Supporting Information

Discovery of Novel Epidermal Growth Factor Receptor (EGFR) Inhibitors Using Computational Approaches

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Table S1. Dataset 1 of EGFR inhibitors for SAR and QSAR study.

Num	SMILES	IC_{50} nM	Subset3 pIC_{50}
1	Brc1cccc(Nc2ncnc3cc4ccccc4cc23)c1	0.003	*
2	CCOc1cc2ncnc(Nc3cccc(Br)c3)c2cc1OCC	0.006	*

3	CN(C)c1cc2c(Nc3cccc(Br)c3)ncnc2cn1	0.006	*
4	Brc1cccc(Nc2ncnc3cc4[nH]cnc4cc23)c1	0.008	*
5	CNc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	0.008	*
6	Cn1cnc2cc3ncnc(Nc4cccc(Br)c4)c3cc21	0.01	*
7	Cn1cnc2cc3c(Nc4cccc(Br)c4)ncnc3cc21	0.025	*
8	C#CCNC/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)c(C#N)cnc2cc1OCC	0.03	10.52
9	COc1cc2ncnc(Nc3ccc(Br)c(Br)c3)c2cc1OC	0.072	*
10	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccn4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	0.08	8.41
11	CN(C)c1cc2ncnc(Nc3cccc(Br)c3)c2cn1	0.091	*
12	CCC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	0.1	9.68
13	Nc1ccc2c(Nc3cccc(Br)c3)ncnc2c1	0.1	*
14	Nc1ccc2cncnc2c1	0.1	*
15	O=C(CCCCCCn1cc(-c2ccc3ncnc(Nc4cccc(Cl)c4F)c3c2)nn1)NO	0.12	*
16	CNc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	0.13	*
17	Nc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	0.13	*
18	CN(C)C/C=C(\F)C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	0.16	9.80
19	C=CC(=O)Nc1nc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1/C=C/CCN1CCOCC1	0.16	*
20	Oc1cc2ncnc(Nc3cccc(Br)c3)c2cc1O	0.17	*
21	CCCOc1cc2ncnc(Nc3cccc(Br)c3)c2cc1OCCC	0.17	*
22	C=CC(=O)N(C)c1cc2c(Nc3cccc(Br)c3)ncnc2cn1	0.17	*
23	CCOc1cc2ncnc(Nc3ccc(OCc4ccccn4)c(Cl)c3)c2cc1NC(=O)/C(F)=C/CN(C)C	0.18	9.74
24	C=CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCC	0.18	9.74
25	OCC(O)CNc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	0.18	*
26	CN(C)C/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	0.19	8.76
27	OCCNc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	0.19	*
28	CNc1cc2c(Nc3cccc(Cl)c3)ncnc2cn1	0.19	*
29	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C(F)=C/CN(C)C	0.2	9.70
30	CC#CC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	0.2	*
31	COc1cc(CO)ccc1-c1cc2c(N[C@H](CO)c3ccccc3)ncnc2[nH]1	0.2	*
32	COc1cc(CO)ccc1-c1cc2c(N[C@H](C)c3ccccc3)ncnc2[nH]1	0.2	*
33	CC1(C)Cc2c(sc(=S)n2-c2ccccc2)-c2c1sc(NC1=C(Cl)C(c3ccc(Cl)cc3)C(C#N)=C(O)O1)c2C#N	0.21	*
34	CN(C)C/C=C/C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	0.22	8.81
35	CN(CCO)c1cc2c(Nc3cccc(Br)c3)ncnc2cn1	0.22	*
36	CN1CCN(CCC(=O)Nc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)CC1	0.23	9.64
37	OCCNc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	0.24	*
38	COc1cc2ncnc(Nc3cccc(C(F)(F)F)c3)c2cc1OC	0.24	*
39	OCCNc1c(Br)cccc1Nc1ncnc2ccncc12	0.2455	*
40	CCOc1cc2ncc(C#N)c(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CNC	0.25	9.60
41	C=CC(=O)Nc1ccc2c(Nc3cccc(Cl)c3)ncnc2c1	0.25	*
42	Nc1ccc2c(Nc3cccc(Cl)c3)ncnc2c1	0.25	*
43	Brc1cccc(Nc2ncnc3cnc(NCCc4c[nH]cn4)nc23)c1	0.25	*
44	CC1(C)Cc2c(sc(=S)n2-c2ccccc2)-c2c(C#N)c(N)cc(C#N)c21	0.25	*
45	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)/C(F)=C/CN1CCOCC1	0.26	9.59

46	C#Cc1cccc(Nc2ncnc3cc(OCCCCn4ccnc4[N+](=O)[O-])c(OC)cc23)c1	0.26	9.59
47	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C(F)=C/CN1CCCCC1	0.27	9.57
48	CCOc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)CCN(C)C	0.27	9.57
49	O=C(CCN1CCCCC1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	0.27	9.57
50	O=C(CCCCCn1cc(-c2ccc3ncnc(Nc4cccc(Cl)c4F)c3c2)nn1)NO	0.27	*
51	O=C(O)CCNc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	0.27	*
52	Nc1ccc2sc3c(Nc4cccc(Br)c4)ncnc3c2c1	0.27	*
53	CC1(C)CC(=O)C(=NNc2ccc(Cl)cc2)c2c1sc(N)c2C#N	0.27	*
54	CN(C)CCC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	0.28	9.55
55	O=C(O)CCCNc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	0.28	*
56	O=C(O)CNc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	0.28	*
57	O=C(O)CCCNc1c(Br)cccc1Nc1ncnc2ccncc12	0.2818	*
58	CNC/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)c(C#N)cnc2cc1OCCF	0.29	9.54
59	CCOc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)CCN1CCOCC1	0.29	9.54
60	C=CC(=O)Nc1cccc(N2C(=O)N(Cc3ccccc3)Cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	0.29	9.54
61	Cc1nc2cc3c(Nc4cccc(Br)c4)ncnc3cc2[nH]1	0.29	*
62	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C(F)=C\CN1CCOCC1	0.3	9.52
63	C=CC(=O)Nc1cccc(N2C(=O)N(c3ccccc3)Cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	0.3	9.52
64	CC#CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cn1	0.3	*
65	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1OC(=O)N1CCN(C)C[C@H]1C	0.3	*
66	COc1cc2ncnc(Nc3cccc(Br)c3)c2cc1OCCCOP(N)(=O)N(CCCl)CCCl	0.3	*
67	OCCc1nc(-c2ccc(F)cc2)c(-c2ccnc3[nH]c(-c4ccccc4)cc23)[nH]1	0.3	*
68	OCCCCc1nc(-c2ccc(F)cc2)c(-c2ccnc3[nH]c(-c4ccccc4)cc23)[nH]1	0.3	*
69	C=CC(=O)Nc1cccc(-c2c[nH]c3nccc(-c4[nH]c(CCCO)nc4-c4ccc(F)cc4)c23)c1	0.3	*
70	C[C@@H](Nc1ncnc2[nH]c(-c3ccc(CO)cc3)cc12)c1ccccc1	0.3	*
71	COc1cc(C=O)ccc1-c1cc2c(N[C@H](CO)c3ccccc3)ncnc2[nH]1	0.3	*
72	C[C@@H](Nc1ncnc2[nH]c(-c3cccc(CO)c3)cc12)c1ccccc1	0.3	*
73	OCc1ccc(-c2cc3c(N[C@H](CO)c4ccccc4)ncnc3[nH]2)c(F)c1	0.3	*
74	COc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2cc1OCCCN1CCNCCNCCNCC1	0.3	*
75	CN(C)C/C=C(/F)C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	0.31	9.51
76	COc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCCn1ccnc1[N+](=O)[O-]	0.31	9.51
77	COc1cc2ncnc(Nc3cccc(Cl)c3)c2cc1OC	0.31	*
78	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCCCCn1ccnc1[N+](=O)[O-]	0.32	9.49
79	COc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCOCCn1ccnc1[N+](=O)[O-]	0.32	9.49
80	COc1cc2c(Nc3cccc(Br)c3)ncnc2cc1OCCCCCn1ccnc1[N+](=O)[O-]	0.33	9.48
81	Brc1cccc(Nc2ncnc3cc4c[nH]nc4cc23)c1	0.34	*
82	OCCN(CCO)CCCNc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	0.35	*
83	Nc1ccc2c(Nc3cccc(I)c3)ncnc2c1	0.35	*
84	COc1cc2c(Nc3cccc(Br)c3)ncnc2cc1OCCCCn1ccnc1[N+](=O)[O-]	0.37	9.43
85	Cn1ncc2cc3c(Nc4cccc(Br)c4)ncnc3cc21	0.37	*
86	O=C(O)/C=C/C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	0.37	*
87	C=CC(=O)Nc1cccc(N2C(=O)N(C(C)C)Cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	0.38	9.42
88	C[C@@H](Nc1ncnc2oc(-c3ccc(NCCN(C)C)cc3)cc12)c1ccccc1	0.4	9.40

89	COc1cc(C(=O)NCCN(C)C)cc(OC)c1-c1cc2c(N[C@H](C)c3ccccc3)ncnc2s1	0.4	9.40
90	C=CC(=O)Nc1ccc2ncnc(N3CCc4ccc(Br)cc43)c2c1	0.4	*
91	OCc1ccc(-c2cc3c(N[C@H](CO)c4ccccc4)ncnc3[nH]2)cc1	0.4	*
92	COC[C@@H](Nc1ncnc2[nH]c(-c3ccccc3)cc12)c1ccccc1	0.4	*
93	Brc1cccc(Nc2ncnc3ccc(NCCCN4CCCCC4)cc23)c1	0.41	9.39
94	C=CC(=O)Nc1cccc(N2C(=O)N(C)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(OC)c4)nc32)c1	0.41	9.39
95	CCOC1=C2C(=CCc3c2sc(N)c3C(=O)Nc2ccc(Cl)cc2)OC(O)=C1C#N	0.41	*
96	C=CC(=O)Nc1ccc2ncnc(Nc3cccc(C)c3)c2c1	0.42	*
97	CC1(C)C2=C(OC(O)=C(C#N)C2c2ccccc2)C(=NNc2ccc(Cl)cc2)c2c1sc(N)c2C#N	0.42	*
98	Nc1sc2c(c1C(=O)Nc1ccc(Cl)cc1)CCC(=O)C2=NNc1ccc(Cl)cc1	0.42	*
99	C=CC(=O)Nc1cccc(N2C(=O)N(C)Cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4)nc32)c1	0.43	9.37
100	C=CS(=O)(=O)c1cc2c(Nc3cccc(Br)c3)ncnc2cn1	0.43	*
101	Brc1cccc(Nc2ncnc3cc4[nH]ncc4cc23)c1	0.44	*
102	Brc1cccc(Nc2ncnc3cc4[nH]ccc4cc23)c1	0.44	*
103	CN(CC(=O)O)c1cc2c(Nc3cccc(Br)c3)ncnc2cn1	0.44	*
104	CN(C)CCCNC(=O)/C=C/C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	0.44	*
105	CNc1cc2c(Nc3cccc(C)c3)ncnc2cn1	0.45	*
106	C=CC(=O)Nc1ccc2c(Nc3cccc(Br)c3)ncnc2c1	0.45	*
107	CCN(CC)CC(O)CNC(=O)c1cc(C)c(/C=C2\C(=O)Nc3ncnc(Nc4ccc(F)c(Cl)c4)c32)[nH]1	0.45	*
108	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCCn1ccnc1[N+](=O)[O-]	0.47	9.33
109	C#Cc1cccc(Nc2ncnc3cc(OCCCCCn4ccnc4[N+](=O)[O-])c(OC)cc23)c1	0.47	9.33
110	COc1cc2ncnc(Nc3cccc(Br)c3)c2cc1NC(=O)[C@@H]1COC(=O)N1	0.47	9.33
111	Cl.Nc1ccc2c(c1)sc1c(Nc3cccc(Br)c3)ncnc12	0.47	*
112	C=CC(=O)Nc1cc2c(Nc3cccc(C)c3)ncnc2cn1	0.48	*
113	C#Cc1cccc(Nc2ncnc3cc(OC)c(OCCCCCn4ccnc4[N+](=O)[O-])cc23)c1	0.49	9.31
114	COc1cc2c(Nc3cccc(Br)c3)ncnc2cc1OCCCn1ccnc1[N+](=O)[O-]	0.49	9.31
115	O=C(O)[C@H]1O[C@@H]1C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	0.49	9.31
116	C#Cc1cccc(Nc2ncnc3cc(OC)c(OCCCCCCn4ccnc4[N+](=O)[O-])cc23)c1	0.5	9.30
117	O=C(O)[C@@H]1O[C@H]1C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	0.5	9.30
118	COc1cc(C(=O)NCCN(C)C)ccc1-c1cc2c(N[C@H](C)c3ccccc3)ncnc2s1	0.5	9.30
119	COc1ccc(C(=O)NCCN(C)C)cc1-c1cc2c(N[C@H](C)c3ccccc3)ncnc2s1	0.5	9.30
120	C=CC(=O)N1CC[C@H](N2C(=O)N(c3ccccc3Cl)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	0.5	9.30
121	CN1CCN(CCC#CC(=O)Nc2cc3c(Nc4ccc(F)c(Cl)c4)ncnc3cn2)CC1	0.5	*
122	C/C=C/C(=O)Nc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	0.5	*
123	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCOP(N)(=O)N(CCCl)CCCl	0.5	*
124	OCCCc1nc(-c2ccc(F)cc2)c(-c2ccnc3[nH]c(-c4ccccc4)cc23)[nH]1	0.5	*
125	NCc1cccc(-c2nc(-c3ccc(F)cc3)c(-c3ccnc4[nH]c(-c5ccccc5)cc34)[nH]2)c1	0.5	*
126	COc1cc(C=O)ccc1-c1cc2c(N[C@H](C)c3ccccc3)ncnc2[nH]1	0.5	*
127	COc1ccccc1-c1cc2c(N[C@H](CO)c3ccccc3)ncnc2[nH]1	0.5	*
128	COc1cc(C=O)ccc1-c1cc2c(NCc3ccccc3)ncnc2[nH]1	0.5	*
129	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCCCn1ccnc1[N+](=O)[O-]	0.51	9.29
130	O=C(CCN1CCOCC1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	0.51	9.29
131	CCOc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)CCN1CCCCC1	0.51	9.29

132	Brc1cccc(Nc2ncnc3cc(NCCCn4ccnc4)ncc23)c1	0.51	*
133	Brc1cccc(Nc2ncnc3ccncc23)c1NCCCn1ccnc1	0.5129	*
134	COc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCCCn1ccnc1[N+](=O)[O-]	0.52	9.28
135	CC1(C)Cc2c(nn(-c3ccc(Cl)cc3)c(=O)c2C#N)-c2c1sc(N)c2C#N	0.52	*
136	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C(F)=C/CN1CCOCC1	0.53	9.28
137	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCCn1c([N+](=O)[O-])cnc1C	0.53	9.28
138	C#Cc1cccc(Nc2ncnc3cc(OCCOCCn4ccnc4[N+](=O)[O-])c(OC)cc23)c1	0.54	9.27
139	C=CC(=O)Nc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	0.54	*
140	C/C=C/C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	0.55	*
141	C#Cc1cccc(Nc2ncnc3cc(OC)c(OCCCCn4ccnc4[N+](=O)[O-])cc23)c1	0.56	9.25
142	CN(CC(O)CO)c1cc2c(Nc3cccc(Br)c3)ncnc2cn1	0.56	*
143	O=C(/C=C/C(=O)Nc1cc2c(Nc3cccc(Br)c3)ncnc2cn1)NCCCn1ccnc1	0.56	*
144	C#Cc1cccc(Nc2ncnc3cc(OCCCCCCn4ccnc4[N+](=O)[O-])c(OC)cc23)c1	0.57	9.24
145	CCOc1cc2ncc(C#N)c(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)Cc1ccc(F)cc1	0.57	9.24
146	C=CC(=O)Nc1cccc(N2C(=O)N(C3CC3)Cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	0.58	9.24
147	C#Cc1cccc(Nc2ncnc3cc(OCCOC)c(OCCOC)cc23)c1	0.6	7.86
148	CCOc1cc2ncc(C#N)c(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	0.6	8.00
149	C[C@@H](Nc1ncnc2oc(-c3ccc(NCCN4CCCCC4)cc3)cc12)c1ccccc1	0.6	9.22
150	C#CC(=O)Nc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	0.6	*
151	O=Cc1ccc(-c2cc3c(N[C@H](CO)c4ccccc4)ncnc3[nH]2)c(F)c1	0.6	*
152	O=C(O)CCNc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	0.61	*
153	O=C(/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cn1)NCCCN1CCOCC1	0.61	*
154	O=C(O)CCNc1c(Br)cccc1Nc1ncnc2ccncc12	0.6166	*
155	CCOC(=O)c1cc(N)c(C(=O)OCC)c2c1C(C)(C)Cc1c-2sc(=S)n1-c1ccccc1	0.62	*
156	Nc1sc2c(c1C(=O)Nc1ccc([N+](=O)[O-])cc1)CCC(=O)C2=NNc1ccc(Cl)cc1	0.62	*
157	O=C(CCCN1CCCCC1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	0.63	9.20
158	COc1ccc(NN=C2C(=O)CCc3c2sc(N)c3C(=O)Nc2ccc(Cl)cc2)cc1	0.63	*
159	CCOC(=O)c1c(NC(=O)CCl)sc2c1-c1sc(=S)n(-c3ccccc3)c1CC2(C)C	0.64	*
160	C#Cc1cccc(Nc2ncnc3cc(OCCCn4ccnc4[N+](=O)[O-])c(OC)cc23)c1	0.65	9.19
161	O=C(CCCCCn1cc(-c2ccc3ncnc(Nc4ccc(F)c(Cl)c4)c3c2)nn1)NO	0.65	*
162	Brc1cccc(Nc2ncnc3cnc(NCCN4CCOCC4)cc23)c1	0.65	*
163	COc1cc2ncnc(Nc3cccc(Br)c3)c2cc1OCCCn1ccnc1[N+](=O)[O-]	0.66	9.18
164	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C(F)=C\CN1CCCCC1	0.67	9.17
165	COc1cc2ncnc(Nc3cccc(Br)c3)c2c(OC)c1OC	0.67	*
166	CCOc1cc2ncc(C#N)c(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)CCN(C)C	0.68	9.17
167	O=C(CCCCCCn1cc(-c2ccc3ncnc(Nc4ccc(F)c(Cl)c4)c3c2)nn1)NO	0.69	*
168	C=CC(=O)Nc1ccc2ncnc(Nc3ccc(F)c(Br)c3)c2c1	0.69	*
169	CNc1cc2ncnc(Nc3cccc(Br)c3)c2cc1N	0.69	*
170	O=C(/C=C/Cl)Nc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	0.69	*
171	CC1(C)Cc2c(sc(=S)n2-c2ccccc2)-c2c1nn(-c1ccc(Cl)cc1)c(=O)c2C#N	0.69	*
172	CC1(C)Cc2c(sc(=S)n2-c2ccccc2)-c2c1sc(NC(=O)CCl)c2C#N	0.69	*
173	OC[C@@H](Nc1ncnc2[nH]c(-c3ccccc3)cc12)c1ccccc1	0.7	*
174	C=CC(=O)Nc1cccc(n2c(=O)n(CCc3ccccc3)c(=O)c3cnc(Nc4ccc(N5CCC(N(C)C)CC5)cc4OC)nc32)c1	0.7	*

175	CN(CC(=O)O)Cc1c[nH]c2cc3ncnc(Nc4cccc(Br)c4)c3cc12	0.72	*
176	C=CC(=O)Nc1cc2c(Nc3ccc(F)c(Br)c3)ncnc2cn1	0.72	*
177	CCN(CC)CCCNC(=O)/C=C/C(=O)Nc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	0.73	*
178	C=CC(=O)Nc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	0.75	*
179	C=CC(=O)Nc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2n1	0.75	*
180	CNc1ncc2ncnc(Nc3cccc(Br)c3)c2n1	0.76	*
181	C=CS(=O)(=O)Nc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	0.76	*
182	COc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCn1ccnc1[N+](=O)[O-]	0.77	9.11
183	C=CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cn1	0.77	*
184	O=C(NCCN1CCCCC1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	0.772	9.11
185	COc1cc2c(Nc3cccc(Br)c3)ncnc2cc1OCCCCCCn1ccnc1[N+](=O)[O-]	0.78	9.11
186	C=CC(=O)Nc1cc2c(Nc3cccc(Br)c3)ncnc2cc1SCCCN(CC)CC	0.78	*
187	Brc1cccc(Nc2ncnc3cnc(NCCc4c[nH]cn4)cc23)c1	0.78	*
188	Nc1ccc2ncncc2c1	0.79	*
189	CCOc1cc2ncc(C#N)c(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)CCF	0.8	9.10
190	C=CC(=O)Nc1cccc(N2C(=O)N(c3ccc4ccccc4c3)Cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	0.8	9.10
191	Cn1ccc2cc3c(Nc4cccc(Br)c4)ncnc3cc21	0.8	*
192	OCCNc1nc(NCc2ccccc2)c2cn[nH]c2n1	0.8	*
193	C[C@@H](Nc1ncnc2[nH]c(-c3cccc(O)c3)cc12)c1ccccc1	0.8	*
194	C[C@@H](Nc1ncnc2[nH]c(-c3ccccc3CO)cc12)c1ccccc1	0.8	*
195	CCOC1=C2C(=CCc3c2sc(N)c3C(=O)Nc2ccc(Cl)cc2)OC(N)=C1C#N	0.8	*
196	C=CC(=O)Nc1cccc(N2C(=O)N(c3cccc4ccccc34)Cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	0.8	*
197	NC(=O)Nc1ccc2ncnc(Nc3ccc(Br)cc3)c2c1	0.803	9.10
198	Nc1cc2ncnc(Nc3cccc(Br)c3)c2cc1N	0.81	9.09
199	Brc1cccc(Nc2ncnc3cnc(NCCN4CCOCC4)nc23)c1	0.81	*
200	O=C(/C=C/C(=O)Nc1cc2c(Nc3cccc(Br)c3)ncnc2cn1)NCCCN1CCOCC1	0.81	*
201	CCOC(=O)c1c(NC2=C(Cl)C(c3ccc(Cl)cc3)C(C#N)=C(O)O2)sc2c1-c1sc(=S)n(-c3ccccc3)c1CC2(C)C	0.81	*
202	COc1cc2c(Nc3cccc(Br)c3)ncnc2cc1OCCOCCn1ccnc1[N+](=O)[O-]	0.82	9.09
203	CC1(C)C2=C(OC(N)=C(C#N)C2c2ccccc2)C(=NNc2ccc(Cl)cc2)c2c1sc(N)c2C#N	0.83	*
204	NC(=O)Nc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	0.854	9.07
205	CC1(C)Cc2c(sc(=S)n2-c2ccccc2)-c2c1sc(N)c2C#N	0.86	*
206	CCOc1cc2ncnc(Nc3ccc(OCc4ccccn4)c(Cl)c3)c2cc1NC(=O)/C(F)=C\CN(C)C	0.89	9.05
207	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCn1ccnc1[N+](=O)[O-]	0.89	9.05
208	COc1cc2ncnc(Nc3cccc(I)c3)c2cc1OC	0.89	*
209	COc1cccc(OC)c1-c1cc2c(N[C@H](CO)c3ccccc3)ncnc2s1	0.9	9.05
210	C[C@@H](Nc1ncnc2sc(-c3cccc(C(=O)NCCN(C)C)c3)cc12)c1ccccc1	0.9	9.05
211	O=C(C#CCCN1CCCCC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cn1	0.9	*
212	O=C(/C=C/CN1CC2CCC1C(=O)C2)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	0.9	*
213	CCOc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CNC1CC1	0.9	*
214	CN(C)C1CCN(c2ccc(Nc3cc4c(N5CCCCC5)nc(Nc5ccccc5)nc4cn3)nc2)CC1	0.9	*
215	CN(C)C1CCN(c2ccc(Nc3cc4c(N5CCOCC5)nc(Nc5ccc(F)cc5F)nc4cn3)nc2)CC1	0.9	*
216	Brc1cccc(Nc2ncnc3cc(NCCc4c[nH]cn4)ncc23)c1	0.91	*
217	C=CC(=O)Nc1ccc2ncnc(Nc3cccc(C(F)(F)F)c3)c2c1	0.91	*

218	C=CC(=O)Nc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	0.91	*
219	Brc1cccc(Nc2ncnc3ccncc23)c1NCCc1c[nH]cn1	0.912	*
220	OCC(O)CNc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	0.92	*
221	OCCN(CCO)CCNc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	0.93	*
222	OCC(O)CNc1c(Br)cccc1Nc1ncnc2ccncc12	0.9333	*
223	C=CC(=O)Nc1nc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OC	0.95	*
224	CN(C)c1ncc2ncnc(Nc3cccc(Br)c3)c2n1	0.95	*
225	C=CC(=O)Nc1nc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCOC	0.97	*
226	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)/C(F)=C\CN1CCOCC1	1	9.00
227	C#Cc1cccc(Nc2ncnc3cc(OCCO)c(OCCOC)cc23)c1	1	9.00
228	COc1cc2ncnc(Nc3cc(Cl)ccc3F)c2cc1OC1CCN(S(C)(=O)=O)CC1	1	*
229	COc1ccccc1-c1cc2c(N[C@H](CO)c3ccccc3)ncnc2s1	1	*
230	CC(C)(O)CC(=O)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21	1	*
231	C=CC(=O)Nc1cccc(-n2c(=O)c(Cc3ccccc3)cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	1	*
232	CS(=O)(=O)CCNCc1ccc(-c2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)o1	1	*
233	Brc1cccc(Nc2ncnc3cnc(NCCCN4CCOCC4)cc23)c1	1	*
234	Oc1cccc(Nc2[nH]nc3ncnc(Nc4cccc(Cl)c4)c23)c1	1	*
235	Cc1cccc(Nc2cc(NCCO)ncn2)c1	1	*
236	Nc1cc2sc3c(Nc4cccc(Br)c4)ncnc3c2cc1F	1	*
237	COc1cc2c(Nc3ccc(NC(=O)Nc4ccc(Cl)cc4)c(Cl)c3)ncnc2cc1OCCCN1CCN(C)CC1	1	*
238	COc1cc2c(Nc3ccc(NC(=O)Nc4ccc(C)c(C)c4)c(Cl)c3)ncnc2cc1OCCCN1CCN(C)CC1	1	*
239	c1ccc(CCCN(c2cc3ncnc(Nc4ccc5[nH]ccc5c4)c3s2)n2ccnc2)cc1	1	*
240	c1csc(-c2cc3nccc(Nc4ccc5[nH]ccc5c4)c3s2)c1	1	*
241	c1ccc(NCCN(c2cc3ncnc(Nc4ccc5[nH]ccc5c4)c3s2)n2cccc2)cc1	1	*
242	c1csc(-c2cc3ncnc(Nc4ccc5[nH]ccc5c4)c3s2)c1	1	*
243	OCc1ccc(-c2cc3ncnc(Nc4ccc5[nH]ccc5c4)c3s2)cc1	1	*
244	NC(=O)C1CCN(Cc2ccc(-c3cc4nccc(Nc5ccc6[nH]ccc6c5)c4s3)cc2)CC1	1	*
245	COc1cc(F)ccc1-c1cc2c(NC(CO)c3ccccc3)ncnc2[nH]1	1	*
246	CN(C)CC=CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	1	*
247	C=CC(=O)Nc1cccc(Nc2cc(-c3[nH]c(SC)nc3-c3ccc(F)cc3)ccn2)c1	1	*
248	C=CC(=O)Nc1ccc(OC)c(Nc2cc(-c3[nH]c(SC)nc3-c3ccc(F)cc3)ccn2)c1	1	*
249	CCC(=O)Nc1ccc(OC)c(Nc2cc(-c3[nH]c(SC)nc3-c3ccc(F)cc3)ccn2)c1	1	*
250	C=CC(=O)Nc1cc(Nc2cc(-c3[nH]c(SC)nc3-c3ccc(F)cc3)ccn2)cc(N2CCOCC2)c1	1	*
251	C=CC(=O)Nc1cc(Nc2cc(-c3[nH]c(SC)nc3-c3ccc(F)cc3)ccn2)cc(N2CCN(C)CC2)c1	1	*
252	C=CC(=O)Nc1cccc(Nc2cc(-c3[nH]c(SC)nc3-c3ccc(F)cc3)ccn2)n1	1	*
253	C=CC(=O)Nc1ccc(OC)c(Nc2cc(-c3[nH]c(SC)nc3-c3ccc4ccccc4c3)ccn2)c1	1	*
254	C=CC(=O)Nc1ccc(OC)c(Nc2cc(-c3[nH]c(SC)nc3C3CCCC3)ccn2)c1	1	*
255	C=CC(=O)Nc1ccc(OC)c(Nc2cc(-c3[nH]c(CCCO)nc3-c3ccc(F)cc3)ccn2)c1	1	*
256	CCC(=O)Nc1ccc(OC)c(Nc2cc(-c3[nH]c(CCCO)nc3-c3ccc(F)cc3)ccn2)c1	1	*
257	C=CC(=O)Nc1ccc(OC)c(Nc2cc(-c3[nH]c(SC)nc3-c3cccs3)ccn2)c1	1	*
258	C=CC(=O)Nc1cccc(Nc2cc(-c3[nH]c(SCCNC(=O)CC)nc3-c3ccccc3)ccn2)c1	1	*
259	C=CC(=O)Nc1ccc(OC)c(Nc2cc(-c3[nH]c(SC)nc3C3CCC3)ccn2)c1	1	*
260	CC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	1.01	9.00

261	O=C(NCCN1CCCCC1)Nc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	1.06	8.97
262	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)[C@@H]1COC(=O)N1	1.06	8.97
263	C#Cc1cccc(Nc2ncnc3cc(OC)c(OCCCn4ccnc4[N+](=O)[O-])cc23)c1	1.08	8.97
264	C[C@@H](Nc1ncnc2oc(-c3ccc(NCCN4CCOCC4)cc3)cc12)c1ccccc1	1.1	8.96
265	CN(C)CCNc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	1.1	*
266	CNc1cc2c(Nc3cccc(C(F)(F)F)c3)ncnc2cn1	1.1	*
267	C=CC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2n1	1.1	*
268	CCO.CNc1ccc2sc3c(Nc4cccc(Br)c4)ncnc3c2c1	1.1	*
269	C=C/C=C/C(=O)Nc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	1.1	*
270	CN(C)CCCNC(=O)/C=C/C(=O)Nc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	1.1	*
271	Cc1cc(C(=O)NCCN2CCOCC2)[nH]c1/C=C1\C(=O)Nc2ncnc(Nc3ccc4c(ccn4Cc4ccccc4)c3)c21	1.1	*
272	CN1CCN(c2ccc(Nc3cc4c(N5CCCCC5)nc(Nc5ccccc5)nc4cn3)nc2)CC1	1.1	*
273	COc1ccccc1-c1cc2c(N[C@H](C)c3ccccc3)ncnc2[nH]1	1.1	*
274	COc1cc2ncnc(Nc3cccc(C(=O)NC45CC6CC(CC(C6)C4)C5)c3)c2cc1OCCCN1CCOCC1	1.12	8.95
275	COc1cc2ncnc(Nc3cccc(Br)c3)c2cc1OCCCn1c([N+](=O)[O-])cnc1C	1.18	8.93
276	CCOc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2cc1NC(=O)[C@H]1COC(=O)N1	1.19	8.92
277	C#Cc1cccc(Nc2ncnc3cc(O[C@H]4CCOC4)c(NC(=O)/C=C/CN(C)C)cc23)c1	1.2	*
278	C#Cc1cccc(Nc2ncnc3cc(OCCOC)c(NC(=O)/C=C/CN(C)C)cc23)c1	1.2	*
279	COCCOc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	1.2	*
280	OCCN(CCO)CCCNc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	1.2	*
281	CN(C)CCCNc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	1.2	*
282	Brc1cccc(Nc2ncnc3cnc(NCCc4ccccn4)cc23)c1	1.2	*
283	C=CC(=O)Nc1ccc2ncnc(Nc3ccc(F)c(Br)c3)c2n1	1.2	*
284	COc1ccc2[nH]c3ncnc(Nc4cccc(Br)c4)c3c2c1	1.2	*
285	C=C(C)C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	1.2	*
286	CC(=O)/C=C/C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	1.2	*
287	CCN(CC)CCNC(=O)c1cc(C)c(/C=C2\C(=O)Nc3ncnc(Nc4ccc(F)c(Cl)c4)c32)[nH]1	1.2	*
288	C=CC(=O)Nc1cccc(-n2c(=O)n(Cc3ccccc3)c(=O)c3cnc(Nc4ccc(N5CCC(N(C)C)CC5)cc4OC)nc32)c1	1.2	*
289	OCCN(CCO)CCCNc1c(Br)cccc1Nc1ncnc2ccncc12	1.202	*
290	C=CC(=O)Nc1cccc(-n2c(=O)cnc3cnc(Nc4ccc(N5CCN(C)CC5)cc4)nc32)c1	1.21	8.92
291	O=C(Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)[C@@H]1O[C@H]1CN1CCCCC1	1.24	8.91
292	Brc1cccc(Nc2ncnc3ccc4cc[nH]c4c23)c1	1.24	*
293	CCOC1=C2C(=CCc3c2sc(N)c3C(=O)Nc2ccc([N+](=O)[O-])cc2)OC(O)=C1C#N	1.24	*
294	CC1(C)Cc2c(sc(=S)n2-c2ccccc2)-c2c1sc(NC1=C(Cl)C(c3ccc(Cl)cc3)C(C#N)=C(N)O1)c2C#N	1.27	*
295	Nc1sc2c(c1C(=O)Nc1ccc(Cl)cc1)CCC(=O)C2=NNc1ccccc1	1.28	*
296	Nc1sc2c(c1C(=O)Nc1ccc(Cl)cc1)CC=C1C2SC(=S)N1c1ccccc1	1.29	*
297	COc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2cc1NC(=O)/C(F)=C\CN(C)C	1.3	8.89
298	N#Cc1ccc(F)c(C(=O)Nc2cc3c(Nc4ccc(F)c(Cl)c4)ncnc3cc2OCCCN2CCOCC2)c1	1.3	8.89
299	O=C(C#CCCN1CCOCC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cn1	1.3	*
300	Cc1cccc(Nc2ncnc3cnc(NCCc4c[nH]cn4)cc23)c1	1.3	*
301	CN(C)CCn1cnc2cc3ncnc(Nc4cccc(Br)c4)c3cc21	1.32	*
302	CCOc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2cc1NC(=O)[C@@H]1COC(=O)N1	1.34	8.87
303	O=C(C#CCO)Nc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	1.4	*

304	O=S(=O)(O)CCNc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	1.4	*
305	CNc1cc2ncnc(Nc3cccc(C)c3)c2cn1	1.4	*
306	C=CS(=O)(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	1.4	*
307	Cc1ccccc1Nc1nc2cc(F)c(N(C)C(=O)/C=C/CN(C)C)cc2n2cncc12	1.4	*
308	C=CC(=O)Nc1cccc(-n2c(=O)c(=O)n(C(C)C)c3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)c1	1.4	*
309	C=CC(=O)Nc1cc(Nc2n[nH]c3cc(-c4cccc5ccccc45)ccc23)c(OC)cc1N(C)CCN(C)C	1.4	*
310	COc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2cc1OCCCN1CCNCCNCC1	1.4	*
311	C=CC(=O)Nc1cccc(N2C(=O)N(c3ccc(-c4ccccc4)cc3)Cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	1.41	8.85
312	O=S(=O)(O)CCNc1c(Br)cccc1Nc1ncnc2ccncc12	1.413	*
313	O=C(NCCN1CCOCC1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	1.43	8.84
314	COc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCCCCn1ccnc1[N+](=O)[O-]	1.44	8.84
315	CN(C)CCCNC(=O)/C=C/C(=O)N(C)c1cc2c(Nc3cccc(Br)c3)ncnc2cn1	1.45	*
316	C=CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)c(C#N)cnc2cc1OCC	1.46	8.84
317	C=CC(=O)Nc1cccc(N2C(=O)N(C)Cc3cnc(Nc4ccc(N5CCCN(C)CC5)cc4OC)nc32)c1	1.47	8.83
318	Nc1sc2c(c1C(=O)Nc1ccc([N+](=O)[O-])cc1)CC=C1C2SC(=S)N1c1ccccc1	1.49	*
319	Fc1cccc(COc2ccc(Nc3ncnc4ccc(NC(=S)NCCCN5CCOCC5)cc34)cc2Cl)c1	1.5	8.82
320	C[C@@H](Nc1ncnc2oc(-c3ccc(O)cc3)cc12)c1ccccc1	1.5	8.82
321	COc1c(CO)cccc1-c1cc2c(N[C@H](C)c3ccccc3)ncnc2s1	1.5	8.82
322	COc1cc(C(N)=O)ccc1-c1cc2c(N[C@H](CO)c3ccccc3)ncnc2s1	1.5	8.82
323	O=C(C#CCCN1CCOCC1)Nc1cc2c(Nc3ccc(F)c(Br)c3)ncnc2cn1	1.5	*
324	C=CC(=O)Nc1ccc2ncnc(Nc3cccc(C)c3F)c2c1	1.5	*
325	C=CC(=O)Nc1cc2c(Nc3cccc(C)c3)ncnc2cc1OCCCN1CCOCC1	1.5	*
326	C=CC(=O)Nc1nc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1	1.5	*
327	O=C(O)CNc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	1.5	*
328	Brc1cccc(Nc2ncnc3cnc(NCc4cccnc4)cc23)c1	1.5	*
329	Cc1cccc(Nc2ncnc3cnc(NCCN4CCOCC4)cc23)c1	1.5	*
330	Nc1ncc2ncnc(Nc3cccc(Br)c3)c2n1	1.5	*
331	CCOC(=O)/C=C/C(=O)Nc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	1.5	*
332	C=CC(=O)N[C@H]1CCN(c2nc(Nc3ccccc3)nc3cnc(Nc4ccc(N5CCN(C)CC5)cn4)cc23)C1	1.5	*
333	CN(C)C1CCN(c2ccc(Nc3cc4c(N5CCOCC5)nc(Nc5ccc(F)cc5)nc4cn3)nc2)CC1	1.5	*
334	COc1ccc(NN=C2C(=O)CCc3c2sc(N)c3C(=O)Nc2ccc([N+](=O)[O-])cc2)cc1	1.51	*
335	O=C(O)CNc1c(Br)cccc1Nc1ncnc2ccncc12	1.514	*
336	C=CC(=O)Nc1cccc(N2C(=O)N(c3ccc(Oc4ccccc4)cc3)Cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	1.52	8.82
337	COc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2cc1NC(=O)/C(F)=C/CN(C)C	1.56	8.81
338	C#CC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	1.6	*
339	OCC(O)Cn1ccc2cc3c(Nc4cccc(Br)c4)ncnc3cc21	1.6	*
340	C=CC(=O)Nc1ccc2c(Nc3cccc(C)c3)ncnc2c1	1.6	*
341	C=CC(=O)Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	1.6	*
342	C=C(C)C(=O)Nc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	1.6	*
343	C=C=CC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	1.6	*
344	C=CC(=O)NCCSc1nc(-c2ccc(F)cc2)c(-c2ccnc(Nc3ccccc3)c2)[nH]1	1.6	*
345	CC1(C)Cc2nn(-c3ccc(Cl)cc3)nc2-c2c1sc1nc(=NO)n(-c3ccccc3)c(O)c21	1.6	*
346	COCCOc1cc2ncnc(Nc3cccc(NC(=O)C45CC6CC(CC(C6)C4)C5)c3)c2cc1OCCOC	1.63	8.79

347	COC[C@H]1Oc2cc3ncnc(Nc4cccc(I)c4)c3cc2O[C@@H]1COC	1.66	*
348	C=CC(=O)Nc1cccc(N2C(=O)N(c3ccc(OCc4ccccc4)cc3)Cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	1.67	8.78
349	C=CC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	1.69	8.77
350	CN(C)CCCC(=O)Nc1ccc2nccc(Nc3cccc(Br)c3)c2c1	1.7	8.77
351	COC(=O)c1ccc2oc3cnnc(Nc4cccc(Cl)c4)c3c2c1	1.7	8.77
352	O=C(C#CCCN1CCOCC1)Nc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	1.7	*
353	CCCC#CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cn1	1.7	*
354	C=CC(=O)Nc1cc2c(Nc3cccc(Br)c3)ncnc2cc1OCCCN1CCN(C)CC1	1.7	*
355	C=CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCOCCCCO	1.7	*
356	Brc1cccc(Nc2ncnc3cc4nccnc4cc23)c1	1.7	*
357	CN(CCO)CCNc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	1.7	*
358	Brc1cccc(Nc2ncnc3cnc(NCCCn4ccnc4)cc23)c1	1.7	*
359	Nc1sc2c(c1C(=O)Nc1ccc([N+](=O)[O-])cc1)CCC(=O)C2=NNc1ccccc1	1.73	*
360	O=C(/C=C/C(F)(F)F)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	1.75	*
361	COc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCN1C[C@H](O)[C@@H](O)[C@H](O)[C@H]1CO	1.79	*
362	COc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1C[C@H](O)[C@@H](O)[C@H](O)[C@H]1CO	1.79	*
363	CCN(CC)CCC#CC(=O)Nc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	1.8	*
364	C#Cc1cccc(Nc2ncnc3cc(OCCOC)c(NC(=O)C=C)cc23)c1	1.8	*
365	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CN1CCCCC1	1.8	*
366	CCOc1cc2ncnc(C#Cc3c[nH]nc3-c3ccc(F)cc3)c2cc1OCC	1.8	*
367	C=CC(=O)Nc1cc2c(Nc3ccc(F)c(Br)c3)ncnc2cc1OCCCN1CCOCC1	1.8	*
368	CN(C)CCCCNc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	1.8	*
369	Cc1cccc(Nc2ncnc3cnc(NCCCN4CCOCC4)cc23)c1	1.8	*
370	Brc1cccc(Nc2ncnc3c2sc2ccccc23)c1	1.8	*
371	Cc1cc(C(=O)N2CCOCC2)[nH]c1/C=C1\C(=O)Nc2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c21	1.8	*
372	COc1ccc(-c2cc3c(N[C@H](C)c4ccccc4F)ncnc3[nH]2)cc1	1.8	*
373	CC[C@@H](Nc1ncnc2[nH]c(-c3ccc(OC)cc3)cc12)c1ccccc1	1.8	*
374	S=C(NCCN1CCOCC1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	1.81	8.74
375	CCOc1cc2ncc(C#N)c(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CNCc1cn(CCF)nn1	1.81	8.74
376	CC1(C)CC(=NN)C(=NNc2ccc(Cl)cc2)c2c1sc(N)c2C#N	1.83	*
377	CN(C)C/C=C/C(=O)Nc1cc2c(Nc3cccc(Br)c3)c(C#N)cnc2cn1	1.9	8.72
378	O=C(CCCCCn1cc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)nn1)NO	1.9	*
379	Brc1cccc(Nc2ncnc3cc(NCCCN4CCOCC4)ncc23)c1	1.9	*
380	OCCn1ccc2ncnc(Nc3ccc(Oc4cccc5[nH]ncc45)c(Cl)c3)c21	1.9	*
381	C=CC(=O)N1CCC[C@H](Nc2nc(Nc3ccccc3)nc3cnc(Nc4ccc(N5CCN(C)CC5)cn4)cc23)C1	1.9	*
382	COc1cccc(-c2cc3c(N[C@H](C)c4ccccc4)ncnc3[nH]2)c1	1.9	*
383	Brc1cccc(Nc2ncnc3ccncc23)c1NCCCN1CCOCC1	1.905	*
384	C=CC(=O)Nc1cccc(N2C(=O)N(C)Cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4C)nc32)c1	1.95	8.71
385	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)[C@H]1NC(=O)O[C@@H]1C	1.98	8.70
386	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1SCCCCCCC(=O)NO	1.99	8.70
387	OC[C@@H](Nc1ncnc2oc(-c3ccc(O)cc3)cc12)c1ccccc1	2	8.70
388	C[C@@H](Nc1ncnc2oc(-c3ccccc3O)cc12)c1ccccc1	2	8.70
389	COc1cccc(OC)c1-c1cc2c(N[C@H](C)c3ccccc3)ncnc2s1	2	8.70

390	CN(C)CCNC(=O)c1ccc(-c2cc3c(N[C@H](CO)c4ccccc4)ncnc3s2)cc1	2	8.70
391	C[C@@H](Nc1ncnc2sc(-c3ccc(C(=O)NCCN(C)C)cc3)cc12)c1ccccc1	2	8.70
392	COc1cc(CO)ccc1-c1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	2	8.70
393	COc1cc(C(N)=O)ccc1-c1cc2c(N[C@H](C)c3ccccc3)ncnc2s1	2	8.70
394	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1OCC1CCN(C)CC1	2	*
395	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1OC1CCN(C)CC1	2	*
396	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1OC1CCN(CC(N)=O)CC1	2	*
397	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1OC1CCN(S(C)(=O)=O)CC1	2	*
398	COC(CN(C)C/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1)OC	2	*
399	O=C(/C=C/CN1CCC2(CC1)OCCO2)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	2	*
400	CCOc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2c2c1OCCO2	2	*
401	CCC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OC	2	*
402	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C(C)C)C(C)C	2	*
403	CN(C)C/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cn1	2	*
404	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCNCCN(C)C	2	*
405	CN(C)Cc1ccc(-c2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)o1	2	*
406	Clc1cccc(Nc2ncnc3cc4c(cc23)OCCOCCOCCO4)c1	2	*
407	Fc1ccc(Nc2ncnc3cc4c(cc23)OCCOCCOCCO4)cc1Cl	2	*
408	C#Cc1cccc(Nc2ncnc3cc4c(cc23)OCCOCCOCCO4)c1	2	*
409	c1ccc(-c2cccc(Nc3ncnc4cc5c(cc34)OCO5)c2)cc1	2	*
410	C=CC(=O)Nc1cc2c(Nc3cccc(C)c3)ncnc2cc1OCCCN1CCN(C)CC1	2	*
411	Nc1ccc2c(Nc3cccc(F)c3)ncnc2c1	2	*
412	Nc1ccc(-c2[nH]nc3ncnc(Nc4cccc(Cl)c4)c23)cc1	2	*
413	Cl.c1ccc(-c2cccc(Nc3ncnc4cc5c(cc34)OCO5)c2)cc1	2	*
414	C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4ccccc34)n2)c(OC)cc1N1CCN(C)CC1	2	*
415	O=C(C#CCO)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	2	*
416	C[C@H](CN(C)C(=O)CO)Oc1cccc2ncnc(Nc3ccc(OCc4ccccn4)c(Cl)c3)c12	2	*
417	CC(=O)NCCNCc1ccc(-c2cc3nccc(Nc4ccc5[nH]ccc5c4)c3s2)cc1	2	*
418	OCCNCc1ccc(-c2cc3nccc(Nc4ccc5[nH]ccc5c4)c3s2)cc1	2	*
419	CCN1CCN(Cc2ccc(-c3cc4c(N[C@H](C)c5ccccc5)ncnc4[nH]3)cc2)CC1	2	*
420	CCCN1CCC(Oc2cc(OC)cc3ncnc(Nc4ccc(F)c(Cl)c4)c23)CC1	2	*
421	CCN1CCC(Oc2cc(OC)cc3ncnc(Nc4ccc(F)c(Cl)c4)c23)CC1	2	*
422	C=CC(=O)Nc1cccc(-n2c(=O)c(=O)n(C(C)C)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	2	*
423	COc1cc2ncnc(Nc3ccc(C(=O)NC45CC6CC(CC(C6)C4)C5)cc3)c2cc1OCCCN1CCOCC1	2.01	8.70
424	CCOc1cc2ncc(C#N)c(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)CCN1CCOCC1	2.02	8.69
425	C#Cc1cccc(Nc2ncnc3ccc(NC(C)=O)cc23)c1	2.04	8.69
426	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)CCCCCCC(=O)NO	2.1	8.68
427	C=CC(=O)Nc1ccc2ncnc(Nc3ccc(Br)cc3F)c2c1	2.1	*
428	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CNC1CC1	2.1	*
429	COCCOc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CN1CCCCC1	2.1	*
430	Cc1cccc(Nc2ncnc3c2sc2ccc(N)cc23)c1	2.1	*
431	CN(C)C1CCN(c2ccc(Nc3cc4c(N5CCC(CO)CC5)nc(Nc5ccccc5)nc4cn3)nc2)CC1	2.1	*
432	COc1cc(CO)ccc1-c1cc2c(NCc3ccccc3)ncnc2[nH]1	2.1	*

433	CSc1nc(-c2ccc(F)cc2)c(-c2ccnc(Nc3cc(N4CCN(C)CC4)cc([N+](=O)[O-])c3)c2)[nH]1	2.1	*
434	O=C(NO)c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)s1	2.2	*
435	C=CC(=O)Nc1ccc2ncnc(Nc3c(F)cccc3Br)c2c1	2.2	*
436	C=CC(=O)Nc1ccc2ncnc(Nc3ccc(Br)cc3C)c2c1	2.2	*
437	C=CC(=O)Nc1cccc(-n2c(=O)c(=O)n(CCC)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	2.2	*
438	CCOc1cc2ncc(C#N)c(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)CCN1CCCCC1	2.21	8.66
439	C#Cc1cccc(Nc2ncnc3ccc(NC(N)=O)cc23)c1	2.22	8.65
440	Fc1ccc(Nc2ncnc3ccc(NC(=S)NCCN4CCOCC4)cc23)cc1Cl	2.25	8.65
441	Fc1cccc(COc2ccc(Nc3ncnc4ccc(NC(=S)NCCN5CCOCC5)cc34)cc2Cl)c1	2.26	8.65
442	C=CC(=O)Nc1ccc2ncnc(Nc3ccc(Br)c(C)c3)c2c1	2.3	*
443	COc1ccc(CNc2cc3c(Nc4cccc(Br)c4)ncnc3cn2)cc1	2.3	*
444	Brc1cccc(Nc2ncnc3cnc(NCCCn4ccnc4)nc23)c1	2.3	*
445	Cc1cccc(Nc2ncnc3cnc(NCCN4CCOCC4)nc23)c1	2.3	*
446	NP(=O)(OCCCCCOc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)N(CCCl)CCCl	2.3	*
447	C=CC(=O)Nc1ccc(OC)c(Nc2cc(-c3[nH]c(SC)nc3C3CC3)ccn2)c1	2.3	*
448	Brc1cccc(Nc2ncnc3cnc(NCCn4ccnc4)nc23)c1	2.344	*
449	C#Cc1cccc(Nc2ncnc3cc(OC)c(OCCCCCCC(=O)NO)cc23)c1	2.4	8.62
450	C#Cc1cccc(Nc2ncnc3cc(OCC)c(NC(=O)/C=C/CN(C)C4CC4)cc23)c1	2.4	*
451	CN(C)/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	2.4	*
452	CN(C)CCCOC(=O)/C=C/C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	2.4	*
453	COc1ncc(-c2ccc3ncnc(Nc4ccc(F)c(Cl)c4)c3c2)cc1NS(C)(=O)=O	2.4	*
454	CC1(C)Cc2c(sc(=S)n2-c2ccccc2)C(=O)C1=NNc1ccc(Cl)cc1	2.44	*
455	C=CC(=O)Nc1cccc(N2C(=O)C3CCCCN3C(=O)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	2.45	8.61
456	O=C(/C=C/c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1)NO	2.5	*
457	C=CC(=O)Nc1ccc2ncnc(Nc3ccc(Br)c(OC)c3)c2c1	2.5	*
458	C[C@@H](Nc1ncnc2[nH]c(-c3ccc(O)cc3)cc12)c1ccccc1	2.5	*
459	C#CCCCOc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OC	2.53	*
460	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)/C(F)=C\CN1CCCCC1	2.55	8.59
461	CCOc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2cc1NC(=O)[C@H]1NC(=O)O[C@@H]1C	2.57	8.59
462	COc1cc2ncnc(Nc3cccc(Br)c3)c2cc1OC	2.6	7.87
463	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)/C(F)=C/CN1CCCCC1	2.6	8.59
464	COc1cc2ncnc(Nc3cccc(Br)c3)c2cc1NC(=O)/C(F)=C/CN(C)C	2.6	8.59
465	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCNCC1)c1cc([N+](=O)[O-])ccc1F	2.6	8.59
466	COc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	2.6	*
467	CN(C)Cc1c[nH]c2cc3ncnc(Nc4cccc(Br)c4)c3cc12	2.6	*
468	CN(CCO)c1cc2ncnc(Nc3cccc(Br)c3)c2cn1	2.6	*
469	CC(C)(N)C(=O)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc5sncc45)c(Cl)c3)c21	2.6	*
470	C/C=C/C(=O)Nc1cc2c(N3CCc4ccccc43)ncnc2cc1OC1CCOC1	2.61	*
471	CN(CCO)c1c(Br)cccc1Nc1ncnc2ccncc12	2.63	*
472	COc1ccc(-c2cc3c(N[C@H](CO)c4ccccc4)ncnc3o2)cc1	2.7	8.57
473	C=CC(=O)Nc1ccc2ncnc(Nc3cccc(CC)c3)c2c1	2.7	*
474	C#Cc1cccc(Nc2ncnc3cc(OC)c(NC(=O)/C=C/CN4CCCCC4)cc23)c1	2.7	*
475	C=CC(=O)Nc1nc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1CCCCN1CCOCC1	2.7	*

476	CO.Nc1cccc2c1sc1c(Nc3cccc(Br)c3)ncnc12	2.7	*
477	CCOC(=O)/C=C/C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	2.7	*
478	C=CC(=O)N(CCCN1CCOCC1)c1cc2c(Nc3cccc(Br)c3)ncnc2cn1	2.7	*
479	C=CC(=O)N[C@@H]1CCN(c2nc(Nc3ccccc3)nc3cnc(Nc4ccc(N5CCN(C)CC5)cn4)cc23)C1	2.7	*
480	Cl.Nc1cccc2c1sc1c(Nc3cccc(Br)c3)ncnc12	2.7	*
481	CN(C)C/C=C/C(=O)NCCSc1nc(-c2ccc(F)cc2)c(-c2ccnc(Nc3ccccc3)c2)[nH]1	2.7	*
482	Nc1ccccc1NC(=O)c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)s1	2.8	*
483	Cc1cccc(Nc2ncnc3cnc(N(C)C)cc23)c1	2.8	*
484	Cc1cc(C(=O)N2CCN(C)CC2)[nH]c1/C=C1\C(=O)Nc2ncnc(Nc3ccc(F)c(Cl)c3)c21	2.8	*
485	O=C1Cc2cccc(Oc3ccc(Nc4ncnc5ccn(CCO)c45)cc3Cl)c2N1	2.8	*
486	COc1ccc(-c2cc3c(N[C@H](C)c4ccc(F)cc4)ncnc3[nH]2)cc1	2.8	*
487	C=CC(=O)Nc1cccc(-n2c(=O)c(=O)[nH]c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	2.8	*
488	C=CC(=O)Nc1cc(Nc2n[nH]c3cc(-c4cncc5ccccc45)ccc23)c(OC)cc1N(C)CCN(C)C	2.8	*
489	Nc1ccccc1NC(=O)c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	2.9	*
490	Brc1cccc(Nc2ncnc3cnc(NCCCN4CCOCC4)nc23)c1	2.9	*
491	CC(=O)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc5sncc45)c(Cl)c3)c21	2.9	*
492	COCCOc1cc2ncnc(Nc3ccc(NC(=O)C45CC6CC(CC(C6)C4)C5)c(C)c3)c2cc1OCCOC	2.92	8.53
493	O=C(NCCN1CCOCC1)Nc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	2.92	8.53
494	CNC(=O)c1cc(Oc2ccc(NC(=O)Nc3ccc(Cl)c(C(F)(F)F)c3)cc2)ccn1	2.96	*
495	Cn1cc(-c2ccc3ncnc(Nc4ccc(F)c(Cl)c4)c3c2)cn1	2.97	8.53
496	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C#Cc1ccc(CNC(C)C)cc1	3	8.52
497	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1/C=C(\F)C(=O)NCCN1CCCC1	3	8.52
498	COc1c(C(=O)NCCN(C)C)cccc1-c1cc2c(N[C@H](C)c3ccccc3)ncnc2s1	3	8.52
499	COc1ccc(C=O)cc1-c1cc2c(N[C@H](C)c3ccccc3)ncnc2s1	3	8.52
500	OCc1cccc(-c2cc3c(N[C@H](CO)c4ccccc4)ncnc3s2)c1	3	8.52
501	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1)c1ccccc1F	3	8.52
502	C=CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1.Cl.Cl	3	*
503	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCC1CCN(C)CC1	3	*
504	COCCN1CCC(Oc2cc3c(Nc4cccc(Cl)c4F)ncnc3cc2OC)CC1	3	*
505	C#Cc1cccc(Nc2ncnc3cc4c(cc23)N(C(=O)/C=C/CN2CCCC2)CCO4)c1	3	*
506	C#Cc1cccc(Nc2ncnc3cc4c(cc23)N(C(=O)/C=C/CN(C)C)CCO4)c1	3	*
507	CS(=O)(=O)CCNC/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	3	*
508	O=C(/C=C/CN1CCOCC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	3	*
509	COCCOc1cc2ncnc(Nc3ccc(Br)cc3F)c2cc1NC(=O)/C=C/CN(C)C	3	*
510	CC(=O)Nc1ccc2ncnc(Nc3ccc(OCc4ccccn4)c(Cl)c3)c2c1	3	*
511	CS(=O)(=O)CCNCc1cc(-c2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)cs1	3	*
512	OCc1ccc(-c2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)o1	3	*
513	N#CCNCc1ccc(-c2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)o1	3	*
514	CCN(CC)[C@@](C)(C#Cc1ncnc2cc(OC)c(OC)cc12)Cc1ccccc1	3	*
515	C=CC(=O)Nc1cc2c(Nc3cccc(Br)c3)ncnc2cc1OCCCn1ccnc1	3	*
516	CN1CCC(Nc2ncc3ncnc(Nc4ccc(F)c(Cl)c4)c3n2)CC1	3	*
517	Cc1cccc(Nc2ncnc3cnc(NCCc4c[nH]cn4)nc23)c1	3	*
518	CN1CCC(Oc2cccc3ncnc(Nc4ccc(F)c(Cl)c4)c23)CC1	3	*

519	O=C1Cc2c(cccc2Oc2ccc(Nc3ncnc4ccn(CCO)c34)cc2Cl)N1	3	*
520	Cl.O=C(NCCn1ccc2ncnc(Nc3ccc(Oc4cccc5sncc45)c(Cl)c3)c21)[C@@H]1CCCN1	3	*
521	C[C@H](COc1cccc2ncnc(Nc3ccc(OCc4ccccn4)c(Cl)c3)c12)N(C)C(=O)CO	3	*
522	CN(CCO)Cc1ccc(-c2cc3nccc(Nc4ccc5[nH]ccc5c4)c3s2)cc1	3	*
523	c1cc(Nc2ccc3[nH]ccc3c2)c2sc(-c3ccc(CNCCN4CCNCC4)cc3)cc2n1	3	*
524	NP(=O)(OCCCOc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)N(CCCl)CCCl	3	*
525	Nc1ccc(-c2cc3c(Nc4cccc(Cl)c4)ncnc3[nH]2)cc1	3	*
526	Nc1ccc(-c2cc3c(Nc4cccc(Cl)c4)ncnc3o2)cc1	3	*
527	C[C@@H](Nc1ncnc2oc(-c3cccc(N)c3)cc12)c1ccccc1	3	*
528	Nc1cccc(-c2cc3c(Nc4cc(Cl)ccc4O)ncnc3o2)c1	3	*
529	CCN(CC)C(C)(C#Cc1ncnc2cc(OC)c(OC)cc12)Cc1ccccc1	3	*
530	CC1CCCCN1CC=CC(=O)N1CCOc2cc3ncnc(Nc4ccc(F)c(Cl)c4)c3cc21	3	*
531	O=C(C=CCN1CCCC1)N1CCOc2cc3ncnc(Nc4ccc(F)c(Cl)c4)c3cc21	3	*
532	COc1cc2ncnc(N3CCc4ccccc43)c2cc1NC(=O)/C=C/CN1CCCC1	3	*
533	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCn1ccnc1[N+](=O)[O-]	3.05	8.52
534	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCN1CCOCC1	3.1	8.48
535	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCCCCC(=O)NO	3.1	8.51
536	CCN(CC)CC#CC(=O)Nc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	3.1	*
537	O=C(C#CCN1CCOCC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cn1	3.1	*
538	CNC1=CC2N=CN(C)/C(=N\c3cccc(Br)c3)C2C=N1	3.1	*
539	Cc1cccc(Nc2ncnc3cnc(N)cc23)c1	3.1	*
540	OCCn1ccc2ncnc(Nc3ccc(Oc4cccc5[nH]ccc45)c(Cl)c3)c21	3.1	*
541	COc1cc2ncnc(Nc3cccc(NC(=O)C45CC6CC(CC(C6)C4)C5)c3)c2cc1OCCCN1CCOCC1	3.11	8.51
542	C=C=CCCCOc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O	3.16	*
543	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(C)CC4)cc3OC)ncc2Cl)c1	3.2	8.32
544	C=CC(=O)Nc1ccc2ncnc(Nc3ccc(CC)cc3)c2c1	3.2	*
545	CN(CC(O)CO)c1cc2ncnc(Nc3cccc(Br)c3)c2cn1	3.2	*
546	CN(CC(O)C(O)C(O)C(O)CO)c1cc2ncnc(Nc3cccc(Br)c3)c2cn1	3.2	*
547	Brc1cccc(Nc2ncnc3cc(NCCN4CCOCC4)ncc23)c1	3.2	*
548	C=C=CC(=O)Nc1cc(Nc2nccc(C3=CNC4C=CC=CC34)n2)c(OC)cc1N(C)CCN(C)C	3.2	*
549	C=C=CC(=O)Nc1cc(Nc2nccc(-c3c[nH]c4ccccc34)n2)c(OC)cc1N(C)CCN(C)C	3.2	*
550	C[C@@H](Nc1ncnc2[nH]c(-c3ccccc3)cc12)c1ccccc1	3.2	*
551	CN(CC(O)CO)c1c(Br)cccc1Nc1ncnc2ccncc12	3.236	*
552	Brc1cccc(Nc2ncnc3ccncc23)c1NCCN1CCOCC1	3.236	*
553	C=CC(=O)NCc1coc(-c2c(N)ncnc2Nc2ccc(OCc3ccccn3)c(Cl)c2)n1	3.3	8.48
554	C#Cc1cccc(Nc2ncnc3cc(OC)c(NC(=O)/C=C/CN(C)C4CC4)cc23)c1	3.3	*
555	Nc1ccc2c(Nc3cccc(C(F)(F)F)c3)ncnc2c1	3.3	*
556	C=CC(=O)N(CCCN1CCOCC1)c1ccc2ncnc(Nc3cccc(Br)c3)c2c1	3.3	*
557	C[C@@H](Nc1[nH]cnc2nc(-c3ccccc3)cc1-2)c1ccccc1	3.3	*
558	Br.Oc1ccc(-c2cc3c(NCc4ccccc4)ncnc3[nH]2)cc1	3.3	*
559	NP(=O)(OCCCC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)N(CCCl)CCCl	3.3	*
560	C=CC(=O)N1CC[C@@H](Nc2nc(Nc3ccccc3)nc3cnc(Nc4ccc(N5CCN(C)CC5)cn4)cc23)C1	3.3	*
561	Cc1ccc(F)cc1Nc1nc2cc(Cl)c(N(C)C(=O)/C=C/CN(C)C)cc2n2cncc12	3.35	*

562	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCCCC(=O)NO	3.4	8.47
563	COC(=O)c1ccc2oc3cnnc(Nc4cccc5ccccc45)c3c2c1	3.4	8.47
564	C=CC(=O)Nc1ccc2ncnc(NC3CCCCC3)c2c1	3.4	*
565	COC(=O)CN(C)Cc1c[nH]c2cc3ncnc(Nc4cccc(Br)c4)c3cc12	3.4	*
566	C[C@@H](Nc1ncnc2[nH]c(-c3ccc(O)cc3)cc12)c1ccc(F)cc1	3.4	*
567	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCn1c([N+](=O)[O-])cnc1C	3.43	8.46
568	OCCN(CCO)Cc1c[nH]c2cc3ncnc(Nc4cccc(Br)c4)c3cc12	3.5	*
569	Cc1cccc(Nc2ncnc3cc(NCCCn4ccnc4)ncc23)c1	3.5	*
570	C=CC(=O)Nc1cccc(N2C(=O)N(C)Cc3cnc(Nc4ccc(N5CCC(N(C)C)CC5)cc4OC)nc32)c1	3.52	8.45
571	Cc1cccc(Nc2ncnc3ccncc23)c1NCCCn1ccnc1	3.548	*
572	C#Cc1cccc(Nc2ncnc3ccc(-c4cnn(C)c4)cc23)c1	3.58	8.45
573	CCOc1cc2ncnc(Nc3ccc(OCC4CC4)c(Cl)c3)c2cc1NC(=O)/C(F)=C/CN(C)C	3.6	8.44
574	CCOc1cc2ncnc(Nc3ccc(C)cc3)c2c2c1OCCO2	3.6	*
575	O=C(CCCCCCn1cc(-c2ccc3ncnc(Nc4ccc(OCc5nccs5)c(Cl)c4)c3c2)nn1)NO	3.6	*
576	COc1ccc(/C=C/C(=O)Nc2cc3c(Nc4ccc(F)c(Cl)c4)ncnc3cc2O[C@H]2CCOC2)c(OC)c1OC	3.6	*
577	C=CC(=O)Nc1cc2c(Nc3cccc(Br)c3)ncnc2cc1OCCCN1CCOCC1	3.6	*
578	C=CC(=O)Nc1ccc2ncnc(Nc3ccc(OCc4ccccc4)cc3)c2c1	3.6	*
579	Clc1ccc(Nc2ncnc3[nH]ccc23)cc1Br	3.63	*
580	Fc1ccc(Nc2ncnc3ccc(NC(=S)NCCN4CCCCC4)cc23)cc1Cl	3.7	8.43
581	Brc1cccc(Nc2ncnc3cc4c(cnn4CCN4CCOCC4)cc23)c1	3.7	*
582	Brc1cccc(Nc2ncnc3cc4c(ccn4CCN4CCOCC4)cc23)c1	3.7	*
583	Br.C[C@@H](Nc1ncnc2[nH]c(-c3ccc(O)cc3)cc12)c1ccccc1	3.7	*
584	COc1ccc(-c2cc3c(NCc4ccccc4)ncnc3[nH]2)cc1	3.7	*
585	C=CC(=O)N1CCc2c(sc3ncnc(Nc4ccc(Br)cc4F)c23)C1	3.71	*
586	Brc1cccc(Nc2ncnc3[nH]ccc23)c1	3.76	*
587	COc1cc2ncnc(Nc3cccc(Br)c3)c2cc1N	3.8	*
588	COc1cc2ncnc(Nc3cccc(F)c3)c2cc1OC	3.8	*
589	COc1ncc2ncnc(Nc3cccc(Br)c3)c2n1	3.8	*
590	Br.C[C@@H](Nc1ncnc2[nH]c(-c3ccc(O)cc3)cc12)c1ccc(F)cc1	3.8	*
591	c1ccc(CNc2ncnc3[nH]c(-c4ccccc4)cc23)cc1	3.8	*
592	C=CC(=O)Nc1cccc(-n2c(=O)n(CCCc3ccccc3)c(=O)c3cnc(Nc4ccc(N5CCC(N(C)C)CC5)cc4OC)nc32)c1	3.8	*
593	C=CC(=O)Nc1cccc(-n2c(=O)cnc3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	3.82	8.42
594	OC[C@@H](Nc1ncnc2oc(-c3ccccc3)cc12)c1ccccc1	3.9	8.41
595	O=C(NO)c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	3.9	*
596	C=CC(=O)Nc1cc2c(Nc3cccc(Br)c3)ncnc2cc1OCCCCN(C)C	3.9	*
597	CN1CCN(NCCCNc2cc3c(Nc4cccc(Br)c4)ncnc3cn2)CC1	3.9	*
598	C=CC(=O)N1CCc2c(sc3ncnc(Nc4cccc(C)c4F)c23)C1	3.95	*
599	CC(=O)Nc1ccc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2c1	3.96	8.40
600	COc1ccc(-c2cc3c(N[C@H](CCO)c4ccccc4)ncnc3o2)cc1	4	8.40
601	COc1ccccc1-c1cc2c(N[C@H](C)c3ccccc3)ncnc2o1	4	8.40
602	COC(=O)c1cc(OC)c(-c2cc3c(N[C@H](C)c4ccccc4)ncnc3s2)c(OC)c1	4	8.40
603	C#Cc1cccc(Nc2ncnc3cc4c(cc23)N(C(=O)/C=C/CN2CCCCC2)CCO4)c1	4	*
604	O=C(/C=C/CN1CCC(F)CC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	4	*

