(O)c(O)cc14</chem>

	spirobi[indene]-5,5',6,6'-tetrol					
	2-cyclopentyl-3-({4-[2-(piperidin-1-yl)ethoxy]phenyl)methyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc2c(Cc3ccc(OCCN4CCCC4)cc3)c(sc2c1)C5CCCC5</chem>
	(1s,4s)-4-(6-methoxy-3-{4-[2-(piperidin-1-yl)ethoxy]benzoyl}-1-benzothiophen-2-yl)cyclohexan-1-ol	1	1	1	0	<chem>COc1ccc2c(C(=O)c3ccc(OCCN4CCCC4)cc3)c(sc2c1)[C@@H]5CC[C@H](O)CC5</chem>
	2-ethyl-3-({4-[2-(piperidin-1-yl)ethoxy]phenyl)methyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>CCc1sc2cc(O)ccc2c1Cc3ccc(OCCN4CCCC4)cc3</chem>
	2-isopropyl-3-({4-[2-(piperidin-1-yl)ethoxy]phenyl)methyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>CC(C)c1sc2cc(O)ccc2c1Cc3ccc(OCCN4CCCC4)cc3</chem>
2203-97-6	solu-cortef	0	1	0	1	<chem>C[C@]12CCC(=O)C=C1CC[C@H]3[C@@H]4CC[C@](O)(C(=O)COC(=O)CCC(=O)O)[C@@]4(C)C[C@H](O)[C@H]23</chem>
	3-({4-[2-(piperidin-1-yl)ethoxy]phenyl)methyl}-2-[(1r,4r)-4-hydroxycyclohexyl]-1-benzothiophen-6-ol	1	1	1	0	<chem>O[C@@H]1CC[C@H](CC1)c2sc3cc(O)ccc3c2Cc4ccc(OCCN5CCCC5)cc4</chem>
	2-cyclopentyl-3-[hydroxy({4-[2-(piperidin-1-yl)ethoxy]phenyl})methyl]-1-	1	1	1	0	<chem>OC(c1ccc(OCCN2CCCC2)cc1)c3c(sc4cc(O)ccc34)C5CCCC5</chem>

	benzothiophen-6-ol					
	2-cyclohexyl-3-({4-[2-(piperidin-1-yl)ethoxy]phenyl)methyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc2c(Cc3ccc(OCCN4CCCCC4)cc3)c(sc2c1)C5CCCCC5</chem>
	2-methyl-3-({4-[2-(piperidin-1-yl)ethoxy]phenyl)methyl}-1-benzothiophen-6-ol	1	1	1	0	<chem>Cc1sc2cc(O)ccc2c1Cc3ccc(OCCN4CCCCC4)cc3</chem>
	(2R)-3-({4-[(2,2-dimethylpropanoyl)oxy]phenyl}-4-methyl-2-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2H-chromen-7-yl 2,2-dimethylpropanoate	1	1	1	0	<chem>CC1=C([C@H](Oc2cc(OC(=O)C(C)(C)C)ccc12)c3ccc(OCCN4CCCCC4)cc3)c5ccc(OC(=O)C(C)(C)C)cc5</chem>
80868-58-2	cholestenone	0	1	0	1	<chem>CC(C)CCC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3CCCC=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>
4339-71-3	piceatannol	1	1	1	0	<chem>Oc1cc(O)cc(\C=C\c2ccc(O)c(O)c2)c1</chem>
	2,2-dichloro-3-[9,10,10-tris(4-methoxyphenyl)dec-9-en-1-yl]-1,3-diaza-2-platinacyclopentane-1,3-diium	1	1	1	0	<chem>COc1ccc(cc1)C(=C(c2ccc(OC)cc2)c3ccc(OC)cc3)CCCCCCCC[NH+]4CC[NH2+][Pt]4(Cl)Cl</chem>
	2,2-dichloro-3-[7,8,8-tris(4-methoxyphenyl)oct-7-en-1-yl]-1,3-diaza-2-platinacyclopentane-1,3-diium	1	1	1	0	<chem>COc1ccc(cc1)C(=C(c2ccc(OC)cc2)c3ccc(OC)cc3)CCCCC[NH+]4CC[NH2+][Pt]4(Cl)Cl</chem>

34334-69-5	cirsiliol	1	1	1	0	<chem>COc1cc2OC(=CC(=O)c2c(O)c1OC)c3ccc(O)c(O)c3</chem>
3988-03-2	bis-(4-bromo-phenyl)-methanone	1	1	1	0	<chem>BrC1ccc(cc1)C(=O)c2ccc(Br)cc2</chem>
548-83-4	galangin	0	1	0	1	<chem>OC1=C(Oc2cc(O)cc(O)c2C1=O)c3ccccc3</chem>
38183-03-8	7,8-dihydroxy-2-phenylchromen-4-one	1	1	1	0	<chem>Oc1ccc2C(=O)C=C(Oc2c1O)c3ccccc3</chem>
87-66-1	pyrogallol	1	1	1	0	<chem>Oc1ccc(O)c1O</chem>
	2-[3-(benzyloxy)-4-methoxyphenyl]-5,7-dihydroxy-3-methoxychromen-4-one	1	1	1	0	<chem>COC1=C(Oc2cc(O)cc(O)c2C1=O)c3ccc(OC)c(OCc4ccccc4)c3</chem>
	4-(2,2-dicyanoethyl)phenol	0	1	0	1	<chem>Oc1ccc(CC(C#N)C#N)cc1</chem>
	2-[(15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-17-yl]ethyl 4-[(4-{7,12,17-triphenyl-21,22,23,24-tetraazapentacyclo[16.2.1.1{3,6}.1{8,11}.1{13,16}]tetracos-1,3,5,7,9,11(23),12,14,16(22),17,19-undecaen-2-yl}phenyl)formamido]butanoate	1	1	1	0	<chem>C[C@]12CC(CCOC(=O)CCNC(=O)c3ccc(cc3)c4c5C=Cc([nH]5)c(c6C=Cc(n6)c(c7ccccc7)c8ccc(n8)c(c9ccccc9)c%10ccc4[nH]%10)c%11ccccc%11)C%12C(CCc%13cc(O)ccc%12%13)C1CCC2O</chem>
	4-{2-methyl-11-azatricyclo[5.3.1.0{4,11}]undeca-1,3,5,7,9-pentaen-3-yl}phenol	1	1	1	0	<chem>Cc1c(c2ccc(O)cc2)c3C=Cc4cccc1n34</chem>

2-ethyl-3-(4-hydroxyphenyl)-11-azatricyclo[5.3.1.0{4,11}]undeca-1,3,5,7,9-pentaen-9-ol	1	1	1	0	<chem>CCc1c(c2ccc(O)cc2)c3C=Cc4cc(O)cc1n34</chem>
4-[2-ethyl-10-(hydroxymethyl)-11-azatricyclo[5.3.1.0{4,11}]undeca-1,3,5,7,9-pentaen-3-yl]phenol	1	1	1	0	<chem>CCc1c(c2ccc(O)cc2)c3C=Cc4ccc(CO)c1n34</chem>
2-ethyl-3-phenyl-11-azatricyclo[5.3.1.0{4,11}]undeca-1,3,5,7,9-pentaen-8-ol	1	1	1	0	<chem>CCc1c(c2cccc2)c3C=Cc4c(O)ccc1n34</chem>
2-ethyl-3-phenyl-11-azatricyclo[5.3.1.0{4,11}]undeca-1,3,5,7,9-pentaen-9-ol	1	1	1	0	<chem>CCc1c(c2cccc2)c3C=Cc4cc(O)cc1n34</chem>
2-ethyl-3-(4-hydroxyphenyl)-11-azatricyclo[5.3.1.0{4,11}]undeca-1,3,5,7,9-pentaen-8-ol	1	1	1	0	<chem>CCc1c(c2ccc(O)cc2)c3C=Cc4c(O)ccc1n34</chem>
4-{11-azatricyclo[5.3.1.0{4,11}]undeca-1,3,5,7,9-pentaen-3-yl}phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2cc3cccc4C=Cc2n34</chem>
4-{14-azatetracyclo[10.2.1.0{4,14}.0{7,13}]pentadeca-1(15),2,4,6-tetraen-15-yl}phenol	1	1	1	0	<chem>Oc1ccc(cc1)C2=C3C=CC4=CC=C5CCCCC2C5N34</chem>
4-{13-azatetracyclo[9.2.1.0{4,13}.0{7,12}]	1	1	1	0	<chem>Oc1ccc(cc1)C2=C3C=CC4=CC=C5CCCCC2C5N34</chem>

	tetradeca-1(14),2,4,6-tetraen-14-yl}phenol					
	4-{2-isopropyl-11-azatricyclo[5.3.1.0{4,11}}undeca-1,3,5,7,9-pentaen-3-yl}phenol	1	1	1	0	<chem>CC(C)c1c(c2ccc(O)cc2)c3C=Cc4cccc1n34</chem>
	4-{2-propyl-11-azatricyclo[5.3.1.0{4,11}}undeca-1,3,5,7,9-pentaen-3-yl}phenol	1	1	1	0	<chem>CCCc1c(c2ccc(O)cc2)c3C=Cc4cccc1n34</chem>
	3-{2-ethyl-11-azatricyclo[5.3.1.0{4,11}}undeca-1,3,5,7,9-pentaen-3-yl}phenol	1	1	1	0	<chem>CCc1c(c2cccc(O)c2)c3C=Cc4cccc1n34</chem>
	4-[2-(pentan-2-yl)-11-azatricyclo[5.3.1.0{4,11}}undeca-3,5,7,9-tetraen-3-yl}phenol	1	1	1	0	<chem>CCCC(C)C1C2C=CC=C3C=CC(=C1c4ccc(O)cc4)N23</chem>
	4-[2-(2-phenylethyl)-11-azatricyclo[5.3.1.0{4,11}}undeca-3,5,7,9-tetraen-3-yl}phenol	1	1	1	0	<chem>Oc1ccc(cc1)C2=C3C=CC4=CC=CC(C2CCc5ccccc5)N34</chem>
	4-{2-butyl-11-azatricyclo[5.3.1.0{4,11}}undeca-3,5,7,9-tetraen-3-yl}phenol	1	1	1	0	<chem>CCCCC1C2C=CC=C3C=CC(=C1c4ccc(O)cc4)N23</chem>
80-08-0	4-(4-aminobenzenesulfonyl)aniline	0	1	0	1	<chem>Nc1ccc(cc1)S(=O)(=O)c2ccc(N)cc2</chem>
11098-97-8	4-{bis[4-(dimethylamino)phenyl]methyl}-	0	1	0	1	<chem>CN(C)c1ccc(cc1)C(c2ccc(cc2)N(C)C)c3ccc(cc3)N(C)C</chem>

	N,N-dimethylaniline					
	N,N'-diphenylguanidine	0	1	0	1	<chem>N=C(Nc1ccccc1)Nc2ccccc2</chem>
	P-phenylazophenol	1	1	1	0	<chem>Oc1ccc(cc1)N=Nc2ccccc2</chem>
1137-41-3	4-benzoylaniline	0	1	0	1	<chem>Nc1ccc(cc1)C(=O)c2ccccc2</chem>
611-98-3	4-(4-aminobenzoyl)aniline	0	1	0	1	<chem>Nc1ccc(cc1)C(=O)c2ccc(N)cc2</chem>
41576-40-3	butter yellow	0	1	0	1	<chem>Cc1ccccc1N=Nc2ccc(N)c(C)c2</chem>
591-35-5	3,5-dichlorophenol	0	1	0	1	<chem>Oc1cc(Cl)cc(Cl)c1</chem>
101-77-9	MDA	0	1	0	1	<chem>Nc1ccc(Cc2ccc(N)cc2)cc1</chem>
54760-75-7	4-[(E)-2-(4-aminophenyl)ethenyl]aniline	0	1	0	1	<chem>Nc1ccc(\C=C\c2ccc(N)cc2)cc1</chem>
68-96-2	hydroxyprogesterone	0	1	0	1	<chem>CC(=O)[C@@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>
	(14R)-15-ethyl-14-ethynyl-14-hydroxytetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-5-one	1	1	1	0	<chem>CCC12CCC3C(CCC4=CC(=O)CCC34)C1CC[C@@]2(O)C#C</chem>
612-96-4	2-phenylquinoline	0	1	0	1	<chem>c1ccc(cc1)c2ccc3ccccc3n2</chem>
855-97-0	2-(3,4-dimethoxyphenyl)-5,7-dimethoxychromen-4-one	0	1	0	1	<chem>COc1cc(OC)c2C(=O)C=C(Oc2c1)c3ccc(OC)c(OC)c3</chem>
4143-62-8	2-(3,4-dimethoxyphenyl)chromen-	0	1	0	1	<chem>COc1ccc(cc1OC)C2=CC(=O)c3ccccc3O2</chem>

	4-one					
58574-03-1	4-(4-hydroxyphenyl)benzoic acid	1	1	1	0	<chem>OC(=O)c1ccc(cc1)c2ccc(O)cc2</chem>
	BBC	0	1	0	1	<chem>CCCCNC(=O)n1c(NC(=O)OC)nc2ccccc12</chem>
57-97-6	7,12-dimethylbenz(a)anthracene	0	1	0	1	<chem>Cc1c2ccccc2c(C)c3c1ccc4ccccc34</chem>
709-24-0	1-(4-fluorophenyl)pentan-1-one	0	1	0	1	<chem>CCCCC(=O)c1ccc(F)cc1</chem>
	(2S)-2-[(2S)-2-amino-3-(4-hydroxyphenyl)propanamido]-3-(4-hydroxyphenyl)propanoic acid	0	1	0	1	<chem>N[C@@H](Cc1ccc(O)cc1)C(=O)N[C@@H](Cc2ccc(O)cc2)C(=O)O</chem>
	(2S)-2-[(2S)-2-amino-3-(4-hydroxyphenyl)propanamido]-3-phenylpropanoic acid	0	1	0	1	<chem>N[C@@H](Cc1ccc(O)cc1)C(=O)N[C@@H](Cc2ccccc2)C(=O)O</chem>
455-24-3	P-CF ₃ benzoic acid	0	1	0	1	<chem>OC(=O)c1ccc(cc1)C(F)(F)F</chem>
5471-51-2	raspberry ketone	0	1	0	1	<chem>CC(=O)CCc1ccc(O)cc1</chem>
575-03-1	7-hydroxy-4-(trifluoromethyl)chromen-2-one	1	1	1	0	<chem>Oc1ccc2C(=CC(=O)Oc2c1)C(F)(F)F</chem>
13020-57-0	P-hydroxybenzophenone	1	1	1	0	<chem>Oc1cccc(c1)C(=O)c2ccccc2</chem>
92-92-2	4-phenylbenzoic acid	0	1	0	1	<chem>OC(=O)c1ccc(cc1)c2ccccc2</chem>
123-30-8	aminophenol	1	1	1	0	<chem>Nc1ccc(O)cc1</chem>
12698-64-5	chlorophenols	0	1	0	1	<chem>Oc1c(Cl)cc(Cl)c(Cl)c1Cl</chem>

1138-52-9	3,5-di-T-butylphenol	0	1	0	1	<chem>CC(C)(C)c1cc(O)cc(c1)C(C)(C)C</chem>
19812-93-2	4-(4-hydroxyphenyl)benzonitrile	1	1	1	0	<chem>Oc1ccc(cc1)c2ccc(cc2)C#N</chem>
467-62-9	tris(4-aminophenyl)methanol	1	1	1	0	<chem>Nc1ccc(cc1)C(O)(c2ccc(N)cc2)c3ccc(N)cc3</chem>
	4-[1-(4-hydroxyphenyl)-2-(pyridin-4-yl)but-1-en-1-yl]phenol	1	1	1	0	<chem>CCC(=C(c1ccc(O)cc1)c2ccc(O)cc2)c3ccncc3</chem>
	4-[1-(4-hydroxyphenyl)-2-(pyridin-2-yl)but-1-en-1-yl]phenol	1	1	1	0	<chem>CCC(=C(c1ccc(O)cc1)c2ccc(O)cc2)c3cccn3</chem>
	4-[1-(4-hydroxyphenyl)-2-(pyridin-4-yl)prop-1-en-1-yl]phenol	1	1	1	0	<chem>CC(=C(c1ccc(O)cc1)c2ccc(O)cc2)c3ccncc3</chem>
	4-[1-(4-hydroxyphenyl)-2-(pyridin-4-yl)ethenyl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)C(=Cc2ccncc2)c3ccc(O)cc3</chem>
	4-[1-(4-hydroxyphenyl)-2-(pyridin-2-yl)ethenyl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)C(=Cc2cccn2)c3ccc(O)cc3</chem>
	4-[1-(4-hydroxyphenyl)-2-(pyridin-2-yl)prop-1-en-1-yl]phenol	1	1	1	0	<chem>CC(=C(c1ccc(O)cc1)c2ccc(O)cc2)c3cccn3</chem>
1322-51-6	phenol, 2-(phenylmethyl)-	0	1	0	1	<chem>Oc1ccccc1Cc2ccccc2</chem>
324-74-3	4-fluorobiphenyl	0	1	0	1	<chem>Fc1ccc(cc1)c2ccccc2</chem>
3218-36-8	4-phenylbenzaldehyde	0	1	0	1	<chem>O=Cc1ccc(cc1)c2ccccc2</chem>
	4-[5-(4-hydroxyphenyl)-2-phenylfuran-3-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2oc(c3ccccc3)c(c2)c4ccc(O)cc4</chem>

	4-[5-(4-hydroxyphenyl)-3-phenylfuran-2-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2oc(c3ccc(O)cc3)c(c2)c4ccccc4</chem>
	4-[2-ethyl-3-(4-hydroxyphenyl)-5-phenylpyrrol-1-yl]phenol	1	1	1	0	<chem>CCc1c(cc(c2ccccc2)n1c3ccc(O)cc3)c4ccc(O)cc4</chem>
	4-[5-(4-hydroxyphenyl)-2-phenylthiophen-3-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2cc(c3ccc(O)cc3)c(s2)c4ccccc4</chem>
	4-[5-(4-hydroxyphenyl)-3-phenylthiophen-2-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)c2cc(c3ccccc3)c(s2)c4ccc(O)cc4</chem>
131589-59-8	3-(4-azido-2,3,5,6-tetrafluorobenzoyl)-2-(4-hydroxyphenyl)-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4c(F)c(F)c(N=[N+]=[N-])c(F)c4F</chem>
131589-60-1	3-(4-azidobenzoyl)-2-(4-hydroxyphenyl)-1-benzothiophen-6-ol	1	1	1	0	<chem>Oc1ccc(cc1)c2sc3cc(O)ccc3c2C(=O)c4ccc(cc4)N=[N+]=[N-]</chem>
	(14R)-15-ethyl-14-ethynyl-14-hydroxytetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-1,6,16-trien-5-one	1	1	1	0	<chem>CCC12C=CC3=C4CCC(=O)C=C4CCC3C1CC[C@@]2(O)C#C</chem>
	(14R)-15-ethyl-14-ethynyl-14-hydroxytetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-1,6-dien-5-one	1	1	1	0	<chem>CCC12CCC3=C4CCC(=O)C=C4CCC3C1CC[C@@]2(O)C#C</chem>
	(9R,14S)-14-hydroxy-9,14,15-trimethyltetracyclo[8.7.0.0{2,7}.0{1	1	1	1	0	<chem>C[C@@@H]1CC2=CC(=O)CCC2=C3CCC4(C)C(CC[C@]4(C)O)C13</chem>

	1,15}}heptadeca-1,6-dien-5-one					
	(14S)-15-ethyl-14-hydroxy-14-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-1,6,16-trien-5-one	1	1	1	0	CCC12C=CC3=C4CCC(=O)C=C4CCC3C1CC[C@]2(C)O
	(9R,14S)-15-ethyl-14-hydroxy-9,14-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-1,6,16-trien-5-one	1	1	1	0	CCC12C=CC3=C4CCC(=O)C=C4C[C@@H](C)C3C1CC[C@]2(C)O
	(9R,14S)-14-hydroxy-9,14,15-trimethyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-1,6,16-trien-5-one	1	1	1	0	C[C@@H]1CC2=CC(=O)CCC2=C3C=CC4(C)C(CC[C@]4(C)O)C13
	(14S)-14-hydroxy-14,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-6-en-5-one	1	1	1	0	C[C@]1(O)CCC2C3CCC4=CC(=O)CCC4C3CCC12C
	(14S)-14-hydroxy-15-propyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-1,6-dien-5-one	1	1	1	0	CCCC12CCC3=C4CCC(=O)C=C4CCC3C1CC[C@@H]2O
	(14S)-15-ethyl-14-hydroxytetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-1,6,16-trien-5-one	1	1	1	0	CCC12C=CC3=C4CCC(=O)C=C4CCC3C1CC[C@@H]2O
	(14S)-15-ethyl-14-hydroxytetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-1,6-dien-5-one	1	1	1	0	CCC12CCC3=C4CCC(=O)C=C4CCC3C1CC[C@@H]2O

(14R)-14-ethynyl-14-hydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-1,6,16-trien-5-one	1	1	1	0	<chem>CC12C=CC3=C4CCC(=O)C=C4CCC3C1CC[C@@]2(O)C#C</chem>
(14S)-14-acetyl-14,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-5-one	1	1	1	0	<chem>CC(=O)[C@@]1(C)CCC2C3CCC4=CC(=O)CCC4C3CCC12C</chem>
(14S)-14-acetyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-1,6-dien-5-one	1	1	1	0	<chem>CC(=O)[C@H]1CCC2C3CCC4=CC(=O)CCC4=C3CCC12C</chem>
(14S)-14-acetyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-5-one	1	1	1	0	<chem>CC(=O)[C@H]1CCC2C3CCC4=CC(=O)CCC4C3CCC12C</chem>
(14S)-14-hydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-1,6,16-trien-5-one	1	1	1	0	<chem>CC12C=CC3=C4CCC(=O)C=C4CCC3C1CC[C@@H]2O</chem>
(14S)-14-hydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-1,6-dien-5-one	1	1	1	0	<chem>CC12CCC3=C4CCC(=O)C=C4CCC3C1CC[C@@H]2O</chem>
(14S)-15-ethyl-14-hydroxytetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-5-one	1	1	1	0	<chem>CCC12CCC3C(CCC4=CC(=O)CCC34)C1CC[C@@H]2O</chem>
(14S)-14-hydroxy-15-propyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-1,6,16-trien-5-one	1	1	1	0	<chem>CCCC12CCC3C(CCC4=CC(=O)CCC34)C1CC[C@@H]2O</chem>