605	NC(=O)Nc1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c2c1	4	*
606	CN(C)Cc1ccc(-c2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)[nH]1	4	*
607	CS(=O)(=O)CCNCc1cc(-c2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)co1	4	*
608	COc1cc2ncnc(/C=C/CCc3ccccc3)c2cc1OC	4	*
609	CNc1ccc2cncnc2c1	4	*
610	COc1cc2ncnc(NCc3ccccc3)c2cc1OC.Cl	4	*
611	CNc1ccc2c(Nc3cccc(Br)c3)ncnc2c1	4	*
612	CNc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	4	*
613	Cc1cccc(Nc2ncnc3cnc(N(C)C)nc23)c1	4	*
614	CN1CCN(c2ccc(Nc3ncc4nc(Nc5ccccc5)n(C5CCCC5)c4n3)cc2)CC1	4	*
615	OCCOCCNCc1ccc(-c2cc3nccc(Nc4ccc5[nH]ccc5c4)c3s2)cc1	4	*
616	NCc1ccc(-c2cc3ncnc(Nc4ccc5[nH]ccc5c4)c3s2)cc1	4	*
617	NC1CCN(Cc2ccn3ncnc(Nc4cccc(Cl)c4)c23)CC1	4	*
618	NC1CCN(Cc2ccn3ncnc(Nc4cccc(Br)c4)c23)CC1	4	*
619	Br.CC[C@@H](Nc1ncnc2[nH]c(-c3ccc(O)cc3)cc12)c1ccccc1	4	*
620	Nc1cccc(-c2cc3c(Nc4cccc(Cl)c4)ncnc3[nH]2)c1	4	*
621	OC[C@@H](Nc1ncnc2[nH]c(-c3ccc(F)cc3)cc12)c1ccccc1	4	*
622	O=C(C=CCN1CCCCC1)N1CCOc2cc3ncnc(Nc4ccc(F)c(Cl)c4)c3cc21	4	*
623	CN(C)CC=CC(=O)N1CCOc2cc3ncnc(Nc4ccc(F)c(Cl)c4)c3cc21	4	*
624	COc1cc2ncnc(N3CCc4ccccc43)c2cc1NC(=O)/C=C/CN1CCC(CO)CC1	4	*
625	CCOc1cc2ncc(C#N)c(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/c1cn(CCF)nn1	4.05	8.39
626	CCOc1cc2ncnc(NC3=CC(=O)C(OCc4cccc(F)c4)=CC3=O)c2cc1NC(=O)/C=C/CN(C)C	4.1	8.39
627	CN(C)[C@H](CS(C)(=O)=O)c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	4.1	*
628	O=C(Nc1ccc(CN2CCCC2)cc1)Nc1ccc2ncnc(Nc3cccc(C(F)(F)F)c3)c2c1	4.1	*
629	Brc1cccc(Nc2ncnc3cc4[nH]nnc4cc23)c1	4.1	*
630	OCCn1ccc2ncnc(Nc3ccc(Oc4cccc5sncc45)c(Cl)c3)c21	4.1	*
631	N#Cc1ccc(Nc2nncc3ccccc23)cc1	4.1	*
632	CC(C)N(CC#CC(=O)Nc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1)C(C)C	4.2	*
633	C#Cc1cccc(Nc2ncnc3cc(OCC)c(NC(=O)/C=C/CNC4CC4)cc23)c1	4.2	*
634	O=C(CCCCCCn1cc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)nn1)NO	4.2	*
635	CCOc1cc2ncnc(C#C[C@@](C)(Cc3ccccc3)N3CCC(C(=O)O)CC3)c2cc1OCC	4.2	*
636	C=CC(=O)N(CCN(C)C)c1cc2c(Nc3cccc(Br)c3)ncnc2cn1	4.2	*
637	CCOC(=O)C1CCN([C@@](C)(C#Cc2ncnc3cc(OCC)c(OCC)cc23)Cc2ccccc2)CC1	4.2	*
638	OC[C@@H](Nc1ncnc2[nH]c(-c3ccc(Br)cc3)cc12)c1ccccc1	4.2	*
639	CCOC(=O)c1c(NC2=C(Cl)C(c3ccc(Cl)cc3)C(C#N)=C(N)O2)sc2c1-c1sc(=S)n(-c3ccccc3)c1CC2(C)C	4.28	*
640	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1)c1cccnc1F	4.3	8.37
641	COc1ccc2ncnc(Nc3cccc(Br)c3)c2n1	4.3	*
642	CNc1ncc2ncnc(Nc3cccc(C)c3)c2n1	4.3	*
643	NP(=O)(OCCOc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)N(CCCl)CCCl	4.3	*
644	C=CC(=O)N1CCc2c(sc3ncnc(Nc4ccc(Br)c(C)c4)c23)C1	4.4	*
645	CCOc1cc2ncnc(Nc3cccc(OC)c3)c2c2c1OCCO2	4.4	*
646	CN(CCCl)CCNN=Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	4.4	*
647	CCOC(=O)c1ccc(Nc2nncc3ccccc23)cc1	4.4	*

648	CN1CCN(c2ccc(Nc3cc4c(N5CCCC5)nc(Nc5ccccc5)nc4cn3)nc2)CC1	4.4	*
649	CN(CCCl)CCN/N=N/c1ccc2ncnc(Nc3cccc(Cl)c3)c2c1.[H+]	4.4	*
650	C=CC(=O)Nc1cccc(N2C(=O)N(C)Cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4OCC)nc32)c1	4.41	8.36
651	C=C=CCCCCCOc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O	4.45	*
652	CCOc1cc2ncnc(Nc3ccc(Oc4ccc(C)nc4)c(Cl)c3)c2cc1NC(=O)/C(F)=C/CN(C)C	4.5	8.35
653	Cc1cc(C(=O)N2CCOCC2)[nH]c1/C=C1\C(=O)Nc2ncnc(Nc3ccc4c(ccn4Cc4ccccc4)c3)c21	4.5	*
654	COCCOc1cc2ncnc(Nc3ccc(NC(=O)C45CC6CC(CC(C6)C4)C5)cc3C)c2cc1OCCOC	4.52	8.34
655	COc1cc2c(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncnc2cc1OCCN1C[C@H](O)[C@@H](O)[C@H](O)[C@H]1CO	4.53	*
656	COc1cc2c(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncnc2cc1OCCCN1C[C@H](O)[C@@H](O)[C@H](O)[C@H]1CO	4.53	*
657	O=C1N[C@H](C(=O)Nc2cc3c(Nc4ccc(F)c(Cl)c4)ncnc3cc2OCCCN2CCOCC2)CO1	4.54	8.34
658	C[C@@H](Nc1ncnc2oc(-c3cccc(O)c3)cc12)c1ccccc1	4.6	8.34
659	C#Cc1cccc(Nc2ncnc3cc(OC)c(OCCCCCC(=O)NO)cc23)c1	4.6	8.34
660	CN(C)C/C=C/C(=O)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21	4.6	*
661	CCN(CC)CC(O)CNc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	4.6	*
662	C=C[S+]([O-])c1cc2c(Nc3cccc(Br)c3)ncnc2cn1	4.6	*
663	Clc1ccc(/C=C/C(=N/Nc2nncc3ccccc23)c2ccccc2)cc1	4.6	*
664	CN(C)C1CCN(c2ccc(Nc3cc4c(N5CCOCC5)nc(Nc5ccccc5)nc4cn3)nc2)CC1	4.6	*
665	C=CC(=O)Nc1cccc(N2C(=O)C(Cc3ccccc3)N(C)C(=O)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	4.68	8.33
666	Oc1ccc2c(Nc3cccc(Br)c3)ncnc2c1	4.7	*
667	Cc1cc(CCC(=O)O)[nH]c1/C=C1\C(=O)Nc2ncnc(Nc3ccc(F)c(Cl)c3)c21	4.7	*
668	COc1ccc(-c2cc3c(N[C@H](C)c4ccccc4)ncnc3[nH]2)cc1	4.7	*
669	C=CC(=O)N1CCC[C@@H](Nc2nc(Nc3ccccc3)nc3cnc(Nc4ccc(N5CCN(C)CC5)cn4)cc23)C1	4.7	*
670	COc1cc2ncnc(Nc3ccc(C(=O)NC45CC6CC(CC(C6)C4)C5)c(C#N)c3)c2cc1OCCCN1CCOCC1	4.71	8.33
671	O=C(/C=C/c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)s1)NO	4.8	*
672	Brc1cccc(Nc2ncnc3cc4[nH]cc(CN5CCOCC5)c4cc23)c1	4.8	*
673	OCC(O)C(O)C(O)C(O)CNc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	4.8	*
674	NCCSc1nc(-c2ccc(F)cc2)c(-c2ccnc(Nc3ccccc3)c2)[nH]1	4.8	*
675	CC1(C)Cc2c(nn(-c3ccc(Cl)cc3)c(=N)c2C#N)-c2c1sc(N)c2C#N	4.8	*
676	C#Cc1cccc(Nc2ncnc3cc(OCCN4C[C@H](O)[C@@H](O)[C@H](O)[C@H]4CO)c(OC)cc23)c1	4.87	*
677	C#Cc1cccc(Nc2ncnc3cc(OCCCN4C[C@H](O)[C@@H](O)[C@H](O)[C@H]4CO)c(OC)cc23)c1	4.87	*
678	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCn1c([N+](=O)[O-])cnc1C	4.9	8.31
679	CN1CCN(CCCNc2cc3ncnc(Nc4cccc(Br)c4)c3cn2)CC1	4.9	*
680	COc1ccc(-c2cc3c(N[C@H](C)c4cccc(F)c4)ncnc3[nH]2)cc1	4.9	*
681	C=CC(=O)Nc1cccc(N2C(=O)N(C)Cc3cnc(Nc4ccc(N(C)C)cc4OC)nc32)c1	4.99	8.30
682	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1)c1cc([N+](=O)[O-])ccc1F	5	7.46
683	COc1cc2ncnc(Nc3cccc(Br)c3)c2cc1NC(=O)/C(F)=C\CN(C)C	5	8.30
684	C#Cc1cccc(Nc2ncnc3cc(OCCOC(=O)c4ccccc4OC(C)=O)c(OCCOC)cc23)c1	5	8.30
685	C[C@@H](Nc1ncnc2sc(-c3cccc(C(N)=O)c3)cc12)c1ccccc1	5	8.30
686	COc1cc(C=O)ccc1-c1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	5	8.30
687	COc1cc(CO)ccc1-c1cc2c(NCc3ccccc3)ncnc2s1	5	8.30
688	COc1ccc(-c2cc3c(N[C@H](C)c4ccccc4)ncnc3s2)c(OC)c1	5	8.30
689	COc1ccc(CO)cc1-c1cc2c(N[C@H](C)c3ccccc3)ncnc2s1	5	8.30
690	C#Cc1cccc(Nc2ncnc3sc(-c4ccc(CO)cc4OC)cc23)c1	5	8.30

691	C#Cc1cccc(Nc2ncnc3cc4c(cc23)N(C(=O)/C=C/CN2CCC(C)CC2)CCO4)c1	5	*
692	C#Cc1cccc(Nc2ncnc3cc4c(cc23)N(C(=O)/C=C/CN2CCCCC2C)CCO4)c1	5	*
693	C#Cc1cccc(Nc2ncnc3cc4c(cc23)N(C(=O)/C=C/CN(CC)CC)CCO4)c1	5	*
694	COc1ccccc1-c1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	5	*
695	O=C(Nc1ccc(CN2CCCCC2)cc1)Nc1ccc2ncnc(Nc3cccc(C(F)(F)F)c3)c2c1	5	*
696	CNCC(O)COc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OC	5	*
697	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCC(O)CN(CCO)CCO	5	*
698	COc1cc2ncnc(Nc3cccc(C)c3)c2cc1OC	5	*
699	C=CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1	5	*
700	CN1CCN(Cc2ccc(-c3cc4ncnc(Nc5ccc(OCc6cccc(F)c6)c(Cl)c5)c4s3)o2)CC1	5	*
701	CCOc1cc2ncnc(/C=C/CCc3ccccc3)c2cc1OCC	5	*
702	Brc1cccc(Nc2ncnc3cc4c(cc23)OCCOCCOCCO4)c1	5	*
703	Brc1cccc(Nc2ncnc3cc4c(cc23)OCCOCOCOCCO4)c1	5	*
704	Nc1ccc(Nc2[nH]nc3ncnc(Nc4cccc(Cl)c4)c23)cc1	5	*
705	Nc1cccc(-c2[nH]nc3ncnc(Nc4cccc(Cl)c4)c23)c1	5	*
706	CN1CCC(Oc2cccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c23)CC1	5	*
707	COc1cc(ON2CCC(C)CC2)c2c(Nc3ccc(OCc4ccccn4)c(Cl)c3)ncnc2c1	5	*
708	CCO/N=C/c1c(N)ncnc1Nc1ccc2c(cnn2Cc2cccc(F)c2)c1	5	*
709	Cc1c[nH]c2ccc(Nc3ncnc4cc(-c5ccccc5)sc34)cc12	5	*
710	CC(=O)NCCNCc1ccc(-c2cc3ncnc(Nc4ccc5[nH]ccc5c4)c3s2)cc1	5	*
711	CN(C)CCc1ccc(-c2cc3ncnc(Nc4ccc5[nH]ccc5c4)c3s2)cc1	5	*
712	Cc1cccc(Nc2ncnn3ccc(CN4CCC(N)CC4)c23)c1	5	*
713	Nc1cccc(-c2cc3c(Nc4cccc(Cl)c4)ncnc3o2)c1	5	*
714	Nc1cccc(-c2cc3c(Nc4cccc([N+](=O)[O-])c4)ncnc3o2)c1	5	*
715	COc1ccc(-c2cc3c(NCc4ccc(F)cc4)ncnc3[nH]2)cc1	5	*
716	CC1CCN(CC=CC(=O)N2CCOc3cc4ncnc(Nc5ccc(F)c(Cl)c5)c4cc32)CC1	5	*
717	C=CC(=O)Nc1cc(Nc2n[nH]c3cc(-c4cccc(F)c4)ccc23)c(OC)cc1N(C)CCN(C)C	5	*
718	CN(C)C/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@@H]1CCOC1	5	*
719	CN(C)CC=CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@@H]1CCOC1	5	*
720	CN(C)C/C=C/C(=O)Nc1cc2c(N3CCc4ccccc43)ncnc2cc1OC1CCOC1	5	*
721	COCCOc1cc2ncnc(Nc3ccc(NC(=O)C45CC6CC(CC(C6)C4)C5)c(C#N)c3)c2cc1OCCOC	5.01	8.30
722	CN1CCN(CCCNc2c(Br)cccc2Nc2ncnc3ccncc23)CC1	5.012	*
723	S=C(NCCN1CCOCC1)Nc1ccc2ncnc(Nc3ccc(Cl)cc3)c2c1	5.06	8.30
724	OCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	5.06	*
725	O=C(O)Cn1ccc2cc3c(Nc4cccc(Br)c4)ncnc3cc21	5.1	*
726	C=C=CC(=O)Nc1cc(Nc2ncc(C)c(C3=CN(C)C4C=CC=CC34)n2)c(OC)cc1N(C)CCN(C)C	5.2	*
727	O=C(CNCc1ccccc1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	5.2	*
728	C=C=CC(=O)Nc1cc(Nc2ncc(C)c(-c3cn(C)c4ccccc34)n2)c(OC)cc1N(C)CCN(C)C	5.2	*
729	C=CC(=O)Nc1cccc(-n2c(=O)c(C)nc3cnc(Nc4ccc(OC)cc4)nc32)c1	5.29	8.28
730	COc1ccc(-c2cc3c(N[C@H](C)c4ccccc4)ncnc3o2)cc1	5.3	8.28
731	O=C(/C=C/CN1CCCCC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	5.3	*
732	C#Cc1cccc(Nc2ncnc3cc(O[C@H]4CCOC4)c(NC(=O)/C=C/CN4CCCCC4)cc23)c1	5.3	*
733	COCCOc1cc2ncnc(Nc3ccc(OCc4ccccn4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	5.4	*

734	Brc1cccc(Nc2ncnc3cc(NCCCCN4CCOCC4)ncc23)c1	5.4	*
735	Cc1cccc(Nc2ncnc3cc(NCCCCN(C)C)ncc23)c1	5.4	*
736	COc1ccc(/C=C/C(=N/Nc2nncc3ccccc23)c2ccc(Cl)cc2)cc1	5.4	*
737	C=CC(=O)N[C@@H]1CCCN(c2nc(Nc3ccccc3)nc3cnc(Nc4ccc(N5CCN(C)CC5)cn4)cc23)C1	5.4	*
738	CN1CCN(c2ccc(Nc3cc4c(N5CCOCC5)nc(Nc5ccccc5)nc4cn3)nc2)CC1	5.4	*
739	CC[C@@H](Nc1ncnc2[nH]c(-c3ccccc3)cc12)c1ccccc1	5.4	*
740	Brc1cccc(Nc2ncnc3ccncc23)c1NCCCCN1CCOCC1	5.495	*
741	Cc1cccc(Nc2ncnc3ccncc23)c1NCCCCN(C)C	5.495	*
742	CCOc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C1CC1	5.5	*
743	CC(C)(C(=O)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc5sncc45)c(Cl)c3)c21)S(C)(=O)=O	5.5	*
744	CN(C)C1CCN(c2ccc(Nc3cc4c(N5CCCC5)nc(Nc5ccccc5)nc4cn3)nc2)CC1	5.5	*
745	CCOc1cc2ncnc(N[C@@H](C)c3ccccc3)c2cc1NC(=O)[C@@H]1COC(=O)N1	5.52	8.26
746	O=C(c1cc2ccccc2[nH]1)c1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	5.54	*
747	C#Cc1cccc(Nc2ncnc3cc(O[C@H]4CCOC4)c(NC(=O)/C=C/CNC4CC4)cc23)c1	5.6	*
748	Cc1cccc(Nc2ncnc3cc(NCCCN4CCN(C)CC4)ncc23)c1	5.6	*
749	C(=C/c1ccccc1)\C(=N\Nc1nncc2ccccc12)c1ccccc1	5.6	*
750	C=CC(=O)N1CCC[C@@H](n2nc(-c3ccc(Oc4ccccc4)cc3)c3c(N)ncnc32)C1	5.6	*
751	COc1cc2ncnc(Nc3ccc(F)c(Br)c3)c2cc1OCCCN1CCNCCNCC1	5.6	*
752	Cc1cccc(Nc2ncnc3ccncc23)c1NCCCN1CCN(C)CC1	5.623	*
753	NP(=O)(OCCCOc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1)N(CCCl)CCCl	5.7	*
754	OCCOCCn1ccc2ncnc(Nc3ccc(Oc4cccc(Cl)c4)c(Cl)c3)c21	5.7	*
755	C=CC(=O)Nc1cccc(N2C(=O)C(Cc3ccc(F)cc3)N(C)C(=O)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	5.78	8.24
756	C=CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	5.8	*
757	COc1cc(Nc2ncnc3ccc(-c4cn(CCCCCC(=O)NO)nn4)cc23)ccc1Oc1ccccc1	5.8	*
758	C=CC(=O)Nc1ccc2ncnc(Nc3ccc(Oc4ccccc4)cc3)c2c1	5.8	*
759	C=C=CC(=O)Nc1cc(Nc2nccc(C3=CN(C)C4C=CC=CC34)n2)c(OC)cc1N1CCC(N2CCN(C)CC2)CC1	5.8	*
760	C=C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4ccccc34)n2)c(OC)cc1N1CCC(N2CCN(C)CC2)CC1	5.8	*
761	Fc1ccccc1CNc1ncnc2[nH]c(-c3ccccc3)cc12	5.8	*
762	Cc1cc(C(=O)N2CC(C)NC(C)C2)[nH]c1/C=C1\C(=O)Nc2ncnc(Nc3ccc(F)c(Cl)c3)c21	5.9	*
763	COc1ccc2[nH]c(C(=O)c3cc4c(Nc5ccc(F)c(Cl)c5)ncnc4s3)cc2c1	5.93	*
764	COCCOc1cc2ncnc(Nc3ccc(NC(=O)C45CC6CC(CC(C6)C4)C5)c(OC)c3)c2cc1OCCOC	5.94	8.23
765	Fc1cc(Nc2ncnc3[nH]ccc23)ccc1Cl	5.98	*
766	Cc1ccc(C(=O)Nc2ccc(CN3CCN(C)CC3)c(C(F)(F)F)c2)cc1NC(=O)c1cnc(Nc2ccccc2)nc1	6	8.22
767	COc1cc(C=O)ccc1-c1cc2c(NCc3ccccc3)ncnc2s1	6	8.22
768	C[C@@H](Nc1ncnc2sc(-c3cccc(C=O)c3)cc12)c1ccccc1	6	8.22
769	COc1cc(F)ccc1-c1cc2c(N[C@H](C)c3ccccc3)ncnc2s1	6	8.22
770	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1CN1CCC[C@@H]1C(N)=O	6	*
771	COCCN1CC(C(N)=O)(N(C)Cc2cc3c(Nc4cccc(Cl)c4F)ncnc3cc2OC)C1	6	*
772	C#Cc1cccc(Nc2ncnc3cc(OC4CCOCC4)c(NC(=O)/C=C/CN(C)C)cc23)c1	6	*
773	CCC(=O)Nc1cc2c(Nc3ccc4[nH]ccc4c3)ncnc2cc1OC	6	*
774	CCOc1cc2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c2cc1NC(=O)/C=C/CN(C)C	6	*
775	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCC(O)CN	6	*
776	CCNCc1ccc(-c2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)[nH]1	6	*

777	Clc1cccc(Nc2[nH]cnc3nc4ccccc4c2-3)c1	6	*
778	Oc1ccc(-c2[nH]nc3ncnc(Nc4cccc(Cl)c4)c23)cc1	6	*
779	Fc1ccc(Nc2nncc3ccccc23)cc1	6	*
780	CN(C)CC#CC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	6	*
781	NC1CCN(Cc2ccn3ncnc(Nc4cccc(F)c4)c23)CC1	6	*
782	Cc1ccc(Nc2ncnn3ccc(CN4CCC(N)CC4)c23)cc1	6	*
783	NC1CCN(Cc2ccn3ncnc(Nc4ccc(F)c(Cl)c4)c23)CC1	6	*
784	NP(=O)(OCCCCOc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1)N(CCCl)CCCl	6	*
785	C=CC(=O)N1CCc2ncnc(Nc3cc(Cl)cc(Cl)c3)c2C1	6	*
786	CN(C)CC=CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OC1CCOC1	6	*
787	C#Cc1cccc(Nc2ncnc3cc(OCC)c(NC(=O)/C=C/CN4CCCCC4)cc23)c1	6.1	*
788	O=C(Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1)C1CCCCC1	6.13	*
789	O=C(O)c1ccc(Nc2nncc3ccccc23)cc1	6.2	*
790	CN(C)C/C=C/C(=O)NCc1cccc(-c2nc(-c3ccc(F)cc3)c(-c3ccnc4[nH]c(-c5ccccc5)cc34)[nH]2)c1	6.2	*
791	C=CC(=O)Nc1cccc(N2C(=O)CN(Cc3ccccc3)C(=O)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	6.26	8.20
792	Oc1cc(O)c2cc(O)c(-c3cc(O)c(O)c(O)c3)[o+]c2c1.[Cl-]	6.27	*
793	CN(C)CCCCOc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)c1cc([N+](=O)[O-])ccc1F	6.3	8.20
794	Clc1ccc(C(/C=C/c2ccccc2)=N\\Nc2nncc3ccccc23)cc1	6.3	*
795	C=C=CC(=O)Nc1cc(Nc2nccc(C3=CN(C)C4C=CC=CC34)n2)c(OC)cc1N1CCC(N(C)C)CC1	6.3	*
796	C=C=CC(=O)Nc1cc(Nc2nccc(C3=CN(C)C4C=CC=CC34)n2)c(OC)cc1N1CCN(C)CC1	6.3	*
797	C=C=CC(=O)Nc1cc(Nc2ncc(OC)c(C3=CN(C)C4C=CC=CC34)n2)c(OC)cc1N(C)CCN(C)C	6.3	*
798	C=C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4ccccc34)n2)c(OC)cc1N1CCC(N(C)C)CC1	6.3	*
799	C=C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4ccccc34)n2)c(OC)cc1N1CCN(C)CC1	6.3	*
800	C=C=CC(=O)Nc1cc(Nc2ncc(OC)c(-c3cn(C)c4ccccc34)n2)c(OC)cc1N(C)CCN(C)C	6.3	*
801	C#Cc1cccc(Nc2ncnc3cc(O[C@H]4CCOC4)c(NC(=O)/C=C/CNC(C)C)cc23)c1	6.4	*
802	Cc1ccc(Oc2ccc(Nc3ncnc4ccc(-c5cn(CCCCCC(=O)NO)nn5)cc34)cc2C)cn1	6.4	*
803	COc1cc2ncnc(Nc3cncc4ccccc34)c2cc1OC	6.4	*
804	CN1CCN(c2cc3c(Nc4cccc(Br)c4)ncnc3cn2)CC1	6.4	*
805	COc1cc2ncnc(Nc3ccc(C(=O)NC45CC6CC(CC(C6)C4)C5)c(Cl)c3)c2cc1OCCCN1CCOCC1	6.42	8.19
806	O=C(/C=C/CN1CCCCC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCF	6.44	*
807	O=C(/C=C/CNC1CC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	6.5	*
808	Nc1cc2c(Nc3cccc(Br)c3)ncnc2cc1Cl	6.5	*
809	Cc1cc(C(=O)NCCN2CCOCC2)[nH]c1/C=C1\C(=O)Nc2ncnc(Nc3ccc(F)c(Cl)c3)c21	6.5	*
810	Cc1ccc(C(/C=C/c2ccc(F)cc2)=N\\Nc2nncc3ccccc23)cc1	6.5	*
811	CN1CCN(CCCOc2cc3ncnc(Nc4ccc(F)c(Cl)c4)c3cc2NC(=O)c2cc([N+](=O)[O-])ccc2F)CC1	6.6	8.18
812	C=CC(=O)Nc1nc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCN(C)CC1	6.6	*
813	C[C@@H](Nc1ncnc2[nH]c(-c3ccc(F)cc3)cc12)c1ccccc1	6.6	*
814	COc1ccc(-c2cc3c(N[C@H](C)c4ccccc4O)ncnc3[nH]2)cc1	6.6	*
815	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCN1CCNCCNCCNCC1	6.6	*
816	Clc1cccc(Nc2ncnc3[nH]ccc23)c1	6.63	*
817	COC(=O)c1ccc2oc3cnnc(Nc4ccc(F)c(Cl)c4)c3c2c1	6.7	8.17
818	CCOc1cc2ncnc(Nc3ccc(C)c(Cl)c3)c2c2c1OCCO2	6.7	*
819	CS(=O)(=O)CC(=O)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc(Cl)c4)c(Cl)c3)c21	6.7	*

820	Cc1cc(C)nc(NS(=O)(=O)c2ccc(Nc3nncc4ccccc34)cc2)n1	6.7	*
821	Clc1ccc(Nc2ncnc3[nH]ccc23)cc1Cl	6.7	*
822	CN(C)C(CS(C)(=O)=O)c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	6.8	*
823	C=CC(=O)Nc1cc(Nc2n[nH]c3ccc(-c4ccc(F)cc4)cc23)c(OC)cc1N(C)CCN(C)C	6.8	*
824	O=C(/C=C/CNC1CC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCC(F)(F)F	6.9	*
825	O=C(CCCCCn1cc(-c2ccc3ncnc(Nc4ccc(OCc5nccs5)c(Cl)c4)c3c2)nn1)NO	6.9	*
826	O=C(Nc1cccc(Oc2ccc(Nc3ncnc4ccn(CCOCCO)c34)cc2Cl)c1)NC1CCCCC1	6.9	*
827	Fc1ccc(/C=C/C(=N/Nc2nncc3ccccc23)c2ccccc2)cc1	6.9	*
828	C=CC(=O)Nc1cccc(-n2c(=O)cnc3cnc(Nc4ccc(N5CCOCC5)cc4)nc32)c1	6.95	8.16
829	C=CC(=O)Nc1cccc(N2C(=O)N(C)Cc3cnc(Nc4ccccc4)nc32)c1	6.95	8.16
830	C=CC(=O)Nc1cccc(N2C(=O)CN(c3ccccc3)C(=O)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	6.99	8.16
831	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C#Cc1ccc(CN(C)C)cc1	7	8.15
832	COc1cccc(-c2cc3c(N[C@H](C)c4ccccc4)ncnc3o2)c1	7	8.15
833	COc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCCCCC(=O)NO	7	8.15
834	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4cccc(Cl)c4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	7	8.15
835	COC(=O)c1ccc(OC)c(-c2cc3c(N[C@H](C)c4ccccc4)ncnc3s2)c1	7	8.15
836	C[C@@H](Nc1ncnc2sc(-c3ccc(C(N)=O)cc3)cc12)c1ccccc1	7	8.15
837	Cc1cc(Nc2ncc3c(n2)N([C@H]2CCN(C(=O)CO)C2)C(=O)N(c2ccccc2Cl)C3)ccc1N1CCN(C)CC1	7	8.15
838	O=C(/C=C/CN1CC2(COC2)C1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	7	*
839	O=C(/C=C/CN1CCC(F)(F)CC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	7	*
840	O=C(Nc1ccc(CN2CCCC2)cc1)c1sc2ncnc3c2c1NC(=O)N3c1ccc(F)c(Cl)c1	7	*
841	CC(C)NC/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	7	*
842	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1)C1=CCCC1	7	*
843	CCOc1cc2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c2cc1NC(=O)/C=C/CN1CCCC1	7	*
844	COCCOc1cc2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c2cc1NC(=O)/C=C/CN(C)C	7	*
845	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCN(C)C	7	*
846	CS(=O)(=O)CCNCc1ccc(-c2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)[nH]1	7	*
847	C=CC(=O)Nc1cccc(-c2c(-c3ccccc3)oc3ncnc(N[C@H](CO)c4ccccc4)c23)c1	7	*
848	CN(C)C/C=C/C(=O)N1CCc2c(sc3ncnc(N[C@H](CO)c4ccccc4)c23)C1	7	*
849	Brc1cccc(Nc2ncnc3cc4c(cc23)OCCSCCO4)c1	7	*
850	CN(C)c1cc2c(Nc3ccc4c(cnn4Cc4ccccc4)c3)ncnc2cn1	7	*
851	Fc1cccc(COc2ccc(Nc3ncnc4cc(C#C[C@H]5CCCN5)sc34)cc2Cl)c1	7	*
852	CNc1ccc2ncncc2c1	7	*
853	Clc1cccc(Nc2[nH]cnc3nnc(NCc4ccccc4)c2-3)c1	7	*
854	COc1ccc(CNc2[nH]nc3ncnc(Nc4cccc(Cl)c4)c23)cc1	7	*
855	CC(C)(O)C(=O)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc5sncc45)c(Cl)c3)c21.CS(=O)(=O)O	7	*
856	CC(C)(CO)C(=O)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc5sncc45)c(Cl)c3)c21	7	*
857	C=CC(=O)NCC(=O)Nc1cccc(Nc2ncc(NC(=O)c3cc(NC(=O)c4cccc(C(F)(F)F)c4)ccc3C)cn2)c1	7	*
858	NC(=O)C1CCN(Cc2ccc(-c3cc4ncnc(Nc5ccc6[nH]ccc6c5)c4s3)cc2)CC1	7	*
859	C#Cc1cccc(Nc2ncnn3ccc(CN4CCC(N)CC4)c23)c1	7	*
860	Fc1cccc(COc2ccc(Nc3ncnc4cc(OCCCN5CCOCC5)c(OCCCN5CCOCC5)cc34)cc2Cl)c1	7	*
861	O=[N+]([O-])c1cccc(-c2cc3c(Nc4cccc(Cl)c4)ncnc3o2)c1	7	*
862	c1nc(Nc2ccc(N3CCOCC3)cc2)cc(Nc2ccc3[nH]ccc3c2)n1	7	*

863	O=C(C=CCN1CCOCC1)N1CCOc2cc3ncnc(Nc4ccc(F)c(Cl)c4)c3cc21	7	*
864	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCC(=O)NO	7.1	8.15
865	NNc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	7.1	*
866	Cc1cccc(Nc2ncnc3cc(NCCc4c[nH]cn4)ncc23)c1	7.2	*
867	C#Cc1cccc(Nc2ncnc3ccc(OCCCOP(N)(=O)N(CCCl)CCCl)cc23)c1	7.2	*
868	NNc1c(Br)cccc1Nc1ncnc2ccncc12	7.244	*
869	CCOC(=O)CCCn1c(=O)oc2cc3ncnc(Nc4cc(C(=O)OCC)ccc4O)c3cc21	7.3	*
870	C=CC(=O)N1CCc2c(sc3ncnc(Nc4ccc(CC)cc4)c23)C1	7.38	*
871	CN(C)CCCCNc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	7.4	*
872	NP(=O)(OCCCCOc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)N(CCCl)CCCl	7.4	*
873	CN(C)CCCCNc1c(Br)cccc1Nc1ncnc2ccncc12	7.413	*
874	CN(C)CCN(C)Cc1c[nH]c2cc3ncnc(Nc4cccc(Br)c4)c3cc12	7.5	*
875	COc1ccc(-c2cc3c(NC(C)c4ccccc4C)ncnc3[nH]2)cc1	7.5	*
876	CCC(=O)N1CC[C@H](N2C(=O)N(c3ccccc3C)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	7.6	8.12
877	Fc1cccc(COc2ccc(Nc3ncnc4cc[nH]c34)cc2Cl)c1	7.7	*
878	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCC(=O)NO	7.8	8.11
879	C=CC(=O)Nc1cccc(-n2c(=O)c(-c3ccccc3)cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	7.8	*
880	O=C1NCc2ccc(Oc3ccc(Nc4ncnc5ccn(CCO)c45)cc3Cl)cc21	7.8	*
881	C#Cc1cccc(Nc2ncnc3cc(OC)c(NC(=O)/C=C/CNC4CC4)cc23)c1	7.9	*
882	CCNc1cc2sc3c(Nc4cccc(Br)c4)ncnc3c2cc1F.CCO	7.9	*
883	Cc1ccc(C(=O)Nc2ccc(CN3CCN(C)CC3)c(C(F)(F)F)c2)cc1NC(=O)c1cnc2[nH]ccc2c1	8	8.10
884	CN1CCN(c2ccc(Nc3ncnc4cc5oc(=O)n(CCOC(=O)CBr)c5cc34)cc2Cl)CC1	8	8.10
885	C[C@@H](Nc1ncnc2sc(-c3ccc(F)c(C=O)c3)cc12)c1ccccc1	8	8.10
886	C[C@@H](Nc1ncnc2sc(-c3cccc(C(=O)O)c3)cc12)c1ccccc1	8	8.10
887	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN1CCCC[C@@H]1C(N)=O	8	*
888	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN(C)[C@@H](C)C(N)=O	8	*
889	CN(C)CCC(=O)Nc1cccc(-c2c(-c3ccccc3)oc3ncnc(N[C@H](CO)c4ccccc4)c23)c1	8	*
890	O=C(/C=C/CNCc1ncccn1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	8	*
891	CCN(CC)C/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	8	*
892	COc1ccccc1-c1cc2c(NC(CO)c3ccccc3)ncnc2s1	8	*
893	CCOc1cc2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c2cc1NC(=O)/C=C/CN1CCCCC1	8	*
894	CNCCOc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OC	8	*
895	COCCNCCOc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OC	8	*
896	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCC(O)Cn1ccnc1	8	*
897	Fc1cccc(COc2ccc(Nc3ncnc4cc(-c5cccs5)sc34)cc2Cl)c1	8	*
898	C=CC(=O)N1CCc2c(sc3ncnc(N[C@H](CO)c4ccccc4)c23)C1	8	*
899	CO/N=C/c1c(N)ncnc1Nc1ccc2c(cnn2Cc2cccc(F)c2)c1	8	*
900	CN(C)/N=C/c1c(N)ncnc1Nc1ccc2c(cnn2Cc2cccc(F)c2)c1	8	*
901	Brc1cccc(Nc2ncnc3cc4c(cc23)OCCCSCCCO4)c1	8	*
902	Oc1ccc(Nc2[nH]nc3ncnc(Nc4cccc(Cl)c4)c23)cc1	8	*
903	COc1cccc(Nc2[nH]nc3ncnc(Nc4cccc(Cl)c4)c23)c1	8	*
904	COc1cccc(CNc2[nH]nc3ncnc(Nc4cccc(Cl)c4)c23)c1	8	*
905	Oc1cc(O)c2c(O)c(-c3cccc(Cl)c3)cnc2c1	8	*

906	CC(C)(CO)NCc1ccc(-c2cc3ncnc(Nc4ccc5[nH]ccc5c4)c3s2)cc1	8	*
907	Br.C[C@@H](Nc1ncnc2[nH]c(-c3ccc(O)cc3)cc12)c1ccccc1F	8	*
908	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CNC(=O)[C@H]1CCCCN1C	8	*
909	C=CC(=O)N1CCc2ncnc(Nc3ccc(OCc4ccccn4)c(Cl)c3)c2C1	8	*
910	C=CC(=O)N1CCc2ncnc(Nc3ccc(SCc4cccc(F)c4)c(Cl)c3)c2C1	8	*
911	C#Cc1cccc(Nc2ncnc3cc(OC4CCN(C)CC4)c(NC(=O)/C=C/CN(C)C)cc23)c1	8.1	*
912	CN(C)C/C=C/C(=O)Nc1cc2c(Nc3ccc(OCc4ccccn4)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	8.1	*
913	CN(C)CCN(C)c1cc2c(Nc3cccc(Br)c3)ncnc2cn1	8.1	*
914	COc1ccc(-c2cc3c(N[C@H](C)c4ccccc4Cl)ncnc3[nH]2)cc1	8.1	*
915	C=CC(=O)Nc1cc(Nc2n[nH]c3ccc(-c4ccc5ccccc5c4)cc23)c(OC)cc1N(C)CCN(C)C	8.1	*
916	C#Cc1cccc(Nc2ncnc3cc(OCCCCCCC(=O)NO)c(OC)cc23)c1	8.2	8.09
917	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1)c1cc([N+](=O)[O-])ccc1Cl	8.3	8.08
918	Clc1cccc(Nc2ncnc3cc4c(cc23)OCCO4)c1	8.3	*
919	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCN1CCNCCNCC1	8.3	*
920	CC1(C)CC(=NNc2ccccc2)C(=NNc2ccc(Cl)cc2)c2c1sc(N)c2C#N	8.31	*
921	CN1CCN(Cc2ccc(NC(=O)Nc3ccc4ncnc(Nc5ccc(OCc6cccc(F)c6)c(Cl)c5)c4c3)cc2)CC1	8.4	*
922	CN(C)CCCCCNc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	8.4	*
923	O=C(Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)c1ccco1	8.4	*
924	O=C(COc1ccc(F)cc1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	8.43	8.07
925	Cc1cc(Nc2ncc3c(n2)N([C@H]2CCN(C(=O)C(C)C)C2)C(=O)N(c2ccccc2Cl)C3)ccc1N1CCN(C)CC1	8.5	8.07
926	CN(C)CCCCCNc1c(Br)cccc1Nc1ncnc2ccncc12	8.511	*
927	C=C=CC(=O)Nc1cc(Nc2nccc(C3=CN(C)C4C=CC=CC34)n2)c(OC)cc1N1CCC(N2CCOCC2)CC1	8.6	*
928	C=C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4ccccc34)n2)c(OC)cc1N1CCC(N2CCOCC2)CC1	8.6	*
929	C=CC(=O)Nc1cccc(-n2c(=O)c(=O)n(C(C)C)c3cnc(Nc4ccc(N5CCN(C)CC5)c(OC)c4)nc32)c1	8.6	*
930	CCOC(=O)CCCn1c(=O)oc2cc3ncnc(Nc4cccc(O)c4)c3cc21	8.7	*
931	NP(=O)(OCCCC(=O)Nc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1)N(CCCl)CCCl	8.7	*
932	C=CC(=O)N1CCc2c(sc3ncnc(Nc4cccc(CC)c4)c23)C1	8.73	*
933	Brc1cccc(Nc2ncnc3cc4c(cnn4CCCN4CCOCC4)cc23)c1	8.8	*
934	CN(C)CCCNc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	8.8	*
935	OCCn1ccc2ncnc(Nc3ccc(Oc4cccc5sccc45)c(Cl)c3)c21	8.8	*
936	C=CC(=O)Nc1cccc(N2C(=O)N(C)Cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC(C)C)nc32)c1	8.81	8.06
937	COCCOc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C1CC1	8.9	*
938	Oc1ccc(NC(=S)Nc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)cc1	8.9	*
939	O=C(NCc1ccccc1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	8.9	*
940	CN1CCN(CC2COc3cc4ncnc(Nc5cccc(Br)c5)c4cc3O2)CC1	8.9	*
941	CN(C)CCCNc1c(Br)cccc1Nc1ncnc2ccncc12	8.913	*
942	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C#Cc1ccc(CN2CCCC2)cc1	9	8.05
943	C#Cc1cccc(Nc2ncnc3cc(OCCOC(=O)C(C)c4ccc(CC(C)C)cc4)c(OCCOC)cc23)c1	9	8.05
944	C=CC(=O)N1CCC[C@H]1C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3F)ncnc2cc1OCCOC	9	8.05
945	CCN1CCN(CCCC#Cc2c(C)ncnc2Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)CC1	9	8.05
946	COC(=O)c1cccc(-c2cc3c(N[C@H](C)c4ccccc4)ncnc3s2)c1OC	9	8.05
947	OC[C@@H](Nc1ncnc2sc(-c3ccccc3)cc12)c1ccccc1	9	8.05
948	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN(C)[C@H](C)C(N)=O	9	*

949	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN(C)C1(C(N)=O)CCN(C)CC1	9	*
950	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN(C)C1(C(N)=O)CN(C(C)C)C1	9	*
951	COc1cc2ncnc(Nc3cc(Cl)ccc3F)c2cc1OCC1CCN(C)CC1	9	*
952	COc1cc2ncnc(Nc3cc(Cl)ccc3F)c2cc1OC1CCN(CC(N)=O)CC1	9	*
953	O=C(/C=C/CN1CCCCC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	9	*
954	COc1ccccc1-c1cc2c(N[C@H](C)c3ccccc3)ncnc2s1	9	*
955	CN(C)C/C=C/C(=O)Nc1cc2c(Nc3ccc(OCc4ccccn4)cc3)ncnc2cc1O[C@H]1CCOC1	9	*
956	NC(=O)Nc1ccc(C(=O)Nc2ccc3ncnc(Nc4ccc(F)c(Cl)c4)c3c2)cc1	9	*
957	CCC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1	9	*
958	Fc1cccc(COc2ccc(Nc3ncnc4sc(-c5cccs5)cc34)cc2Cl)c1	9	*
959	CCN(CC)C/C=C/C(=O)N1CCc2c(sc3ncnc(N[C@H](CO)c4ccccc4)c23)C1	9	*
960	COc1cc2ncnc(C#C[C@](C)(O)Cc3ccccc3)c2cc1OC	9	*
961	Nc1ncnc(Nc2ccc3c(cnn3Cc3cccc(F)c3)c2)c1/C=N/N1CCN(CCO)CC1	9	*
962	CNc1cc2c(Nc3ccccc3)ncnc2cn1	9	*
963	COCC#CC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	9	*
964	OCCCNCc1ccc(-c2cc3nccc(Nc4ccc5[nH]ccc5c4)c3s2)cc1	9	*
965	O=C(c1ccccc1)c1cc2ncnc(Nc3ccc4[nH]ccc4c3)c2s1	9	*
966	NC1CCN(Cc2ccn3ncnc(Nc4ccccc4)c23)CC1	9	*
967	Br.C[C@@H](Nc1ncnc2[nH]c(-c3ccc(O)cc3)cc12)c1cccc(F)c1	9	*
968	Cc1ccc(NC(=O)CSc2nc3cc4ccccc4cc3c(=O)n2-c2ccc(S(N)(=O)=O)cc2)cc1	9	*
969	Nc1cccc(-c2cc3c(Nc4ccc(Cl)cc4F)ncnc3o2)c1	9	*
970	COc1cc2ncnc(C#CC(C)(O)Cc3ccccc3)c2cc1OC	9	*
971	C=CC(=O)N1CCc2ncnc(Nc3cccc(Br)c3)c2C1	9	*
972	C=CC(=O)N1CCc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2C1	9	*
973	CN1CCN(CC=CC(=O)N2CCOc3cc4ncnc(Nc5ccc(F)c(Cl)c5)c4cc32)CC1	9	*
974	S=C(NCCN1CCOCC1)Nc1ccc2ncnc(Nc3ccc(Cl)c(Cl)c3)c2c1	9.05	8.04
975	COc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2cc1OCCCCCCC(=O)NO	9.08	8.04
976	COc1ccc(/C=C/C(=O)Nc2cc3c(Nc4ccc(F)c(Cl)c4)ncnc3cc2O[C@H]2CCOC2)cc1	9.1	*
977	O=C(/C=C/c1ccccc1)Nc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	9.1	*
978	CNC(=S)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	9.1	*
979	C=CC(=O)Nc1cccc(N2C(=O)CN(C)C(=O)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	9.14	8.04
980	CN(C)CCCOc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)c1cc([N+](=O)[O-])ccc1F	9.2	8.04
981	C#Cc1cccc(Nc2ncnc3cc(OCC)c4c(c23)OCCO4)c1	9.2	*
982	OCCN(CCO)CCNc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	9.2	*
983	NP(=O)(Oc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)N(CCCl)CCCl	9.2	*
984	Cl.Cn1ccc2ncnc(Nc3ccc(Oc4cccc(Cl)c4)c(Cl)c3)c21	9.2	*
985	O=C(COc1ccccc1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	9.25	8.03
986	Cc1cccc(Nc2ncnc3cc(NCCCN4CCOCC4)ncc23)c1	9.3	*
987	C=CC(=O)Nc1cc(Nc2n[nH]c3cc(-c4cn(C)c5ccccc45)ccc23)c(OC)cc1N(C)CCN(C)C	9.3	*
988	OCCN(CCO)CCNc1c(Br)cccc1Nc1ncnc2ccncc12	9.333	*
989	Cc1cccc(Nc2ncnc3ccncc23)c1NCCCN1CCOCC1	9.333	*
990	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCCC(=O)NO	9.4	8.03
991	CCO.Nc1ccc2sc3c(Nc4ccccc4)ncnc3c2c1	9.4	*

992	Nc1ccc2sc3c(Nc4ccccc4)ncnc3c2c1	9.4	*
993	COc1ccc(NN=C2C(=O)CCc3c2sc(N)c3C(=O)Nc2ccccc2)cc1	9.42	*
994	CCOc1cc2ncnc(Nc3ccc(Oc4ccc(C)nc4)c(Cl)c3)c2cc1NC(=O)/C(F)=C\CN(C)C	9.5	8.02
995	NS(=O)(=O)c1ccc(NC(=S)Nc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)cc1	9.5	*
996	OCCN(CCO)CC1COc2cc3ncnc(Nc4cccc(I)c4)c3cc2O1	9.5	*
997	OCCn1ccc2ncnc(Nc3ccc(Oc4cccc(Cl)c4)c(Cl)c3)c21	9.5	*
998	O=C(/C=C/CNC1CC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OC(F)F	9.6	*
999	COCCOc1cc2ncnc(Nc3ccc(C(=O)NC45CC6CC(CC(C6)C4)C5)cc3)c2cc1OCCOC	9.61	8.02
1000	C=CC(=O)Nc1ccc2ncc(C#N)c(Nc3cccc(Br)c3)c2c1	9.7	6.82
1001	CCOc1cc2ncnc(Nc3cccc([N+](=O)[O-])c3)c2c2c1OCCO2	9.7	*
1002	C=CC(=O)Nc1ccc2ncnc(Nc3ccc(S(=O)(=O)Nc4ccccn4)cc3)c2c1	9.8	*
1003	CC(C(=O)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc(Cl)c4)c(Cl)c3)c21)S(C)(=O)=O	9.8	*
1004	CC(C)(O)CC(=O)NCCc1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c2c1	9.8	*
1005	O=C(/C=C/CN1CCCCC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCC(F)F	9.87	*
1006	C=CC(=O)N1CC[C@H](Nc2nc(Nc3ccccc3)nc3cnc(Nc4ccc(N5CCN(C)CC5)cn4)cc23)C1	9.9	*
1007	CS(=O)(=O)CCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	10	7.82
1008	O=C(CBr)OCCn1c(=O)oc2cc3ncnc(Nc4ccc(N5CCOCC5)c(Cl)c4)c3cc21	10	8.00
1009	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4cccc5ccccc45)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	10	8.00
1010	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN1CCC[C@@H]1C(N)=O	10	*
1011	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN1C[C@H](OC)C[C@@H]1C(N)=O	10	*
1012	COCCN(Cc1cc2c(Nc3cccc(Cl)c3F)ncnc2cc1OC)[C@@H](C)C(N)=O	10	*
1013	COCC[C@@H](C(N)=O)N(C)Cc1cc2c(Nc3cccc(Cl)c3F)ncnc2cc1OC	10	*
1014	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OC1CCN(C)CC1	10	*
1015	O=C(/C=C/CNCC1COC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	10	*
1016	COCCOc1cc2ncnc(Nc3ccc(OCc4ccccn4)cc3)c2cc1NC(=O)/C=C/CN(C)C	10	*
1017	COCCOc1cc2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c2cc1NC(=O)/C=C/CN1CCCC1	10	*
1018	Cc1ccc(Oc2ccc(Nc3ncnc4ccc(-c5cn(CCCCCCC(=O)NO)nn5)cc34)cc2C)cn1	10	*
1019	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCN1CCN(C)CC1	10	*
1020	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCN1CCOCC1	10	*
1021	Fc1cccc(COc2ccc(Nc3ncnc4cc(-c5ccco5)sc34)cc2Cl)c1	10	*
1022	CCOc1cc2ncnc(C#Cc3[nH]ccc3-c3ccccc3)c2cc1OCC	10	*
1023	COc1cc2ncnc(NCc3ccccc3)c2cc1OC	10	*
1024	COc1ccc2c(Nc3cccc(Br)c3)ncnc2c1	10	*
1025	COc1cc2ncnc(NC3CC3c3ccccc3)c2cc1OC	10	*
1026	Nc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	10	*
1027	COc1ccc2cncnc2c1	10	*
1028	COc1cc2ncnc(Sc3cccc(Cl)c3)c2cc1OC	10	*
1029	Cc1c(-c2ccccc2)[nH]c2ncnc(Nc3cccc(Cl)c3)c12	10	*
1030	ClCCNc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	10	*
1031	COc1cc(OC2CCNCC2)c2c(Nc3ccc(F)c(Cl)c3)ncnc2c1	10	*
1032	CCN1CCN(CC/C=C/c2ccc3c(Nc4ccc(Sc5nccn5C)c(Cl)c4)c(C#N)cnc3c2)CC1	10	*
1033	Nc1c(Br)cccc1Nc1ncnc2ccncc12	10	*
1034	COc1cc2ncnc(Sc3cccc(NC(=S)Nc4ccc(F)c(C(F)(F)F)c4)c3)c2cc1OC	10	*

1035	COc1cc2ncnc(Sc3cccc(NC(=S)Nc4ccc(Br)c(C(F)(F)F)c4)c3)c2cc1OC	10	*
1036	C=CC(=O)Cc1cc(Nc2ncc3ncn(-c4ccc(F)c(Br)c4)c3n2)c(OC)cc1N(C)CCN(C)C	10	*
1037	O=[N+]([O-])c1ccc(-c2cc3c(Nc4cccc(Cl)c4)ncnc3o2)cc1	10	*
1038	C[C@@H](Nc1ncnc2oc(-c3cccc([N+](=O)[O-])c3)cc12)c1ccccc1	10	*
1039	Nc1ccc(-c2cc3c(Nc4ccc(Cl)cc4F)ncnc3o2)cc1	10	*
1040	CC(C)(C)C(Nc1ncnc2[nH]c(-c3ccccc3)cc12)c1ccccc1	10	*
1041	c1nc(Nc2ccc(N3CCOCC3)cc2)cc(Oc2ccc3[nH]ccc3c2)n1	10	*
1042	COC[C@H]1Oc2cc3ncnc(Nc4cccc(Cl)c4)c3cc2O[C@@H]1COC	10.08	*
1043	C=CC(=O)Nc1cccc(N2C(=O)C(C(C)CC)N(C)C(=O)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	10.18	7.99
1044	C=CC(=O)Nc1cccc(N2C(=O)C(CC(C)C)N(C)C(=O)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	10.18	*
1045	S=C(Nc1cccnc1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	10.2	*
1046	Nc1sc2c(c1C(=O)Nc1ccccc1)CCC(=O)C2=NNc1ccc(Cl)cc1	10.37	*
1047	COCCOc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCCCCC(=O)NO	10.4	7.98
1048	CN(C)C1CCN(c2ccc(Nc3cc4c(N5CCC(CO)CC5)nc(Nc5ccc(F)cc5)nc4cn3)nc2)CC1	10.4	*
1049	O=C(Nc1ccc(F)c(Cl)c1)c1ccc(OCCCN2CCOCC2)cc1O	10.4	*
1050	C=C=CC(=O)Nc1cc(Nc2nccc(C3=CN(C)C4C=C(F)C=CC34)n2)c(OC)cc1N(C)CCN(C)C	10.5	*
1051	C=CC(=O)Nc1cccc(-c2c[nH]c3nccc(-c4[nH]c(-c5ccccc5)nc4-c4ccc(F)cc4)c23)c1	10.5	*
1052	C=C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4cc(F)ccc34)n2)c(OC)cc1N(C)CCN(C)C	10.5	*
1053	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCN1C[C@H](O)[C@@H](O)[C@H](O)[C@H]1CO	10.71	*
1054	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCN1C[C@H](O)[C@@H](O)[C@H](O)[C@H]1CO	10.71	*
1055	O=C(c1cc2ccccc2s1)c1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	10.8	*
1056	Cc1ccc(S(=O)(=O)O)cc1.NS(=O)(=O)CCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	10.8	*
1057	Cc1ccc(S(=O)(=O)O)cc1.Fc1cccc(COc2ccc(Nc3ncnc4ccc(-c5ccc(CN6CCNCC6)o5)cc34)cc2Cl)c1	10.8	*
1058	CS(=O)(=O)C[C@@H](N)c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	10.8	*
1059	C#Cc1cccc(Nc2ncnc3cc(OC)c4c(c23)OCCO4)c1	10.9	*
1060	C[C@@H](Nc1ncnc2oc(-c3ccccc3)cc12)c1ccccc1	11	7.96
1061	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C#CCCCN1CCCC1	11	7.96
1062	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4Cl)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	11	7.96
1063	C#Cc1cccc(Nc2ncnc3ccc(OCCCCNCCS(C)(=O)=O)cc23)c1	11	*
1064	CC(C)(C(=O)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc(Cl)c4)c(Cl)c3)c21)S(C)(=O)=O.Cc1ccc(S(=O)(=O)O)cc1	11	*
1065	CC(C)(C(=O)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc(Cl)c4)c(Cl)c3)c21)S(C)(=O)=O	11	*
1066	CN(C)c1ccc2cncnc2c1	11	*
1067	CN(C)c1ccc2c(Nc3cccc(Br)c3)ncnc2c1	11	*
1068	Brc1cccc(Nc2ncnc3ccsc23)c1	11	*
1069	Cc1cccc(Nc2ncnc3c2sc2ccc([N+](=O)[O-])cc23)c1.Cl	11	*
1070	C=CC(=O)Nc1cccc(Nc2ncc(NC(=O)c3cc(NC(=O)c4cccc(C(F)(F)F)c4)ccc3C)cn2)c1	11	*
1071	CN(C)N=Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	11	*
1072	C#Cc1cccc(Nc2ncnc3ccc(OCCCCOP(N)(=O)N(CCCl)CCCl)cc23)c1	11	*
1073	OCCSc1nc(-c2ccc(F)cc2)c(-c2ccnc(Nc3ccccc3)c2)[nH]1	11	*
1074	CCOc1cc2ncnc(Nc3ccc(OCC4CC4)c(Cl)c3)c2cc1NC(=O)/C(F)=C\CN(C)C	11.2	7.95
1075	O=C(/C=C/CN1CCCCC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1	11.35	*
1076	CC(=O)N1CCN(Cc2ccc(-c3ccc4ncnc(Nc5ccc(OCc6cccc(F)c6)c(Cl)c5)c4c3)o2)CC1.Cc1ccc(S(=O)(=O)O)cc1	11.4	*
1077	S=C(NCc1ccccc1)Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	11.4	*

1078	CC1(C)OOC2(CCC(C(=O)Nc3ccc4ncnc(Nc5cccc(Cl)c5)c4c3)CC2)OO1	11.42	*
1079	COc1cc(Nc2ncnc3ccc(-c4cn(CCCCCCC(=O)NO)nn4)cc23)ccc1Oc1ccccc1	11.6	*
1080	CCOc1cc2ncnc(C#CC(C)(Cc3ccccc3)N3CCC(C(=O)O)CC3)c2cc1OCC	11.7	*
1081	CNC1CC2OC(C)(C1OC)n1c3ccccc3c3c4c(c5c6ccccc6n2c5c31)C(=O)NC4	11.8	*
1082	COc1cc2c(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncnc2cc1OCCCCn1ccnc1[N+](=O)[O-]	11.9	7.92
1083	C=Cc1cccc(Nc2ncnc3cc(OCCOC)c(OCCOC)cc23)c1	11.9	*
1084	Nc1ccc(C(=O)Nc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)cc1	11.9	*
1085	CC(=O)Nc1cccc(C#Cc2cncnc2Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1	12	*
1086	C#Cc1cccc(Nc2ncnc3cc4c(cc23)N(C(=O)/C=C/CN2CCOCC2)CCO4)c1	12	*
1087	O=C(/C=C/CN1CCOCC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cn1	12	*
1088	CS(=O)(=O)CCNCc1ccc(-c2cc3c(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)ncnc3s2)o1	12	*
1089	C[C@@H](Nc1ncnc2sc3c(c12)CCN(C(=O)/C=C/CN(C)C)C3)c1ccccc1	12	*
1090	CC[C@@H](Nc1ncnc2sc3c(c12)CCN(C(=O)/C=C/CN(C)C)C3)c1ccccc1	12	*
1091	CCOc1cc2ncnc(C#Cc3nccn3-c3ccccc3)c2cc1OCC	12	*
1092	CN/N=C/c1c(N)ncnc1Nc1ccc2c(cnn2Cc2cccc(F)c2)c1	12	*
1093	OCC(O)Cn1ncc2cc3c(Nc4cccc(Br)c4)ncnc3cc21	12	*
1094	OCCN(CCO)c1cc2ncnc(Nc3cccc(Br)c3)c2cn1	12	*
1095	COC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	12	*
1096	CCNc1ccc2c(Nc3cccc(Br)c3)ncnc2c1	12	*
1097	CCN(CC)CC#CC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	12	*
1098	CO/N=C/c1c(N)ncnc1Nc1ccc(OCc2cccc(F)c2)c(Cl)c1	12	*
1099	Nc1ncnc(Nc2ccc3c(cnn3Cc3cccc(F)c3)c2)c1/C=N/O	12	*
1100	C[C@@H](Nc1ncnc2[nH]c(-c3ccc(C#N)cc3)cc12)c1ccccc1	12	*
1101	Cc1ccccc1NC(=O)CSc1nc2cc3ccccc3cc2c(=O)n1-c1ccc(S(N)(=O)=O)cc1	12	*
1102	C=CC(=O)N[C@H]1CCCN(c2nc(Nc3ccccc3)nc3cnc(Nc4ccc(N5CCN(C)CC5)cn4)cc23)C1	12	*
1103	C=CC(=O)N1CCc2ncnc(Nc3ccc(F)c(Cl)c3)c2C1	12	*
1104	C=CC(=O)NCCSc1nc(-c2ccccc2)c(-c2ccnc(Nc3ccccc3)c2)[nH]1	12	*
1105	OCCN(CCO)c1c(Br)cccc1Nc1ncnc2ccncc12	12.02	*
1106	C=CC(=O)Nc1cccc(-n2c(=O)cnc3cnc(Nc4ccc(C(N)=O)cc4)nc32)c1	12.1	7.92
1107	CC(=O)N1CC[C@H](N2C(=O)N(c3ccccc3Cl)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	12.1	7.92
1108	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCNCCN	12.1	*
1109	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CN1CCCCCC1	12.13	*
1110	CCOc1cc2ncnc(NC3=CC(=O)C(OCc4cccc(Cl)c4)=CC3=O)c2cc1NC(=O)/C=C/CN(C)C	12.2	7.91
1111	Cl.O=[N+]([O-])c1ccc2sc3c(Nc4cccc(Br)c4)ncnc3c2c1	12.3	*
1112	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccn4)c(Cl)c3)c2cc1NC(=O)CCN(C)C	12.5	7.90
1113	C=CC(=O)Nc1cccc(-n2c(=O)cnc3cnc(Nc4ccc(NC(C)=O)cc4)nc32)c1	12.5	7.90
1114	CN1CCN(Cc2ccc(-c3ccc4ncnc(Nc5ccc(OCc6cccc(F)c6)c(Cl)c5)c4c3)o2)CC1.Cc1ccc(S(=O)(=O)O)cc1	12.5	*
1115	COc1cccc2c1sc1c(Nc3cccc(Br)c3)ncnc12.Cl	12.6	*
1116	COc1cc2ncnc(N[C@H](C)c3ccccc3)c2cc1OCCCCCCC(=O)NO	12.8	7.89
1117	C=CC(=O)Nc1cccc(-n2c(=O)cnc3cnc(Nc4ccccc4)nc32)c1	12.8	7.89
1118	CC(=O)Nc1ccc(C(=O)Nc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)cc1	12.8	*
1119	CCOc1cc2ncnc(Nc3ccc(Oc4ccc(C)nc4)c(Cl)c3)c2cc1NC(=O)/C(F)=C/CN1CCCCC1	12.9	7.89
1120	C[C@@H](Nc1ncnc2oc(-c3ccc(F)cc3)cc12)c1ccccc1	13	7.89

1121	C=CC(=O)N1CCC[C@H]1C(=O)Nc1cc2c(Nc3cccc(Cl)c3F)ncnc2cc1OCCOC	13	7.89
1122	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C#CCCN1CCOCC1	13	7.89
1123	COc1cccc(-c2cc3c(N[C@H](C)c4ccccc4)ncnc3s2)c1OC	13	7.89
1124	C[C@@H](Nc1ncnc2sc(-c3ccc(CO)cc3F)cc12)c1ccccc1	13	7.89
1125	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1)c1cccc([N+](=O)[O-])c1F	13	7.89
1126	CN1CCN(CCOc2cc3ncnc(Nc4ccc(F)c(Cl)c4)c3cc2NC(=O)c2cc([N+](=O)[O-])ccc2F)CC1	13	7.89
1127	CS(=O)CCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1.Cc1ccc(S(=O)(=O)O)cc1	13	*
1128	COc1cc2ncnc(C#CC(C)(C)Cc3ccccc3)c2cc1OC	13	*
1129	Fc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	13	*
1130	CNc1ncc2ncnc(Nc3ccccc3)c2n1	13	*
1131	CCN1CCN(C(=O)c2cc(C)c(/C=C3\C(=O)Nc4ncnc(Nc5ccc(F)c(Cl)c5)c43)[nH]2)CC1	13	*
1132	CO/N=C/c1c(N)ncnc1Nc1ccc2c(ccn2Cc2cccc(F)c2)c1	13	*
1133	C=CC(=O)Nc1cccc(-n2c(=O)n(CCC)c(=O)c3cnc(Nc4ccc(N5CCC(N(C)C)CC5)cc4OC)nc32)c1	13	*
1134	COCCOc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2c2c1OCCO2	13.1	*
1135	Fc1c(Br)cccc1Nc1ncnc2ccncc12	13.18	*
1136	CS(=O)(=O)C[C@H](N)c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	13.5	*
1137	C=C=CC(=O)Nc1cc(Nc2nccc(C3=CN(C)C4C=CC=CC34)n2)c(OC)cc1N1CCOCC1	13.5	*
1138	C=C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4ccccc34)n2)c(OC)cc1N1CCOCC1	13.5	*
1139	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCNCCN	13.6	*
1140	Oc1ccc(-c2nc(-c3ccccc3)c(-c3ccnc4[nH]c(-c5ccccc5)cc34)[nH]2)cc1	13.6	*
1141	C=CC(=O)Nc1cccc(-n2c(=O)cnc3cnc(Nc4ccc(OC)cc4)nc32)c1	13.8	7.86
1142	C=C=CC(=O)Nc1cc(Nc2nccc(C3=CN(C)C4C=CC=CC34)n2)c(OC)cc1OCCN1CCN(C)CC1	13.9	*
1143	C=C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4ccccc34)n2)c(OC)cc1OCCN1CCN(C)CC1	13.9	*
1144	COC[C@@H](Nc1ncnc2oc(-c3ccc(OC)cc3)cc12)c1ccccc1	14	7.85
1145	COc1cc(CO)ccc1-c1cc2c(Nc3ccccc3)ncnc2s1	14	7.85
1146	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1)c1cccc([N+](=O)[O-])c1Cl	14	7.85
1147	O=C(/C=C/CN1CCCCC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cn1	14	*
1148	COc1cc2ncnc(C#CCCc3ccccc3)c2cc1OC	14	*
1149	O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1	14	*
1150	OCC(CO)Nc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	14	*
1151	COc1cc2c(Nc3ccc(NC(=O)Nc4ccccc4)c(Cl)c3)ncnc2cc1OCCCN1CCN(C)CC1	14	*
1152	CN(C/C=C/C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)CCO	14	*
1153	CN(C)N=Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	14	*
1154	COCCO/N=C/c1c(N)ncnc1Nc1ccc2c(cnn2Cc2cccc(F)c2)c1	14	*
1155	CC(C)O/N=C/c1c(N)ncnc1Nc1ccc2c(cnn2Cc2cccc(F)c2)c1	14	*
1156	C[C@@H](Nc1ncnc2[nH]c(-c3ccc(C#N)cc3)cc12)c1ccc(F)cc1	14	*
1157	COc1ccc(-c2cc3c(NC(C)c4cccc(C)c4)ncnc3[nH]2)cc1	14	*
1158	COc1ccc(-c2cc3c(N[C@H](C)c4ccc(C)cc4)ncnc3[nH]2)cc1	14	*
1159	OCC#Cc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	14.1	*
1160	OCN(CO)c1c(Br)cccc1Nc1ncnc2ccncc12	14.13	*
1161	C=CC(=O)Nc1cccc(-n2c(=O)cnc3cnc(Nc4ccc(N(CC)CC)cc4)nc32)c1	14.5	7.84
1162	CCNC(CS(C)(=O)=O)c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	14.7	*
1163	C=C=CC(=O)Nc1cc(Nc2ncc(OCC)c(C3=CN(C)C4C=CC=CC34)n2)ccc1N(C)CCN(C)C	14.7	*

1164	C=C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4ccccc34)n2)c(OCC)cc1N(C)CCN(C)C	14.7	*
1165	COC(=O)N1CCc2ncnc(Nc3cccc(Cl)c3)c2C1	14.8	7.83
1166	C#CCOc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OC	14.8	*
1167	O=C(Nc1ccncc1)Nc1cc(-c2cncnc2)cc(C(F)(F)F)c1	14.83	*
1168	C#Cc1cccc(Nc2ncnc3cc(OCCOC)c(OCCOC)cc23)c1.Cl	15	7.82
1169	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCN1CCC2(COC2)C1	15	7.82
1170	C#Cc1cccc(Nc2ncnc3cc(OC)c(OCCCCC(=O)NO)cc23)c1	15	7.82
1171	CC1(C)CC(C(=O)Nc2ccc3ncnc(Nc4ccc(F)c(Cl)c4)c3c2)CC(C)(C)N1[O]	15	7.82
1172	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccc5ccccc5c4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	15	7.82
1173	CCCCC#CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cn1	15	*
1174	CCN(CC)CC#CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cn1	15	*
1175	CS(=O)(=O)CCNC(=O)NCc1cccc(C#Cc2cncnc2Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)n1	15	*
1176	Nc1ccccc1NC(=O)CCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)cc1	15	*
1177	C=CC(=O)Nc1cccc(-n2c(=O)ccc3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	15	*
1178	Fc1cccc(COc2ccc(Nc3ncnc4sc(-c5ccco5)cc34)cc2Cl)c1	15	*
1179	CCOc1cc2ncnc(/C=C/c3ccccc3)c2cc1OCC	15	*
1180	COc1cc2ncnc(C#CCOc3ccccc3)c2cc1OC	15	*
1181	CS(=O)(=O)CC(=O)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21	15	*
1182	Brc1cccc(Nc2ncnc3cc4c(cc23)OCO4)c1	15	*
1183	Nc1cc2ncnc(Nc3cccc(C(F)(F)F)c3)c2cn1	15	*
1184	COc1cc2ncnc(Nc3cccc(Br)c3)c2cc1[N+](=O)[O-]	15	*
1185	COc1cc2c(Nc3ccc(NC(=O)Nc4ccccc4C)c(Cl)c3)ncnc2cc1OCCCN1CCN(C)CC1	15	*
1186	OCCOCCn1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21	15	*
1187	CC(C)[C@@H](Nc1ncnc2[nH]c(-c3ccccc3)cc12)c1ccccc1	15	*
1188	COc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2cc1OCCCCCCn1ccnc1[N+](=O)[O-]	15.1	7.82
1189	C=CC(=O)Nc1cccc(-n2c(=O)cnc3cnc(Nc4ccc(N5CCCC5)cc4)nc32)c1	15.3	7.82
1190	Oc1ccc(C=Nc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)cc1	15.3	*
1191	COc1cc2ncnc(Nc3cc(C(=O)NC45CC6CC(CC(C6)C4)C5)ccc3C)c2cc1OCCCN1CCOCC1	15.4	7.81
1192	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1S(=O)(=O)CCCCCCC(=O)NO	15.4	7.81
1193	O=C(Nc1ccc(F)c(Cl)c1)c1ccc(OCCCN2CCCCC2)cc1O	15.4	*
1194	C=CC(=O)Cc1cc(Nc2ncc3ncn(-c4ccc(Cl)cc4)c3n2)c(OC)cc1N(C)CCN(C)C	15.6	*
1195	C#Cc1cccc(Nc2ncnc3ccc(-c4ccc(CO)o4)cc23)c1	15.69	*
1196	C=CC(=O)Nc1cccc(-n2c(=O)cnc3cnc(Nc4ccc(N5CCCCC5)cc4)nc32)c1	15.7	7.80
1197	CCC(=O)N1CC[C@H](N2C(=O)N(c3ccccc3Cl)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	15.7	7.80
1198	S=C(Nc1ccccc1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	15.8	*
1199	S=C(Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)Nc1ccccc1Cl	15.8	*
1200	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCN1CC2(COC2)C1	16	7.80
1201	CCC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	16	7.80
1202	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN1CCSCC1	16	7.80
1203	C#Cc1cccc(Nc2ncnc3cc4c(cc23)N(C(=O)/C=C/CN2CCN(C)CC2)CCO4)c1	16	*
1204	C=CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	16	*
1205	C=CC(=O)Nc1cccc(-n2c(=O)c(C)cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	16	*
1206	COCCOc1cc2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c2cc1NC(=O)/C=C/CN1CCN(C)CC1	16	*

1207	Nc1ncnc(Nc2ccc3c(cnn3Cc3cccc(F)c3)c2)c1/C=N/N1CCOCC1	16	*
1208	CN1CCN(/N=C/c2c(N)ncnc2Nc2ccc3c(cnn3Cc3cccc(F)c3)c2)CC1	16	*
1209	CN(CC(=O)O)c1cc2ncnc(Nc3cccc(Br)c3)c2cn1	16	*
1210	CO/N=C/c1c(N)ncnc1Nc1ccc(OCc2ccccc2)c(Cl)c1	16	*
1211	C=CC(=O)Nc1cc(Nc2n[nH]c3cc(-c4cccc(C(F)(F)F)c4)ccc23)c(OC)cc1N(C)CCN(C)C	16	*
1212	C=CC(=O)NCc1cccc(Nc2cc(-c3[nH]c(SC)nc3-c3ccc(F)cc3)ccn2)c1	16	*
1213	C=CC(=O)NCCCSc1nc(-c2ccc(F)cc2)c(-c2ccnc(Nc3ccccc3)c2)[nH]1	16	*
1214	O=[N+]([O-])c1ccc(C=Nc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)cc1	16.2	*
1215	CN(CC(=O)O)c1c(Br)cccc1Nc1ncnc2ccncc12	16.22	*
1216	C=CC(=O)Nc1cccc(N2C(=O)N(C)Cc3cnc(Nc4ccc(N5CCOCC5)cc4OC)nc32)c1	16.4	7.79
1217	COc1cc2c(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncnc2cc1OCCCCCn1ccnc1[N+](=O)[O-]	16.6	7.78
1218	O=C(c1cc2ccccc2[nH]1)c1cc2c(Nc3cccc(Cl)c3)ncnc2s1	16.6	*
1219	C#Cc1cccc(Nc2ncnc3cc(OC4CCOC4)c4c(c23)OCCO4)c1	16.7	*
1220	C=C=CCOc1cc2c(Nc3cccc(Cl)c3)ncnc2cc1O	16.9	*
1221	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C	17	7.77
1222	CCCCN(CC#CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cn1)CCCC	17	*
1223	Fc1cccc(COc2ccc(Nc3ncncc3C#Cc3ccccn3)cc2Cl)c1	17	*
1224	Cn1ccnc1S(=O)(=O)CCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(C(F)(F)F)c4)c3c2)o1	17	*
1225	COc1ccccc1-c1cc2c(NCc3ccccc3)ncnc2s1	17	*
1226	CCC(=O)Nc1cc2c(Nc3ccc4c(cnn4Cc4ccccc4)c3)ncnc2cc1OC	17	*
1227	Cc1cccc(Nc2ncnc3cnc(N)nc23)c1	17	*
1228	COc1cc2c(Nc3ccc(NC(=O)Nc4ccc(Cl)cc4)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1	17	*
1229	Br.Cc1ccccc1C(C)Nc1ncnc2[nH]c(-c3ccc(O)cc3)cc12	17	*
1230	CC(C)(C)OC(=O)NCC(=O)Nc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	17	*
1231	C=CC(=O)Nc1cccc(NC(=O)Nc2ccnc(Nc3ccc(N4CCN(C)CC4)cc3OC)n2)c1	17	*
1232	C=CC(=O)Cc1cc(Nc2ncc3ncn(-c4ccc(I)cc4)c3n2)c(OC)cc1N(C)CCN(C)C	17	*
1233	COc1cc2ncnc(Nc3ccc(OCc4ccccc4)cc3)c2cc1OC	17	*
1234	COc1cc2ncnc(Nc3ccc(OCc4ccccc4Br)c(Cl)c3)c2cc1OC	17	*
1235	C=CC(=O)Nc1ccc(OC)c(Nc2cc(-c3cnc(SC)[nH]3)ccn2)c1	17	*
1236	CC/C=C/C(=O)Nc1cc2c(N3CCc4ccccc43)ncnc2cc1OC	17	*
1237	S=C(NCc1ccccc1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	17.2	*
1238	CN(C)CCC(=O)N(C)c1ccc2ncnc(Nc3cccc(Br)c3)c2c1	17.4	7.76
1239	O=C(Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)c1ccncc1	17.5	*
1240	CCC(=O)N1CC[C@H](N2C(=O)N(c3ccccc3F)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	17.6	7.75
1241	CS(=O)(=O)CC(N)c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	17.6	*
1242	C=CC(=O)NCc1cccc(-c2nc(-c3ccc(F)cc3)c(-c3ccnc4[nH]c(-c5ccccc5)cc34)[nH]2)c1	17.6	*
1243	C#CCCCOc1cc2c(Nc3cccc(Cl)c3)ncnc2cc1OC	17.7	*
1244	Brc1cccc(Nc2ncnc3cc4c(cc23)OCCO4)c1	17.8	*
1245	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1/C=C(\F)C(=O)NCCN1CCOCC1	18	7.74
1246	CC(C)S(=O)(=O)CCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	18	*
1247	CS(=O)(=O)CCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5ccccc5)c(Cl)c4)c3c2)o1	18	*
1248	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1OCCCN1CCOCC1	18	*
1249	O=C(/C=C/c1cccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)c1)NO	18	*

1250	O=C(/C=C/c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)cc1)NO	18	*
1251	CSC1CCN(C/C=C/C(=O)Nc2cc3c(Nc4ccc(F)c(Cl)c4)ncnc3s2)CC1	18	*
1252	C#Cc1cccc(Nc2ncnc3sc(-c4ccccc4OC)cc23)c1	18	*
1253	CCC1=C2C(Nc3ccc4c(cnn4Cc4ccccc4)c3)=NC=NC2N=C1NC(=O)OCCN1CCNCC1	18	*
1254	CCC1=C2C(Nc3ccc4c(cnn4Cc4ccccc4)c3)=NC=NC2N=C1NC(=O)O[C@H]1CC[C@H](N)CC1	18	*
1255	CC(C(=O)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21)S(C)(=O)=O	18	*
1256	Clc1ccc2ncnc(Nc3cccc(Br)c3)c2n1	18	*
1257	C#Cc1cccc(Nc2ncnc3c2/C(=C/c2[nH]c(C(=O)NCCN4CCOCC4)cc2C)C(=O)N3)c1	18	*
1258	C=CC(=O)Nc1cccc(NC(=O)Nc2nc(Nc3ccc(N4CCC(N5CCOCC5)CC4)cc3OC)ncc2C(F)(F)F)c1	18	*
1259	COc1cc2ncnc(Nc3ccc4[nH]c(Cc5ccccc5)nc4c3)c2cc1OC	18	*
1260	Clc1cc(Nc2ncnc3cc[nH]c23)ccc1OCc1ccccn1	18	*
1261	C=CC(=O)N1CCc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c2C1	18	*
1262	Cc1ccc(Nc2cc(Oc3ccc4[nH]ccc4c3)ncn2)cc1S(N)(=O)=O	18	*
1263	O=C(Nc1ccncc1)Nc1cc(-c2cncnc2)ccc1OC(F)(F)F	18.04	*
1264	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CN1CCC(F)CC1	18.08	*
1265	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCBr	18.1	*
1266	C=CC(=O)Cc1cc(Nc2ncc3ncn(-c4ccc(F)cc4)c3n2)c(OC)cc1N(C)CCN(C)C	18.2	*
1267	Brc1cccc(Nc2ncnc3cc(OCCCN4CCOCC4)c4c(c23)OCCO4)c1	18.48	*
1268	O=C(c1cc2ccccc2[nH]1)c1cc2c(Nc3ccc(OCc4cccc(F)c4)cc3Cl)ncnc2s1	18.5	*
1269	CCOc1cc2ncnc(NC3=CC(=O)C(OCc4ccccc4)=CC3=O)c2cc1NC(=O)/C=C/CN(C)C	18.7	7.73
1270	C#Cc1cccc(Nc2ncnc3sc(C(=O)c4cc5ccccc5[nH]4)cc23)c1	18.7	*
1271	CS(=O)(=O)NCCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1.Cc1ccc(S(=O)(=O)O)cc1	18.7	*
1272	C=CC(=O)Nc1ccc2ncnc(Nc3ccccc3CC)c2c1	18.9	*
1273	C=C=CC(=O)Nc1cc(Nc2nccc(C3=CN(C)C4C=CC=CC34)n2)c(OC)cc1N1CCC(N(C)C)C1	18.9	*
1274	C=C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4ccccc34)n2)c(OC)cc1N1CCC(N(C)C)C1	18.9	*
1275	O=C(CCOc1ccccc1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	19	7.72
1276	O=C(CCl)OCCn1c(=O)oc2cc3ncnc(Nc4ccc(N5CCOCC5)c(Cl)c4)c3cc21	19	7.72
1277	C#Cc1cccc(Nc2ccnc3cc(OC)c(OC)cc23)c1	19	7.72
1278	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1/C=C(\F)C(=O)NCCS(C)(=O)=O	19	7.72
1279	C[C@@H](Nc1ncnc2sc(-c3ccc(C(=O)O)cc3)cc12)c1ccccc1	19	7.72
1280	CS(=O)(=O)CCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1.Cc1ccc(S(=O)(=O)O)cc1.Cc1ccc(S(=O)(=O)O)cc1.O	19	8.01
1281	O=S(=O)(CCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1)c1ccccc1	19	*
1282	O=S(=O)(CCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(C(F)(F)F)c4)c3c2)o1)c1ccccn1	19	*
1283	COc1ccccc1-c1cc2c(NC(C)c3ccccc3)ncnc2s1	19	*
1284	CN1CCN(C/C=C/C(=O)Nc2cc3c(Nc4ccc(F)c(Cl)c4)ncnc3cn2)CC1	19	*
1285	Clc1cccc(Nc2[nH]cnc3nnc(-c4ccccc4)c2-3)c1	19	*
1286	Cc1cncc(Cn2ncc3cc(Nc4ncnn5ccc(CN6CCC(N)CC6)c45)ccc32)c1	19	*
1287	C=CC(=O)N1CCC[C@H]1CSc1nc(-c2ccc(F)cc2)c(-c2ccnc(Nc3ccccc3)c2)[nH]1	19	*
1288	O=C(Nc1ccc(Cl)cc1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	19.3	*
1289	S=C(Nc1ccc(Cl)cc1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	19.5	*
1290	COc1ccc(C(=O)Nc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)cc1OC	19.5	*
1291	CN(C)c1ccc2sc3c(Nc4cccc(Br)c4)ncnc3c2c1	19.8	*

1292	O=C(Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)c1ccenc1	19.8	*
1293	CN1CCN(c2ccc(Nc3ncnc4cc5oc(=O)n(CCOC(=O)CCl)c5cc34)cc2Cl)CC1	20	7.70
1294	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)CCO	20	7.70
1295	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN1CCOCC1	20	7.70
1296	COc1cc(C=O)ccc1-c1cc2c(Nc3ccccc3)ncnc2s1	20	7.70
1297	COC(=O)c1ccc(-c2cc3c(N[C@H](C)c4ccccc4)ncnc3s2)c(OC)c1	20	7.70
1298	CS(=O)(=O)CCNCCCCOc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	20	*
1299	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1CN1CCC[C@H]1C(N)=O	20	*
1300	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN(C)CC(N)=O	20	*
1301	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN(C)C1CCNC1=O	20	*
1302	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN(C)[C@@H](CO)C(N)=O	20	*
1303	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN(C)C1(C(N)=O)CN(C)C1	20	*
1304	O=C(/C=C/CNC1CCOCC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	20	*
1305	CCOC(=O)CCCn1c(=O)oc2cc3ncnc(Nc4ccc(O)cc4)c3cc21	20	*
1306	C=CC(=O)Nc1cccc(-n2c(=O)c(-c3ccccc3)c(C)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	20	*
1307	C=CC(=O)N1CCc2c(sc3ncnc(N[C@H](C)c4ccccc4)c23)C1	20	*
1308	CCC1=C2C(Nc3ccc4c(cnn4Cc4ccccc4)c3)=NC=NC2N=C1NC(=O)O[C@H]1CC[C@@](C)(N)CC1	20	*
1309	C=CC(=O)N(C)c1nc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1	20	*
1310	CNc1ccc2ncnc(Nc3cccc(Br)c3)c2n1	20	*
1311	COc1cc2ncnc(Oc3cccc(Cl)c3)c2cc1OC	20	*
1312	COc1cccc2sc3c(Nc4cccc(Br)c4)ncnc3c12.Cl	20	*
1313	CCc1c(C(=O)O)cn2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c12	20	*
1314	COc1cc2c(Nc3ccc(NC(=O)c4ccccc4Cl)cc3)ncnc2cc1OCCCN1CCN(C)CC1	20	*
1315	O=C(C#CCN1CCOCC1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	20	*
1316	CO/N=C/c1c(N)ncnc1Nc1ccc2c(cnn2Cc2cccc(C#N)c2)c1	20	*
1317	C#Cc1cccc(Nc2ncnn3ccc(COC[C@@H]4CNCCO4)c23)c1	20	*
1318	Cc1ccccc1Nc1ncnn2ccc(CN3CCC(N)CC3)c12	20	*
1319	COc1cc2ncnc(Oc3cccc(NC(=S)Nc4ccc(Cl)c(C(F)(F)F)c4)c3)c2cc1OC	20	*
1320	COc1cc2ncnc(Sc3cccc(NC(=S)Nc4cc(C(F)(F)F)cc(C(F)(F)F)c4)c3)c2cc1OC	20	*
1321	COc1cc2ncnc(Nc3ccc(Br)c(O)c3)c2cc1OC	20	*
1322	COc1ccc(Nc2ncnc3oc(-c4ccc(N)cc4)cc23)cc1O	20	*
1323	Cc1ccc(Nc2ncnc3oc(-c4cccc(N)c4)cc23)cc1O	20	*
1324	O=[N+]([O-])c1ccc(-c2cc3c(Nc4ccc(Cl)cc4F)ncnc3o2)cc1	20	*
1325	Cc1cccc(Oc2ccc(Nc3ncnc4cc[nH]c34)cc2Cl)c1	20	*
1326	Cc1nc(C)c(C=C2CN(C)CC(=C/c3nc(C)c(C)nc3C)/C2=N/O)nc1C	20	*
1327	COc1cc(Br)c(C=C2CN(C)CC(=Cc3nc(C)c(C)nc3C)C2=NO)cc1OC	20	*
1328	C=CC(=O)Nc1cccc(-n2c(=O)n(C(C)C)c(=O)c3cnc(Nc4ccc(N5CCC(N(C)C)CC5)cc4OC)nc32)c1	20	*
1329	Cc1cccc(NNc2ncnc3[nH]ccc23)c1	20.01	*
1330	COc1cc2c(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncnc2cc1OCCOCCn1ccnc1[N+](=O)[O-]	20.1	7.70
1331	Fc1ccc(Nc2ncnc3cc(OC4CCOC4)c4c(c23)OCCO4)cc1Cl	20.5	*
1332	S=C(Nc1cccc(Cl)c1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	20.6	*
1333	C/C=C\c1ccc(Nc2ncnc3cc(OCCCN4CCOCC4)c(OCCCN4CCOCC4)cc23)cc1	20.7	*
1334	C/C=C/c1ccc(Nc2ncnc3cc(OCCCN4CCOCC4)c(OCCCN4CCOCC4)cc23)cc1	20.72	*

1335	OCc1ccc(-c2cc3c(Nc4ccccc4)ncnc3s2)cc1	21	7.68
1336	COc1c(C=O)cccc1-c1cc2c(N[C@H](C)c3ccccc3)ncnc2s1	21	7.68
1337	CC(=O)N1CCN(CCCOc2cc3ncnc(Nc4ccc(F)c(Cl)c4)c3cc2NC(=O)c2cc([N+](=O)[O-])ccc2F)CC1	21	7.68
1338	NCc1cccc(C#Cc2cncnc2Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)n1	21	*
1339	CCCS(=O)(=O)CCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	21	*
1340	C#Cc1cccc(Nc2ncnc3cc(OCCOC)c4c(c23)OCCO4)c1	21	*
1341	C=C(C)C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1	21	*
1342	CCC(=O)Nc1cc2c(Nc3ccc4c(ccn4Cc4ccccc4)c3)ncnc2cc1OC	21	*
1343	CCOc1cc2ncnc(Nc3ccc(NS(=O)(=O)c4ccccc4)cc3)c2cc1NC(=O)/C=C/CN1CCCC1	21	*
1344	O=C(/C=C/CN1CCOCC1)N1CCc2c(sc3ncnc(N[C@H](CO)c4ccccc4)c23)C1	21	*
1345	CCC1=C2C(Nc3ccc4c(cnn4Cc4ccccc4)c3)=NC=NC2N=C1NC(=O)OC[C@@H]1COCCN1	21	*
1346	O=C(Nc1cccc(Nc2cc(Nc3cccc(C(F)(F)F)c3)ncn2)c1)C1CC1	21	*
1347	CN(C)CCCn1ccc2cc3c(Nc4cccc(Br)c4)ncnc3cc21	21	*
1348	COc1cc(OC2CCN(C)CC2)c2c(Nc3ccc(F)c(Cl)c3)ncnc2c1	21	*
1349	CC(C)(C)C(=O)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc5sncc45)c(Cl)c3)c21.CS(=O)(=O)O	21	*
1350	O=C1NCc2cccc(Oc3ccc(Nc4ncnc5ccn(CCO)c45)cc3Cl)c21	21	*
1351	Cc1ccc(S(=O)(=O)O)cc1.O=S(=O)(CCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1)CC(F)(F)F	21.1	*
1352	CN(C)CCOC(=O)N1CCc2ncnc(Nc3cccc(C(F)(F)F)c3)c2C1	21.4	7.67
1353	Nc1ccc(-c2cc3c(Nc4ccc(Oc5cccc(C(F)(F)F)c5)c(Cl)c4)ncnc3s2)cc1	21.4	*
1354	Clc1cccc(Nc2ncnc3cc(OCCCN4CCOCC4)c4c(c23)OCCO4)c1	21.95	*
1355	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C#Cc1ccc(CNCCS(C)(=O)=O)cc1	22	7.66
1356	CC[C@@H](Nc1ncnc2oc(-c3ccc(OC)cc3)cc12)c1ccccc1	22	7.66
1357	COc1ccc(-c2cc3c(NC(CC(N)=O)c4ccccc4)ncnc3o2)cc1	22	7.66
1358	C/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1	22	*
1359	CCC1=C2C(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)=NC=NC2N=C1NC(=O)OC[C@@H]1COCCN1	22	*
1360	Cc1c(NC(=O)OC[C@@H]2COCCN2)cn2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c12	22	*
1361	CN(C)CCn1cnc2cc3c(Nc4cccc(Br)c4)ncnc3cc21	22	*
1362	O=C1Nc2ncnc(Nc3ccc(F)c(Cl)c3)c2/C1=C/c1ccc(C(=O)NCCN2CCOCC2)[nH]1	22	*
1363	C[C@@H](Oc1cccc2ncnc(Nc3ccc(OCc4ccccn4)c(Cl)c3)c12)C(=O)N(C)C	22	*
1364	CCc1cc(Nc2nccc(-c3c(-c4cccc(C(=O)Nc5c(F)cccc5F)c4)nc4ccccn34)n2)c(OC)cc1N1CCC(N2CCN(S(C)(=O)=O)CC2)CC1	22	*
1365	O=S(=O)(Nc1nccs1)c1ccc(NC(=S)Nc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)cc1	22	*
1366	COc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2cc1OCCCOP(N)(=O)N(CCCl)CCCl	22	*
1367	CCc1cccc(NC(=O)CSc2nc3cc4ccccc4cc3c(=O)n2-c2ccc(S(N)(=O)=O)cc2)c1	22	*
1368	Clc1cccc(Nc2ncnc3cc4c(cc23)OC(CCN(N2CCOCC2)N2CCOCC2)CO4)c1	22	*
1369	OCCNCCn1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21	22	*
1370	CCC(=O)Nc1cccc(Nc2cc(-c3[nH]c(SC)nc3-c3ccc(F)cc3)ccn2)c1	22	*
1371	C=CC(=O)Nc1cccc(N2C(=O)C(C)N(C)C(=O)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	22.12	7.66
1372	Cc1cc(Nc2ncc3c(n2)N([C@H]2CCN(C(=O)CC(C)C)C2)C(=O)N(c2ccccc2Cl)C3)ccc1N1CCN(C)CC1	22.2	7.65
1373	C=C=CC(=O)Nc1cc(Nc2nccc(-c3cnn4ccccc34)n2)c(OC)cc1N(C)CCN(C)C	22.4	*
1374	C=CC(=O)Cc1cc(Nc2ncc3nc(Nc4ccccc4)n(C)c3n2)c(OC)cc1N(C)CCN(C)C	22.4	*
1375	Cc1cccc(NC(=O)c2ccc(OCCCN3CCCCC3)cc2O)c1	22.4	*

1376	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2c2c1OCCO2	22.5	*
1377	C=C=CC(=O)Nc1cc(Nc2nccc(C3=CN(C)C4C=CC=CC34)n2)ccc1N(C)CCN(C)C	22.8	*
1378	C=C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4ccccc34)n2)ccc1N(C)CCN(C)C	22.8	*
1379	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccco4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	23	7.64
1380	CNC(=O)NCc1cccc(C#Cc2cncnc2Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)n1	23	*
1381	COC[C@@H](Nc1ncnc2sc(-c3ccccc3OC)cc12)c1ccccc1	23	*
1382	C#Cc1cccc(Nc2ncnc3sc(Br)cc23)c1	23	*
1383	CCOC(=O)C(=CNc1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c2c1)C(=O)OCC	23	*
1384	CCOc1cc2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c2cc1NC(=O)/C=C/CN1CCN(C)CC1	23	*
1385	CCOc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2cc1NC(=O)/C=C/CN1CCN(C)CC1	23	*
1386	CCC1=C2C(Nc3ccc4c(cnn4Cc4ccccc4)c3)=NC=NC2N=C1NC(=O)OCC1CCNCC1	23	*
1387	Clc1cccc(Nc2ncnc3ccccc23)c1	23	*
1388	CCCCN1C(=O)CS/C1=N/Nc1nncc2ccccc12	23	*
1389	Nc1ncnc(Nc2ccc3c(cnn3Cc3cccc(F)c3)c2)c1/C=N/OCc1ccccc1	23	*
1390	CO/N=C/c1c(N)ncnc1Nc1ccc2c(cnn2Cc2cccc(Cl)c2)c1	23	*
1391	O=S1CCN(Cc2ccc(-c3cc4c(Nc5ccc(OCc6cccc(F)c6)cc5)ncnc4cn3)o2)CC1	23	*
1392	Nc1ccc(-c2ccc(C(=O)Nc3cccc(Cl)c3)c(O)c2)cc1	23	*
1393	O=C(Nc1ccc([N+](=O)[O-])cc1Cl)c1ccc(OCCCN2CCCCC2)cc1O	23	*
1394	O=C(CCNc1ccc(S(=O)(=O)Nc2nccs2)cc1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	23.1	*
1395	CCC(=O)N1CC[C@@H](N2C(=O)N(c3ccccc3Cl)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	23.4	7.63
1396	O=C(COc1c(F)c(F)c(F)c(F)c1F)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	23.6	7.63
1397	C#Cc1cccc(Nc2ncnc3cc(OC(C)C)c4c(c23)OCCO4)c1	23.7	*
1398	C=C=CCOc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O	23.8	*
1399	CS(=O)(=O)CCNCc1ccc(-c2ccc3ncnc(Nc4ccc(F)c(Cl)c4)c3c2)o1	23.99	*
1400	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1/C=C/c1ccc(CNC(C)C)cc1	24	7.62
1401	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCN1CC2(C1)CS(=O)(=O)C2	24	7.62
1402	COc1ccc(-c2cc3c(N[C@H](C)c4cccc(F)c4)ncnc3o2)cc1	24	7.62
1403	COc1ccc(-c2cc3c(N[C@H](C)c4ccccc4F)ncnc3o2)cc1	24	7.62
1404	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/Cc1c[nH]cn1	24	7.62
1405	COc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	24	7.62
1406	CS(=O)(=O)c1cccc(C(=O)Nc2cc3c(Nc4ccc(F)c(Cl)c4)ncnc3cc2OCCCN2CCOCC2)c1F	24	7.62
1407	CS(=O)(=O)CCNCCCCOc1ccc2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c2c1	24	*
1408	CS(=O)(=O)CCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)cc4)c3c2)o1	24	*
1409	O=C(c1cc2cc(O)ccc2[nH]1)c1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	24	*
1410	CN(C)CCCNC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	24	*
1411	CN(C)C/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	24	*
1412	Cc1cccc(Nc2ncnc3ccc(N=NN(C)C)cc23)c1	24	*
1413	CO/N=C/c1c(N)ncnc1Nc1cccc(Br)c1	24	*
1414	CN(C)CCCNN(NCCCN(C)C)C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	24	*
1415	C=CC(=O)Nc1cc(C(C)C)cc(-n2c(=O)cc(C)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	24	*
1416	CSc1nc(-c2ccc(F)cc2)c(-c2ccnc(Nc3ccccc3)c2)[nH]1	24	*
1417	CC#Cc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2s1	24	*
1418	Fc1ccc(Nc2ncnc3cc(OCC4CCCO4)c4c(c23)OCCO4)cc1Cl	24.1	*

1419	Nc1cccc(-c2cc3c(-c4[nH]c(-c5ccccc5)nc4-c4ccc(F)cc4)ccnc3[nH]2)c1	24.1	*
1420	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccn4)c(Cl)c3)c2cc1NC(=O)CCN1CCCCC1	24.8	7.61
1421	COc1cc(NC(=O)Nc2ccccn2)cc(-c2c[nH]cn2)c1OC	24.81	*
1422	C=CC(=O)Nc1cccc(N2C(=O)C(C(C)C)N(C)C(=O)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	24.83	7.61
1423	CCOc1cc2ncnc(NC3=CC(=O)C(OCc4cccc(C)c4)=CC3=O)c2cc1NC(=O)/C=C/CN(C)C	24.9	7.60
1424	Cc1cc(Nc2ncc3c(n2)N([C@H]2CCN(C(=O)C4CCCCC4)C2)C(=O)N(c2ccccc2Cl)C3)ccc1N1CCN(C)CC1	24.9	7.60
1425	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCN1CC(O)C1	25	7.60
1426	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN(C)C1(C(N)=O)CCN(C(C)C)CC1	25	*
1427	O=S(=O)(CCOCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1)c1ccccc1	25	*
1428	CS(=O)(=O)CCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5ccccc5)c(Br)c4)c3c2)o1	25	*
1429	CN(C)C/C=C/C(=O)Nc1cc2c(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncnc2cn1	25	*
1430	CS(=O)(=O)CCNCc1ccc(-c2cc3c(Nc4ccc(OCc5ccccc5)cc4)ncnc3cn2)o1	25	*
1431	COc1cc2ncnc(Nc3cccc(F)c3)c2cc1OC.Cl	25	*
1432	Cc1[nH]c2ncnc(Nc3cccc(Br)c3)c2c1C	25	*
1433	O=[N+]([O-])c1cc2c(Nc3cccc(Br)c3)ncnc2cc1Cl	25	*
1434	Brc1cccc(Nc2ncnc3ccc(NN=NCc4ccccc4)cc23)c1	25	*
1435	CSCCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1.Cc1ccc(S(=O)(=O)O)cc1	25.1	*
1436	Fc1ccc(NC(=S)Nc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)cc1Cl	25.3	*
1437	O=C(Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)N1CCOCC1	25.3	*
1438	C=C=CC(=O)Nc1cc(Nc2nccc(C3=CN(C)C4C=CC=CC34)n2)c(OC)cc1N(CC)CCN(C)C	25.4	*
1439	C=C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4ccccc34)n2)c(OC)cc1N(CC)CCN(C)C	25.4	*
1440	Cc1cc(Nc2ncc3c(n2)N([C@H]2CCN(C(=O)C4CCCC4)C2)C(=O)N(c2ccccc2Cl)C3)ccc1N1CCN(C)CC1	25.5	7.59
1441	O=C1N[C@H](C(=O)Nc2cc3c(Nc4ccc(F)c(Cl)c4)ncnc3cc2OCCN2CCCCC2)CO1	25.53	7.59
1442	Nc1cc(Br)ccc1Nc1ncnc2ccncc12	25.7	*
1443	Fc1ccc(Nc2ncnc3cc(OCCCN4CCOCC4)c4c(c23)OCCO4)cc1Cl	25.86	*
1444	C#CCOc1cc2c(Nc3cccc(Cl)c3)ncnc2cc1OC	25.9	*
1445	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCN1CC(O)C1	26	7.59
1446	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN1CCC1	26	7.59
1447	C[C@@H](Nc1ncnc2sc(-c3cccc(S(C)(=O)=O)c3)cc12)c1ccccc1	26	7.59
1448	CS(=O)(=O)CCOCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	26	*
1449	Nc1ccccc1NC(=O)/C=C/c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	26	*
1450	Cc1ccc(S(=O)(=O)O)cc1.Fc1cccc(COc2ccc(Nc3ncnc4ccc(-c5ccc(CN6CCOCC6)o5)cc34)cc2Cl)c1	26	*
1451	C#Cc1cccc(N2C(=O)Nc3c(C(=O)Nc4ccc(CN5CCCC5)cc4)sc4ncnc2c34)c1	26	*
1452	COCCn1c(=O)oc2cc3ncnc(Nc4ccc(F)c(F)c4)c3cc21	26	*
1453	COc1cc2ncnc(C#Cc3ccccc3-c3ccccc3)c2cc1OC	26	*
1454	COC[C@@H]1CCCN1/N=C/c1c(N)ncnc1Nc1ccc2c(cnn2Cc2cccc(F)c2)c1	26	*
1455	Clc1cccc(CNc2[nH]nc3ncnc(Nc4cccc(Cl)c4)c23)c1	26	*
1456	Oc1cccc(-c2[nH]nc3ncnc(Nc4cccc(Cl)c4)c23)c1	26	*
1457	ClCCNc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	26	*
1458	O[C@H]1CNCCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)C1	26	*
1459	Br.Oc1ccc(-c2cc3c(NCc4ccc(F)cc4)ncnc3[nH]2)cc1	26	*
1460	NP(=O)(OCCCC(=O)Nc1ccc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2c1)N(CCCl)CCCl	26	*
1461	C=CC(=O)Nc1cc(F)cc(-n2c(=O)cc(C)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	26	*

1462	NS(=O)(=O)c1ccc(-n2c(SCC(=O)Nc3ccccc3F)nc3cc4ccccc4cc3c2=O)cc1	26	*
1463	Cc1nnc(-c2ccc3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c3c2)o1	26	*
1464	C=CC(=O)Nc1cc(Nc2n[nH]c3cc(-c4ccc(F)cc4)ccc23)c(OC)cc1N(C)CCN(C)C	26	*
1465	COc1cccc(Nc2cc(Nc3cc(OC)ccc3OC)ncn2)c1	26	*
1466	COC(=O)N1CCc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c2C1	26.2	7.58
1467	O=C(Nc1ccccn1)Nc1cc(-c2cncnc2)ccc1OC(F)(F)F	26.56	*
1468	Cc1cc(Nc2ncc3c(n2)N([C@H]2CCN(C(=O)CN(C)C)C2)C(=O)N(c2ccccc2Cl)C3)ccc1N1CCN(C)CC1	26.6	7.58
1469	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C1CC1	26.9	*
1470	S=C(Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)N1CCOCC1	26.9	*
1471	C#Cc1cccc(Nc2ncnc3cc(OCCOC(=O)Cc4c(C)n(C(=O)c5ccc(Cl)cc5)c5ccc(OC)cc45)c(OCCOC)cc23)c1	27	7.57
1472	C#Cc1cccc(Nc2ncnc3cc(OCCOC(=O)CC4=C(C)/C(=C/c5ccc([S+](C)[O-])cc5)c5ccc(F)cc54)c(OCCOC(=O)CC4=C(C)/C(=C/c5ccc([S+](C)[O-])cc5)c5ccc(F)cc54)cc23)c1	27	7.57
1473	COc1ccc(-c2cc3c(N[C@H](C)c4ccc(F)cc4)ncnc3o2)cc1	27	7.57
1474	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1)c1ccccc1	27	7.57
1475	CS(=O)(=O)CCNCCCCOc1ccc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2c1	27	*
1476	CS(=O)(=O)CCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5ccccc5)cc4)c3c2)o1	27	*
1477	CS(=O)(=O)CCN(CC#N)Cc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	27	*
1478	O=C(NCCO)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	27	*
1479	COc1ccccc1-c1cc2c(N[C@H](C)c3ccc(F)cc3)ncnc2s1	27	*
1480	c1ccc(-c2cccc(Nc3ncnc4cc5c(cc34)OCCCO5)c2)cc1	27	*
1481	C=CC(=O)Nc1ccc2ncnc(Nc3ccc(OCCN(C)C)c(Br)c3)c2c1	27	*
1482	Brc1cccc(Nc2ncnc3ccccc23)c1	27	*
1483	COc1cc2ncnc(NC3CC3c3ccccc3)c2cc1OCCCN(C)C	27	*
1484	c1ccc2ncncc2c1	27	*
1485	Cc1[nH]c2ncnc(Nc3cccc(Cl)c3)c2c1C	27	*
1486	Cl.c1ccc(-c2cccc(Nc3ncnc4cc5c(cc34)OCCCO5)c2)cc1	27	*
1487	C[C@@H](Nc1ncnc2[nH]c(-c3ccc(F)cc3)cc12)c1ccc(F)cc1	27	*
1488	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N(NCO)NCCO	27	*
1489	NP(=O)(OCCCCOc1ccc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2c1)N(CCCl)CCCl	27	*
1490	Clc1ccccc1Oc1ccc(Nc2ncnc3cc[nH]c23)cc1Cl	27	*
1491	Cl.Cn1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21	27	*
1492	CCOC(=O)CCCC(=O)Nc1cc(Nc2cccc(Cl)c2)ncn1	27	*
1493	O=C(O)CCCC(=O)Nc1cc(Nc2cccc(Cl)c2)ncn1	27	*
1494	CCC(=O)Nc1cccc(-c2cc3c(-c4[nH]c(-c5ccccc5)nc4-c4ccc(F)cc4)ccnc3[nH]2)c1	27.2	*
1495	C#Cc1cccc(Nc2ncnc3cc(OCC4CCCO4)c4c(c23)OCCO4)c1	27.3	*
1496	CCC(=O)N1CC[C@H](N2C(=O)N(c3ccccc3OC)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	27.4	7.56
1497	C=C=CC(=O)Nc1cc(Nc2nccc(C3=CN(C)C4C=CC=CC34)n2)c(OC)cc1N(C)CCN(C)C	27.9	*
1498	C=C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4ccccc34)n2)c(OC)cc1N(C)CCN(C)C	27.9	*
1499	COC[C@@H](Nc1ncnc2oc(-c3ccccc3)cc12)c1ccccc1	28	7.55
1500	C/C(=C\c1c(C)ncnc1Nc1ccc(OCc2cccc(F)c2)c(Cl)c1)C(=O)NCCN1CCOCC1	28	7.55
1501	O=C(Nc1cc2c(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1)c1cc([N+](=O)[O-])ccc1F	28	7.55
1502	CCOC(=O)N1CCN(Cc2ccc(-c3ccc4ncnc(Nc5ccc(OCc6cccc(F)c6)c(Cl)c5)c4c3)o2)CC1.Cc1ccc(S(=O)(=O)O)cc1	28	*

1503	O=C(/C=C/CN1CCC(F)(F)C1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	28	*
1504	CN(C)C(=O)O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1	28	*
1505	CCC1=C2C(Nc3ccc4c(cnn4Cc4ccccc4)c3)=NC=NC2N=C1NC(=O)OCCN1CCCCC1	28	*
1506	CC(=O)Nc1cc2ncnc(Nc3cccc(Br)c3)c2cc1[N+](=O)[O-]	28	*
1507	CC1(C)[C@@H](O[C@@H]2O[C@H](C(=O)O)[C@@H](O)[C@H](O)[C@H]2O)CC[C@@]2(C)[C@H]1CC[C@]1(C)[C@@H]2C(=O)C=C2[C@@H]3C[C@@](C)(C(=O)O)CC[C@]3(C)CC[C@]21C	28	*
1508	C=CC(=O)Nc1cccc(-n2c(=O)c(=O)n(C(C)C)c3cnc(Nc4ccc(N5CCC(N6CCN(C)CC6)CC5)cc4OC)nc32)c1	28	*
1509	C=CC(=O)N1CCC[C@@H]1CSc1nc(-c2ccc(F)cc2)c(-c2ccnc(Nc3ccccc3)c2)[nH]1	28	*
1510	c1cnc2ccc(Nc3ncnc4ccc(-c5cnn(C6CCNCC6)c5)cc34)cc2c1	28.2	7.55
1511	COCC1COc2cc3ncnc(Nc4cccc(I)c4)c3cc2O1	28.2	*
1512	OCCNCC1COc2cc3ncnc(Nc4cccc(Br)c4)c3cc2O1	28.2	*
1513	COc1cc2ncnc(Nc3ccc(Br)cc3F)c2cc1OCCCN1CCNCCNCC1	28.2	*
1514	S=C(NCc1ccc(Cl)cc1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	28.3	*
1515	COc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2cc1OCCCCn1ccnc1[N+](=O)[O-]	28.5	7.55
1516	C=C=CCCCOc1cc2c(Nc3cccc(Cl)c3)ncnc2cc1O	28.5	*
1517	Cc1cc(Nc2ncc3c(n2)N([C@H]2CCN(C(=O)C4CC4)C2)C(=O)N(c2ccccc2Cl)C3)ccc1N1CCN(C)CC1	28.7	7.54
1518	CS(=O)(=O)CCNC(CS(C)(=O)=O)c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	28.7	*
1519	C#Cc1cc(Nc2ncnc3cc(OC)c(OCCCCCCC(=O)NO)cc23)ccc1F	28.8	7.54
1520	C#Cc1cccc(Nc2ncnc3cc(OC)c(OC)cc23)c1	28.8	*
1521	COC[C@H]1Oc2cc3ncnc(Nc4cccc(Br)c4)c3cc2O[C@@H]1COC	28.89	*
1522	CN1CCN(CCOC(=O)N2CCc3ncnc(Nc4cccc(C(F)(F)F)c4)c3C2)CC1	28.9	7.54
1523	CCCC(=O)N1CC[C@H](N2C(=O)N(c3ccccc3Cl)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	28.9	7.54
1524	C=Cc1ccc(-c2cc3c(N[C@H](C)c4ccccc4)ncnc3o2)cc1	29	7.54
1525	Nc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	29	7.54
1526	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1)c1cccc(F)c1F	29	7.54
1527	Nc1ccccc1NC(=O)/C=C/c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)cc1	29	*
1528	CN(C)CCCC(=O)Nc1cccc(-c2c(-c3ccccc3)oc3ncnc(N[C@H](CO)c4ccccc4)c23)c1	29	*
1529	O=C(/C=C/CN1CCS(=O)(=O)CC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	29	*
1530	CCNC(=O)Nc1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c2c1	29	*
1531	CCC1=C2C(Nc3ccc4c(cnn4Cc4ccccc4)c3)=NC=NC2N=C1NC(=O)OCC1CCCNC1	29	*
1532	Brc1cccc(Nc2ncnc3ccc4[nH]cnc4c23)c1	29	*
1533	CC(=O)Nc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	29	*
1534	Clc1cccc(Nc2[nH]cnc3nc4c(c2-3)CCCC4)c1	29	*
1535	CN(C)c1ccc(Nc2[nH]nc3ncnc(Nc4cccc(Cl)c4)c23)cc1	29	*
1536	Cc1cc(C(=O)O)[nH]c1/C=C1\C(=O)Nc2ncnc(Nc3ccc(F)c(Cl)c3)c21	29	*
1537	C[C@@H](Nc1ncnc2[nH]c(-c3ccc(Br)cc3)cc12)c1ccc(F)cc1	29	*
1538	Brc1cccc(Nc2ncnc3ccc4nc[nH]c4c23)c1	29	*
1539	CS(=O)(=O)CCNCc1ccc(-c2ccc3ncnc(Nc4ccc(S(=O)(=O)c5ccccc5)cc4)c3c2)o1	29	*
1540	CC(C)Oc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2c2c1OCCO2	29.1	*
1541	C=C=CC(=O)Nc1cc(Nc2nccc(C3=CN(C)C4C=CC=CC34)n2)c(OC)cc1O[C@H]1CCOC1	29.1	*
1542	C=C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4ccccc34)n2)c(OC)cc1O[C@H]1CCOC1	29.1	*
1543	Fc1ccc(-c2nc(Nc3cc(Br)cc4cc(-c5cccc(Cl)c5)oc34)c3cc(Br)ccc3n2)cc1	29.3	*
1544	Cc1cc(Nc2ncc3c(n2)N([C@H]2CCN(C(=O)C(C)(C)C)C2)C(=O)N(c2ccccc2Cl)C3)ccc1N1CCN(C)CC1	29.4	7.53

1545	C=CC(=O)Nc1cccc(N2C(=O)N(C)Cc3cnc(Nc4ccc(N5CCCCC5)cc4OC)nc32)c1	29.5	7.53
1546	CC(=O)Nc1c(Br)cccc1Nc1ncnc2ccncc12	29.51	*
1547	C=C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4ccccc34)n2)c(C)cc1N(C)CCN(C)C	29.9	*
1548	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C#Cc1ccc(CN2CCCC2)s1	30	7.52
1549	Cc1ccc(C(=O)Nc2ccc(CN3CCN(C)CC3)c(C(F)(F)F)c2)cc1NC(=O)c1cnc2[nH]ncc2c1	30	7.52
1550	C#Cc1cccc(Nc2ccnc3cc(OCCOC)c(OCCOC)cc23)c1	30	7.52
1551	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C(C)C)C(C)C	30	7.52
1552	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c3s2)C1)N1CCOCC1	30	7.52
1553	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1)c1cccc(C(F)(F)F)c1F	30	7.52
1554	Nc1ccc(C#Cc2cncnc2Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)cc1	30	*
1555	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN1CCC[C@H]1C(N)=O	30	*
1556	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN1CCN(C)CC1C(N)=O	30	*
1557	CNC(=O)[C@@H](C)N(C)Cc1cc2c(Nc3cccc(Cl)c3F)ncnc2cc1OC	30	*
1558	COC[C@@H](C(N)=O)N(C)Cc1cc2c(Nc3cccc(Cl)c3F)ncnc2cc1OC	30	*
1559	CCC1=C2C(Nc3ccc4c(cnn4Cc4ccccc4)c3)=NC=NC2N=C1NC(=O)OCC1CCCCN1	30	*
1560	Nc1ncnc(Nc2ccc3c(cnn3Cc3cccc(F)c3)c2)c1/C=N/N1CCCCC1	30	*
1561	O=C(OCCCc1ccccc1)c1cc(NCc2cc(O)ccc2O)ccc1O	30	*
1562	COc1ccc2ncncc2c1	30	*
1563	COc1cc2ncnc(Nc3cccc(Cl)c3)c2cc1OC.Cl	30	*
1564	COc1ccc(Nc2[nH]nc3ncnc(Nc4cccc(Cl)c4)c23)cc1	30	*
1565	COc1cccc(Nc2ncc3cc(-c4c(Cl)cccc4Cl)c(=O)n(C)c3n2)c1	30	*
1566	Fc1ccc(Nc2ncnc3ccccc23)cc1Cl	30	*
1567	O=C(O)COCc1ccn2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c12	30	*
1568	c1cc(Nc2ccc3[nH]ccc3c2)c2sc(-c3ccc(CN4CCOCC4)cc3)cc2n1	30	*
1569	Nc1ccc(-c2cc3c(Nc4cccc(N)c4)ncnc3o2)cc1	30	*
1570	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CNC(=O)C1CN(C)CCN1C	30	*
1571	C=CC(=O)Nc1cc(Nc2n[nH]c3cc(-c4ccncc4)ccc23)c(OC)cc1N(C)CCN(C)C	30	*
1572	CN(C)[C@@H](CS(C)(=O)=O)c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	30.4	*
1573	C=C=CC(=O)Nc1cc(Nc2nccc(C3=CN(C)C4C=CC=CC34)n2)c(OC)cc1OCCN1CCOCC1	30.4	*
1574	Oc1cccc(-c2nc(-c3ccc(F)cc3)c(-c3ccnc4[nH]c(-c5ccccc5)cc34)[nH]2)c1	30.4	*
1575	C=C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4ccccc34)n2)c(OC)cc1OCCN1CCOCC1	30.4	*
1576	COc1cc2c(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncnc2cc1OCCCn1ccnc1[N+](=O)[O-]	30.5	7.52
1577	COc1ccc(CNC(=O)c2ccccc2NC(=O)c2ccco2)cc1	30.5	*
1578	C=C=CC(=O)Nc1cc(Nc2nccc(C3=CN(C)C4C=C(Cl)C=CC34)n2)c(OC)cc1N(C)CCN(C)C	30.6	*
1579	C=C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4cc(Cl)ccc34)n2)c(OC)cc1N(C)CCN(C)C	30.6	*
1580	C#Cc1cccc(Nc2ncnc3cc(OCCOC(=O)CC4=C(C)/C(=C\c5ccc([S+](C)[O-])cc5)c5ccc(F)cc54)c(OCCOC)cc23)c1	31	7.51
1581	CC1(C)CC(C(=O)Nc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)CC(C)(C)N1[O]	31	7.51
1582	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4OC)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	31	7.51
1583	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN1CCCCC1	31	7.51
1584	COC(=O)CCCC(=O)Nc1cccc(C#Cc2cncnc2Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1	31	*
1585	CCNC(=O)Nc1ccc(C(=O)Nc2ccc3ncnc(Nc4ccc(F)c(Cl)c4)c3c2)cc1	31	*
1586	COC[C@H]1CCCN1/N=C/c1c(N)ncnc1Nc1ccc2c(cnn2Cc2cccc(F)c2)c1	31	*

1587	CCS(=O)(=O)CC(=O)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21	31	*
1588	Brc1cccc(Nc2[nH]cnc3nc4ccccc4c2-3)c1	31	*
1589	Brc1cccc(Nc2ncnc3[nH]c4ccccc4c23)c1	31	*
1590	O=S(CCO)CCn1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21	31	*
1591	COc1ccc(Nc2cc(Oc3ccc4[nH]ccc4c3)ncn2)cc1N1CCOCC1	31	*
1592	Fc1ccc(-c2nc(Nc3cc(Br)cc4cc(-c5ccc(OC(F)(F)F)cc5)oc34)c3cc(Br)ccc3n2)cc1	31.1	*
1593	O=C(Nc1ccccc1C(=O)N/N=C/c1ccc(O)cc1O)c1ccco1	31.2	*
1594	COc1ccc(-c2c3c4cc(OCCCN(C)C)c(OCCCN(C)C)cc4oc(=O)c3n3ccc4cc(O)c(OC)cc4c23)cc1O.O=C(O)C(F)(F)F	31.8	*
1595	Fc1ccc(Nc2ncnc3ccc(-c4cnn(C5CCNCC5)c4)cc23)cc1Cl	31.9	7.50
1596	C#Cc1cccc(Nc2ncnc3cc(OCCOC(=O)c4ccc(C(=O)Nc5ccc6c(c5)C(C)(C)CCC6(C)C)cc4)c(OCCOC)cc23)c1	32	7.49
1597	COc1cc2ncc(C#N)c(Nc3ccc(Sc4ncc(-c5ccccc5)s4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	32	7.49
1598	Nc1nccc(C#Cc2cncnc2Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)n1	32	*
1599	CCN(CC)CCCNC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	32	*
1600	CCNC(=O)O[C@H]1CN[C@@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1	32	*
1601	CCNC(=O)O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1	32	*
1602	CN(C)c1ccc2ncnc(Nc3cccc(Br)c3)c2n1	32	*
1603	NC1CCN(Cc2ccn3ncnc(Nc4ccc(OCc5cncn5)c(Cl)c4)c23)CC1	32	*
1604	Fc1cccc(COc2ccc(Nc3ncnc4nn5ccccc5c34)cc2Cl)c1	32	*
1605	CC(C)CO/N=C/c1c(N)ncnc1Nc1ccc2c(cnn2Cc2cccc(F)c2)c1	32	*
1606	CCN(CC)CCCNN(NCCCN(CC)CC)C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	32	*
1607	O=C(CN1CCCC1)Nc1ccc2ncnc(Nc3ccc(Cl)cc3)c2c1	32	*
1608	CN1CCN(CC(=O)Nc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)CC1	32	*
1609	O=C(Nc1cccc(Cl)c1)c1c(O)cc(O)cc1O	32	*
1610	C=CC(=O)Nc1ccc(OC)c(Nc2cc(-c3[nH]c(SC)nc3C)ccn2)c1	32	*
1611	c1ccc2c(c1)CCN2c1ncnc2cc3c(cc12)ncn3CCN1CCCC1	32	*
1612	C#Cc1cccc(Nc2ncnc3cc(O[C@H]4CCOC4)c(NC(=O)C=C)cc23)c1	32.2	*
1613	O=C(Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1)C1CCC2(CC1)OOC1(O2)C2CC3CC(C2)CC1C3	32.35	*
1614	C=CCCCCOc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OC	32.6	*
1615	C#CCCCCCOc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OC	32.7	*
1616	Cc1ccc(C(=O)Nc2ccc(CN3CCN(C)CC3)c(C(F)(F)F)c2)cc1NC(=O)c1cnc(NC2CCCC2)nc1	33	7.48
1617	C#Cc1cccc(Nc2ncnc3cc(OCCOC(=O)Cc4c(C)n(C(=O)c5ccc(Cl)cc5)c5ccc(OC)cc45)c(OCCOC(=O)Cc4c(C)n(C(=O)c5ccc(Cl)cc5)c5ccc(OC)cc45)cc23)c1	33	7.48
1618	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc5c(cnn5Cc5cc(F)ccc5F)c4)c3s2)C1)N1CCOCC1	33	7.48
1619	OCc1ccc(C#Cc2cncnc2Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)o1	33	*
1620	Nc1ccccc1NC(=O)c1ccc(COc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)cc1	33	*
1621	COc1cc2ncnc(C#C[C@@](C)(Cc3ccccc3)N3CCC(C(=O)O)CC3)c2cc1OC	33	*
1622	Fc1cccc(Cn2ncc3cc(Nc4ncnn5ccc(CN6CCCNCC6)c45)ccc32)c1	33	*
1623	CC(C)(C)NC(=O)c1cccc(Oc2ccc(Nc3ncnc4ccn(CCO)c34)cc2Cl)c1	33	*
1624	CO/N=C/c1c(N)ncnc1Nc1ccc(OCc2cc(F)cc(F)c2)c(Cl)c1	33	*
1625	Nc1ccc(-c2nn(C3CCCC3)c3ncnc(N)c23)cc1O	33	*
1626	C[C@@H](Nc1ncnc2[nH]c(-c3ccccc3)cc12)c1ccc(F)cc1	33	*
1627	OCCCCCn1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21	33	*

1628	COc1cc2ncnc(C#CC(C)(Cc3ccccc3)N3CCC(C(=O)O)CC3)c2cc1OC	33	*
1629	COc1cc(Nc2nccc(N(C)c3ccc4[nH]ccc4c3)n2)cc(N2CCOCC2)c1	33	*
1630	C=CC(=O)Nc1cc(Nc2n[nH]c3ccc(-c4cccc5ccccc45)cc23)c(OC)cc1N(C)CCN(C)C	33	*
1631	CCC(=O)NCCSc1nc(-c2ccc(F)cc2)c(-c2ccnc(Nc3ccccc3)c2)[nH]1	33	*
1632	CCC/C=C/C(=O)Nc1cc2c(N3CCCc4ccccc43)ncnc2cc1OC	33	*
1633	C=CC(=O)Nc1cc(Cl)cc(-n2c(=O)cc(C)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	33.1	*
1634	C=CC(=O)NCc1cccc(-c2cc3c(-c4[nH]c(-c5ccccc5)nc4-c4ccc(F)cc4)ccnc3[nH]2)c1	33.2	*
1635	C=CC(=O)Nc1cccc(N2C(=O)C(Cc3ccc(OC)cc3)N(C)C(=O)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	33.95	7.47
1636	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCN1CC(OC)C1	34	7.47
1637	C#Cc1cccc(Nc2ncnc3cc(OCCOC(=O)c4ccccc4OC(C)=O)c(OCCOC(=O)c4ccccc4OC(C)=O)cc23)c1	34	7.47
1638	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C#CCCCN1CCOCC1	34	7.47
1639	CCOc1cc2ncc(C#N)c(Nc3ccc(NCc4cccc5ccccc45)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	34	7.47
1640	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	34	7.47
1641	CN(C)CCCCC(=O)Nc1cccc(-c2c(-c3ccccc3)oc3ncnc(N[C@H](CO)c4ccccc4)c23)c1	34	*
1642	CC(C)N1CCN(C/C=C/C(=O)Nc2cc3c(Nc4ccc(F)c(Cl)c4)ncnc3s2)CC1	34	*
1643	Brc1cccc(Nc2ncnc3cccnc23)c1	34	*
1644	OCCn1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21	34	*
1645	NC1CCN(Cc2ccn3ncnc(Nc4cc(Cl)cc(Cl)c4)c23)CC1	34	*
1646	C=CC(=O)Nc1cccc(-n2c(=O)n(C(C)C)c(=O)c3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)c1	34	*
1647	C#Cc1cccc(Nc2ncnc3ccc(-c4ccc(CNCCS(C)(=O)=O)o4)cc23)c1	34.16	*
1648	O=C(Nc1cccc(C(F)(F)F)c1)c1ccc(OCCCN2CCOCC2)cc1O	34.6	*
1649	CNC(CS(C)(=O)=O)c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	34.8	*
1650	CCCCCCCCCCCCCCCCNC(=O)COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1	35	7.46
1651	CCN1CCN(C/C=C/C(=O)Nc2cc3c(Nc4ccc(F)c(Cl)c4)ncnc3s2)CC1	35	*
1652	CCNC(=O)Nc1ccc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2c1	35	*
1653	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCN(CCO)CCO	35	*
1654	Brc1cccc(Nc2ncnc3ccncc23)c1	35	*
1655	CN(C)CCNc1ncc2ncnc(Nc3cccc(Br)c3)c2n1	35	*
1656	Brc1cccc(Nc2ncnc3sccc23)c1	35	*
1657	NCC1CCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)CC1	35	*
1658	NC1CCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)CC1	35	*
1659	CN(CCOc1cccc2ncnc(Nc3ccc(OCc4ccccn4)c(Cl)c3)c12)C(=O)CO	35	*
1660	Clc1cccc(Oc2ccc(Nc3ncnc4cc[nH]c34)cc2Cl)c1	35	*
1661	CN(c1ccc2[nH]ccc2c1)c1cc(Nc2ccc(N3CCOCC3)cc2)ncn1	35	*
1662	O=C(Nc1cccc(C(F)(F)F)c1)c1ccc(OCCCN2CCCCC2)cc1O	35.2	*
1663	S=C(Nc1ccc(Br)cc1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	35.4	*
1664	COc1cc2c(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncnc2cc1OCCCCCCn1ccnc1[N+](=O)[O-]	35.5	7.45
1665	COCC1COc2cc3ncnc(Nc4cccc(Br)c4)c3cc2O1	35.5	*
1666	CCC(=O)N1CC[C@H](N2C(=O)N(c3cccc(F)c3)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	35.8	7.45
1667	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCN1CC2(CCO2)C1	36	7.44
1668	OC[C@@H](Nc1ncnc2sc(Br)cc12)c1ccccc1	36	*
1669	CCC(=O)Nc1cc2c(Nc3ccc(OCc4ccccc4)cc3)ncnc2cc1OC	36	*
1670	CCOc1cc2ncnc(Nc3ccc4c(ccn4S(=O)(=O)c4ccccc4)c3)c2cc1NC(=O)/C=C/CN1CCCC1	36	*

1671	O=C(NCCO)C1=Cc2c(ncnc2Nc2ccc(Oc3cccc4sccc34)c(Cl)c2)NCC1	36	*
1672	CN(CCO)c1cc2c(Nc3ccc4c(cnn4Cc4ccccc4)c3)ncnc2cn1	36	*
1673	NC1CCN(Cc2ccn3ncnc(Nc4ccc(OCc5ccccn5)c(Cl)c4)c23)CC1	36	*
1674	Cn1ncc2c(Oc3ccc(Nc4ncnc5ccn(CCO)c45)cc3Cl)cccc21	36	*
1675	COc1ccc(N2C(=O)CS/C2=N/Nc2nncc3ccccc23)cc1	36	*
1676	C=CC(=O)Nc1cccc(NC(=O)Nc2ccnc(Nc3ccc(N4CCC(N(CC)CC)CC4)cc3OC)n2)c1	36	*
1677	CN1CCN(N(CCC2COc3cc4ncnc(Nc5cccc(Br)c5)c4cc3O2)N2CCN(C)CC2)CC1	36	*
1678	COCCOc1cc2ncnc(Nc3ccc(Cl)c([N+](=O)[O-])c3)c2c2c1OCCO2	36.2	*
1679	Cc1cccc(Nc2ncnc3ccc(NC(=S)NCc4ccccc4)cc23)c1	36.8	*
1680	C=CC(=O)Nc1cc(-n2c(=O)cc(C)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)ccc1C	36.9	*
1681	C=CC(=O)Nc1cccc(Oc2cc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncn2)c1	37	7.43
1682	O=C(/C=C/CN1CCCC1)Nc1cc2c(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncnc2cn1	37	*
1683	CCC1=C2C(Nc3ccc4c(cnn4Cc4ccccc4)c3)=NC=NC2N=C1NC(=O)OCCC1CCNCC1	37	*
1684	O=[N+]([O-])c1cccc(-c2[nH]nc3ncnc(Nc4cccc(Cl)c4)c23)c1	37	*
1685	CN(C)CCNN=Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	37	*
1686	O=C(CN1CCCCC1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	37	*
1687	CN(C)CCN/N=N/c1ccc2ncnc(Nc3cccc(Cl)c3)c2c1.[H+]	37	*
1688	COc1cccc(Nc2cc(NC(=O)CCCC(=O)O)ncn2)c1	37	*
1689	CN(C)C/C=C/C(=O)Nc1ccc2ncc(C#N)c(Nc3cccc(Br)c3)c2c1	37.2	6.82
1690	C=CC(=O)Nc1cccc(N2C(=O)C(Cc3ccc(Cl)cc3)N(C)C(=O)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	37.37	7.43
1691	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccn4)c(Cl)c3)c2cc1NC(=O)CCN1CCOCC1	37.5	7.43
1692	CCOc1cc2ncnc(Nc3ccc(OCC4CC4)c(Cl)c3)c2cc1NC(=O)[C@@H]1COC(=O)N1	37.81	7.42
1693	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C#C/C=N/OCCN1CCOCC1	38	7.42
1694	O=C(/C=C/CN1CC(O)C1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	38	*
1695	C[C@@H](Nc1ncnc2sc(Br)cc12)c1ccccc1	38	*
1696	CCOc1cc2ncnc(Nc3ccc4c(ccn4S(=O)(=O)c4ccccc4)c3)c2cc1NC(=O)/C=C/CN(C)C	38	*
1697	O=C(NCCO)C1=Cc2c(ncnc2Nc2ccc(Oc3cccc(C(F)(F)F)c3)c(Cl)c2)NCC1	38	*
1698	COc1cc(O)c2c(O)c(-c3cccc(Cl)c3)cnc2c1	38	*
1699	NC1CCN(Cc2ccn3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c23)CC1	38	*
1700	CN(C)CCN=NNc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	38	*
1701	Cc1cc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c2n1CCOCCO	38	*
1702	COc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2cc1OCCCn1ccnc1[N+](=O)[O-]	38.3	7.42
1703	C=C=Cc1cccc(Nc2ncnc3cc(OC)c(OC)cc23)c1	38.7	*
1704	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(C(C)=O)CC4)cc3OC(F)F)ncc2SC)c1	38.8	*
1705	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(CC(=O)N5CCN(CCOc6no[n+]([O-])c6S(=O)(=O)c6ccccc6)CC5)CC4)cc3OC)ncc2Cl)c1	39	7.41
1706	O=C(Nc1cc2c(Nc3ccc(OCc4ccccn4)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1)c1cc([N+](=O)[O-])ccc1F	39	7.41
1707	COc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	39	*
1708	CN=NNc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	39	*
1709	CCOc1cc2ncnc(Nc3ccc(Oc4ccc(C)nc4)c(Cl)c3)c2cc1NC(=O)/C(F)=C\CN1CCCCC1	39.2	7.41
1710	CC(C)NC(CS(C)(=O)=O)c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	39.2	*
1711	COc1c(Br)cccc1Nc1ncnc2ccncc12	39.81	*
1712	CCCCN(CC#CC(=O)Nc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1)CCCC	40	*

1713	OCc1cccc(C#Cc2cncnc2Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)n1	40	*
1714	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN(C)[C@H](C)C(=O)N(C)C	40	*
1715	CCN1CCN(Cc2ccc(-c3cc4c(N[C@@H](C)c5ccccc5)ncnc4[nH]3)cc2)CC1	40	*
1716	O=C(CCl)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	40	*
1717	CN(C)C(=O)O[C@@H]1CN[C@@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1	40	*
1718	O=C(O[C@@H]1CN[C@@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1)N1CCOCC1	40	*
1719	CS(=O)(=O)CCNC(=O)O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1	40	*
1720	NC(=O)O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1	40	*
1721	Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	40	*
1722	Clc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	40	*
1723	CN(C)CCn1ncc2cc3c(Nc4cccc(Br)c4)ncnc3cc21	40	*
1724	CN(C)CCN(C)c1cc2ncnc(Nc3cccc(Br)c3)c2cn1	40	*
1725	Cc1cccc(Nc2ncnc3cc(N)ncc23)c1	40	*
1726	Nc1cc2ncnc(Nc3cccc([N+](=O)[O-])c3)c2cn1	40	*
1727	CC(=O)Nc1ccc2c(Nc3cccc(Br)c3)ncnc2c1	40	*
1728	Brc1cccc(Nc2ncnc3c2sc2ncsc23)c1.CO	40	*
1729	CCc1c(NC(=O)OCCn2ccnc2)cn2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c12	40	*
1730	CCc1c(C(=O)NCCCn2ccnc2)cn2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c12	40	*
1731	COc1cn2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c2c1CN1CCC(N)CC1	40	*
1732	COc1cc2ncnc(Oc3cccc(NC(=S)Nc4ccc(F)c(C(F)(F)F)c4)c3)c2cc1OC	40	*
1733	Brc1cccc(Nc2ncnc3c2sc2ncsc23)c1	40	*
1734	COc1cc2ncnc(Nc3ccc(C)c(O)c3)c2cc1OC	40	*
1735	Cc1ccc(Nc2ncnc3oc(-c4ccc(N)cc4)cc23)cc1O	40	*
1736	O=S(=O)(CCO)CCn1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21	40	*
1737	Cc1nc(C)c(C=C2CN(C)CC(=Cc3nc(C)c(C)nc3C)C2=O)nc1C	40	*
1738	CN1CC(=Cc2ccc(N(C)C)cc2[N+](=O)[O-])C(=N/O)/C(=C/c2ccc(N(C)C)cc2[N+](=O)[O-])C1	40	*
1739	Cc1c2oc3c(C)ccc(C(=O)N[C@@H]4C(=O)N[C@H](C(C)C)C(=O)N5CCC[C@H]5C(=O)N(C)CC(=O)N(C)[C@@H](C(C)C)C(=O)O[C@@H]4C)c3nc-2c(C(=O)N[C@@H]2C(=O)N[C@H](C(C)C)C(=O)N3CCC[C@H]3C(=O)N(C)CC(=O)N(C)[C@@H](C(C)C)C(=O)O[C@@H]2C)c(N)c1=O	40	*
1740	Clc1ccc(-c2nc(Nc3cc(Br)cc4cc(-c5ccccc5)oc34)c3cc(Br)ccc3n2)cc1	40.4	*
1741	Fc1ccc(-c2nc(Nc3cc(Br)cc4cc(-c5cccc(Cl)c5)[nH]c34)c3ccccc3n2)cc1	40.7	*
1742	CN(C)CCN(C)c1c(Br)cccc1Nc1ncnc2ccncc12	40.74	*
1743	Nc1c(Nc2ncnc3ccncc23)cccc1[N+](=O)[O-]	40.74	*
1744	Cc1cccc(Nc2ncnc3ccncc23)c1N	40.74	*
1745	COc1cc2ncc(C#N)c(Nc3ccc(Sc4nccn4C)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	41	7.39
1746	C[C@@H](Nc1ncnc2sc(-c3ccc(S(C)(=O)=O)cc3)cc12)c1ccccc1	41	7.39
1747	CS(=O)(=O)CCNC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	41	*
1748	CN(C)C/C=C/C(=O)Nc1cc2c(Nc3ccc4c(cnn4Cc4ccccc4)c3)ncnc2cn1	41	*
1749	CN(C)CCn1ccc2cc3c(Nc4cccc(Br)c4)ncnc3cc21	41	*
1750	Cc1cc(C)c(/C=C2\C(=O)Nc3ncnc(Nc4ccc(F)c(Cl)c4)c32)[nH]1	41	*
1751	CS(=O)(=O)CCNN(NCS(C)(=O)=O)C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	41	*
1752	C=CC(=O)Cc1cc(Nc2ncc3nc(Nc4ccccc4)n(C(C)C)c3n2)c(OC)cc1N(C)CCN(C)C	41	*