	5]]heptadec-6-en-5-one					
	(14S)-14-hydroxy-15-propyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-1,6,16-trien-5-one	1	1	1	0	CCCC12C=CC3=C4CCC(=O)C=C4CCC3C1CC[C@@H]2O
	(14S)-14-hydroxy-14,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-1,6-dien-5-one	1	1	1	0	C[C@]1(O)CCC2C3CCC4=CC(=O)CCC4=C3CCC12C
	(14S)-14-acetyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-1,6,16-trien-5-one	1	1	1	0	CC(=O)[C@H]1CCC2C3CCC4=CC(=O)CCC4=C3C=CC12C
	(14S)-14-acetyl-14,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-1,6,16-trien-5-one	1	1	1	0	CC(=O)[C@@]1(C)CCC2C3CCC4=CC(=O)CCC4=C3C=CC12C
	(14R)-14-ethynyl-14-hydroxy-15-propyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-1,6,16-trien-5-one	1	1	1	0	CCCC12C=CC3=C4CCC(=O)C=C4CCC3C1CC[C@@]2(O)C#C
	(14R)-14-ethynyl-14-hydroxy-15-propyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-1,6-dien-5-one	1	1	1	0	CCCC12CCC3=C4CCC(=O)C=C4CCC3C1CC[C@@]2(O)C#C
	(14R)-14-ethynyl-14-hydroxy-15-propyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-6-en-5-one	1	1	1	0	CCCC12CCC3C(CCC4=CC(=O)CCC34)C1CC[C@@]2(O)C#C

566-48-3	formestane	0	1	0	1	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=C(O)C(=O)CC[C@]34C)[C@@H]1CCC2=O</chem>
	6-methyl-2-phenylchromen-4-one	0	1	0	1	<chem>Cc1ccc2OC(=CC(=O)c2c1)c3ccccc3</chem>
	3-{4-[3-(piperidin-1-yl)propoxy]phenyl}-2',3'-dihydro-1,1'-spirobi[indene]-5,5'-diol	1	1	1	0	<chem>Oc1ccc2c(CCC23C=C(c4ccc(OCCCN5CCCCC5)cc4)c6cc(O)ccc36)c1</chem>
	3-{4-[2-(4-methylpiperidin-1-yl)ethoxy]phenyl}-2',3'-dihydro-1,1'-spirobi[indene]-5,5'-diol	1	1	1	0	<chem>CC1CCN(CCOc2ccc(cc2)C3=CC4(CCc5cc(O)ccc45)c6ccc(O)cc36)CC1</chem>
	3-{4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}-2',3'-dihydro-1,1'-spirobi[indene]-5,5'-diol	1	1	1	0	<chem>Oc1ccc2c(CCC23C=C(c4ccc(OCCN5CCCC5)cc4)c6cc(O)ccc36)c1</chem>
	3-{4-[2-(diethylamino)ethoxy]phenyl}-2',3'-dihydro-1,1'-spirobi[indene]-5,5'-diol	1	1	1	0	<chem>CCN(CC)CCOc1ccc(cc1)C2=CC3(CCc4cc(O)ccc34)c5ccc(O)cc25</chem>
	3-[4-(4-propylpiperazin-1-yl)phenyl]-2',3'-dihydro-1,1'-spirobi[indene]-5,5'-diol	1	1	1	0	<chem>CCCN1CCN(CC1)c2ccc(cc2)C3=CC4(CCc5cc(O)ccc45)c6ccc(O)cc36</chem>
	3-[4-(4-methylpiperazin-1-yl)phenyl]-2',3'-dihydro-1,1'-spirobi[indene]-5,5'-diol	1	1	1	0	<chem>CN1CCN(CC1)c2ccc(cc2)C3=CC4(CCc5cc(O)ccc45)c6ccc(O)cc36</chem>
	3-{4-[4-(2-methylpropyl)piperazin-	1	1	1	0	<chem>CC(C)CN1CCN(CC1)c2ccc(cc2)C3=CC4(CCc5cc(O)ccc45)c6cc</chem>

	1-yl]phenyl}-2',3'-dihydro-1,1'-spirobi[indene]-5,5'-diol					c(O)cc36
	3-[4-(4-ethylpiperazin-1-yl)phenyl]-2',3'-dihydro-1,1'-spirobi[indene]-5,5'-diol	1	1	1	0	CCN1CCN(CC1)c2ccc(cc2)C3=CC4(CCC5cc(O)ccc45)c6ccc(O)cc36
	3-{3-[2-(piperidin-1-yl)ethoxy]phenyl}-2',3'-dihydro-1,1'-spirobi[indene]-5,5'-diol	1	1	1	0	Oc1ccc2c(CCC23C=C(c4ccc(OCCN5CCCCC5)c4)c6cc(O)ccc36)c1
	3-{2-methyl-4-[2-(piperidin-1-yl)ethoxy]phenyl}-2',3'-dihydro-1,1'-spirobi[indene]-5,5'-diol	1	1	1	0	Cc1cc(OCCN2CCCCC2)ccc1C3=CC4(CCC5cc(O)ccc45)c6ccc(O)cc36
	3-{4-[2-(dimethylamino)ethoxy]phenyl}-2',3'-dihydro-1,1'-spirobi[indene]-5,5'-diol	1	1	1	0	CN(C)CCOc1ccc(cc1)C2=CC3(CCC4cc(O)ccc34)c5ccc(O)cc25
	3-[4-(4-isopropylpiperazin-1-yl)phenyl]-2',3'-dihydro-1,1'-spirobi[indene]-5,5'-diol	1	1	1	0	CC(C)N1CCN(CC1)c2ccc(cc2)C3=CC4(CCC5cc(O)ccc45)c6ccc(O)cc36
	3-{3-fluoro-4-[2-(piperidin-1-yl)ethoxy]phenyl}-2',3'-dihydro-1,1'-spirobi[indene]-5,5'-diol	1	1	1	0	Oc1ccc2c(CCC23C=C(c4ccc(OCCN5CCCCC5)c(F)c4)c6cc(O)ccc36)c1
	3-{4-[3-(piperidin-1-yl)propyl]phenyl}-2',3'-dihydro-1,1'-	1	1	1	0	Oc1ccc2c(CCC23C=C(c4ccc(CCCN5CCCCC5)cc4)c6cc(O)ccc36)c1

	spirobi[indene]-5,5'-diol					
26964-24-9	6-methoxy-2-phenylchromen-4-one	0	1	0	1	<chem>COc1ccc2OC(=CC(=O)c2c1)c3ccccc3</chem>
	3-{4-[2-(piperidin-1-yl)ethoxy]phenyl}-2',3'-dihydro-1,1'-spirobi[indene]-5,5'-diol	1	1	1	0	<chem>Oc1ccc2c(CCC23C=C(c4ccc(OCCN5CCCCC5)cc4)c6cc(O)ccc36)c1</chem>
	3-[4-(4-ethylazepan-1-yl)phenyl]-2',3'-dihydro-1,1'-spirobi[indene]-5,5'-diol	1	1	1	0	<chem>CCC1CCCN(CC1)c2ccc(cc2)C3=CC4(CCC5cc(O)ccc45)c6ccc(O)cc36</chem>
	3-[4-(piperidin-1-yl)phenyl]-2',3'-dihydro-1,1'-spirobi[indene]-5,5'-diol	1	1	1	0	<chem>Oc1ccc2c(CCC23C=C(c4ccc(cc4)N5CCCCC5)c6cc(O)ccc36)c1</chem>
26088-14-2	4-[9-(4-hydroxyphenyl)fluoren-9-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)C2(c3ccc(O)cc3)c4ccccc4c5ccccc25</chem>
15499-84-0	4-[9-(4-aminophenyl)fluoren-9-yl]aniline	0	1	0	1	<chem>Nc1ccc(cc1)C2(c3ccc(N)cc3)c4ccccc4c5ccccc25</chem>
	4-[(3R,4S)-4-(4-hydroxyphenyl)hexan-3-yl]benzonitrile	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(cc2)C#N</chem>
	1-{4-[(3R,4S)-4-(4-hydroxyphenyl)hexan-3-yl]phenyl}ethanone	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(cc2)C(=O)C</chem>

4-[(3S,4R)-4-[4-(hydroxymethyl)phenyl]hexan-3-yl]phenol	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(CO)cc2</chem>
4-[(3R,4S)-4-(4-hydroxyphenyl)hexan-3-yl]benzenesulfonyl azide	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(cc2)S(=O)(=O)N=[N+]=[N-]</chem>
4-[(3S,4R)-4-[4-(2-hydroxypropoxy)phenyl]hexan-3-yl]phenol	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(OCC(C)O)cc2</chem>
3-{4-[(3R,4S)-4-(4-hydroxyphenyl)hexan-3-yl]phenoxy}propane-1,2-diol	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(OCC(O)CO)cc2</chem>
4-[(3S,4R)-4-[4-(prop-2-en-1-yloxy)phenyl]hexan-3-yl]phenol	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(OCC=C)cc2</chem>
4-[(3S,4R)-4-[4-(2-hydroxyethoxy)phenyl]hexan-3-yl]phenol	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(OCCO)cc2</chem>
4-[(3S,4R)-4-(4-aminophenyl)hexan-3-yl]phenol	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(N)cc2</chem>
4-[(3R,4S)-4-(4-hydroxyphenyl)hexan-3-yl]phenoxyacetic acid	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(OCC(=O)O)cc2</chem>
4-[(3S,4R)-4-{4-[2-(2-	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(OCCOCCCl)cc2</chem>

	chloroethoxy)ethoxy]phenyl]hexan-3-yl]phenol					
	4-[(3S,4R)-4-(4-azidophenyl)hexan-3-yl]phenol	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(cc2)N=[N+]=[N-]</chem>
	4-[(3S,4R)-4-[4-(ethoxymethyl)phenyl]hexan-3-yl]phenol	1	1	1	0	<chem>CCOCc1ccc(cc1)[C@H](CC)[C@H](CC)c2ccc(O)cc2</chem>
	ethyl 2-{4-[(3R,4S)-4-(4-hydroxyphenyl)hexan-3-yl]phenoxy}acetate	1	1	1	0	<chem>CCOC(=O)COc1ccc(cc1)[C@H](CC)[C@H](CC)c2ccc(O)cc2</chem>
	4-[(3S,4R)-4-(4-hydroxyphenyl)hexan-3-yl]-2-(prop-2-en-1-yl)phenol	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)c(CC=C)c1)c2ccc(O)cc2</chem>
	hexestrol monomethyl ether	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(OC)cc2</chem>
	4-[(3S,4R)-4-(4-hydroxyphenyl)hexan-3-yl]-2-(3-hydroxypropyl)phenol	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)c(CCO)c1)c2ccc(O)cc2</chem>
	4-[(3R,4S)-4-(4-hydroxyphenyl)hexan-3-yl]benzoic acid	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(cc2)C(=O)O</chem>
	4-[(3S,4R)-4-(4-nitrophenyl)hexan-3-yl]phenol	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(cc2)[N+](=O)[O-]</chem>

	1-{4-[(3R,4S)-4-(4-hydroxyphenyl)hexan-3-yl]phenoxy}propan-2-one	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(OCC(=O)C)cc2</chem>
	1-diazo-3-{4-[(3R,4S)-4-(4-hydroxyphenyl)hexan-3-yl]phenoxy}propan-2-one	1	1	1	0	<chem>CC[C@H]([C@H](CC)c1ccc(O)cc1)c2ccc(OCC(=O)C=[N+]=[N-])cc2</chem>
427-51-0	cypoterone acetate	0	1	0	1	<chem>CC(=O)O[C@@]1(CC[C@H]2[C@@H]3C=C(Cl)C4=CC(=O)[C@@H]5C[C@@H]5[C@]4(C)[C@H]3CC[C@]12C)C(=O)C</chem>
1965-09-9	phenol, 4,4'-oxybis-	1	1	1	0	<chem>Oc1ccc(Oc2ccc(O)cc2)cc1</chem>
	7-hydroxy-3-phenylchromen-2-one	0	1	0	1	<chem>Oc1ccc2C=C(C(=O)Oc2c1)c3ccccc3</chem>
	enilconazole	0	1	0	1	<chem>Clc1ccc(C(Cn2ccnc2)OCC=C)c(Cl)c1</chem>
	1H-3,1-benzoxazine-2,4-dione	0	1	0	1	<chem>O=C1Nc2ccccc2C(=O)O1</chem>
	(2R)-15'-methylspiro[oxolane-2,14'-tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadecane]-1',6',16'-triene-5,5'-dione	1	1	1	0	<chem>CC12C=CC3=C4CCC(=O)C=C4CCC3C1CC[C@@]25CCC(=O)O5</chem>
	(2R)-15'-methylspiro[1,5S[4]-oxathiolane-2,14'-tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadecane]-1',6',16'-triene-5,5'-dione	1	1	1	0	<chem>CC12C=CC3=C4CCC(=O)C=C4CCC3C1CC[C@@]25CCS(=O)O5</chem>
	(2R)-15'-methylspiro[1,5S[4]-oxathiolane-2,14'-	1	1	1	0	<chem>CC12CCC3=C4CCC(=O)C=C4CCC3C1CC[C@@]25CCS(=O)O5</chem>

tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadecane]-1',6'-diene-5,5'-dione						
(14S)-14-hydroxy-8,8,14,15-tetramethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-1,6,16-trien-5-one	1	1	1	0		CC1(C)CC2C3CC[C@](C)(O)C3(C)C=CC2=C4CCC(=O)C=C14
(2R)-15'-methylspiro[oxolane-2,14'-tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadecan]-6'-ene-5,5'-dione	1	1	1	0		CC12CCC3C(CCC4=CC(=O)CCC34)C1CC[C@@]25CCC(=O)O5
(14S)-14-hydroxy-4,4,14,15-tetramethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-1,6,16-trien-5-one	1	1	1	0		CC1(C)CC2=C3C=CC4(C)C(CC[C@]4(C)O)C3CCC2=CC1=O
15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-1,6,16-trien-5-one	1	1	1	0		CC12CCCC1C3CCC4=CC(=O)CCC4=C3C=C2
(14S)-14,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-1,6,16-trien-14-ol	1	1	1	0		C[C@]1(O)CCC2C3CCC4=CCCCC4=C3C=CC12C
(14S)-14-hydroxy-6,14,15-trimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-1,6,16-trien-5-one	1	1	1	0		CC1=C2CCC3C4CC[C@](C)(O)C4(C)C=CC3=C2CCC1=O
15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-1,6,16-trien-5-one	1	1	1	0		CC12C=CC3=C4CCC(=O)C=C4CCC3C1CCC2=O

	15}}heptadeca-1,6,16-triene-5,14-dione					
	(2R)-15'-methylspiro[oxolane-2,14'-tetracyclo[8.7.0.0{2,7}.0{11,15}}heptadecane]-1',6'-diene-5,5'-dione	1	1	1	0	<chem>CC12CCC3=C4CCC(=O)C=C4CCC3C1CC[C@@]25CCC(=O)O5</chem>
500-66-3	olivetol	0	1	0	1	<chem>CCCCCc1cc(O)cc(O)c1</chem>
	(14S)-14-hydroxy-4,14,15-trimethyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-1,6,16-trien-5-one	1	1	1	0	<chem>CC1CC2=C3C=CC4(C)C(CC[C@]4(C)O)C3CCC2=CC1=O</chem>
	(14S)-14-hydroxy-14,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-1,6,16-trien-4-one	1	1	1	0	<chem>C[C@]1(O)CCC2C3CCC4=CCC(=O)CC4=C3C=CC12C</chem>
	(3S)-3,3a-dimethyl-1H,2H,7H,8H,9H,9aH,9bH-cyclopenta[a]naphthalen-3-ol	1	1	1	0	<chem>C[C@]1(O)CCC2C3CCCC=C3C=CC12C</chem>
	1-[(4-hydroxyphenyl)methyl]-3H-imidazole-2-thione	0	1	0	1	<chem>Oc1ccc(CN2C=CNC2=S)cc1</chem>
	briten	0	1	0	1	<chem>COP(=O)(OC)C(O)C(Cl)(Cl)Cl</chem>
121509-79-3	4,4-oxydianiline	0	1	0	1	<chem>Nc1ccc(Oc2ccc(N)cc2)cc1</chem>
	2-(aziridin-1-yl)ethyl (2R,3S)-2,3-bis(4-hydroxyphenyl)pentanoate	1	1	1	0	<chem>CC[C@@H]([C@@H](C(=O)OCCN1CC1)c2ccc(O)cc2)c3ccc(O)cc3</chem>

79642-44-7	1-(2-{4-[(1Z)-1,2-diphenylbut-1-en-1-yl]phenoxy}ethyl)aziridine	1	1	1	0	<chem>CC\C(=C(/c1ccccc1)\c2ccc(OCCN3CC3)cc2)\c4ccccc4</chem>
	4-[(2R,3S)-1-{[3-(dimethylamino)propyl]sulfanyl}-2-(4-hydroxyphenyl)pentan-3-yl]phenol	1	1	1	0	<chem>CC[C@@H]([C@@H](CSCCN(C)C)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	4-[(2R,3S)-1-{[3-(aziridin-1-yl)propyl]sulfanyl}-2-(4-hydroxyphenyl)pentan-3-yl]phenol	1	1	1	0	<chem>CC[C@@H]([C@@H](CSCCN1CC1)c2ccc(O)cc2)c3ccc(O)cc3</chem>
	(6R,7S)-1-(aziridin-1-yl)-6,7-bis(4-hydroxyphenyl)nonan-5-one	1	1	1	0	<chem>CC[C@@H]([C@@H](C(=O)CCCCN1CC1)c2ccc(O)cc2)c3ccc(O)cc3</chem>
	(6R,7S)-1-(dimethylamino)-6,7-bis(4-hydroxyphenyl)nonan-5-one	1	1	1	0	<chem>CC[C@@H]([C@@H](C(=O)CCCCN(C)C)c1ccc(O)cc1)c2ccc(O)cc2</chem>
	4-[(2R,3S)-1-{[2-(aziridin-1-yl)ethyl]sulfanyl}-2-(4-hydroxyphenyl)pentan-3-yl]phenol	1	1	1	0	<chem>CC[C@@H]([C@@H](CSCCN1CC1)c2ccc(O)cc2)c3ccc(O)cc3</chem>
	4-[(3S,4R)-8-(aziridin-1-yl)-4-(4-hydroxyphenyl)octan-3-yl]phenol	1	1	1	0	<chem>CC[C@@H]([C@@H](CCCCN1CC1)c2ccc(O)cc2)c3ccc(O)cc3</chem>
	3-(aziridin-1-yl)propyl (2R,3S)-2,3-bis(4-hydroxyphenyl)pentanoate	1	1	1	0	<chem>CC[C@@H]([C@@H](C(=O)OCCCN1CC1)c2ccc(O)cc2)c3ccc(O)cc3</chem>
	(2R,3S)-1-(aziridin-1-yl)-2,3-bis(4-hydroxyphenyl)pentan-1-one	1	1	1	0	<chem>CC[C@@H]([C@@H](C(=O)N1CC1)c2ccc(O)cc2)c3ccc(O)cc3</chem>

3704-09-4	mibolerone	1	1	1	0	<chem>C[C@@H]1CC2=CC(=O)CC[C@@H]2[C@H]3CC[C@@]4(C)[C@@H](CC[C@]4(C)O)[C@H]13</chem>
973-67-1	5,6,7-trimethoxyflavone	0	1	0	1	<chem>COc1cc2OC(=CC(=O)c2c(OC)c1OC)c3ccccc3</chem>
95-56-7	2-bromophenol	0	1	0	1	<chem>Oc1ccccc1Br</chem>
591-20-8	M-bromophenol	0	1	0	1	<chem>Oc1cccc(Br)c1</chem>
	2-oxoquinoline	0	1	0	1	<chem>O=C1Nc2ccccc2C=C1</chem>
579-39-5	bis(4-fluorophenyl)ethane-1,2-dione	0	1	0	1	<chem>Fc1ccc(cc1)C(=O)C(=O)c2ccc(F)cc2</chem>
1226-42-2	bis(4-methoxyphenyl)ethane-1,2-dione	0	1	0	1	<chem>COc1ccc(cc1)C(=O)C(=O)c2ccc(OC)cc2</chem>
40101-17-5	bis(3-methoxyphenyl)ethane-1,2-dione	0	1	0	1	<chem>COc1cccc(c1)C(=O)C(=O)c2cccc(OC)c2</chem>
17078-27-2	bis[4-(dimethylamino)phenyl]ethane-1,2-dione	0	1	0	1	<chem>CN(C)c1ccc(cc1)C(=O)C(=O)c2ccc(cc2)N(C)C</chem>
35578-47-3	bis(4-bromophenyl)ethane-1,2-dione	0	1	0	1	<chem>BrC1ccc(cc1)C(=O)C(=O)c2ccc(Br)cc2</chem>
3457-48-5	bis(4-methylphenyl)ethane-1,2-dione	0	1	0	1	<chem>Cc1ccc(cc1)C(=O)C(=O)c2ccc(C)cc2</chem>
611-95-0	benzoic acid, 4-benzoyl-	0	1	0	1	<chem>OC(=O)c1ccc(cc1)C(=O)c2ccccc2</chem>

402-45-9	α,α,α -trifluoro-P-cresol	1	1	1	0	<chem>Oc1ccc(cc1)C(F)(F)F</chem>
	4-{12-[(4-hydroxyphenyl)methyl]-1\$I{5},2\$I{5},3\$I{5},4\$I{5},5\$I{5},6\$I{5},7\$I{5},8\$I{5},9\$I{5},10\$I{5}-decaboranonadecacyclo[5.4.1.0{1,3}.0{1,4}.0{2,6}.0{2,7}.0{2,12}.0{3,5}.0{3,6}.0{4,9}.0{4,11}.0{5,8}.0{5,9}.0{6,8}.0{7,10}.0{8,10}.0{9,11}.0{10,12}.0{11,12}]dodecan-11-yl}phenol	1	1	1	0	<chem>Oc1ccc(CC2345B678B9%10%11B%12%13%14B9%15%16B%12%17%18B%13%19%20B6%10%14B27%19C3%17%20(c%21ccc(O)cc%21)B4%15%18B58%11%16)cc1</chem>
	4-{12-[2-(4-hydroxyphenyl)ethyl]-1\$I{5},2\$I{5},3\$I{5},4\$I{5},5\$I{5},6\$I{5},7\$I{5},8\$I{5},9\$I{5},10\$I{5}-decaboranonadecacyclo[5.4.1.0{1,3}.0{1,4}.0{2,6}.0{2,7}.0{2,12}.0{3,5}.0{3,6}.0{4,9}.0{4,11}.0{5,8}.0{5,9}.0{6,8}.0{7,10}.0{8,10}.0{9,11}.0{10,12}.0{11,12}]dodecan-11-yl}phenol	1	1	1	0	<chem>Oc1ccc(CCC2345B678B9%10%11B%12%13%14B9%15%16B%12%17%18B%13%19%20B6%10%14B27%19C3%17%20(c%21ccc(O)cc%21)B4%15%18B58%11%16)cc1</chem>
	4-[(2E)-2-[2-(4-hydroxyphenyl)ethylidene]adaman tan-1-yl]phenol	1	1	1	0	<chem>Oc1ccc(C\\C=C\\2/C3CC4CC(C3)CC2(C4)c5ccc(O)cc5)cc1</chem>
	4-[11-(4-hydroxyphenyl)-1\$I{5},2\$I{5},3\$I{5},4\$I{5},5\$I{5},6\$I{5},7\$I{5},8\$I{5},9\$I{5},10\$I{5}-decaboranonadecacyclo[5.4.1.0{1,3}.0{1,4}.0{2,6}.0{2,7}.0{2,12}.0{3,5}.0{3,6}.0{4,9}.0{4,11}.0{5,8}.0{5,9}.0	1	1	1	0	<chem>Oc1ccc(cc1)C2345B678B9%10%11B%12%13%14B9%15%16B%12%17%18B%13%19%20B6%10%14B27%19C3%17%20(c%21ccc(O)cc%21)B4%15%18B58%11%16</chem>

	{6,8}.0{7,10}.0{8,10}.0{9,11}.0{10,12}.0{11,12}]dodecan-12-yl]phenol					
	4-[3-(4-hydroxyphenyl)bicyclo[2.2.2]oct-2-en-2-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)C2=C(C3CCC2CC3)c4ccc(O)cc4</chem>
	4-[(2E)-2-[(4-hydroxyphenyl)methylidene]adamantan-1-yl]phenol	1	1	1	0	<chem>Oc1ccc(\C=C\2/C3CC4CC(C3)CC2(C4)c5ccc(O)cc5)cc1</chem>
	4-[2-(4-hydroxyphenyl)-4,4,5,5-tetramethylcyclohex-1-en-1-yl]phenol	1	1	1	0	<chem>CC1(C)CC(=C(CC1(C)C)c2ccc(O)cc2)c3ccc(O)cc3</chem>
106-37-6	dibromobenzene	0	1	0	1	<chem>Brc1ccc(Br)cc1</chem>
	3-chloro-4-[4-(2-chloro-4-hydroxyphenyl)-1-(4-hydroxyphenyl)imidazol-2-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)n2cc(nc2c3ccc(O)cc3Cl)c4ccc(O)cc4Cl</chem>
	4-[5-ethyl-1,4-bis(4-hydroxyphenyl)imidazol-2-yl]phenol	1	1	1	0	<chem>CCc1c(nc(c2ccc(O)cc2)n1c3ccc(O)cc3)c4ccc(O)cc4</chem>
1224-92-6	3b-hydroxy-5a-androstane	1	1	1	0	<chem>C[C@@]12CCCC[C@H]1[C@@H]3CC[C@H]4C[C@@H](O)CC[C@]4(C)[C@H]3CC2</chem>

1137-42-4	4-hydroxybenzophenone	1	1	1	0	<chem>Oc1ccc(cc1)C(=O)c2ccccc2</chem>
520-85-4	medroxyprogesterone	0	1	0	1	<chem>C[C@H]1C[C@@H]2[C@H](CC[C@@]3(C)[C@H]2CC[C@]3(O)C(=O)C)[C@@]4(C)CCC(=O)C=C14</chem>
18951-43-4	4-[(E)-2-(4-aminophenyl)ethenyl]phenol	1	1	1	0	<chem>Nc1ccc(\C=C\c2ccc(O)cc2)cc1</chem>
	ammo	0	1	0	1	<chem>CC1(C)C(C=C(Cl)Cl)C1C(=O)OC(C#N)c2cccc(Oc3ccccc3)c2</chem>
611-94-9	(4-methoxyphenyl)(phenyl)methanone	0	1	0	1	<chem>COc1ccc(cc1)C(=O)c2ccccc2</chem>
	4-(4-ethylphenyl)benzoic acid	0	1	0	1	<chem>CCc1ccc(cc1)c2ccc(cc2)C(=O)O</chem>
2168-06-1	3,3,3-tris(4-chlorophenyl)propanoic acid	0	1	0	1	<chem>OC(=O)CC(c1ccc(Cl)cc1)(c2ccc(Cl)cc2)c3ccc(Cl)cc3</chem>
437-64-9	genkwanin	1	1	1	0	<chem>COc1cc(O)c2C(=O)C=C(Oc2c1)c3ccc(O)cc3</chem>
14064-83-6	4-[(E)-2-(4-nitrophenyl)ethenyl]phenol	0	1	0	1	<chem>Oc1ccc(\C=C\c2ccc(cc2)[N+](=O)[O-])cc1</chem>
	3,6-dihydroxy-2-phenylchromen-4-one	0	1	0	1	<chem>OC1=C(Oc2ccc(O)cc2C1=O)c3ccccc3</chem>
14392-69-9	1-(4-hydroxyphenyl)nonan-1-one	1	1	1	0	<chem>CCCCCCCCC(=O)c1ccc(O)cc1</chem>
	9a-[(4-chlorophenyl)methyl]-7-hydroxy-4-methyl-2,9-dihydro-1H-fluoren-3-one	1	1	1	0	<chem>CC1=C2c3ccc(O)cc3CC2(Cc4ccc(Cl)cc4)CCC1=O</chem>

87-82-1	hexabromobenzene	0	1	0	1	<chem>BrC1c(Br)c(Br)c(Br)c(Br)c1Br</chem>
	(1S,10S,11S,14R,15S,17S)-17-methoxy-15-methyl-14-[(E)-2-phenylethenyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	<chem>CO[C@H]1C[C@@]2(C)[C@@H](CC[C@@]2(O)\C=C\c3ccc3)[C@@H]4CCc5cc(O)ccc5[C@@H]14</chem>
	(1S,10S,11S,14R,15S,17S)-17-methoxy-15-methyl-14-[(E)-2-[2-(trifluoromethyl)phenyl]ethenyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	<chem>CO[C@H]1C[C@@]2(C)[C@@H](CC[C@@]2(O)\C=C\c3ccc3C(F)(F)F)[C@@H]4CCc5cc(O)ccc5[C@@H]14</chem>
	(1S,10S,11S,14R,15S,17S)-17-methoxy-15-methyl-14-[(E)-2-[4-(trifluoromethyl)phenyl]ethenyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	<chem>CO[C@H]1C[C@@]2(C)[C@@H](CC[C@@]2(O)\C=C\c3ccc(cc3)C(F)(F)F)[C@@H]4CCc5cc(O)ccc5[C@@H]14</chem>
	(1S,10R,11S,14R,15S)-15-methyl-14-[(E)-2-[2-(trifluoromethyl)phenyl]ethenyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)\C=C\c5ccccc5C(F)(F)F</chem>
	(1S,10R,11S,14R,15S)-15-methyl-14-[(E)-2-[3-(trifluoromethyl)phenyl]ethenyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]hepta	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)\C=C\c5cccc(c5)C(F)(F)F</chem>

	deca-2,4,6-triene-5,14-diol					
98-29-3	4-tert-butylcatechol	1	1	1	0	<chem>CC(C)(C)c1ccc(O)c(O)c1</chem>
	3-chloro-4-[4-(2-chloro-4-hydroxyphenyl)-1-(4-hydroxyphenyl)-5-methylimidazol-2-yl]phenol	1	1	1	0	<chem>Cc1c(nc(c2ccc(O)cc2Cl)n1c3ccc(O)cc3)c4ccc(O)cc4Cl</chem>
	3-chloro-4-[5-ethyl-1,4-bis(4-hydroxyphenyl)imidazol-2-yl]phenol	1	1	1	0	<chem>CCc1c(nc(c2ccc(O)cc2Cl)n1c3ccc(O)cc3)c4ccc(O)cc4</chem>
6990-06-3	ramycin	0	1	0	1	<chem>C[C@@H]1[C@H](O)CC[C@@]2(C)[C@H]1CC[C@@]3(C)[C@H]2[C@H](O)C[C@H]4\C(=C(/CCC=C(C)C)\C(=O)O)\[C@H](C[C@]34C)OC(=O)C</chem>
4143-64-0	2-(3,4-dihydroxyphenyl)chromen-4-one	1	1	1	0	<chem>Oc1ccc(cc1O)C2=CC(=O)c3ccccc3O2</chem>
3440-24-2	2-(3,4-dihydroxyphenyl)-7,8-dihydroxychromen-4-one	1	1	1	0	<chem>Oc1ccc(cc1O)C2=CC(=O)c3ccc(O)c(O)c3O2</chem>
622-62-8	P-ethoxyphenol	0	1	0	1	<chem>CCOc1ccc(O)cc1</chem>
18979-50-5	phenol, 4-propoxy-	0	1	0	1	<chem>CCCOc1ccc(O)cc1</chem>
831-82-3	4-phenoxyphenol	1	1	1	0	<chem>Oc1ccc(Oc2ccccc2)cc1</chem>
4130-42-1	2,6-di-tert-butyl-4-ethylphenol	0	1	0	1	<chem>CCc1cc(c(O)c(c1)C(C)(C)C)C(C)(C)C</chem>

732-26-3	2,4,6-tri(tert-butyl)phenol	0	1	0	1	<chem>CC(C)(C)c1cc(c(O)c(c1)C(C)(C)C(C)(C)C</chem>
57-24-9	strychnos	0	1	0	1	<chem>O=C1C[C@@H]2OCC=C3CN4CC[C@]56[C@@H]4C[C@@H]3[C@H]2[C@@H]5N1c7ccccc67</chem>
26087-47-8	IBP	0	1	0	1	<chem>CC(C)OP(=O)(OC(C)C)SCc1ccccc1</chem>
	benzyladenine	0	1	0	1	<chem>C(Nc1ncnc2[nH]cnc12)c3ccccc3</chem>
130785-52-3	4-{2-[4-hydroxy-3-(prop-2-en-1-yl)phenyl]propan-2-yl}-2-(prop-2-en-1-yl)phenol	1	1	1	0	<chem>CC(C)(c1ccc(O)c(CC=C)c1)c2ccc(O)c(CC=C)c2</chem>
94-59-7	sassafras	0	1	0	1	<chem>C=CCc1ccc2OCOc2c1</chem>
1818-12-8	(1S,10R,11S,14S,15S)-4,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	<chem>Cc1cc2[C@H]3CC[C@]4(C)[C@@H](O)CC[C@H]4[C@@H]3CCc2cc1O</chem>
	3-(1,3-benzoxazol-2-yl)-7-hydroxychromen-2-one	0	1	0	1	<chem>Oc1ccc2C=C(C(=O)Oc2c1)c3oc4ccccc4n3</chem>
	3-(1,3-benzothiazol-2-yl)-7-hydroxychromen-2-one	1	1	1	0	<chem>Oc1ccc2C=C(C(=O)Oc2c1)c3nc4ccccc4s3</chem>
480-44-4	acacetin	0	1	0	1	<chem>COc1ccc(cc1)C2=CC(=O)c3c(O)cc(O)cc3O2</chem>
4376-18-5	monomethyl phthalate	0	1	0	1	<chem>COC(=O)c1ccccc1C(=O)O</chem>
21643-38-9	benzoic acid, 4-hexyl-	0	1	0	1	<chem>CCCCCc1ccc(cc1)C(=O)O</chem>

	warfarin	0	1	0	1	<chem>CC(=O)CC(C1=C(O)c2cccc2OC1=O)c3cccc3</chem>
	dicoumarol	0	1	0	1	<chem>OC1=C(CC2=C(O)c3cccc3OC2=O)C(=O)Oc4cccc14</chem>
17230-88-5	danazol	1	1	1	0	<chem>C[C@]12Cc3cnoc3C=C1CC[C@@H]4[C@@H]2CC[C@@]5(C)[C@H]4CC[C@@]5(O)C#C</chem>
94-74-6	zelan	0	1	0	1	<chem>Cc1cc(Cl)ccc1OCC(=O)O</chem>
	3-{2-[(1S,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]]heptadeca-2,4,6-trien-14-yl]ethynyl}-2-phenylchromen-4-one	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)C#CC5=C(Oc6cccc6C5=O)c7cccc7</chem>
	8-{2-[(1S,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]]heptadeca-2,4,6-trien-14-yl]ethynyl}-2-phenylchromen-4-one	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)C#Cc5cccc6C(=O)C=C(Oc56)c7cccc7</chem>
	(1S,10R,11S,14S,15S)-14-{2-[2-(2-methoxyphenyl)-1H-indol-3-yl]ethynyl}-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	<chem>COc1cccc1c2[nH]c3cccc3c2C#C[C@]4(O)CC[C@H]5[C@@H]6CCc7cc(O)ccc7[C@H]6CC[C@]45C</chem>
	(1S,10R,11S,14S,15S)-14-{2-[2-(2-hydroxyphenyl)-1H-indol-3-yl]ethynyl}-15-	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)C#Cc5c([nH]c6cccc56)c7cccc7O</chem>

	methylnetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol					
	2-[4-(benzyloxy)phenyl]-3-{2-[(1S,10R,11S,14S,15S)-5,14-dihydroxy-15-methylnetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-yl]ethynyl}-1-benzofuran-6-yl 4-methylbenzenesulfonate	1	1	1	0	Cc1ccc(cc1)S(=O)(=O)Oc2ccc3c(C#C[C@]4(O)CC[C@H]5[C@@H]6CCc7cc(O)ccc7[C@H]6CC[C@]45C)c(oc3c2)c8ccc(OCc9ccccc9)cc8
	3-{8-[(1S,10R,11S,14S,15S)-5,14-dihydroxy-15-methylnetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-yl]octa-1,7-diyn-1-yl}-2-phenylchromen-4-one	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)C#CCCCC#CC5=C(Oc6ccccc6C5=O)c7ccccc7
	8-{8-[(1S,10R,11S,14S,15S)-5,14-dihydroxy-15-methylnetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-yl]octa-1,7-diyn-1-yl}-2-phenylchromen-4-one	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)C#CCCCC#Cc5ccccc6C(=O)C=C(Oc56)c7ccccc7
	2-[4-(benzyloxy)phenyl]-3-{8-[(1S,10R,11S,14S,15S)-5,14-dihydroxy-15-methylnetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-yl]octa-1,7-diyn-1-yl}-2-phenylchromen-4-one	1	1	1	0	Cc1ccc(cc1)S(=O)(=O)Oc2ccc3c(C#CCCCC#C[C@]4(O)CC[C@H]5[C@@H]6CCc7cc(O)ccc7[C@H]6CC[C@]45C)c(oc3c2)c8ccc(OCc9ccccc9)cc8

	15]]heptadeca-2,4,6-trien-14-yl]octa-1,7-diyn-1-yl]-1-benzofuran-6-yl 4-methylbenzenesulfonate					
6678-14-4	2-[(1S,2R,10S,11S,14R,15S,17S)-14,17-dihydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-14-yl]-2-oxoethyl octanoate	0	1	0	1	CCCCCCCC(=O)OCC(=O)[C@@]1(O)CC[C@H]2[C@@H]3CC C4=CC(=O)CC[C@]4(C)[C@H]3[C@@H](O)C[C@]12C
174491-50-0	glyphosine	0	1	0	1	OC(=O)CN(CP(=O)(O)O)CP(=O)(O)O
1424-00-6	proviron	1	1	1	0	C[C@H]1CC(=O)C[C@@H]2CC[C@H]3[C@@H]4CC[C@H](O)[C@@]4(C)CC[C@@H]3[C@@]12C
121-14-2	2,4-dinitrotoluene	0	1	0	1	Cc1ccc(cc1[N+](=O)[O-])[N+](=O)[O-]
57164-27-9	liothyronine	0	1	0	1	N[C@@H](Cc1cc(I)c(Oc2ccc(O)c(I)c2)c(I)c1)C(=O)O
	(1R,5R)-8-methyl-8-azabicyclo[3.2.1]octan-3-yl 3-hydroxy-2-phenylpropanoate	0	1	0	1	CN1[C@@H]2CC[C@@H]1CC(C2)OC(=O)C(CO)c3ccccc3
136684-50-9	(bromodiphenylmethyl)benzene	0	1	0	1	BrC(c1ccccc1)(c2ccccc2)c3ccccc3
76-83-5	triphenylmethyl chloride	0	1	0	1	ClC(c1ccccc1)(c2ccccc2)c3ccccc3
1553-56-6	3-ketolithocholic acid	0	1	0	1	C[C@H](CCC(=O)O)[C@H]1CC[C@H]2[C@@H]3CC[C@@H]4CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C

595-91-5	triphenylacetic acid	0	1	0	1	<chem>OC(=O)C(c1ccccc1)(c2ccccc2)c3ccccc3</chem>
	tebuconazole	0	1	0	1	<chem>CC(C)(C)C(O)(CCc1ccc(Cl)cc1)Cn2cncn2</chem>
5597-50-2	methyl 3-(4-hydroxyphenyl)propanoate	0	1	0	1	<chem>COC(=O)CCc1ccc(O)cc1</chem>
39475-55-3	terial	1	1	1	0	<chem>CCOP(=S)(OCC)Oc1nc(Cl)c(Cl)cc1Cl</chem>
	hordenine	0	1	0	1	<chem>CN(C)CCc1ccc(O)cc1</chem>
	enterolactone	1	1	1	0	<chem>Oc1cccc(C[C@H]2COC(=O)[C@@H]2Cc3cccc(O)c3)c1</chem>
855-96-9	eupatorin	0	1	0	1	<chem>COc1ccc(cc1O)C2=CC(=O)c3c(O)c(OC)c(OC)cc3O2</chem>
90297-42-0	2-tert-butyl-6-[(3-tert-butyl-2-hydroxy-5-methylphenyl)methyl]-4-methylphenol	0	1	0	1	<chem>Cc1cc(Cc2cc(C)cc(c2O)C(C)(C)C)c(O)c(c1)C(C)(C)C</chem>
2150-43-8	methyl 3,4-dihydroxybenzoate	0	1	0	1	<chem>COC(=O)c1ccc(O)c(O)c1</chem>
3943-89-3	ethyl 3,4-dihydroxybenzoate	0	1	0	1	<chem>CCOC(=O)c1ccc(O)c(O)c1</chem>
52441-13-1	ethyl gallate	0	1	0	1	<chem>CCOC(=O)c1cc(O)c(O)c(O)c1</chem>
2664-60-0	dodecyl 4-hydroxybenzoate	1	1	1	0	<chem>CCCCCCCCCCCCOC(=O)c1ccc(O)cc1</chem>
86-50-0	azinthos	0	1	0	1	<chem>COP(=S)(OC)SCN1N=Nc2ccccc2C1=O</chem>
150-68-5	monuron	0	1	0	1	<chem>CN(C)C(=O)Nc1ccc(Cl)cc1</chem>
1689-83-4	ioxynil	0	1	0	1	<chem>Oc1c(I)cc(cc1I)C#N</chem>

1689-84-5	bromoxynil	0	1	0	1	<chem>Oc1c(Br)cc(cc1Br)C#N</chem>
	triphenyltin hydroxide	1	1	1	0	<chem>O[Sn](c1ccccc1)(c2ccccc2)c3ccccc3</chem>
	4-[1-(4-hydroxyphenyl)-1-phenylethyl]phenol	1	1	1	0	<chem>CC(c1ccccc1)(c2ccc(O)cc2)c3ccc(O)cc3</chem>
	4-(2-{4-[2-(4-hydroxyphenyl)propan-2-yl]phenyl}propan-2-yl)phenol	1	1	1	0	<chem>CC(C)(c1ccc(O)cc1)c2ccc(cc2)C(C)(C)c3ccc(O)cc3</chem>
	penconazole	0	1	0	1	<chem>CCCC(Cn1cncn1)c2ccc(Cl)cc2Cl</chem>
66230-04-4	(R)-cyano(3-phenoxyphenyl)methyl (2R)-2-(4-chlorophenyl)-3-methylbutanoate	0	1	0	1	<chem>CC(C)[C@@H](C(=O)O[C@@H](C#N)c1ccc(Oc2ccccc2)c1)c3ccc(Cl)cc3</chem>
7488-70-2	levothyroxine	0	1	0	1	<chem>N[C@@H](Cc1cc(I)c(Oc2cc(I)c(O)c(I)c2)c(I)c1)C(=O)O</chem>
136-77-6	oxana	0	1	0	1	<chem>CCCCCCC1ccc(O)cc1O</chem>
	(1S,10S,11S,14S,15S,17S)-15-methyl-17-[9-(4,4,5,5,5-pentafluoropentanesulfinyl)nonyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	<chem>C[C@]12C[C@H](CCCCCCCCC[S+])([O-])CCCC(F)(F)C(F)(F)F[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O</chem>
	(1S,10S,11S,14S,15S,17S)-15-methyl-17-[4,4,5,5,6,6,7,7-octafluoro-9-(4,4,5,5,5-pentafluoropentanesulfinyl)nonyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	<chem>C[C@]12C[C@H](CCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)CC[S+])([O-])CCCC(F)(F)C(F)(F)F[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O</chem>

	adeca-2(7),3,5-triene-5,14-diol					
5613-46-7	4-[2-(4-hydroxy-3,5-dimethylphenyl)propan-2-yl]-2,6-dimethylphenol	1	1	1	0	<chem>Cc1cc(cc(C)c1O)C(C)(C)c2cc(C)c(O)c(C)c2</chem>
1096-84-0	squoxin	1	1	1	0	<chem>Oc1ccc2ccccc2c1Cc3c(O)ccc4ccccc34</chem>
88-58-4	2,5-di-tert-butylhydroquinone	0	1	0	1	<chem>CC(C)(C)c1cc(O)c(cc1O)C(C)(C)C</chem>
120-78-5	MBTS	1	1	1	0	<chem>S(Sc1nc2ccccc2s1)c3nc4ccccc4s3</chem>
	difenoconazole	0	1	0	1	<chem>CC1COC(Cn2cncn2)(O1)c3ccc(Oc4ccc(Cl)cc4)cc3Cl</chem>
29752-43-0	(2S,3S,4aS)-2,3,7-trihydroxy-9-methoxy-4a-methyl-2H,3H,4H-benzo[c]chromen-6-one	0	1	0	1	<chem>COc1cc(O)c2C(=O)O[C@@]3(C)C[C@H](O)[C@@H](O)C=C3c2c1</chem>
298-02-2	rampart	0	1	0	1	<chem>CCOP(=S)(OCC)SCSCC</chem>
2540-82-1	formothion	0	1	0	1	<chem>COP(=S)(OC)SCC(=O)N(C)C=O</chem>
631-64-1	acetic acid, dibromo-	0	1	0	1	<chem>OC(=O)C(Br)Br</chem>
	(1R,10S)-8-oxatetracyclo[8.7.0.0{2,7}.0{12,17}]heptadeca-2,4,6,12(17),13,15-hexaene-5,6,10,14,15-pentol	1	1	1	0	<chem>Oc1cc2C[C@@]3(O)COc4c(O)c(O)ccc4[C@H]3c2cc1O</chem>
6259-76-3	hexyl 2-hydroxybenzoate	0	1	0	1	<chem>CCCCCOC(=O)c1ccccc1O</chem>