1753	COc1cc(Nc2nccc(Nc3ccc4[nH]ccc4c3)n2)cc(N2CCOCC2)c1	41	*
1754	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(CC(=O)N5CCC(Oc6no[n+]([O-])c6S(=O)(=O)c6ccccc6)CC5)CC4)cc3OC)ncc2Cl)c1	42	7.38
1755	COc1cc2ncc(C#N)c(Nc3ccc(Sc4nccs4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	42	7.38
1756	Fc1cccc(COc2ccc(Nc3ncncc3C#Cc3cc[nH]n3)cc2Cl)c1	42	*
1757	Nc1cccc(C#Cc2cncnc2Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1	42	*
1758	c1ccc(-c2cccc(Nc3ncnc4cc5c(cc34)OCCO5)c2)cc1	42	*
1759	O=C1CS/C(=N/Nc2nncc3ccccc23)N1c1ccc(Cl)cc1	42	*
1760	C=C=CC(=O)Nc1cc(Nc2nccc(C3=CN(C)C4C=CC=CC34)n2)c(OC)cc1N(C)CCN1CCOCC1	42	*
1761	Brc1cccc(Nc2ncnc3cc4c(cc23)OC(CCN(N2CCOCC2)N2CCOCC2)CO4)c1	42	*
1762	C=C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4ccccc34)n2)c(OC)cc1N(C)CCN1CCOCC1	42	*
1763	COc1ccc(-c2cc3c(N[C@H](C)c4ccc(Br)cc4)ncnc3[nH]2)cc1	42	*
1764	Cc1ccc(C(=O)Nc2ccc(CN3CCN(C)CC3)c(C(F)(F)F)c2)cc1NC(=O)c1cnc(N)nc1	43	7.37
1765	Cc1ccc(C(=O)Nc2ccc(CN3CCN(C)CC3)c(C(F)(F)F)c2)cc1NC(=O)c1cnc(NC(C)C)nc1	43	7.37
1766	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1)c1cc(F)ccc1[N+](=O)[O-]	43	7.37
1767	CS(=O)(=O)CCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(Br)c5)cc4)c3c2)o1	43	*
1768	Cc1ccc(Nc2nccc(N(C)c3ccc4[nH]ccc4c3)n2)cc1S(N)(=O)=O	43	*
1769	C=CC(=O)Nc1cccc(-c2cc3c(-c4[nH]c(-c5ccccc5)nc4-c4ccc(F)cc4)ccnc3[nH]2)c1	43.2	*
1770	FC(F)(F)c1cccc(Nc2ncnc3[nH]ccc23)c1	43.57	*
1771	O=C(c1cc2ccccc2[nH]1)c1cc2c(Nc3ccc(F)cc3)ncnc2s1	43.7	*
1772	C=CC(=O)Nc1ccc2ncnc(Nc3ccc(S(=O)(=O)Nc4nccs4)cc3)c2c1	43.7	*
1773	COCCOc1cc2ncnc(Nc3ccc(F)c([N+](=O)[O-])c3)c2c2c1OCCO2	43.8	*
1774	Cc1ccc(C(=O)Nc2ccc(CN3CCN(C)CC3)c(C(F)(F)F)c2)cc1NC(=O)c1cnc(NC2CC2)nc1	44	7.36
1775	C[C@@H](Nc1ncnc2oc(-c3ccc(C#N)cc3)cc12)c1ccccc1	44	7.36
1776	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1F)c1cc([N+](=O)[O-])ccc1F	44	7.36
1777	CC(C)N(CC#CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cn1)C(C)C	44	*
1778	CCC1=C2C(Nc3ccc4c(cnn4Cc4ccccc4)c3)=NC=NC2N=C1NC(=O)OCCn1ccnc1	44	*
1779	COC(=O)C1=Cc2c(ncnc2Nc2ccc(Oc3cccc4sccc34)c(Cl)c2)NCC1	44	*
1780	Brc1cccc(Nc2ncnc3cc4ncsc4cc23)c1	44	*
1781	Fc1ccc2ncnc(Nc3cccc(Br)c3)c2n1	44	*
1782	CCN(CC)CCOc1ccc(Nc2ncc3cc(-c4c(Cl)cccc4Cl)c(=O)n(C)c3n2)cc1	44	*
1783	CO/N=C/c1c(N)ncnc1Nc1ccc2c(cnn2Cc2ccccc2)c1	44	*
1784	OCCCc1nc(-c2ccc(F)cc2)c(-c2ccnc3[nH]ccc23)[nH]1	44	*
1785	OCCSCCn1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21	44	*
1786	Cn1cc(-c2ccc3ncnc(Nc4ccc5ncccc5c4)c3c2)cn1	44.1	7.36
1787	C=CS(=O)(=O)Nc1cc2c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c(C#N)cnc2cc1OCC	45	7.35
1788	CCOc1cc2ncc(C#N)c(Nc3ccc(NCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	45	7.35
1789	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C#Cc1ccc(CNCCS(C)(=O)=O)o1	45	7.35
1790	C=CC(=O)Nc1ccc2ncnc(Nc3ccc(CN(C)C)c(Br)c3)c2c1	45	*
1791	CN(C)CCNc1cc2ncnc(Nc3cccc(Br)c3)c2cn1	45	*
1792	OCCNCc1ccn2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c12	45	*
1793	O=C1CS/C(=N/Nc2nncc3ccccc23)N1c1ccccc1	45	*
1794	Br.Oc1ccc(-c2cc3c(NCc4ccccc4F)ncnc3[nH]2)cc1	45	*

1795	C=CC(=O)Nc1cccc(NC(=O)Nc2ccnc(Nc3ccc(N4CCC(N(C)C)CC4)cc3OC)n2)c1	45	*
1796	C=CC(=O)NCCSc1nc(-c2ccc(F)c(C(F)(F)F)c2)c(-c2ccnc(Nc3ccccc3)c2)[nH]1	45	*
1797	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CN1CCCC(F)C1	45.34	*
1798	COc1cc2ncnc(N3CCc4ccccc43)c2cc1NC(=O)/C=C/CN1CCCCC1	45.4	*
1799	O=C(Nc1cccc(Br)c1)c1ccc(OCCCN2CCCCC2)cc1O	45.7	*
1800	CN(C)CCNc1c(Br)cccc1Nc1ncnc2ccncc12	45.71	*
1801	C=CC(=O)N1CCc2c(sc3ncnc(N[C@H](CC)c4ccccc4)c23)C1	46	*
1802	Brc1cccc(Nc2[nH]cnc3nc4c(c2-3)CCCC4)c1	46	*
1803	C=CC(=O)Nc1cc(Nc2ncc(F)c(Nc3ccccc3S(=O)(=O)C(C)C)n2)c(OC)cc1N(C)CCN(C)C	46	*
1804	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(C(=O)CC)CC4)cc3OC(F)F)ncc2SC)c1	46.4	*
1805	C=CC(=O)Nc1cc(-n2c(=O)cc(C)c3cnc(Nc4ccc(N5CCN(C)CC5)nc4)nc32)cc(C(F)(F)F)c1	46.8	*
1806	Cc1ccc(C(=O)Nc2ccc(CN3CCN(C)CC3)c(C(F)(F)F)c2)cc1NC(=O)c1cnc(NC2CCCCC2)nc1	47	7.33
1807	CC(C)(C(=O)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21)S(C)(=O)=O	47	*
1808	CS(=O)(=O)CCNC(=O)C1=Cc2c(ncnc2Nc2ccc(Oc3cccc4sccc34)c(Cl)c2)NCC1	47	*
1809	Nc1ccc2sc3c(Nc4cccc(C(F)(F)F)c4)ncnc3c2c1	47	*
1810	NC1CCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5ccccn5)c4)c23)CC1	47	*
1811	CCN1C(=O)CS/C1=N/Nc1nncc2ccccc12	47	*
1812	COc1ccccc1CO/N=C/c1c(N)ncnc1Nc1ccc2c(cnn2Cc2cccc(F)c2)c1	47	*
1813	COc1ccc(-c2cc3c(N[C@H](C)c4ccc([N+](=O)[O-])cc4)ncnc3[nH]2)cc1	47	*
1814	COc1ccc(-c2c3c4cc(OC)c(OCCCNC(=N)N)cc4oc(=O)c3n3ccc4cc(O)c(OC)cc4c23)cc1O.O=C(O)C(F)(F)F	47	*
1815	Nc1cnc(C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)cn1	47	*
1816	C=CC(=O)Nc1cccc(-n2c(=O)cnc3cnc(Nc4ccc(Cl)cc4)nc32)c1	47.1	7.33
1817	CS(=O)(=O)Nc1ccc(-c2cc3c(Nc4ccc(Oc5cccc(C(F)(F)F)c5)c(Cl)c4)ncnc3s2)cc1	47.1	*
1818	CCOc1cc2ncnc(NC3=CC(=O)C(OCc4cccs4)=CC3=O)c2cc1NC(=O)/C=C/CN(C)C	47.5	7.32
1819	CC(=O)Nc1ccc(-c2cc3c(Nc4ccc(Oc5cccc(C(F)(F)F)c5)c(Cl)c4)ncnc3s2)cc1	47.7	*
1820	COc1ccc(-c2c3c4cc(O)c(OCCCN(C)C)cc4oc(=O)c3n3ccc4cc(O)c(OC)cc4c23)cc1O.O=C(O)C(F)(F)F	47.8	*
1821	N#CCC(=O)Nc1cccc(Oc2cc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncn2)c1	48	7.32
1822	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCN1CC2(CSC2)C1	48	7.32
1823	CCCCCCCCCCCCCCCCOC(=O)COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1	48	7.32
1824	OCc1ccc(-c2cc3c(NCc4ccccc4)ncnc3s2)cc1	48	7.32
1825	CN(C)CC(=O)Nc1cccc(-c2c(-c3ccccc3)oc3ncnc(N[C@H](CO)c4ccccc4)c23)c1	48	*
1826	CN[C@@H]1C[C@H]2O[C@@](C)([C@@H]1OC)n1c3ccccc3c3c4c(c5c6ccccc6n2c5c31)C(=O)NC4	48	*
1827	Cl.O=[N+]([O-])c1ccc2c(c1)sc1c(Nc3cccc(Br)c3)ncnc12	48	*
1828	OCCNC1CCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)CC1	48	*
1829	Fc1cccc(COc2ccc(Nc3ncnn4ccc(CN5CCCNCC5)c34)cc2Cl)c1	48	*
1830	CO/N=C/c1c(N)ncnc1Nc1ccc2[nH]c(Cc3cccc(F)c3)nc2c1	48	*
1831	C=CC(=O)Nc1cc(Nc2n[nH]c3cc(-c4cccc(N(C)C)c4)ccc23)c(OC)cc1N(C)CCN(C)C	48	*
1832	CCOC(=O)c1ccc(Nc2cc(NC(=O)CCCC(=O)O)ncn2)cc1	48	*
1833	COc1cc(NC(=O)Nc2ccccn2)cc(-c2cccnc2)c1OC	48.81	*
1834	S=C(Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)Nc1ccc(Cl)cc1Cl	48.9	*
1835	Nc1ccccc1NC(=O)/C=C/c1cccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)c1	49	*
1836	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCN(C)C	49	*
1837	COc1ccc(/N=C/c2c(N)ncnc2Nc2ccc3c(cnn3Cc3cccc(F)c3)c2)cc1	49	*

1838	C=CC(=O)Nc1cccc(NC(=O)Nc2ccnc(Nc3ccc(N(C)CCN(C)C)cc3OC)n2)c1	49	*
1839	OCCOCCn1ccc2ncnc(Nc3ccc(Oc4cccc(OC(F)(F)F)c4)c(Cl)c3)c21	49	*
1840	Cc1ccc(NC(/C=C/c2ccccc2)n2c(-c3cc(CCn4c(-c5ccccc5)nc5ccccc5c4=O)ccc3Cl)nc3ccccc32)cc1	49	*
1841	CN1CCN(c2ccc(Nc3nccc(Nc4ccc5[nH]ccc5c4)n3)cc2)CC1	49	*
1842	Oc1ccc(-c2nc(-c3ccc(F)cc3)c(-c3ccnc4[nH]c(-c5ccccc5)cc34)[nH]2)cc1	49.2	*
1843	O=C1OC[C@H]2OC(=O)c3cc(O)c(O)c(O)c3-c3c(O)c(O)c(O)c4c3C(=O)O[C@H]([C@H]3OC(=O)c5c-4c(O)c(O)c(O)c5[C@H]3O)[C@@H]2OC(=O)c2cc(O)c(O)c(O)c2-c2c1cc(O)c(O)c2O	49.9	*
1844	Clc1ccc(C2=NN(c3ccccc3)C(c3ccc4ccccc4c3)C2)cc1Cl	50	7.30
1845	CN(C)CCOc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)c1cc([N+](=O)[O-])ccc1F	50	7.30
1846	CS(=O)(=O)CCC(=O)Nc1cccc(C#Cc2cncnc2Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1	50	*
1847	CNC(=O)[C@H]1CCCN1Cc1cc2c(Nc3cccc(Cl)c3F)ncnc2cc1OC	50	*
1848	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN1CCOCC1C(N)=O	50	*
1849	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN1CC(C(N)=O)C1	50	*
1850	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN(C)[C@@H](CN(C)C)C(N)=O	50	*
1851	O=S(=O)(CCCCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5ccccc5)c(Cl)c4)c3c2)o1)c1ccccc1	50	*
1852	CNC(=O)O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1	50	*
1853	O=C(O[C@H]1CN[C@@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1)N1CCOCC1	50	*
1854	CCN(C)C(=O)O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1	50	*
1855	CCNC(=O)O[C@@H]1CN[C@@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1	50	*
1856	CCS(=O)(=O)N[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1	50	*
1857	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5ccccn5)c(Cl)c4)c3s2)C1)N1CCOCC1	50	*
1858	O=C(NOCc1ccccc1)c1cc(NCc2cc(O)ccc2O)ccc1O	50	*
1859	Cl.Clc1cccc(Nc2ncnc3ccccc23)c1	50	*
1860	COc1cc2ncnc(Nc3ccccc3)c2cc1OC.Cl	50	*
1861	CCOC(=O)c1cn2ncnc(Nc3ccc4[nH]ncc4c3)c2c1CC	50	*
1862	CC1(N)CCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)CC1	50	*
1863	N[C@H]1CCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)C1	50	*
1864	Clc1cc(Nc2ncnc3nn4ccccc4c23)ccc1OCc1ccccc1	50	*
1865	COc1cc2ncnc(Oc3cccc(NC(=S)Nc4ccc(Br)c(C(F)(F)F)c4)c3)c2cc1OC	50	*
1866	COc1cc(Nc2ncnc3cc(OC)c(OC)cc23)ccc1Br	50	*
1867	Nc1cccc(-c2cc3c(Nc4cc(Cl)cc(Cl)c4)ncnc3o2)c1	50	*
1868	CC(C)(O)C(=O)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21	50	*
1869	Cl.Cn1ccc2ncnc(Nc3ccc(Oc4cccc(OC(F)(F)F)c4)c(Cl)c3)c21	50	*
1870	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CNC(=O)C1COCCN1C	50	*
1871	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CNC(=O)C1CN(C)C1	50	*
1872	CCOC(OCC)c1ccc(C=C2CN(C)CC(=C\c3ccc(C(OCC)OCC)cc3)/C2=N\O)cc1	50	*
1873	Fc1ccc(Nc2ncnc3ccc(C#CCN4CCOCC4)cc23)cc1Cl	50.3	*
1874	C=CC(=O)Nc1cc(Nc2nccc(NC(=O)c3cccc(OC)c3)n2)c(OC)cc1N1CCC(C(N)=O)CC1	50.5	*
1875	C=CC(=O)Nc1cc2c(Nc3ccc(OCc4ccccn4)c(Cl)c3)c(C#N)cnc2cc1OCC	50.7	7.29
1876	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1)c1cccc([N+](=O)[O-])c1	50.9	7.29
1877	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(CC(=O)NCCOc5no[n+]([O-])c5S(=O)(=O)c5ccccc5)CC4)cc3OC)ncc2Cl)c1	51	7.29
1878	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccc(Cl)cc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	51	7.29

1879	COc1cc2ncnc(Nc3cc(Cl)ccc3F)c2cc1OCCCN1CCOCC1	51	*
1880	Brc1cccc(Nc2ncnc3cnccc23)c1	51	*
1881	O=C1CS/C(=N/Nc2nncc3ccccc23)N1	51	*
1882	COc1cc2c(Nc3ccc(NC(=O)Nc4ccc(C)c(C)c4)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1	51	*
1883	N#Cc1ccccc1Oc1ccc(Nc2ncnc3cc[nH]c23)cc1Cl	51	*
1884	COc1ccc(-n2c(-c3ccccc3)c(-c3ccccc3)c3cc4c(cc3c2=O)C(c2ccccc2)NC(=O)N4)cc1	51	*
1885	COc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2cc1OCCCCCn1ccnc1[N+](=O)[O-]	51.2	7.29
1886	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(CC(=O)OCC#CCOc5no[n+]([O-])c5S(=O)(=O)c5ccccc5)CC4)cc3OC)ncc2Cl)c1	52	7.28
1887	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCN1CC2(CSC2)C1	52	7.28
1888	Nc1ncnc(Nc2ccc3c(cnn3Cc3cccc(F)c3)c2)c1/C=N/NCC(F)(F)F	52	*
1889	CNc1ccc2c(Nc3cccc(Br)c3)ncnc2n1	52	*
1890	CCCCNC(=S)NNc1nncc2ccccc12	52	*
1891	Br.Oc1ccc(-c2cc3c(NCc4cccc(F)c4)ncnc3[nH]2)cc1	52	*
1892	OCCC1COc2cc3ncnc(Nc4cccc(Cl)c4)c3cc2O1	52	*
1893	Brc1cccc(Nc2ncnc3cc4c(cc23)OC(CCN(N2CCCCC2)N2CCCCC2)CO4)c1	52	*
1894	Fc1ccc(-c2nc(Nc3cc(Br)cc4cc(-c5ccc(F)cc5)oc34)c3cc(Br)ccc3n2)cc1	52.2	*
1895	Fc1ccc(-c2nc(Nc3cc(Br)cc4cc(-c5ccc(F)cc5)[nH]c34)c3ccccc3n2)cc1	52.5	*
1896	CCCN1CC[C@H](N2C(=O)N(c3ccccc3Cl)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	52.8	7.28
1897	O=C(Nc1cc2c(Nc3ccc(F)c(F)c3)ncnc2cc1OCCCN1CCOCC1)c1cc([N+](=O)[O-])ccc1F	53	7.28
1898	Fc1ccc(Nc2ncnc3sc(Br)cc23)cc1Cl	53	*
1899	CCOC(=O)CCCn1c(=O)oc2cc3ncnc(Nc4ccc(OCc5ccc(Cl)cc5)c(Cl)c4)c3cc21	53	*
1900	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	53	*
1901	CC(C)S(=O)(=O)CC(=O)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21	53	*
1902	Nc1ccc2ncnc(Nc3cccc(Br)c3)c2n1	53	*
1903	O=C(O)Cn1ncc2cc3c(Nc4cccc(Br)c4)ncnc3cc21	53	*
1904	Nc1cc2ncnc(Nc3cccc(Br)c3)c2cc1[N+](=O)[O-]	53	*
1905	COc1ccc(NC(=S)NNc2nncc3ccccc23)cc1	53	*
1906	COc1cc(Nc2c(C#N)cnc3cc(OCCCN4CCN(C)CC4)c(OC)cc23)c(Cl)cc1Cl	53	*
1907	O=C(O)CCCC(=O)Nc1cc(N2CCOCC2)ncn1	53	*
1908	O=C1COc2cc3ncnc(Nc4ccc(F)c(Cl)c4)c3cc2N1CCCN1CCOCC1	53.1	*
1909	C=CC(=O)Nc1ccc2ncnc(Nc3ccc(S(=O)(=O)NC(=N)N)cc3)c2c1	53.3	*
1910	C=CC(=O)Nc1ccc2ncnc(Nc3ccc(OC)cc3OC)c2c1	53.6	*
1911	Fc1cccc(COc2ccc(Nc3ncnc4sc(-c5ccc(CNCc6ccccc6)o5)cc34)cc2Cl)c1	54	*
1912	O=C(O)c1ccc(S(=O)(=O)Oc2ccc(/C=C/[N+](=O)[O-])cc2)cc1O	54	*
1913	COc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1nccc(Nc2ccc3ccccc3c2)n1	54	*
1914	C=CC(=O)Nc1cc(Nc2ncc(I)c(Nc3ccccc3P(C)(C)=O)n2)c(OC)cc1N(C)CCN(C)C	54	*
1915	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C#Cc1cccc(CN(C)C)c1	55	7.26
1916	COc1ccccc1-c1cc2c(N[C@H](C)c3cccs3)ncnc2s1	55	*
1917	Brc1cccc(Nc2ncnc3cc4c(cc23)OCCOCCO4)c1	55	*
1918	COc1ccc2ncnc(Nc3ccccc3)c2c1	55	*
1919	Cc1ccc(Nc2nccc(N(C)c3ccc4[nH]cc(C)c4c3)n2)cc1S(N)(=O)=O	55	*
1920	NCCCSc1nc(-c2ccc(F)cc2)c(-c2ccnc(Nc3ccccc3)c2)[nH]1	55	*

1921	S=C(Nc1cncc(Cl)c1)Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	55.5	*
1922	CC[C@H](C)[C@@H](NC(=O)OC(C)(C)C)C(=O)Nc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	55.5	*
1923	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCN1CC2(COC2)C1	56	7.25
1924	C[C@@H](Nc1ncnc2oc(-c3ccc(Br)cc3)cc12)c1ccccc1	56	7.25
1925	CC(C)(C)S(=O)(=O)CC(=O)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21	56	*
1926	COc1cc2ncnc(NCc3ccccc3)c2cc1O	56	*
1927	Fc1cccc(Nc2ncnc3ccccc23)c1	56	*
1928	O=C(N/N=C/c1ccc(O)cc1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	56	*
1929	COc1ccc(Nc2nccc(Nc3ccc4[nH]ccc4c3)n2)cc1N1CCOCC1	56	*
1930	CS(=O)(=O)c1ccc(F)c(C(=O)Nc2cc3c(Nc4ccc(F)c(Cl)c4)ncnc3cc2OCCCN2CCOCC2)c1	57	7.24
1931	O=C(/C=C/CN1CCCC1)Nc1cc2c(Nc3ccc4c(cnn4Cc4ccccc4)c3)ncnc2cn1	57	*
1932	CCN(CC)CCCOc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OC	57	*
1933	O=C(C#CCN1CCCCC1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	57	*
1934	COc1cc(N2CCC(N3CCN(S(C)(=O)=O)CC3)CC2)ccc1Nc1nccc(-c2c(-c3cccc(C(=O)Nc4c(F)cccc4F)c3)nc3ccccn23)n1	57	*
1935	CO/N=C/c1c(N)ncnc1Nc1ccc2c(c1)CCN2Cc1cccc(F)c1	57	*
1936	C=CC(=O)Nc1cc(Br)cc(-n2c(=O)cc(C)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	57	*
1937	COc1cc(O)c(C(=O)Nc2cccc(Cl)c2)cc1O	57	*
1938	C=CC(=O)Nc1ccc(OC)c(Nc2cc(-c3[nH]c(SC)nc3C(C)(C)C)ccn2)c1	57	*
1939	C#Cc1cccc(Nc2ncnc3cc(OC4CCOCC4)c4c(c23)OCCO4)c1	57.8	*
1940	COc1ccccc1Cc1nc2ccc(-c3nn([C@H]4CC[C@H](C5CCN(C)CC5)CC4)c4ncnc(N)c34)cc2[nH]1	58	*
1941	COCCCN1CCC([C@H]2CC[C@H](n3nc(-c4ccc5nc(Cc6ccccc6Cl)[nH]c5c4)c4c(N)ncnc43)CC2)CC1	58	*
1942	CC(=O)N1CCC[C@@H]1C#Cc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2s1	58	*
1943	COc1ccc2c(NCc3ccccc3)ncnc2c1	58	*
1944	c1ccc(Nc2nc[nH]c3nnc(Nc4ccccc4)c2-3)cc1	58	*
1945	Cl.O=[N+]([O-])c1ccc2sc3c(Nc4ccccc4)ncnc3c2c1	58	*
1946	Clc1cccc(Nc2ncnc3cc4c(cc23)OC(CCN(N2CCCCC2)N2CCCCC2)CO4)c1	58	*
1947	Fc1ccc(Nc2ncnc3cc(OC4CCOCC4)c4c(c23)OCCO4)cc1Cl	58.8	*
1948	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(CC(=O)NCCCOc5no[n+]([O-])c5S(=O)(=O)c5ccccc5)CC4)cc3OC)ncc2Cl)c1	59	7.23
1949	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(CC(=O)OCCOc5no[n+]([O-])c5S(=O)(=O)c5ccccc5)CC4)cc3OC)ncc2Cl)c1	59	7.23
1950	C[C@@H](Nc1ncnc2sc(-c3ccc(C=O)cc3F)cc12)c1ccccc1	59	7.23
1951	COc1cc2ncnc(Nc3ccc(OCc4ccccn4)c(C)c3)c2cc1OC	59	*
1952	COCOCC#CC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	59	*
1953	COc1ccc(Nc2ncc3ncc(=O)n(-c4ccc(NC(=O)/C=C/CN(C)C)cc4)c3n2)cc1	59.1	7.23
1954	O=C1OC[C@H]2OC(=O)c3cc(O)c(O)c(O)c3-c3c(O)c(O)c(O)c4c3C(=O)O[C@H]([C@H]3OC(=O)c5c-4c(O)c(O)c(O)c5[C@@H]3[C@]3(O)OC[C@@H](O)[C@H](O)[C@H]3O)[C@@H]2OC(=O)c2cc(O)c(O)c(O)c2-c2c1cc(O)c(O)c2O	59.2	*
1955	O=C(Nc1ccccc1C(=O)N/N=C/c1ccccc1)c1ccco1	59.3	*
1956	CS(=O)(=O)N1CCN(Cc2ccc(-c3ccc4ncnc(Nc5ccc(OCc6cccc(F)c6)c(Cl)c5)c4c3)o2)CC1.Cc1ccc(S(=O)(=O)O)cc1	59.9	*
1957	Cc1ccc(C2=NN(c3ccccc3)C(c3ccc4ccccc4c3)C2)cc1	60	7.22

1958	Cc1ccc(C2=NN(c3nc(-c4ccc(Cl)cc4)cs3)C(c3ccc(F)cc3)C2)cc1C	60	7.22
1959	CC(=O)NCc1cccc(C#Cc2cncnc2Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1	60	*
1960	CCOc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2cc1NC(=O)/C=C/CN1CCCC1	60	*
1961	CCOC(=O)N[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1	60	*
1962	O=C(Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)C1CCSS1	60	*
1963	CCOC(=O)c1cn2ncnc(Nc3cccc(Br)c3)c2c1CC	60	*
1964	N[C@@H]1CCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)C1	60	*
1965	NS(=O)(=O)c1ccc(-n2c(SCC(=O)Nc3ccc([N+](=O)[O-])cc3[N+](=O)[O-])nc3cc4ccccc4cc3c2=O)cc1	60	*
1966	Nc1cccc(-c2nc3c(Nc4cccc(Cl)c4)ncnc3o2)c1	60	*
1967	COc1cc(Br)c(C=C2CN(C)CC(=Cc3nc(C)c(C)nc3C)C2=O)cc1OC	60	*
1968	Fc1cc(F)cc(NC(=S)Nc2ccc3ncnc(Nc4cccc(Cl)c4)c3c2)c1	60.1	*
1969	C=CC(=O)Oc1ccc(-n2c(=O)cnc3cnc(Nc4ccc(OC)cc4)nc32)cc1	60.4	7.22
1970	FC(F)(F)c1cccc(NC(=S)Nc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)c1	60.7	*
1971	Nc1cc(Nc2cccc(Oc3cc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)ncn3)c2)ncn1	61	7.21
1972	O=c1oc2cc3ncnc(Nc4ccc(OCc5ccc(Cl)cc5)c(Cl)c4)c3cc2n1CCCN1CCOCC1	61	*
1973	NC(=O)Nc1ccc2ncnc(Nc3ccc(Cl)cc3)c2c1	61	*
1974	CCC(=O)Nc1cc2c(Nc3ccc4c(ccn4Cc4ccccn4)c3)ncnc2cc1OC	61	*
1975	COCCN(CCOC)CCOc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OC	61	*
1976	Fc1cccc(Cn2ncc3cc(Nc4ncnn5ccc(COC[C@@H]6CNCCO6)c45)ccc32)c1	61	*
1977	Fc1ccccc1Oc1ccc(Nc2ncnc3cc[nH]c23)cc1Cl	61	*
1978	CS(=O)(=O)O.O=C(CCO)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21	61	*
1979	FC(F)(F)Oc1ccc(-c2cc3cc(Br)cc(Nc4nc(-c5ccc(Cl)cc5)nc5ccc(Br)cc45)c3o2)cc1	61.5	*
1980	O=C1OC[C@H]2OC(=O)c3cc(O)c(O)c(O)c3-c3c(O)c(O)c(O)c4c3C(=O)O[C@H]([C@H]3OC(=O)c5c-4c(O)c(O)c(O)c5[C@@H]3O)[C@@H]2OC(=O)c2cc(O)c(O)c(O)c2-c2c1cc(O)c(O)c2O	61.8	*
1981	O=C(Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)c1ccc([N+](=O)[O-])cc1	61.8	*
1982	COCCN(C)C/C=C/C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	62	*
1983	CCCN(CC#CC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)CCC	62	*
1984	Br.C[C@@H](Nc1ncnc2[nH]c(-c3ccc(O)cc3)cc12)c1ccc(Br)cc1	62	*
1985	Brc1cccc(Nc2ncnc3cc4c(cc23)OC(CCN(N2CCCC2)N2CCCC2)CO4)c1	62	*
1986	COc1ccc(NC(c2ccccc2)n2c(-c3cc(CCn4c(-c5ccccc5)nc5ccccc5c4=O)ccc3Cl)nc3ccccc32)cc1	62	*
1987	Nc1ccccc1C#Cc1cncnc1Nc1ccc(OCc2cccc(F)c2)c(Cl)c1	63	*
1988	CCN(CC)C(=O)O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1	63	*
1989	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1)N1CCNCC1	63	*
1990	CCC(=O)O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1	63	*
1991	CNC1CCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)CC1	63	*
1992	C[C@@H](Nc1ncnc2[nH]c(-c3ccc(Br)cc3)cc12)c1ccccc1	63	*
1993	Ic1cccc(Nc2ncnc3cc4c(cc23)OCCO4)c1	63	*
1994	O=C1COc2cc3ncnc(Nc4cccc(Cl)c4)c3cc2N1CCCN1CCOCC1	63.1	*
1995	Brc1cccc(Nc2ncnc3cc4c(cc23)OC(CN2CCOCC2)CO4)c1	63.1	*
1996	c1ccc(Cc2ccc(Nc3ncnc4[nH]ccc34)cc2)cc1	63.29	*
1997	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCO	63.4	*
1998	Oc1cccc(Nc2ncnc3ccc(NC(=S)NCc4ccccc4)cc23)c1	63.6	*
1999	O=C(Nc1cccc(Cl)c1)c1ccc(OCCCN2CCCCC2)cc1O	63.9	*

2000	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccc(F)cc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	64	7.19
2001	COC(=O)Cn1cc(-c2cccc(Cl)c2)c(=O)c2c(O)cc(OC)cc21	64	*
2002	S=C(NNc1nncc2ccccc12)Nc1ccc(Cl)cc1	64	*
2003	NCCCOCc1ccn2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c12	64	*
2004	Brc1cccc(Nc2ncnc3ccc(NN=NCCN4CCOCC4)cc23)c1	64	*
2005	COc1cc(O)c(C(=O)Nc2cccc(Cl)c2)cc1OC	64	*
2006	CN1CCN(N(CCC2COc3cc4ncnc(Nc5cccc(Cl)c5)c4cc3O2)N2CCN(C)CC2)CC1	64	*
2007	C[C@H](N)C#Cc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2s1	64	*
2008	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1)N1CCOCC1	65	7.14
2009	O=C(COc1ccccc1)Nc1cccc(Oc2cc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncn2)c1	65	7.19
2010	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1/C=N/OCCCN1CCOCC1	65	7.19
2011	CC1(C)CC(C(=O)Nc2ccc3ncnc(Nc4cccc(Cl)c4)c3c2)CC(C)(C)N1[O]	65	7.19
2012	CCC(=O)Nc1cc2c(Nc3ccc(Oc4ccccc4)cc3)ncnc2cc1OC	65	*
2013	CCC(=O)Nc1cc2c(Nc3ccc(NS(=O)(=O)c4ccccc4)cc3)ncnc2cc1OC	65	*
2014	S=C(NNc1nncc2ccccc12)Nc1ccccc1	65	*
2015	COCC1CCCN1CC#CC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	65	*
2016	COCCOCC#CC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	65	*
2017	CCN1CCN(CC#CC(=O)Nc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)CC1	65	*
2018	OCCn1cnc2cc3c(N4CCc5ccccc54)ncnc3cc21	65	*
2019	C=CC(=O)Nc1cc(Nc2ncc(Cl)c(Nc3ccccc3P(C)(C)=O)n2)c(OC)cc1N(C)CCN(C)C	65	*
2020	C=C=CCCCCOc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O	65.5	*
2021	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCn1ccnc1	66	*
2022	COc1ccccc1Nc1ncc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1	66	*
2023	CN1CCN(CCCOc2cc(OC3CCOCC3)c3c(Nc4ccc(F)c(Cl)c4)ncnc3c2)CC1	66	*
2024	C=CC(=O)Nc1cc(-n2c(=O)cc(C)c3cnc(Nc4ccc(N5CCN(C)C(C)C5)cc4OC)nc32)cc(C(F)(F)F)c1	66	*
2025	CCN(CC)N(CCC1COc2cc3ncnc(Nc4cccc(Cl)c4)c3cc2O1)N(CC)CC	66	*
2026	Fc1ccc(Nc2ncnc3cc4c(cc23)OC(CCN(N2CCOCC2)N2CCOCC2)CO4)cc1Cl	66	*
2027	Fc1ccc(Nc2ncnc3cc4c(cc23)OC(CCN(N2CCCCC2)N2CCCCC2)CO4)cc1Cl	66	*
2028	COc1ccc(-c2cc(NC(=O)Nc3ccccn3)cc(OC)c2OC)cn1	66.59	*
2029	Cc1ccc(Nc2ncnc3cc4oc(=O)n(CCCN5CCOCC5)c4cc23)cc1	67	*
2030	CCC(=O)Nc1cc2c(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncnc2cc1OC	67	*
2031	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OC[C@H](O)CN1CCOCC1	67	*
2032	Nc1ncnc2c1c(-c1ccc(Cl)c(O)c1)nn2C1CCCC1	67	*
2033	FC(F)(F)c1cccc(Oc2ccc(Nc3ncnc4cc[nH]c34)cc2Cl)c1	67	*
2034	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1/C=N/OCCN1CCOCC1	68	7.17
2035	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)CCOC	68	7.17
2036	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)c1cc([N+](=O)[O-])ccc1F	68	7.17
2037	COc1ccc2ncnc(Nc3ccc(OCc4ccccc4)cc3)c2c1	68	*
2038	O=C(NCCN1CCCC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	68	*
2039	CN(C)Cc1ccc(-c2cc3c(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)ncnc3s2)[nH]1	68	*
2040	Fc1cccc(COc2ccc(Nc3ncnc4cc(-c5ccc[nH]5)sc34)cc2Cl)c1	68	*
2041	CNc1cc2ncnc(Nc3cccc(Br)c3)c2cc1[N+](=O)[O-]	68	*
2042	OC1CCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)CC1	68	*

2043	O=C(/C=C/CN1CCC(N2CCCCC2)CC1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	68	*
2044	C[C@H](c1cccc(F)c1)n1ncc2cc(Nc3ncnn4ccc(COC[C@@H]5CNCCO5)c34)ccc21	68	*
2045	c1ccc(-c2cc3ncnc(Nc4ccc5[nH]ccc5c4)c3s2)cc1	68	*
2046	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N(NCCN1CCCC1)NCN1CCCC1	68	*
2047	C=CC(=O)Nc1cccc(-n2c(=O)c(=O)n(C(C)C)c3cnc(Nc4ccc(OCCN(C)C)cc4OC)nc32)c1	68	*
2048	COc1ccc(OC)c(Nc2cc(NC(=O)CCCC(=O)O)ncn2)c1	68	*
2049	C[C@H](N)C#Cc1cc2c(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncnc2s1	69	*
2050	CCOc1cc2ncnc(Nc3ccc(NS(=O)(=O)c4ccccc4)cc3)c2cc1NC(=O)/C=C/CN1CCOCC1	69	*
2051	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCNC(C)(CO)CO	69	*
2052	CC1(C)[C@@H](O[C@@H]2O[C@H](C(=O)O)[C@@H](O)[C@H](O)[C@H]2O)CC[C@@]2(C)[C@H]1CC[C@]1(C)[C@@H]2C(=O)C=C2[C@H]3C[C@@](C)(C(=O)O)CC[C@]3(C)CC[C@]21C	69	*
2053	COc1ccc(C2CC(c3ccc(C)c(C)c3)=NN2C(N)=S)cc1	70	7.15
2054	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN1CCC1C(N)=O	70	*
2055	O=C(Oc1ccccc1)c1cc(NCc2cc(O)ccc2O)ccc1O	70	*
2056	Nc1cc2ncnc(Nc3cccc(O)c3)c2cn1	70	*
2057	CCc1c(C(=O)NC)cn2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c12	70	*
2058	NC1CCN(Cc2ccn3ncnc(Nc4ccc(OCc5cccc[n+]5[O-])c(Cl)c4)c23)CC1	70	*
2059	CO/N=C/c1c(N)ncnc1Nc1ccc(F)c(Cl)c1	70	*
2060	COc1ccc(Nc2ncnn3ccc(CN4CCC(N)CC4)c23)cc1Cl	70	*
2061	COc1cc2ncnc(Sc3cccc(NC(=S)Nc4cccc(C(F)(F)F)c4)c3)c2cc1OC	70	*
2062	CN/N=N/c1ccc2ncnc(Nc3cccc(Br)c3)c2c1	70	*
2063	Nc1ccc(-c2nc3c(Nc4cccc(O)c4)ncnc3o2)cc1	70	*
2064	Clc1cccc(Nc2ncnc3cc4c(cc23)OC(CCN(N2CCCC2)N2CCCC2)CO4)c1	70	*
2065	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CNC(=O)C1CCN1C	70	*
2066	O=C(O)CCCC(=O)Nc1cc(Nc2cccc(Br)c2)ncn1	70	*
2067	Nc1c(O)cccc1Nc1ncnc2ccncc12	70.79	*
2068	C#Cc1cc2c(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncnc2s1	71	*
2069	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCN1CCCC1	71	*
2070	ClCCN(CCNN=Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1)Cc1ccccc1	71	*
2071	C=CCN(C)CC#CC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	71	*
2072	COCCN=NNc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	71	*
2073	O=C(CN1CCCC1)Nc1ccc2ncnc(Nc3ccc(OCc4cccc(F)c4)cc3)c2c1	71	*
2074	O=C(Nc1cccc(Cl)c1)c1ccc(O)cc1O	71	*
2075	O=C1OC[C@H]2OC(=O)c3cc(O)c(O)c(O)c3-c3c(O)c(O)c(O)c4c3C(=O)O[C@H]([C@H]3OC(=O)c5c-4c(O)c(O)c(O)c5[C@@H]3[C@]3(O)OC[C@@H](O)[C@H](O)[C@@H]3O)[C@@H]2OC(=O)c2cc(O)c(O)c(O)c2-c2c1cc(O)c(O)c2O	71.2	*
2076	CCC(=O)N1CC[C@H](N2C(=O)N(c3ccc(F)cc3)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	71.6	7.15
2077	O=C(Nc1nccs1)Nc1cc(-c2cncnc2)ccc1OC(F)(F)F	71.71	*
2078	O=C(Nc1cc(-c2cncnc2)cc(C(F)(F)F)c1)Nc1nccs1	71.82	*
2079	C#Cc1cccc(Nc2ncnc3cc(OCCOC(=O)C(C)c4ccc5cc(OC)ccc5c4)c(OCCOC)cc23)c1	72	7.14
2080	COc1cc2ncnc(NCc3ccc(Cl)c(F)c3)c2cc1OCCCCCCC(=O)NO	72	7.14
2081	COc1cc2ncc(C#N)c(Nc3ccc(NCc4cccnc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	72	7.14
2082	Brc1cccc(Nc2[nH]cnc3c4ccccc4nc2-3)c1.Cl	72	*

2083	Brc1cccc(Nc2ncnc3c2[nH]c2ccccc23)c1.Cl	72	*
2084	CN1CCN(N(CCC2COc3cc4ncnc(Nc5ccc(F)c(Cl)c5)c4cc3O2)N2CCN(C)CC2)CC1	72	*
2085	Cc1ccc(NC(c2ccccc2)n2c(-c3cc(CCn4c(-c5ccccc5)nc5ccccc5c4=O)ccc3Cl)nc3ccccc32)cc1	72	*
2086	CN(C)c1nc2cc3c(N4CCc5ccccc54)ncnc3cc2o1	72	*
2087	COc1cc2ncnc(N3CCCc4ccccc43)c2cc1NC(=O)/C=C/CN(C)C	72	*
2088	C=CC(=O)Nc1cc2c(Nc3ccc(OCc4cccc(F)c4)cc3)ncnc2cc1O[C@H]1CCOC1	72.2	*
2089	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(CC(=O)NCC(C)Oc5no[n+]([O-])c5S(=O)(=O)c5ccccc5)CC4)cc3OC)ncc2Cl)c1	73	7.14
2090	CCN(CC)C/C=C/C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	73	*
2091	Fc1cccc(Cn2ncc3cc(Nc4ncnn5ccc(COC6CCNCC6)c45)ccc32)c1	73	*
2092	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C#Cc1ncc(CN2CCCC2)s1	74	7.13
2093	COc1ccc(-c2cc3c(NCc4ccccc4)ncnc3o2)cc1	74	7.13
2094	CS(=O)(=O)CCNCCCCOc1ccc2ncnc(Nc3ccc(OCc4ccccc4)cc3)c2c1	74	*
2095	O=C(NCCCCOc1ccc2ncnc(Nc3ccc(OCc4ccccc4)cc3)c2c1)C(F)(F)F	74	*
2096	Fc1cccc(COc2ccc(Nc3ncncc3C#Cc3cccnc3)cc2Cl)c1	74	*
2097	O=C(/C=C/CN1CCOCC1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	74	*
2098	COCCOc1cc2ncnc(Nc3ccc(C)c([N+](=O)[O-])c3)c2c2c1OCCO2	74.6	*
2099	C=C(CN1CCOCC1)C(=O)Nc1cc2c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c(C#N)cnc2cc1OCC	75	7.12
2100	CS(=O)(=O)CCNC(=O)C1=Cc2c(ncnc2Nc2ccc(Oc3cccc(C(F)(F)F)c3)c(Cl)c2)NCC1	75	*
2101	COc1cc2c(Nc3ccc(Cl)cc3F)ncnc2cc1OCCCN1CCN(C)CC1.Cl	75	*
2102	NP(=O)(OCCCOc1ccc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2c1)N(CCCl)CCCl	75	*
2103	OCc1nc(C#Cc2cncnc2Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)cs1	76	*
2104	CCN=C(S)NNc1nncc2ccccc12	76	*
2105	C=CC(=O)Nc1ccc2ncnc(Nc3ccc(S(N)(=O)=O)cc3)c2c1	76.5	*
2106	O=C(CBr)OCCn1c(=O)oc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3cc21	77	7.11
2107	Fc1cccc(COc2ccc(Nc3ncncc3C#Cc3nccn3)cc2Cl)c1	77	*
2108	CCC1=C2C(Nc3ccc4c(cnn4Cc4ccccc4)c3)=NC=NC2N=C1NC(=O)OCCN1CCOCC1	77	*
2109	NC(=S)NNc1nncc2ccccc12	77	*
2110	COc1ccc(-c2cc3c(N[C@@H](C)c4ccccc4)ncnc3[nH]2)cc1	77	*
2111	C=CC(=O)Nc1cccc(N2C(=O)C(c3ccccc3)N(C)C(=O)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	77.19	7.11
2112	CS(=O)(=O)CC(NC1CCCCC1)c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	77.2	*
2113	Fc1ccc(Nc2ncnc3cc4c(cc23)OCCO4)cc1	77.6	*
2114	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN1CCCC1	78	7.11
2115	O=c1oc2cc3ncnc(Nc4ccc(F)c(Cl)c4)c3cc2n1CCCN1CCOCC1	78	*
2116	C#Cc1cccc(Nc2ncnc3ccc(OCc4ccc(C(=O)Nc5ccccc5N)cc4)cc23)c1	78	*
2117	COc1cc2c(Nc3ccc(NC(=O)Nc4ccc(F)c(Cl)c4)c(Cl)c3)ncnc2cc1OCCCN1CCN(C)CC1	78	*
2118	O=C(Nc1cc(-c2cccnc2)cc(C(F)(F)F)c1)Nc1nccs1	78.17	*
2119	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C#Cc1ccc(CN2CCCC2)o1	79	7.10
2120	C=CCOc1ccc2ncnc(Nc3ccc(OCc4ccccc4)cc3)c2c1	79	*
2121	Fc1cccc(COc2ccc(Nc3ncncc3C#Cc3ccccc3)cc2Cl)c1	79	*
2122	CNC(=O)c1cccc(C#Cc2cncnc2Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1	79	*
2123	CCC(=O)Nc1cc2c(Nc3ccc4[nH]ncc4c3)ncnc2cc1OC	79	*
2124	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCCN1CCCCC1	79	*

2125	CN(C)C(=O)O[C@@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1	79	*
2126	CN(C)C(=O)O[C@H]1CN[C@@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1	79	*
2127	O=C(O[C@@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1)N1CCOCC1	79	*
2128	C=CC(=O)Nc1cccc(-n2c(=O)n(C(C)C)c(=O)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	79	*
2129	Oc1ccc(CN(Cc2cccc(Cl)c2O)C(=S)Nc2ccccc2)cc1	80	7.10
2130	COc1ccc(NC(=O)c2ccc(N(CCCl)CCCl)cc2)cc1	80	7.10
2131	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc5c(cnn5Cc5ccccc5)c4)c3s2)C1)N1CCOCC1	80	7.10
2132	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN1CC[C@H](C(N)=O)C1	80	*
2133	CS(=O)(=O)CCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(C(F)(F)F)c4)c3c2)o1	80	*
2134	Brc1cc2c(Nc3ccccc3)ncnc2s1	80	*
2135	COc1cc2ncnc(C#CC(C)(C)N(C)c3ccccc3)c2cc1OC	80	*
2136	O=C(OCc1ccccc1)c1cc(NCc2cc(O)ccc2O)ccc1O	80	*
2137	Ic1cccc(Nc2ncnc3ccccc23)c1	80	*
2138	Cn1c(=O)c(-c2c(Cl)cccc2Cl)cc2cnc(Nc3ccc(CCCC(=O)O)cc3)nc21	80	*
2139	COc1ccc2c(c1)sc1c(Nc3cccc(Br)c3)ncnc12	80	*
2140	C=CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)c(C#N)cnc2cc1OCCCN1CCOCC1	80	*
2141	C=CC(=O)Nc1cccc(NC(=O)Nc2ccnc(Nc3ccc(N4CCC(N5CCN(C)CC5)CC4)cc3OC)n2)c1	80	*
2142	CS(=O)(=O)O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1	81	*
2143	Cc1ccn2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c12	81	*
2144	COc1ccc(NC(/C=C/c2ccccc2)n2c(-c3cc(CCn4c(-c5ccccc5)nc5ccccc5c4=O)ccc3Cl)nc3ccccc32)cc1	81	*
2145	CC1(C)[C@@H](O[C@H]2O[C@H](C(=O)O)[C@@H](O)[C@H](O)[C@H]2O[C@@H]2O[C@H](C(=O)O)[C@@H](O)[C@H](O)[C@H]2O)CC[C@@]2(C)[C@H]1CC[C@]1(C)[C@@H]2C(=O)C=C2[C@@H]3C[C@@](C)(C(=O)O)CC[C@]3(C)CC[C@]21C	81	*
2146	C=CC(=O)Nc1cccc(-n2c(=O)c(=O)n(CC)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	81	*
2147	COc1ccc(Nc2cc(NC(=O)c3ccccc3)ncn2)cc1	81	*
2148	CCOc1cc2ncc(C#N)c(Nc3ccc4c(ccn4S(=O)(=O)c4ccccc4)c3)c2cc1NC(=O)/C=C/CN(C)C	82	7.09
2149	O=C(NCCN1CCOCC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	82	*
2150	CCOc1cc2ncnc(Nc3ccc(NS(=O)(=O)c4ccccc4)cc3)c2cc1NC(=O)/C=C/CN1CCN(C)CC1	82	*
2151	C=CC(=O)Nc1ccc(-c2c(-c3ccccc3)oc3ncnc(N[C@H](CO)c4ccccc4)c23)cc1	82	*
2152	Clc1ncc2ncnc(Nc3cccc(Br)c3)c2n1	82	*
2153	COc1cc2ncnc(Nc3cccc(NC(=O)Nc4ccc(Cl)c(C(F)(F)F)c4)c3)c2cc1OCCCN1CCOCC1	82	*
2154	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N(NCCN1CCOCC1)NCN1CCOCC1	82	*
2155	C=CC(=O)Nc1cccc(-n2c(=O)n(C)c(=O)c3cnc(Nc4ccccc4)nc32)c1	82	*
2156	CC(C)Oc1cc2ncnc(Nc3ccc(F)c([N+](=O)[O-])c3)c2c2c1OCCO2	82.5	*
2157	OCC(Nc1ncnc2sc(Br)cc12)c1ccccc1	83	*
2158	Fc1cccc(Cn2ncc3cc(Nc4ncnn5ccc(COC[C@H]6CNCCO6)c45)ccc32)c1	83	*
2159	O=C(Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1)C1CCC2(CC1)OOC1(CCCCC1)OO2	83.82	*
2160	Fc1cccc(Nc2ncnc3cc(OCCCN4CCOCC4)c4c(c23)OCCO4)c1	83.88	*
2161	COc1cc2ncnc(NC3CC3c3ccccc3)c2cc1OC(C)=O	84	*
2162	CN(C)c1ccc2ncnc(Nc3cccc(Br)c3)c2c1	84	*
2163	Clc1cccc(Nc2[nH]nc3ncnc(Nc4ccccc4)c23)c1	84	*
2164	O=S(=O)(Nc1ccccn1)c1ccc(Nc2nncc3ccccc23)cc1	84	*
2165	COc1cc(-c2nn(C3CCCC3)c3ncnc(N)c23)ccc1N	84	*

2166	O=C(CCCCCCOc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1)NO	84.2	7.07
2167	O=C(Nc1ccc([N+](=O)[O-])cc1Cl)c1ccc(OCCCN2CCOCC2)cc1O	84.8	*
2168	Clc1ccc(Nc2ncnc3[nH]ccc23)cc1	84.92	*
2169	Cc1ccc(Br)c2c(C#N)cc(C(=O)C3CC3)n12	85	7.07
2170	C#Cc1cncnc1Nc1ccc(OCc2cccc(F)c2)c(Cl)c1	85	*
2171	CCCN(CCS(C)(=O)=O)Cc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	85	*
2172	Brc1cccc(Nc2ncnc3cc4c(cc23)OCCCO4)c1	85	*
2173	Cc1cncc(COc2ccc(Nc3ncnn4ccc(CN5CCC(N)CC5)c34)cc2Cl)c1	85	*
2174	COC[C@H]1CCCN1C/C=C/C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	85	*
2175	CC(C)N(C)CC#CC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	85	*
2176	Nc1ncnc2c1c(-c1ccc3cc[nH]c3c1)nn2C1CCCC1	85	*
2177	O=C1NCc2cc3c(=O)n(-c4ccc(Cl)cc4)c(-c4ccccc4)c(-c4ccccc4)c3cc2N1	85	*
2178	NS(=O)(=O)c1ccc(NC(=O)c2ccccc2NC(=O)c2ccco2)cc1	85.4	*
2179	O=C(Nc1cccc(Br)c1)c1ccc(OCCCN2CCOCC2)cc1O	85.8	*
2180	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C#CCOc1ccc(CNC(C)C)cc1	86	7.07
2181	O=C(C#CCN1CCOCC1)Nc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	86	*
2182	CCC(=O)Nc1cc2c(Nc3ccc4c(ccn4Cc4ccco4)c3)ncnc2cc1OC	86	*
2183	CCC(=O)Nc1cc2c(N[C@H](C)c3ccccc3)ncnc2cc1OC	86	*
2184	O=S(=O)(Nc1ncccn1)c1ccc(Nc2nncc3ccccc23)cc1	86	*
2185	Cc1ccn2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c12	86	*
2186	C=CC(=O)Nc1cccc(NC(=O)Nc2ccnc(Nc3ccc(N4CCC(N5CCOCC5)CC4)cc3OC)n2)c1	86	*
2187	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCN1CCCC1	87	*
2188	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(/C=C/c4cc(C)cc(C)c4)cc3)ncc2Cl)c1	87	*
2189	C#CCCCCOc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OC	87.1	*
2190	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(C(C)=O)CC4)cc3OC)ncc2SC)c1	87.5	*
2191	O=S(=O)(Nc1nccs1)c1ccc(Nc2nncc3ccccc23)cc1	88	*
2192	CC(C)n1nc(-c2ccc3cc(O)ccc3c2)c2c(N)ncnc21	88	*
2193	Fc1ccc(Nc2ncnc3ccc(C#CCN4CCCCC4)cc23)cc1Cl	88.7	*
2194	CN1CCN(C/C=C/C(=O)N2CCc3c(sc4ncnc(N[C@H](CO)c5ccccc5)c34)C2)CC1	89	*
2195	CCC(=O)ON[C@H](CS(C)(=O)=O)c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	89.6	*
2196	O=C1COc2cc3ncnc(Nc4cccc(Br)c4)c3cc2N1CCCN1CCOCC1	89.6	*
2197	CCOC(=O)C1=C(N)N(c2ccccc2)C2=C(C(=O)CCC2)C1c1cc2ccccc2n2nnnc12	90	7.05
2198	O=C1CSC(N/N=C/c2cc(Br)ccc2O)=N1	90	7.05
2199	O=C(Nc1cccc2ccccc12)c1ccc(N(CCCl)CCCl)cc1	90	7.05
2200	O=C(NS(=O)(=O)c1ccc(Cl)cc1)c1cncc(Br)c1	90	7.05
2201	COc1cc2ncc(C#N)c(Nc3cccc(Br)c3)c2cc1NC(=O)C#CCN(C)C	90	7.05
2202	CS(=O)(=O)CCN(Cc1ccccc1)Cc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	90	*
2203	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc5c(ccn5Cc5ccccc5)c4)c3s2)C1)N1CCOCC1	90	*
2204	O=C(Oc1cccc(O)c1)c1cc(NCc2cc(O)ccc2O)ccc1O	90	*
2205	O=C(Oc1ccc2ccccc2c1)c1cc(NCc2cc(O)ccc2O)ccc1O	90	*
2206	Nc1cc2ncnc(Nc3ccc(Br)cc3)c2cn1	90	*
2207	Cn1c(=O)c(-c2c(Cl)cccc2Cl)cc2cnc(Nc3cccc(CO)c3)nc21	90	*
2208	COc1cc2c(Nc3ccc(Cl)cc3F)ncnc2cc1OC/C=C/CN1CCCC1.Cl	90	*

2209	CCOC(=O)c1cn2ncnc(Nc3ccc(F)c(Cl)c3)c2c1CC	90	*
2210	Fc1cccc(Cn2ncc3cc(Nc4ncnn5ccc(CN6CCNCC6)c45)ccc32)c1	90	*
2211	CCCN(C/C=C/C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)CCC	90	*
2212	NCCOCc1ccn2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c12	90	*
2213	COc1ccc(/C=C/C(=O)c2cc(Br)cc3cc(-c4ccc(F)cc4)oc23)cc1	90	*
2214	COc1cc2c(Oc3ccc(NC(=O)c4cc(-c5ccc(C)cc5)ccn4)cc3F)ccnc2cc1OCCCN1CCN(C)CC1	90.05	*
2215	Clc1ccc(-c2nc(Nc3cc(Br)cc4cc(-c5cccc(Cl)c5)oc34)c3cc(Br)ccc3n2)cc1	90.2	*
2216	O=C(Nc1ccccn1)Nc1cc(-c2ccccnc2)ccc1OC(F)(F)F	90.57	*
2217	CCOc1cc2ncnc(NC3=CC(=O)C(OCc4ccccn4)=CC3=O)c2cc1NC(=O)/C=C/CN(C)C	90.8	7.04
2218	CC(=O)Nc1cccc(C#Cc2cncnc2Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)n1	91	*
2219	CS(=O)(=O)CCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(C(F)(F)F)c5)cc4)c3c2)o1	91	*
2220	COCCOc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)cc3)c2cc1NC(=O)/C=C/CN(C)C	91	*
2221	C=CS(=O)(=O)N1CCc2c(sc3ncnc(N[C@H](CO)c4ccccc4)c23)C1	91	*
2222	COC(=O)c1ccc2oc3cnnc(Nc4ccc(C)cc4)c3c2c1	91.2	7.04
2223	O=C(NCCN1CCOCC1)Nc1ccc(-c2cc3c(Nc4ccc(Oc5cccc(C(F)(F)F)c5)c(Cl)c4)ncnc3s2)cc1	91.7	*
2224	CC1(C)[C@@H](O[C@H]2O[C@H](C(=O)O)[C@@H](O)[C@H](O)[C@H]2O[C@@H]2O[C@H](C(=O)O)[C@@H](O)[C@H](O)[C@H]2O)CC[C@@]2(C)[C@H]1CC[C@]1(C)[C@@H]2C(=O)C=C2[C@H]3C[C@@](C)(C(=O)O)CC[C@]3(C)CC[C@]21C	92	*
2225	CCCCC(=O)ON[C@H](CS(C)(=O)=O)c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	92.8	*
2226	c1ccc(CNc2ncnc3oc(-c4ccccc4)cc23)cc1	93	7.03
2227	CS(=O)(=O)CCNCCCCOc1ccc2ncnc(Nc3ccc(S(=O)(=O)c4ccccc4)cc3)c2c1	93	*
2228	CN(C)CCCN(C)C/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	93	*
2229	CCN(CC)CCOc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OC	93	*
2230	c1ccc2c(c1)CCCN2c1ncnc2cc3oc(N4CCCCC4)nc3cc12	93	*
2231	Ic1cccc(Nc2ncnc3cc4c(cc23)OC(CN2CCOCC2)CO4)c1	93.3	*
2232	Ic1cccc(Nc2ncnc3cc4c(cc23)OC(CNCCN2CCOCC2)CO4)c1	93.3	*
2233	O=S(=O)(CCO)c1cc2c(Nc3cccc(Br)c3)ncnc2cn1	93.5	*
2234	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1/C=C/c1ccc(CNCCS(C)(=O)=O)cc1	94	7.03
2235	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCN1CC(OC)C1	94	7.03
2236	CCC(=O)Nc1cc2c(Nc3ccc4c(cnn4Cc4ccccn4)c3)ncnc2cc1OC	94	*
2237	CN(C)c1ccc(Nc2ncnc3cc(-c4ccccc4)sc23)cc1	94	*
2238	COc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(Cl)c(N(C)c2ccc3ccccc3c2)n1	94	*
2239	CC(O)C#Cc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	94.5	*
2240	O=C(Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1)C1CCC2(CC1)OCC1(OO2)C2CC3CC(C2)CC1C3	94.72	*
2241	Cn1cnc(-c2ccc(OC(F)(F)F)c(NC(=O)Nc3ccncc3)c2)c1	94.82	*
2242	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OC[C@@H](O)CN1CCOCC1	95	*
2243	O=c1c(-c2cccc(Cl)c2)coc2cc(O)cc(O)c12	95	*
2244	O=C(C#CCN1CCSCC1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	95	*
2245	Br.Cc1cccc(C(C)Nc2ncnc3[nH]c(-c4ccc(O)cc4)cc23)c1	95	*
2246	CS(=O)(=O)CCNCc1ccc(-c2cc3c(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)ncnc3s2)s1	96	*
2247	Clc1cccc(Nc2[nH]cnc3nc(-c4ccccc4)c(-c4ccccc4)c2-3)c1	96	*
2248	COc1ccc(-c2[nH]nc3ncnc(Nc4cccc(Cl)c4)c23)cc1	96	*
2249	C=C=Cc1cccc(Nc2ncnc3cc(OCCOC)c(OCCOC)cc23)c1	96	*

2250	C=CC(=O)Nc1cccc(-n2c(=O)cc(-c3ccccc3)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	97	*
2251	CC(C)N(CC#CC(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)C(C)C	97	*
2252	O=C(CO)N1CCC[C@@H]1COc1cccc2ncnc(Nc3ccc(OCc4ccccn4)c(Cl)c3)c12	97	*
2253	C=CC(=O)Nc1cccc(-n2c(=O)cc(C)c3cnc(Nc4ccc(N5CC(C)N(C)C(C)C5)cc4OC)nc32)c1	97	*
2254	C=CC(=O)Nc1cc(-n2c(=O)cc(C)c3cnc(Nc4ccc(N5CC(C)N(C)C(C)C5)cc4OC)nc32)cc(C(F)(F)F)c1	97	*
2255	C=CC(=O)Nc1cc(Nc2n[nH]c3cc(-c4cccnc4)ccc23)c(OC)cc1N(C)CCN(C)C	97	*
2256	FC(F)(F)c1cccc(Nc2ncnc3cc(OCCCN4CCOCC4)c4c(c23)OCCO4)c1	97.18	*
2257	O=C(Nc1ccncc1)Nc1cc(-c2cccnc2)ccc1OC(F)(F)F	97.22	*
2258	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1/C=C/c1ccc(CNC2CC2)cc1	98	7.01
2259	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(CC(C)O)CC(C)O	98	7.01
2260	Brc1cccc(Nc2ncnc3ccc(NCc4ccc5c(c4)OCCCO5)cc23)c1	98	7.01
2261	Oc1ccc2ncnc(Nc3ccc(OCc4ccccc4)cc3)c2c1	98	*
2262	C=CC(=O)Nc1cccc(-n2c(=O)cc(C(C)C)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	98	*
2263	CCOc1cc2ncnc(Nc3ccc(OCc4ccccn4)cc3)c2cc1NC(=O)/C=C/CN1CCCC1	98	*
2264	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCN1CCCCC1	98	*
2265	O=C(CN1CCOCC1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	98	*
2266	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(CC(=O)OCCCOc5no[n+]([O-])c5S(=O)(=O)c5ccccc5)CC4)cc3OC)ncc2Cl)c1	99	7.00
2267	CCc1ccc(C(=O)Nc2ccc(CN3CCN(C)CC3)c(C(F)(F)F)c2)cc1NC(=O)c1cnc2[nH]ccc2c1	99	7.00
2268	NC(=O)Nc1ccc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2c1	99	8.69
2269	Cc1c(OCC(F)(F)F)ccnc1COc1cccc(Nc2ncnc3cc4oc(=O)n(CCCN5CCOCC5)c4cc23)c1	99	*
2270	O=C1COc2cc3ncnc(Nc4cccc(Br)c4)c3cc2N1CCCN1CCCCC1	99	*
2271	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1)N1CCCC1	99	*
2272	O=C(Nc1cccc(Nc2ncnc3cc(OCCCN4CCN(CCO)CC4)ccc23)c1)Nc1ccc(Cl)c(C(F)(F)F)c1	99	*
2273	Fc1cc(Br)ccc1Nc1ncnc2cc3c(cc12)OC(CCN(N1CCOCC1)N1CCOCC1)CO3	99	*
2274	COc1cc2ncnc(NCc3ccccc3)c2cc1OCCCCCCC(=O)NO	99.4	7.00
2275	COc1ccc(C2=NN(c3ccccc3)C(c3cccc4ccccc34)C2)cc1	100	7.00
2276	CCOc1cc2ncc(C#N)c(Nc3ccc4c(ccn4Cc4ccccc4)c3)c2cc1NC(=O)/C=C/CN(C)C	100	7.00
2277	CCOc1cc2ncc(C#N)c(Nc3ccc(O[C@H](C)c4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	100	7.00
2278	COc1cc(Nc2ncnc3ccc(-c4ccc(CNCCS(C)(=O)=O)o4)cc23)ccc1OCc1cccc(F)c1	100	*
2279	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCNC(C)(C)C	100	*
2280	CC(C)(C)ONC(=O)c1cc(NCc2cc(O)ccc2O)ccc1O	100	*
2281	CC(=O)Nc1cc2ncnc(NCc3ccccc3)c2cn1	100	*
2282	COc1cc2ncnc(Nc3ccc(O)cc3)c2cc1OC.Cl	100	*
2283	COc1ccc2ncnc(Nc3cc(OC)c(OC)c(OC)c3)c2c1.Cl	100	*
2284	Nc1ccc2c(Nc3ccccc3)ncnc2c1	100	*
2285	COc1cc2ncnc(N(C)c3cccc(Cl)c3)c2cc1OC.Cl	100	*
2286	COc1cc2c(Nc3ccc(Br)cc3F)ncnc2cc1OC[C@H]1CCCN(C)C1	100	*
2287	COc1cc2c(Nc3ccc(Cl)cc3F)ncnc2cc1OC[C@@H]1CCCN(C)C1	100	*
2288	COc1cc2c(Nc3ccc(Cl)cc3F)ncnc2cc1OCCCN1CCOCC1	100	*
2289	COc1cc2c(Nc3cc(O)c(Cl)cc3F)ncnc2cc1OCC1CCN(C)CC1.Cl	100	*
2290	COc1cc2c(Nc3ccc(Cl)cc3F)ncnc2cc1OCCCN1CCCC1.Cl	100	*
2291	COc1cc2c(Nc3ccc(Br)cc3F)ncnc2cc1OC/C=C/CN1CCCC1.Cl	100	*