2417-04-1	4-(4-hydroxy-3,5-dimethylphenyl)-2,6-dimethylphenol	1	1	1	0	<chem>Cc1cc(cc(C)c1O)c2cc(C)c(O)c(C)c2</chem>
434-64-0	octafluorotoluene	0	1	0	1	<chem>Fc1c(F)c(F)c(c(F)c1F)C(F)(F)F</chem>
67747-09-5	prochloraz	0	1	0	1	<chem>CCCN(CCOc1c(Cl)cc(Cl)cc1Cl)C(=O)n2ccnc2</chem>
1816-85-9	(1S,2R,10S,11S,14S,15S,17S)-14,17-dihydroxy-2,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-5-one	0	1	0	1	<chem>C[C@]12C[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
1045-69-8	testosterone, acetate	0	1	0	1	<chem>CC(=O)O[C@H]1CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>
641-38-3	alternariol	1	1	1	0	<chem>Cc1cc(O)cc2OC(=O)c3c(O)cc(O)cc3c12</chem>
13609-67-1	hydrocortisone 17-butyrate	0	1	0	1	<chem>CCCC(=O)O[C@@]1(CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3[C@@H](O)C[C@]12C)C(=O)CO</chem>
81-23-2	dehydrocholic	0	1	0	1	<chem>C[C@H](CCC(=O)O)[C@H]1CC[C@H]2[C@H]3[C@H](CC(=O)[C@]12C)[C@@]4(C)CCC(=O)C[C@H]4CC3=O</chem>
27987-13-9	benzyl chloride	0	1	0	1	<chem>ClCc1ccccc1</chem>
	isoxsuprine hydrochloride	0	1	0	1	<chem>Cl.CC(COc1ccccc1)NC(C)C(O)c2ccc(O)cc2</chem>
	(3S,4R)-3-phenyl-4-(4-{[2-(pyrrolidin-1-yl)ethyl]sulfanyl}phenyl)-3,4-dihydro-2H-1-benzopyran-7-ol	1	1	1	0	<chem>Cl.Oc1ccc2[C@H]([C@H](COc2c1)c3ccccc3)c4ccc(SCCN5CCC5)cc4</chem>

	hydrochloride					
	ethyl 4-[(3R,4S)-4-(4-hydroxyphenyl)hexan-3-yl]benzenecarboximate hydrochloride	1	1	1	0	Cl.CCOC(=N)c1ccc(cc1)[C@H](CC)[C@H](CC)c2ccc(O)cc2
	propiconazole	0	1	0	1	CCCC1COC(Cn2cncn2)(O1)c3ccc(Cl)cc3Cl
3604-87-3	14-(3,6-dihydroxy-6-methylheptan-2-yl)-4,5,11-trihydroxy-2,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-9-en-8-one	0	1	0	1	C[C@@H]([C@H](O)CCC(C)(C)O)[C@@H]1CC[C@@]2(O)C3=CC(=O)[C@H]4C[C@H](O)[C@@H](O)C[C@]4(C)[C@H]3CC[C@@]12C
	2-(2,4-dihydroxyphenyl)-4-hydroxy-5-(2-hydroxy-3-methylbut-3-en-1-yl)-6-methoxy-1-benzofuran-3-carbaldehyde	1	1	1	0	COc1cc2oc(c(C=O)c2c(O)c1CC(O)C(=C)C)c3ccc(O)cc3O
	4-hydroxy-2-(4-hydroxy-2-methoxyphenyl)-6-methoxy-5-(3-methylbut-2-en-1-yl)-1-benzofuran-3-carbaldehyde	1	1	1	0	COc1cc2oc(c(C=O)c2c(O)c1CC=C(C)C)c3ccc(O)cc3OC
	2-(2,4-dihydroxyphenyl)-4-hydroxy-6-methoxy-5-(3-methylbut-2-en-1-yl)-1-benzofuran-3-carbaldehyde	1	1	1	0	COc1cc2oc(c(C=O)c2c(O)c1CC=C(C)C)c3ccc(O)cc3O
	2-(2,4-dihydroxyphenyl)-4-hydroxy-5-(3-hydroxy-3-methylbutyl)-6-methoxy-1-benzofuran-3-	1	1	1	0	COc1cc2oc(c(C=O)c2c(O)c1CCC(C)(C)O)c3ccc(O)cc3O

	carbaldehyde					
	4,6-dihydroxy-2-(4-hydroxy-2-methoxyphenyl)-5-(2-hydroxy-3-methylbut-3-en-1-yl)-1-benzofuran-3-carbaldehyde	1	1	1	0	<chem>COc1cc(O)ccc1c2oc3cc(O)c(CC(O)C(=C)C)c(O)c3c2C=O</chem>
	4-hydroxy-2-(4-hydroxy-2-methoxyphenyl)-5-(3-hydroxy-3-methylbutyl)-6-methoxy-1-benzofuran-3-carbaldehyde	1	1	1	0	<chem>COc1cc2oc(c(C=O)c2c(O)c1CCC(C)(C)O)c3ccc(O)cc3OC</chem>
2545-08-6	α -catechin	1	1	1	0	<chem>O[C@@H]1Cc2c(O)cc(O)cc2O[C@@H]1c3ccc(O)c(O)c3</chem>
97-74-5	monex	1	1	1	0	<chem>CN(C)C(=S)SC(=S)N(C)C</chem>
119739-80-9	chlorferone	0	1	0	1	<chem>CC1=C(Cl)C(=O)Oc2cc(O)ccc12</chem>
101-53-1	benzophenol	1	1	1	0	<chem>Oc1ccc(Cc2ccccc2)cc1</chem>
19471-12-6	3-[(3-aminophenyl)methyl]aniline	0	1	0	1	<chem>Nc1cccc(Cc2cccc(N)c2)c1</chem>
5384-21-4	4-[(4-hydroxy-3,5-dimethylphenyl)methyl]-2,6-dimethylphenol	1	1	1	0	<chem>Cc1cc(Cc2cc(C)c(O)c(C)c2)cc(C)c1O</chem>
	(5-benzylfuran-3-yl)methyl (1S,3S)-2,2-dimethyl-3-(2-methylprop-1-en-1-yl)cyclopropane-1-carboxylate	0	1	0	1	<chem>CC(=C[C@H]1[C@H](C(=O)OCc2coc(Cc3ccccc3)c2)C1(C)C)C</chem>

	14-hydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-3,6-dien-5-one pentamethylcyclopentadiene ruthenium	1	1	1	0	[Ru].CC1C(=C(C)C(=C1C)C)C.C[C@]23CCC4C(CCC5=CC(=O)C=CC45)C2CC[C@@H]3O
37350-34-8	citral	0	1	0	1	CC(=CCC\C=C\C=O)\C)C
	(4aS,4bR,10bS,12aS)-9-chloro-8-hydroxy-12a-methyl-2,3,4,4a,4b,5,6,10b,11,12-decahydrochrysen-1-one	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)c(Cl)cc34)[C@@H]1CCCC2=O
	(4aS,4bR,10bS,12aS)-8-hydroxy-9-methoxy-12a-methyl-2,3,4,4a,4b,5,6,10b,11,12-decahydrochrysen-1-one	1	1	1	0	COc1cc2[C@H]3CC[C@@]4(C)[C@H](CCCC4=O)[C@@H]3CCc2cc1O
	tin-san	1	1	1	0	CCCC[Sn](Cl)(CCCC)CCCC
56718-71-9	4-(2-methoxyethyl)phenol	0	1	0	1	COCCc1ccc(O)cc1
38350-87-7	4-heptylbenzoic acid	0	1	0	1	CCCCCCCc1ccc(cc1)C(=O)O
501-97-3	hydroxyphenyl propionic acid	0	1	0	1	OC(=O)CCc1ccc(O)cc1
11111-10-7	everone	0	1	0	1	CCCCCCC(=O)O[C@H]1CC[C@H]2[C@@H]3CCCC4=CC(=O)C[C@]4(C)[C@H]3CC[C@]12C
	dobutamine hydrochloride	1	1	1	0	Cl.CC(CCC1ccc(O)cc1)NCCc2ccc(O)c(O)c2

	β-HC	0	1	0	1	<chem>CCCCC(=O)O[C@@]1(CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3[C@@H](O)C[C@]12C)C(=O)CO</chem>
434-07-1	anadrol	1	1	1	0	<chem>C[C@]1(O)CC[C@H]2[C@@H]3CC[C@H]4CC(=O)\C(=C/O)\C[C@]4(C)[C@H]3CC[C@]12C</chem>
	procaine hydrochloride	0	1	0	1	<chem>Cl.CCN(CC)CCOC(=O)c1ccc(N)cc1</chem>
3093-35-4	halog	0	1	0	1	<chem>CC1(C)O[C@@H]2C[C@H]3[C@@H]4CCC5=CC(=O)CC[C@]5(C)[C@@]4(F)[C@@H](O)C[C@]3(C)[C@@]2(O1)C(=O)CCl</chem>
1524-88-5	flurandrenolide	0	1	0	1	<chem>CC1(C)O[C@@H]2C[C@H]3[C@@H]4C[C@H](F)C5=CC(=O)CC[C@]5(C)[C@H]4[C@@H](O)C[C@]3(C)[C@@]2(O1)C(=O)CO</chem>
	4-[(1R,2S)-1-hydroxy-2-{[2-(4-hydroxyphenyl)ethyl]amino}propyl]phenol hydrochloride	0	1	0	1	<chem>Cl.C[C@H](NCCC1ccc(O)cc1)[C@H](O)c2ccc(O)cc2</chem>
152-43-2	quinnestrol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(OC5CCCC5)ccc34)[C@@H]1CC[C@@]2(O)C#C</chem>
	(2S)-2-[(2S)-2-amino-3-hydroxypropanamido]-3-(4-hydroxyphenyl)propanoic acid	0	1	0	1	<chem>N[C@@H](CO)C(=O)N[C@@H](Cc1ccc(O)cc1)C(=O)O</chem>
7698-93-3	4-[[[(1S,10R,11S,14S,15S)-5-hydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]]heptadeca-2(7),3,5-trien-14-yl]oxy]-4-oxobutanoic acid	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2OC(=O)CCC(=O)O</chem>

608-71-9	pentabromophenol	0	1	0	1	<chem>Oc1c(Br)c(Br)c(Br)c(Br)c1Br</chem>
491-45-2	2-(3,5-dihydroxyphenyl)benzene-1,3,5-triol	0	1	0	1	<chem>Oc1cc(O)c(c(O)c1)c2cc(O)cc(O)c2</chem>
117-82-8	bis(methoxyethyl)phthalate	0	1	0	1	<chem>COCCOC(=O)c1cccc1C(=O)OCCOC</chem>
95-76-1	3,4-dichloroaniline	0	1	0	1	<chem>Nc1ccc(Cl)c(Cl)c1</chem>
1746-81-2	monolinuron	0	1	0	1	<chem>CON(C)C(=O)Nc1ccc(Cl)cc1</chem>
	phenothrin	0	1	0	1	<chem>CC(=CC1C(C(=O)OCc2cccc(Oc3ccccc3)c2)C1(C)C)C</chem>
131-17-9	diallylphthalate	0	1	0	1	<chem>C=CCOC(=O)c1cccc1C(=O)OCC=C</chem>
15950-66-0	2,3,4-trichlorophenol	0	1	0	1	<chem>Oc1ccc(Cl)c(Cl)c1Cl</chem>
79762-84-8	3-methylbutyl 4-(dimethylamino)benzoate	0	1	0	1	<chem>CC(C)CCOC(=O)c1ccc(cc1)N(C)C</chem>
33089-61-1	bipin	0	1	0	1	<chem>CN(\C=N\c1ccc(C)cc1C)\C=N\c2ccc(C)cc2C</chem>
	pararosaniline	1	1	1	0	<chem>Nc1ccc(cc1)C(=C2C=CC(=N)C=C2)c3ccc(N)cc3</chem>
	(10S)-5,6,10,15-tetrahydroxy-8-oxatetracyclo[8.7.0.0{2,7}.0{12,17}]heptadeca-1(17),2(7),3,5,12,15-hexaen-14-one	1	1	1	0	<chem>OC1=CC2=C3c4ccc(O)c(O)c4OC[C@]3(O)CC2=CC1=O</chem>
92-66-0	4-bromobiphenyl	0	1	0	1	<chem>Brc1ccc(cc1)c2ccccc2</chem>
117-84-0	dioctyl phthalate	0	1	0	1	<chem>CCCCCCCCOC(=O)c1cccc1C(=O)OCCCCCCCC</chem>

	methyl[sulfanyl(carbonothioyl)]amine	0	1	0	1	CNC(=S)S
1889-71-0	1-(4-chlorophenyl)-2-phenylethanone	0	1	0	1	Clc1ccc(cc1)C(=O)Cc2ccccc2
42019-78-3	4-(4-chlorobenzoyl)phenol	1	1	1	0	Oc1ccc(cc1)C(=O)c2ccc(Cl)cc2
3144-54-5	2,4-dihydroxy pentyl ketone	1	1	1	0	CCCCC(=O)c1ccc(O)cc1O
596-27-0	3,3-bis(4-hydroxy-3-methylphenyl)-2-benzofuran-1-one	1	1	1	0	Cc1cc(ccc1O)C2(OC(=O)c3ccccc23)c4ccc(O)c(C)c4
94271-03-1	DETA	0	1	0	1	CCN(CC)C(=O)c1cccc(C)c1
933-75-5	2,3,6-trichlorophenol	0	1	0	1	Oc1c(Cl)ccc(Cl)c1Cl
18144-43-9	isopropyl 4-aminobenzoate	0	1	0	1	CC(C)OC(=O)c1ccc(N)cc1
	1-[(S)-(4-chlorophenyl)(phenyl)methyl]-4-methylpiperazine	0	1	0	1	CN1CCN(CC1)[C@@H](c2ccccc2)c3ccc(Cl)cc3
37693-01-9	clofoctol	0	1	0	1	CC(C)(C)CC(C)(C)c1ccc(O)c(Cc2ccc(Cl)cc2Cl)c1
732-11-6	percolate	0	1	0	1	COP(=S)(OC)SCN1C(=O)c2ccccc2C1=O
6088-51-3	ddd (analytical)	1	1	1	0	Oc1ccc2cc(SSc3ccc4cc(O)ccc4c3)ccc2c1
50-84-0	2,4-dichlorobenzoic acid	0	1	0	1	OC(=O)c1ccc(Cl)cc1Cl
52222-87-4	6-benzoylnaphthalen-2-ol	1	1	1	0	Oc1ccc2cc(ccc2c1)C(=O)c3ccccc3

530-44-9	4-benzoyl-N,N-dimethylaniline	0	1	0	1	<chem>CN(C)c1ccc(cc1)C(=O)c2ccccc2</chem>
123113-74-6	acetochlor	0	1	0	1	<chem>CCOCN(C(=O)CCl)c1c(C)cccc1CC</chem>
533-31-3	sesamol	0	1	0	1	<chem>Oc1ccc2OCOc2c1</chem>
80-06-8	dimite	0	1	0	1	<chem>CC(O)(c1ccc(Cl)cc1)c2ccc(Cl)cc2</chem>
92-91-1	4-acetyl biphenyl	0	1	0	1	<chem>CC(=O)c1ccc(cc1)c2ccccc2</chem>
130-80-3	4-[(3E)-4-[4-(propanoyloxy)phenyl]hex-3-en-3-yl]phenyl propanoate	1	1	1	0	<chem>CCC(=O)Oc1ccc(cc1)\C=C(/CC)\c2ccc(OC(=O)CC)cc2)\CC</chem>
77-47-4	hexachlorocyclopentadiene	1	1	1	0	<chem>ClC1=C(Cl)C(Cl)(Cl)C(=C1Cl)Cl</chem>
	21-deoxyhydrocortisone	0	1	0	1	<chem>CC(=O)[C@@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3[C@@H](O)C[C@]12C</chem>
342009-25-0	dimethylcarbamyl chloride	0	1	0	1	<chem>CN(C)C(=O)Cl</chem>
1929-82-4	nitrapyrin	0	1	0	1	<chem>Clc1cccc(n1)C(Cl)(Cl)Cl</chem>
25057-89-0	leader	0	1	0	1	<chem>CC(C)N1C(=O)c2ccccc2NS1(=O)=O</chem>
933-78-8	2,3,5-trichlorophenol	0	1	0	1	<chem>Oc1cc(Cl)cc(Cl)c1Cl</chem>
95-33-0	N-(1,3-benzothiazol-2-ylsulfanyl)cyclohexanamine	1	1	1	0	<chem>C1CCC(CC1)NSc2nc3ccccc3s2</chem>

62229-77-0	deltamethrin	0	1	0	1	<chem>CC1(C)[C@@H](C=C(Br)Br)[C@H]1C(=O)O[C@H](C#N)c2cc cc(Oc3ccccc3)c2</chem>
108-45-2	developer C	0	1	0	1	<chem>Nc1cccc(N)c1</chem>
131-54-4	2-(2-hydroxy-4-methoxybenzoyl)-5-methoxyphenol	0	1	0	1	<chem>COc1ccc(C(=O)c2ccc(OC)cc2O)c(O)c1</chem>
2524-37-0	ethyl 2,4-dihydroxy-6-methylbenzoate	1	1	1	0	<chem>CCOC(=O)c1c(C)cc(O)cc1O</chem>
	β -estradiol 17-acetate	1	1	1	0	<chem>CC(=O)O[C@H]1CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@H]3 CC[C@]12C</chem>
101-61-1	tetra-base	0	1	0	1	<chem>CN(C)c1ccc(Cc2ccc(cc2)N(C)C)cc1</chem>
	(E)-N-{{4-(dimethylamino)phenyl}imino}sulfamic acid	0	1	0	1	<chem>CN(C)c1ccc(cc1)N=NS(=O)(=O)O</chem>
2764-72-9	7 <i>S</i> {5},10 <i>S</i> {5}-diazatricyclo[8.4.0.0{2,7}]tetradeca-1(10),2(7),3,5,11,13-hexaene-7,10-bis(ylum)	0	1	0	1	<chem>C1C[n+]2ccccc2c3cccc[n+]13</chem>
	(1 <i>S</i> ,10 <i>R</i> ,11 <i>S</i> ,13 <i>R</i> ,14 <i>S</i> ,15 <i>S</i>)-13-bromo-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1C[C @@H](Br)[C@H]2O</chem>

	(1S,10R,11S,13R,14S,15S)-13-chloro-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1C[C@@H](Cl)[C@H]2O</chem>
	(1S,10R,11S,13R,15S)-13-bromo-5-methoxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-one	1	1	1	0	<chem>COc1ccc2[C@H]3CC[C@@]4(C)[C@@H](C[C@@H](Br)C4=O)[C@@H]3CCc2c1</chem>
	(1S,10R,11S,13S,14R,15S)-13-iodo-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1C[C@H](I)[C@@H]2O</chem>
101021-11-8	(1S,10R,11S,14S,15S)-4-fluoro-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)c(F)cc34)[C@@H]1C[C@@H]2O</chem>
	(1S,10R,11S,14S,15S)-6-fluoro-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4c(F)c(O)ccc34)[C@@H]1C[C@@H]2O</chem>
62633-99-2	(1S,10R,11S,13S,14S,15S)-13-ethyl-15-methyltetracyclo[8.7.0.0{2,7}.0{11,	1	1	1	0	<chem>CC[C@H]1C[C@H]2[C@@H]3CCc4cc(O)ccc4[C@H]3CC[C@]2(C)[C@H]1O</chem>

	15]]heptadeca-2(7),3,5-triene-5,14-diol					
	(1S,2R,11S,14S,15R,16R)-14-methylpentacyclo[14.2.1.0{1,14}.0{2,11}.0{5,10}]nonadeca-5(10),6,8-triene-7,15-diol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@]15CC[C@H](C5)[C@H]2O
	10-[(1S,10S,11S,14S,15S,17S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-17-yl]decyl 4-methylbenzenesulfonate	1	1	1	0	Cc1ccc(cc1)S(=O)(=O)OCCCCCCCCC[C@H]2C[C@]3(C)[C@@H](O)CC[C@H]3[C@@H]4CCc5cc(O)ccc5[C@@H]24
	2-bromo-N-{2-[(1S,10S,11S,14S,15S,17R)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-17-yl]ethyl}acetamide	1	1	1	0	C[C@]12C[C@H](CCNC(=O)CBr)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@H]2O
	N-{3-[(1S,10R,11S,14R,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-yl]propyl}acetamide	1	1	1	0	CC(=O)NCCC[C@]1(O)CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@H]3CC[C@]12C
	(1S,9R,10R,11S,14S,15S)-9-[6-({4-[(4-{4-[bis(2-chloroethyl)amino]phenyl}butyl)am	1	1	1	0	C[C@]12CC[C@H]3[C@@H]([C@H](CCCCCNCCCCNCCCCc4ccc(cc4)N(CCCl)CCCl)Cc5cc(O)ccc35)[C@@H]1CC[C@@H]2O

	ino]butyl}amino)hexyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-2(7),3,5-triene-5,14-diol					
	(2R,2'S,3R,3'R,4R,4'R,5S,5'S,6S,6'S)-2'-[(1S,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-2,4,6-trien-14-yl]-2,3,4,5,6-pentamethyl-1-ruthena-1,1'-spirobi[pentacyclo[2.2.0.0{1,3}.0{1,5}.0{2,6}}hexan]-1-ylum triflate	0	1	0	1	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)[C@@]56[C@H]7[C@H]8[C@H]9[C@@H]5[Ru+][6789%10%11%12%13[C@@]%14(C)[C@]%10(C)[C@]%11(C)[C@]%12(C)[C@@]%13%14C.[O-]S(=O)(=O)C(F)(F)F
	(1S,10R,11S,14S,15S)-15-methyl-14-(2-phenylethynyl)tetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)C#Cc5ccccc5
	(1S,10R,11S,14S,15S)-6-(2-aminoethyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4c(CCN)c(O)ccc34)[C@@H]1CC[C@@H]2O