2292	COCCOc1cc2ncnc(Nc3ccc(Cl)cc3F)c2cc1OC	100	*
2293	COc1cc2c(Nc3ccc(Br)cc3F)ncnc2cc1OCCCN1CCN(C)CC1.Cl	100	*
2294	Cc1ccn2ncnc(Nc3ccc(F)c(Cl)c3)c12	100	*
2295	CN(C)C1CCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)CC1	100	*
2296	CN=NNc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	100	*
2297	Cc1cc2cc(Nc3ncnc4cc(-c5ccccc5)sc34)ccc2[nH]1	100	*
2298	C/C=C\C(=O)Nc1cccc(Nc2ncnc3cc(OC)c(OCCCN4CCOCC4)cc23)c1	100	*
2299	COc1ccc(Nc2ncnc3oc(-c4ccc([N+](=O)[O-])cc4)cc23)cc1O	100	*
2300	OCCN(CCO)N(CCC1COc2cc3ncnc(Nc4cccc(Br)c4)c3cc2O1)N(CCO)CCO	100	*
2301	C=CC(=O)Nc1cc2c(Nc3ccc(OCc4ccccn4)cc3)ncnc2cc1O[C@H]1CCOC1	100.1	*
2302	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(CC(=O)OCCOCCOc5no[n+]([O-])c5S(=O)(=O)c5ccccc5)CC4)cc3OC)ncc2Cl)c1	101	7.00
2303	C=CC(=O)Nc1cc2c(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncnc2cc1OCCOC	102.2	*
2304	COCCOc1cc2ncnc(Nc3ccc(NC(=O)/C=C/CN(C)C)c(C(F)(F)F)c3)c2cc1NC(=O)/C=C/CN(C)C	102.3	*
2305	CC(C)Oc1cc2ncnc(Nc3ccc(Cl)c([N+](=O)[O-])c3)c2c2c1OCCO2	102.6	*
2306	COc1ccc(-c2ccc(OC(F)(F)F)c(NC(=O)Nc3ccncc3)c2)cn1	102.93	*
2307	CS(=O)(=O)CCNCCCOc1ccc2ncnc(Nc3ccc(OCc4ccccc4)cc3)c2c1	104	*
2308	CO/N=C/c1c(N)ncnc1Nc1ccc2c(cnn2Cc2ccc(F)cc2)c1	104	*
2309	C=CC(=O)Nc1cc2c(Nc3ccc(Cl)c(C(F)(F)F)c3)ncnc2cc1O[C@H]1CCOC1	104.7	*
2310	Nc1cccc2c(Nc3cccc(Br)c3)ncnc12	105	*
2311	CCCCOc1cc2ncnc(Nc3cccc(Br)c3)c2cc1OCCCC	105	*
2312	C/C=C\C(=O)Nc1ccccc1Nc1ncnc2cc(OC)c(OCCCN3CCOCC3)cc12	105	*
2313	COc1ccc(-c2cc3c(N[C@H](C)c4ccccc4OC)ncnc3[nH]2)cc1	105	*
2314	COc1cc2ncnc(Nc3cc(Cl)ccc3F)c2cc1OC1CCN(C)CC1	106	*
2315	CCCCCCOc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OC	106	*
2316	O=C(/C=C/CN1CCCCC1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	106	*
2317	C=CC(=O)Nc1cc(Nc2ncc(F)c(Nc3ccccc3P(C)(C)=O)n2)c(OC)cc1N(C)CCN(C)C	106	*
2318	C=C(CN1CCOCC1)C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	107	*
2319	CC(=O)Nc1cccc(Oc2cc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncn2)c1	108	6.97
2320	COc1ccccc1-c1cc2c(NCc3ccncc3)ncnc2s1	108	*
2321	C=CC(=O)Nc1cc(Nc2nccc(NC(=O)c3ccc(C(F)(F)F)cc3)n2)c(OC)cc1N(C)CCN(C)C	108.7	*
2322	Fc1cccc(COc2ccc(Nc3ncnc4sc(C#CC5CCCN5)cc34)cc2Cl)c1	109	*
2323	Fc1cccc(COc2ccc(Nc3ncnc4cc(C#C[C@@H]5CCCN5)sc34)cc2Cl)c1	109	*
2324	N#CCCSc1nc(-c2ccc(F)cc2)c(-c2ccnc(Nc3ccccc3)c2)[nH]1	109	*
2325	Fc1cccc(COc2ccc(Nc3ncnc4sc(C#C[C@H]5CCCN5)cc34)cc2Cl)c1	109	*
2326	O=C(/C=C/CN1CC[S+]([O-])CC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	109.4	*
2327	Clc1ccc(C2=NN(c3ccccc3)C(c3ccc4ccccc4c3)C2)cc1	110	6.96
2328	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccc(F)cc4F)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	110	6.96
2329	CS(=O)(=O)Nc1cccc(C#Cc2cncnc2Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1	110	*
2330	COC(=O)C1=Cc2c(ncnc2Nc2ccc(Oc3cccc(C(F)(F)F)c3)c(Cl)c2)NCC1	110	*
2331	O=C(Oc1cccc2ccccc12)c1cc(NCc2cc(O)ccc2O)ccc1O	110	*
2332	Cc1ccc(Nc2[nH]cnc3nc4c(c2-3)CCCC4)cc1	110	*
2333	O=C(CO)NC1CCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)CC1	110	*

2334	Fc1cccc(Cn2ncc3cc(Nc4ncnn5ccc(CNC6CCNCC6)c45)ccc32)c1	110	*
2335	CN(CCO)Cc1ccn2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c12	110	*
2336	NS(=O)(=O)c1ccc(-n2c(SCC(=O)Nc3cnc4ccccc4c3)nc3cc4ccccc4cc3c2=O)cc1	110	*
2337	COc1cc2c(Nc3ccc(NC(=O)c4ccccc4)cc3)ncnc2cc1OCCCN1CCOCC1	110	*
2338	CN(CO)/N=N/c1ccc2ncnc(Nc3cccc(Br)c3)c2c1	110	*
2339	Clc1cc(Nc2ncnc3cc[nH]c23)ccc1Oc1ccccc1	110	*
2340	OCCn1ccc2ncnc(Nc3ccc(Oc4cccc(OC(F)(F)F)c4)c(Cl)c3)c21	110	*
2341	CCCCCCC(=O)ON[C@H](CS(C)(=O)=O)c1ccc(-c2ccc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3c2)o1	110.2	*
2342	c1ccc(Oc2ccc(Nc3ncnc4[nH]ccc34)cc2)cc1	110.97	*
2343	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4cccc(C)c4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	111	6.95
2344	C=CC(=O)Nc1cccc(-n2c(=O)n(CC)c(=O)c3cnc(Nc4ccc(N5CCC(N(C)C)CC5)cc4OC)nc32)c1	111	*
2345	Fc1ccc(-c2nc(Nc3cc(Br)cc4cc(-c5ccccc5)oc34)c3cc(Br)ccc3n2)cc1	111.3	*
2346	O=C(Nc1ccc(-c2cc3c(Nc4ccc(Oc5cccc(C(F)(F)F)c5)c(Cl)c4)ncnc3s2)cc1)NC1CC1	112	*
2347	COc1cc2c(Nc3ccc(Br)cc3F)ncnc2cc1OCC1CCN(C)CC1	112.4	6.95
2348	Fc1c(NC(=S)Nc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)cccc1C(F)(F)F	112.4	*
2349	COc1cc2ncnc(Nc3cc(Br)cc(Br)c3)c2cc1OC	113	*
2350	Nc1c(-c2ccc(F)cc2)c(-c2ccncc2)nn1-c1c(Cl)cc(Cl)cc1Cl	113	*
2351	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1/C=C/C(=O)NCCN1CCOCC1	114	6.94
2352	COCCN1CCC(Oc2cc3c(Nc4cc(Cl)ccc4F)ncnc3cc2OC)CC1	114	*
2353	C=CC(=O)Nc1cccc(-n2c(=O)cc(CC)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	114	*
2354	OCCCC#Cc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	114.2	*
2355	CN(C)C/C=C/C(=O)Nc1cccc(-n2c(=O)cnc3cnc(Nc4ccccc4)nc32)c1	115	6.94
2356	Fc1cccc(COc2ccc(Nc3ncnc4sc(-c5ccc[nH]5)cc34)cc2Cl)c1	115	*
2357	CCO[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1	115	*
2358	CN1CCC=C(C(=O)Nc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)C1	115	*
2359	C=CC(=O)Nc1cc2c(Nc3ccc(NC(=O)C=C)c(C(F)(F)F)c3)ncnc2cc1OCCOC	115.1	*
2360	O=C1COc2cc3ncnc(Nc4cccc(Cl)c4)c3cc2N1CCCN1CCCCC1	115.9	*
2361	CCC(=O)Nc1cc2c(Nc3ccc(OCc4ccccn4)cc3)ncnc2cc1OC	116	*
2362	Cc1nc(Nc2cccc(Br)c2)c2cc(NCCN3CCOCC3)ncc2n1	117	*
2363	Fc1ccc(Nc2ncnn3cccc23)cc1Cl	118	*
2364	C=CC(=O)Nc1cccc(-n2c(=O)n(C(C)C)c(=O)c3cnc(Nc4ccc(N5CCN(C)CC5)c(OC)c4)nc32)c1	119	*
2365	COc1ccc(C2=NN(c3ccccc3)C(c3ccc4ccccc4c3)C2)cc1	120	6.92
2366	COc1ccc(Oc2nc3ccc(C)cc3cc2/C=N/NC(=O)Cn2c([N+](=O)[O-])cnc2C)cc1	120	6.92
2367	CNc1ncc(C(=O)Nc2cc(C(=O)Nc3ccc(CN4CCN(C)CC4)c(C(F)(F)F)c3)ccc2C)cn1	120	6.92
2368	Cc1ccc(C2=NN(C3=NC(=O)CS3)C(c3ccc4ccccc4c3)C2)cc1C	120	6.92
2369	Oc1ccc(CN(Cc2cccc(Br)c2O)C(=S)Nc2ccccc2)cc1	120	6.92
2370	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1/C=C/c1ccc(CN2CCOCC2)cc1	120	6.92
2371	O=C(/C=C/c1cccc([N+](=O)[O-])c1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	120	6.92
2372	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cscn5)c(Cl)c4)c3s2)C1)N1CCOCC1	120	6.92
2373	CC(c1cccc(F)c1)n1ncc2cc(Nc3ncnc4cc(C#C[C@@H]5C[C@@H](OC(=O)N6CCOCC6)CN5)sc34)ccc21	120	6.92
2374	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN(CCN(C)C)[C@@H](C)C(N)=O	120	*
2375	O=c1oc2cc3ncnc(Nc4ccc5[nH]ncc5c4)c3cc2n1CCCN1CCOCC1	120	*
2376	C=CC(=O)Nc1cccc(-n2c(=O)cc(C3CC3)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	120	*

2377	Brc1cccc(Nc2ncnc3cc4c(cc23)Oc2ccccc2O4)c1	120	*
2378	CS(=O)(=O)N1CCC[C@@H]1C#Cc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2s1	120	*
2379	CN(C)c1ccc2ncncc2c1	120	*
2380	Nc1cc2ncnc(Nc3cccc(Cl)c3)c2cn1	120	*
2381	COc1ccc2c(Nc3ccccc3)ncnc2c1	120	*
2382	CCc1c(C(N)=O)cn2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c12	120	*
2383	CCOC(=O)c1cc2c(Nc3ccc4c(cnn4Cc4ccccc4)c3)ncnn2c1	120	*
2384	OCc1ccn2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c12	120	*
2385	C[C@H](c1ccccc1)n1ncc2cc(Nc3ncnn4ccc(COC[C@@H]5CNCCO5)c34)ccc21	120	*
2386	S=C(Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1)Nc1ncc(Cl)s1	120	*
2387	Cc1nnc(NC(=S)Nc2ccc3ncnc(Nc4cccc(Cl)c4)c3c2)s1	120	*
2388	N#CC1=C(c2ccccc2)Nc2c(c(-c3cccs3)nn2-c2ccccc2)C12C(=O)Nc1ccc(Br)cc12	120	*
2389	Nc1ccc(C(=O)Nc2cccc(Cl)c2)c(O)c1	120	*
2390	CN1CCN(N(CCC2COc3cc4ncnc(Nc5ccc(Br)cc5F)c4cc3O2)N2CCN(C)CC2)CC1	120	*
2391	CCN(CC)N(CCC1COc2cc3ncnc(Nc4ccc(Br)cc4F)c3cc2O1)N(CC)CC	120	*
2392	OCCC1COc2cc3ncnc(Nc4ccc(Br)cc4F)c3cc2O1	120	*
2393	CN(CCN(CCN1CCOCC1)CCN(C)/N=N/c1ccc2ncnc(Nc3cccc(Br)c3)c2c1)/N=N/c1ccc2ncnc(Nc3cccc(Br)c3)c2c1	120	*
2394	Cc1nc(Nc2ncc(C(=O)Nc3c(C)cccc3Cl)s2)cc(N2CCN(CCOC(=O)CCC(=O)OCCN(C)Cc3ccc(C(=O)Nc4ccc5ncnc(Nc6cccc(Cl)c6)c5c4)cc3)CC2)n1	120	*
2395	O=C(/C=C/c1ccc(OC(F)(F)F)cc1)c1cc(Br)cc2cc(-c3cccc(F)c3)oc12	120	*
2396	Nc1c(Cl)cccc1Nc1ncnc2ccncc12	120.23	*
2397	COc1ccc2ncnc(Nc3ccccc3)c2c1.Cl	120.23	*
2398	CCNCc1ccc(-c2cc3c(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)ncnc3s2)[nH]1	121	*
2399	C=CC(=O)Nc1cccc(-n2c(=O)n(C(C)C)c(=O)c3cnc(Nc4ccc(N(C)CCN(C)C)cc4OC)nc32)c1	121	*
2400	O=C(Nc1nccs1)Nc1cc(-c2cccnc2)ccc1OC(F)(F)F	121.09	*
2401	C=CC(=O)Nc1cc2c(Nc3ccc(Br)cc3F)ncnc2cc1O[C@H]1CCOC1	121.1	*
2402	CCOc1cc2ncnc(Nc3ccc4c(ccn4S(=O)(=O)c4ccccc4)c3)c2cc1NC(=O)/C=C/CN1CCOCC1	122	*
2403	Fc1cc(Br)ccc1Nc1ncnc2cc3c(cc12)OC(CCN(N1CCCCC1)N1CCCCC1)CO3	122	*
2404	Fc1ccc(-c2nc(Nc3cc(Br)cc4cc(-c5cccc(F)c5)oc34)c3cc(Br)ccc3n2)cc1	122.5	*
2405	CN1CCN(C/C=C/C(=O)Nc2cc3c(Nc4ccc(F)c(Cl)c4)ncnc3s2)CC1	124	*
2406	Fc1cc2c(Nc3cccc(Br)c3)ncnc2cn1	124	*
2407	O=C(CO)NCCn1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21	124	*
2408	CCOc1cc2ncc(C#N)c(Nc3ccc(Sc4nc(-c5ccccc5)cs4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	125	6.90
2409	CCNC(=O)O[C@@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1	125	*
2410	N#CC(C#N)=C(N)/C(C#N)=C/c1ccc(O)cc1	125	*
2411	COc1ccc(OC)c(Nc2cc(NCCc3cccs3)ncn2)c1	125	*
2412	C=CC(=O)Nc1cc(Nc2nccc(NC(=O)c3ccc(C(F)(F)F)cc3)n2)c(OC)cc1N1CCC(C(N)=O)CC1	125.1	*
2413	Brc1ccc(Nc2ncnc3[nH]ccc23)cc1	125.33	*
2414	COc1cc2ncnc(N[C@@H](C)c3ccc(F)cc3)c2cc1OCCCCCCC(=O)NO	125.6	6.90
2415	Fc1ccc(-c2cc3cc(Br)cc(Nc4nc(-c5ccc(Cl)cc5)nc5ccc(Br)cc45)c3o2)cc1	125.7	*
2416	COc1cc2ncnc(Nc3cccc(SC)c3)c2cc1OC	126.7	*
2417	COc1cc2ncnc(Nc3cccc(-c4ccccc4)c3)c2cc1OC	126.7	*

2418	C#Cc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	126.9	*
2419	CCC(=O)Nc1cc2c(Nc3ccc4c(ccn4S(=O)(=O)c4ccccc4)c3)ncnc2cc1OC	127	*
2420	CN1CCN(c2ccc(Nc3nc(Nc4ccc5[nH]ccc5c4)c4cn[nH]c4n3)cc2)CC1	127	*
2421	C=CC(=O)Nc1cc(Nc2nccc(NC(=O)c3ccccc3)n2)c(OC)cc1N(C)C	127.2	*
2422	O=C(Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1)C1CCC2(CC1)OCC1(O2)C2CC3CC(C2)CC1C3	127.8	*
2423	COc1cc2ncnc(Nc3ccccc3Br)c2cc1OC	128	*
2424	C=CC(=O)Nc1cc(Nc2nccc(NC(=O)c3ccc(OC)c(OC)c3)n2)c(OC)cc1N1CCC(C(N)=O)CC1	128	*
2425	CCOC(=O)/C=C/C(=O)Nc1cccc(Oc2cc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncn2)c1	129	6.89
2426	COc1cc(N2CCN(C)CC2)ccc1Nc1ncc(Cl)c(Oc2cccc(COc3no[n+]([O-])c3S(=O)(=O)c3ccccc3)c2)n1	130	6.89
2427	CCNc1ncc(C(=O)Nc2cc(C(=O)Nc3ccc(CN4CCN(C)CC4)c(C(F)(F)F)c3)ccc2C)cn1	130	6.89
2428	Cc1ccc(C2=NN(C(N)=S)C(c3ccc(O)cc3)C2)cc1C	130	6.89
2429	COc1cc2ncc(C#N)c(Nc3ccc4c(cnn4Cc4ccccc4)c3)c2cc1NC(=O)/C=C/CN(C)C	130	6.89
2430	CCCN(CC#CC(=O)Nc1ccc2ncc(C#N)c(Nc3cccc(Br)c3)c2c1)CCC	130	6.89
2431	CCOC(=O)CCCn1c(=O)oc2cc3ncnc(Nc4ccc5[nH]ncc5c4)c3cc21	130	*
2432	CCN(CC)[C@@](C)(CCc1ncnc2cc(OC)c(OC)cc12)Cc1ccccc1	130	*
2433	COCCN1CCC[C@@H]1C#Cc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2s1	130	*
2434	O=C(OCCc1ccccc1)c1cc(NCc2cc(O)ccc2O)ccc1O	130	*
2435	COc1cccc(Nc2ncnc3cc(N)ncc23)c1	130	*
2436	Clc1cccc(Nc2[nH]nc3ncnc(Nc4cccc(Br)c4)c23)c1	130	*
2437	Cc1cccc(Nc2[nH]cnc3nnc(Nc4cccc(Cl)c4)c2-3)c1	130	*
2438	CN1CCCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)CC1	130	*
2439	CC1CNCCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)C1	130	*
2440	COc1cc2c(Nc3ccc(NC(=O)c4ccccc4)cc3)ncnc2cc1OCCCN1CCN(C)CC1	130	*
2441	Cc1cc(NS(=O)(=O)c2ccc(Nc3nncc4ccccc34)cc2)no1	130	*
2442	Fc1cccc(Cn2ncc3cc(Nc4ncnn5ccc(COCC6CCNCC6)c45)ccc32)c1	130	*
2443	FC(F)(F)c1nnc(NC(=S)Nc2ccc3ncnc(Nc4cccc(Cl)c4)c3c2)s1	130	*
2444	CC(=O)OCN(C)/N=N/c1ccc2ncnc(Nc3cccc(Br)c3)c2c1	130	*
2445	CCN(CC)C(C)(CCc1ncnc2cc(OC)c(OC)cc12)Cc1ccccc1	130	*
2446	COc1cc2ncnc(-c3c[nH]c4ccc(Br)cc34)c2cc1OC	131	*
2447	COC[C@@H]1CCCN1C/C=C/C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	131	*
2448	COc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(F)c(Nc2ccc3ccccc3c2)n1	131	*
2449	O=C(Nc1cc(N2CCOCC2)ncn1)c1ccc(F)cc1	131	*
2450	COc1cc(NC(=O)Nc2ccncc2)cc(-c2cccnc2)c1OC	131.09	*
2451	COc1cccc(Nc2ncnc3ccncc23)c1N	131.83	*
2452	COc1cc2ncnc(Nc3ccc(Oc4ccccc4)cc3)c2cc1NC(=O)/C=C/CN1CCCCC1	132	*
2453	Cl.Cn1c2ccccc2c2ncnc(Nc3cccc(Br)c3)c21	132	*
2454	O=C1Nc2cc3c(-c4ccccc4)c(-c4ccccc4)n(-c4ccc(Cl)cc4)c(=O)c3cc2C(c2ccccc2)N1	132	*
2455	COC(=O)c1ccc2oc3cnnc(Nc4ccccc4C)c3c2c1	132.5	6.88
2456	Fc1cccc(-c2cc3cc(Br)cc(Nc4nc(-c5ccc(Cl)cc5)nc5ccc(Br)cc45)c3o2)c1	132.9	*
2457	S=C(Nc1ccc(Cl)c(Cl)c1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	133.1	*
2458	CN(C)C/C=C/C(=O)Nc1cc2c(Nc3ccc(OCc4cccc(F)c4)cc3)ncnc2cc1O[C@H]1CCOC1	133.9	*
2459	C=CC(=O)Nc1cc(Nc2nccc(NC(=O)c3cccc4ccccc34)n2)c(OC)cc1N1CCN(C)CC1	133.9	*
2460	C=CC(=O)Nc1cc2c(Nc3ccc(OCc4ccccn4)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	134.9	*

2461	CCC(=O)Nc1cc2c(NCc3ccccc3)ncnc2cc1OC	136	*
2462	CCN1CCC(Nc2ccc3c(c2)C(=C(c2ccc(Cl)cc2)c2ncc[nH]2)C(=O)N3)CC1	137	*
2463	FC(F)(F)c1csc(NC(=S)Nc2ccc3ncnc(Nc4cccc(Cl)c4)c3c2)n1	137	*
2464	C=CC(=O)Nc1cccc(-n2c(=O)n(C)c(=O)c3cnc(Nc4ccc(N5CCC(N(C)C)CC5)cc4OC)nc32)c1	137	*
2465	O=C1COc2cc3ncnc(Nc4ccc(F)c(Cl)c4)c3cc2N1CCCN1CCCCC1	137.9	*
2466	CS(=O)(=O)CCNCc1ccc(-c2cc3c(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)ncnc3s2)[nH]1	138	*
2467	CCN(CC)CCN(C)C/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	139	*
2468	C#Cc1cccc(Nc2ncnc3cc4c(cc23)N(CCCN2CCOCC2)C(=O)CO4)c1	139	*
2469	COc1cccc2ncnc(Nc3cccc(Br)c3)c12	139	*
2470	Clc1ccc(C2=NN(c3ccccc3)C(c3cccc4ccccc34)C2)cc1Cl	140	6.85
2471	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4cc(F)cc(F)c4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	140	6.85
2472	O=c1oc2cc3ncnc(Nc4ccc(OCc5ccccc5)cc4)c3cc2n1CCCN1CCOCC1	140	*
2473	CCOC(=O)CCCn1c(=O)oc2cc3ncnc(Nc4ccc(F)c(F)c4)c3cc21	140	*
2474	CCOc1cc2ncnc(/C=C/CCCc3ccccc3)c2cc1OCC	140	*
2475	COC(=O)N1CCC[C@@H]1C#Cc1cc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2s1	140	*
2476	CN1CCC(Oc2cccc3ncnc(Nc4ccc(OCc5ccccn5)c(Cl)c4)c23)CC1	140	*
2477	NC(=O)C1CCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)CC1	140	*
2478	NS(=O)(=O)c1ccc(Nc2nncc3ccccc23)cc1	140	*
2479	NC(=O)COCc1ccn2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c12	140	*
2480	Cc1cc2cc(Nc3ccnc4cc(-c5ccc(CN(C)CCO)cc5)sc34)ccc2[nH]1	140	*
2481	CC(C)C[C@@H](NC(=O)OC(C)(C)C)C(=O)Nc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	140	*
2482	COc1cc2ncnc(Oc3cccc(NC(=S)Nc4cccc(C(F)(F)F)c4)c3)c2cc1OC	140	*
2483	COc1ccc(-n2c(-c3ccccc3)c(-c3ccccc3)c3cc4c(cc3c2=O)CNC(=O)N4)cc1	140	*
2484	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CNC1CC(F)(F)C1	141	*
2485	CCOC(=O)O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)c3s2)C1	141	*
2486	Cc1cccc(NC(=O)c2ccc(OCCCN3CCOCC3)cc2O)c1	142.1	*
2487	C=CC(=O)Nc1ccccc1Nc1nc(Nc2ccc(OCC(=O)N3CCOCC3)cc2)ncc1Cl	142.9	*
2488	C=CC(=O)Nc1cccc(NC(=O)Nc2ccnc(Nc3ccc(N4CCN(C)CC4)cc3)n2)c1	143	*
2489	CCC(=O)N1CC[C@H](N2C(=O)N(c3cccc(Cl)c3)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	144	6.84
2490	S=C(Nc1cc(Cl)cc(Cl)c1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	146.3	*
2491	Nc1nc(Nc2cccc(Br)c2)c2c(n1)[nH]c1ccccc12	147	*
2492	CN(C)C/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(C#N)c3)ncnc2cc1O[C@H]1CCOC1	147.4	*
2493	C=CC(=O)Nc1cc(Nc2nccc(NC(=O)c3cccc(OC)c3)n2)c(OC)cc1N1CCN(C)CC1	147.4	*
2494	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5CCN(C(C)=O)CC5)c(C)c4)nc32)C1	148	6.83
2495	COc1cc2ncnc(Nc3ccc(Cc4ccccn4)cc3)c2cc1NC(=O)/C=C/CN1CCCC1	148	*
2496	C=CC(=O)Nc1cc(Nc2nccc(NC(=O)c3ccc(OC)c(OC)c3)n2)c(OC)cc1N(C)C	148.8	*
2497	CN(C)C/C=C/C(=O)N1CCc2c(sc3ncnc(N[C@H](CO)Cc4ccccc4)c23)C1	149	*
2498	C=CC(=O)Nc1cc(Nc2nccc(Nc3ccccc3P(C)(C)=O)n2)c(OC)cc1N(C)CCN(C)C	149	*
2499	COc1cc2c(cc1OC)Nc1ncnc(N[C@H](C)c3ccccc3)c1NC2	150	6.82
2500	COCC1CCCN1CC#CC(=O)Nc1ccc2ncc(C#N)c(Nc3cccc(Br)c3)c2c1	150	6.82
2501	COC[C@@H]1CCCN1CC#CC(=O)Nc1ccc2ncc(C#N)c(Nc3cccc(Br)c3)c2c1	150	6.82
2502	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc5c(ccn5S(=O)(=O)c5ccsc5)c4)c3s2)C1)N1CCOCC1	150	6.82
2503	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN[C@H](C)C(N)=O	150	*

2504	C[C@@H](Nc1ncnc2sc(Br)cc12)c1ccc(F)cc1	150	*
2505	Cc1ccc(S(=O)(=O)N2CCOc3cc4ncnc(Nc5cccc(Br)c5)c4cc3OCC2)cc1	150	*
2506	CN1CCN(CCCNc2ncc3cc(-c4c(Cl)cccc4Cl)c(NC(=O)NC(C)(C)C)nc3n2)CC1	150	*
2507	Cn1c(=O)c(-c2c(Cl)cccc2Cl)cc2cnc(Nc3cccc(O)c3)nc21	150	*
2508	NC1CCN(Cc2ccn3ncnc(Nc4ccc(OCc5cccnc5)c(Cl)c4)c23)CC1	150	*
2509	COc1cc2c(Nc3ccc(NC(=O)c4cccc(Cl)c4)cc3)ncnc2cc1OCCCN1CCN(C)CC1	150	*
2510	Cc1nnc(-c2cn3ncnc(Nc4cnc5[nH]ccc5c4)c3c2C(C)C)o1	150	*
2511	CN(C)C/C=C/C(=O)Nc1ccc2c(C#N)cnc(Nc3cccc(Br)c3)c2c1	150	*
2512	Nc1nccc(-c2c(-c3ccc(F)cc3)ncn2C2CCCCC2)n1	150	*
2513	N#CC1=C(c2ccccc2)Nc2c(c(-c3cccs3)nn2-c2ccccc2)C12C(=O)Nc1ccc(Cl)cc12	150	*
2514	CN(CCN(CCN1CCOCC1)CCN(C)/N=N/c1ccc2ncnc(Nc3cccc(Cl)c3)c2c1)/N=N/c1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	150	*
2515	N#Cc1cccc(Oc2ccc(Nc3ncnc4cc[nH]c34)cc2Cl)c1	150	*
2516	Fc1cccc(Oc2ccc(Nc3ncnc4cc[nH]c34)cc2Cl)c1	150	*
2517	FC(F)(F)c1ccccc1Oc1ccc(Nc2ncnc3cc[nH]c23)cc1Cl	150	*
2518	COc1ccc(-c2cc3cc(Br)cc(C(=O)/C=C/c4ccc(F)cc4)c3o2)cc1	150	*
2519	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN1CCCC1COC	151	6.82
2520	Cc1cc2c(Nc3ccc(F)c(Cl)c3)ncnn2c1	151	*
2521	C=CC(=O)Nc1cc(Nc2ncc(Cl)c(Nc3ccccc3S(=O)(=O)C(C)C)n2)c(OC)cc1N(C)CCN(C)C	151	*
2522	CC(C)(O)C#Cc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	151.5	*
2523	COc1cc2ncnc(N(C)c3cccc(Br)c3)c2cc1OC	152	*
2524	O=C1NCc2cc3c(=O)n(-c4ccccc4)c(-c4ccccc4)c(-c4ccccc4)c3cc2N1	152	*
2525	C=CC(=O)Nc1cc(Nc2nccc(NC(=O)c3ccc(C(F)(F)F)cc3)n2)c(OC)cc1N1CCN(C)CC1	152.2	*
2526	CCC(=O)N1CC[C@H](N2C(=O)N(c3ccc(OC)cc3)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	153	6.82
2527	COc1ccccc1-c1cc2c(N[C@H](C)c3ccccn3)ncnc2s1	153	*
2528	C=CC(=O)Nc1cc(Nc2nccc(NC(=O)c3cccc(OC)c3)n2)c(OC)cc1N(C)CCN(C)C	153.5	*
2529	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(C(=O)CC)CC4)cc3OC)ncc2SC)c1	153.7	*
2530	CCN1CCN(C(=O)/C(F)=C/c2c(C)ncnc2Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)CC1	156	6.81
2531	CC(Nc1ncnc2sc(Br)cc12)c1ccccc1	156	*
2532	C=CC(=O)Nc1cc(Nc2nccc(NC(=O)c3ccccc3)n2)c(OC)cc1N1CCN(C)CC1	156.5	*
2533	C=CC(=O)Nc1cc(Nc2nccc(NC(=O)c3ccc(OC)c(OC)c3)n2)c(OC)cc1N1CCN(C)CC1	157.5	*
2534	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCN1CC2(C1)CS(=O)(=O)C2	158	6.80
2535	Cl.O=[N+]([O-])c1cccc2c1sc1c(Nc3cccc(Br)c3)ncnc12	158	*
2536	CC(C)n1nc(-c2ccc(Cl)c(O)c2)c2c(N)ncnc21	158	*
2537	C=CC(=O)Nc1cccc(NC(=O)Nc2ccnc(Nc3ccc(N4CCN(CCF)CC4)cc3OC)n2)c1	158	*
2538	COC(=O)c1ccc2oc3cnnc(NCc4ccccc4)c3c2c1	158.5	6.80
2539	CN(C)c1cc2ncnc(Nc3cccc(Br)c3)c2cc1N	159	*
2540	COCCOc1cc2ncnc(Nc3cccc(OC)c3)c2c2c1OCCO2	159.9	*
2541	COc1ccc(C2=NN(C(N)=S)C(c3cccc4ccccc34)C2)cc1	160	6.80
2542	CC(C)c1ccc(C(=O)Nc2ccc(CN3CCN(C)CC3)c(C(F)(F)F)c2)cc1NC(=O)c1cnc2[nH]ccc2c1	160	6.80
2543	O=C(CBr)OCCn1c(=O)oc2cc3ncnc(Nc4ccc(Oc5cccc(C(F)(F)F)c5)c(Cl)c4)c3cc21	160	6.80
2544	CS(=O)(=O)CCNCc1ccc(-c2ccc3ncnc(Nc4ccc(OCc5ccccc5)c(C(F)(F)F)c4)c3c2)o1	160	*
2545	CCOC(=O)CCCn1c(=O)oc2cc3ncnc(Nc4ccc(OC(C)C)cc4)c3cc21	160	*

2546	Nc1[nH]cnc2nnc(Nc3cccc(Cl)c3)c1-2	160	*
2547	NCCCCOCc1ccn2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c12	160	*
2548	COc1cc2ncc(C#N)c(Nc3ccc(F)c(C(F)(F)F)c3)c2cc1OC.Cl	160	*
2549	Cc1ccc(Nc2ncnc3cc4c(cc23)N(CCCN2CCOCC2)C(=O)CO4)cc1Cl	162.7	*
2550	CCOc1cc2ncc(C#N)c(Nc3cc(Cl)c(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	163	6.79
2551	CCOc1cc2ncnc(Nc3ccc(OCc4ccccn4)cc3)c2cc1NC(=O)/C=C/CN1CCN(C)CC1	164	*
2552	C=CC(=O)NCc1cn(Cc2cccc(Nc3cc(-c4[nH]c(SC)nc4-c4ccc(F)cc4)ccn3)c2)nn1	164	*
2553	CCOc1cc2ncc(C#N)c(Nc3ccc(OCCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	165	6.78
2554	O=C(NCCN1CCCCC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	165	*
2555	CCN(CCO)CCCOc1ccc2c(Nc3cccc(NC(=O)Nc4ccc(F)c(Cl)c4)c3)ncnc2c1	165	*
2556	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N(NCCN1CCCCC1)NCN1CCCCC1	165	*
2557	Cn1cnc(-c2cc(NC(=O)Nc3ccncc3)cc(C(F)(F)F)c2)c1	165.6	*
2558	C=CC(=O)Nc1cc(-n2c(=O)cc(C)c3cnc(Nc4cnn(C5CCN(C)CC5)c4)nc32)cc(C(F)(F)F)c1	166.2	*
2559	CCOc1cc2ncnc(NC3=CC(=O)C(OCc4ccc(F)c(F)c4)=CC3=O)c2cc1NC(=O)/C=C/CN(C)C	166.7	6.78
2560	C=CC(=O)Nc1cc2c(Nc3ccc(F)c(C#N)c3)ncnc2cc1O[C@H]1CCOC1	167.3	*
2561	N#Cc1cccc(Oc2ccc(Nc3ncnc4cc(OCCCN5CCOCC5)c(NC(=O)c5cc([N+](=O)[O-])ccc5F)cc34)cc2Cl)c1	169	6.77
2562	C=CC(=O)Nc1cccc(-n2c(=O)cc(C)c3cnc(Nc4ccc(N5CCN(C)C(C)C5)cc4OC)nc32)c1	169.2	*
2563	O=C(Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1)C1CCC2(CC1)OCC1(CO2)C2CC3CC(C2)CC1C3	169.4	*
2564	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN1CCC[C@H]1CC(N)=O	170	*
2565	COc1ccccc1-c1cc2c(NCc3cccs3)ncnc2s1	170	*
2566	C=CC(=O)Nc1cccc(-n2c(=O)cc(C)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OCC)nc32)c1	170	*
2567	COc1cc2ncnc(NCc3cccc(C)c3)c2cc1OC	170	*
2568	Cc1[nH]c2ncnc(Nc3cc(Cl)cc(Cl)c3)c2c1C	170	*
2569	COc1cc(O)c2c(=O)c(-c3cccc(Cl)c3)cn(C)c2c1	170	*
2570	Cc1cc(C(=O)N2CCOCC2)[nH]c1/C=C1\C(=O)Nc2ncnc(Nc3ccc(F)c(Cl)c3)c21	170	*
2571	CCc1c(C(=O)OCCCn2ccnc2)cn2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c12	170	*
2572	CN1CCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)CC1	170	*
2573	NC(=O)CN1CCC(n2cc(-c3cccc(O)c3)c3c(N)ncnc32)CC1	170	*
2574	COc1cc(-c2nn(C(C)C)c3ncnc(N)c23)ccc1NC(=O)OC(C)(C)C	170	*
2575	CCNc1cc(Nc2cccc(Cl)c2)ncn1	170	*
2576	O=C(/C=C/c1ccc(F)cc1)c1cc(Br)cc2cc(-c3ccccc3)oc12	170	*
2577	O=C(/C=C/c1ccccc1)c1cc(Br)cc2cc(-c3cccc(Cl)c3)oc12	170	*
2578	O=C(Nc1cc2c(Nc3ccc(OCC4CC4)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1)c1cc([N+](=O)[O-])ccc1F	172	6.76
2579	C=CC(=O)Nc1cc(Nc2ncc(F)c(Nc3ccccc3S(=O)(=O)N(C)C)n2)c(OC)cc1N(C)CCN(C)C	172	*
2580	COc1ccccc1-c1cc2c(Nc3ccccc3)ncnc2s1	173	*
2581	COc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(C#N)c(Nc2ccc3ccccc3c2)n1	173	*
2582	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(C(=O)C(C)C)CC4)cc3OC)ncc2SC)c1	173.6	*
2583	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(CC(=O)OCCCCOc5no[n+]([O-])c5S(=O)(=O)c5ccccc5)CC4)cc3OC)ncc2Cl)c1	174	6.76
2584	CCC(=O)Nc1cc2c(Nc3ccc4c(c3)CCN4Cc3ccccc3)ncnc2cc1OC	175	*
2585	CC(C)n1nc(-c2ccc3[nH]ccc3c2)c2c(N)ncnc21	176	*
2586	c1cc(Nc2ccc3[nH]ccc3c2)nc(Nc2ccc(OCCCCN3CCOCC3)cc2)n1	178	*
2587	CC(=O)Nc1ccc(-c2c(-c3ccccc3)oc3ncnc(N[C@H](CO)c4ccccc4)c23)cc1	179	*

2588	CC(C)n1nc(-c2ccc3c(ccn3C(=O)OC(C)(C)C)c2)c2c(N)ncnc21	179	*
2589	Cc1ccc(Oc2nc3ccc(C)cc3cc2/C=N/NC(=O)Cn2c([N+](=O)[O-])cnc2C)cc1	180	6.74
2590	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(NCc4cccc(Oc5ccccc5)c4)c3s2)C1)N1CCOCC1	180	6.74
2591	O=C(/C=C/CN1CCCC1)Nc1cc2c(Nc3ccc(Oc4ccccc4)cc3)ncnc2cn1	180	*
2592	C=C(CN(C)C)C(=O)c1ccc(OCc2ccccc2)cc1.Cl	180	*
2593	Cc1[nH]c(/C=C2\C(=O)Nc3ncnc(Nc4ccc(F)c(Cl)c4)c32)c(C)c1CCC(=O)O	180	*
2594	C[C@@H](Oc1cccc2ncnc(Nc3ccc4c(cnn4Cc4ccccn4)c3)c12)C(=O)N(C)C	180	*
2595	COc1cc2ncc(C#N)c(Nc3cccc(Cl)c3)c2cc1OC	180	*
2596	c1cc(Nc2nccc(Nc3ccc4[nH]ccc4c3)n2)cc(N2CCOCC2)c1	180	*
2597	C=CC(=O)Nc1cccc(-n2c(=O)n(C)c(=O)c3cnc(Nc4ccc(N5CCN(C(C)=O)CC5)cc4OC)nc32)c1	180	*
2598	C=CC(=O)Nc1cc(Nc2nccc(NC(=O)c3ccccc3)n2)c(OC)cc1N1CCC(C(N)=O)CC1	180.6	*
2599	C=CC(=O)Nc1cc(-n2c(=O)cc(C)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)cc(C(F)(F)F)c1	181.9	*
2600	COc1ccccc1-c1cc2c(NCc3ccccn3)ncnc2s1	183	*
2601	CC[C@@H](Nc1ncnc2sc(Br)cc12)c1ccccc1	183	*
2602	C=CC(=O)Nc1cccc(NC(=O)Nc2ccnc(Nc3ccc(N(CC)CC)cc3OC)n2)c1	183	*
2603	Fc1ccc(-c2nc(SCCN3CCOCC3)[nH]c2-c2ccnc(Nc3ccccc3)c2)cc1	183	*
2604	O=C(CBr)OCCn1c(=O)oc2cc3ncnc(Nc4ccc(N5CCCCC5)c(Cl)c4)c3cc21	184	6.74
2605	Cc1ccc(Nc2ncnc3cc(OC(C)C)c4c(c23)OCCO4)cc1[N+](=O)[O-]	184.5	*
2606	COc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)cc3)c2cc1NC(=O)/C=C/CN(C)C	185	6.73
2607	Cc1ccc(-n2c(-c3ccccc3)c(-c3ccccc3)c3cc4c(cc3c2=O)C(c2ccccc2)NC(=O)N4)cc1	185	*
2608	CC(=O)CCCSc1nc(-c2ccc(F)cc2)c(-c2ccnc(Nc3ccccc3)c2)[nH]1	185	*
2609	OCCC#Cc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	185.8	*
2610	Cc1cccc(Nc2ncnc3cc4c(cc23)N(CCCN2CCOCC2)C(=O)CO4)c1	186.9	*
2611	COc1cc(OC2CCOC2)c2c(Nc3ccc(F)c(Cl)c3)ncnc2c1	187	*
2612	C=CC(=O)Nc1cc(Nc2nccc(NC(=O)c3ccc(OC)c(OC)c3)n2)c(OC)cc1N(C)CCN(C)C	187.2	*
2613	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4nc5ccccc5s4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	188	6.73
2614	CCN(CCO)CCCOc1ccc2c(Nc3cccc(NC(=O)Nc4ccc(Cl)c(C(F)(F)F)c4)c3)ncnc2c1	188	*
2615	O=C(Nc1ccncc1)Nc1cc(-c2cccnc2)cc(C(F)(F)F)c1	189.49	*
2616	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C#Cc1ccc(CN2CCCC2)c(F)c1	190	6.72
2617	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCN1CC2(CCO2)C1	190	6.72
2618	O=C(/C=C/c1cccc([N+](=O)[O-])c1)Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	190	6.72
2619	Cc1ccc(C2=NN(c3nc(-c4ccc(Cl)cc4)cs3)C(c3ccc(Cl)cc3)C2)cc1C	190	6.72
2620	COc1cc2ncc(C#N)c(Nc3cccc(Br)c3)c2cc1OC	190	6.72
2621	C#Cc1cccc(Nc2ncnc3cc4oc(=O)n(CCOC)c4cc23)c1	190	*
2622	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(Oc5ccccn5)c(Cl)c4)c3s2)C1)N1CCOCC1	190	*
2623	Cn1c(=O)c(-c2c(Cl)cccc2Cl)cc2cnc(Nc3cccc(C(=O)O)c3)nc21	190	*
2624	COc1cn2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c2c1CN1CCCNCC1	190	*
2625	NC1CCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5ccccc5)c4)c23)CC1	190	*
2626	COC1CNCCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)C1	190	*
2627	Fc1cccc(Cn2ncc3cc(Nc4ncnn5ccc(COC[C@H]6CCCNC6)c45)ccc32)c1	190	*
2628	CC(C)(N)c1cc(C(=O)N[C@@H]2CCc3ccc(Oc4ccnc5c4CCC(=O)N5)cc3C2)cc(C(F)(F)F)c1	190	*
2629	COc1ccc(C(Nc2ccc(C)cc2)n2c(-c3cc(CCn4c(-c5ccccc5)nc5ccccc5c4=O)ccc3Cl)nc3ccccc32)cc1	190	*
2630	COc1ccc(-c2c3c4cc(OCCN(C)C)c(OCCN(C)C)cc4oc(=O)c3n3ccc4cc(O)c(OC)cc4c23)cc1O.O=C(O)C(F)(F)F	190.6	*

2631	c1ccc(CNc2ncnc3c2sc2ccccc23)cc1	191	*
2632	C[C@@H](CN(C)C(=O)CO)Oc1cccc2ncnc(Nc3ccc(OCc4ccccn4)c(Cl)c3)c12	191	*
2633	COc1cc2c(Nc3ccc(NC(=O)Nc4ccccc4)cc3)ncnc2cc1OCCCN1CCN(C)CC1	194	*
2634	COC[C@@H]1CCCN1C/C=C\C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	194	*
2635	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4cccc(C#N)c4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	195	6.71
2636	C=CC(=O)Nc1cc2c(Nc3ccc(F)c(C#N)c3)ncnc2cc1OCCOC	195.8	*
2637	O=C(Nc1cccc(Cl)c1)c1ccc(OCCCN2CCOCC2)cc1O	195.8	*
2638	COCCCNC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	197	*
2639	COCCCNN(NCCCOC)C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	197	*
2640	C[C@@H](Nc1ncnc2[nH]c(-c3ccccc3O)cc12)c1ccccc1	198	*
2641	Cc1ccc(C2=NN(c3ccccc3)C(c3cccc4ccccc34)C2)cc1	200	6.70
2642	CCOC(=O)C1=C(N)N(c2cccnc2)C2=C(C(=O)CCC2)C1c1cc2cc(OC)ccc2n2nnnc12	200	6.70
2643	COc1cc2c(cc1OC)Nc1ncnc(NCc3ccccc3)c1NC2	200	6.70
2644	Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	200	7.02
2645	CCN(CC)[C@@](C)(C#Cc1ncnc2cc(OC)c(OC)cc12)Cc1ccncc1	200	*
2646	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(C(C)=O)CC4)cc3OC)ncc2C(F)(F)F)c1	200	*
2647	COc1ccc2ncnc(NCc3ccccc3)c2c1	200	*
2648	COc1cc2ncnc(Nc3nccc4ccccc34)c2cc1OC	200	*
2649	Cc1[nH]c2ncnc(Nc3cccc(C#N)c3)c2c1C	200	*
2650	CCn1c(=O)c(-c2c(Cl)cccc2Cl)cc2cnc(Nc3ccccc3)nc21	200	*
2651	CCN(CC)CCNC(=O)c1c(C)[nH]c(/C=C2\C(=O)Nc3ncnc(Nc4ccc(F)c(Cl)c4)c32)c1C	200	*
2652	COc1cc2c(Nc3ccc(Br)cc3F)ncnc2cc1OC[C@@H]1CCCN(C)C1	200	*
2653	COc1cc2c(Nc3ccc(Cl)cc3F)ncnc2cc1OCCN1CCN(C)CC1	200	*
2654	COc1cc2c(Nc3ccc(Br)cc3F)ncnc2cc1OCCC1CCN(C)CC1	200	*
2655	COc1cc2c(Nc3ccc(Br)cc3F)ncnc2cc1OCCC1CCNCC1	200	*
2656	Cc1ccc(Nc2ncnn3cc(C)c(C)c23)cc1O	200	*
2657	CCc1c(C(=O)N(C)C)cn2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c12	200	*
2658	CCOC(=O)c1cn2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c2c1C	200	*
2659	CCOC(=O)c1cn2ncnc(NCc3ccccc3)c2c1CC	200	*
2660	CCOC(=O)c1cn2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c2c1C(C)C	200	*
2661	CS(=O)(=O)CCNC1CCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)CC1	200	*
2662	Fc1ccc(Nc2ncnc3nn4ccccc4c23)cc1Cl	200	*
2663	O[C@@H]1CNCCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)C1	200	*
2664	Cc1ccn2ncnc(Nc3ccc4c(cnn4Cc4ccccn4)c3)c12	200	*
2665	CN=NNc1ccc2ncnc(Nc3cccc(C)c3)c2c1	200	*
2666	CN/N=N/c1ccc2ncnc(Nc3cccc(C)c3)c2c1	200	*
2667	Nc1cccc(-c2nc3c(Nc4cccc(O)c4)ncnc3o2)c1	200	*
2668	Nc1ccc(-c2nc3c(Nc4ccc(O)cc4)ncnc3o2)cc1	200	*
2669	Cl.Nc1ccc(-c2nc3c(Nc4cccc(Cl)c4)ncnc3o2)cc1	200	*
2670	CCN(CC)C(C)(C#Cc1ncnc2cc(OC)c(OC)cc12)Cc1ccncc1	200	*
2671	CN(c1ccc2[nH]ccc2c1)c1ccnc(Nc2ccc(OCCCCN3CCOCC3)cc2)n1	200	*
2672	COCCOc1cc2ncnc(Nc3ccc(F)cc3)c2c2c1OCCO2	200.3	*
2673	COc1cc(N2CCN(C)CC2)ccc1Nc1ncc(Cl)c(Oc2cccc(NC(=O)CCN3CCN(CCOc4no[n+]([O-])c4S(=O)(=O)c4ccc	201	6.70

	cc4)CC3)c2)n1		
2674	CN(C)C/C=C/C(=O)Nc1cc2c(Nc3ccc(Oc4ccccc4)cc3)ncnc2cn1	201	*
2675	Nc1cccc(-c2c(-c3ccccc3)oc3ncnc(N[C@H](CO)c4ccccc4)c23)c1	203	*
2676	CN(C)CCn1cnc2c(Cl)c3c(Nc4cccc(Br)c4)ncnc3cc21	203	*
2677	O=C(/C=C/CN1CCSCC1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	203	*
2678	C=CC(=O)Nc1cc(Nc2ncc(Cl)c(Nc3ccccc3S(=O)(=O)N(C)C)n2)c(OC)cc1N(C)CCN(C)C	204	*
2679	CCC(=O)Nc1cc2c(Nc3ccc(Cc4ccccn4)cc3)ncnc2cc1OC	205	*
2680	COc1cc2ncnc(Nc3cccc(C#CC(C)(C)O)c3)c2cc1OC	205.8	*
2681	CC(C)n1nc(-c2ccc3c(N)n[nH]c3c2)c2c(N)ncnc21	207	*
2682	C=CC(=O)Nc1cc(C)cc(-n2c(=O)cc(C)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	208.4	*
2683	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5CCCN(C)CC5)c(C)c4)nc32)C1	209	6.68
2684	COc1cc2ncnc(-c3c[nH]c4cc(F)c(Cl)cc34)c2cc1OC	209	*
2685	NC(=S)N1N=C(c2ccc(Cl)c(Cl)c2)CC1c1cccc2ccccc12	210	6.68
2686	Cc1ncc([N+](=O)[O-])n1C/C(=N/NC(=O)c1ccc(O)cc1)c1ccc(Br)cc1	210	6.68
2687	COc1cc2ncc(C#N)c(Nc3ccc(NCNc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	210	6.68
2688	C=CC(=O)Nc1cccc(-n2c(=O)cc(N(C)C)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	210	*
2689	C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4ccccc34)n2)c(OC)cc1N(C)CCN(C)C	210	*
2690	CN1CCN(CCCCNc2ncc3cc(-c4c(Cl)cccc4Cl)c(=O)n(C)c3n2)CC1	210	*
2691	Cc1cc(/C=C2\C(=O)Nc3ncnc(Nc4ccc(F)c(Cl)c4)c32)[nH]c1C(=O)N1CCN(C)CC1	210	*
2692	CCc1c(NC(=O)OCc2ccccc2)cn2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c12	210	*
2693	CS(=O)(=O)N1CCCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)CC1	210	*
2694	Fc1cccc(Cn2ncc3cc(Nc4ncnn5ccc(COCC6CNCCOC6)c45)ccc32)c1	210	*
2695	Cc1ccn2ncnc(Nc3ccc4[nH]ncc4c3)c12	210	*
2696	FC(F)(F)Oc1ccccc1Oc1ccc(Nc2ncnc3cc[nH]c23)cc1Cl	210	*
2697	CN(CCn1ccc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21)C(=O)CO	210	*
2698	c1cc(Nc2ccc3[nH]ccc3c2)nc(Nc2ccc(OCCN3CCOCC3)cc2)n1	210	*
2699	C#Cc1cccc(Nc2ncnc3cc4c(cc23)N(CCCN2CCCCC2)C(=O)CO4)c1	211.4	*
2700	COc1cc2c(Nc3ccc(NC(=O)Nc4ccccc4)c(Cl)c3)ncnc2cc1OCCN1CCCCC1	212	*
2701	COc1cc2ncc(C#N)c(Nc3ccc(Cc4nc(-c5ccccc5)cs4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	214	6.67
2702	O=C(/C=C/N1CCOCC1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	215	*
2703	Fc1ccc(-c2nc(-c3ccccc3)[nH]c2-c2ccnc3[nH]c(-c4ccccc4)cc23)cc1	215	*
2704	COc1ccc(-c2c3c4cc(OC)c(OCCCN(C)C)cc4oc(=O)c3n3ccc4cc(O)c(OC)cc4c23)cc1O.O=C(O)C(F)(F)F	215.4	*
2705	Clc1cccc(Nc2ncnc3ccc(NCc4ccc5c(c4)OCCCO5)cc23)c1	216	6.67
2706	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5C[C@@H]6CN(C)C[C@@H]6C5)c(C)c4)nc32)C1	216	6.67
2707	C=CC(=O)Nc1cccc(Nc2nc(Nc3ccc(/C=C/c4cc(OC)cc(OC)c4)cc3)ncc2Cl)c1	216.1	*
2708	C=CC(=O)N1CCC(Sc2nc(-c3ccc(F)cc3)c(-c3ccnc(Nc4ccccc4)c3)[nH]2)C1	217	*
2709	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5CC6(CCN(C)CC6)C5)c(C)c4)nc32)C1	218	6.66
2710	CC(=O)Nc1cccc(-c2c(-c3ccccc3)oc3ncnc(N[C@H](CO)c4ccccc4)c23)c1	218	*
2711	COc1ccccc1-c1cc2c(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncnc2s1	220	*
2712	Nc1nc(N)c2c(Nc3cccc(Cl)c3)[nH]nc2n1	220	*
2713	COc1ccc(Nc2ncc3cc(-c4c(Cl)cccc4Cl)c(=O)n(C)c3n2)cc1	220	*
2714	Cn1c(=O)c(-c2c(Cl)cccc2Cl)cc2cnc(Nc3ccc(CC(=O)O)cc3)nc21	220	*

2715	O=C(O)C1CCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)CC1	220	*
2716	CC(C)n1nc(-c2ccc3cc[nH]c3c2)c2c(N)ncnc21	220	*
2717	O=C(Nc1cccc(Cl)c1)c1cc(O)ccc1O	220	*
2718	FC(F)(F)Oc1cccc(Oc2ccc(Nc3ncnc4cc[nH]c34)cc2Cl)c1	220	*
2719	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN1CCC(O)CC1	221	6.66
2720	C=C(CN(C)C)C(=O)Nc1cc2c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c(C#N)cnc2cc1OCC	223	6.65
2721	C=CC(=O)Nc1cccc(-n2c(=O)c(=O)n(C(C)C)c3cnc(Nc4ccc(N(C)CCN(C)C)cc4OC)nc32)c1	223	*
2722	C/C=C\C(=O)Nc1ccccc1Nc1ncnc2cc(OCCCOC)c(OCCCOC)cc12	223.6	*
2723	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5CCC6(CCN(C)CC6)CC5)c(C)c4)nc32)C1	224.5	6.65
2724	COc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1OC1CCN(C)CC1	225	*
2725	C=CC(=O)Nc1cccc(NC(=O)Nc2ccnc(Nc3ccc(N4CCOCC4)cc3OC)n2)c1	225	*
2726	COc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(C)c(Nc2ccc3ccccc3c2)n1	225	*
2727	COc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(OC)c(Nc2ccc3ccccc3c2)n1	225	*
2728	CCNC(=O)Nc1ccc2ncnc(Nc3ccc(OCc4ccccn4)c(Cl)c3)c2c1	227	*
2729	C=CC(=O)Nc1cccc(-n2c(=O)n(C(C)C)c(=O)c3cnc(Nc4ccc(OCCN(C)C)cc4OC)nc32)c1	227	*
2730	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc5c(cnn5S(=O)(=O)c5cccc(F)c5)c4)c3s2)C1)N1CCOCC1	230	6.64
2731	CCOC(=O)c1ccc(O)c(Nc2ncnc3cc4oc(=O)n(CCCN5CCOCC5)c4cc23)c1	230	*
2732	Nc1cc2ncnc(NCc3ccccc3N)c2cn1	230	*
2733	C=C(CN(C)C)C(=O)c1ccc(OS(=O)(=O)c2ccc(C(=O)O)cc2)cc1	230	*
2734	Cc1[nH]c2ncnc(Nc3cccc(Cl)c3)c2c1-c1ccccc1	230	*
2735	COc1cc(Nc2c(C#N)cnc3cc(-c4coc(CN5CCN(C)CC5)c4)c(OC)cc23)c(Cl)cc1Cl	230	*
2736	COc1cc2c(Nc3ccc(NC(=O)c4cccc(Cl)c4)cc3)ncnc2cc1OCCCN1CCOCC1	230	*
2737	COc1cc2ncc(C#N)c(Nc3ccc(C(C)C)cc3)c2cc1OC	230	*
2738	N#Cc1cc2ncnc(Nc3ccc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c2n1CCOCCO	230	*
2739	C#CCNC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	232	*
2740	C#CCNN(NCC#C)C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	232	*
2741	CCOC(C)Oc1cc2ncnc(Nc3ccc(F)c([N+](=O)[O-])c3)c2c2c1OCCO2	232.3	*
2742	CN1CCN(C(=O)c2ccc(-c3ccc4ncnc(Nc5ccc(OCc6cccc(F)c6)c(Cl)c5)c4c3)o2)CC1.Cc1ccc(S(=O)(=O)O)cc1	232.4	*
2743	COc1cc2c(Nc3ccc(NC(=O)Nc4ccc(Cl)cc4)cc3)ncnc2cc1OCCCN1CCN(C)CC1	235	*
2744	Nc1ncnc2c1c(-c1ccc(Br)c(O)c1)nn2C1CCCC1	236	*
2745	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccnc5ccccc45)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	238	6.62
2746	Brc1cccc(Nc2ncnc3ccc(NN=NCc4ccccn4)cc23)c1	238	*
2747	O=C1Nc2cc3c(-c4ccccc4)c(-c4ccccc4)n(-c4ccccc4)c(=O)c3cc2C(c2ccccc2)N1	238	*
2748	COc1ccc(N2Cc3cnc(Nc4ccccc4)nc3N([C@@H]3CC[C@@H](O)C3)C2=O)cc1	239	*
2749	Cc1ccc(C2=NN(C3=NC(=O)CS3)C(c3ccc(Br)cc3)C2)cc1	240	6.62
2750	c1ccc(C2=NN(c3ccccc3)C(c3ccc4ccccc4c3)C2)cc1	240	6.62
2751	COc1cc(N2CCC(O)CC2)ccc1Nc1ncc(Cl)c(Oc2cccc(COc3no[n+]([O-])c3S(=O)(=O)c3ccccc3)c2)n1	240	6.62
2752	O=C(CCl)OCCn1c(=O)oc2cc3ncnc(Nc4ccc(N5CCCCC5)c(Cl)c4)c3cc21	240	6.62
2753	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C#Cc1ccc(CN2CCOCC2)cc1	240	6.62
2754	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc5c(c4)c(F)cn5Cc4ccccc4)c3s2)C1)N1CCOCC1	240	6.62
2755	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(Cc5ccccc5)cc4)c3s2)C1)N1CCOCC1	240	6.62
2756	C=CC(=O)Nc1cccc(-n2c(=O)cc(C)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	240	*

2757	Nc1cc2ncnc(Nc3ccccc3Br)c2cn1	240	*
2758	CCN(CC)CCCCNc1ncc2cc(-c3c(Cl)cccc3Cl)c(NC(=O)NC(C)(C)C)nc2n1	240	*
2759	O=C1CCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)CCN1	240	*
2760	NS(=O)(=O)c1ccc(-n2c(SCC(=O)Nc3cc(Cl)c(Cl)cc3Cl)nc3cc4ccccc4cc3c2=O)cc1	240	*
2761	COc1ccc(O)c(C(=O)Nc2cccc(Cl)c2)c1	240	*
2762	c1cc(Nc2ccc3[nH]ccc3c2)nc(Nc2ccc(N3CCOCC3)cc2)n1	240	*
2763	C=CC(=O)Nc1cccc(-n2c(=O)n(C(C)C)c(=O)c3cnc(Nc4ccc(N5CCC(N6CCN(C)CC6)CC5)cc4OC)nc32)c1	240	*
2764	Brc1cc2c(NCc3ccccc3)ncnc2s1	241	*
2765	C=CC(=O)Nc1cc(Nc2ncc(I)c(Nc3ccccc3S(=O)(=O)N(C)C)n2)c(OC)cc1N(C)CCN(C)C	244	*
2766	O=C1COc2cc3ncnc(Nc4cccc(F)c4)c3cc2N1CCCN1CCOCC1	245.1	*
2767	Nc1ccccc1Nc1ncnc2cc(Br)ncc12	245.47	*
2768	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN1C(C)CCCC1C	247	6.61
2769	COCC(C)Oc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2c2c1OCCO2	247.2	*
2770	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(C(=O)C(F)(F)F)CC4)cc3OC)ncc2SC)c1	247.8	*
2771	CC(C)n1nc(-c2cc(O)cc(Br)c2)c2c(N)ncnc21	249	*
2772	COc1ccc(-c2c3c4cc(O)c(OC)cc4oc(=O)c3n3ccc4cc(O)c(OC)cc4c23)cc1O	249.1	*
2773	CCOc1cc2ncc(C#N)c(Nc3ccc(N(C)Cc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	250	6.60
2774	CC(C)N(CC#CC(=O)Nc1ccc2ncc(C#N)c(Nc3cccc(Br)c3)c2c1)C(C)C	250	6.60
2775	COc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1.Cl	250	*
2776	Nc1cc2ncnc(Nc3ccccc3)c2cn1	250	*
2777	COc1ccc(Nc2ncc3cc(-c4c(Cl)cccc4Cl)c(=O)n(C)c3n2)cc1C	250	*
2778	CN(C)/C=C/C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	250	*
2779	Cc1ccn2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c12	250	*
2780	Cc1cc2cc(Nc3ccnc4cc(-c5ccc(CNCCN6CCNCC6)cc5)sc34)ccc2[nH]1	250	*
2781	Nc1ccccc1Nc1ncnc2ccncc12	251.19	*
2782	COc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(Br)c(Nc2ccc3ccccc3c2)n1	254	*
2783	c1ccc(Nc2ncnc3[nH]ccc23)cc1	254.13	*
2784	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/c1cn(C)cn1	255	6.59
2785	CCC(=O)N1CC[C@H](N2C(=O)N(c3cccc(OC(F)F)c3)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	257	6.59
2786	Fc1cccc(COc2ccc(Nc3ncnc4sc(Br)cc34)cc2Cl)c1	257	*
2787	OC[C@@H](Nc1ncnc2oc(-c3ccccc3)c(-c3ccc4c(c3)OCO4)c12)c1ccccc1	258	*
2788	CC#CC(=O)Nc1ccc2ncc(C#N)c(Nc3cccc(Br)c3)c2c1	258.9	6.21
2789	Nc1cc2ncnc(Nc3cccc(I)c3)c2cn1	260	*
2790	Cn1c(=O)c(-c2c(Cl)cccc2Cl)cc2cnc(Nc3ccccc3)nc21	260	*
2791	Nc1ncnc2c1c(-c1cnc3[nH]ccc3c1)nn2C1CCCC1	260	*
2792	COc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(Cl)c(Nc2ccc3ccccc3c2)n1	260	*
2793	COC[C@@H](Nc1ncnc2sc(Br)cc12)c1ccccc1	262	*
2794	CS(=O)(=O)CCN(CCCCOc1ccc2ncnc(Nc3ccc(OCc4ccccc4)cc3)c2c1)C(=O)C(F)(F)F	263	*
2795	COc1ccc2c(Nc3cccc(Br)c3)ncnc2n1	263	*
2796	c1ccc(Nc2[nH]cnc3nc4ccccc4c2-3)cc1	264	*
2797	c1ccc(Nc2ncnc3[nH]c4ccccc4c23)cc1	264	*
2798	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N1CCC(N2CCCC2)CC1	265	*
2799	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N(N1CCC(N2CCCC2)CC1)N1CCC(N2CCCC2)	265	*

	CC1		
2800	CSc1nc(-c2ccc(F)cc2)c(-c2ccnc(Nc3cc(F)cc([N+](=O)[O-])c3)c2)[nH]1	265	*
2801	CO/N=C/c1c(N)ncnc1Nc1ccc2c(cnn2Cc2cccc(OC)c2)c1	267	*
2802	COc1cc2ncnc(NCc3ccc(F)cc3)c2cc1OCCCCCCCC(=O)NO	268	6.57
2803	C/C=C\C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	269	*
2804	COc1ccc(Oc2nc3ccccc3cc2/C=N/NC(=O)Cn2c([N+](=O)[O-])cnc2C)cc1	270	6.57
2805	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C#CCCNCc1ccccc1	270	6.57
2806	C=CC(=O)Nc1cccc(-n2c(=O)cc(C)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OCCC)nc32)c1	270	*
2807	CC(C)(C)OC(=O)Nc1ccc(-c2[nH]nc3ncnc(Nc4cccc(Cl)c4)c23)cc1	270	*
2808	COc1ccc(-c2nn(C3CCC(C)C3)c3ncnc(N)c23)cc1O	270	*
2809	COc1ccc(-c2cc3c(NC(C)c4ccc(C(F)(F)F)cc4)ncnc3[nH]2)cc1	270	*
2810	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(C)CC4)cc3OC)ncc2SC)c1	271.6	*
2811	Brc1cccc(Nc2ncnc3c2ccc2[nH]cnc23)c1	272	*
2812	Brc1cccc(Nc2ncnc3c2ccc2nc[nH]c23)c1	272	*
2813	C=CC(=O)Nc1cccc(NC(=O)Nc2ccnc(Nc3ccc(N4CCCCC4)cc3OC)n2)c1	273	*
2814	COc1ccccc1-c1cc2c(NCc3cccnc3)ncnc2s1	275	*
2815	C[C@@H](Nc1ncnc2sc(-c3ccccc3C(N)=O)cc12)c1ccccc1	276	6.56
2816	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4cccs4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	277	6.56
2817	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(Oc5ccnc6ccc(F)cc56)c(Cl)c4)c3s2)C1)N1CCOCC1	280	6.55
2818	CN1CCC(Oc2cccc3ncnc(Nc4ccc(OCc5cscn5)c(Cl)c4)c23)CC1	280	*
2819	CN(C)CCN(C)C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	281	*
2820	CN(C)CCN(C)N(C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N(C)CCN(C)C	281	*
2821	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN1CCC(O)(O)CC1	282	6.55
2822	CCOc1cc2ncnc(NC3=CC(=O)C(OC(CF)CF)=CC3=O)c2cc1NC(=O)/C=C/CN(C)C	283.3	6.55
2823	CCOc1cc2ncc(C#N)c(Nc3ccc(OCC4CCCCC4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	285	6.55
2824	COc1cc2ncnc(Nc3ccc(NC(=O)Nc4ccc(Cl)c(C(F)(F)F)c4)cc3)c2cc1OCCCN1CCOCC1	285	*
2825	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5CCC(N(C)C)CC5)c(C)c4)nc32)C1	286	6.54
2826	COc1ccc(OC)c(Nc2cc(Nc3ccc(N4CCN(C)CC4)cc3)ncn2)c1	288	*
2827	COc1cccc(Oc2ccc(Nc3ncnc4cc[nH]c34)cc2Cl)c1	290	*
2828	COc1cc(NC(=O)Nc2ccncc2)cc(-c2cncnc2)c1OC	290.46	*
2829	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(CC(=O)OCCCCCCOc5no[n+]([O-])c5S(=O)(=O)c5ccccc5)CC4)cc3OC)ncc2Cl)c1	292	6.53
2830	COc1cccc(-c2cn(C3CCN(CCN(C)CCO)CC3)c3ncnc(N)c23)c1	295	*
2831	COc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(Cl)c(Nc2ccc3[nH]ccc3c2)n1	295	*
2832	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5CCC6(CCN(C)C6)C5)c(C)c4)nc32)C1	295.7	6.53
2833	Fc1ccc(C2=NN(c3ccccc3)C(c3ccc4ccccc4c3)C2)cc1	300	6.52
2834	O=C(CBr)OCCn1c(=O)oc2cc3ncnc(Nc4ccc(F)c(F)c4)c3cc21	300	6.52
2835	COc1cc2c(cc1OC)Oc1ncnc(Nc3cccc(Br)c3)c1NC2	300	6.52
2836	COc1cc2c(cc1OC)Oc1ncnc(Nc3cccc(Cl)c3F)c1NC2	300	6.52
2837	COc1cc2c(cc1OC)Nc1ncnc(NCc3ccc(F)c(Cl)c3)c1NC2	300	6.52
2838	CONC(=O)c1cc(NCc2cc(O)ccc2O)ccc1O	300	*
2839	O=C1NC(=O)c2cc(Nc3ccccc3)c(Nc3ccccc3)cc21	300	*
2840	COc1cc2ncnc(NC3CC3c3ccccc3)c2cc1OCCN1CCOCC1	300	*

2841	CCOC(=O)C1CCN(CCC(=O)c2ccc(OCc3ccccc3)cc2)CC1.Cl	300	*
2842	COc1cc2c(Nc3ccc(Cl)cc3F)ncnc2cc1OCC1CCN(C)CC1.Cl	300	*
2843	COc1cc2c(Nc3ccc(Cl)cc3F)ncnc2cc1OCCC1CCN(C)CC1	300	*
2844	COc1cc2c(Nc3ccc(Cl)cc3F)ncnc2cc1OCC1CCNCC1.Cl	300	*
2845	COc1cc2c(Nc3cc(O)c(C)cc3F)ncnc2cc1OCC1CCN(C)CC1.Cl	300	*
2846	COc1cc2c(Nc3c(F)cc(Br)cc3F)ncnc2cc1OCC1CCN(C)CC1	300	*
2847	COc1cc2c(Nc3ccc(Cl)cc3F)ncnc2cc1OCCN(C)c1ccncc1	300	*
2848	COc1cc2c(Nc3ccc(NC(=O)c4cccc(Cl)c4)cc3)ncnc2cc1OCCN1CCCCC1	300	*
2849	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5CCN(C6COC6)CC5)c(C)c4)nc32)C1	302	6.52
2850	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N1CCC(CCO)CC1	304	*
2851	CN(C)C/C=C/C(=O)Nc1cc2c(Nc3ccc(Cc4ccccn4)cc3)ncnc2cn1	304	*
2852	CS(=O)(=O)CCNCc1cc(-c2cc3c(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)ncnc3s2)cs1	304	*
2853	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N(N1CCC(CCO)CC1)N1CCC(CCO)CC1	304	*
2854	CO/N=C/c1c(N)ncnc1Nc1ccc2[nH]ncc2c1	306	*
2855	C=CC(=O)Nc1cc(Nc2nccc(Nc3ccccc3S(=O)(=O)N(C)C)n2)c(OC)cc1N(C)CCN(C)C	307	*
2856	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OCCNC(C)C	310	*
2857	O=C(O)c1ccc(S(=O)(=O)Oc2ccc(/C=C/[N+](=O)[O-])cc2)c(O)c1	310	*
2858	c1ccc(Nc2ncnc3[nH]c4c(c23)CCCC4)cc1	310	*
2859	COCCNCCN1CCC(n2cc(-c3cccc(OC)c3)c3c(N)ncnc32)CC1	310	*
2860	COc1ccc(C2=C(C#N)C3(C(=O)Nc4ccc(Br)cc43)c3c(-c4cccs4)nn(-c4ccccc4)c3N2)cc1	310	*
2861	CCOC(=O)c1c(C)cn2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c12	310	*
2862	Cn1cnc(-c2cc(NC(=O)Nc3nccs3)cc(C(F)(F)F)c2)c1	310.76	*
2863	C=CC(=O)Nc1cc(Nc2n[nH]c3cc(-c4ccc5ccccc5c4)ccc23)c(OC)cc1N(C)CCN(C)C	312	*
2864	CC(C)Oc1cc2ncnc(Nc3ccc(F)c(C#N)c3)c2c2c1OCCO2	313.6	*
2865	C=CC(=O)Nc1cccc(-n2c(=O)n(C)c(=O)c3cnc(Nc4ccc(N5CCSCC5)cc4OC)nc32)c1	314	*
2866	CCCCCCCCCCCCCCNC(=O)COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1	316	6.50
2867	COc1cc(NC(=O)Nc2nccs2)cc(-c2cccnc2)c1OC	317.12	*
2868	C=CC(=O)Nc1cc(Nc2nccc(NC(=O)c3ccccc3)n2)c(OC)cc1N(C)CCN(C)C	317.6	*
2869	Nc1ncnc2c1c(-c1ccc(F)c(O)c1)nn2C1CCCC1	318	*
2870	Fc1cccc(COc2ccc(Nc3ccncn3)cc2Cl)c1	320	6.04
2871	COc1ccc(-c2nnc(-n3c(-c4ccccc4)nc4cc(Cl)ccc4c3=O)s2)cc1	320	6.49
2872	c1ccc(CNc2ncnc3ccccc23)cc1	320	*
2873	O=c1[nH]cc(F)c(=O)[nH]1	320	*
2874	O=c1nc(O)c(F)c[nH]1	320	*
2875	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN1CCOCCOCCOCC1	321	6.49
2876	CN(C)c1ccc2c(Nc3cccc(Br)c3)ncnc2n1	324	*
2877	Nc1ncnc2c1c(-c1ccc(Br)c(O)c1)nn2C1CCC1	324	*
2878	Clc1ccc(Nc2cc(Nc3cccc(Cl)n3)ncn2)cc1	324	*
2879	CN1CCN(c2ccc(Nc3ncc(Br)c(Nc4ccc5c(ccn5Cc5cccc(F)c5)c4)n3)cc2)CC1	325	*
2880	O=C(CO)N1CCC[C@H]1COc1cccc2ncnc(Nc3ccc(OCc4ccccn4)c(Cl)c3)c12	327	*
2881	O=C(CCl)OCCn1c(=O)oc2cc3ncnc(Nc4ccc(F)c(Cl)c4)c3cc21	330	6.48
2882	COCOC#CC(=O)Nc1ccc2ncc(C#N)c(Nc3cccc(Br)c3)c2c1	330	6.48
2883	COCOCC#CC(=O)Nc1ccc2ncc(C#N)c(Nc3cccc(Br)c3)c2c1	330	6.48

2884	Clc1cccc(Nc2nc[nH]c3nnc(Nc4cccc(Cl)c4)c2-3)c1	330	*
2885	COc1cc(Nc2ncc3cc(-c4c(Cl)cccc4Cl)c(=O)n(C)c3n2)cc(OC)c1	330	*
2886	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N1CCN(CCO)CC1	331	*
2887	Fc1ccc(Nc2ncnc3ccc(C#Cc4ccccc4)cc23)cc1Cl	331	*
2888	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N(N1CCN(CCO)CC1)N1CCN(CCO)CC1	331	*
2889	COc1cc2ncnc(-c3c[nH]c4cc(F)c(Cl)cc34)c2cc1OCCCN1CCOCC1	333	*
2890	CN=NNc1ccc2ncnc(NCc3ccccc3)c2c1	335	*
2891	COc1ccc(OC)c(Nc2cc(Nc3ccc(F)cc3)ncn2)c1	336	*
2892	Cc1ccc(C2CC(c3ccc(C)c(C)c3)=NN2C(N)=S)cc1	340	6.47
2893	CCOc1cc2ncc(C#N)c(Nc3ccc4c(c3)CCN4Cc3ccccc3)c2cc1NC(=O)/C=C/CN(C)C	340	6.47
2894	COCCn1c(=O)oc2cc3ncnc(Nc4ccc(OCc5nccc(OCC(F)(F)F)c5C)cc4)c3cc21	340	*
2895	COCc1ccn2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c12	340	*
2896	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4cccnc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	341	6.47
2897	C=CC(=O)Nc1cccc(-n2c(=O)n(C)c(=O)c3cnc(Nc4ccc(N5CCOCC5)cc4OC)nc32)c1	341	*
2898	COc1cc2ncc(C(=O)NC3CC(C)(C)N([O])C(C)(C)C3)c(Nc3cccc(Br)c3)c2cc1OC	342	6.47
2899	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN1CC1C(=O)OC	343	6.46
2900	CCC(=O)Nc1cc2c(Nc3ccc(C(O)c4ccccc4)cc3)ncnc2cc1OC	343	*
2901	c1ccc(Nc2ncnc3ccccc23)cc1	344	*
2902	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)cc3)c2cc1NC(=O)/C=C/CN(C)C	345	6.46
2903	Cc1ccc(Nc2ncnn3ccc(C)c23)cc1O	346	*
2904	CCOc1cc2ncnc(NC3=CC(=O)C(OCc4cccc(OC)c4)=CC3=O)c2cc1NC(=O)/C=C/CN(C)C	346.9	6.46
2905	COc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	348	*
2906	C=CC(=O)Nc1cccc(NC(=O)Nc2ccnc(Nc3ccc(OC)cc3OC)n2)c1	348	*
2907	CCc1cccc(Nc2ncnc3cc(OCCOC)c(OCCOC)cc23)c1	348.7	*
2908	NC(=S)N1N=C(c2ccc(Br)cc2)CC1c1ccc2ccccc2c1	350	6.46
2909	C=CC(=O)N1CCN(c2ccc(Nc3ncc(Cl)c(Oc4cccc(COc5no[n+]([O-])c5S(=O)(=O)c5ccccc5)c4)n3)c(OC)c2)CC1	350	6.46
2910	Cc1ccc(C(/C=C/c2ccccc2)=N\NC(N)=S)cc1	350	6.46
2911	C=CC(=O)Nc1cccc(Nc2nc(Nc3ccc(N4CCN(C(C)=O)CC4)cc3OC)ncc2C(F)(F)F)c1	350	*
2912	COc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1OC.Cl	350	*
2913	O=C1CN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)CCN1	350	*
2914	COc1cccc(-c2cn(C3CCN(CC(N)=O)CC3)c3ncnc(N)c23)c1	350	*
2915	N#Cc1cnc2cc(O)c(O)cc2c1Nc1cccc(Br)c1	350	*
2916	CCOC(C)Oc1cc2ncnc(Nc3ccc(F)c(C#N)c3)c2c2c1OCCO2	351.8	*
2917	OC[C@@H](Nc1ncnc2oc(-c3ccccc3)c(-c3ccoc3)c12)c1ccccc1	352	*
2918	O=C1COc2cc3ncnc(Nc4ccc(Cl)cc4)c3cc2N1CCCN1CCOCC1	353.7	*
2919	O=[N+]([O-])c1cccc2ncnc(Nc3cccc(Br)c3)c12	355	*
2920	COCCOc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CN1CC[S+]([O-])CC1	356.6	*
2921	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN1CCN(C)CC1	360	6.44
2922	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3Cl)Cc3cnc(Nc4ccc(N5CCN(C6COC6)CC5)c(C)c4)nc32)C1	360	6.44
2923	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN1CCCC1	360	*
2924	CC(COC(=O)c1cc(NCc2cc(O)ccc2O)ccc1O)Cc1ccccc1	360	*
2925	CN(C)CCC(=O)c1ccc(OCc2ccccc2)c(O)c1.Cl	360	*
2926	FC(F)(F)c1cccc(Nc2[nH]cnc3nc4c(c2-3)CCCC4)c1	360	*

2927	Cn1ncc2cc(Nc3ncnn4ccc(CN5CCC(N)CC5)c34)ccc21	360	*
2928	N#CC1=C(c2ccc(Cl)cc2)Nc2c(c(-c3cccs3)nn2-c2ccccc2)C12C(=O)Nc1ccccc12	360	*
2929	COc1cc2ncc(C#N)c(Nc3ccccc3C(C)C)c2cc1OC	360	*
2930	COc1ccc(C(=O)Nc2cccc(Cl)c2)c(O)c1	360	*
2931	CCOc1ccc(NC(=O)/C=C/c2ccc3c(c2)OCCCCO3)cc1	360	*
2932	CCOc1cc2ncc(C#N)c(Nc3cc(Cl)c(OCc4cccc(F)c4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	362	6.44
2933	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	362	6.44
2934	COc1cc(NC(=O)Nc2nccs2)cc(-c2cn(C)cn2)c1OC	362	*
2935	CCOC(C)Oc1cc2ncnc(Nc3ccc(C)c([N+](=O)[O-])c3)c2c2c1OCCO2	363.3	*
2936	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1OCCCN1CCOCC1)c1cc(F)cc(F)c1F	365	6.44
2937	CCC(=O)N1CC[C@H](N2C(=O)N(c3cccc(C)c3)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	365	6.44
2938	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C(C)C)c4)nc32)C1	365	6.44
2939	CCN(CC)CCNC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	365	*
2940	COc1ccc(N2Cc3cnc(Nc4ccccc4)nc3N([C@H]3CC[C@H](O)C3)C2=O)cc1	365	*
2941	CCN(CC)CCNN(NCN(CC)CC)C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	365	*
2942	CC1CCC(n2nc(-c3ccc(F)c(O)c3)c3c(N)ncnc32)C1	366	*
2943	CCOC(=O)CNc1cccc(Oc2cc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncn2)c1	370	6.43
2944	Cc1ccc(C2=NN(c3nc(-c4ccc(Cl)cc4)cs3)C(c3ccc(Br)cc3)C2)cc1C	370	6.43
2945	COc1cc2nccc(Nc3cccc(Br)c3)c2cc1OC	370	*
2946	Nc1cnc(C#Cc2cc3c(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)ncnc3s2)cn1	372	*
2947	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3Cl)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	373	6.43
2948	C=CC(=O)Nc1ccc(-n2c(=O)cnc3cnc(Nc4ccc(Cl)cc4)nc32)cc1	373.5	6.43
2949	CN(C)CCOc1ccc(Nc2ncnc3cc(OCCCN4CCOCC4)c(NC(=O)c4cc([N+](=O)[O-])ccc4F)cc23)cc1Cl	374	6.43
2950	C=CC(=O)Nc1cnc2ncc(C#N)c(Nc3cccc(Br)c3)c2c1	374.8	6.43
2951	CCC(=O)N1CC[C@H](N2C(=O)N(c3ccc(C)cc3)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	377	6.42
2952	O=C(Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1)C1CCC2(CC1)OOC1(OO2)C2CC3CC(C2)CC1C3	379.7	*
2953	CCOc1cc2ncc(C#N)c(Nc3ccc(O[C@@H]4CCc5ccccc54)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	380	6.42
2954	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OC	380	*
2955	COc1ccc(Nc2ncnc3cc4oc(=O)n(CCCN5CCOCC5)c4cc23)cc1	380	*
2956	C#Cc1cccc(Nc2ncnc3cc4oc(=O)n(CCCN5CCOCC5)c4cc23)c1	380	*
2957	Cc1cccc(Nc2ncnc3cnc(Cl)nc23)c1	380	*
2958	CC(=O)NC1CCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)CC1	380	*
2959	Cn1c(=O)c(-c2c(Cl)cccc2Cl)cc2cnc(Nc3ccc(F)cc3)nc21	380	*
2960	CCN(CC)CCOc1ccc(Nc2cc(NC(=O)Nc3c(Cl)cccc3Cl)ncn2)cc1	380	*
2961	CC(C)n1nc(-c2cnc3[nH]ccc3c2)c2c(N)ncnc21	380	*
2962	O[C@H]1CC[C@H](Nc2ncc3nc(Nc4c(F)cc(F)cc4F)n([C@H]4CCOC4)c3n2)CC1	380	*
2963	CCC(=O)N1CC[C@H](N2C(=O)N(c3ccc(Cl)cc3)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	383	6.42
2964	CCC(=O)Nc1cc2c(Nc3ccc(NCc4ccccc4)cc3)ncnc2cc1OC	383	*
2965	Nc1nc(Nc2cccc(Br)c2)c2cc[nH]c2n1	383.7	*
2966	C=CC(=O)Nc1cccc(Nc2nc(Nc3ccc(/C=C/c4ccc(C)cc4C)cc3)ncc2F)c1	386.7	*
2967	C=CC(=O)Nc1cc(Nc2n[nH]c3cc(-c4ccc(N(C)C)cc4)ccc23)c(OC)cc1N(C)CCN(C)C	387	*
2968	COCCOc1cc2ncnc(Nc3ccc(F)c(C#N)c3)c2c2c1OCCO2	387.8	*
2969	CCC(=O)Nc1cc2c(Nc3ccc(Cc4ccncc4)cc3)ncnc2cc1OC	388	*

2970	Cn1nc(-c2ccc3ccccc3c2)c2c(N)ncnc21	388	*
2971	C=CC(=O)Nc1cccc(Nc2nc(Nc3ccc(/C=C/c4cc(Cl)cc(Cl)c4)cc3)ncc2F)c1	388.1	*
2972	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCCN(C(C)=O)CC4)cc3OC)ncc2SC)c1	389.4	*
2973	Cc1ncc([N+](=O)[O-])n1CC(=O)NS(=O)(=O)c1ccc(F)cc1	390	6.41
2974	C#Cc1cccc(Nc2ncnc3cc(OCCOC(=O)C(C)c4ccc5cc(OC)ccc5c4)c(OCCOC(=O)C(C)c4ccc5cc(OC)ccc5c4)cc23)c1	390	6.41
2975	Cc1ccc(Oc2ccc(Nc3ncnc4cc(OCCCN5CCOCC5)c(NC(=O)c5cc([N+](=O)[O-])ccc5F)cc34)cc2Cl)cn1	390	6.41
2976	COc1cc2ncnc(NC3CC3c3ccccc3)c2cc1O	390	*
2977	Cc1cc(Nc2ncc3cc(-c4c(Cl)cccc4Cl)c(=O)n(C)c3n2)ccc1F	390	*
2978	CC(C)(C)OC(=O)n1ccc2cc(-c3nn(C4CCCC4)c4ncnc(N)c34)ccc21	391	*
2979	OC[C@@H](Nc1ncnc2oc(-c3ccccc3)c(-c3ccccc3)c12)c1ccccc1	393	*
2980	CN1CCN(c2ccc(Nc3ncc(Br)c(Nc4ccc5[nH]ncc5c4)n3)cc2)CC1	393	*
2981	CC/C=C\C(=O)Nc1cccc(Nc2ncnc3cc(OC)c(OCCCN4CCOCC4)cc23)c1	393.9	*
2982	C=CC(=O)Nc1ccc(-n2c(=O)cnc3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)cc1	395	6.40
2983	c1ccc(-c2c(-c3ccc(OCCN4CCCC4)cc3)oc3ncnc(NCCN4CCNCC4)c23)cc1	397	*
2984	COc1cc(/C=C(\C#N)C(N)=O)cc(CSc2ccccc2)c1O	398.11	*
2985	COc1cc(/C=C2\CCC/C(=C\c3ccc(O)c(O)c3)C2=O)cc(OC)c1	400	6.38
2986	COc1cc2ncc(C#N)c(Nc3ccc(NCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	400	6.40
2987	CCOc1cc2ncc(C#N)c(Nc3ccc(O[C@H]4CCc5ccccc54)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	400	6.40
2988	Cc1cc(Oc2ccc(Nc3ncnc4cc(C#C[C@@H]5C[C@@H](OC(=O)N6CCOCC6)CN5)sc34)cc2Cl)no1	400	6.40
2989	O=C(OCCCCc1ccccc1)c1cc(NCc2cc(O)ccc2O)ccc1O	400	*
2990	CC(CCOC(=O)c1cc(NCc2cc(O)ccc2O)ccc1O)c1ccccc1	400	*
2991	CCOC(=O)c1cc(NCc2cc(O)ccc2O)ccc1O	400	*
2992	O=C(NO)c1cc(NCc2cc(O)ccc2O)ccc1O	400	*
2993	CNC(=O)c1ccc(S(=O)(=O)Oc2ccc(/C=C/[N+](=O)[O-])cc2)cc1	400	*
2994	COc1cc2c(Nc3ccc(Cl)cc3F)ncnc2cc1OCCN1CCOCC1	400	*
2995	COc1cc2c(Nc3ccc(Br)cc3F)ncnc2cc1OCCn1ccnn1	400	*
2996	NC(=O)CN1CCC(n2cc(-c3cccc(O)c3)c3c(N)ncnc32)C1	400	*
2997	C[C@@H](c1cccc(F)c1)n1ncc2cc(Nc3ncnn4ccc(COC[C@@H]5CNCCO5)c34)ccc21	400	*
2998	Cc1nc(Nc2ncc(C(=O)Nc3c(C)cccc3Cl)s2)cc(N2CCN(CCOC(=O)CCC(=O)Nc3ccc4ncnc(Nc5cccc(Cl)c5)c4c3)CC2)n1	400	*
2999	COc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(Cl)c(Nc2ccc(Cl)c(Cl)c2)n1	400	*
3000	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4F)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	401	6.40
3001	COc1cc2ncnc(Nc3cccc(C#CCCO)c3)c2cc1OC	402.1	*
3002	COc1cc2ncc(C#N)c(Nc3ccc(Sc4ncccn4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	403	6.39
3003	COC(=O)/C=C/CNC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	404	*
3004	COC(=O)/C=C\CNN(NC/C=C\C(=O)OC)C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	404	*
3005	O=C(/C=C/CN1CCCC1)Nc1cc2c(Nc3ccc(Cc4ccccn4)cc3)ncnc2cn1	405	*
3006	CN1CCN(c2ccc(Nc3ncc(Br)c(Nc4ccc5nccnc5c4)n3)cc2)CC1	408	*
3007	COC(=O)c1cccc(Nc2ncnc3ccc(-c4cnc(OC)c(NS(C)(=O)=O)c4)cc23)c1	409	*
3008	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(C(=O)C(C)(C)C)CC4)cc3OC)ncc2SC)c1	409.7	*
3009	NC(=S)N/N=C(/C=C/c1cccc2ccccc12)c1ccccc1	410	6.39
3010	Cc1c(C(=O)N2CCN(C)CC2)c[nH]c1/C=C1\C(=O)Nc2ncnc(Nc3ccc(F)c(Cl)c3)c21	410	*

3011	CNC(=O)c1nc(-c2ccc(Cl)c(S(=O)(=O)Nc3cccc(F)c3C)c2)cnc1N	410	*
3012	COc1cc2ncnc(Nc3cccc(C#N)c3)c2cc1OC	412.8	*
3013	CCC(=O)N1CC[C@H](N2C(=O)N(c3cccc(OC)c3Cl)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	413	6.38
3014	C[C@@H](Nc1ncnc2sc(Br)cc12)c1cccs1	415	*
3015	Cc1ccc(Nc2ncnc3cc(OC(C)C)c4c(c23)OCCO4)cc1C#N	416.1	*
3016	CCC(=O)N1CC[C@H](N2C(=O)N(c3cccc(OC)c3)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	417	6.38
3017	C[C@H](Nc1[nH]cnc2c3ccccc3nc1-2)c1ccccc1.Cl	419	*
3018	C[C@@H](Nc1ncnc2c1[nH]c1ccccc12)c1ccccc1.Cl	419	*
3019	Cc1ccc2nc(Oc3ccc(F)cc3)c(/C=N/NC(=O)Cn3c([N+](=O)[O-])cnc3C)cc2c1	420	6.38
3020	O=C(Nn1c(-c2ccccc2)nc2ccccc2c1=O)c1ccc(Br)cc1	420	6.38
3021	Oc1cccc(Nc2[nH]cnc3nc4c(c2-3)CCCC4)c1	420	*
3022	CCOc1cc2ncc(C#N)c(Nc3cccc(Br)c3)c2cc1OCC	420	*
3023	OCCOCCn1ccc2ncnc(Nc3cnc(Oc4cccc(C(F)(F)F)c4)c(Cl)c3)c21	420	*
3024	CCC(=O)N1CC[C@H](N2C(=O)N(c3cccc(OC)c3F)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	421	6.38
3025	CCC(=O)Nc1cc2c(Nc3ccc4c(ccn4CC(C)C)c3)ncnc2cc1OC	421	*
3026	COc1cc2ncc(C(=O)NC3CC(C)(C)N([O])C(C)(C)C3)c(Nc3ccc(F)c(Cl)c3)c2cc1OC	422	6.37
3027	Cc1ncc([N+](=O)[O-])n1C/C(=N/NC(=O)c1ccc(N)cc1)c1ccc(Br)cc1	430	6.37
3028	COc1cc2ncnc(NNc3ccc(F)c(Cl)c3)c2cc1OC	430	*
3029	COc1cn2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c2c1COC[C@@H]1CNCCO1	430	*
3030	N#CC1=C(c2ccccc2)Nc2c(c(-c3cccs3)nn2-c2ccccc2)C12C(=O)Nc1ccccc12	430	*
3031	OC[C@@H](Nc1ncnc2oc(-c3ccccc3)c(-c3ccco3)c12)c1ccccc1	434	*
3032	O=C1COc2cc3ncnc(Nc4ccc(F)cc4)c3cc2N1CCCN1CCOCC1	434.1	*
3033	COc1ccc(-c2nn(C3CCCC3)c3ncnc(N)c23)cc1O	437	*
3034	Nc1cccc2ncnc(Nc3cccc(Br)c3)c12	439	*
3035	CCOC(=O)c1ccc(O)c(Nc2ncnc3cc4oc(=O)n(CCOC)c4cc23)c1	440	*
3036	COc1cccc2ncnc(Nc3ccc(OCc4ccccn4)c(Cl)c3)c12	440	*
3037	COc1cccc(-c2cn(C3CCN(CC(N)=O)C3)c3ncnc(N)c23)c1	440	*
3038	COc1cc2sc3c(Nc4cccc(Br)c4)ncnc3c2cc1OC.Cl	444	*
3039	C=CC(=O)Nc1cc(-n2c(=O)cc(C)c3cnc(Nc4cnn(CCN(C)C)c4)nc32)cc(C(F)(F)F)c1	444.7	*
3040	CCOc1cc2ncc(C#N)c(Nc3ccc(Oc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	445	6.35
3041	N#CC(C#N)=CNc1ccc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2c1	445	*
3042	C=CC(=O)Nc1cccc(Nc2nc(Nc3ccc(CN4CCOCC4)cc3)ncc2Cl)c1	448.7	*
3043	Cc1ccc(NC(=O)/C=C/CN(C)C)cc1C(=O)Nc1ccc(OCc2cccc(F)c2)c(Cl)c1	450	6.35
3044	COc1cc2ncnc(Nc3cccc(Cl)c3F)c2cc1CN1CCC[C@@H]1C(=O)N(C)C	450	*
3045	CC(C)(C)NC(=O)Nc1nc2nc(N)ncc2cc1-c1c(Cl)cccc1Cl	450	*
3046	CCN(CC)CCNC(=O)c1cc(C)c(/C=C2\C(=O)Nc3ncnc(Nc4ccc(Cl)cc4F)c32)[nH]1	450	*
3047	COc1cc2c(Nc3c(F)cc(Br)cc3F)ncnc2cc1OCC1CCNCC1	450	*
3048	COc1cc2c(Nc3c(F)cc(Cl)cc3F)ncnc2cc1OCC1CCN(C)CC1	450	*
3049	Br.Cc1ccc([C@@H](C)Nc2ncnc3[nH]c(-c4ccc(O)cc4)cc23)cc1	450	*
3050	OC[C@@H](Nc1ncnc2oc(-c3ccccc3)c(Br)c12)c1ccccc1	452	*
3051	CC/C=C\C(=O)Nc1ccccc1Nc1ncnc2cc(OC)c(OCCCN3CCOCC3)cc12	452.4	*
3052	COc1ccc(-c2cc(NC(=O)Nc3ccncc3)cc(OC)c2OC)cn1	455.17	*
3053	Cc1cccc(Nc2ncnc3cc4c(cc23)N(CCCN2CCCCC2)C(=O)CO4)c1	456.2	*

3054	Clc1ccc(Nc2nnc(Cc3ccncc3)c3ccccc23)cc1	457.7	6.34
3055	O=C(CBr)OCCn1c(=O)oc2cc3ncnc(Nc4ccc(F)c(Cl)c4)c3cc21	460	6.34
3056	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1/C=C/c1ccc(CNCCS(C)(=O)=O)o1	460	6.34
3057	COc1cc2ncnc(Nc3cccc(Cl)c3)c2cc1B(O)O	460	*
3058	O=C1COc2cc3ncnc(Nc4cccc(F)c4)c3cc2N1CCCN1CCCCC1	460	*
3059	c1ccc(CNc2[nH]cnc3c4ccccc4nc2-3)cc1	460	*
3060	Cl.O=[N+]([O-])c1ccc2sc3c(Nc4cccc(C(F)(F)F)c4)ncnc3c2c1	460	*
3061	CC(C)S(=O)(=O)c1ccccc1Nc1nc(N/N=C/c2cccc(C(F)(F)F)c2)ncc1Cl	460	*
3062	COC(=O)COCc1ccn2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c12	460	*
3063	c1ccc(CNc2ncnc3c2[nH]c2ccccc23)cc1	460	*
3064	C=CC(=O)Nc1cccc(NC(=O)Nc2ccnc(Nc3ccc(N(C)C)cc3)n2)c1	462	*
3065	COc1cc2nc(N)nc(Nc3cccc(Br)c3)c2cc1OC	463	*
3066	CCCCCCCCCCCCCCCCCCCNC(=O)COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1	464	6.33
3067	CN1CCN(C(=O)Nc2cc3c(Nc4ccc(F)c(Cl)c4)ncnc3cc2O[C@H]2CCOC2)CC1	464	*
3068	CN(C)CCCN(C)C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	464	*
3069	CN(C)CCCN(C)N(C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N(C)CCCN(C)C	464	*
3070	CN1CCN(N(C(=O)Nc2cc3c(Nc4ccc(F)c(Cl)c4)ncnc3cc2O[C@H]2CCOC2)N2CCN(C)CC2)CC1	464	*
3071	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5CCCCC5)c(C)c4)nc32)C1	467	6.33
3072	COCCn1c(=O)oc2cc3ncnc(Nc4ccc(F)c(Cl)c4)c3cc21	470	*
3073	C=C(CN(C)C)C(=O)c1ccc(OS(=O)(=O)c2ccc(C(=O)O)c(O)c2)cc1	470	*
3074	CCOC(=O)c1cn2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c2c1C	470	*
3075	Clc1ccccc1Nc1ncnc2[nH]ccc12	470.67	*
3076	COCCOc1cc2ncnc(-c3c[nH]c4cc(F)c(Cl)cc34)c2cc1OCCOC	472	*
3077	C=CC(=O)Nc1cc(CC)cc(-n2c(=O)cc(C)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	472.1	*
3078	Nc1cccc(Oc2cc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncn2)c1	473	6.33
3079	C#Cc1cccc(Nc2ncnc3cc(OC(C)COC)c4c(c23)OCCO4)c1	473.6	*
3080	C=CC(=O)Nc1cccc(-n2c(=O)c(=O)n(C)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	474	*
3081	COc1ccc(-c2cc(NC(=O)Nc3nccs3)cc(C(F)(F)F)c2)cn1	476.66	*
3082	COCCNC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	479	*
3083	COCCNN(NCOC)C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	479	*
3084	CC(C)(C)n1nc(-c2ccc(Cl)cc2)c2c(N)ncnc21	480	*
3085	Cc1ccc(Nc2ncc3cc(-c4c(Cl)cccc4Cl)c(=O)n(C)c3n2)cc1	480	*
3086	CN(C)N=Nc1ccc2ncnc(NCc3ccccc3)c2c1	482	*
3087	Brc1ccc(C2=NN(c3ccccc3)C(c3cccc4ccccc34)C2)cc1	490	6.31
3088	COc1cc2ncnc(Nc3cccc(Cl)c3)c2cc1B1OC(C)(C)C(C)(C)O1	490	*
3089	CCn1c(=O)c(-c2c(Cl)cccc2Cl)cc2cnc(Nc3ccncc3)nc21	490	*
3090	COc1cc2ncnc(Nc3cc(NC(=O)c4ccccc4)c(F)cc3F)c2cc1OC	490	*
3091	CCc1c(CO)cn2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c12	490	*
3092	COCCOCc1ccn2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c12	490	*
3093	N#Cc1c(-c2ccc3ncc(C(N)=O)c(Nc4cccc(Br)c4)c3c2)csc1N	490	*
3094	C=CC(=O)Nc1ccccc1Nc1nc(Nc2ccc(OCCN3CCOCC3)cc2)ncc1Cl	491	*
3095	COc1ccc(-c2ccc(OC(F)(F)F)c(NC(=O)Nc3nccs3)c2)cn1	495.3	*
3096	C/C=C\C(=O)Nc1ccc(Nc2ncnc3cc(OCCCOC)c(OCCCOC)cc23)cc1	497.5	*

3097	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4nccn4C)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	500	6.30
3098	COc1cc2c(cc1OC)Oc1ncnc(Nc3ccc4ccccc4c3)c1NC2	500	6.30
3099	Cc1ccc2[nH]c(C(=O)NC(CO)Cc3ccccc3)c(Cl)c2c1	500	6.30
3100	N#CC(C#N)=C1CCc2cc(O)c(O)cc21	500	*
3101	COc1cc2ncnc(Nc3cc(OC)c(OC)c(OC)c3)c2cc1OC.Cl	500	*
3102	N#CC(C#N)=C(N)/C(C#N)=C/c1cc(O)c(O)c(Br)c1	500	*
3103	COc1cc(/C=C/[N+](=O)[O-])ccc1OS(=O)(=O)c1ccc(C(=O)OC[C@H]2O[C@@H](n3cnc4c(N)ncnc43)[C@H](O)[C@@H]2O)cc1	500	*
3104	Cc1nc2nc[nH]c(N(C)c3cccc(Cl)c3)c-2c1C	500	*
3105	COc1cc2c(Nc3ccc(Br)cc3F)ncnc2cc1OCC1CCN(C)CC1.Cl	500	*
3106	COc1cc2c(Nc3c(F)cc(Cl)cc3F)ncnc2cc1OCC1CCNCC1	500	*
3107	COc1cc2c(Nc3ccc(C)cc3F)ncnc2cc1OCC1CCNCC1	500	*
3108	Fc1cccc(Cn2ncc3cc(Nc4ncnn5ccc(CN6CCCC6)c45)ccc32)c1	500	*
3109	COc1cc2c(Nc3ccc(NC(=O)Nc4cccc(Cl)c4)cc3)ncnc2cc1OCCCN1CCN(C)CC1	500	*
3110	CN(C)C(=O)CN1CCC(n2cc(-c3cccc(O)c3)c3c(N)ncnc32)CC1	500	*
3111	c1ccc(Cn2ncc3cc(Nc4ncnn5ccc(COC[C@@H]6CNCCO6)c45)ccc32)nc1	500	*
3112	Cc1cc2cc(Nc3ccnc4cc(-c5ccc(CNCCCO)cc5)sc34)ccc2[nH]1	500	*
3113	C=CC(=O)Nc1cccc(Nc2nc(Nc3ccc(CN4CCOCC4)cc3)ncc2F)c1	500	*
3114	COc1cc2c(Nc3ccc(NC(=O)Nc4ccccc4C)cc3)ncnc2cc1OCCCN1CCN(C)CC1	502	*
3115	COCCOc1ccc(Nc2ncnc3cc(OCCCN4CCOCC4)c(NC(=O)c4cc([N+](=O)[O-])ccc4F)cc23)cc1Cl	503	6.30
3116	CCN(CC)CCN(C)C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	505	*
3117	CCN(CC)CCN(C)N(C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N(C)CCN(CC)CC	505	*
3118	C=CC(=O)Nc1cccc(Nc2nc(Nc3ccc(Cn4ccnc4)cc3OC)ncc2Cl)c1	506	*
3119	CCC(=O)Nc1cc2c(Nc3ccc(Oc4ccc5c(c4)OCO5)cc3)ncnc2cc1OC	509	*
3120	CCOC(=O)C1=C(N)N(c2cccnc2)C2=C(C(=O)CC(C)(C)C2)C1c1c(C)nn(-c2ccc(C)cc2)c1Cl	510	6.29
3121	O=C(CCl)OCCn1c(=O)oc2cc3ncnc(Nc4ccc(Oc5cccc(C(F)(F)F)c5)c(Cl)c4)c3cc21	510	6.29
3122	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1B(O)O	510	*
3123	Cn1c(=O)c(-c2c(Cl)cccc2Cl)cc2cnc(Nc3cccnc3)nc21	510	*
3124	Cc1ccc(Nc2ncnn3cccc23)cc1O	510	*
3125	O=C1NCc2cc(Oc3ccc(Nc4ncnc5ccn(CCO)c45)cc3Cl)ccc21	510	*
3126	COc1ccc2cc(-c3nn(C(C)C)c4ncnc(N)c34)ccc2c1.Cl	510	*
3127	Cc1ccc(C2=C(C#N)C3(C(=O)Nc4ccc(Br)cc43)c3c(-c4cccs4)nn(-c4ccccc4)c3N2)cc1	510	*
3128	CN(C)C/C=C/C(=O)Nc1cc2c(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	510.2	*
3129	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(CC)c4)nc32)C1	518	6.29
3130	O=C1COc2cc3ncnc(Nc4ccccc4)c3cc2N1CCCN1CCOCC1	518.6	*
3131	CCOc1cc2ncc(C#N)c(Nc3ccc(Cn4ccnc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	519	6.28
3132	CCC(=O)Nc1cc2c(Nc3ccc4c(c3)CCN4Cc3ccccn3)ncnc2cc1OC	519	*
3133	Cc1ccc(C2=NN(C(N)=S)C(c3ccc4ccccc4c3)C2)cc1	520	6.28
3134	COc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1B1OC(C)(C)C(C)(C)O1	520	*
3135	O=C1CCN(C/C=C/C(=O)Nc2cc3c(Nc4ccc(F)c(Cl)c4)ncnc3cc2O[C@H]2CCOC2)CC1	520.2	*
3136	CCC(=O)Nc1cc2c(Nc3ccc(NS(=O)(=O)c4ccccc4)nc3)ncnc2cc1OC	522	*
3137	COc1ccc(/C=C/C(=O)Nc2cccc(Oc3cc(Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)ncn3)c2)cc1OC	523	6.28
3138	COc1cc(N2CCN(C)CC2)ccc1Nc1ncc(Cl)c(Oc2cccc(NC(=O)CCN3CCCC3)c2)n1	525	6.28

3139	C=CC(=O)NCc1cccc(-c2cc3ccncc3[nH]2)c1	525	*
3140	COc1cc2c(Oc3ccc(NC(=O)c4cn(-c5ccccc5Cl)nn4)cc3F)ccnc2cc1OCCCN1CCCCC1	529.4	6.28
3141	NC(=S)N1N=C(c2ccc(Cl)cc2)CC1c1ccc2ccccc2c1	530	6.28
3142	O=c1c2ccc(Cl)cc2nc(-c2ccccc2)n1-c1nnc(C2CC2)s1	530	6.28
3143	NCCCn1ccc2c(-c3ccnc(Nc4cccc(OC(F)(F)C(F)F)c4)n3)cccc21	530	*
3144	NC1CCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5ccncc5)c4)c23)CC1	530	*
3145	CCC(=O)Nc1cc2c(Nc3ccc(Oc4cccnc4)cc3)ncnc2cc1OC	531	*
3146	COc1cc2ncnc(-c3c[nH]c4cc(F)c(C)cc34)c2cc1OC	533	*
3147	C[C@H](Nc1ncnc2c1sc1ccccc12)c1ccccc1	538	*
3148	C[C@@H](Nc1ncnc2c1sc1ccccc12)c1ccccc1	538	*
3149	Cn1ccc2cc(-c3nn(C4CCCC4)c4ncnc(N)c34)ccc21	539	*
3150	C=CC(=O)Nc1cccc(Nc2nc(Nc3ccc(/C=C/c4cc(C)cc(C)c4)cc3)ncc2F)c1	539.2	*
3151	O=[N+]([O-])c1ccc2c(Nc3cccc(I)c3)ncnc2c1	540	*
3152	Nc1ncnc2c1c(-c1cnc3ccccc3c1)nn2C1CCCC1	540	*
3153	O=C(CN1CCC(CCO)CC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	542	*
3154	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N1CC(O)C1	543	*
3155	NC(=O)Nc1ccc2ncnc(Nc3ccc(Oc4ccc(Cl)c(Cl)c4)c(Cl)c3)c2c1	543	*
3156	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N(N1CC(O)C1)N1CC(O)C1	543	*
3157	COC(CCNC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)OC	544	*
3158	COC(CCNN(NCCC(OC)OC)C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)OC	544	*
3159	COc1ccc(N2Cc3cnc(Nc4ccc(F)cc4)nc3N([C@@H]3CC[C@@H](O)C3)C2=O)cc1	545	*
3160	C=CC(=O)Nc1cc(-n2c(=O)cc(C)c3cnc(Nc4nc5c(s4)CN(C)CC5)nc32)cc(C(F)(F)F)c1	549.6	*
3161	Cc1ccc(C(=O)Nc2ccc(CN3CCN(C)CC3)c(C(F)(F)F)c2)cc1NC(=O)c1cccnc1	550	6.26
3162	N#Cc1cnc2ccc(NC(=O)C#CCN3CCSCC3)cc2c1Nc1cccc(Br)c1	550	6.26
3163	Cc1[nH]c2ncnc(Nc3cccc(F)c3)c2c1C	550	*
3164	CC(C)n1nc(-c2ccc(Br)c(O)c2)c2c(N)ncnc21	550	*
3165	CN1CCN(c2ccc(Nc3ncc(Cl)c(Nc4ccc5[nH]ccc5c4)n3)cc2)CC1	557	*
3166	O=C1CSC(N/N=C/c2cc(Cl)ccc2O)=N1	560	6.25
3167	Oc1ccc(CN(Cc2cc(Cl)cc(Cl)c2O)C(=S)Nc2ccccc2)cc1	560	6.25
3168	C=C(CN(C)C)C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)c(C#N)cnc2cc1OCC	560	6.25
3169	COCCn1c(=O)oc2cc3ncnc(Nc4cccc(C(C)=O)c4)c3cc21	560	*
3170	Cc1[nH]c2ncnc(Nc3ccc(F)cc3)c2c1C	560	*
3171	Fc1cccc(COc2ccc(Nc3ncnn4ccc(COC[C@@H]5CNCCO5)c34)cc2Cl)c1	560	*
3172	CCN1CCC(=O)/C(=C/c2ccc(CC3CCCC3)cc2)C1	560	*
3173	C=CC(=O)Nc1cc2c(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	560.4	*
3174	Clc1cccc(Nc2ncnc3ccc(NCc4ccc5c(c4)OCO5)cc23)c1	570	6.24
3175	O=c1oc2cc3ncnc(Nc4ccc(F)c(F)c4)c3cc2n1CCCN1CCOCC1	570	*
3176	CC1(C)OB(c2ccc3ncnc(Nc4ccc(F)c(Cl)c4)c3c2)OC1(C)C	570	*
3177	Cc1cccc(Nc2[nH]cnc3nc(C)c(C)c2-3)c1	570	*
3178	CC(C)S(=O)(=O)c1ccccc1Nc1nc(N/N=C/c2ccc(F)cc2)ncc1Cl	570	*
3179	Nc1ncnc2c1c(-c1ccc3[nH]ncc3c1)nn2C1CCCC1	571	*
3180	COCCOc1cc2ncnc(Nc3ccc(Cl)c(C(F)(F)F)c3)c2cc1NC(=O)/C=C/CN(C)C	573.6	*
3181	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccc(OCc5ccccc5)cc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	574	6.24

3182	Nc1ccc2ncnc(Nc3cccc(C(F)(F)F)c3)c2c1	574	*
3183	Cc1ccc(C(=O)Nc2ccc(CN3CCN(C)CC3)c(C(F)(F)F)c2)cc1NC(=O)c1ccccn1	575	6.24
3184	Nc1ncnc2c1c(-c1ccc3occc3c1)nn2C1CCCC1	575	*
3185	CC(C)n1nc(-c2cc(O)cc(F)c2)c2c(N)ncnc21	576	*
3186	FC(F)(F)c1cccc(Nc2ncnc3ccccc23)c1	577	*
3187	Nc1cc2ncnc(NCc3ccccc3)c2cn1	578	*
3188	CC(=O)N(C)/N=N/c1ccc2ncnc(Nc3cccc(C)c3)c2c1	578	*
3189	CC(C)n1nc(-c2cccc(C(=O)NC3=NCCS3)c2)c2c(N)ncnc21	579	*
3190	Cc1ccc(NC(=O)c2ccc(N(CCCl)CCCl)cc2)cc1	580	6.24
3191	O=C(Nc1ccc(Oc2ccnc3[nH]ccc23)c(F)c1)c1nnn(-c2ccc(F)cc2)c1C(F)(F)F	582.17	*
3192	COc1ccc(/C=N/Nc2ncc(Cl)c(Nc3ccccc3S(=O)(=O)C(C)C)n2)cc1	587	*
3193	COc1cc2c(NCc3ccccc3)ncnc2cc1O	588	*
3194	OC[C@@H](Nc1ncnc2oc(-c3ccccc3)c(Cl)c12)c1ccccc1	589	*
3195	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1-c1cccc(CN2CCOCC2)c1	590	6.23
3196	NC(=S)N/N=C(/C=C/c1ccccc1)c1ccc(Cl)cc1	590	6.23
3197	CC1(C)OB(c2ccc3ncnc(Nc4cccc(Cl)c4)c3c2)OC1(C)C	590	*
3198	Cc1cc(-c2cnc(Nc3cc(Cl)cc(Cl)c3)nc2NC2CCC(N(C)C)CC2)on1	590	*
3199	Fc1ccc(Oc2ncnc3ccccc23)cc1Cl	590	*
3200	N#Cc1ccc(Oc2ccc(Nc3ncnc4cc[nH]c34)cc2Cl)cc1	590	*
3201	C=CC(=O)Nc1ccccc1Nc1nc(Nc2ccc(NC(=O)CN3CCOCC3)cc2)ncc1Cl	592.1	*
3202	CCC(=O)Nc1cc2c(Nc3ccc(NS(=O)(=O)c4ccccc4)c(F)c3)ncnc2cc1OC	593	*
3203	CC(C)S(=O)(=O)c1ccccc1Nc1nc(N/N=C/c2ccc(C(F)(F)F)cc2)ncc1Cl	593	*
3204	Cc1ccc(Nc2ncnc3cc4c(cc23)N(CCCN2CCOCC2)C(=O)CO4)cc1	594.5	*
3205	COc1ccc(-c2c3c4cc(OC)c(OCCN(C)C)cc4oc(=O)c3n3ccc4cc(O)c(OC)cc4c23)cc1O.O=C(O)C(F)(F)F	595.4	*
3206	Cc1ccc(NC(=O)c2ccc(CN3CCN(C)CC3)cc2)cc1C(=O)Nc1ccc(OCc2cccc(F)c2)c(Cl)c1	600	6.22
3207	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(OC)c4)nc32)C1	600	6.22
3208	OCCN1CCN(Cc2ccc(-c3cc4c(N[C@H](CO)c5ccccc5)ncnc4s3)cc2)CC1	600	*
3209	OC[C@@H](Nc1ncnc2sc(-c3ccc(CN4CCNCC4)cc3)cc12)c1ccccc1	600	*
3210	COc1cc2ncnc(Nc3ccc4c(c3)CCC4)c2cc1OC.Cl	600	*
3211	Nc1ncnc2c1ncn2[C@@H]1O[C@H](COC(=O)c2ccc(S(=O)(=O)Oc3ccc(/C=C/[N+](=O)[O-])cc3)cc2)[C@@H](O)[C@H]1O	600	*
3212	O=C(NCCc1ccc(O)c(Br)c1)/C(Cc1cc(Br)c(O)c(Oc2ccc(CCNC(=O)/C(Cc3cc(Br)c(O)c(-c4cc(C/C(=N\O)C(=O)NCCc5ccc(O)c(Br)c5)cc(Br)c4O)c3)=N/O)cc2Br)c1)=N/O	600	*
3213	c1nc(Nc2ccc3[nH]ccc3c2)c2sccc2n1	600	*
3214	Cc1nc(Nc2ncc(C(=O)Nc3c(C)cccc3Cl)s2)cc(N2CCN(CCOC(=O)c3cnc(C(=O)Nc4ccc5ncnc(Nc6cccc(Cl)c6)c5c4)cn3)CC2)n1	600	*
3215	COc1cccc(/C=N/Nc2ncc(Cl)c(Nc3ccccc3S(=O)(=O)C(C)C)n2)c1	601	*
3216	c1ccc(CNc2ncnc3cccnc23)cc1	603	*
3217	C=CC(=O)Nc1cccc(Nc2nc(Nc3ccc(/C=C/c4cc(C)cc(C)c4)cc3)ncc2Cl)c1	606.5	*
3218	Cc1cccc(C)c1-c1cc2cnc(N)nc2nc1NC(=O)NC(C)(C)C	610	*
3219	CCOC(=O)c1cn2ncnc(Nc3ccc(Oc4ccccc4)cc3)c2c1CC	610	*
3220	CC(C)n1nc(-c2ccc3ncccc3c2)c2c(N)ncnc21	610	*
3221	Fc1cc(Nc2nccc(Nc3ccc4[nH]ccc4c3)n2)cc(N2CCOCC2)c1	610	*

3222	COC(=O)CNC(=O)c1ccc(Nc2ncnc3cc(OCCCN4CCN(C)CC4)c(OC)cc23)cc1	611	*
3223	COc1cc2ncnc(N[C@@H](C)c3ccc(Cl)cc3)c2cc1OCCCCCCCC(=O)NO	614	6.21
3224	COc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(Cl)c(Nc2ccc3ncccc3c2)n1	615	*
3225	Cc1ncc([N+](=O)[O-])n1CCOC(=O)/C=C/c1ccc(-c2ccccc2)cc1	620	6.21
3226	CN(C)CCCOCc1ccn2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c12	620	*
3227	COc1cc2ncc(C#N)c(Nc3ccc(Br)c(C)c3)c2cc1OC	620	*
3228	COc1cc2ncc(C(=O)NC3CC(C)(C)N([O])C(C)(C)C3)c(Nc3cccc(Cl)c3)c2cc1OC	623	6.21
3229	O=C(Cc1cc(F)c(F)cc1F)Nc1cccc(Oc2cc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncn2)c1	627	6.20
3230	COc1ccccc1-c1cc2c(N[C@@H](CO)c3ccccc3)ncnc2s1	629	*
3231	Cc1ccc(C2=NN(c3nc(-c4ccc(Cl)cc4)cs3)C(c3ccc([N+](=O)[O-])cc3)C2)cc1C	630	6.20
3232	Brc1cccc(Nc2ncnc3ccc(NCc4ccc5c(c4)OCO5)cc23)c1	630	6.20
3233	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(Sc5cccc(F)c5)c(Cl)c4)c3s2)C1)N1CCOCC1	630	6.20
3234	COc1ccc(NC(=O)c2cc(I)ccc2O)cc1	630	*
3235	CN(C)CCNC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	635	*
3236	CN(C)CCNN(NCN(C)C)C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1	635	*
3237	COc1cc(N2CCN(C)CC2)ccc1Nc1ncc(Cl)c(Oc2cccc(NC(=O)CCN(C)C)c2)n1	638	6.20
3238	CC(C)n1nc(-c2ccc3c(C=O)c[nH]c3c2)c2c(N)ncnc21	638	*
3239	CCc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C	640	6.19
3240	Fc1cccc(Cn2ncc3cc(Nc4ncnn5ccc(COC[C@@H]6COCCN6)c45)ccc32)c1	640	*
3241	CN1C(=O)c2ccc(NC(=O)CSc3nc4cc5ccccc5cc4c(=O)n3-c3ccc(S(N)(=O)=O)cc3)cc2C1=O	640	*
3242	C=CC(=O)Nc1cccc(NC(=O)Nc2nc(Nc3ccc(N4CCC(N5CCOCC5)CC4)cc3OC)ncc2Cl)c1	641	*
3243	C=CC(=O)Nc1cccc(NC(=O)Nc2ccnc(Nc3ccc(N4CCOCC4)cc3)n2)c1	644	*
3244	N#C/C(=C\c1cc(O)c(O)c(CSCc2ccccc2)c1)C(N)=O	645.65	*
3245	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C#Cc1ccccc1	650	6.19
3246	Cc1ccc(C2=NN(C3=NC(c4ccccc4)CS3)C(c3ccc4ccccc4c3)C2)cc1C	650	6.19
3247	CCOc1cc2ncc(C#N)c(Nc3ccc(Oc4ccncc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	650	6.19
3248	CN(C)C/C=C/C(=O)Nc1ccc2ncc(C#N)c(Nc3ccc(F)c(Cl)c3)c2c1	650	6.19
3249	OB(O)c1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	650	*
3250	COc1cc2nccc(Oc3cccc(NC(=O)c4ccc(C(C)(C)C)cc4)c3)c2cc1OC	650	*
3251	Cc1cc2c(Nc3ccc(C)c(O)c3)ncnn2c1	654	*
3252	Cc1cc2cc(Nc3ccnc4cc(-c5ccc(CNCCOCCO)cc5)sc34)ccc2[nH]1	657	*
3253	NC(=S)N1N=C(c2ccc(Cl)c(Cl)c2)CC1c1ccc2ccccc2c1	660	6.18
3254	CN(C)C/C=C/C(=O)Nc1ccc(-c2cncc(C#N)c2Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)cc1	660	6.18
3255	CCOC(=O)CCCn1c(=O)oc2cc3ncnc(Nc4ccc(C(=O)OCc5ccc(Cl)cc5)cc4)c3cc21	660	*
3256	COc1cc2ncnc(Nc3cc4ccccc4cn3)c2cc1OC	660	*
3257	CCOc1cc2ncnc(C#C[C@](C)(Cc3ccccc3)N3CCC(C(=O)O)CC3)c2cc1OCC	662	*
3258	CCOC(=O)C1CCN([C@](C)(C#Cc2ncnc3cc(OCC)c(OCC)cc23)Cc2ccccc2)CC1	662	*
3259	Cc1ccc(-c2nn(C(C)C)c3ncnc(N)c23)cc1O	663	*
3260	Cc1ccc(Nc2ncnc3[nH]ccc23)cc1	667.13	*
3261	COc1cc2c(Nc3ccc(NC(=O)Nc4ccc(C)c(C)c4)cc3)ncnc2cc1OCCCN1CCN(C)CC1	668	*
3262	Oc1c(Cl)cccc1CN(Cc1ccc(F)cc1)C(=S)Nc1ccccc1	670	6.17
3263	COc1ccc(Nc2ncnc3cc(N)ncc23)cc1	670	*
3264	C=C(CN(C)C)C(=O)c1ccc(OCc2ccccc2)c(O)c1.Cl	670	*

3265	Cn1c(=O)c(-c2c(Cl)cccc2Cl)cc2cnc(Nc3cccc(Br)c3)nc21	670	*
3266	COCCOc1cc(OC2CCOCC2)c2c(Nc3ccc(F)c(Cl)c3)ncnc2c1	671	*
3267	CCC(=O)Nc1cccc(-c2c[nH]c3nccc(-c4[nH]c(CCCO)nc4-c4ccc(F)cc4)c23)c1	673	*
3268	C=CC(=O)Nc1cccc(-c2c[nH]c3nccc(-c4[nH]c(CCCO)nc4C4CC4)c23)c1	673	*
3269	COc1ccc(Nc2ncnc3ccncc23)c(N)c1	676.08	*
3270	Clc1ccc(C2=NN(c3ccccc3)C(c3cccc4ccccc34)C2)cc1	680	6.17
3271	CN1CCN(Cc2ccc(NC(=O)c3cccc(NC(=O)c4cnc5[nH]ccc5c4)c3)cc2C(F)(F)F)CC1	680	6.17
3272	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc5c(ccn5Cc5cscn5)c4)c3s2)C1)N1CCOCC1	680	6.17
3273	C=CC(=O)Nc1cccc(-c2c[nH]c3nccc(-c4[nH]c(CCCO)nc4C(F)(F)F)c23)c1	680	*
3274	Fc1ccc2c(Nc3cccc(Br)c3)ncnc2n1	684	*
3275	Brc1cccc(Nc2ncnc3ncccc23)c1	688	*
3276	CN1CCC(Oc2cccc3ncnc(Nc4ccc(OCc5cnccn5)c(Cl)c4)c23)CC1	690	*
3277	O=c1oc2c(O)c(O)cc3c(=O)oc4c(O)c(O)cc1c4c23	690	*
3278	COc1cc2c(Nc3ccc(NC(=O)c4ccc(C)cc4)cc3)ncnc2cc1OCCCN1CCN(C)CC1	690	*
3279	COc1cc2c(Oc3ccc(NC(=O)c4cn(-c5ccccc5OC)cn4)cc3F)ccnc2cc1OCCCN1CCN(C)CC1	690	*
3280	C[C@@H](c1ccccc1)n1ncc2cc(Nc3ncnn4ccc(COC[C@@H]5CNCCO5)c34)ccc21	690	*
3281	CCCCCCCCCCCCCCCCCCOC(=O)COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1	692	6.16
3282	CCOC(=O)N1CCN(CCC(=O)Nc2cccc(Oc3nc(Nc4ccc(N5CCN(C)CC5)cc4OC)ncc3Cl)c2)CC1	698	6.16
3283	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N1CCC(F)CC1	699	*
3284	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N(N1CCC(F)CC1)N1CCC(F)CC1	699	*
3285	NC(=S)N/N=C(/C=C/c1ccc(OCc2ccccc2)cc1)c1ccccc1	700	6.15
3286	COc1cc2c(cc1OC)Oc1ncnc(Oc3cccc(Br)c3)c1NC2	700	6.15
3287	N#C/C(=C\c1ccc(O)c(O)c1)C(=O)NCCCc1ccccc1	700	*
3288	CC(C)(C)CCOC(=O)c1cc(NCc2cc(O)ccc2O)ccc1O	700	*
3289	O=C1NC(=O)c2cc(Nc3ccc(F)cc3)c(Nc3ccc(F)cc3)cc21	700	*
3290	C=C(CN(C)C)C(=O)c1ccc(OS(=O)(=O)c2ccc(C(=O)N(C)C)cc2)cc1.Cl	700	*
3291	CCOC(=O)CCCc1ccc(Nc2ncc3cc(-c4c(Cl)cccc4Cl)c(=O)n(C)c3n2)cc1	700	*
3292	CCOc1ccc2cc(-c3nn(C(C)C)c4ncnc(N)c34)ccc2c1.Cl	700	*
3293	Cc1ccc(NC(=O)c2ccc(CN3CCN(C)CC3)cc2)cc1-c1ccc2ccncc2c1	700	*
3294	CN(C)c1ccc(C=C2CNCC(=C\c3ccc(N(C)C)cc3[N+](=O)[O-])/C2=N\O)c([N+](=O)[O-])c1	700	*
3295	COc1cc(/C=C(\C#N)C(N)=O)cc(CSc2ccccc2C(=O)O)c1O	707.95	*
3296	Brc1ccc(C2=NN(c3ccccc3)C(c3ccc4ccccc4c3)C2)cc1	710	6.15
3297	O=C1NC(=O)N(CCc2ccccc2)/C1=C/c1ccc(O)cc1	710	*
3298	CC(=O)N1CCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)CC1	710	*
3299	Fc1ccc(-c2nc(-c3ccccc3)[nH]c2-c2ccnc3[nH]ccc23)cc1	712	*
3300	CCC(=O)Nc1cc2c(Nc3ccc4c(ccn4Cc4cccnc4)c3)ncnc2cc1OC	714	*
3301	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5CCN(C)C(C)C5)c(C)c4)nc32)C1	715	6.15
3302	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)NC[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO	719	6.14
3303	OC[C@@H](Nc1ncnc2sc3c(c12)CCCC3)c1ccccc1	720	*
3304	COc1cc(Nc2c(C#N)cnc3cc(C#CCCN4CCN(C)CC4)c(OC)cc23)c(Cl)cc1Cl	720	*
3305	O=C(COc1cc(F)c(F)c(F)c1)Nc1cccc(Oc2cc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncn2)c1	721	6.14
3306	O=C(Nc1cc2c(Nc3ccc(F)cc3)ncnc2cc1OCCCN1CCOCC1)c1cc([N+](=O)[O-])ccc1F	722	6.14

3307	CC(=O)Nc1ccc2c(c1)C(c1ccccc1Cl)=Nc1c[nH]nc1N2	726	*
3308	COc1cc2ncnc(N=Nc3ccc(F)c(Cl)c3)c2cc1OC	730	*
3309	COc1cc2c(Nc3ccc(NC(=O)c4ccccc4Cl)cc3)ncnc2cc1OCc1ccccc1	730	*
3310	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(S(C)(=O)=O)CC4)cc3OC)ncc2SC)c1	730.5	*
3311	COc1ccc(-c2cc3c(NCc4cccc(F)c4)ncnc3[nH]2)cc1	731	*
3312	Brc1cccc(Nc2ncnc3c2sc2ncccc23)c1	732	*
3313	Nc1ncnc2c1c(-c1ccc3[nH]ccc3c1)nn2C1CCCC1	734	*
3314	CNC(=O)c1ncc(C#Cc2cc(C(=O)Nc3ccc(CN4CCN(CCO)CC4)c(C(F)(F)F)c3)ccc2C)n1C	736	*
3315	CNC(=O)c1nc(-c2ccc(Cl)c(S(=O)(=O)Nc3cccc(F)c3F)c2)cnc1N	739	*
3316	Brc1cccc(Nc2ncnc3c2oc2ccccc23)c1	740	*
3317	COC(=O)CN1CCC(n2cc(-c3cccc(O)c3)c3c(N)ncnc32)C1	740	*
3318	COc1cc(N2CCN(C)CC2)ccc1Nc1nccc(Oc2cccc([N+](=O)[O-])c2)n1	740	*
3319	COc1cc2ncc(C#N)c(Nc3cccc(F)c3)c2cc1OC	740	*
3320	Cn1c2ccccc2c2c(Nc3cccc(Br)c3)ncnc21	742	*
3321	CCC(=O)Nc1cc2c(Nc3ccc(CCc4ccccc4)cc3)ncnc2cc1OC	747	*
3322	CC(C)c1ccc(NC(=O)c2ccc(N(CCCl)CCCl)cc2)cc1	750	6.12
3323	COc1cccc(-c2cn(C3CCN(CC(=O)N(C)C)CC3)c3ncnc(N)c23)c1	750	*
3324	Nc1cccc(Oc2ccnc(Nc3ccccc3O)n2)c1	750	*
3325	Nc1ncnc2c1c(-c1cc(O)cc(F)c1)nn2C1CCCC1	751	*
3326	Cc1oc2ncnc(Nc3cccc(Br)c3)c2c1C(=O)O	752	*
3327	Brc1cccc(Oc2ncnc3ccccc23)c1	756	*
3328	COc1cc2c(Nc3ccc(NC(=O)c4ccc(C)cc4)cc3)ncnc2cc1OCCCN1CCOCC1	760	*
3329	Nc1ncnc2c1c(-c1ccc3cn[nH]c3c1)nn2C1CCCC1	760	*
3330	COc1cc2ncc(C#N)c(Nc3cccc(SC)c3)c2cc1OC.Cl	760	*
3331	COC(=O)CNC(=O)c1ccc(Nc2ncnc3cc(OCCCN4CCOCC4)c(OC)cc23)cc1	763	*
3332	C=CC(=O)Nc1ccccc1Nc1nc(Nc2ccc(OCCCN3CCOCC3)cc2)ncc1Cl	766.6	*
3333	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(C#N)c3)c2cc1NC(=O)/C=C/CN(C)C	768	6.11
3334	CCOc1ccc(-c2nn(C3CCCC3)c3ncnc(N)c23)cc1O	768	*
3335	CCOc1cc2ncc(C#N)c(Nc3ccc(O[C@@H](C)c4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	770	6.11
3336	COc1cc2ncc(C#N)c(Nc3ccc(-n4ccnc4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	770	6.11
3337	O=C(CN1CCN(CCO)CC1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	770	*
3338	Nc1ccc2ncnc(Nc3ccccc3)c2c1	770	*
3339	Nc1ncnc2c1c(-c1ccc(F)c(O)c1)nn2C1CCCCCC1	775	*
3340	COc1ccc(OC)c(Nc2cc(Nc3ccc(S(N)(=O)=O)cc3)ncn2)c1	779	*
3341	CCOC(=O)CCCn1c(=O)oc2cc3ncnc(Nc4ccc(OCc5nccc(OCC(F)(F)F)c5C)cc4)c3cc21	780	*
3342	O=C(O)/C=C/c1cc(CO)ccc1CO	780	*
3343	COc1cc2ncnc(Nc3cnc4ccccc4n3)c2cc1OC	780	*
3344	O=C1CNCCN(Cc2ccn3ncnc(Nc4ccc5c(cnn5Cc5cccc(F)c5)c4)c23)C1	780	*
3345	Clc1cccc(Nc2ncnc3ccc(NCc4ccc5c(c4)OCCO5)cc23)c1	790	6.10
3346	COc1cc2ncc(C#N)c(Nc3cccc(Br)c3)c2cc1NC(=O)/C=C/CN(C)C	790	6.10
3347	COCC#CC(=O)Nc1cc2c(Nc3cccc(Br)c3)c(C#N)cnc2cc1OC	790	6.10
3348	CN1CCC(O)(c2nc(-c3ccc(F)cc3)c(-c3ccncc3)o2)CC1	797	*
3349	CN(C)CCCC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	799	*