2-({6-[(1S,9R,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-9-yl]hexyl}amino)ethyl N-(3-{4-[bis(2-chloroethyl)amino]phenyl}propyl)carbamate	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H]([C@H](CCCCCNCCOC(=O)NC CCc4ccc(cc4)N(CCCl)CCl)Cc5cc(O)ccc35)[C@@H]1CC[C@H]2O</chem>
4-(4-{4-[bis(2-chloroethyl)amino]phenyl}butanamide)-N-{6-[(1S,9R,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-9-yl]hexyl}butanamide	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H]([C@H](CCCCCNC(=O)CCCNC(=O)CCc4ccc(cc4)N(CCCl)CCl)Cc5cc(O)ccc35)[C@@H]1CC[C@@H]2O</chem>
(Z)-1-(3-{4-[bis(2-chloroethyl)amino]phenyl}propyl)-2-{6-[(1S,9R,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-9-yl]hexyl}guanidine	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H]([C@H](CCCCC\\N=C(\\N)/NC CCc4ccc(cc4)N(CCCl)CCl)Cc5cc(O)ccc35)[C@@H]1CC[C@@H]2O</chem>
2-chloro-N-(2-{4-[(1R,10S,11S,14S,15S,17S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-17-	1	1	1	0	<chem>C[C@]12C[C@@H]([C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O)c5ccc(OCCNC(=O)CCl)cc5</chem>

	yl]phenoxy}ethyl)acetamide					
	2-bromo-N-(2-{4- [(1R,10S,11S,14S,15S,17S)-5,14- dihydroxy-15- methyltetracyclo[8.7.0.0{2,7}.0{11, 15}]heptadeca-2,4,6-trien-17- yl]phenoxy}ethyl)-N- methylacetamide	1	1	1	0	CN(CCOc1ccc(cc1)[C@H]2C[C@]3(C)[C@@H](O)CC[C@H]3 [C@@H]4CCc5cc(O)ccc5[C@@H]24)C(=O)CBr
	2-chloro-N-(2-{4- [(1R,10S,11S,14S,15S,17S)-5,14- dihydroxy-15- methyltetracyclo[8.7.0.0{2,7}.0{11, 15}]heptadeca-2,4,6-trien-17- yl]phenoxy}ethyl)-N- methylacetamide	1	1	1	0	CN(CCOc1ccc(cc1)[C@H]2C[C@]3(C)[C@@H](O)CC[C@H]3 [C@@H]4CCc5cc(O)ccc5[C@@H]24)C(=O)CCl
	2-chloro-N-(3-{4- [(1R,10S,11S,14S,15S,17S)-5,14- dihydroxy-15- methyltetracyclo[8.7.0.0{2,7}.0{11, 15}]heptadeca-2,4,6-trien-17- yl]phenyl}prop-2-yn-1-yl)-N- methylacetamide	1	1	1	0	CN(CC#Cc1ccc(cc1)[C@H]2C[C@]3(C)[C@@H](O)CC[C@H] 3[C@@H]4CCc5cc(O)ccc5[C@@H]24)C(=O)CCl
	2-{4-[(1R,10S,11S,14S,15S,17S)- 5,14-dihydroxy-15- methyltetracyclo[8.7.0.0{2,7}.0{11,	1	1	1	0	C[C@]12C[C@@H]([C@H]3[C@@H](CCc4cc(O)ccc34)[C@ @H]1CC[C@@H]2O)c5ccc(OCCOS(=O)(=O)C)cc5

	15}}heptadeca-2,4,6-trien-17-yl]phenoxy}ethyl methanesulfonate					
	2-chloro-N-(3-{4-[(1R,10S,11S,14S,15S,17S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-2,4,6-trien-17-yl]phenyl}prop-2-yn-1-yl)acetamide	1	1	1	0	<chem>C[C@]12C[C@@H]([C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O)c5ccc(cc5)C#CCNC(=O)CCI</chem>
	(1R,10S,11S,14S,15S,17S)-17-[4-(2-iodoethoxy)phenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	<chem>C[C@]12C[C@@H]([C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O)c5ccc(OCCI)cc5</chem>
	(1S,10R,11S,13S,14R)-13-bromo-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	<chem>CC12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1C[C@H](Br)[C@@H]2O</chem>
	(1S,10R,11S,13S)-13-bromo-5-methoxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-2,4,6-trien-14-one	1	1	1	0	<chem>COc1ccc2[C@H]3CCC4(C)[C@@H](C[C@H](Br)C4=O)[C@@H]3CCc2c1</chem>
4091-75-2	(1S,10R,11S,13R,15S)-13-chloro-5-methoxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,	1	1	1	0	<chem>COc1ccc2[C@H]3CC[C@@]4(C)[C@@H](C[C@@H](Cl)C4=O)[C@@H]3CCc2c1</chem>

	15]]heptadeca-2,4,6-trien-14-one					
	(1S,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-2(7),3,5-triene-4-carbaldehyde	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)c(C=O)cc34)[C@@H]1CC[C@@H]2O
	(1S,2R,11S,14S,15S,16R)-14-methylpentacyclo[14.2.1.0{1,14}.0{2,11}.0{5,10}]nonadeca-5(10),6,8-triene-7,15-diol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@]15CC[C@H](C5)[C@@H]2O
	(1S,10S,11S,14S,15S,17S)-17-(but-3-en-1-yl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	C[C@]12C[C@H](CCC=C)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O
	2-[(1S,10S,11S,14S,15S,17R)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-2,4,6-trien-17-yl]ethyl methanesulfonate	1	1	1	0	C[C@]12C[C@H](CCOS(=O)(=O)C)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O
	2-[(1S,10R,11S,14R,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadeca-2,4,6-trien-14-yl]ethyl methanesulfonate	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)CCOS(=O)(=O)C

(1S,10S,11S,14S,15S,17S)-17-(4-bromobutyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	C[C@]12C[C@H](CCCCBr)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O
(1S,10R,11S,14S,15S)-14-{1-ferra-1,1'-spirobi[pentacyclo[2.2.0.0{1,3}.0{1,5}.0{2,6}]hexane]-6-yl}-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)C56C7C8C9C5[Fe]6789%10%11%12%13C%14C%10C%11C%12C%13%14
6-[(1S,9R,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-9-yl]hexyl N-(3-{4-[bis(2-chloroethyl)amino]phenyl}propyl)carbamate	1	1	1	0	C[C@]12CC[C@H]3[C@@H]([C@H](CCCCCOC(=O)NCCCCc4ccc(cc4)N(CCCl)CCCl)Cc5cc(O)ccc35)[C@@H]1CC[C@@H]2O
4-{4-[bis(2-chloroethyl)amino]phenyl}-N-{6-[(1S,9R,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-9-yl]hexyl}butanamide	1	1	1	0	C[C@]12CC[C@H]3[C@@H]([C@H](CCCCCNC(=O)CCCCc4cc(cc4)N(CCCl)CCCl)Cc5cc(O)ccc35)[C@@H]1CC[C@@H]2O

2-bromo-N-(5-{4-[(1R,10S,11S,14S,15S,17S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-17-yl]phenoxy}pentyl)-N-methylacetamide	1	1	1	0	CN(CCCCCOc1ccc(cc1)[C@H]2C[C@]3(C)[C@@H](O)CC[C@H]3[C@@H]4CCc5cc(O)ccc5[C@@H]24)C(=O)CBr
(1S,10R,11S,15S)-5-hydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-8,14-dione	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CC(=O)c4cc(O)ccc34)[C@@H]1CCC2=O
(1S,10S,11S,14R,15S,17S)-17-methoxy-15-methyl-14-[(E)-2-[3-(trifluoromethyl)phenyl]ethenyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	CO[C@H]1C[C@@]2(C)[C@@H](CC[C@@]2(O)\C=C\c3ccc(c3)C(F)(F)F)[C@@H]4CCc5cc(O)ccc5[C@@H]14
(1S,10R,11S,13S,14S,15S)-4,13,15-trimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	C[C@H]1C[C@H]2[C@@H]3CCc4cc(O)c(C)cc4[C@H]3CC[C@]2(C)[C@H]1O
(4-{[(1S,10R,11S,14R,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-14-yl]methyl}phenyl)chromiumtricarba	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)Cc5ccc(cc5)[Cr](C=O)(C=O)C=O

	Idehyde					
	rhodium(2+) ion (1S,10R,11S,14S,15S)-5-(2-hydroxyethoxy)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-14-ol pentamethylcyclopentadiene ditetrafluoroborate	1	1	1	0	[Rh+2].CC1C(=C(C)C(=C1C)C)C.C[C@]23CC[C@H]4[C@@H](CCc5cc(OCCO)ccc45)[C@@H]2CC[C@H]3O.F[B-](F)(F)F.F[B-](F)(F)F
	estradiol hexafluoro- $\text{S}l\{5\}$ -phosphanuide pentamethylcyclopentadiene ruthenium	1	1	1	0	[Ru].CC1C(=C(C)C(=C1C)C)C.C[C@]23CC[C@H]4[C@@H](CCc5cc(O)ccc45)[C@@H]2CC[C@H]3O.F[P-](F)(F)(F)(F)F
	(3-{2-[(1S,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-14-yl]ethynyl}phenyl)chromiumtricarbonyl aldehyde	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@]2(O)C#Cc5cccc(c5)[Cr](C=O)(C=O)C=O
	(1R,10S,11S,14S,15S,17S)-17-{4-[(5-iodopentyl)oxy]phenyl}-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-triene-5,14-diol	1	1	1	0	C[C@]12C[C@@H]([C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O)c5ccc(OCCCCCl)cc5

2-bromo-N-{4-[(1S,10S,11S,14S,15S,17S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-17-yl]butyl}acetamide	1	1	1	0	C[C@]12C[C@H](CCCCNC(=O)CBr)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O
(1S,9R,10R,11S,14S,15S)-9-{6-[(4-{4-[bis(2-chloroethyl)amino]phenyl}butyl)amino]hexyl}-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	C[C@]12CC[C@H]3[C@@H]([C@H](CCCCCNCCCCc4ccc(cc4)N(CCCl)CCl)Cc5cc(O)ccc35)[C@@H]1CC[C@@H]2O
4-[(1S,10S,11S,14S,15S,17S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-17-yl]butyl methanesulfonate	1	1	1	0	C[C@]12C[C@H](CCCCOS(=O)(=O)C)[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O
(Z)-1-(3-{4-[bis(2-chloroethyl)amino]phenyl}propyl)-2-[2-({6-[(1S,9R,10R,11S,14S,15S)-5,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-9-yl]hexyl)amino)ethyl]guanidine	1	1	1	0	C[C@]12CC[C@H]3[C@@H]([C@H](CCCCCNCC\N=C(\N)/NCCCc4ccc(cc4)N(CCCl)CCl)Cc5cc(O)ccc35)[C@@H]1CC[C@@H]2O

	rhodium(2+) ion estradiol pentamethylcyclopentadiene ditriflate	1	1	1	0	[Rh+2].CC1C(=C(C)C(=C1C)C)C.C[C@]23CC[C@H]4[C@@H](CCc5cc(O)ccc45)[C@@H]2CC[C@@H]3O.[O-]S(=O)(=O)C(F)(F)F.[O-]S(=O)(=O)C(F)(F)F
	2-bromo-N-(5-{4-[(1R,10S,11S,14S,15S,17S)-5,14-dihydroxy-15-methyltetraacyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-17-yl]phenoxy}pentyl)acetamide	1	1	1	0	C[C@]12C[C@@H]([C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1CC[C@@H]2O)c5ccc(OCCCCCNC(=O)CBr)cc5
65195-55-3	avermectin B1a	0	1	0	1	CC[C@H](C)[C@H]1O[C@@]2(C[C@@H]3C[C@@H](C\C=C(/C)\[C@@H](O[C@H]4C[C@H](OC)[C@@H](O[C@H]5C[C@H](OC)[C@@H](O)[C@H](C)O5)[C@H](C)O4)[C@@H](C)\C=C\C=C\6/CO[C@@H]7[C@H](O)C(=C[C@@H](C(=O)O3)[C@]67O)C)O2)C=C[C@@H]1C
25913-05-7	4-(4-fluorobenzoyl)phenol	1	1	1	0	Oc1ccc(cc1)C(=O)c2ccc(F)cc2
1702-17-6	clopyralid	0	1	0	1	OC(=O)c1nc(Cl)ccc1Cl
14548-48-2	4-(4-chlorobenzoyl)pyridine	0	1	0	1	Clc1ccc(cc1)C(=O)c2ccncc2
113-38-2	β -estradiol dipropionate	1	1	1	0	CCC(=O)O[C@H]1CC[C@H]2[C@@H]3CCc4cc(OC(=O)CC)cc4[C@H]3CC[C@]12C
4956-37-0	estradiol enanthate	1	1	1	0	CCCCCCC(=O)O[C@H]1CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@H]3CC[C@]12C
84-62-8	diphenyl phthalate	0	1	0	1	O=C(Oc1ccccc1)c2ccccc2C(=O)Oc3ccccc3

	3-acetyl-4-hydroxy-6-methylpyran-2-one	0	1	0	1	<chem>CC(=O)C1=C(O)C=C(C)OC1=O</chem>
24758-49-4	4-(4-benzoylphenyl)morpholine	0	1	0	1	<chem>O=C(c1ccccc1)c2ccc(cc2)N3CCOCC3</chem>
	(1S,10R,11S,15S)-5,6-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2,4,6-trien-14-one	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4c(O)c(O)ccc34)[C@@H]1CCC2=O</chem>
5817-39-0	reverse triiodothyronine	0	1	0	1	<chem>N[C@@H](Cc1ccc(Oc2cc(I)c(O)c(I)c2)c(I)c1)C(=O)O</chem>
118-82-1	ionox 220	0	1	0	1	<chem>CC(C)(C)c1cc(Cc2cc(c(O)c(c2)C(C)(C)C(C)(C)C(C)(C)cc(c1O)C(C)(C)C</chem>
978-86-9	4-(triphenylmethyl)phenol	0	1	0	1	<chem>Oc1ccc(cc1)C(c2ccccc2)(c3ccccc3)c4ccccc4</chem>
26249-12-7	1,2-dibromobenzene	0	1	0	1	<chem>BrC1CCCCC1Br</chem>
349-58-6	3,5-bis(trifluoromethyl)phenol	0	1	0	1	<chem>Oc1cc(cc(c1)C(F)(F)F)C(F)(F)F</chem>
769-92-6	4-tert-butylaniline	0	1	0	1	<chem>CC(C)(C)c1ccc(N)cc1</chem>
85-29-0	(2-chlorophenyl)(4-chlorophenyl)methanone	0	1	0	1	<chem>Clc1ccc(cc1)C(=O)c2ccccc2Cl</chem>
33228-44-3	benzenamine, 4-pentyl-	0	1	0	1	<chem>CCCCCc1ccc(N)cc1</chem>
	rimsulfuron	0	1	0	1	<chem>CCS(=O)(=O)c1cccnc1S(=O)(=O)NC(=O)Nc2nc(OC)cc(OC)n2</chem>
90-98-2	4,4'-dichlorobenzophenone	0	1	0	1	<chem>Clc1ccc(cc1)C(=O)c2ccc(Cl)cc2</chem>
13608-87-2	1-(2,3,4-trichlorophenyl)ethanone	0	1	0	1	<chem>CC(=O)c1ccc(Cl)c(Cl)c1Cl</chem>

120-61-6	dimethyl terephthalate	0	1	0	1	<chem>COC(=O)c1ccc(cc1)C(=O)OC</chem>
299-84-3	ronnel	1	1	1	0	<chem>COP(=S)(OC)Oc1cc(Cl)c(Cl)cc1Cl</chem>
	selectin	0	1	0	1	<chem>CSc1nc(NC(C)C)nc(NC(C)C)n1</chem>
	stannane,(benzoyloxy)tributyl	1	1	1	0	<chem>CCCC[Sn](CCCC)(CCCC)OC(=O)c1ccccc1</chem>
133-07-3	folpet	1	1	1	0	<chem>ClC(Cl)(Cl)SN1C(=O)c2ccccc2C1=O</chem>
120-95-6	2,4-di-t-pentylphenol	0	1	0	1	<chem>CCC(C)(C)c1ccc(O)c(c1)C(C)(C)CC</chem>
94-82-6	butyrac	0	1	0	1	<chem>OC(=O)CCCOc1ccc(Cl)cc1Cl</chem>
84087-01-4	quinclorac	0	1	0	1	<chem>OC(=O)c1c(Cl)ccc2cc(Cl)cnc12</chem>
37331-41-2	savall	0	1	0	1	<chem>CCOP(=S)(OCC)Oc1cnc2ccccc2n1</chem>
2050-47-7	benzene, 1,1'-oxybis 4-bromo-	0	1	0	1	<chem>BrC1ccc(Oc2ccc(Br)cc2)cc1</chem>
919-86-8	DSM	0	1	0	1	<chem>CCSCCSP(=O)(OC)OC</chem>
3669-41-8	1-(2,4-dihydroxyphenyl)-2-phenylethanone	1	1	1	0	<chem>Oc1ccc(C(=O)Cc2ccccc2)c(O)c1</chem>
26718-65-0	mevinphos (trans)	0	1	0	1	<chem>COC(=O)\C=C(/C)\OP(=O)(OC)OC</chem>
2491-32-9	1-(4-hydroxyphenyl)-2-phenylethanone	1	1	1	0	<chem>Oc1ccc(cc1)C(=O)Cc2ccccc2</chem>
1470-79-7	4-(4-hydroxybenzoyl)benzene-1,3-diol	1	1	1	0	<chem>Oc1ccc(cc1)C(=O)c2ccc(O)cc2O</chem>

	desethylatrazine	1	1	1	0	<chem>CC(C)Nc1nc(N)nc(Cl)n1</chem>
	(2S)-flavanone	0	1	0	1	<chem>O=C1C[C@H](Oc2cccc12)c1cccc1</chem>
136-83-4	nonylphenol	1	1	1	0	<chem>CCCCCCCCCc1cccc1O</chem>
6164-98-3	CDM	0	1	0	1	<chem>CN(C)\C=N\c1ccc(Cl)cc1C</chem>
1459-93-4	dimethyl isophthalate	0	1	0	1	<chem>COC(=O)c1cccc(c1)C(=O)OC</chem>
68648-92-0	dinonyl phthalate	0	1	0	1	<chem>CCCCCCCCCOC(=O)c1cccc1C(=O)OCCCCCCCCC</chem>
	2-[(2S)-butan-2-yl]-4,6-dinitrophenol	0	1	0	1	<chem>CC[C@H](C)c1cc(cc(c1O)[N+](=[O-])=O)[N+](=[O-])=O</chem>
51235-04-2	velpar	0	1	0	1	<chem>CN(C)c1nc(=O)n(C2CCCCC2)c(=O)n1C</chem>
	(R)-methoprene	0	1	0	1	<chem>COC(C)(C)CCC[C@@H](C)C\C=C\C(\C)=C\C(=O)OC(C)C</chem>
29082-74-4	octachlorostyrene	0	1	0	1	<chem>ClC(Cl)=C(Cl)c1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl</chem>
7005-72-3	4-chlorophenyl phenyl ether	0	1	0	1	<chem>Clc1ccc(Oc2ccccc2)cc1</chem>
	(1S)-4-oxo-3-(prop-2-en-1-yl)cyclopent-2-en-1-yl (1S,2R)-2-(2-methylprop-1-en-1-yl)cyclopropane-1-carboxylate	0	1	0	1	<chem>CC(C)=C[C@H]1C[C@@H]1C(=O)O[C@H]1CC(=O)C(CC=C)=C1</chem>
843-55-0	4-[1-(4-hydroxyphenyl)cyclohexyl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)C1(CCCCC1)c1ccc(O)cc1</chem>
1844-01-5	4-[(4-hydroxyphenyl)diphenylmethyl]phe	1	1	1	0	<chem>Oc1ccc(cc1)C(c1ccccc1)(c1ccccc1)c1ccc(O)cc1</chem>

	nol					
	4-(4-hydroxybenzoyl)benzene-1,2,3-triol	1	1	1	0	<chem>Oc1ccc(cc1)C(=O)c1ccc(O)c(O)c1O</chem>
787-70-2	4-(4-carboxyphenyl)benzoic acid	0	1	0	1	<chem>OC(=O)c1ccc(cc1)-c1ccc(cc1)C(O)=O</chem>
1518-83-8	4-cyclopentylphenol	1	1	1	0	<chem>Oc1ccc(cc1)C1CCCC1</chem>
72495-97-7	P-cyclohexylphenol	1	1	1	0	<chem>Oc1ccc(cc1)C1CCCCC1</chem>
1470-94-6	5-indanol	0	1	0	1	<chem>Oc1ccc2CCc2c1</chem>
632-51-9	tetraphenylethylene	1	1	1	0	<chem>c1ccc(cc1)C(=C(c1ccccc1)c1ccccc1)c1ccccc1</chem>
	(2S)-2-[4-(2-[4-[(2S)-oxiran-2-ylmethoxy]phenyl]propan-2-yl)phenoxy]methyl]oxirane	0	1	0	1	<chem>CC(C)(c1ccc(OC[C@@H]2CO2)cc1)c1ccc(OC[C@@H]2CO2)cc1</chem>
	16b-hydroxyestrone	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@@H]1C[C@H](O)C2=O</chem>
	1,6-bis(2S)-2-ethylhexyl hexanedioate	0	1	0	1	<chem>CCCC[C@H](CC)COC(=O)CCCCC(=O)OC[C@@H](CC)CCCC</chem>
34-74-2	monobutyl phthalate	0	1	0	1	<chem>CCCCOC(=O)c1ccccc1C(O)=O</chem>
	2-({[(2S)-2-ethylhexyl]oxy}carbonyl)benzoic acid	1	1	1	0	<chem>CCCC[C@H](CC)COC(=O)c1ccccc1C(O)=O</chem>
	(S)-(ethyl 4-nitrophenyl	0	1	0	1	<chem>CCO[P@](=S)(Oc1ccc(cc1)[N+])([O-])=O)c1ccccc1</chem>

	phenyl(sulfanylidene)phosphonite)					
564-35-2	11-ketotestosterone	0	1	0	1	<chem>C[C@]12CC(=O)[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>
	(1R,2R,4S,6R,7R,10S,11R)-6-acetyl-7,11-dimethyl-5-oxapentacyclo[8.8.0.0{2,7}.0{4,6}.0{11,16}]octadec-15-en-14-one	0	1	0	1	<chem>CC(=O)[C@]12O[C@H]1C[C@@H]1[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@@]21C</chem>
	(R)-(4-chlorophenyl)(phenyl)methanol	0	1	0	1	<chem>O[C@H](c1ccccc1)c1ccc(Cl)cc1</chem>
	2-[(1S,2S,10S,11R,14R,15R,17R)-17-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-14-yl]-2-oxoethyl propanoate	0	1	0	1	<chem>CCC(=O)OCC(=O)[C@@H]1CC[C@@H]2[C@@H]3CCC4=CC(=O)CC[C@@]4(C)[C@H]3[C@H](O)C[C@@]12C</chem>
	(1S,2R,10R,11R,14R,15R,17R)-1-fluoro-14,17-dihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-5-one	0	1	0	1	<chem>C[C@@]12C[C@@H](O)[C@]3(F)[C@H](CCC4=CC(=O)CC[C@@]34C)[C@H]1CC[C@]2(O)C(=O)CO</chem>
	(1S,2R,10S,11R,14R,15R)-14-[(1S)-1-hydroxyethyl]-2,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-5-one	0	1	0	1	<chem>C[C@H](O)[C@@H]1CC[C@@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@@]12C</chem>

(1S,2R,10R,11R,14R,15R)-14-hydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-5-one	0	1	0	1	<chem>C[C@@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@H]1CC[C@]2(O)C(=O)CO</chem>
(1R,2R,10S,11R,14S,15R)-2,15-dimethyl-5-oxotetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-14-yl 4-methylpentanoate	0	1	0	1	<chem>CC(C)CCC(=O)O[C@H]1CC[C@@H]2[C@H]3CCC4=CC(=O)CC[C@]4(C)[C@@H]3CC[C@@]12C</chem>
(1S,10R,11R,15R)-5-hydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5,8-tetraen-14-one	1	1	1	0	<chem>C[C@@]12CC[C@H]3[C@@H](C=Cc4cc(O)ccc34)[C@H]1CC[C2=O</chem>
(1R,2R,8R,10R,11R,14R,15R,17R)-14-acetyl-17-hydroxy-2,8,15-trimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-5-one	0	1	0	1	<chem>C[C@@H]1C[C@@H]2[C@H]3CC[C@@H](C(C)=O)[C@]3(C)C[C@@H](O)[C@H]2[C@@]2(C)CCC(=O)C=C12</chem>
(1S,10R,11R,14S,15R)-5-hydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-14-yl 3-cyclopentylpropanoate	1	1	1	0	<chem>C[C@@]12CC[C@H]3[C@@H](CCc4cc(O)ccc34)[C@H]1CC[C@@H]2OC(=O)CCC1CCCC1</chem>
(1R,2S,10R,11R,15R,17R)-17-hydroxy-2,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-5-one	0	1	0	1	<chem>C[C@@]12C[C@@H](O)[C@@H]3[C@H](CCC4=CC(=O)CC[C@@]34C)[C@H]1CCC2=O</chem>

	1,15]]heptadec-6-ene-5,14-dione					
	(1R,2S,10R,11R,15R)-2,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15]]heptadec-6-ene-5,14,17-trione	0	1	0	1	<chem>C[C@@]12CC(=O)[C@@H]3[C@H](CCC4=CC(=O)CC[C@@]34C)[C@H]1CCC2=O</chem>
	(1R,2R,10S,11R,14S,15R)-14-ethynyl-14-hydroxy-2,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15]]heptadec-6-en-5-one	0	1	0	1	<chem>C[C@@]12CC[C@@H]3[C@H](CCC4=CC(=O)CC[C@]34C)[C@H]1CC[C@]2(O)C#C</chem>
	2-[(1S,2S,10S,11R,14R,15R,17R)-17-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.0.0{2,7}.0{11,15]]heptadec-6-en-14-yl]-2-oxoethyl acetate	0	1	0	1	<chem>CC(=O)OCC(=O)[C@@H]1CC[C@@H]2[C@@H]3CCC4=CC(=O)CC[C@@]4(C)[C@H]3[C@H](O)C[C@@]12C</chem>
	2-[(1R,2S,10R,11R,14R,15R)-2,15-dimethyl-5,17-dioxotetracyclo[8.7.0.0{2,7}.0{11,15]]heptadec-6-en-14-yl]-2-oxoethyl acetate	0	1	0	1	<chem>CC(=O)OCC(=O)[C@@H]1CC[C@@H]2[C@H]3CCC4=CC(=O)CC[C@@]4(C)[C@@H]3C(=O)C[C@@]12C</chem>
	(1R,2S,10S,11R,15R)-2-(hydroxymethyl)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15]]heptadec-6-ene-5,14-dione	0	1	0	1	<chem>C[C@@]12CC[C@@H]3[C@H](CCC4=CC(=O)CC[C@]34CO)[C@H]1CCC2=O</chem>
	(1R,2S,10R,11R,14R,15R)-14-hydroxy-14-(2-hydroxyacetyl)-2,15-	0	1	0	1	<chem>C[C@@]12CC(=O)[C@@H]3[C@H](CCC4=CC(=O)CC[C@@]3</chem>

	dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-ene-5,17-dione					34C)[C@H]1CC[C@]2(O)C(=O)CO
	(1R,2S,5R,7S,10S,11R,15R)-5-hydroxy-2,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadecan-14-one	0	1	0	1	C[C@@]12CC[C@@H]3[C@H](CC[C@H]4C[C@H](O)CC[C@]34C)[C@H]1CCC2=O
	2-[(1S,2R,10S,11R,14R,15R)-2,15-dimethyl-5-oxotetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-14-yl]-2-oxoethyl acetate	0	1	0	1	CC(=O)OCC(=O)[C@@H]1CC[C@@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@@]12C
	(1S,2R,7R,10R,11R,14R,15R)-14-acetyl-2,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadecan-5-one	0	1	0	1	CC(=O)[C@@H]1CC[C@@H]2[C@@H]3CC[C@@H]4CC(=O)CC[C@@]4(C)[C@H]3CC[C@@]12C
	(1R,2R,8R,10S,11S,14R,15S)-8,14-dihydroxy-2,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-5-one	0	1	0	1	C[C@]12CC[C@@H]3[C@H](C[C@@H](O)C4=CC(=O)CC[C@]34C)[C@@H]1CC[C@H]2O
	(2R,3R)-1-[(1R,2R,8aR)-1-ethyl-8a-methyl-6-oxo-1,2,3,4,7,8-hexahydronaphthalen-2-yl]-2-methyl-4-oxopentan-3-yl hexanoate	0	1	0	1	CCCCC(=O)O[C@H]([C@H](C)C[C@H]1CCC2=CC(=O)CC[C@]2(C)[C@@H]1CC)C(C)=O

	(1S,2R,10S,11R,14R,15R)-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-5-one	0	1	0	1	<chem>C[C@@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@H]1CC[C@H]2C(=O)CO</chem>
	(1R)-1-[(2R,4aR,4bR,9R,10aR)-2,4b,9-trimethyl-7-oxo-3,4,4a,5,6,9,10,10a-octahydro-1H-phenanthren-2-yl]-2-oxopropyl acetate	0	1	0	1	<chem>C[C@@H]1C[C@@H]2C[C@@](C)(CC[C@H]2[C@@]2(C)CC(C(=O)C=C12)[C@@H](OC(C)=O)C(C)=O</chem>
	(1S,2S,10S,11R,14R,15R,17R)-14-acetyl-17-hydroxy-2,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-5-one	0	1	0	1	<chem>CC(=O)[C@@H]1CC[C@@H]2[C@@H]3CCC4=CC(=O)CC[C@@]4(C)[C@H]3[C@H](O)C[C@@]12C</chem>
	(1S,10R,11R,14S,15R)-5-hydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-14-yl pentanoate	1	1	1	0	<chem>CCCCC(=O)O[C@H]1CC[C@@H]2[C@@H]3CCc4cc(O)ccc4[C@H]3CC[C@@]12C</chem>
84-77-5	didecyl phthalate	0	1	0	1	<chem>CCCCCCCCCOC(=O)c1cccc1C(=O)OCCCCCCCCC</chem>
1482-70-8	5 α -androstane-3,11,17-trione	0	1	0	1	<chem>C[C@]12CC(=O)[C@H]3[C@@H](CC[C@H]4CC(=O)CC[C@]34C)[C@@H]1CCC2=O</chem>
	(2S,3R)-2-ethylhexane-1,3-diol	0	1	0	1	<chem>CCC[C@@H](O)[C@@H](CC)CO</chem>
	1-(chloromethyl)-4-[(E)-2-	0	1	0	1	<chem>ClCc1ccc(\C=C\c2ccccc2)cc1</chem>

	phenylethenyl]benzene					
	propylthiourea	0	1	0	1	CCCNC(N)=S
96-29-7	2-butanone oxime	0	1	0	1	CC\C(C)=N\O
	tri-N-butyltin fluoride	1	1	1	0	CCCC[Sn](F)(CCCC)CCCC
	chlorotripropyl stannane	1	1	1	0	CCC[Sn](Cl)(CCC)CCC
	omethoate	0	1	0	1	CNC(=O)CSP(=O)(OC)OC
63042-18-2	(1S,10R,11S,14S,15S)-14-(butanoyloxy)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-5-yl benzoate	0	1	0	1	CCCC(=O)O[C@H]1CC[C@H]2[C@@H]3CCc4cc(OC(=O)c5ccccc5)ccc4[C@H]3CC[C@]12C
41164-36-7	{[(1S,10R,11S,14S,15S)-14-hydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-5-yl]oxy}acetic acid	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(OCC(O)=O)ccc34)[C@@H]1CC[C@@H]2O
	{[(1S,10R,11S,13R,14R,15S)-13,14-dihydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-5-yl]oxy}acetic acid	1	1	1	0	C[C@]12CC[C@H]3[C@@H](CCc4cc(OCC(O)=O)ccc34)[C@@H]1C[C@@H](O)[C@@H]2O

3758-34-7	(1S,10R,11S,14S,15S)-5-hydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-14-yl propanoate	1	1	1	0	<chem>CCC(=O)O[C@H]1CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@H]3CC[C@]12C</chem>
	(1S,10R,11S,13R,14R,15S)-5-(benzyloxy)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-13,14-diol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(OCc5ccccc5)ccc34)[C@@H]1C[C@@H](O)[C@@H]2O</chem>
	(1S,10R,11S,13R,14R,15S)-14-(acetyloxy)-5-hydroxy-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-13-yl acetate	1	1	1	0	<chem>CC(=O)O[C@@H]1C[C@H]2[C@@H]3CCc4cc(O)ccc4[C@H]3CC[C@]2(C)[C@H]1OC(C)=O</chem>
	(1S,10R,11S,13R,14R,15S)-5,14-bis(acetyloxy)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-13-yl acetate	1	1	1	0	<chem>CC(=O)O[C@@H]1C[C@H]2[C@@H]3CCc4cc(OC(C)=O)ccc4[C@H]3CC[C@]2(C)[C@H]1OC(C)=O</chem>
	(1S,10R,11S,13R,14R,15S)-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-4,5,13,14-tetrol	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(O)c(O)cc34)[C@@H]1C[C@@H](O)[C@@H]2O</chem>
	([(1S,8Z,10R,11S,14S,15S)-5,14-dihydroxy-15-	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](C\C=C\N\OCC(O)=O)c4cc(O)ccc34)[C@@H]1CC[C@@H]2O</chem>

	methylnitratetetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-8-ylidene]amino}oxy)acetic acid					
	4-[[[(1S,10R,11S,15S)-15-methyl-14-oxotetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-trien-5-yl]oxy]-4-oxobutanoic acid	1	1	1	0	<chem>C[C@]12CC[C@H]3[C@@H](CCc4cc(OC(=O)CCC(O)=O)ccc34)[C@@H]1CCC2=O</chem>
	(4R)-4-[(1R,2S,7R,10S,11S,14R,15R)-2,15-dimethyl-5,9,16-trioxotetracyclo[8.7.0.0{2,7}.0{11,15}]heptadecan-14-yl]pentanoic acid	0	1	0	1	<chem>C[C@H](CCC(O)=O)[C@H]1CC[C@H]2[C@@H]3[C@@H](C(=O)[C@]12C)[C@@]1(C)CCC(=O)C[C@@H]1CC3=O</chem>
	(1S,2S,7S,10S,11S,14S,15S)-14-acetyl-2,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadecane-5,17-dione	0	1	0	1	<chem>CC(=O)[C@H]1CC[C@H]2[C@@H]3CC[C@H]4CC(=O)CC[C@]4(C)[C@H]3C(=O)C[C@]12C</chem>
	(1S,2R,10R,11S,14R,15S)-14-acetyl-2,15-dimethyl-5-oxotetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-14-yl acetate	0	1	0	1	<chem>CC(=O)O[C@@]1(CC[C@H]2[C@@H]3CCCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C)C(C)=O</chem>
	2-[(1R,2S,10S,11S,14R,15S)-1-fluoro-14-hydroxy-2,15-dimethyl-5,17-dioxotetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-14-yl]-2-oxoethyl	0	1	0	1	<chem>CC(=O)OCC(=O)[C@@]1(O)CC[C@H]2[C@@H]3CCCC4=CC(=O)CC[C@]4(C)[C@@]3(F)C(=O)C[C@]12C</chem>

	acetate					
	(1S,2R,10S,11S,14S,15R,17S)-14-{2-[(3-carboxypropanoyl)oxy]acetyl}-17-hydroxy-2-methyl-5-oxotetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-ene-15-carboxylic acid	0	1	0	1	<chem>C[C@]12CCC(=O)C=C1CC[C@H]1[C@@H]3CC[C@H](C(=O)COC(=O)CCC(O)=O)[C@]3(C[C@H](O)[C@H]21)C(O)=O</chem>
	(1S,2R,6S,7R,10R,11S,15S)-2,15-dimethyl-5,14-dioxotetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-3-en-6-yl acetate	0	1	0	1	<chem>CC(=O)O[C@H]1[C@@H]2CC[C@H]3[C@@H]4CCC(=O)[C@@]4(C)CC[C@@H]3[C@@]2(C)C=CC1=O</chem>
2268-98-6	(1S,2R,10S,11S,14S,15S,17R)-14-acetyl-2,15-dimethyl-5-oxotetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-17-yl acetate	0	1	0	1	<chem>CC(=O)O[C@@H]1C[C@@]2(C)[C@@H](CC[C@@H]2C(C)=O)[C@@H]2CCC3=CC(=O)CC[C@]3(C)[C@@H]12</chem>
10215-74-4	4-{2-[(1S,2R,10S,11S,14S,15S)-2,15-dimethyl-5-oxotetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-14-yl]-2-oxoethoxy}-4-oxobutanoic acid	0	1	0	1	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2C(=O)COC(=O)CCC(O)=O</chem>
	(1S,2R,10S,11S,14S,15S,17S)-17-hydroxy-2,15-dimethyl-14-(2-[[2S,3R,4S,5S,6R]-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)acetyl)tetracyclo[8.7.0.0{2,7}	0	1	0	1	<chem>C[C@]12C[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2C(=O)CO[C@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O</chem>

	.0{11,15}}heptadec-6-en-5-one					
1105-02-8	2-[(1S,2R,10S,11S,14S,15S,17S)-17-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-6-en-14-yl]-2-oxoethoxysulfonic acid	0	1	0	1	<chem>C[C@]12C[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2C(=O)COS(O)(=O)=O</chem>
	(1S,2R,8R,10S,11S,14R,15S)-8,14-dihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-6-ene-5,17-dione	0	1	0	1	<chem>C[C@]12CC(=O)[C@H]3[C@@H](C[C@@H](O)C4=CC(=O)CC[C@]34C)[C@@H]1CC[C@]2(O)C(=O)CO</chem>
	(1S,2R,10S,11S,13R,14S,15S)-14-acetyl-2,13,15-trimethyltetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-6-en-5-one	0	1	0	1	<chem>C[C@@H]1C[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1C(C)=O</chem>
1662-06-2	17 α ,20 β -dihydroxyprogesterone	0	1	0	1	<chem>C[C@@H](O)[C@@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>
	2-[(1S,2R,10R,11S,14R,15S)-14-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.0.0{2,7}.0{11,15}}heptadec-6-en-14-yl]-2-oxoethyl acetate	0	1	0	1	<chem>CC(=O)OCC(=O)[C@@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>
30330-56-4	testosterone glucuronide	0	1	0	1	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O[C@@H]1O[C@@H]([C@@H](O)[C@H]</chem>

						<chem>](O)[C@H]1O)C(O)=O</chem>
	(1S,2R,4R,10R,11S,14S,15S)-4,14-dihydroxy-2,15-dimethyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadec-6-en-5-one	0	1	0	1	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)[C@H](O)C[C@]34C)[C@@H]1CC[C@H]2O</chem>
	2-(adamantan-1-yl)-4-methylphenol	0	1	0	1	<chem>Cc1ccc(O)c(c1)C12CC3CC(CC(C3)C1)C2</chem>
3228-03-3	3-isopropyl-5-methylphenol	0	1	0	1	<chem>CC(C)c1cc(C)cc(O)c1</chem>
1879-09-0	2-tert-butyl-4,6-dimethylphenol	0	1	0	1	<chem>Cc1cc(C)c(O)c(c1)C(C)(C)C</chem>
	4-[(2R)-butan-2-yl]-2,6-di-tert-butylphenol	0	1	0	1	<chem>CC[C@@H](C)c1cc(c(O)c(c1)C(C)(C)C)C(C)(C)C</chem>
1083-27-8	hexyl P-hydroxybenzoate	1	1	1	0	<chem>CCCCCOC(=O)c1ccc(O)cc1</chem>
6521-29-5	pentyl 4-hydroxybenzoate	1	1	1	0	<chem>CCCCCOC(=O)c1ccc(O)cc1</chem>
4191-73-5	isopropyl 4-hydroxybenzoate	1	1	1	0	<chem>CC(C)OC(=O)c1ccc(O)cc1</chem>
6521-30-8	3-methylbutyl 4-hydroxybenzoate	1	1	1	0	<chem>CC(C)CCOC(=O)c1ccc(O)cc1</chem>
3780-50-5	4-(octyloxy)phenol	0	1	0	1	<chem>CCCCCCCCOc1ccc(O)cc1</chem>
18979-53-8	phenol, 4-(pentyloxy)-	1	1	1	0	<chem>CCCCCOc1ccc(O)cc1</chem>
24305-56-4	4-dodecylbenzene-1,3-diol	1	1	1	0	<chem>CCCCCCCCCCCCc1ccc(O)cc1O</chem>
2138-20-7	1,3-benzenediol, 4-cyclohexyl-	1	1	1	0	<chem>Oc1ccc(C2CCCCC2)c(O)c1</chem>

1138-60-9	isopropyl gallate	1	1	1	0	<chem>CC(C)OC(=O)c1cc(O)c(O)c(O)c1</chem>
84375-71-3	hexyl 4-hydroxy-3-methoxybenzoate	0	1	0	1	<chem>CCCCCOC(=O)c1ccc(O)c(OC)c1</chem>
7781-98-8	ethyl-3-hydroxybenzoate	0	1	0	1	<chem>CCOC(=O)c1cccc(O)c1</chem>
3337-59-5	methyl 3,5-dichloro-4-hydroxybenzoate	0	1	0	1	<chem>COC(=O)c1cc(Cl)c(O)c(Cl)c1</chem>
10210-17-0	4-(3-hydroxypropyl)phenol	1	1	1	0	<chem>OCCCC1ccc(O)cc1</chem>
	4-(4-hydroxyphenyl)cyclohexan-1-one	0	1	0	1	<chem>Oc1ccc(cc1)C1CCC(=O)CC1</chem>
17362-17-3	3-(4-hydroxyphenyl)propanenitrile	0	1	0	1	<chem>Oc1ccc(CCC#N)cc1</chem>
1124-04-5	2-chloro-4,5-dimethylphenol	0	1	0	1	<chem>Cc1cc(O)c(Cl)cc1C</chem>
7463-51-6	4-bromo-3,5-dimethylphenol	1	1	1	0	<chem>Cc1cc(O)cc(C)c1Br</chem>
576-55-6	2,3,4,5-tetrabromo-6-methylphenol	0	1	0	1	<chem>Cc1c(O)c(Br)c(Br)c(Br)c1Br</chem>
	5-ethyl-5-(4-hydroxyphenyl)-1,3-diazinane-2,4,6-trione	0	1	0	1	<chem>CCC1(C(=O)NC(=O)NC1=O)c1ccc(O)cc1</chem>
54548-50-4	6-chloro-m-cresol	0	1	0	1	<chem>Cc1ccc(Cl)c(O)c1</chem>
14199-15-6	methyl 2-(4-hydroxyphenyl)acetate	1	1	1	0	<chem>COC(=O)Cc1ccc(O)cc1</chem>
108-36-1	1,3-dibromobenzene	0	1	0	1	<chem>Brc1cccc(Br)c1</chem>