3350	CCOc1cc2ncnc(NC3=CC(=O)C(OC)=CC3=O)c2cc1NC(=O)/C=C/CN(C)C	799.3	6.10
3351	COc1cccc(CNc2ncnc3c2NCc2cc(OC)c(OC)cc2N3)c1	800	6.10
3352	CCOc1cc(N)c(C(=O)Nc2ccc(F)c(Cl)c2)cc1NC(=O)c1ccc(CN2CCN(C)CC2)cc1	800	6.10
3353	CCOc1cc(N)c(C(=O)Nc2ccc(OCc3ccccn3)c(Cl)c2)cc1NC(=O)/C=C/CN(C)C	800	6.10
3354	O=C(NC(CO)Cc1ccccc1)c1cc2cc(Cl)ccc2[nH]1	800	6.10
3355	CCCCOC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1.Cl	800	*
3356	OB(O)c1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	800	*
3357	CCCCOC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1	800	*
3358	Nc1ncnc2c1c(-c1ccccc1)nn2-c1ccccc1	800	*
3359	COc1cc2c(Nc3ccc(C#N)cc3F)ncnc2cc1OC/C=C/CN1CCCC1	800	*
3360	COc1cc2c(Nc3ncc(CC(=O)Nc4cccc(F)c4)s3)ncnc2cc1OCCCN1CCC(CO)CC1	800	*
3361	COC(=O)CN1CCC(n2cc(-c3cccc(O)c3)c3c(N)ncnc32)CC1	800	*
3362	C=CC(=O)Nc1cc2c(Nc3cccc(Br)c3)c(C#N)cnc2cc1OC	810	6.09
3363	O=[N+]([O-])c1ccc2c(Nc3cccc(Cl)c3)ncnc2c1	810	*
3364	c1cncc(Cn2ncc3cc(Nc4ncnn5ccc(COC[C@@H]6CNCCO6)c45)ccc32)c1	810	*
3365	CCOC(=O)C(=CNc1ccc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2c1)C(=O)OCC	812	*
3366	COc1cc2c(Nc3ccc(NC(=O)Nc4ccc(C)c(C)c4)c(Cl)c3)ncnc2cc1OCCN1CCCCC1	817	*
3367	COc1ccc(C2CC(c3ccc(C)c(C)c3)=NN2c2nc(-c3ccc(Cl)cc3)cs2)cc1	820	6.09
3368	O=[N+]([O-])c1cccc(-c2c(-c3ccccc3)oc3ncnc(N[C@H](CO)c4ccccc4)c23)c1	820	*
3369	COc1cc2ncnc(Nc3nnc4ccccc4n3)c2cc1OC	820	*
3370	COc1cc2ncnc(N3CCc4ccccc43)c2cc1OC	820	*
3371	Cc1cccc(Nc2[nH]cnc3nc4c(c2-3)CCCC4)c1	820	*
3372	COc1cc2ncc(C#N)c(Nc3cccc(N)c3)c2cc1OC	820	*
3373	O=C(Nc1cccc(Cl)c1)c1ccc(O)c(O)c1O	820	*
3374	O=C(/C=C/c1ccc(F)cc1)Nc1cccc(Oc2cc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncn2)c1	821	6.09
3375	O=C1COc2cc3ncnc(Nc4ccc(Br)cc4)c3cc2N1CCCN1CCOCC1	823.9	*
3376	O=C1COc2cc3ncnc(Nc4cccc(C(F)(F)F)c4)c3cc2N1CCCN1CCOCC1	829.2	*
3377	Cc1ccc(C2=NN(C(N)=S)C(c3ccc(F)cc3)C2)cc1C	830	6.08
3378	CN(CCCOc1ccc2ncnc(Nc3ccc(OCc4ccccc4)cc3)c2c1)CCS(C)(=O)=O	830	*
3379	COC(=O)CN1CCC(n2cc(-c3cccc(OC)c3)c3c(N)ncnc32)C1	830	*
3380	Nc1cc2ncnc(Nc3cccc(F)c3)c2cn1	840	*
3381	COc1cc2ncc(C#N)c(Nc3cccc(Br)c3C)c2cc1OC	840	*
3382	COc1cccc(Nc2ncnc3ccccc23)c1	842	*
3383	COc1ccc(-c2c3c4cc(OCCN(C)C)c(OC)cc4oc(=O)c3n3ccc4cc(O)c(OC)cc4c23)cc1O.O=C(O)C(F)(F)F	842.3	*
3384	COc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(Cl)c(Nc2cnc3ccccc3c2)n1	848	*
3385	CCOc1cc([N+](=O)[O-])c(C(=O)Nc2ccc(OCc3ccccn3)c(Cl)c2)cc1NC(=O)/C=C/CN(C)C	850	6.07
3386	O=C(CCc1c(SSc2[nH]c3ccccc3c2CCC(=O)NCc2ccccc2)[nH]c2ccccc12)NCc1ccccc1	850	*
3387	C#Cc1cccc(Nc2c(C#N)cnc3cc(OCCOC)c(OCCOC)cc23)c1	850	*
3388	COc1cc2ncc(C#N)c(Nc3cccc(N(C)C)c3)c2cc1OC.Cl	850	*
3389	COc1ccc(NC(=O)/C=C/c2ccc3c(c2)OCCCCO3)cc1	850	*
3390	Nc1c(F)cccc1Nc1ncnc2ccncc12	851.14	*
3391	COc1cc(Nc2nccc(Nc3cnc4ccccc4c3)n2)cc(OC)c1OC	853	*
3392	CN1CCN(C/C=C/C(=O)Nc2cc3c(Nc4ccc(Cc5ccccn5)cc4)ncnc3cn2)CC1	857	*

3393	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N1CCC(F)(F)CC1	859	*
3394	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N(N1CCC(F)(F)CC1)N1CCC(F)(F)CC1	859	*
3395	COc1cccc(Nc2[nH]cnc3nc4c(c2-3)CCCC4)c1	860	*
3396	C=CC(=O)Nc1cc(Nc2ncc(I)c(Nc3ccccc3S(=O)(=O)C(C)C)n2)c(OC)cc1N(C)CCN(C)C	865	*
3397	C=C=Cc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1	865.2	*
3398	CC(C)(C)c1ccc(Nc2ncnc3cc4oc(=O)n(CCOC(=O)CBr)c4cc23)cc1	870	6.06
3399	Oc1ccc(CN(Cc2cc(Br)cc(Br)c2O)C(=S)Nc2ccccc2)cc1	870	6.06
3400	Oc1ccc(CNc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)cc1	870	6.06
3401	Clc1cccc(Nc2[nH]nc3ncnc(NCc4ccccc4)c23)c1	870	*
3402	COc1cc2ncc(C#N)c(Nc3cccc([N+](=O)[O-])c3)c2cc1OC	870	*
3403	COc1cc(OC2CCN(C(C)=O)CC2)c2c(Nc3ccc(F)c(Cl)c3)ncnc2c1	873	*
3404	CCN(CC)CCC(=O)Nc1cccc(Oc2nc(Nc3ccc(N4CCN(C)CC4)cc3OC)ncc2Cl)c1	877	6.06
3405	C#Cc1cccc(Nc2ncnc3cc(OCCOC(=O)c4ccc(C(=O)Nc5ccc6c(c5)C(C)(C)CCC6(C)C)cc4)c(OCCOC(=O)c4ccc(C(=O)Nc5ccc6c(c5)C(C)(C)CCC6(C)C)cc4)cc23)c1	880	6.06
3406	CC(C)Nc1ncnn2ccc(CN3CCC(N)CC3)c12	880	*
3407	S=C=Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	880	*
3408	CCC(=O)Nc1cc2c(Nc3ccc(Oc4cccc(F)c4)cc3)ncnc2cc1OC	881	*
3409	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N1CCCC(F)(F)C1	884	*
3410	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N(N1CCCC(F)(F)C1)N1CCCC(F)(F)C1	884	*
3411	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5C[C@H](C)N(C)[C@H](C)C5)c(C)c4)nc32)C1	888.2	6.05
3412	CCC(=O)N1CC[C@H](N2C(=O)N(c3cccc(OC(F)(F)F)c3)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C)c4)nc32)C1	889	6.05
3413	O=C1NCc2c(Oc3ccc(Nc4ncnc5ccn(CCO)c45)cc3Cl)cccc21	890	*
3414	COc1cc(/C=C(\C#N)C(N)=O)cc(CSCc2ccccc2)c1O	891.25	*
3415	CCCCCOc1ccc(Nc2c(C#N)cnc3cc(OCC)c(NC(=O)/C=C/CN(C)C)cc23)cc1Cl	894	6.05
3416	O=[N+]([O-])c1ccc2ncnc(Nc3cccc(Br)c3)c2c1	897	*
3417	CC(C)S(=O)(=O)c1ccccc1Nc1nc(N/N=C/c2ccc(OC(F)(F)F)cc2)ncc1Cl	898	*
3418	CCOc1cc([N+](=O)[O-])c(C(=O)Nc2ccc(OCc3ccccn3)c(Cl)c2)cc1NC(=O)c1ccc(CN2CCN(C)CC2)cc1	900	6.05
3419	CCc1ccc2[nH]c(C(=O)NC(CO)Cc3ccccc3)c(C(F)(F)F)c2c1	900	6.05
3420	CCOC(=O)Nc1cc(Nc2ncnc3cc(OC)c(OC)cc23)ccc1Cl.Cl	900	*
3421	CCCOC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1C.Cl	900	*
3422	CCOC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1C.Cl	900	*
3423	CCOC(=O)Nc1cc(Nc2ncnc3cc(OC)c(OC)cc23)ccc1Cl	900	*
3424	CCOC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1C	900	*
3425	CCCOC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1C	900	*
3426	COc1cc2nc(Cl)nc(Nc3ccc(C(N)=O)cc3)c2cc1OC	900	*
3427	CCCCCCNC(=O)c1cc(NCc2cc(O)ccc2O)ccc1O	900	*
3428	Clc1ccc2c(c1Nc1ncnc3cc(OCCCN4CCCC4)cc(OC4CCOCC4)c13)OCO2	900	*
3429	C#Cc1cccc(NC(=O)c2cc(OCCCCCCC(=O)NO)ccc2O)c1	900	*
3430	Cc1cc(Nc2ncc(Cl)c(Nc3ccccc3S(=O)(=O)C(C)C)n2)c(OC(C)C)cc1C1CCNCC1	900	*
3431	C=CC(=O)Nc1cc(Nc2cc[nH]n2)nc(-c2ccccc2)n1	900	*
3432	C=CC(=O)Nc1ccccc1Oc1nc(Nc2cc(C)[nH]n2)cc(N2CCN(C)CC2)n1	900	*
3433	COc1cccc(-c2cn(C3CCN(CCO)CC3)c3ncnc(N)c23)c1	900	*

3434	O=c1c(O)c(-c2ccc(O)c(O)c2)oc2cc(O)cc(O)c12	900	*
3435	COc1ccc(Nc2ncnc3oc(-c4cccc(N)c4)nc23)cc1O	900	*
3436	Cc1nc(Nc2ncc(C(=O)Nc3c(C)cccc3Cl)s2)cc(N2CCN(CCOC(=O)OCCN3CCN(N=Nc4ccc5ncnc(Cc6cccc(Br)c6)c5c4)CC3)CC2)n1	900	*
3437	CCOC(OCC)c1ccc(C=C2CNCC(=C\c3ccc(C(OCC)OCC)cc3)/C2=N\O)cc1	900	*
3438	Cc1oc2ncnc(Nc3cccc(Cl)c3)c2c1C(=O)O	901	*
3439	COc1cc(Nc2cc(Nc3ccc(Cl)cc3)ncn2)cc(OC)c1OC	901	*
3440	COc1cc(-c2nn(C(C)C)c3ncnc(N)c23)ccc1O	908	*
3441	CCOC(=O)C1=C(N)N(c2ccccnc2)C2=C(C(=O)CCC2)C1c1c(C)nn(-c2ccc(C)cc2)c1Cl	910	6.04
3442	CC#CC(=O)Nc1cc2c(Nc3cccc(Br)c3)c(C#N)cnc2cc1OC	910	6.04
3443	Cc1cccc(Nc2ncnc3ccccc23)c1	910	*
3444	COc1cc2ncnc(NC3CCc4ccccc43)c2cc1OC	910	*
3445	Cn1c(=O)c(-c2c(Cl)cccc2Cl)cc2cnc(Nc3ccncc3)nc21	910	*
3446	Clc1cccc(Nc2ncnc3ccc(NCc4ccc5c(c4)OCCCCO5)cc23)c1	920	6.04
3447	O=C(Nc1ccccc1Br)c1cc(I)ccc1O	920	*
3448	COc1cc2ncnc(Nc3cccc(C#Cc4ccccc4)c3)c2cc1OC	921	*
3449	CC(C)n1nc(-c2ccc(O)cc2)c2c(N)ncnc21	922	*
3450	C=CC(=O)Nc1cccc(N2C(=O)N(C)Cc3cnc(NC)nc32)c1	929	6.03
3451	COCCOCC#CC(=O)Nc1ccc2ncc(C#N)c(Nc3cccc(Br)c3)c2c1	930	6.03
3452	N#C/C(=C\c1ccc(O)c(O)c1)C(=O)NCCc1ccccc1	930	*
3453	COCCN(C)CCN1CCC(n2cc(-c3cccc(OC)c3)c3c(N)ncnc32)CC1	930	*
3454	CC(C)n1nc(-c2ccc3[nH]c(=O)[nH]c3c2)c2c(N)ncnc21	937	*
3455	NC(=S)N1N=C(c2ccc(Cl)cc2)CC1c1cccc2ccccc12	940	6.03
3456	O=C(Nc1ccc(Br)cc1)c1ccc(N(CCCl)CCCl)cc1	940	6.03
3457	O=C(/C=C/c1ccccc1[N+](=O)[O-])Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	940	6.03
3458	Nc1ccc2c(Nc3cccc(Br)c3)ncnc2n1	940	*
3459	COc1cc(/C=C(\C#N)S(=O)(=O)/C(C#N)=C/c2cc(O)c(O)c(OC)c2)cc(O)c1O	940	*
3460	CCOCc1cn2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c2c1CC	950	*
3461	CCCc1c(C(=O)OCC)cn2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c12	950	*
3462	Cc1cccc(Nc2ncnc3ccc(/N=N/N(C)CCN(CCN4CCOCC4)CCN(C)/N=N/c4ccc5ncnc(Nc6cccc(C)c6)c5c4)cc23)c1	950	*
3463	Cc1oc2ncnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2c1C(=O)NCCO	951	*
3464	CC(C)n1nc(-c2cccc(O)c2)c2c(N)ncnc21	954	*
3465	Cc1cc(O)ccc1-c1nn(C(C)C)c2ncnc(N)c12	954	*
3466	CC(C)n1nc(-c2ccc3c(ccn3C)c2)c2c(N)ncnc21	955	*
3467	O=C(Nc1ccccc1)N(Cc1ccc(O)cc1)Cc1cccc(Cl)c1O	960	6.02
3468	COCC#CC(=O)Nc1ccc2ncc(C#N)c(Nc3cccc(Br)c3)c2c1	960	6.02
3469	O=C1Cc2cc(Oc3ccc(Nc4ncnc5ccn(CCO)c45)cc3Cl)ccc2N1	960	*
3470	C=CC(=O)Nc1cccc(Nc2nc(Nc3ccc(OCCN4CCOCC4)cc3)ncc2Cl)c1	961.3	*
3471	CC(C)n1nc(-c2ccc3occc3c2)c2c(N)ncnc21	964	*
3472	Cc1cccc(C)c1-c1cc(C)c2nc(Nc3ccc(OCCN4CCCC4)cc3)nnc2c1	965	*
3473	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N1CC(F)C1	967	*
3474	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N(N1CC(F)C1)N1CC(F)C1	967	*
3475	O=C1CSC(N/N=C/c2cc(F)ccc2O)=N1	970	6.01

3476	Cc1ccc(C2=NN(c3nc(-c4ccc(Cl)cc4)cs3)C(c3ccc(O)cc3)C2)cc1C	970	6.01
3477	C=CC(=O)Nc1cccc(-n2c(=O)cc(CCC)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	970	*
3478	COc1ccc(N(CCNN=Nc2ccc3ncnc(Nc4cccc(Cl)c4)c3c2)CC(C)Cl)cc1	970	*
3479	O=C(Cc1nc2ccccc2[nH]1)N1N=C(c2ccc(Cl)cc2)CC1c1ccc(Cl)cc1	970	*
3480	C=CC(=O)Nc1cccc(NC(=O)Nc2ccnc(Nc3ccc(C(=O)N4CCN(C)CC4)cc3OC)n2)c1	972	*
3481	COc1cccc2c(Nc3cccc(Br)c3)ncnc12	974	*
3482	COc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(Cl)c(Nc2ccc(Cl)cc2)n1	976	*
3483	Oc1c(Br)cccc1CN(Cc1ccc(F)cc1)C(=S)Nc1ccccc1	980	6.01
3484	C=CC(=O)Nc1cccc(Nc2cc(Nc3ccc(SCC(=O)N4CCOCC4)cc3)ccc2Cl)c1	980	*
3485	CCOc1cc2ncc(C#N)c(Nc3ccc(F)c(Cl)c3)c2cc1OCC	980	*
3486	C=CC(=O)Nc1cccc(Nc2nc(Nc3ccc(Cn4ccnc4)cc3)ncc2F)c1	987	*
3487	Nc1ccc2c(c1)C(c1ccccc1Cl)=Nc1c[nH]nc1N2	989	*
3488	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/c1cccc2cccnc12	990	6.00
3489	O=c1oc2cc3ncnc(Nc4ccc(OCc5ccc(Cl)cc5)cc4)c3cc2n1CCCN1CCOCC1	990	*
3490	C=CC(=O)Nc1cccc(Nc2cc(Nc3ccc(S(=O)CC(=O)N4CCOCC4)cc3)ccc2Cl)c1	992.9	*
3491	C=CC(=O)Nc1cccc(Oc2nc(Nc3ccc(CC(=O)N4CCOCC4)cc3)ncc2Cl)c1	996	*
3492	C=CC(=O)Nc1cccc(Nc2nc(Nc3ccc(/C=C/c4ccc(C)cc4C)cc3)ncc2Cl)c1	996.1	*
3493	COc1cc2c(cc1OC)Oc1ncnc(Sc3cccc(Cl)c3)c1NC2	1000	6.00
3494	CCOc1cc(N)c(C(=O)Nc2ccc(OCc3ccccn3)c(Cl)c2)cc1NC(=O)c1ccc(CN2CCN(C)CC2)cc1	1000	6.00
3495	CCCOC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1Cl.Cl	1000	*
3496	CCOC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1Cl.Cl	1000	*
3497	CCCOC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1Cl	1000	*
3498	CCOC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1Cl	1000	*
3499	C=CC(=O)Nc1cccc(Nc2nc(Nc3ccc(Cn4ccnc4)cc3)ncc2Cl)c1	1000	*
3500	CN1C(=S)C(C(=O)Nc2ccccc2)c2ccccc21	1000	*
3501	CC(C)(C)OC(=O)c1cc(NCc2cc(O)ccc2O)ccc1O	1000	*
3502	CC(C)c1ccc(COC(=O)c2cc(NCc3cc(O)ccc3O)ccc2O)cc1	1000	*
3503	O=C(Cc1cc(NCc2cc(O)ccc2O)ccc1O)NOCc1ccccc1	1000	*
3504	O=[N+]([O-])c1ccc2c(Nc3cccc(Br)c3)ncnc2c1	1000	*
3505	O=C(O)c1ccc(S(=O)(=O)Oc2ccc(/C=C/[N+](=O)[O-])cc2)cc1	1000	*
3506	Nc1cc2ncnc(NCc3cccc(Br)c3)c2cn1	1000	*
3507	Cn1c(=O)c(-c2c(Cl)cccc2Cl)cc2cnc(NCCCCCC(=O)O)nc21	1000	*
3508	CCN(CC)CCCCNc1ncc2cc(-c3c(Cl)cccc3Cl)c(NC(=O)Nc3cccc3)nc2n1	1000	*
3509	COc1cc2c(Nc3ccc(C)cc3F)ncnc2cc1OCC1CCN(C)CC1	1000	*
3510	COc1cc2ncnc(Nc3ccc(Cl)c(NC(=O)c4cccc(N(C)C)c4)c3)c2cc1OC	1000	*
3511	COc1cc(/C=C(\C#N)C(N)=O)cc(CSCc2ccccc2Cl)c1O	1000	*
3512	Cc1cccc(Nc2ncnc3ccc(N)cc23)c1	1000	*
3513	Cc1cc2cc(Nc3ccnc4cc(-c5ccc(CNCCO)cc5)sc34)ccc2[nH]1	1000	*
3514	CC(C)n1nc(-c2cnc3ccccc3c2)c2c(N)ncnc21	1000	*
3515	Clc1cccc(Nc2ncnc3c2sc2ncccc23)c1	1000	*
3516	Nc1ccc(-c2ccc(C(=O)Nc3cccc(O)c3)c(O)c2)cc1	1000	*
3517	CCOC(=O)c1c(OC)cn2ncnc(Nc3ccc4c(cnn4Cc4cccc(F)c4)c3)c12	1000	*
3518	C=CC(=O)Nc1cccc(N2C(=O)C3CCCN3C(=O)c3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)c1	1000	*

3519	CN1CCN(c2ccc(Nc3ncc(F)c(Nc4ccc5[nH]ccc5c4)n3)cc2)CC1	1000	*
3520	Cc1cnc(Nc2ccc(N3CCN(C)CC3)cc2)nc1Nc1ccc2[nH]ccc2c1	1000	*
3521	CN1CCN(c2ccc(Nc3ncc(Br)c(Nc4ccc5[nH]ccc5c4)n3)cc2)CC1	1000	*
3522	CN1CCN(c2ccc(Nc3ncc(C(F)(F)F)c(Nc4ccc5[nH]ccc5c4)n3)cc2)CC1	1000	*
3523	CN1CCN(c2ccc(Nc3ncc([N+](=O)[O-])c(Nc4ccc5[nH]ccc5c4)n3)cc2)CC1	1000	*
3524	COc1cnc(Nc2ccc(N3CCN(C)CC3)cc2)nc1Nc1ccc2[nH]ccc2c1	1000	*
3525	COc1ccc(-c2c3c4cc(OC)c(O)cc4oc(=O)c3n3ccc4cc(O)c(OC)cc4c23)cc1O	1000	*
3526	COc1ccc(-c2c3c4cc(OC)c(OC)cc4oc(=O)c3n3ccc4cc(O)c(OC)cc4c23)cc1O	1000	*
3527	COc1ccc(- c2c3c4cc(OCCCN5CCOCC5)c(OCCCN5CCOCC5)cc4oc(=O)c3n3ccc4cc(O)c(OC)cc4c23)cc1O.CS(=O)(=O)O	1000	*
3528	COc1ccc(-c2c3c4cc(OC)c(OCCNC(=N)N)cc4oc(=O)c3n3ccc4cc(O)c(OC)cc4c23)cc1O.O=C(O)C(F)(F)F	1000	*
3529	C=CC(=O)Nc1cccc(N2C(=O)N(C)Cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4F)nc32)c1	1000	*
3530	COc1cc(N2CCN(C)CC2)ccc1Nc1ncc2c(n1)N(c1cccc(N)c1)C(=O)N(C)C2	1000	*
3531	Br.CC(Nc1ncnc2[nH]c(-c3ccc(O)cc3)cc12)c1cccc2ccccc12	1008	*
3532	CCCCCCCCCCCCCCOC(=O)COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1	1010	6.00
3533	C=CC(=O)Nc1cccc(Oc2cc(Nc3ccc(SCCCN4CCOCC4)cc3)ccc2Cl)c1	1012	*
3534	O=C(/C=C/c1ccccc1[N+](=O)[O-])Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	1020	5.99
3535	Brc1cccc(Nc2ncnc3ccc(NCc4ccc5c(c4)OCCO5)cc23)c1	1020	5.99
3536	CCOC(=O)C(=CNc1ccc2ncnc(Nc3ccc(OCc4ccccn4)c(Cl)c3)c2c1)C(=O)OCC	1020	*
3537	CC(C)[C@@H](NC(=O)OC(C)(C)C)C(=O)Nc1ccc2ncnc(Nc3ccc(F)c(Cl)c3)c2c1	1021	*
3538	CC(C)Nc1ncnc2oc(-c3ccc(OCCN4CCCC4)cc3)c(-c3ccccc3)c12	1029	*
3539	CCOC(=O)C1=C(N)N(c2cccnc2)C2=C(C(=O)CC(C)(C)C2)C1c1c(C)nn(-c2ccc(Cl)cc2)c1Cl	1030	5.99
3540	C=CC(=O)Nc1cccc(Nc2cc(Nc3ccc(S(=O)CCCN4CCOCC4)cc3)ccc2Cl)c1	1035	*
3541	C=CC(=O)Nc1cccc(Nc2nc(Nc3ccc(/C=C/c4cc(Cl)cc(Cl)c4)cc3)ncc2Cl)c1	1037	*
3542	COc1ccc(C2=NN(C(N)=S)C(c3ccc4ccccc4c3)C2)cc1	1040	5.98
3543	Cc1ccc(C2CC(c3ccc(C)c(C)c3)=NN2c2nc(-c3ccc(Cl)cc3)cs2)cc1	1040	5.98
3544	COCCNC/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	1040	*
3545	COc1cc2ncc(C#N)c(Nc3ccc(F)c(Cl)c3)c2cc1OCCCN1CCOCC1	1040	*
3546	CC(C)n1nc(-c2ccc(O)c(F)c2)c2c(N)ncnc21	1040	*
3547	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc5c(Oc6ccccn6)cccc5c4)c3s2)C1)N1CCOCC1	1050	5.98
3548	COc1cccc(CNC(=O)CSc2nc3cc4ccccc4cc3c(=O)n2-c2ccc(S(N)(=O)=O)cc2)c1OC	1050	*
3549	Fc1ccc(C2=NN(c3ccccc3)C(c3cccc4ccccc34)C2)cc1	1070	5.97
3550	O=C(Nc1ccccc1)N(Cc1ccc(O)cc1)Cc1cccc(Br)c1O	1070	5.97
3551	Cc1ccc(C2=NN(C3=NC(=O)CS3)C(c3ccccc3)C2)cc1	1080	5.97
3552	Cc1[nH]c2ncnc(NCc3ccccc3)c2c1C	1080	*
3553	COc1cc(N2CCN(C)CC2)ccc1Nc1ncc(Cl)c(Oc2ccc(COc3no[n+]([O-])c3S(=O)(=O)c3ccccc3)cc2)n1	1090	5.96
3554	OC[C@@H](Nc1ncnc2sc3c(c12)CCC3)c1ccccc1	1090	*
3555	COC(=O)C1=C(N)N(c2cccnc2)C2=C(C(=O)CCC2)C1c1cc2ccccc2n2nnnc12	1100	5.96
3556	Cc1cc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)ncn1	1100	5.96
3557	COc1cc2c(cc1OC)Oc1ncnc(Nc3cc(Cl)ccc3F)c1NC2	1100	5.96
3558	C=CC(=O)Nc1ccc(-n2c(=O)cnc3cnc(Nc4ccc(N5CCN(C)CC5)cc4)nc32)cc1	1100	5.96
3559	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4)nc32)C1	1100	5.96
3560	CCN(CC)[C@@](C)(C#Cc1ncnc2cc(OC)c(OC)cc12)CC1CCCCC1	1100	*

3561	N#C/C(=C\c1ccc(O)c(O)c1)C(=O)Nc1ccccc1Cl	1100	*
3562	N#C/C(=C\c1ccc(O)c(O)c1)C(=O)NCCCCc1ccccc1	1100	*
3563	C=C(CN1CCCCC1)C(=O)c1ccc(OCc2ccccc2)cc1.Cl	1100	*
3564	C=C(CN1CCOCC1)C(=O)c1ccc(OCc2ccccc2)cc1.Cl	1100	*
3565	CCc1c(CC(N)=O)cn2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c12	1100	*
3566	O=C(CCCCCC(=O)Nc1ccc(O)c(C(=O)Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1)NO	1100	*
3567	C=CC(=O)Nc1cccc(-c2nc(Nc3cc[nH]n3)c3ccccc3n2)c1	1100	*
3568	Cc1ccc(Oc2ccc(Nc3ncnc4cccc(O[C@H](C)C(=O)N(C)C)c34)cc2C)cn1	1100	*
3569	CC(C)n1nc(-c2ccc3[nH]ncc3c2)c2c(N)ncnc21	1100	*
3570	COCCOc1cc2ncc(C#N)c(Nc3cccc(Br)c3)c2cc1OCCOC	1100	*
3571	CCN(CC)C(C)(C#Cc1ncnc2cc(OC)c(OC)cc12)CC1CCCCC1	1100	*
3572	Cc1nc(Nc2ncc(C(=O)Nc3c(C)cccc3Cl)s2)cc(N2CCN(CCOC(=O)OCCN3CCN(CCNc4ccc5ncnc(Nc6cccc(Br)c6)c5c4)CC3)CC2)n1	1100	*
3573	Cc1nc(C)c(C=C2CC(C)CC(=Cc3nc(C)c(C)nc3C)C2=O)nc1C	1100	*
3574	CN1CCN(c2ccc(Nc3ncc(Br)c(Nc4ccc5cn[nH]c5c4)n3)cc2)CC1	1100	*
3575	COc1ccc(C(=O)Nc2ccc(Nc3ncnc4cc(OCCCN5CCN(C)CC5)c(OC)cc34)cc2)cc1	1110	*
3576	Cc1ccc2nc(/C=C/c3ccc(N(C)C)cc3)cc(-c3nnc(N)s3)c2c1	1110	*
3577	O=C(Nc1ccccc1)N(Cc1ccc(O)cc1)Cc1cc(Br)cc(Br)c1O	1120	5.95
3578	C#Cc1cccc(NC(=O)c2cc(NC(=O)CCCCCC(=O)NO)c(OC)cc2O)c1	1120	*
3579	COc1cccc(-c2cn(C3CCNC3)c3ncnc(N)c23)c1	1120	*
3580	CO/N=C/c1c(N)ncnc1NCc1ccc(F)c(Cl)c1	1123	*
3581	O=C(/C=C/Cn1cccn1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	1124	*
3582	COC/C=C/C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	1132	*
3583	Brc1cccc(Nc2ncnc3ccc(NCc4ccc5c(c4)OCCCCO5)cc23)c1	1140	5.94
3584	Nc1ncnc2c1c(-c1ccc(Cl)c(O)c1)nn2C1CCC1	1150	*
3585	Cc1ccc(C2=NN(C3=NC(=O)CS3)C(c3ccc(C)cc3)C2)cc1	1160	5.94
3586	CCOc1ccc(-c2nn(C3CCCCC3)c3ncnc(N)c23)cc1OC	1160	*
3587	COc1cc(O)c2c(c1)CCN(c1cccc(C(=O)N3CCCCC3)c1)C2=O	1180	*
3588	Cc1ccc(C(=O)NS(=O)(=O)c2ccc(Cl)cc2)c(Cl)n1	1190	5.92
3589	C=C(CNc1cc2c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c(C#N)cnc2cc1OCC)C(=O)O	1191	5.92
3590	CN(C)CCCNC/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	1196	*
3591	Fc1cccc(COc2ccc(Nc3cc(-c4ccccc4)ncn3)cc2Cl)c1	1200	5.92
3592	COc1cc2c(cc1OC)Oc1ncnc(Nc3ccc(F)c(Cl)c3)c1NC2	1200	5.92
3593	COc1cc2c(cc1OC)Oc1ncnc(Nc3ccc4c[nH]nc4c3)c1NC2	1200	5.92
3594	COc1cc2c(cc1OC)Oc1ncnc(Oc3cccc(Cl)c3F)c1NC2	1200	5.92
3595	CCOc1ccc(C(=O)Nc2ccc(OCc3ccccn3)c(Cl)c2)cc1NC(=O)/C=C/CN(C)C	1200	5.92
3596	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(Cl)c4)nc32)C1	1200	5.92
3597	C#Cc1cccc(Nc2ncnc3ccc(S(=O)(=O)n4ccc(/C=C/C(=O)NO)c4)cc23)c1	1200	*
3598	CCOC(=O)CCCn1c(=O)oc2cc3ncnc(Nc4ccc(Cl)cc4)c3cc21	1200	*
3599	CCN(CC)[C@@](C)(C#Cc1ncnc2cc(OC)c(OC)cc12)CCc1ccccc1	1200	*
3600	O=C(OCC1CCCCC1)c1cc(NCc2cc(O)ccc2O)ccc1O	1200	*
3601	COc1cc(/C=C(\C#N)C(N)=C(C#N)C#N)cc(O)c1O	1200	*
3602	COc1cccc(Nc2[nH]cnc3nc(C)c(C)c2-3)c1	1200	*

3603	CC(C)n1nc(-c2cc(F)c3cn[nH]c3c2)c2c(N)ncnc21	1200	*
3604	Cc1ccc(O)c(C(=O)Nc2cccc(Cl)c2)c1	1200	*
3605	CCN(CC)C(C)(C#Cc1ncnc2cc(OC)c(OC)cc12)CCc1ccccc1	1200	*
3606	O=[N+]([O-])c1cccc(Oc2cc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncn2)c1	1204	5.92
3607	O=C(/C=C/c1ccc(Cl)cc1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	1210	5.92
3608	COc1cc2c(c(OC)c1)C(=O)N(c1cccc(C(=O)N3CCCCC3)c1)CC2	1230	*
3609	Cc1ccccc1Nc1ncnc2[nH]ccc12	1230	*
3610	O=C1CSC(N/N=C/c2cc(Br)cc(Br)c2O)=N1	1240	5.91
3611	Nc1cc2ncnc(Nc3ccccc3[N+](=O)[O-])c2cn1	1250	*
3612	Cc1[nH]c2ncnc(Nc3cccc(O)c3)c2c1C	1250	*
3613	Cc1cc2cc(Nc3ccnc4cc(-c5ccc(CN6CCOCC6)cc5)sc34)ccc2[nH]1	1250	*
3614	NS(=O)(=O)c1ccc(-n2c(SCC(=O)Nc3ccc(N4CCOCC4)cc3)nc3cc4ccccc4cc3c2=O)cc1	1250	*
3615	COc1ccc(C2=NN(C3=NC(=O)CS3)C(c3ccc(Br)cc3)C2)cc1	1260	5.90
3616	CCNC(=O)Nc1nc2nc(NCCCCN(CC)CC)ncc2cc1-c1c(Cl)cccc1Cl	1260	*
3617	O=C(Nc1cccc(Br)c1)Nc1ccc(Oc2ncnc3sc4c(c23)CCCC4)cc1Cl	1260	*
3618	Cc1ncc([N+](=O)[O-])n1CCOC(=O)/C=C/c1ccc(OCc2ccccc2)cc1	1270	5.90
3619	CCCCCCCCCCCCCNC(=O)COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1	1270	5.90
3620	CC#CC(=O)N1CCc2c(sc3ncnc(N[C@H](CO)c4ccccc4)c23)C1	1270	*
3621	COc1cc(O)c2c(=O)c(-c3cccc(Cl)c3)coc2c1	1270	*
3622	CCN(CC)CCNC(=O)c1[nH]c2cnnc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)c2c1C	1280	5.89
3623	O=C(Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1)c1cccc2c1OCCO2	1290	5.89
3624	Cn1c2ccccc2c2ccc(NC(=O)CSc3nc4cc5ccccc5cc4c(=O)n3-c3ccc(S(N)(=O)=O)cc3)cc21	1290	*
3625	COC(=O)C1=C(N)N(c2cccnc2)C2=C(C(=O)CCC2)C1c1cc2cc(OC)ccc2n2nnnc12	1300	5.89
3626	COc1cc2c(cc1OC)Oc1ncnc(Sc3cccc(Br)c3)c1NC2	1300	5.89
3627	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(F)c4)nc32)C1	1300	5.89
3628	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N(C)CCN(C)C)c(C)c4)nc32)C1	1300	5.89
3629	C#Cc1cccc(Nc2ncnc3ccc(S(=O)(=O)n4ccc(/C=C/C(=O)Nc5ccccc5N)c4)cc23)c1	1300	*
3630	COCCn1c(=O)oc2cc3ncnc(Nc4ccc(OCc5ccc(Cl)cc5)c(Cl)c4)c3cc21	1300	*
3631	N#C/C(=C\c1ccc(O)c(O)c1)C(=O)c1ccccc1	1300	*
3632	O=C(OC/C=C/c1ccccc1)c1cc(NCc2cc(O)ccc2O)ccc1O	1300	*
3633	CC(C)(C)NC(=O)c1ccc(S(=O)(=O)Oc2ccc(/C=C/[N+](=O)[O-])cc2)cc1	1300	*
3634	N#C/C(=C\c1ccc(O)c(O)c1)C(=O)NCCCCCCCCCCCNC(=O)/C(C#N)=C/c1ccc(O)c(O)c1	1300	*
3635	COc1ccc(Nc2ncc3cc(-c4c(Cl)cccc4Cl)c(=O)n(C)c3n2)cn1	1300	*
3636	O=C(NCCc1ccc(O)c(Br)c1)/C(Cc1cc(Br)c(O)c(-c2cc(C/C(=N/O)C(=O)NCCc3ccc(O)c(Br)c3)cc(Br)c2O)c1)=N\O	1300	*
3637	CN1CCN(CCC(=O)Nc2ccc3c(C#N)cnc(Nc4cccc(Br)c4)c3c2)CC1	1300	*
3638	COc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(Cl)c(Nc2cccc(Cl)c2)n1	1300	*
3639	CN1CCN(c2ccc(Nc3ncc(Br)c(Nc4ccc5ccn(C)c5c4)n3)cc2)CC1	1300	*
3640	N#C/C(=C\c1ccc(O)c(O)c1)C(N)=S	1310	*
3641	Cc1ccc(C2=NN(C3=NC(=O)CS3)C(c3cccc4ccccc34)C2)cc1C	1320	5.88
3642	Cc1ccc(C(=O)Nc2ccc(CN3CCN(C)CC3)c(C(F)(F)F)c2)cc1NC(=O)c1ccc(O)nc1	1330	5.88
3643	Fc1ccc(Nc2ncnc3sc4c(c23)CCCC4)cc1Cl	1330	*
3644	COc1cc2c(Nc3ccc(NC(=O)c4ccc(Cl)cc4)cc3)ncnc2cc1OCCCN1CCN(C)CC1	1330	*

3645	COc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(Cl)c(Nc2ccccc2)n1	1330	*
3646	Oc1c(Cl)cc(Cl)cc1CN(Cc1ccc(F)cc1)C(=S)Nc1ccccc1	1340	5.87
3647	O=C1CSC(N2N=C(c3ccccc3)CC2c2ccc(Br)cc2)=N1	1350	5.87
3648	CCCCCCCCCCCCCCCCCCCCCNC(=O)COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1	1350	5.87
3649	COc1cc2c(Nc3ccc(NC(=O)c4ccc(Cl)cc4)cc3)ncnc2cc1OCCCN1CCOCC1	1350	*
3650	Cc1ccc(C2=NN(C(N)=S)C(c3ccc(Cl)cc3)C2)cc1C	1360	5.87
3651	CCNC(=O)Nc1nc2nc(N)ncc2cc1-c1c(Cl)cccc1Cl	1360	*
3652	OCCCNc1cncc(-c2cncc(Nc3cccc(Cl)c3)n2)c1	1360	*
3653	COc1cc2ncnc(Nc3cccc(C#CCCCO)c3)c2cc1OC	1362.6	*
3654	COc1ccc2ncnc(Nc3cccc(Br)c3)c2c1OC	1370	*
3655	Cc1c2ccc(N(C)c3ccnc(Nc4ccc(S(=O)(=O)NC(=N)N)cc4)n3)cc2nn1C	1370	*
3656	Brc1cc2c(NCc3cccs3)ncnc2s1	1374	*
3657	COc1cc(O)c2c(=O)n(-c3cccc(C(=O)N4CCCCC4)c3)ccc2c1	1380	*
3658	COc1cc(OC2CCOCC2)c2c(Nc3ccc(F)c(Cl)c3)ncnc2c1	1384	*
3659	CCOc1ccc(Nc2ncnc3cc4oc(=O)n(CCCN5CCOCC5)c4cc23)cc1	1400	*
3660	CC(C)(C)OC(=O)NCCNC(=O)c1ccc(S(=O)(=O)Oc2ccc(/C=C/[N+](=O)[O-])cc2)cc1	1400	*
3661	CCN(CC)CCCNc1ncc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1	1400	*
3662	CCOc1ccc(-c2nn(C3CCCC3)c3ncnc(N)c23)cc1OC	1400	*
3663	COc1cccc(-c2nn(C(C)C)c3ncnc(N)c23)c1	1400	*
3664	Nc1ncnc2c1c(-c1ccc(Cl)c(O)c1)nn2[C@@H]1CCOC1	1400	*
3665	CC(C)n1nc(-c2ccc(F)c(O)c2)c2c(N)ncnc21	1400	*
3666	Nc1ncnc2c1c(-c1ccc3[nH]c(=O)ccc3c1)nn2C1CCCC1	1400	*
3667	Nc1ncnc2c1c(-c1cccc3[nH]ccc13)nn2C1CCCC1	1400	*
3668	CN(C)C/C=C/C(=O)Nc1ccc(F)c(Nc2ncc(Cl)c(Nc3ccc4ccccc4c3)n2)c1	1400	*
3669	CN1CCN(c2ccc(Nc3ncc(Br)c(Nc4ccc5cc[nH]c5c4)n3)cc2)CC1	1400	*
3670	Cc1cc(C(=O)N2CCOCC2)[nH]c1/C=C1\C(=O)Nc2ncnc(Nc3ccc4c(c3)CCC4)c21	1410	*
3671	O=C(CCCCCC(=O)Nc1ccc(O)c(C(=O)Nc2cccc(F)c2)c1)NO	1410	*
3672	O=C(CCCCCC(=O)Nc1ccc(O)c(C(=O)Nc2ccc(Cl)c(C(F)(F)F)c2)c1)NO	1410	*
3673	COc1cc2ncc(C#N)c(Nc3cccc(C(F)(F)F)c3)c2cc1OC	1450	*
3674	O=C1CSC(N/N=C/c2cc(Cl)cc(Cl)c2O)=N1	1460	5.84
3675	CCOC(=O)C(=CNC(=O)Nc1ccc(C(=O)Nc2ccc3ncnc(Nc4ccc(F)c(Cl)c4)c3c2)cc1)C(=O)OCC	1460	*
3676	c1ccc(CNc2ncnc3ccncc23)cc1	1460	*
3677	CCOc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(Cl)c(Nc2ccc3ccccc3c2)n1	1460	*
3678	COC(=O)CN1CCC(n2cc(-c3cccc(OC)c3)c3c(N)ncnc32)CC1	1470	*
3679	COc1cc2ncc(C#N)c(Nc3ccc(C)c(Cl)c3)c2cc1OC.Cl	1480	*
3680	O=C(Nc1ccc(Cl)cc1)c1ccc(N(CCCl)CCCl)cc1	1490	5.83
3681	COc1cc(/C=C2\CCC/C(=C\c3ccccc3Cl)C2=O)cc(OC)c1	1500	5.46
3682	Clc1cccc(Nc2ncnc3ccc(NCc4ccc(Br)s4)cc23)c1	1500	5.82
3683	COc1cc2c(cc1OC)Nc1ncnc(Nc3cccc(Br)c3)c1NC2	1500	5.82
3684	Cc1ncc(C#N)c(Nc2ccc(OCc3ccccn3)c(Cl)c2)c1C#Cc1ccc(CNCCS(C)(=O)=O)o1	1500	5.82
3685	CCOc1cc(N)c(C(=O)Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)cc1NC(=O)/C=C/CN(C)C	1500	5.82
3686	COc1ccc(-c2nc3sc(-c4ccc(Cl)cc4)cn3n2)cc1	1500	5.82
3687	CCOC(=O)CCCn1c(=O)oc2cc3ncnc(Nc4cc(C)cc(C)c4)c3cc21	1500	*

3688	COC(=O)c1ccc(S(=O)(=O)Oc2ccc(/C=C/[N+](=O)[O-])cc2)cc1	1500	*
3689	Cc1cccc2c(CCC(=O)O)c(SSc3[nH]c4c(C)cccc4c3CCC(=O)O)[nH]c12	1500	*
3690	Cl.O=C(CCN1CCOCC1)c1ccc(OCc2ccccc2)cc1	1500	*
3691	C=C(CN1CCNCC1)C(=O)c1ccc(OCc2ccccc2)cc1.Cl	1500	*
3692	CN(C)CCC(=O)c1ccc(OCc2ccccc2)cc1.Cl	1500	*
3693	O=C1N/C=C\c2ccc(c(Br)c2)Oc2cc(cc(Br)c2O)CCNC(=O)/C(=N/O)Cc2ccc(c(Br)c2)Oc2cc(cc(Br)c2O)C/C1=N\O	1500	*
3694	Cc1c(Cl)cccc1NC(=O)c1ccccc1O	1500	*
3695	Cc1ncc([N+](=O)[O-])n1CC(=O)NS(=O)(=O)c1ccc(Cl)cc1	1510	5.82
3696	Nc1ccccc1-c1nnc(SCc2ccccc2)o1	1510	5.82
3697	CCOC(=O)C(Cc1ccccc1)NC(=O)/C(C#N)=C/c1ccc(O)c(O)c1	1530	*
3698	Nc1ncnc2c1c(-c1cccc(O)c1)cn2C1CCNC1	1530	*
3699	N#C/C(=C\c1ccc(O)c(O)c1)C(=O)c1ccccc1Cl	1540	*
3700	Nc1cccc(Nc2ncnc3cc(N)ncc23)c1	1550	*
3701	COc1cc(O)c(C(=O)Nc2ccc(F)c(Cl)c2)cc1NC(=O)CCCCCC(=O)NO	1560	*
3702	COc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(Cl)c(Nc2cccc3ccccc23)n1	1560	*
3703	CCOc1cc2ncc(C#N)c(Nc3ccc(OCc4ccccc4)c(Cl)c3)c2cc1NC(=O)/C=C/c1ccccc1N(C)C	1569	5.80
3704	NC(=S)N/N=C(/C=C/c1ccc([N+](=O)[O-])cc1)c1ccccc1	1570	5.80
3705	Nc1ncnc2c1c(-c1ccc(Cl)c(O)c1)nn2[C@H]1CCOC1	1580	*
3706	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N1CCC(F)(F)C1	1581	*
3707	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N(N1CCC(F)(F)C1)N1CCC(F)(F)C1	1581	*
3708	CCCCCCCCCCCCCCCCCCCCOC(=O)COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1	1589	5.80
3709	COc1cc(/C=C2\CCC/C(=C\c3ccccc3)C2=O)cc(OC)c1	1600	5.34
3710	COc1cc2c(cc1OC)Sc1ncnc(Sc3cccc(Br)c3)c1NC2	1600	5.80
3711	CCOc1cc2ncc(C#N)c(Nc3cccc(Br)c3)c2cc1NC(=O)/C=C/CN(C)C	1600	5.80
3712	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4OC)nc32)C1	1600	5.80
3713	N#C/C(=C\c1ccc(O)c(O)c1)C(=O)NC1CCCCC1	1600	*
3714	CCc1c(CC(=O)O)cn2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c12	1600	*
3715	c1ccc(-c2cc3ncnc(Nc4ccc5[nH]ncc5c4)c3s2)cc1	1600	*
3716	CCOC(=O)C1=C(C)OC(N)=C(C#N)C1c1ccc(OC2CCCC2)cc1	1600	*
3717	CN(C)c1ccc(C=C2COCC(=C\c3ccc(N(C)C)cc3[N+](=O)[O-])/C2=N\O)c([N+](=O)[O-])c1	1600	*
3718	C/C=C/C(=O)Nc1ccc2ncc(C#N)c(Nc3cccc(Br)c3)c2c1	1620	5.79
3719	O=C(O)CCC1C(S)=Nc2ccccc21	1620	*
3720	Cc1ccc(O)cc1-n1c(=O)c2c(c3c(N)ncnc31)CCCC2	1620	*
3721	O=C(Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)c1cccc2c1OCCO2	1630	5.79
3722	CNS(=O)(=O)c1ccc(Nc2nc(Cl)nc3cc(OC)c(OC)cc23)cc1	1630	*
3723	Fc1cc(Nc2nccc(Nc3ccc4[nH]ccc4c3)n2)ccc1N1CCOCC1	1630	*
3724	Clc1ccc(CNc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)cc1	1640	5.79
3725	Fc1ccc(Nc2ncnc3ccc(C#Cc4cccs4)cc23)cc1Cl	1640.6	*
3726	COc1cc2ncnc(Nc3cccc(C#CCO)c3)c2cc1OC	1643.6	*
3727	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(Sc5ccccn5)cc4)c3s2)C1)N1CCOCC1	1650	5.78
3728	Cc1ccc(C2=NN(C3=NC(=O)CS3)C(c3ccc(Cl)cc3)C2)cc1	1660	5.78
3729	Nc1cc2ncnc(NCc3ccccc3Br)c2cn1	1670	*

3730	CCC(C)n1nc(-c2ccc(C)c(O)c2)c2c(N)ncnc21	1670	*
3731	O=C(/C=C/c1ccccc1)Nc1cccc(Oc2cc(Nc3ccc(OCc4cccc(F)c4)c(Cl)c3)ncn2)c1	1671	5.78
3732	O=c1c2ccc(Cl)cc2nc(-c2ccccc2)n1-c1nnc(-c2ccccc2)s1	1680	5.77
3733	COc1cc(C2=C(c3c[nH]c4ccc(I)cc34)C(=O)NC2=O)cc(OC)c1OC	1688	*
3734	COc1cc(/C=C(\C#N)C(N)=O)cc(CSc2cccc3ccccc23)c1O	1698.24	*
3735	COc1cc(-c2nc3sc(-c4ccc(Cl)cc4)cn3n2)cc(OC)c1OC	1700	5.77
3736	CC1=C2C=C(Cl)C=CC2N2C=C(Cc3ccccc3)NC(=O)C12	1700	5.77
3737	O=c1oc2cc3ncnc(Nc4ccc(OCc5ccccn5)cc4)c3cc2n1CCCN1CCOCC1	1700	*
3738	COc1ccc(CCNC(=O)/C(C#N)=C/c2ccc(O)c(O)c2)cc1OC	1700	*
3739	COc1ccc(NC(=O)/C(C#N)=C/c2ccc(O)c(O)c2)c(OC)c1	1700	*
3740	C=CC(=O)Nc1cccc(Oc2nc(Nc3n[nH]c4ccccc34)cc(N3CCN(C)CC3)n2)c1	1700	*
3741	Cc1cc(Nc2cc(N3CCN(C)CC3)nc(Oc3ccc(NC(=O)/C=C/CN(C)C)cc3)n2)n[nH]1	1700	*
3742	COc1cc2c(Oc3ccc(-c4cnc(Cc5ccccc5)n(C)c4=O)cc3F)ccnc2cc1OCCCN1CCOCC1	1700	*
3743	COc1cc2c(Oc3ccc(-c4cnc(Nc5ccc(F)cc5)n(C)c4=O)cc3F)ccnc2cc1OCCCN1CCOCC1	1700	*
3744	COc1ccc(C2=NN(C(=O)Cc3nc4ccccc4[nH]3)C(c3ccc(Cl)cc3)C2)cc1	1700	*
3745	CC(=O)Nc1ccc(C(=O)Nc2cccc(Cl)c2)c(O)c1	1700	*
3746	COc1cc(Nc2nccc(-c3ccc(N4CCNCC4)nc3)n2)cc(OC)c1OC	1704	*
3747	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N1CCC2(CC1)OCCO2	1715	*
3748	O=C(Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2cc1O[C@H]1CCOC1)N(N1CCC2(CC1)OCCO2)N1CCC2(CC1)OCCO2	1715	*
3749	O=C1CSC(N/N=C/c2ccc(Br)cc2)=N1	1720	5.76
3750	O=C(Nc1ccc(F)cc1)c1ccc(N(CCCl)CCCl)cc1	1720	5.76
3751	CCCCCCCCCCCCOC(=O)COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1	1720	5.76
3752	Cc1ccc(C2=NN(c3nc(-c4ccccc4)cs3)C(c3ccc(F)cc3)C2)cc1C	1730	5.76
3753	CC(=O)c1ccc2ncc(C(N)=O)c(Nc3ccc(OCc4ccccc4)cc3)c2c1	1730	*
3754	COc1cc(/C=C(\C#N)C(N)=O)cc(CSc2ccc(C)cc2)c1O	1737.8	*
3755	Oc1c(Br)cc(Br)cc1CN(Cc1ccc(F)cc1)C(=S)Nc1ccccc1	1760	5.75
3756	Nc1ncnc2c1c(-c1cccc(O)c1F)nn2C1CCCC1	1770	*
3757	CN(C)c1cccc(Nc2ncnc3cc(N)ncc23)c1	1790	*
3758	Oc1ccc(-c2nc(-c3ccco3)c(-c3ccnc4[nH]c(-c5ccccc5)cc34)[nH]2)cc1	1790	*
3759	COc1cc2ncc(C#N)c(Nc3ccc(C)c(Br)c3)c2cc1OC	1790	*
3760	C=CCOC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	1792	*
3761	COC(=O)c1ccc(S(=O)(=O)Oc2ccc(/C=C/[N+](=O)[O-])cc2)cc1O	1800	*
3762	Cl.O=C(CCN1CCCCC1)c1ccc(OCc2ccccc2)cc1	1800	*
3763	N#C/C(=C\c1ccc(O)c(O)c1)C(=O)NCC1CCCC(CNC(=O)/C(C#N)=C/c2ccc(O)c(O)c2)C1	1800	*
3764	FC(F)C(F)(F)Oc1cccc(Nc2nccc(-c3c[nH]c4ccccc34)n2)c1	1800	*
3765	COc1ccc(Nc2ncnc3cccc(OC4CCN(C)CC4)c23)cc1Cl	1800	*
3766	CC(C)(C)c1ccc(OC[C@@H](Cn2ccnc2[N+](=O)[O-])OC(=O)c2ccc(NC=C3C(=O)C=CC3=O)cc2)cc1	1800	*
3767	O=C(CCCCCC(=O)Nc1ccc(O)c(C(=O)Nc2ccc(Cl)c(Cl)c2)c1)NO	1800	*
3768	Cc1ccn2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c12	1800	*
3769	CC(C)CC(C)NC(=O)CSc1nc2cc3ccccc3cc2c(=O)n1-c1ccc(S(N)(=O)=O)cc1	1810	*
3770	CN(C)c1cccc(Nc2ncnc3ccncc23)c1N	1819.7	*
3771	Cc1ccc(C2=NN(c3nc(-c4ccccc4)cs3)C(c3ccc(Br)cc3)C2)cc1C	1840	5.74
3772	O=C(Nc1ccccc1)N(Cc1ccc(O)cc1)Cc1cc(Cl)cc(Cl)c1O	1860	5.73

3773	COc1ccccc1-c1cc2c(N[C@@H](C)c3ccccc3)ncnc2s1	1860	*
3774	Oc1ccc(CNc2ccc3ncnc(Nc4cccc(Cl)c4)c3c2)cc1	1870	5.73
3775	Cc1ncc([N+](=O)[O-])n1C/C(=N/NC(=O)c1ccccc1N)c1ccc(Br)cc1	1890	5.72
3776	COc1cc(/C=C2\CCC/C(=C\c3ccc(S(C)(=O)=O)cc3)C2=O)cc(OC)c1	1900	5.71
3777	Cc1[nH]c2ncnc(Nc3ccccc3)c2c1C	1900	*
3778	Cc1[nH]c2ncnc(Nc3cccc(C(F)(F)F)c3)c2c1C	1900	*
3779	Cc1ccc(Oc2ccc(Nc3ncnc4cc[nH]c34)cc2C)cn1	1900	*
3780	COc1cc(Br)c(C=C2CC(C)CC(=Cc3nc(C)c(C)nc3C)C2=O)cc1OC	1900	*
3781	CCOC(OCC)c1ccc(C=C2COCC(=C\c3ccc(C(OCC)OCC)cc3)/C2=N\O)cc1	1900	*
3782	CCN(CC)C/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)c(C#N)cnc2cc1OC	1910	5.72
3783	Cc1ccc(C(=O)Nc2ccc(CN3CCN(C)CC3)c(C(F)(F)F)c2)cc1NC(=O)c1cncnc1	1920	5.72
3784	Cc1ccc(C2=NN(c3nc(-c4ccccc4)cs3)C(c3ccc(O)cc3)C2)cc1C	1920	5.72
3785	Cc1ccc(-c2nc3cc(NC(=O)CCl)ccc3[nH]2)cc1	1929	*
3786	O=C1CSC(N/N=C/c2ccc(Cl)cc2)=N1	1940	5.71
3787	Nc1cc2ncnc(NCc3cccc(C(F)(F)F)c3)c2cn1	1950	*
3788	O=C(Nc1ccccc1)N(Cc1ccc(F)cc1)Cc1cccc(Cl)c1O	1980	5.70
3789	COc1cc(/C=C2\CCC/C(=C\c3cc(OC)cc(OC)c3)C2=O)cc(OC)c1	2000	5.69
3790	CCOc1cc([N+](=O)[O-])c(C(=O)Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)cc1NC(=O)/C=C/CN(C)C	2000	5.70
3791	COc1ccc(Nc2cc3c(cc2Nc2ccccc2)C(=O)NC3=O)cc1	2000	*
3792	CN(C)c1cc2ncnc(Nc3cccc(Br)c3)c2cc1[N+](=O)[O-]	2000	*
3793	CN(c1ccccc1)c1[nH]cnc2ncnc1-2	2000	*
3794	CCn1cnc2c(Nc3cccc(Cl)c3)nc(N[C@@H]3CCCC[C@@H]3N)nc21	2000	*
3795	COc1cc(Nc2c(C#N)cnc3cc(-c4ccc(CN5CCN(C)CC5)cn4)sc23)c(Cl)cc1Cl	2000	*
3796	O=C1NCCc2cc(Br)c(O)c(c2)Oc2c(Br)cc(cc2Br)CCNC(=O)/C(=N/O)Cc2cc(Br)c(O)c(c2)Oc2c(Br)cc(cc2Br)C/C1=N\O	2000	*
3797	Cc1cc(Nc2cc(N3CCN(C)CC3)nc(Oc3ccc(NC(=O)/C=C/C(F)(F)F)cc3)n2)n[nH]1	2000	*
3798	Cc1ccc(Oc2ccc(Nc3ncnc4cccc(O[C@H](C)C(=O)N(C)CCO)c34)cc2C)cn1	2000	*
3799	CN(C)c1ccc(C=C2CCCC(=C\c3ccc(N(C)C)cc3[N+](=O)[O-])/C2=N\O)c([N+](=O)[O-])c1	2000	*
3800	Cc1ccc(C2=NN(C3=NC(=O)CS3)C(c3ccc(F)cc3)C2)cc1	2010	5.70
3801	Nc1ncnc2c1c(-c1ccc(Cl)c(O)c1)nn2CC1CCNC1	2010	*
3802	O=C1CSC(N2N=C(c3ccc(Br)cc3)CC2c2ccc(Br)cc2)=N1	2030	5.69
3803	c1ccc(CNc2ncnc3cnccc23)cc1	2030	*
3804	Cc1ccc(Nc2nccc(Oc3ccc4[nH]ccc4c3)n2)cc1S(N)(=O)=O	2042	*
3805	CN(C)C/C=C/C(=O)Nc1cnc2ncc(C#N)c(Nc3cccc(Br)c3)c2c1	2043.6	5.69
3806	Cc1ccc(C2=NN(C(N)=S)C(c3cccc4ccccc34)C2)cc1	2060	5.69
3807	COc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(C(F)(F)F)c(Nc2ccc3ccccc3c2)n1	2070	*
3808	C[C@@H](Nc1ncnc2sc(Br)cc12)c1ccccn1	2079	*
3809	NC(=S)N/N=C(/C=C/c1cccc(F)c1)c1ccccc1	2080	5.68
3810	O=C(NS(=O)(=O)c1ccc(Br)cc1)c1cncc(Br)c1	2080	5.68
3811	CCOC(=O)C1=C(N)N(c2cccnc2)C2=C(C(=O)CCC2)C1c1c(C)nn(-c2ccccc2)c1Cl	2090	5.68
3812	Nc1ncnn2ccc(C(=O)Nc3ccc(NC(=O)Nc4cccc(F)c4)cc3)c12	2090	*
3813	COc1cc(/C=C2\CCC/C(=C\c3ccccc3F)C2=O)cc(OC)c1	2100	5.67
3814	N#C/C(=C\c1ccc(O)c(O)c1)C(=O)N1CCc2ccccc21	2100	*

3815	Cc1ccc(SCC(CN(C)C)C(=O)c2ccc(OCc3ccccc3)cc2)cc1C.Cl	2100	*
3816	Cc1ccc(Nc2[nH]cnc3nc(C)c(C)c2-3)cc1	2100	*
3817	CN1CCC(Oc2cccc3ncnc(Nc4ccc(OCc5ccccn5)cc4)c23)CC1	2100	*
3818	C[C@@H]1CN(c2nc(C(F)(F)F)no2)CCN1c1ncc(OCc2ccc(CS(C)(=O)=O)cc2F)cn1	2100	*
3819	COc1cccc(-c2cn(C3CCN(C(=O)OC(C)(C)C)C3)c3ncnc(N)c23)c1	2100	*
3820	Nc1ncnc2c1c(-c1ccc3ncccc3c1)nn2C1CCCC1	2100	*
3821	NCCn1c(-c2ccccc2)nc2cc(Cl)ccc2c1=O	2110	5.68
3822	Cl.c1ccc(Nc2[nH]cnc3c4ccccc4nc2-3)cc1	2110	*
3823	Cl.c1ccc(Nc2ncnc3c2[nH]c2ccccc23)cc1	2110	*
3824	COc1cc(OC)c2c(=O)n(-c3cccc(C(=O)N4CCCCC4)c3)ccc2c1	2120	*
3825	CC(C)n1nc(-c2ccc(N)c(O)c2)c2c(N)ncnc21	2120	*
3826	CCCCCCCCCCNC(=O)COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1	2140	5.67
3827	COc1cc(Nc2nccc(-c3ccc(Cl)cc3)n2)cc(OC)c1OC	2145	*
3828	O=C(/C=C/CN1CC2(CCOCC2)C1)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	2159	*
3829	Cc1ccc(C2=NOC(c3ccc(OC4CCCC4)cc3)C2)cc1	2160	*
3830	Cc1ncc([N+](=O)[O-])n1CC(=O)NS(=O)(=O)c1ccc(Br)cc1	2170	5.66
3831	Cc1ccc(C2=NN(C(N)=S)C(c3ccc(Br)cc3)C2)cc1C	2170	5.66
3832	NC(=S)N/N=C(/C=C/c1ccc(F)cc1)c1ccc(Br)cc1	2170	5.66
3833	O=C1CSC(N/N=C/c2ccc(F)cc2)=N1	2180	5.66
3834	O=C(/C=C/c1ccc2c(c1)OCCCCO2)NCc1ccccc1F	2180	*
3835	COc1ccc(-c2nn(C(C)C)c3ncnc(N)c23)cc1O	2190	*
3836	COc1cc(/C=C2\CCC/C(=C\c3cccc(Cl)c3)C2=O)cc(OC)c1	2200	*
3837	COc1cc2ncnc(Nc3ccc(Cl)c(NC(=O)c4ccccc4)c3)c2cc1OC	2200	*
3838	ClCCN(CCNN=Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1)c1ccc(Cl)cc1	2200	*
3839	CCCC(Cc1coc2nc(N)nc(N)c12)c1ccccc1OC	2200	*
3840	CC(C)(C)OC(=O)N1CCC(n2cc(-c3cccc(O)c3)c3c(N)ncnc32)C1	2200	*
3841	N#Cc1cnc(Nc2cccc(Br)c2)c2cc(NC(=O)[C@@H]3CCC(=O)N3)ccc12	2200	*
3842	COc1cc2ncc(C#N)c(Nc3cccc(N=[N+]=[N-])c3)c2cc1OC	2210	*
3843	O=C(CCCCCC(=O)Nc1ccc(O)c(C(=O)Nc2ccc(F)c(F)c2)c1)NO	2220	*
3844	Cc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(Cl)c(Nc2ccc3ccccc3c2)n1	2220	*
3845	NC(=S)N1N=C(c2ccccc2)CC1c1cccc2ccccc12	2230	5.65
3846	CN(C)c1ccc(/C=C/c2cc(C(=O)O)c3cc(Br)ccc3n2)cc1	2230	*
3847	O=C(Nc1ccccc1)N(Cc1ccc(F)cc1)Cc1cccc(Br)c1O	2240	5.65
3848	Cc1c(C(=O)c2ccc(Cl)cc2)c2ccc(OC(F)(F)F)cc2n1Cc1cccc(O[C@H](C)C(=O)O)c1	2240	*
3849	Cn1ccc2cc(Nc3ccnc(Nc4ccc(N5CCOCC5)cc4)n3)ccc21	2240	*
3850	C#Cc1cccc(NC(=O)c2cc(NC(=O)CCCCCCC(=O)NO)ccc2O)c1	2250	*
3851	O=C1CSC(N2N=C(c3ccc(Cl)cc3)CC2c2ccc(Br)cc2)=N1	2280	5.64
3852	COc1cc(N2CCN(C)CC2)ccc1Nc1ncc(Cl)c(Oc2ccc(CCCOc3no[n+]([O-])c3S(=O)(=O)c3ccccc3)cc2)n1	2280	5.64
3853	N#Cc1cnc2ccc(NC(=O)/C=C/CN3CCOCC3)cc2c1Nc1ccc(F)c(Cl)c1	2290	5.64
3854	c1ccc2ncc(Nc3ccnc(Nc4ccc(OCCCN5CCCCC5)cc4)n3)cc2c1	2290	*
3855	CN1CCN(Cc2ccc(C(=O)Nc3ccc(-c4cncc(C#N)c4Nc4ccc(OCc5ccccn5)c(Cl)c4)cc3)cc2)CC1	2300	5.64
3856	CCOC(=O)CCCn1c(=O)oc2cc3ncnc(Nc4ccc(OCc5ccccn5)cc4)c3cc21	2300	*
3857	N#C/C(=C\c1ccc(O)c(O)c1)C(=O)c1ccc([N+](=O)[O-])cc1	2300	*

3858	COC[C@@H](Cn1ccnc1[N+](=O)[O-])OC(=O)c1ccc(NC=C2C(=O)C=CC2=O)cc1	2300	*
3859	O=C1Cc2ccc(Oc3ccc(Nc4ncnc5ccn(CCO)c45)cc3Cl)cc2N1	2300	*
3860	COc1ccc(-c2nn(C3CCC3)c3ncnc(N)c23)cc1OC	2300	*
3861	Nc1ncnc2c1c(-c1cccc(O)c1)cn2[C@H]1C[C@@H](CN2CCC2)C1	2300	*
3862	COc1cc2ncc(C#N)c(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	2320	5.63
3863	O=C(CCCCCC(=O)Nc1ccc(O)c(C(=O)Nc2ccccc2)c1)NO	2340	*
3864	COc1cc2ncnc(Nc3cccc(NC(=O)Nc4cccc(C)c4)c3)c2cc1OCCCN1CCOCC1	2350	*
3865	Cc1ccc(C2=NN(c3nc(-c4ccccc4)cs3)C(c3ccc(Cl)cc3)C2)cc1C	2360	5.63
3866	C[C@H]1CN=C(Nc2ccc3ncnc(Nc4ccc(OCc5nccs5)c(Cl)c4)c3c2)O1	2360	*
3867	COc1ccc(C2=NN(C3=NC(=O)CS3)C(c3ccccc3)C2)cc1	2370	5.63
3868	COc1cc2nc(Cl)nc(Nc3ccc(S(N)(=O)=O)cc3)c2cc1OC	2370	*
3869	C[C@@H]1CN=C(Nc2ccc3ncnc(Nc4ccc(OCc5nccs5)c(Cl)c4)c3c2)O1	2370	*
3870	NC(=S)N/N=C(/C=C/c1ccccc1)c1ccccc1	2380	5.62
3871	COc1cc(N2CCN(C)CC2)ccc1Nc1ncc(Cl)c(Oc2cccc(NC(=O)CCN3CCN(CCO)CC3)c2)n1	2388	5.62
3872	O=C(/C=C/c1ccc(Br)s1)Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	2400	5.62
3873	O=C1NC(Cc2ccccc2)=CN2C1C=C1C=C(Cl)C=CC12	2400	5.62
3874	Clc1cc(Nc2ncnc3cccc(OC4CCOCC4)c23)ccc1OCc1ccccn1	2400	*
3875	COc1cc(Nc2nn3c(N[C@H](CO)Cc4ccccc4)cc(C4CC4)nc3c2C(N)=O)cc(OC)c1	2400	*
3876	COc1cc(-c2nc(=O)c3c([nH]2)sc2ccc(C)cc23)ccc1OCC(=O)O	2400	*
3877	Cc1nc(C)c(C=C2CC(C)CC(=C/c3nc(C)c(C)nc3C)/C2=N/O)nc1C	2400	*
3878	N#Cc1ccc(Nc2ncnc3cc(OCCCN4CCOCC4)c(NC(=O)c4cc([N+](=O)[O-])ccc4F)cc23)cc1Cl	2426	5.62
3879	COc1ccc(-c2cc3c(N[C@H](C)c4ccc(OC)cc4)ncnc3[nH]2)cc1	2454	*
3880	Nc1cc2ncnc(NCc3ccc(Br)cc3)c2cn1	2460	*
3881	C=CC(=O)Nc1cc(Nc2nccc(Nc3ccccc3S(=O)(=O)C(C)C)n2)c(OC)cc1N(C)CCN(C)C	2480	*
3882	CN1CCN(Cc2ccc(C(=O)Nc3ccc(-c4cncc(C#N)c4Nc4ccc(OCc5cccc(F)c5)c(Cl)c4)cc3)cc2)CC1	2500	5.60
3883	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5CCN(C)CC5)cc4C)nc32)C1	2500	5.60
3884	N#CC(C#N)=C1C(=O)Nc2cc(O)c(O)cc21	2500	*
3885	O=C1NC(=O)c2cc(Nc3ccc(O)cc3)c(Nc3ccc(O)cc3)cc21	2500	*
3886	Cc1ccc(Nc2cc3c(cc2Nc2ccc(C)cc2)C(=O)NC3=O)cc1	2500	*
3887	N#CC(C#N)=C(N)/C(C#N)=C/c1ccc(O)c(O)c1	2500	*
3888	COc1cc(/C=C(\C)[N+](=O)[O-])ccc1OS(=O)(=O)c1ccc(C(=O)O)cc1	2500	*
3889	Cc1[nH]c2ncnc(Oc3cccc(Cl)c3)c2c1C	2500	*
3890	COc1cc2nccc(Oc3cccc(Br)c3)c2cc1OC	2500	*
3891	CC(C)n1nc(-c2ccc3cn[nH]c3c2)c2c(N)ncnc21	2500	*
3892	Cc1nc(C)c(C=C2CN(C(C)C)CC(=Cc3nc(C)c(C)nc3C)C2=O)nc1C	2500	*
3893	CCOC(OCC)c1ccc(C=C2CCCC(=Cc3ccc(C(OCC)OCC)cc3)C2=NO)cc1	2500	*
3894	c1ccc(C2=NN(c3ccccc3)C(c3cccc4ccccc34)C2)cc1	2520	5.60
3895	Nc1ncnc2c1c(-c1cccc(O)c1)cn2C1CCN(CCO)CC1	2540	*
3896	Clc1ncc2ncnc(Nc3ccccc3)c2n1	2550	*
3897	Cc1[nH]c(-c2ccccc2)c(-c2ccccc2)c1-c1nnc(C)c2nn(-c3ccc(Cl)cc3)cc12	2550	*
3898	Cc1[nH]c(-c2ccccc2)c(-c2ccccc2)c1C(=O)c1cn(-c2ccccc2)nc1-c1ccccc1	2560	*
3899	Cc1ncc([N+](=O)[O-])n1C/C(=N/NC(=O)c1ccccc1O)c1ccc(Br)cc1	2580	5.59
3900	C[C@@H](COc1cccc2ncnc(Nc3ccc(OCc4ccccn4)c(Cl)c3)c12)N(C)C(=O)CO	2580	*