615-54-3	1,2,4-tribromobenzene	0	1	0	1	<chem>Brc1ccc(Br)c(Br)c1</chem>
626-39-1	1,3,5-tribromobenzene	0	1	0	1	<chem>Brc1cc(Br)cc(Br)c1</chem>
636-28-2	1,2,4,5-tetrabromobenzene	0	1	0	1	<chem>Brc1cc(Br)c(Br)cc1Br</chem>
328-84-7	3,4-dichlorobenzotrifluoride	0	1	0	1	<chem>FC(F)(F)c1ccc(Cl)c(Cl)c1</chem>
94-99-5	2,4-dichlorobenzylchloride	0	1	0	1	<chem>ClCc1ccc(Cl)cc1Cl</chem>
320-60-5	2,4-dichloro-1-(trifluoromethyl)benzene	0	1	0	1	<chem>FC(F)(F)c1ccc(Cl)cc1Cl</chem>
	1-butyl-4-chlorobenzene	0	1	0	1	<chem>CCCCc1ccc(Cl)cc1</chem>
51554-95-1	1-bromo-4-pentylbenzene	0	1	0	1	<chem>CCCCCc1ccc(Br)cc1</chem>
	1-bromo-4-heptylbenzene	0	1	0	1	<chem>CCCCCCCc1ccc(Br)cc1</chem>
	1-bromo-4-butylbenzene	0	1	0	1	<chem>CCCCc1ccc(Br)cc1</chem>
95-73-8	2,4-dichlorotoluene	0	1	0	1	<chem>Cc1ccc(Cl)cc1Cl</chem>
5216-25-1	4-chlorobenzotrichloride	0	1	0	1	<chem>Clc1ccc(cc1)C(Cl)(Cl)Cl</chem>
3972-65-4	4-tert-butyl-1-bromobenzene	0	1	0	1	<chem>CC(C)(C)c1ccc(Br)cc1</chem>
5798-75-4	ethyl 4-bromobenzoate	0	1	0	1	<chem>CCOC(=O)c1ccc(Br)cc1</chem>
6575-05-9	2,4,6-trichlorobenzonitrile	0	1	0	1	<chem>Clc1cc(Cl)c(C#N)c(Cl)c1</chem>
	(S)-(4-bromo-2-chlorophenyl ethyl propylsulfanylphosphonate)	0	1	0	1	<chem>CCCS[P@@](=O)(OCC)Oc1ccc(Br)cc1Cl</chem>

2432-90-8	didodecylphthalate	0	1	0	1	CCCCCCCCCCCCCOC(=O)c1cccc1C(=O)OCCCCCCCCCCC
523-31-9	dibenzyl phthalate	1	1	1	0	O=C(OCc1cccc1)c1cccc1C(=O)OCc1cccc1
117-83-9	palatinol	0	1	0	1	CCCCOCCOC(=O)c1cccc1C(=O)OCCOCCCC
85-70-1	butylglycolyl butyl phthalate	0	1	0	1	CCCCOC(=O)COC(=O)c1cccc1C(=O)OCCCC
	1,2,4-tris(2R)-2-ethylhexyl benzene-1,2,4-tricarboxylate	0	1	0	1	CCCC[C@@H](CC)COC(=O)c1ccc(C(=O)OC[C@H](CC)CCCC)c(c1)C(=O)OC[C@H](CC)CCCC
1528-49-0	1,2,4-trihexyl benzene-1,2,4-tricarboxylate	0	1	0	1	CCCCCOC(=O)c1ccc(C(=O)OCCCCC)c(c1)C(=O)OCCCCC
131918-42-8	1,2,4-tris(7-methyloctyl) benzene-1,2,4-tricarboxylate	0	1	0	1	CC(C)CCCCCOC(=O)c1ccc(C(=O)OCCCCC(C)C)c(c1)C(=O)OCCCCC(C)C
2694-54-4	1,2,4-tris(prop-2-en-1-yl) benzene-1,2,4-tricarboxylate	0	1	0	1	C=CCOC(=O)c1ccc(C(=O)OCC=C)c(c1)C(=O)OCC=C
636-09-9	1,4-diethyl benzene-1,4-dicarboxylate	0	1	0	1	CCOC(=O)c1ccc(cc1)C(=O)OCC
154204-78-1	1,4-bis(prop-2-en-1-yl) benzene-1,4-dicarboxylate	0	1	0	1	C=CCOC(=O)c1ccc(cc1)C(=O)OCC=C
	1,4-bis(2R)-2-ethylhexyl benzene-1,4-dicarboxylate	0	1	0	1	CCCC[C@@H](CC)COC(=O)c1ccc(cc1)C(=O)OC[C@H](CC)CCCC
1539-04-4	1,4-diphenyl benzene-1,4-dicarboxylate	0	1	0	1	O=C(Oc1cccc1)c1ccc(cc1)C(=O)Oc1cccc1

104-13-2	benzenamine, 4-butyl-	0	1	0	1	<chem>CCCCc1ccc(N)cc1</chem>
33228-45-4	aniline, (p-hexyl)-	0	1	0	1	<chem>CCCCCCc1ccc(N)cc1</chem>
3575-31-3	benzoic acid, 4-octyl-	0	1	0	1	<chem>CCCCCCCCc1ccc(cc1)C(O)=O</chem>
6853-57-2	4-pentylbenzaldehyde	0	1	0	1	<chem>CCCCC1ccc(C=O)cc1</chem>
	(2R)-2-ethylhexyl 4-(dimethylamino)benzoate	0	1	0	1	<chem>CCCC[C@@H](CC)COC(=O)c1ccc(cc1)N(C)C</chem>
527-54-8	3,4,5-trimethylphenol	0	1	0	1	<chem>Cc1cc(O)cc(C)c1C</chem>
67845-93-6	hexadecyl 3,5-di-tert-butyl-4-hydroxybenzoate	0	1	0	1	<chem>CCCCCCCCCCCCCCCCOC(=O)c1cc(c(O)c(c1)C(C)(C)C(C)(C)C</chem>
451-46-7	ethyl 4-fluorobenzoate	0	1	0	1	<chem>CCOC(=O)c1ccc(F)cc1</chem>
99-77-4	ethyl-P-nitrobenzoate	0	1	0	1	<chem>CCOC(=O)c1ccc(cc1)[N+](=[O-])=O</chem>
16245-79-7	4-octylaniline	0	1	0	1	<chem>CCCCCCCCc1ccc(N)cc1</chem>
2033-89-8	3,4-dimethoxyphenol	0	1	0	1	<chem>COc1ccc(O)cc1OC</chem>
94-12-2	risocaine	0	1	0	1	<chem>CCCOC(=O)c1ccc(N)cc1</chem>
455-19-6	4-(trifluoromethyl)benzaldehyde	0	1	0	1	<chem>FC(F)(F)c1ccc(C=O)cc1</chem>
120-48-9	n-butyl 4-nitrobenzoate	0	1	0	1	<chem>CCCCOC(=O)c1ccc(cc1)[N+](=[O-])=O</chem>
828-27-3	4-(trifluoromethoxy)phenol	1	1	1	0	<chem>Oc1ccc(OC(F)(F)F)cc1</chem>
13036-02-7	1,3-dimethyl 5-hydroxybenzene-	0	1	0	1	<chem>COC(=O)c1cc(O)cc(c1)C(=O)OC</chem>

	1,3-dicarboxylate					
	(2R)-2-ethylhexyl 2-hydroxybenzoate	0	1	0	1	<chem>CCCC[C@@H](CC)COC(=O)c1ccccc1O</chem>
20834-61-1	2-bromo-4,6-di-tert-butylphenol	0	1	0	1	<chem>CC(C)(C)c1cc(Br)c(O)c(c1)C(C)(C)C</chem>
56424-77-2	ethyl 2-(2-ethoxy-2-oxoethoxy)benzoate	0	1	0	1	<chem>CCOC(=O)COc1ccccc1C(=O)OCC</chem>
	2,4-dinitro-6-[(2R)-octan-2-yl]phenyl but-2-enoate	0	1	0	1	<chem>CCCCCC[C@@H](C)c1cc(cc(c1OC(=O)C=CC)[N+])([O-])=O[N+](O-)=O</chem>
15165-67-0	(2R)-2-(2,4-dichlorophenoxy)propanoic acid	0	1	0	1	<chem>C[C@@H](Oc1ccc(Cl)cc1Cl)C(O)=O</chem>
	ethyl (E)-2-(2-phenylethyl)diazen-1-yl ethoxy(sulfanylidene)phosphonite	0	1	0	1	<chem>CCOP(=S)(OCC)O\N=N\CCc1ccccc1</chem>
	[(R)-4-tert-butyl-2-chlorophenoxy(methoxy)phosphoryl](methyl)amine	0	1	0	1	<chem>CN[P@@](=O)(OC)Oc1ccc(cc1Cl)C(C)(C)C</chem>
12778-41-5	nexion	1	1	1	0	<chem>COP(=S)(OC)Oc1cc(Cl)c(Br)cc1Cl</chem>
	ethyl 3-[[[[(2,2-dimethyl-1,3-dihydroinden-5-yl)oxy]carbonyl](methyl)amino)sulfanyl](isopropyl)amino}propanoate	0	1	0	1	<chem>CCOC(=O)CCN(SN(C)C(=O)Oc1ccc2CC(C)(C)Cc2c1)C(C)C</chem>

700-13-0	2,3,5-trimethylbenzene-1,4-diol	0	1	0	1	<chem>Cc1cc(O)c(C)c(C)c1O</chem>
17138-28-2	ethyl 2-(4-hydroxyphenyl)acetate	0	1	0	1	<chem>CCOC(=O)Cc1ccc(O)cc1</chem>
85482-67-3	4-[(2S)-2-(methylamino)propyl]phenol	0	1	0	1	<chem>CN[C@@H](C)Cc1ccc(O)cc1</chem>
470-90-6	chlorfenvinphos	0	1	0	1	<chem>CCOP(=O)(OCC)O\C(=C/Cl)c1ccc(Cl)cc1Cl</chem>
2051-61-8	chlorobiphenyl	0	1	0	1	<chem>Clc1cccc(c1)-c1ccccc1</chem>
398-23-2	4,4'-difluorobiphenyl	0	1	0	1	<chem>Fc1ccc(cc1)-c1ccc(F)cc1</chem>
3001-15-8	1-iodo-4-(4-iodophenyl)benzene	1	1	1	0	<chem>Ic1ccc(cc1)-c1ccc(I)cc1</chem>
29558-77-8	4-(4-bromophenyl)phenol	1	1	1	0	<chem>Oc1ccc(cc1)-c1ccc(Br)cc1</chem>
613-37-6	4-methoxybiphenyl	0	1	0	1	<chem>COc1ccc(cc1)-c1ccccc1</chem>
6807-17-6	4-[2-(4-hydroxyphenyl)-4-methylpentan-2-yl]phenol	1	1	1	0	<chem>CC(C)CC(C)(c1ccc(O)cc1)c1ccc(O)cc1</chem>
81-92-5	phenolphthalol	1	1	1	0	<chem>OCc1ccccc1C(c1ccc(O)cc1)c1ccc(O)cc1</chem>
	4-[(1R,2R,6R,7R)-8-(4-hydroxyphenyl)tricyclo[5.2.1.0{2,6}]decan-8-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)C1(C[C@H]2C[C@@H]1[C@@H]1CCC[C@H]21)c1ccc(O)cc1</chem>
	4-(2-{3-[2-(4-hydroxyphenyl)propan-2-yl]phenyl}propan-2-yl)phenol	1	1	1	0	<chem>CC(C)(c1ccc(O)cc1)c1cccc(c1)C(C)(C)c1ccc(O)cc1</chem>

	(5R)-5-(4-hydroxyphenyl)-5-phenylimidazolidine-2,4-dione	0	1	0	1	<chem>Oc1ccc(cc1)[C@]1(NC(=O)NC1=O)c1ccccc1</chem>
	2-[(4-hydroxy-2-methylphenyl)[(1E)-2-methyl-4-oxocyclohexa-2,5-dien-1-ylidene]methyl]benzenesulfonic acid	1	1	1	0	<chem>CC1=CC(=O)C=C\C1=C(\c1ccc(O)cc1C)c1ccccc1S(O)(=O)=O</chem>
	4-[(3R)-1,3-bis(5-tert-butyl-4-hydroxy-2-methylphenyl)butyl]-2-tert-butyl-5-methylphenol	1	1	1	0	<chem>C[C@H](CC(c1cc(c(O)cc1C)C(C)(C)C)c1cc(c(O)cc1C)C(C)(C)C)c1cc(c(O)cc1C)C(C)(C)C</chem>
88-24-4	2-tert-butyl-6-[(3-tert-butyl-5-ethyl-2-hydroxyphenyl)methyl]-4-ethylphenol	0	1	0	1	<chem>CCc1cc(Cc2cc(CC)cc(c2O)C(C)(C)C)c(O)c(c1)C(C)(C)C</chem>
7500-76-7	4,4'-dimethoxytrityl cation	0	1	0	1	<chem>COc1ccc(cc1)C(c1ccccc1)c1ccc(OC)cc1</chem>
3010-81-9	tris(4-methoxyphenyl)methanol	0	1	0	1	<chem>COc1ccc(cc1)C(O)(c1ccc(OC)cc1)c1ccc(OC)cc1</chem>
2642-82-2	DDOH	0	1	0	1	<chem>OCC(c1ccc(Cl)cc1)c1ccc(Cl)cc1</chem>
90-97-1	bis(4-chlorophenyl)methanol	0	1	0	1	<chem>OC(c1ccc(Cl)cc1)c1ccc(Cl)cc1</chem>
2172-51-2	3,3,3-tris(4-chlorophenyl)propanenitrile	0	1	0	1	<chem>Clc1ccc(cc1)C(CC#N)(c1ccc(Cl)cc1)c1ccc(Cl)cc1</chem>
2990-17-2	1-bromo-4-[1-(4-bromophenyl)-2,2,2-trichloroethyl]benzene	0	1	0	1	<chem>ClC(Cl)(Cl)C(c1ccc(Br)cc1)c1ccc(Br)cc1</chem>

5216-53-5	1-bromo-4-[1-(4-bromophenyl)-2,2-dichloroethyl]benzene	0	1	0	1	<chem>ClC(Cl)C(c1ccc(Br)cc1)c1ccc(Br)cc1</chem>
27064-94-4	1-[chloro(4-fluorophenyl)methyl]-4-fluorobenzene	0	1	0	1	<chem>Fc1ccc(cc1)C(Cl)c1ccc(F)cc1</chem>
22856-62-8	4-[2-(4-amino-2-methylphenyl)ethyl]-3-methylaniline	1	1	1	0	<chem>Cc1cc(N)ccc1CCc1ccc(N)cc1C</chem>
4073-98-7	4-[(4-amino-3,5-dimethylphenyl)methyl]-2,6-dimethylaniline	0	1	0	1	<chem>Cc1cc(Cc2cc(C)c(N)c(C)c2)cc(C)c1N</chem>
	4-[(3S,4S)-4-[4-(propanoyloxy)phenyl]hexan-3-yl]phenyl propanoate	1	1	1	0	<chem>CC[C@@H]([C@H](CC)c1ccc(OC(=O)CC)cc1)c1ccc(OC(=O)CC)cc1</chem>
90-96-0	bis(4-methoxyphenyl)methanone	0	1	0	1	<chem>COc1ccc(cc1)C(=O)c1ccc(OC)cc1</chem>
131-55-5	4-(2,4-dihydroxybenzoyl)benzene-1,3-diol	1	1	1	0	<chem>Oc1ccc(C(=O)c2ccc(O)cc2O)c(O)c1</chem>
136-36-7	resorcinol monobenzoate	0	1	0	1	<chem>Oc1cccc(OC(=O)c2ccccc2)c1</chem>
	4-[(E)-2-(pyridin-2-yl)diazen-1-yl]benzene-1,3-diol	0	1	0	1	<chem>Oc1ccc(\N=N\c2ccncc2)c(O)c1</chem>
	4-[(1s,3s,5s,7s)-3-(4-hydroxyphenyl)adamantan-1-yl]phenol	1	1	1	0	<chem>Oc1ccc(cc1)[C@@]12C[C@@H]3C[C@@H](C[C@@](C3)(C1)c1ccc(O)cc1)C2</chem>

2664-63-3	DFS	1	1	1	0	<chem>Oc1ccc(Sc2ccc(O)cc2)cc1</chem>
78-30-8	tr cresyl phosphate	1	1	1	0	<chem>Cc1ccccc1OP(=O)(Oc1ccccc1C)Oc1ccccc1C</chem>
17606-31-4	ruban	0	1	0	1	<chem>CN(C)C(CSS(=O)(=O)c1ccccc1)CSS(=O)(=O)c1ccccc1</chem>
	(S)-(4-bromo-2,5-dichlorophenyl methyl phenyl(sulfanylidene)phosphonite)	1	1	1	0	<chem>CO[P@](=S)(Oc1cc(Cl)c(Br)cc1Cl)c1ccccc1</chem>
34123-59-6	tolkan	0	1	0	1	<chem>CC(C)c1ccc(NC(=O)N(C)C)cc1</chem>
	2-(4-hydroxyphenyl)pyrimidin-5-ol	0	1	0	1	<chem>Oc1ccc(cc1)-c1ncc(O)cn1</chem>
	2,4-dihydroxyazobenzene	1	1	1	0	<chem>Oc1ccc(\N=N\c2ccccc2)c(O)c1</chem>
93487-18-4	2-[[2-hydroxy-5-(2,4,4-trimethylpentan-2-yl)phenyl]sulfanyl]-4-(2,4,4-trimethylpentan-2-yl)phenol	1	1	1	0	<chem>CC(C)(C)CC(C)(C)c1ccc(O)c(Sc2cc(ccc2O)C(C)(C)CC(C)(C)C)c1</chem>
	azo violet	0	1	0	1	<chem>Oc1ccc(\N=N\c2ccc(cc2)[N+](=[O-])=O)c(O)c1</chem>
	2,3,5,6-tetrafluoro-4-(pentafluorophenyl)phenol	1	1	1	0	<chem>Oc1c(F)c(F)c(c(F)c1F)-c1c(F)c(F)c(F)c(F)c1F</chem>
728-87-0	bis(4-methoxyphenyl)methanol	0	1	0	1	<chem>COc1ccc(cc1)C(O)c1ccc(OC)cc1</chem>
1144-74-7	(4-nitrophenyl)(phenyl)methanone	0	1	0	1	<chem>[O-][N+](=O)c1ccc(cc1)C(=O)c1ccccc1</chem>
434-90-2	decafluorobiphenyl	0	1	0	1	<chem>Fc1c(F)c(F)c(c(F)c1F)-c1c(F)c(F)c(F)c(F)c1F</chem>

1016-78-0	(3-chlorophenyl)(phenyl)methanone	0	1	0	1	<chem>Clc1cccc(c1)C(=O)c1ccccc1</chem>
134-85-0	(4-chlorophenyl)(phenyl)methanone	0	1	0	1	<chem>Clc1ccc(cc1)C(=O)c1ccccc1</chem>
90-90-4	(4-bromophenyl)(phenyl)methanone	0	1	0	1	<chem>BrC1ccc(cc1)C(=O)c1ccccc1</chem>
	1-chloro-4-[(R)-chloro(phenyl)methyl]benzene	0	1	0	1	<chem>Cl[C@H](c1ccccc1)c1ccc(Cl)cc1</chem>
	1-[(R)-(4-chlorophenyl)(phenyl)methyl]piperazine	0	1	0	1	<chem>Clc1ccc(cc1)[C@H](N1CCNCC1)c1ccccc1</chem>
2051-90-3	diphenyldichloromethane	0	1	0	1	<chem>ClC(Cl)(c1ccccc1)c1ccccc1</chem>
345-83-5	(4-fluorophenyl)(phenyl)methanone	0	1	0	1	<chem>Fc1ccc(cc1)C(=O)c1ccccc1</chem>
342-25-6	(2-fluorophenyl)(4-fluorophenyl)methanone	0	1	0	1	<chem>Fc1ccc(cc1)C(=O)c1ccccc1F</chem>
1607-57-4	(2-bromo-1,2-diphenylethenyl)benzene	1	1	1	0	<chem>BrC(=C(c1ccccc1)c1ccccc1)c1ccccc1</chem>
	triphenyltin	1	1	1	0	<chem>c1ccc(cc1)[SnH](c1ccccc1)c1ccccc1</chem>
457-68-1	1-fluoro-4-[(4-fluorophenyl)methyl]benzene	0	1	0	1	<chem>Fc1ccc(Cc2ccc(F)cc2)cc1</chem>

2835-78-1	benzophenone, 3-amino-	0	1	0	1	<chem>Nc1cccc(c1)C(=O)c1ccccc1</chem>
2005-08-5	4-chlorophenyl benzoate	0	1	0	1	<chem>Clc1ccc(OC(=O)c2ccccc2)cc1</chem>
32555-96-7	4-[(E)-2-phenylethenyl]benzaldehyde	0	1	0	1	<chem>O=Cc1ccc(\C=C\c2ccccc2)cc1</chem>
1868-00-4	bis[3-(trifluoromethyl)phenyl]methanone	0	1	0	1	<chem>FC(F)(F)c1cccc(c1)C(=O)c1cccc(c1)C(F)(F)F</chem>
85118-07-6	(3,4-difluorophenyl)(phenyl)methanone	0	1	0	1	<chem>Fc1ccc(cc1F)C(=O)c1ccccc1</chem>
	bis(3-fluorophenyl)methanone	0	1	0	1	<chem>Fc1cccc(c1)C(=O)c1cccc(F)c1</chem>
	2-(4-chlorophenyl)-1,1-diphenylethanol	1	1	1	0	<chem>OC(Cc1ccc(Cl)cc1)(c1ccccc1)c1ccccc1</chem>
21084-22-0	[3-(trifluoromethyl)phenyl][4-(trifluoromethyl)phenyl]methanone	0	1	0	1	<chem>FC(F)(F)c1ccc(cc1)C(=O)c1cccc(c1)C(F)(F)F</chem>
49757-42-8	1-[chlorobis(4-methoxyphenyl)methyl]-4-methoxybenzene	1	1	1	0	<chem>COc1ccc(cc1)C(Cl)(c1ccc(OC)cc1)c1ccc(OC)cc1</chem>
1171-47-7	4-[2-(4-carboxyphenyl)-1,1,1,3,3,3-hexafluoropropan-2-yl]benzoic acid	1	1	1	0	<chem>OC(=O)c1ccc(cc1)C(c1ccc(cc1)C(O)=O)(C(F)(F)F)C(F)(F)F</chem>
	1-[1,1,1,3,3,3-hexafluoro-2-(4-methylphenyl)propan-2-yl]-4-	1	1	1	0	<chem>Cc1ccc(cc1)C(c1ccc(C)cc1)(C(F)(F)F)C(F)(F)F</chem>

	methylbenzene					
1095-78-9	4-[2-(4-aminophenyl)-1,1,1,3,3,3-hexafluoropropan-2-yl]aniline	1	1	1	0	<chem>Nc1ccc(cc1)C(c1ccc(N)cc1)(C(F)(F)F)C(F)(F)F</chem>
39634-42-9	4-[4-(trifluoromethyl)phenoxy]phenol	1	1	1	0	<chem>Oc1ccc(Oc2ccc(cc2)C(F)(F)F)cc1</chem>
106246-33-7	4-[(4-amino-2-chloro-3,5-diethylphenyl)methyl]-3-chloro-2,6-diethylaniline	1	1	1	0	<chem>CCc1cc(Cc2cc(CC)c(N)c(CC)c2Cl)c(Cl)c(CC)c1N</chem>
19811-05-3	(2,4-dichlorophenyl)(phenyl)methanone	0	1	0	1	<chem>Clc1ccc(C(=O)c2ccccc2)c(Cl)c1</chem>
	[3-(4-fluorobenzoyl)phenyl](4-fluorophenyl)methanone	0	1	0	1	<chem>Fc1ccc(cc1)C(=O)c1cccc(c1)C(=O)c1ccc(F)cc1</chem>
3016-97-5	(4-benzoylphenyl)(phenyl)methanone	0	1	0	1	<chem>O=C(c1ccccc1)c1ccc(cc1)C(=O)c1ccccc1</chem>
	4-(2-{3-[2-(4-aminophenyl)propan-2-yl]phenyl}propan-2-yl)aniline	1	1	1	0	<chem>CC(C)(c1ccc(N)cc1)c1cccc(c1)C(C)(C)c1ccc(N)cc1</chem>
5447-02-9	3,4-bis(benzyloxy)benzaldehyde	1	1	1	0	<chem>O=Cc1ccc(OCc2ccccc2)c(OCc2ccccc2)c1</chem>
	L-thyronine	0	1	0	1	<chem>N[C@H](Cc1ccc(Oc2ccc(O)cc2)cc1)C(O)=O</chem>
611-79-0	3-(3-aminobenzoyl)aniline	0	1	0	1	<chem>Nc1cccc(c1)C(=O)c1cccc(N)c1</chem>
2001-29-8	1-(4-bromophenyl)-2-phenylethanone	0	1	0	1	<chem>BrC1CCC(CC1)C(=O)Cc1ccccc1</chem>

	[4-(benzyloxy)phenyl](phenyl)methanone	0	1	0	1	<chem>O=C(c1ccccc1)c1ccc(OCc2ccccc2)cc1</chem>
	(2E)-1,4-bis(4-fluorophenyl)but-2-ene-1,4-dione	1	1	1	0	<chem>Fc1ccc(cc1)C(=O)\C=C\C(=O)c1ccc(F)cc1</chem>
42187-33-7	(3,4-dimethylphenyl)(3-nitrophenyl)methanone	0	1	0	1	<chem>Cc1ccc(cc1C)C(=O)c1ccc(c1)[N+][O-]=O</chem>
	methyl 4-[(Z)-2-[4-(methoxycarbonyl)phenyl]ethenyl]benzoate	0	1	0	1	<chem>COC(=O)c1ccc(\C=C/c2ccc(cc2)C(=O)OC)cc1</chem>
100-31-2	4-[(E)-2-(4-carboxyphenyl)ethenyl]benzoic acid	0	1	0	1	<chem>OC(=O)c1ccc(\C=C\c2ccc(cc2)C(O)=O)cc1</chem>
10192-62-8	4-{2-[4-(acetyloxy)phenyl]propan-2-yl}phenyl acetate	0	1	0	1	<chem>CC(=O)Oc1ccc(cc1)C(C)(C)c1ccc(OC(C)=O)cc1</chem>
	4-{2-[4-(carboxymethoxy)phenyl]propan-2-yl}phenoxyacetic acid	0	1	0	1	<chem>CC(C)(c1ccc(OCC(O)=O)cc1)c1ccc(OCC(O)=O)cc1</chem>
2772-45-4	2,4-bis(2-phenylpropan-2-yl)phenol	1	1	1	0	<chem>CC(C)(c1ccccc1)c1ccc(O)c(c1)C(C)(C)c1ccccc1</chem>
127774-72-5	4-[(4-amino-3,5-diethylphenyl)methyl]-2,6-diethylaniline	0	1	0	1	<chem>CCc1cc(Cc2cc(CC)c(N)c(CC)c2)cc(CC)c1N</chem>

519-73-3	triphenylmethane	1	1	1	0	<chem>c1ccc(cc1)C(c1ccccc1)c1ccccc1</chem>
40615-36-9	1-[chloro(4-methoxyphenyl)benzyl]-4-methoxybenzene	0	1	0	1	<chem>COc1ccc(cc1)C(Cl)(c1ccccc1)c1ccc(OC)cc1</chem>
466-37-5	tetraphenylethanone	1	1	1	0	<chem>O=C(c1ccccc1)C(c1ccccc1)(c1ccccc1)c1ccccc1</chem>
900-91-4	3,3,3-triphenylpropanoic acid	0	1	0	1	<chem>OC(=O)CC(c1ccccc1)(c1ccccc1)c1ccccc1</chem>
	1-(triphenylmethyl)pyridin-1-ium	0	1	0	1	<chem>c1ccc(cc1)C(c1ccccc1)(c1ccccc1)[n+]1ccccc1</chem>
4471-22-1	N-(triphenylmethyl)aniline	0	1	0	1	<chem>N(c1ccccc1)C(c1ccccc1)(c1ccccc1)c1ccccc1</chem>
1596-67-4	thyronine	0	1	0	1	<chem>N[C@@H](Cc1ccc(Oc2ccc(O)cc2)cc1)C(O)=O</chem>
	(2S)-2-amino-3-[4-(2,4-dinitrophenoxy)phenyl]propanoic acid	0	1	0	1	<chem>N[C@@H](Cc1ccc(Oc2ccc(cc2[N+])([O-])=O)[N+])([O-])=O)cc1)C(O)=O</chem>
1450-63-1	tetraphenyl butadiene	1	1	1	0	<chem>C(C=C(c1ccccc1)c1ccccc1)=C(c1ccccc1)c1ccccc1</chem>
	(2R)-1,2,3,4-tetrahydronaphthalen-2-ol	0	1	0	1	<chem>O[C@@H]1CCc2ccccc2C1</chem>
145-50-6	(4E)-4-[(4-hydroxynaphthalen-1-yl)(phenyl)methylidene]naphthalen-1-one	1	1	1	0	<chem>Oc1ccc(\C(=C2/C=CC(=O)c3ccccc23)c2ccccc2)c2ccccc12</chem>
6949-73-1	2-hydroxy-9-fluorenone	1	1	1	0	<chem>Oc1ccc2-c3ccccc3C(=O)c2c1</chem>
	2,3-dimethyl naphthalene-2,3-	0	1	0	1	<chem>COC(=O)c1cc2ccccc2cc1C(=O)OC</chem>

	dicarboxylate					
41175-50-2	1-azatricyclo[7.3.1.0{5,13}]trideca-5(13),6,8-trien-6-ol	0	1	0	1	<chem>Oc1ccc2CCCN3CCCc1c23</chem>
580-16-5	6-hydroxyquinoline	0	1	0	1	<chem>Oc1ccc2ncccc2c1</chem>
7061-81-6	2,4,7-trichloro-9H-fluorene	0	1	0	1	<chem>Clc1ccc-2c(Cc3cc(Cl)cc(Cl)c-23)c1</chem>
6297-11-6	2,7-dichlorofluoren-9-one	0	1	0	1	<chem>Clc1ccc2-c3ccc(Cl)cc3C(=O)c2c1</chem>
	(2E)-3-(2,4-dimethoxyphenyl)-1-(6-hydroxy-2,3,4-trimethoxyphenyl)prop-2-en-1-one	0	1	0	1	<chem>COc1ccc(\C=C\C(=O)c2c(O)cc(OC)c(OC)c2OC)c(OC)c1</chem>
6948-88-5	4-[hydroxy(4-hydroxynaphthalen-1-yl)benzyl]naphthalen-1-ol	1	1	1	0	<chem>Oc1ccc(c2cccc12)C(O)(c1cccc1)c1ccc(O)c2cccc12</chem>
4709-68-6	9-(diphenylmethylidene)fluorene	0	1	0	1	<chem>c1ccc(cc1)C(=C1c2cccc2-c2cccc12)c1cccc1</chem>
596-01-0	naphtholphthalein	1	1	1	0	<chem>Oc1ccc(c2cccc12)C1(OC(=O)c2cccc12)c1ccc(O)c2cccc12</chem>
49652-64-4	3-[2-(diethylamino)ethyl]-7-hydroxy-4-methylchromen-2-one	0	1	0	1	<chem>CCN(CC)CCc1c(C)c2ccc(O)cc2oc1=O</chem>
	(R)-(2-chlorophenyl)(4-chlorophenyl)pyrimidin-5-ylmethanol	1	1	1	0	<chem>O[C@](c1ccc(Cl)cc1)(c1cncnc1)c1cccc1Cl</chem>
	(2R)-4-(4-chlorophenyl)-2-phenyl-2-(1,2,4-triazol-1-ylmethyl)butanenitrile	0	1	0	1	<chem>Clc1ccc(CC[C@@](Cn2cncn2)(C#N)c2cccc2)cc1</chem>

	(1R,9R,14R,22S)-2,5,8,15,18,21-hexaoxatricyclo[20.4.0.0{9,14}]hexacosane	0	1	0	1	C1CC[C@H]2OCCOCCO[C@H]3CCCC[C@H]3OCCOCCO[C@H]2C1
19315-93-6	2,6-dihydroxyquinoline	0	1	0	1	Oc1ccc2nc(O)ccc2c1
	3-(5-chloro-1,3-benzoxazol-2-yl)-7-hydroxy-2-oxochromene-4-carbonitrile	1	1	1	0	Oc1ccc2c(C#N)c(-c3nc4cc(Cl)ccc4o3)c(=O)oc2c1
	(1S)-1-(2-fluorophenyl)-1-(4-fluorophenyl)-2-(1,2,4-triazol-1-yl)ethanol	0	1	0	1	O[C@@](Cn1cncn1)(c1ccc(F)cc1)c1ccccc1F
	(3aS,7aS)-2-[(1,1,2,2-tetrachloroethyl)sulfanyl]-3a,4,7,7a-tetrahydroisindole-1,3-dione	1	1	1	0	ClC(Cl)C(Cl)(Cl)SN1C(=O)[C@H]2CC=CC[C@@H]2C1=O
56048-49-8	(2S,6S)-2,6-dimethyl-4-tridecylmorpholine	0	1	0	1	CCCCCCCCCCCCCN1C[C@H](C)O[C@@H](C)C1
	ametryn	0	1	0	1	CCNc1nc(NC(C)C)nc(SC)n1
	diethyl [(1S)-2-chloro-1-(1,3-dioxoisindol-2-yl)ethyl]sulfanyl(sulfanylidene)phosphonite	1	1	1	0	CCOP(=S)(OCC)S[C@@H](CCl)N1C(=O)c2ccccc2C1=O
	bensulfuron-methyl (PH7)	0	1	0	1	COC(=O)c1ccccc1CS(=O)(=O)NC(=O)Nc1nc(OC)cc(OC)n1

1120-71-4	2,2-dioxide-1,2-oxathiolane	0	1	0	1	<chem>O=S1(=O)CCCO1</chem>
100646-51-3	ethyl (2R)-2-{4-[(6-chloroquinoxalin-2-yl)oxy]phenoxy}propanoate	0	1	0	1	<chem>CCOC(=O)[C@@H](C)Oc1ccc(Oc2cnc3cc(Cl)ccc3n2)cc1</chem>
	(2R)-2-(4-chlorophenyl)-2-(1,2,4-triazol-1-ylmethyl)hexanenitrile	0	1	0	1	<chem>CCCC[C@@](Cn1cncn1)(C#N)c1ccc(Cl)cc1</chem>
64529-56-2	ethiozin	0	1	0	1	<chem>CCSc1nnc(c(=O)n1N)C(C)(C)C</chem>
	(2S,3S)-2-(4-chlorophenyl)-3-cyclopropyl-1-(1,2,4-triazol-1-yl)butan-2-ol	0	1	0	1	<chem>C[C@@H](C1CC1)[C@@](O)(Cn1cncn1)c1ccc(Cl)cc1</chem>
	(2R)-2-(2,4-dichlorophenyl)-1-(1,2,4-triazol-1-yl)hexan-2-ol	0	1	0	1	<chem>CCCC[C@](O)(Cn1cncn1)c1ccc(Cl)cc1Cl</chem>
	(1R,2R,8R,9S)-1,9,10,11,12,12-hexachloro-4,6-dioxo-5 λ {6}-thiatricyclo[7.2.1.0{2,8}]dodec-10-ene-5,5-dione	0	1	0	1	<chem>ClC1=C(Cl)[C@]2(Cl)[C@H]3COS(=O)(=O)OC[C@@H]3[C@@]1(Cl)C2(Cl)Cl</chem>
	5-amino-2-(2,4,6-trichlorophenyl)-4H-pyrazol-3-one	1	1	1	0	<chem>NC1=NN(C(=O)C1)c1c(Cl)cc(Cl)cc1Cl</chem>
	(14R,15S)-15-methyl-14-[(E)-2-(2-methylphenyl)ethenyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	<chem>Cc1ccccc1\C=C\[C@]1(O)CCC2C3CCc4cc(O)ccc4C3CC[C@]12C</chem>

(14R,15S)-15-methyl-14-[(E)-2-(3-methylphenyl)ethenyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	<chem>Cc1cccc(\C=C\[C@]2(O)CCC3C4CCc5cc(O)ccc5C4CC[C@]23C)c1</chem>
(14R,15S)-15-methyl-14-[(E)-2-(4-methylphenyl)ethenyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	<chem>Cc1ccc(\C=C\[C@]2(O)CCC3C4CCc5cc(O)ccc5C4CC[C@]23C)cc1</chem>
(14R,15S)-15-methyl-14-[(E)-2-[2-(trifluoromethyl)phenyl]ethenyl]tetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	<chem>C[C@]12CCC3C(CCc4cc(O)ccc34)C1CC[C@@]2(O)\C=C\c1cccc1C(F)(F)F</chem>
(14R,15S)-14-[(E)-2-(2,3-dimethylphenyl)ethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	<chem>Cc1cccc(\C=C\[C@]2(O)CCC3C4CCc5cc(O)ccc5C4CC[C@]23C)c1C</chem>
(14R,15S)-14-[(E)-2-(2,4-dimethylphenyl)ethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	<chem>Cc1ccc(\C=C\[C@]2(O)CCC3C4CCc5cc(O)ccc5C4CC[C@]23C)c(C)c1</chem>
(14R,15S)-14-[(E)-2-(2,5-dimethylphenyl)ethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	<chem>Cc1ccc(C)c(\C=C\[C@]2(O)CCC3C4CCc5cc(O)ccc5C4CC[C@]23C)c1</chem>

	15]]heptadeca-2(7),3,5-triene-5,14-diol					
	(14R,15S)-14-[(E)-2-(2,6-dimethylphenyl)ethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	Cc1cccc(C)c1\\C=C\\[C@]1(O)CCC2C3CCc4cc(O)ccc4C3CC[C@]12C
	(14R,15S)-14-[(E)-2-(3,4-dimethylphenyl)ethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	Cc1ccc(\\C=C\\[C@]2(O)CCC3C4CCc5cc(O)ccc5C4CC[C@]23C)cc1C
	(14R,15S)-14-[(E)-2-(3,5-dimethylphenyl)ethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	Cc1cc(C)cc(\\C=C\\[C@]2(O)CCC3C4CCc5cc(O)ccc5C4CC[C@]23C)c1
	(14R,15S)-14-[(E)-2-[2,5-bis(trifluoromethyl)phenyl]ethenyl]-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}}]heptadeca-2(7),3,5-triene-5,14-diol	1	1	1	0	C[C@]12CCC3C(CCc4cc(O)ccc34)C1CC[C@@]2(O)\\C=C\\c1cc(ccc1C(F)(F)F)C(F)(F)F
	(14R,15S)-14-[(E)-2-[3,5-bis(trifluoromethyl)phenyl]ethenyl]	1	1	1	0	C[C@]12CCC3C(CCc4cc(O)ccc34)C1CC[C@@]2(O)\\C=C\\c1cc(cc(c1)C(F)(F)F)C(F)(F)F

	-15-methyltetracyclo[8.7.0.0{2,7}.0{11,15}]heptadeca-2(7),3,5-triene-5,14-diol					
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Table S2. Description of 13 ToxCast ER pathway related assays

Assay Name	Assay Description
ACEA_T47D_80hr_Positive	Cell growth assay
ATG_ERE_CIS	Attagene multiplexed ER reporter gene assay
ATG_ERRa_Trans	Attagene multiplexed GAL4 reporter construct with human ER α ligand binding domain assay
NVS_NR_bER	Bovine ER binding assay
NVS_NR_hER	Human ER binding assay
NVS_NR_mERa	Murine ER α binding assay
OT_ER_ERaERa_1440	Odyssey Thera ER α -ER α dimerization assay in agonist mode
OT_ER_ERaERb_1440	Odyssey Thera ER α -ER β dimerization assay in agonist mode
OT_ER_ERbERb_1440	Odyssey Thera ER β -ER β dimerization assay in agonist mode
Tox21_ERa_BLA_Agonist_ratio	ER α β -lactamase reporter gene assay in human HEK-293 cells in agonist mode
Tox21_ERa_BLA_Antagonist_ratio	ER α β -lactamase reporter gene assay in human HEK-293 cells in antagonist mode
Tox21_ERa_LUC_BG1_Agonist	ER α luciferase reporter gene assay in human BG-1 ovarian cells in agonist mode
Tox21_ERa_LUC_BG1_Antagonist	ER α luciferase reporter gene assay in human BG-1 ovarian cells in antagonist mode

Table S3. Comparison of data from EADB (treated as “truth”) and ToxCast for the 162 chemicals found in both data sets: sensitivity, specificity, accuracy and balanced accuracy across 13 ER pathway related assays. The assays correlated with EADB data that were used in external validation are determined using the criterion of balance accuracy > 0.7 and are marked in bold font.

ToxCast Assay Name	Sensitivity	Specificity	Accuracy	Balanced Accuracy
OT_ER_ERbERb_1440	0.72	0.9009	0.8447	0.8105
Tox21_ERa_BLA_Agonist_ratio	0.76	0.8571	0.8272	0.8086
OT_ER_ERaERa_1440	0.64	0.9730	0.8696	0.8065
OT_ER_ERaERb_1440	0.76	0.8378	0.8137	0.7989
Tox21_ERa_LUC_BG1_Agonist	0.72	0.8393	0.8025	0.7796
ACEA_T47D_80hr_Positive	0.66	0.8839	0.8148	0.7720
NVS_NR_hER	0.52	0.9554	0.8210	0.7377
ATG_ERE_CIS	0.66	0.7232	0.7037	0.6916
NVS_NR_bER	0.38	0.9911	0.8025	0.6855
NVS_NR_mERa	0.38	0.9821	0.7963	0.6811
Tox21_ERa_BLA_Antagonist_ratio	0.26	0.9464	0.7346	0.6032
ATG_ERRa_TRANS	0	0.9821	0.6790	0.4911
Tox21_ERa_LUC_BG1_Antagonist	0	0.9821	0.6790	0.4911

Table S4. External validation of DF model: total number of compounds tested, number of compounds tested as active and inactive in each assay, and the corresponding model prediction accuracy, sensitivity, specificity, area under the curve (AUC) and balanced accuracy.

Assay Name	Total	Active	Inactive	Accuracy	Sensitivity	Specificity	AUC	Balanced accuracy
OT_ER_ERbERb_1440	1633	120	1513	0.7789	0.3500	0.8130	0.6312	0.5815
Tox21_ERa_BLA_Agonist_ratio	1641	169	1472	0.7642	0.3313	0.8139	0.6012	0.5726
OT_ER_ERaERa_1440	1634	71	1563	0.7883	0.3521	0.8081	0.6384	0.5801
OT_ER_ERaERb_1440	1633	122	1511	0.7789	0.3525	0.8134	0.6358	0.5829
Tox21_ERa_LUC_BG1_Agonist	1641	218	1423	0.7294	0.2385	0.8046	0.5376	0.5216
ACEA_T47D_80hr_Positive	1608	211	1397	0.7438	0.2701	0.8153	0.5892	0.5427
NVS_NR_hER	1641	94	1547	0.7977	0.4894	0.8164	0.7430	0.6529

Table S5. Results of external validations presented in relative metrics to the prediction using experimental data

Assay Name	Relative Accuracy	Relative Sensitivity	Relative Specificity	Relative Balanced accuracy
OT_ER_ERbERb_1440	0.9221	0.4861	0.9024	0.7174
Tox21_ERa_BLA_Agonist_ratio	0.9238	0.4359	0.9495	0.7081
OT_ER_ERaERa_1440	0.9065	0.5501	0.8305	0.7192
OT_ER_ERaERb_1440	0.9572	0.4638	0.9708	0.7296
Tox21_ERa_LUC_BG1_Agonist	0.9089	0.3312	0.9586	0.6691
ACEA_T47D_80hr_Positive	0.9128	0.4092	0.9223	0.7029
NVS_NR_hER	0.9716	0.9411	0.8545	0.8850

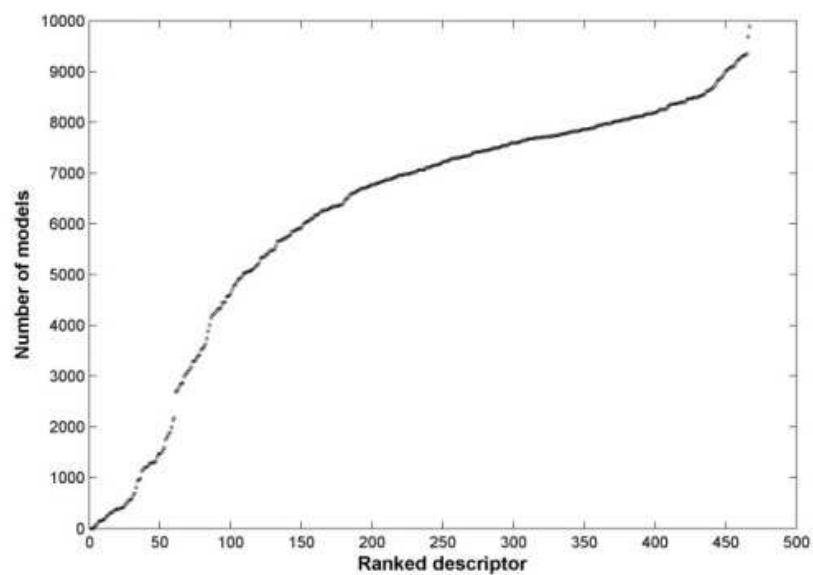


Figure S1. Results of descriptor analysis: The x-axis depicts the rank of the descriptors based on their frequency values. The y-axis gives the number of models that utilized the descriptors.