3901	CN1CCN(CCOc2cc(OC3CCOCC3)c3c(Nc4c(Cl)ccc5c4OCO5)ncnc3c2)CC1	2590	5.59
3902	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc(OCc5cccc(F)c5)nc4)c3s2)C1)N1CCOCC1	2600	5.59
3903	O=c1c(-c2ccc(O)cc2)coc2cc(O)cc(O)c12	2600	*
3904	NC(=O)C1=C(N)C(=O)C=C(Nc2ccccc2O)C1=O	2600	*
3905	CC(C)n1nc(-c2ccc(C#N)c(O)c2)c2c(N)ncnc21	2600	*
3906	Nc1ncnc2c1c(-c1ccc(F)c(O)c1)nn2[C@@H]1CCOC1	2600	*
3907	Cc1cccc(Nc2c(C(N)=O)cnc3ccc(C(=O)/C=C/c4ccc(-c5ccc(S(N)(=O)=O)cc5)o4)cc23)c1	2610	*
3908	Cc1ccc(C(=O)NS(=O)(=O)c2ccc(Br)cc2)c(Cl)n1	2640	5.58
3909	CN(C)C/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)c(C#N)cnc2cc1OC(F)(F)F	2640	5.58
3910	Cc1ccc(C2CC(c3ccc(C)c(C)c3)=NN2c2nc(-c3ccccc3)cs2)cc1	2670	5.57
3911	Nc1ncnc2c1c(-c1ccc(O)cc1)cn2C1CCNC1	2670	*
3912	Cc1ccc(NC(=O)c2cc(I)ccc2O)cc1	2680	*
3913	C=C(CN1CCOCC1)C(=O)Nc1ccc2ncc(C#N)c(Nc3ccc(F)c(Cl)c3)c2c1	2700	5.57
3914	Cc1oc2ncnc(Nc3cccc(Cl)c3)c2c1C(=O)NCCO	2700	*
3915	Nc1ncnc2c1c(-c1ccc(Cl)c(O)c1)nn2CC1CCCNC1	2720	*
3916	Cc1cccc(C)c1Nc1ncc(-c2ccc(OCC3CCCN(C)C3)cc2)n2cncc12.Cl	2730	*
3917	COc1cc2ncc(C#N)c(Nc3ccc(C)cc3)c2cc1OC	2730	*
3918	O=C(Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1)C1COc2ccccc2O1	2750	5.56
3919	COc1ccc(C2=NN(C3=NC(=O)CS3)C(c3ccc4ccccc4c3)C2)cc1	2800	5.55
3920	COc1cc(-c2nc3sc(-c4ccccc4)cn3n2)cc(OC)c1OC	2800	5.55
3921	COc1cc(/C=C/[N+](=O)[O-])ccc1OS(=O)(=O)c1ccc(C(=O)O)cc1	2800	*
3922	COc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1OC	2800	*
3923	COc1cc2ncnc(Nc3cccc(NC(=O)c4ccccc4)c3F)c2cc1OC	2800	*
3924	COC(=O)c1c(OCCN2CCCCC2)c2ccccc2c2oc3c(c12)C(=O)c1ccccc1C3=O	2800	*
3925	CC(=O)c1cccc(-c2nn(C(C)C)c3ncnc(N)c23)c1	2800	*
3926	O=C(Nc1cccc(Cl)c1)c1ccc(Br)cc1O	2800	*
3927	O=C(/C=C/c1cccc2ccccc12)Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	2810	5.55
3928	COc1cc2ncnc(Sc3cccc(NC(=S)Nc4ccc(Cl)cc4)c3)c2cc1OC	2860	*
3929	COc1cccc(CNc2ncnc3cc(N)ncc23)c1	2870	*
3930	COc1cc(NC(=O)/C=C/CN(C)C)cc2c(Nc3cccc(Br)c3)c(C#N)cnc12	2880	5.54
3931	Cc1[nH]c(-c2ccccc2)c(-c2ccccc2)c1-c1ccc(NC(=O)c2ccccc2)c(=O)o1	2890	*
3932	COc1cc2c(cc1OC)Sc1ncnc(Sc3cccc(Cl)c3)c1NC2	2900	5.54
3933	Cc1ccc2c(CCC(=O)O)c(SSc3[nH]c4cc(C)ccc4c3CCC(=O)O)[nH]c2c1	2900	*
3934	O=C1NCCc2ccc(O)c(c2)Oc2c(Br)cc(cc2Br)CCNC(=O)/C(=N/O)Cc2cc(Br)c(O)c(c2)Oc2c(Br)cc(cc2Br)C/C1=N\O	2900	*
3935	C=CC(=O)Nc1cccc(Oc2nc(Nc3n[nH]c4ccc(Br)cc34)cc(N3CCN(C)CC3)n2)c1	2900	*
3936	Nc1ncnc2c1c(-c1ccc(F)c(O)c1)nn2C1CNC1	2900	*
3937	Nc1ncnc2c1c(-c1ccc(F)c(O)c1)nn2C1CCC1	2900	*
3938	Cn1nc(-c2ccc3cc[nH]c3c2)c2c(N)ncnc21	2900	*
3939	COc1cc(Br)c(C=C2CC(C)CC(=Cc3nc(C)c(C)nc3C)C2=NO)cc1OC	2900	*
3940	COc1cc2c(Nc3ccc(NC(=O)Nc4ccccc4)cc3)ncnc2cc1OCc1ccccc1	2933	*
3941	COc1ccc(Nc2ncnc3[nH]ccc23)cc1	2936.67	*
3942	Cc1ncc([N+](=O)[O-])n1CC(=O)NS(=O)(=O)c1ccccc1	2940	5.53

3943	COc1cc(N2CCN(C)CC2)ccc1Nc1ncc(Cl)c(Oc2ccc(CCOc3no[n+]([O-])c3S(=O)(=O)c3ccccc3)cc2)n1	2940	5.53
3944	Fc1ccc(Nc2ncnc3sccc23)cc1Cl	2980	*
3945	C[C@@H](Nc1ncnc2oc(-c3ccccc3)c(-c3ccccc3)c12)c1ccccc1	2991	*
3946	CN1CCN(Cc2ccc(C(=O)Nc3ccc(-c4cncc(C#N)c4Nc4ccc(F)c(Cl)c4)cc3)cc2)CC1	3000	5.52
3947	CC(C)Oc1cccc(Nc2ncnc3cc4oc(=O)n(CCCN5CCOCC5)c4cc23)c1	3000	*
3948	O=CN/C=C/c1cc(O)ccc1O	3000	*
3949	Cc1cc(C)cc(COC(=O)c2cc(NCc3cc(O)ccc3O)ccc2O)c1	3000	*
3950	O=P(O)(O)Cc1cc(NCc2cc(O)ccc2O)ccc1O	3000	*
3951	COC(=O)Cc1cc(NCc2cc(O)ccc2O)ccc1O	3000	*
3952	COc1cc(Nc2ncnc3cc(OC)c(OC)cc23)cc(OC)c1.Cl	3000	*
3953	N#CC(C#N)=Cc1cc(O)c(O)c(O)c1	3000	*
3954	COc1cc2ncnc(N(C)c3ccc(Cl)cc3)c2cc1OC.Cl	3000	*
3955	COc1cc2ncnc(N3CCc4ccccc43)c2cc1OC.Cl	3000	*
3956	O=[N+]([O-])c1cccc(Oc2ccnc(Oc3cccc([N+](=O)[O-])c3)n2)c1	3000	*
3957	NC(=S)N1N=C(c2ccccc2)CC1c1ccc2ccccc2c1	3010	5.52
3958	N#C/C(=C\c1ccc(O)c(O)c1)C(=O)NCc1ccc(O)cc1	3019.95	*
3959	COc1ccc(-c2nn(C(C)C)c3ncnc(N)c23)cc1OC	3020	*
3960	Cc1ccc(C2CC(c3ccccc3)=NN2C2=NC(=O)CS2)cc1	3030	5.52
3961	N#CC(C#N)=CNc1ccc2ncnc(Nc3ccc(OCc4ccccn4)c(Cl)c3)c2c1	3050	*
3962	C=CC(=O)N1CCc2c(sc3ncnc(N[C@@H](CO)c4ccccc4)c23)C1	3057	*
3963	Cc1ccc(C2=NN(C(N)=S)C(c3ccc([N+](=O)[O-])cc3)C2)cc1C	3060	5.51
3964	C#Cc1cccc(-n2ccc3cc(OC)cc(O)c3c2=O)c1	3060	*
3965	CNC(=O)c1nn(C)c2c1C(C)(C)Cc1cnc(Nc3ccc(N4CCN(C)CC4)cc3)nc1-2	3069	*
3966	COc1ccc(C2CC(c3ccc(C)c(C)c3)=NN2c2nc(-c3ccccc3)cs2)cc1	3080	5.51
3967	N#C/C(=C\c1ccc(O)c(O)c1)C(=O)c1cccs1	3100	*
3968	Cn1c(SSc2c(CCC(=O)O)c3ccccc3n2C)c(CCC(=O)O)c2ccccc21	3100	*
3969	O=C1N=C(N2CCC[C@H]2C(=O)Nc2ccc3ncnc(Nc4cccc(Cl)c4)c3c2)S/C1=C/c1cccc(Br)n1	3100	*
3970	C=CC(=O)Nc1ccc(Oc2nc(Nc3cc(C)[nH]n3)cc(N3CCN(C)CC3)n2)cc1	3100	*
3971	COc1cc(Br)c(C=C2CN(C(C)C)CC(=Cc3nc(C)c(C)nc3C)C2=O)cc1OC	3100	*
3972	CCCCCCCCCCOC(=O)COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1	3110	5.51
3973	Brc1ccc(CNc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)cc1	3130	5.50
3974	COc1cc(N2CCC(O)CC2)ccc1Nc1ncc(Cl)c(Oc2ccc(COc3no[n+]([O-])c3S(=O)(=O)c3ccccc3)cc2)n1	3150	5.50
3975	COc1cc2ncc(C#N)c(Nc3cc(Cl)c(O)c(Cl)c3)c2cc1OC	3150	*
3976	O=C(O[C@H]1CN[C@H](C#Cc2cc3ncnc(Nc4ccc5c(ccn5CCc5ccccc5)c4)c3s2)C1)N1CCOCC1	3160	*
3977	Cc1ccc2nc(Oc3ccccc3)c(/C=N/NC(=O)Cn3c([N+](=O)[O-])cnc3C)cc2c1	3170	5.50
3978	COc1cc2ncnc(Sc3cccc(NC(=S)Nc4ccc(F)c(F)c4)c3)c2cc1OC	3170	*
3979	O=C1CSC(N2N=C(c3ccc(Br)cc3)CC2c2ccccc2)=N1	3200	5.49
3980	C#Cc1cccc(Nc2ncnc3c2NCc2cc(OC)c(OC)cc2O3)c1	3200	5.49
3981	COc1cc2ncnc(Nc3ccc(C)c(NC(=O)c4ccccc4)c3)c2cc1OC	3200	*
3982	CCOC(=O)c1nn(-c2ccc(Cl)cc2)cc1C(=O)c1c(C)[nH]c(-c2ccccc2)c1-c1ccccc1	3200	*
3983	Cc1nnc(-n2c(-c3ccccc3)nc3cc(Cl)ccc3c2=O)s1	3210	5.49
3984	Oc1ccccc1CNc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	3220	5.49
3985	CCOC(=O)c1nn(-c2ccccc2)cc1C(=O)c1c(C)[nH]c(-c2ccccc2)c1-c1ccccc1	3220	*

3986	Cc1ncc([N+](=O)[O-])n1CCOC(=O)/C=C/c1ccc(Br)cc1	3240	5.49
3987	C[C@@H](Nc1ncnc2sc3c(c12)CCCC3)c1ccccc1	3240	*
3988	Cc1ccc(C2=NN(C3=NC(=O)CS3)C(c3ccc4ccccc4c3)C2)cc1	3250	5.49
3989	Cc1ccc2c(Nc3ccc(F)c(Cl)c3)ncnn12	3250	*
3990	Cc1ccc(/C=N/NC2=NC(=O)CS2)cc1	3260	5.49
3991	O=C(NS(=O)(=O)c1ccc(F)cc1)c1cncc(Br)c1	3270	5.49
3992	NC(=S)N1N=C(c2ccc(F)cc2)CC1c1ccc2ccccc2c1	3280	5.48
3993	Cc1cc(Oc2ncnc3sc4c(c23)CCCC4)ccc1NC(=O)Nc1cccc(Br)c1	3290	*
3994	O=C(O)c1cc(CCc2cc(O)ccc2O)ccc1O	3300	*
3995	CN(C)CCOc1ccc(/C=C/c2cc(-c3cc4c(=O)[nH]cnc4[nH]3)ccn2)cc1	3300	*
3996	COc1ccc(-c2nn(C3CCCC3)c3ncnc(N)c23)cc1OC	3300	*
3997	C#Cc1cccc(NC(=O)c2cc(NC(=O)CCCCCC(=O)NO)ccc2O)c1	3310	*
3998	O=C(Nc1cccc(Nc2ncnc3cc(OCCCN4CCOCC4)ccc23)c1)Nc1ccc(F)c(Cl)c1	3315	*
3999	COc1cc2ncc(C=O)c(Nc3cccc(Br)c3)c2cc1OC	3370	*
4000	O=C1CSC(N2N=C(c3ccccc3)CC2c2ccccc2)=N1	3380	5.47
4001	COc1cc(/C=C(\C#N)C(N)=O)cc(CSc2ccccn2)c1O	3388.44	*
4002	CN1CCN(CC(=O)Nc2cc3c(Nc4ccc(F)c(Cl)c4)ncnc3s2)CC1	3399	*
4003	Clc1cccc(Nc2ncnc3ccc(NCc4cccs4)cc23)c1	3400	5.47
4004	COc1cc2c(cc1OC)Oc1ncnc(Nc3ccc(F)cc3Cl)c1NC2	3400	5.47
4005	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5CCN(C)CC5)c(C(F)(F)F)c4)nc32)C1	3400	5.47
4006	Oc1cc2c(cc1O)[C@@H]1c3ccc(O)c(O)c3OC[C@]1(O)C2	3400	*
4007	Cc1ccc(S(=O)(=O)NC(=O)Cn2c([N+](=O)[O-])cnc2C)cc1	3430	5.46
4008	O=C(/C=C/c1ccc([N+](=O)[O-])cc1)Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	3450	5.46
4009	Cc1ccc(-n2cc3c(-c4c[nH]c(-c5ccccc5)c4-c4ccccc4)nnc(O)c3n2)cc1	3450	*
4010	Cc1cccc(CN(Cc2ccc(O)cc2)C(=S)Nc2ccccc2)c1O	3460	5.46
4011	Cc1[nH]c(/C=C2\C(=O)Nc3ccc(C(=O)NNc4ccccc4)cc32)c(C)c1CCC(=O)O	3480	*
4012	O=C1CSC(N2N=C(c3ccccc3)CC2c2ccc(Cl)cc2)=N1	3490	5.46
4013	O=C(/C=C/c1ccc(Br)cc1)Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	3490	5.46
4014	O=C1NN(c2ccc(F)c(Cl)c2)C(=O)/C1=C\c1cccc(OC(=O)c2cccs2)c1	3500	5.46
4015	CCOc1ccc(C(=O)Nc2ccc(OCc3ccccn3)c(Cl)c2)cc1NC(=O)c1ccc(CN2CCN(C)CC2)cc1	3500	5.46
4016	CN(C)C/C=C/C(=O)Nc1ccc(-c2cncc(C#N)c2Nc2ccc(F)c(Cl)c2)cc1	3500	5.46
4017	Cn1c([Se][Se]c2c(C(=O)O)c3ccccc3n2C)c(C(=O)O)c2ccccc21	3500	*
4018	O=C(/C=C/c1ccccc1)N1CCc2c(sc3ncnc(N[C@H](CO)c4ccccc4)c23)C1	3503	*
4019	C#Cc1cccc(-n2ccc3cc(OC)cc(OC)c3c2=O)c1	3510	*
4020	O=C(/C=C/c1ccc2c(c1)OCCCCO2)Nc1ccc(Br)cc1	3520	*
4021	O=C(CCCCCC(=O)Nc1ccc(O)c(C(=O)Nc2ccc(F)c(Cl)c2)c1)NO	3530	*
4022	Oc1ccccc1CNc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	3540	5.45
4023	Cc1[nH]c(-c2ccccc2)c(-c2ccccc2)c1C(=O)c1cn(-c2ccccc2)nc1C(=O)Nc1ccccc1	3560	*
4024	COc1cc2ncnc(Sc3cccc(NC(=S)Nc4ccc(Cl)cc4Cl)c3)c2cc1OC	3560	*
4025	CCCCCCCCCNC(=O)COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1	3580	5.45
4026	CC(=O)NC[C@H]1CC[C@H](c2nc(-c3cc4ccccc4[nH]3)c3c(N)nccn32)CC1	3580	*
4027	O=C(/C=C/c1cccnc1Cl)Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	3600	5.44
4028	COc1ccc(C(=O)n2nc(-c3cccnc3)nc2N)cc1	3600	5.44

4029	COc1ccc2c(C(=O)Nc3ccccc3)c(SSc3c(C(=O)Nc4ccccc4)c4ccc(OC)cc4n3C)n(C)c2c1	3600	*
4030	C=CC(=O)Nc1cccc(Oc2nc(Nc3n[nH]c4ccccc34)cc(N3CCN(C(C)=O)CC3)n2)c1	3600	*
4031	Oc1nnc(-c2c[nH]c(-c3ccccc3)c2-c2ccccc2)c2cn(-c3ccccc3)nc12	3600	*
4032	O=C(/C=C/c1ccccc1)Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	3610	5.44
4033	Cc1ncc([N+](=O)[O-])n1CCOC(=O)/C=C/c1ccc(Cl)cc1	3620	5.44
4034	COc1cccc(-c2nn(C(C)C)c3ncnc(N)c23)c1OC	3660	*
4035	Cc1c(C(=O)c2coc3ccc(O)cc23)[nH]c(-c2ccccc2)c1-c1ccccc1	3670	*
4036	O=C(Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1)C1COc2ccccc2O1	3680	5.43
4037	C[C@H](Nc1ncnc2cc3oc(=O)n(CCCN4CCOCC4)c3cc12)c1ccccc1	3700	*
4038	CCC(=O)Nc1cccc(-c2nc(Nc3cc[nH]n3)c3ccccc3n2)c1	3700	*
4039	COc1ccccc1Nc1ncnc2cc(N)ncc12	3710	*
4040	COc1cc2ncnc(Nc3ccccc3N)c2cn1	3715.35	*
4041	CC(C)n1nc(-c2cccc(O)c2F)c2c(N)ncnc21	3720	*
4042	NC(=S)N/N=C(/C=C/c1cccc([N+](=O)[O-])c1)c1ccccc1	3740	5.43
4043	CC#CC(=O)Nc1cnc2ncc(C#N)c(Nc3ccc(F)c(Cl)c3)c2c1	3762.4	5.42
4044	Cc1[nH]c(-c2ccccc2)c(-c2ccccc2)c1C(=O)c1cn(-c2ccc(Cl)cc2)nc1C(=O)Nc1ccccc1	3780	*
4045	Cc1[nH]c(/C=C2\C(=O)Nc3ccc(S(=O)(=O)Cc4c(Cl)cccc4Cl)cc32)c(C)c1C(=O)N1CCC[C@@H]1CN1CCCC1	3800	*
4046	COc1cc2ncc(C#N)c(Nc3cccc(Br)c3)c2cc1NC(=O)/C=C/CN1CCOCC1	3830	5.42
4047	Cc1ccc(C2=NN(c3nc(-c4ccccc4)cs3)C(c3ccc([N+](=O)[O-])cc3)C2)cc1C	3850	5.41
4048	COc1cc(-c2nn(C(C)C)c3ncnc(N)c23)ccc1N	3850	*
4049	COc1cc(-c2nn(C(C)C)c3ncnc(N)c23)ccc1F	3860	*
4050	Cc1ccc(C2=NN(C(N)=S)C(c3ccccc3Cl)C2)cc1C	3870	5.41
4051	Cc1ncc([N+](=O)[O-])n1CCOC(=O)/C=C/c1cccc2ccccc12	3880	5.41
4052	Brc1cc2c(NCc3ccncc3)ncnc2s1	3883	*
4053	Cc1[nH]c(-c2ccccc2)c(-c2ccccc2)c1-c1nnc(C)c2nn(-c3ccccc3)cc12	3890	*
4054	COc1cc(/C=C2\CCC/C(=C\c3ccc(N(C)C)cc3)C2=O)cc(OC)c1	3900	5.40
4055	Cc1ccc(C(=O)Nc2ccc(CN3CCN(C)CC3)c(C(F)(F)F)c2)cc1NC(=O)c1cnccn1	3900	5.41
4056	CCC1=C2C=C(C(F)(F)F)C=CC2N2C=C(Cc3ccccc3)NC(=O)C12	3900	5.41
4057	CCCOc1cc2ncnc(Nc3ccc(NC(=O)OCC)c(C)c3)c2cc1OC.Cl	3900	*
4058	CN(C)CC(CNNC(N)=O)C(=O)c1ccc(OCc2ccccc2)cc1.Cl	3900	*
4059	Cc1cc(Nc2cc(N3CCN(C)CC3)nc(Oc3cccc([N+](=O)[O-])c3)n2)n[nH]1	3900	*
4060	Cc1nc(C)c(C=C2CN(C(C)C)CC(=C/c3nc(C)c(C)nc3C)/C2=N/O)nc1C	3900	*
4061	Cc1ccc2c(C)nc(Nc3nc(O)cc(CSc4nnnn4-c4ccccc4)n3)nc2c1	3920	*
4062	O=C(Nc1ccc(Nc2ncnc3sc4c(c23)CCCC4)cc1)Nc1cccc(Br)c1	3950	*
4063	Cc1ccc(C2=NN(C3=NC(c4ccccc4)CS3)C(c3cccc4ccccc34)C2)cc1C	3960	5.40
4064	COc1ccc(N(CCCl)CCNN=Nc2ccc3ncnc(Nc4cccc(Cl)c4)c3c2)cc1	3960	*
4065	COC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1C.Cl	4000	*
4066	COC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1C	4000	*
4067	N#C/C(=C\c1ccc(O)c(O)c1)C(N)=O	4000	*
4068	CCOP(=O)(Cc1cc(NCc2cc(O)ccc2O)ccc1O)OCC	4000	*
4069	COc1cc2ncnc(N(C)c3ccccc3)c2cc1OC.Cl	4000	*
4070	CNC(=O)c1ccc(S(=O)(=O)Oc2ccc(/C=C(\C)[N+](=O)[O-])cc2OC)cc1	4000	*
4071	COc1cc2ncnc(N(C)c3ccc(C)cc3)c2cc1OC.Cl	4000	*

4072	COc1cc(O)c2c(=O)c(-c3cccc(Cl)c3)cn(CCc3ccccc3)c2c1	4000	*
4073	O=[N+]([O-])c1cccc(Oc2ccnc(Nc3ccccc3O)n2)c1	4000	*
4074	C=CC(=O)NCc1cccc(-c2nc(C3CC3)c(-c3ccnc4[nH]c(-c5ccccc5)cc34)[nH]2)c1	4050	*
4075	Clc1cccc(Nc2ncnc3ccc(NCc4cccc(Br)n4)cc23)c1	4100	5.39
4076	O=C(O)c1cc(N(Cc2ccccc2O)Cc2cc(O)ccc2O)ccc1O	4100	*
4077	c1ccc(CCNc2ncnc3ccccc23)cc1	4100	*
4078	CCN(CC)CCn1c2ccccc2c2c(Nc3cccc(Br)c3)ncnc21	4100	*
4079	CN(C)CCCC(=O)Nc1ccc2c(C#N)cnc(Nc3cccc(Br)c3)c2c1	4100	*
4080	CCN(CC)CCn1c2ccccc2c2c(Nc3cccc(Br)c3)ncnc21.Cl	4100	*
4081	Cc1ncc([N+](=O)[O-])n1CCOC(=O)/C=C/c1ccc(F)cc1	4120	5.39
4082	O=C1CSC(N2N=C(c3ccc(Br)cc3)CC2c2ccc(Cl)cc2)=N1	4120	5.39
4083	Cc1ncnc(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)c1C#CCN1CCOCC1	4130	5.38
4084	Cc1nn(-c2ccc(Cl)cc2)c(Cl)c1C1C(C#N)=C(N)N(c2cccnc2)C2=C1C(=O)CCC2	4150	5.38
4085	O=C(Nc1ccccc1)N(Cc1ccc(F)cc1)Cc1cc(Cl)cc(Cl)c1O	4150	5.38
4086	COc1cc2ncnc(Oc3cccc(NC(=S)Nc4ccc(Cl)cc4)c3)c2cc1OC	4170	*
4087	COc1cc2ncc(C#N)c(Nc3ccccc3Br)c2cc1OC	4180	*
4088	O=C(O)CCc1c(SSc2[nH]c3ccccc3c2CCC(=O)O)[nH]c2ccccc12	4200	*
4089	CONC(=O)c1cc(Nc2ncnn3cc(NC(=O)OCCCS(C)(=O)=O)c(C(C)C)c23)c(F)cc1F	4200	*
4090	O=C(CCCCCC(=O)Nc1ccc(O)c(C(=O)Nc2cccc(C(F)(F)F)c2)c1)NO	4200	*
4091	Cc1ccc(C2=NN(C(N)=S)C(c3ccccc3Br)C2)cc1C	4210	5.38
4092	COc1ccc(C2CC(c3ccc(C)cc3)=NN2C2=NC(=O)CS2)cc1	4240	5.37
4093	Nc1cc2ncnc(NCc3ccccc3[N+](=O)[O-])c2cn1	4250	*
4094	COc1ccc(C2CC(c3ccccc3)=NN2C2=NC(=O)CS2)cc1	4270	5.37
4095	CCN(CC)CCn1c2ccc(OC)cc2c2c(Nc3cccc(Br)c3)ncnc21	4270	*
4096	CCN(CC)CCn1c2ccc(OC)cc2c2c(Nc3cccc(Br)c3)ncnc21.Cl	4270	*
4097	O=C(/C=C/c1ccccc1Br)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	4280	5.37
4098	CN(C)CCN(C)CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	4286	*
4099	COC(=O)C1=C(N)N(c2cccnc2)C2=C(C(=O)CCC2)C1c1cc2cc(C)ccc2n2nnnc12	4300	5.37
4100	COc1cccc2c1C(=O)c1c(O)ccc(O)c1C2=O	4300	*
4101	COc1cc2nc(Cl)nc(Nc3ccc(O)cc3)c2cc1OC	4300	*
4102	N#C/C(=C\c1ccc(O)c(O)c1)C(=O)N1CCN(c2ccccc2)CC1	4300	*
4103	Cn1c(SSc2c(C(=O)Nc3ccccc3)c3cc(Cl)ccc3n2C)c(C(=O)Nc2ccccc2)c2cc(Cl)ccc21	4300	*
4104	COc1ccc(-c2nn(C(C)C)c3ncnc(N)c23)cc1	4300	*
4105	Cc1nc(Nc2ncc(C(=O)Nc3c(C)cccc3Cl)s2)cc(N2CCN(CCOC(=O)c3ccc(C(=O)Nc4ccc5ncnc(Nc6cccc(Cl)c6)c5c4)nc3)CC2)n1	4300	*
4106	COCOc1cc(-c2nn(C(C)C)c3ncnc(N)c23)ccc1Br	4320	*
4107	CN(C)CCCCCC(=O)Nc1cccc(-c2c(-c3ccccc3)oc3ncnc(N[C@H](CO)c4ccccc4)c23)c1	4327	*
4108	O=C(Nc1ccccc1Cl)c1cc(I)ccc1O	4370	*
4109	Oc1nnc(-c2c[nH]c(-c3ccccc3)c2-c2ccccc2)c2cn(-c3ccc(Cl)cc3)nc12	4390	*
4110	CCCCNc1ncc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1	4400	*
4111	CC(C)n1nc(-c2cc3cc(O)ccc3[nH]2)c2c(N)ncnc21	4400	*
4112	Clc1ccc(CNc2ccc3ncnc(Nc4cccc(Cl)c4)c3c2)cc1	4410	5.36
4113	CC(=O)c1nn(-c2ccc(Cl)cc2)cc1C(=O)c1c(C)[nH]c(-c2ccccc2)c1-c1ccccc1	4480	*

4114	Cc1ccc(-n2cc(C(=O)c3c(C)[nH]c(-c4ccccc4)c3-c3ccccc3)c(C(=O)Nc3ccccc3)n2)cc1	4490	*
4115	CCOc1cc(N)c(C(=O)Nc2ccc(F)c(Cl)c2)cc1NC(=O)/C=C/CN(C)C	4500	5.35
4116	C[C@@H](Nc1ncnc2cc3oc(=O)n(CCCN4CCOCC4)c3cc12)c1ccccc1	4500	*
4117	CCNc1ncc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1	4500	*
4118	CN1CCN(CCCCCNc2ncc3cc(-c4c(Cl)cccc4Cl)c(=O)n(C)c3n2)CC1	4500	*
4119	COc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(Cl)c(Nc2ccccc2Cl)n1	4560	*
4120	COc1cc(/C=C2\CCC/C(=C\c3ccc(O)cc3)C2=O)cc(OC)c1	4600	5.33
4121	COc1cc2c(cc1OC)Oc1ncnc(Oc3cccc(Br)c3)c1N(C)C2	4600	5.34
4122	COc1ccc(C(=O)n2nc(-c3ccncc3)nc2N)cc1	4600	5.34
4123	CCN(CC)CCNC(=O)c1c([Se][Se]c2[nH]c3ccccc3c2C(=O)NCCN(CC)CC)[nH]c2ccccc12	4600	*
4124	N=C(N)SCCCn1c(=O)c2c(c1=O)n1c3ccccc3cc1c1cccc3ccn2c31	4600	*
4125	CC(C)n1nc(-c2cccc3[nH]ccc23)c2c(N)ncnc21	4600	*
4126	Br.CC(Nc1ncnc2[nH]c(-c3ccc(O)cc3)cc12)c1ccc(C(F)(F)F)cc1	4608	*
4127	COc1cc2c(Nc3ccc(NC(=O)c4ccccc4)cc3)ncnc2cc1OCCN1CCCCC1	4610	*
4128	COc1cc2c(Nc3ccc(NC(=O)Nc4cccc(Cl)c4)cc3)ncnc2cc1OCc1ccccc1	4649	*
4129	CN1CCC(=O)/C(=C/c2ccc(CC3CCCC3)cc2)C1	4660	*
4130	CC(=O)c1nn(-c2ccccc2)cc1C(=O)c1c(C)[nH]c(-c2ccccc2)c1-c1ccccc1	4670	*
4131	O=C(Nc1ccccc1)N(Cc1ccc(F)cc1)Cc1cc(Br)cc(Br)c1O	4680	5.33
4132	COc1ccc(C2=NN(c3nc(-c4ccc(Cl)cc4)cs3)C(c3ccc(C)cc3)C2)cc1	4680	5.33
4133	O=C(/C=C/c1cccnc1)Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	4700	5.33
4134	O=C(CCl)OCCn1c(=O)oc2cc3ncnc(Nc4ccc(F)c(F)c4)c3cc21	4700	5.33
4135	CCN(CC)CCNC(=O)c1c([Se][Se]c2c(C(=O)NCCN(CC)CC)c3ccccc3n2C)n(C)c2ccccc12	4700	*
4136	Nc1cc2ncnc(Nc3ccc(C(F)(F)F)cc3)c2cn1	4700	*
4137	COc1cc2ncnc(Nc3ccc(C(C)(F)F)cc3)c2cc1OC	4700	*
4138	O=C1CSC(N/N=C/c2ccc(O)cc2)=N1	4710	5.33
4139	COc1ccc2c(c1)SCc1cnc(-c3ccccc3)nc1-2	4720	5.33
4140	Nc1cc(C(F)(F)F)ccc1Nc1ncnc2ccncc12	4786.3	*
4141	O=C1CSC(N2N=C(c3ccc(F)cc3)CC2c2ccc(Br)cc2)=N1	4790	5.32
4142	COc1cc(/C=C2\CCC/C(=C\c3cc(C(C)(C)C)c(O)c(C(C)(C)C)c3)C2=O)cc(OC)c1	4800	5.32
4143	N#CC1=C(N)N(c2cccnc2)C2=C(C(=O)CCC2)C1c1cc2ccccc2n2nnnc12	4800	5.32
4144	COc1cc(N2CCN(C)CC2)ccc1Nc1ncc(Cl)c(Oc2cccc(NC(=O)/C(C#N)=C/c3ccc(SC)cc3)c2)n1	4800	5.32
4145	COc1cc2ncnc(Nc3ccc(NC(=O)OC(C)C)cc3)c2cc1OC	4800	*
4146	CCCCNC(=O)c1ccc(S(=O)(=O)Oc2ccc(/C=C/[N+](=O)[O-])cc2)cc1	4800	*
4147	Nc1ncnc2c1c(-c1ccc(F)c(O)c1)nn2[C@H]1CCOC1	4800	*
4148	C[C@H](CN)n1nc(-c2ccc(Cl)c(O)c2)c2c(N)ncnc21	4800	*
4149	CN(C)C/C=C/C(=O)Nc1cccc(Nc2ncc(Cl)c(Nc3ccc4ccccc4c3)n2)c1	4800	*
4150	CCN(CC)C(C)/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)c(C#N)cnc2cc1OC	4840	5.32
4151	O=C1CSC(N2N=C(c3ccccc3)CC2c2ccc(F)cc2)=N1	4860	5.31
4152	CN(C)c1ccc(Nc2ncnc3cc(N)ncc23)cc1	4860	*
4153	COc1cc2ncnc(Oc3cccc(NC(=S)Nc4ccc(F)c(F)c4)c3)c2cc1OC	4880	*
4154	CN(C)C/C=C/C(=O)N1CCc2c(sc3ncnc(NCCO)c23)C1	4884	*
4155	CN(C)c1ccc(Nc2ncnc3ccncc23)c(N)c1	4897.79	*
4156	COc1cccc2ncnc(NCc3ccccc3)c12	4900	*

4157	CN(C)Cc1cc(C(=O)N[C@@H]2CCc3ccc(Oc4ccnc5c4CCC(=O)N5)cc3C2)cc(C(F)(F)F)c1	4900	*
4158	COc1cc(Br)c(C=C2CN(C(C)C)CC(=Cc3nc(C)c(C)nc3C)C2=NO)cc1OC	4900	*
4159	COc1ccc(C2=NN(c3nc(-c4ccccc4)cs3)C(c3ccc(Cl)cc3)C2)cc1	4940	5.31
4160	CCCCCCCCCOC(=O)COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1	4960	5.30
4161	COC(=O)CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	4997	*
4162	CCOc1cc([N+](=O)[O-])c(C(=O)Nc2ccc(F)c(Cl)c2)cc1NC(=O)c1ccc(CN2CCN(C)CC2)cc1	5000	5.30
4163	Cc1ccc(NC(=O)/C=C/CN(C)C)cc1C(=O)Nc1nccc(-c2cccnc2)n1	5000	5.30
4164	CCOc1cc(N)c(C(=O)Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)cc1NC(=O)c1ccc(CN2CCN(C)CC2)cc1	5000	5.30
4165	CCOC(=O)Nc1cc(Nc2ncnc3cc(OC)c(OC)cc23)ccc1C.Cl	5000	*
4166	CCOC(=O)Nc1cc(Nc2ncnc3cc(OC)c(OC)cc23)ccc1C	5000	*
4167	Cn1c(SSc2c(C(=O)Nc3ccccc3)c3cc([N+](=O)[O-])ccc3n2C)c(C(=O)Nc2ccccc2)c2cc([N+](=O)[O-])ccc21	5000	*
4168	Oc1cc2cc(-c3ccncc3)cnc2cc1O	5000	*
4169	O=C(Oc1ccc(-c2ccccc2)cc1)c1cc(NCc2cc(O)ccc2O)ccc1O	5000	*
4170	CC(C)(C)ONC(=O)Cc1cc(NCc2cc(O)ccc2O)ccc1O	5000	*
4171	O=C(O)c1cc(/N=C/c2cc(O)ccc2O)ccc1O	5000	*
4172	O=[N+]([O-])c1ccc2ncnc(Nc3ccccc3)c2c1	5000	*
4173	CC(C)n1nc(-c2ccc3c(c2)CCO3)c2c(N)ncnc21	5000	*
4174	O=[N+]([O-])c1cccc(-c2cc3c(Nc4ccc(Cl)cc4F)ncnc3o2)c1	5000	*
4175	c1ccc(Cc2nc3cc(Nc4ncnc5nn6ccccc6c45)ccc3[nH]2)cc1	5010	*
4176	CSc1cn2c(-c3cn[nH]c3)cnc2c(Nc2cc(C)ns2)n1	5048	*
4177	COc1ccc(C2=NN(c3nc(-c4ccc(Cl)cc4)cs3)C(c3ccc(F)cc3)C2)cc1	5070	5.29
4178	COc1cc2ncnc(N[C@@H](C)c3ccccc3)c2cc1OCCCCCCC(=O)NO	5077	5.29
4179	C=CCn1nc(-c2ccc(OCC)c(OC)c2)c2c(N)ncnc21	5080	*
4180	CSCCCNc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	5100	5.29
4181	COCCn1c(=O)oc2cc3ncnc(Nc4ccc(OC)cc4)c3cc21	5100	*
4182	Cc1cccc(C)c1NC(=O)/C(C#N)=C/c1ccc(O)c(O)c1	5100	*
4183	COc1cc(Nc2nccc(-c3ccc(NCCN)nc3)n2)cc(OC)c1OC	5100	*
4184	CCN(CC)CCOc1c(C(=O)OC)c2c3c(oc2c2ccccc12)C(=O)c1ccccc1C3=O	5100	*
4185	Cc1c(C(=O)c2coc3c2cc(O)c2ccccc23)[nH]c(-c2ccccc2)c1-c1ccccc1	5100	*
4186	O=C(Nc1cccc(O)c1)c1ccc(-c2ccc([N+](=O)[O-])cc2)cc1O	5100	*
4187	NC(=S)N/N=C(/C=C/c1ccc(-c2ccccc2)cc1)c1ccccc1	5110	5.29
4188	Fc1ccccc1-c1nnc(SCc2ccccc2)o1	5110	5.29
4189	Cc1ncc([N+](=O)[O-])n1CC(=O)N/N=C/c1cc2ccccc2nc1Oc1ccc(Cl)cc1	5120	5.29
4190	C=CC(=O)Nc1ccc(-n2c(=O)cnc3cnc(Nc4ccc(OC)cc4)nc32)cc1	5129	5.29
4191	COc1cc(-c2nn(C(C)C)c3ncnc(N)c23)cc(OC)c1OC	5140	*
4192	N#Cc1cnc2cc3c(cc2c1Nc1cccc(Br)c1)OCCCO3	5150	*
4193	O=C(/C=C/c1ccc([N+](=O)[O-])cc1)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	5160	5.29
4194	C#Cc1cccc(NC(=O)c2cc(NC(=O)CCCCCC(=O)NO)ccc2OC)c1	5160	*
4195	COc1ccccc1NC(=O)/C=C/c1ccccc1	5160	*
4196	O=C(Cc1ccc(F)cc1)NS(=O)(=O)c1ccc(F)cc1	5170	5.29
4197	Cc1ccc(C2=NN(C(N)=S)C(c3ccccc3F)C2)cc1C	5190	5.28
4198	C#Cc1cccc(Nc2ncnc3cc4oc(=O)n(CCOC(=O)CBr)c4cc23)c1	5200	5.28
4199	Cc1cc(Nc2ncc(C(=O)Nc3c(C)cccc3Cl)s2)nc(C)n1	5200	*

4200	COc1cc2ncc(C#N)c(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/C(C)N(C)C	5220	5.28
4201	CN(C)CCCN(C)CC(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	5222	*
4202	COc1cc(/C=C(\C#N)C(N)=O)cc(CSc2nc3ccccc3o2)c1O	5248.07	*
4203	Nc1cc2ncnc(Nc3ccccc3N)c2cn1	5250	*
4204	Cc1ccc(C2=NN(C3=NC(c4ccccc4)CS3)C(c3ccc4ccccc4c3)C2)cc1	5260	5.28
4205	NC(=S)N1N=C(c2ccc(Cl)c(Cl)c2)CC1c1ccc(O)cc1	5270	5.28
4206	Cc1cccc2nc(NC(=O)c3cccc(C(F)(F)F)c3)n([C@H]3CC[C@H](O)CC3)c12	5270	*
4207	CN(C)c1ccc(/C=C/C(=O)c2ccc3ncc(C(N)=O)c(Nc4ccc(Cl)cc4)c3c2)cc1	5283	*
4208	COc1cc(/C=C2\CCC/C(=C\c3ccc(OC)c(O)c3)C2=O)cc(OC)c1	5300	5.27
4209	Nc1nn2c(=O)cc(-c3ccccc3)[nH]c2c1N=Nc1ccc2c(c1)OCO2	5300	5.28
4210	CC(=O)Oc1ccc2c(c1)c(C(=O)Nc1ccccc1)c(SSc1c(C(=O)Nc3ccccc3)c3cc(OC(C)=O)ccc3n1C)n2C	5300	*
4211	CCn1cnc2c(Nc3cccc(Cl)c3)nc(N[C@H]3CCC[C@@H](N)C3)nc21	5300	*
4212	Cc1cc(C(=O)NCCN2CCOCC2)[nH]c1/C=C1\C(=O)N(C)c2ncnc(Nc3ccc(F)c(Cl)c3)c21	5310	*
4213	COc1cc(-c2nn(C(C)C)c3ncnc(N)c23)ccc1NC(C)CO	5320	*
4214	CCCCCCCCNC(=O)COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1	5330	5.27
4215	O=C1CSC(N2N=C(c3ccc(Cl)cc3)CC2c2ccccc2)=N1	5340	5.27
4216	COc1ccc(C2=NN(C3=NC(=O)CS3)C(c3ccc(Cl)cc3)C2)cc1	5350	5.27
4217	COc1ccc(C2=NN(c3nc(-c4ccccc4)cs3)C(c3ccc(O)cc3)C2)cc1	5350	5.27
4218	COc1cc2ncnc(Sc3cccc(NC(=S)Nc4ccc(F)cc4)c3)c2cc1OC	5350	*
4219	COc1cc(NC(=O)/C=C/CN2CCOCC2)cc2c(Nc3cccc(Br)c3)c(C#N)cnc12	5390	5.27
4220	COc1ccc2c(c1)cc(C1C(C#N)=C(N)N(c3cccnc3)C3=C1C(=O)CCC3)c1nnnn12	5400	5.27
4221	NCCNC(=O)c1ccc(S(=O)(=O)Oc2ccc(/C=C/[N+](=O)[O-])cc2)cc1	5400	*
4222	O=[N+]([O-])c1cc(NCc2cc(O)ccc2O)ccc1O	5400	*
4223	COc1c(NC(=O)Nc2ccc(-c3ccc(CN4CCOCC4)nc3)c3ccccc23)cc(C(C)(C)C)cc1NS(C)(=O)=O	5400	*
4224	Cc1ccc(-n2cc3c(-c4c(C)[nH]c(-c5ccccc5)c4-c4ccccc4)nnc(C)c3n2)cc1	5430	*
4225	COc1ccc(C2=NN(C3=NC(=O)CS3)C(c3ccc(C)cc3)C2)cc1	5460	5.26
4226	COc1cc(OC)c2c(=O)n(-c3ccc(F)c(Cl)c3)ccc2c1	5490	*
4227	CCOc1cc([N+](=O)[O-])c(C(=O)Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)cc1NC(=O)c1ccc(CN2CCN(C)CC2)cc1	5500	5.26
4228	COc1cc(C(=O)n2nc(-c3ccc(Cl)cc3)nc2N)cc(OC)c1OC	5500	5.26
4229	CCCOc1cc2ncnc(Nc3ccc(NC(=O)OCC)c(Cl)c3)c2cc1OC.Cl	5500	*
4230	COCCn1c(=O)oc2cc3ncnc(Nc4ccc(OC)c(OC)c4)c3cc21	5500	*
4231	Brc1cccc(Nc2ccnc3ccccc23)c1	5500	*
4232	CCN(c1ccccc1)c1ncnc2cc(OC)c(OC)cc12.Cl	5500	*
4233	CONC(=O)c1cc(Nc2ncnn3cc(NC(=O)OCC4CCCO4)c(C(C)C)c23)c(F)cc1F	5500	*
4234	C/C1=C/CC[C@]23O[C@H]2[C@@H](OC3=O)C2=C(C1)C(=O)C(O)=CC2=O	5500	*
4235	COc1ccc(C2=NN(C3=NC(=O)CS3)C(c3cccc4ccccc34)C2)cc1	5530	5.26
4236	CC(C)(C)NC(=O)Nc1nc2nc(N)ncc2cc1-c1ccccc1	5530	*
4237	Cc1ccc(C(=O)Nc2ccc(CN3CCN(C)CC3)c(C(F)(F)F)c2)cc1NC(=O)c1cnc(N(C)C)nc1	5540	5.26
4238	COc1ccc(C2=NN(c3nc(-c4ccccc4)cs3)C(c3ccc(Br)cc3)C2)cc1	5560	5.25
4239	Cc1ccc(C2CC(c3ccc(Br)cc3)=NN2C2=NC(=O)CS2)cc1	5580	5.25
4240	C=CC(=O)Nc1ccc(-n2c(=O)cnc3cnc(Nc4ccc(N5CCOCC5)cc4)nc32)cc1	5585	5.25
4241	COc1cc(/C=C2\CCC/C(=C\c3ccc(F)cc3)C2=O)cc(OC)c1	5600	5.25
4242	O=C1NN(c2ccc(F)cc2)C(=O)/C1=C\c1cccc(OCc2ccccc2F)c1	5600	5.25

4243	COc1cc2c(cc1OC)Oc1ncnc(Nc3ccc4ncsc4c3)c1NC2	5600	5.25
4244	COc1cc(N2CCN(C)CC2)ccc1Nc1ncc(Cl)c(Oc2cccc(NC(=O)/C=C/C3CC3)c2)n1	5600	5.25
4245	COc1ccc(-c2nc3sc(-c4ccccc4)cn3n2)cc1	5600	5.25
4246	COc1cc2ncnc(C#Cc3ccccc3)c2cc1OC	5600	*
4247	C=C(CN(C)C)C(=O)c1ccccc1.Cl	5600	*
4248	Cn1c(=O)c(-c2c(Cl)cccc2Cl)cc2cnc(N)nc21	5600	*
4249	COc1cc2ncnc(Nc3cccc(NC(=O)c4ccccc4)c3)c2cc1OC	5600	*
4250	Clc1cccc(Nc2ncnc3ccc(NCc4ccc(Br)cc4)cc23)c1	5670	5.25
4251	NC(=S)N1N=C(c2ccc(Br)cc2)CC1c1cccc2ccccc12	5680	5.25
4252	COc1cc2ncnc(Nc3ccc(Br)cc3F)c2cc1OC	5700	*
4253	C#Cc1cccc(Nc2ncnc3cc4oc(=O)n(CCCC(=O)OCC)c4cc23)c1	5700	*
4254	CC(=O)N1CCc2ccc(Nc3nc(Nc4ccc(N5CCN(C)CC5)cc4)ncc3Br)cc21	5700	*
4255	COc1ccc(C2=NN(c3nc(-c4ccccc4)cs3)C(c3ccc(F)cc3)C2)cc1	5710	5.24
4256	Cc1ccccc1-c1nnc(SCc2ccccc2)o1	5720	5.24
4257	COc1ccc(C2CC(c3ccc(Cl)c(Cl)c3)=NN2C(N)=S)cc1	5740	5.24
4258	Cc1ncc([N+](=O)[O-])n1CCOC(=O)/C=C/c1ccc2ccccc2c1	5760	5.24
4259	COc1ccc(/C=N/NC2=NC(=O)CS2)cc1	5780	5.24
4260	COc1cc(C2=C(c3c[nH]c4ccc(Br)cc34)C(=O)NC2=O)cc(OC)c1OC	5797	*
4261	CCOC(=O)c1ccc(Nc2ncnc3cc4oc(=O)n(CCCN5CCOCC5)c4cc23)cc1	5800	*
4262	COc1cc2ncnc(Nc3ccc(NC(=O)OC(C)C)c(C)c3)c2cc1OC	5800	*
4263	Cc1cc(C)c(O)c(CN(Cc2ccc(O)cc2)C(=S)Nc2ccccc2)c1	5830	5.23
4264	CCCCCCCCOC(=O)COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1	5840	5.23
4265	COc1cc2c(cc1OC)Sc1ncnc(Nc3cccc(Br)c3)c1NC2	5900	5.23
4266	COc1cc2ncnc(Oc3ccc(Br)c(F)c3)c2cc1OC	5900	*
4267	O=[N+]([O-])c1ccc2c(NCc3ccccc3)ncnc2c1	5900	*
4268	Nc1ccc(Nc2ncnc3cc(N)ncc23)cc1	5900	*
4269	COc1cc2ncnc(Oc3cccc(NC(=S)Nc4ccc(F)cc4)c3)c2cc1OC	5900	*
4270	O=C(Cc1ccc(F)cc1)NS(=O)(=O)c1ccc(Cl)cc1	5930	5.23
4271	COc1ccc(C2=NN(C3=NC(=O)CS3)C(c3ccc(F)cc3)C2)cc1	5950	5.23
4272	CCOc1ccc(-c2nn(C(C)C)c3ncnc(N)c23)cc1OC	5950	*
4273	Cc1ccc(Nc2nccc(N(C)c3ccc4c(C)n(C)nc4c3)n2)cc1S(N)(=O)=O	5950	*
4274	CC(C)n1nc(-c2cc(C=O)co2)c2c(N)ncnc21	5960	*
4275	CCOc1ccc(C(=O)Nc2nccc(-c3cccnc3)n2)cc1NC(=O)/C=C/CN(C)C	6000	5.22
4276	Cc1ccc(NC(=O)c2ccc(CN3CCN(C)CC3)cc2)cc1C(=O)Nc1nccc(-c2cccc(F)c2)n1	6000	5.22
4277	CCOc1cc([N+](=O)[O-])c(C(=O)Nc2ccc(F)c(Cl)c2)cc1NC(=O)/C=C/CN(C)C	6000	5.22
4278	O=C(O)Cc1cc(NCc2cc(O)ccc2O)ccc1O	6000	*
4279	COc1cc(C=C(C#N)C#N)cc(O)c1O	6000	*
4280	COc1cc2nccc(Oc3ccc(N(C)C(=O)c4ccc(C(C)(C)C)cc4)cc3)c2cc1OC	6000	*
4281	COc1cccc(/C=C/C(=O)Nc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)c1	6020	5.22
4282	COc1cccc(/C=C2\CCC/C(=C\c3cc(OC)cc(OC)c3)C2=O)c1	6100	5.21
4283	CNC(=O)c1c([Se][Se]c2c(C(=O)NC)c3ccccc3n2C)n(C)c2ccccc12	6100	*
4284	O=[N+]([O-])c1ccc2c(Nc3cccc(F)c3)ncnc2c1	6100	*
4285	Cc1ccc(C(=O)N/N=C(/Cn2c([N+](=O)[O-])cnc2C)c2ccc(Br)cc2)cc1	6130	5.21

4286	CCOC(=O)C1=C(N)N(c2cccnc2)C2=C(C(=O)CCC2)C1c1c(C)nn(-c2ccc(Cl)cc2)c1Cl	6150	5.21
4287	COC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1Cl.Cl	6150	*
4288	COC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1Cl	6150	*
4289	C#Cc1cccc(NC(=O)c2cccc(NC(=O)CCCCCC(=O)NO)c2)c1	6170	*
4290	CCN(CC)CCCNc1ncc2cc(-c3c(Cl)cccc3Cl)c(NC(=O)NC(C)(C)C)nc2n1	6200	*
4291	CCC(=O)N1CC[C@H](N2C(=O)N(c3cc(OC)ccc3F)Cc3cnc(Nc4ccc(N5CCOCC5)c(C)c4)nc32)C1	6265	5.20
4292	CC#CC(=O)Nc1cnc2ncc(C#N)c(Nc3cccc(Br)c3)c2c1	6266.2	5.20
4293	NC(=S)N1N=C(c2ccc(Cl)c(Cl)c2)CC1c1ccc(F)cc1	6270	5.20
4294	COc1ccc(C2=NN(c3nc(-c4ccc(Cl)cc4)cs3)C(c3ccc(OC)cc3)C2)cc1	6270	5.20
4295	CCCCCCCNC(=O)COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1	6280	5.20
4296	Fc1ccc(-c2nn3ccccc3c2-c2ccncc2)cc1	6300	*
4297	O=C1CSC(N2N=C(c3ccccc3)CC2c2ccc3ccccc3c2)=N1	6310	5.20
4298	COc1ccc(C2=NN(c3nc(-c4ccc(Cl)cc4)cs3)C(c3ccc(Br)cc3)C2)cc1	6310	5.20
4299	COc1ccc(-c2nn(C(C)(C)C)c3ncnc(N)c23)cc1OC	6340	*
4300	COc1cc2ncc(C#N)c(Nc3cccc(O)c3)c2cc1OC	6360	*
4301	O=C(CBr)OCCn1c(=O)oc2cc3ncnc(Nc4ccc(OCc5ccc(Cl)cc5)cc4)c3cc21	6400	5.19
4302	CCCCOC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1Cl.Cl	6400	*
4303	CCCCOC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1Cl	6400	*
4304	O=C(Cc1ccc(F)cc1)NS(=O)(=O)c1ccc(Br)cc1	6410	5.19
4305	C/C=C(\C)C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)ncnc2s1	6414	*
4306	NC(=S)N1N=C(c2ccc(Cl)c(Cl)c2)CC1c1ccccc1Br	6430	5.19
4307	CCn1nc(-c2ccc(OC)c(O)c2)c2c(N)ncnc21	6450	*
4308	O=C1CSC(N2N=C(c3ccc(Br)cc3)CC2c2ccc(F)cc2)=N1	6480	5.19
4309	COc1cc(C(=O)n2nc(-c3cc(OC)c(OC)c(OC)c3)nc2N)cc(OC)c1OC	6500	5.19
4310	COc1cccc2c(C(=O)Nc3ccccc3)c(SSc3c(C(=O)Nc4ccccc4)c4cccc(OC)c4n3C)n(C)c12	6500	*
4311	Cc1cccc(N(C)c2ncnc3cc(C)c(C)cc23)c1.Cl	6500	*
4312	Cc1cccc(/C=C2/SC(N3CCC[C@H]3C(=O)Nc3ccc4ncnc(Nc5cccc(Cl)c5)c4c3)=NC2=O)n1	6500	*
4313	COc1ccc(C2=NN(C(=O)Cc3nc4ccccc4[nH]3)C(c3ccc(Br)cc3)C2)cc1	6500	*
4314	COc1cc2nccc(Oc3ccc(NC(=O)NC4CC4)c(Cl)c3)c2cc1C(N)=O	6500	*
4315	NC(=S)N1N=C(c2ccc(Cl)c(Cl)c2)CC1c1ccccc1F	6560	5.18
4316	COc1cccc(/C=C/C(=O)Nc2ccc3ncnc(Nc4cccc(Cl)c4)c3c2)c1	6630	5.18
4317	COc1cc2ncc(C#N)c(Nc3ccc(Br)cc3)c2cc1OC	6650	*
4318	Cc1ccc(C2CC(c3ccc(Cl)cc3)=NN2C2=NC(=O)CS2)cc1	6670	5.18
4319	Cc1cc(C)c(C)c(-c2cc3cnc(N)nc3nc2NC(=O)NC(C)(C)C)c1C	6680	*
4320	O=C(O)CCCC1C(S)=Nc2ccccc21	6700	*
4321	CN1C(=S)C(CCC(=O)O)c2ccccc21	6700	*
4322	CN(C)C/C=C/C(=O)Nc1cccc(Oc2nc(Nc3n[nH]c4ccccc34)cc(N3CCN(C)CC3)n2)c1	6700	*
4323	CC(C)n1nc(-c2ccc3[nH]c(=O)ccc3c2)c2c(N)ncnc21	6700	*
4324	O=C(Cc1ccc(F)cc1)NS(=O)(=O)c1ccccc1	6740	5.17
4325	COCOc1cc2ncc(C#N)c(Nc3cccc(Br)c3)c2cc1OCOC	6750	*
4326	COc1cc(C=C(C#N)C#N)cc(CSc2ccccc2)c1O	6760.83	*
4327	COc1cccc(NC(=O)/C=C/c2ccc3c(c2)OCCCCO3)c1	6780	*
4328	N#Cc1cnc2cc3c(cc2c1Nc1cccc(Br)c1)OCO3	6790	*

4329	O=C(Cn1c(-c2ccccc2)cc(=O)n2ncnc12)NNC(=S)Nc1ccccc1	6800	5.17
4330	COc1cc(/C=C2\CCC/C(=C\c3cccc(Br)c3)C2=O)cc(OC)c1	6800	5.41
4331	CC(=O)c1cccc(Nc2ncnc3cc4oc(=O)n(CCCN5CCOCC5)c4cc23)c1	6800	*
4332	CN1CCN(c2ccc(Nc3ncc(Br)c(Nc4ccc5c(c4)CCC5)n3)cc2)CC1	6800	*
4333	Cc1ncc([N+](=O)[O-])n1CCOC(=O)/C=C/c1ccc(C(C)C)cc1	6820	5.17
4334	O=C1CSC(N/N=C/c2ccc([N+](=O)[O-])cc2)=N1	6820	5.17
4335	NC(=S)N1N=C(c2ccc(Cl)c(Cl)c2)CC1c1ccc(Br)cc1	6850	5.16
4336	COC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1	6900	*
4337	CNC(=O)c1c(SSc2c(C(=O)NC)c3ccccc3n2C)n(C)c2ccccc12	6900	*
4338	CCN(CC)CCn1c([Se][Se]c2c(C(=O)NC)c3ccccc3n2CCN(CC)CC)c(C(=O)NC)c2ccccc21	6900	*
4339	CC(C)n1nc(-c2cc(F)c(O)cc2F)c2c(N)ncnc21	6900	*
4340	N#Cc1cnc(Nc2cccc(Br)c2)c2cc(NC(=O)CCN3CCOCC3)ccc12	6900	*
4341	Cc1cc(=O)n(-c2ccc(F)cc2)nc1C(=O)Nc1ccc(Oc2ncnc3ccsc23)c(F)c1	6900	*
4342	COc1ccc(C2=NN(c3nc(-c4ccccc4)cs3)C(c3ccc(OC)cc3)C2)cc1	6920	5.16
4343	Cc1nc(NC2CCCCC2)c2c(C)c(C)[nH]c2n1	6920	*
4344	CCOC(=O)C1=C(N)N(c2cccnc2)C2=C(C(=O)CCC2)C1c1cc2cc(C)ccc2n2nnnc12	7000	5.15
4345	COc1cc(N2CCN(C)CC2)ccc1Nc1ncc(Cl)c(Oc2cccc(NC(=O)/C(C#N)=C/c3ccc(F)cc3)c2)n1	7000	5.15
4346	O=CN/C=C/c1ccc(O)c(O)c1	7000	*
4347	N#CC(C#N)=C1CCc2c1ccc(O)c2O	7000	*
4348	CC(C)CCCC(C)CCOC(=O)c1cc(NCc2cc(O)ccc2O)ccc1O	7000	*
4349	CCOC(=O)Cc1cc(NCc2cc(O)ccc2O)ccc1O	7000	*
4350	Clc1ccc(CNc2ncnc3ccccc23)cc1	7000	*
4351	O=C(NCc1ccccc1)[C@H](Cc1c([Se][Se]c2[nH]c3ccccc3c2C[C@@H](NC(=O)C(F)(F)F)C(=O)NCc2ccccc2)[nH]c2ccccc12)NC(=O)C(F)(F)F	7000	*
4352	C[C@@H](NC(=O)[C@@H](C)NC(=O)c1ccc(S(=O)(=O)Oc2ccc(/C=C/[N+](=O)[O-])cc2)cc1)C(=O)O	7000	*
4353	Cc1cc(C)c(C)c(-c2cc3cnc(NCCCN4CCN(C)CC4)nc3nc2NC(=O)NC(C)(C)C)c1C	7000	*
4354	CC(C)n1nc(-c2ccc3nc(NN)ccc3c2)c2c(N)ncnc21	7000	*
4355	CCCOC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1.Cl	7050	*
4356	CCCOC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1	7050	*
4357	COc1cc(/C=C2\CCC/C(=C\c3ccc(Br)cc3)C2=O)cc(OC)c1	7100	5.15
4358	COc1cc2c(cc1OC)Oc1ncnc(Nc3ccc(F)cc3)c1NC2	7100	5.15
4359	c1cc(Nc2nccc(-c3ccncc3)n2)cc(OCCn2ccnc2)c1	7100	*
4360	COCCOc1cc2ncnc(Nc3c(Cl)ccc4c3OCO4)c2cc1NC(=O)[C@@H]1CCCN1	7130	5.15
4361	COc1cc(N2CCN(C)CC2)ccc1Nc1ncc(Cl)c(Oc2cccc(NC(=O)/C(C#N)=C/C3CC3)c2)n1	7200	5.14
4362	Clc1ccc(-c2cn3nc(-c4ccccc4)nc3s2)cc1	7200	5.14
4363	CN(c1ccccc1)c1ncnc2cc3oc(=O)n(CCCN4CCOCC4)c3cc12	7200	*
4364	COC(=O)Nc1cc(Nc2ncnc3cc(OC)c(OC)cc23)ccc1C.Cl	7200	*
4365	COC(=O)Nc1cc(Nc2ncnc3cc(OC)c(OC)cc23)ccc1C	7200	*
4366	COc1ccc(/C=C/C(=O)Nc2ccc3ncnc(Nc4cccc(Br)c4)c3c2)cc1	7220	5.14
4367	CCCCCCCOC(=O)COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1	7230	5.14
4368	O=C(/C=C/c1ccc2c(c1)OCCCCO2)Nc1ccc([N+](=O)[O-])cc1	7250	*
4369	NC(=S)N1N=C(c2ccc(Cl)c(Cl)c2)CC1c1ccccc1Cl	7280	5.14
4370	CCN(CC)[C@@](C)(C#Cc1ncnc2cc(OC)c(OC)cc12)c1ccccc1	7300	*

4371	CN(C)CC(CSc1ccccc1)C(=O)c1ccc(OCc2ccccc2)cc1.Cl	7300	*
4372	O=C(Nc1ccc(Cl)cc1)c1ccccc1NCc1ccncc1	7300	*
4373	CCN(CC)C(C)(C#Cc1ncnc2cc(OC)c(OC)cc12)c1ccccc1	7300	*
4374	NC(=S)N1N=C(c2ccc(Cl)c(Cl)c2)CC1c1ccc(Cl)cc1	7320	5.14
4375	O=C(/C=C/c1ccccc1)Nc1ccccc1F	7370	*
4376	Cc1ccc(C2CC(c3ccc(Cl)c(Cl)c3)=NN2C(N)=S)cc1	7380	5.13
4377	COc1cc2ncc(C#N)c(Nc3cccc(C(C)=O)c3)c2cc1OC	7380	*
4378	COc1cc2c(cc1OC)Oc1ncnc(Nc3cccc(C)c3)c1NC2	7400	5.13
4379	COc1cc(C(=O)Nc2nc(-c3cccc(Cl)c3)n[nH]2)cc(OC)c1OC	7400	5.13
4380	NC(Cc1c(SSc2[nH]c3ccccc3c2CC(N)C(=O)NCc2ccccc2)[nH]c2ccccc12)C(=O)NCc1ccccc1	7400	*
4381	O=C(CCc1c(SSc2[nH]c3ccccc3c2CCC(=O)NCc2ccc(C(=O)O)cc2)[nH]c2ccccc12)NCc1ccc(C(=O)O)cc1	7400	*
4382	CCNCc1cn2ncnc(Nc3ccc4c(cnn4Cc4ccccc4)c3)c2c1CC	7400	*
4383	O=C1N=C(N2CCC[C@H]2C(=O)Nc2ccc3ncnc(Nc4cccc(Cl)c4)c3c2)S/C1=C/c1cccnc1Cl	7400	*
4384	OCCCCNc1cncc(-c2cncc(Nc3cccc(Cl)c3)n2)c1	7400	*
4385	CC(C)n1nc(-c2ccc3nc[nH]c(=O)c3c2)c2c(N)ncnc21	7400	*
4386	CC(C)(C)c1ccc(-c2nnc(SCc3ccccc3)o2)cc1	7440	5.13
4387	COc1cc(N2CCN(C)CC2)ccc1Nc1ncc(Cl)c(Oc2cccc(NC(=O)CCN3CCN(C)CC3)c2)n1	7442	5.13
4388	O=C1CSC(N/N=C/c2cccc(Br)c2)=N1	7460	5.13
4389	COc1ccc(C2=NN(c3nc(-c4ccccc4)cs3)C(c3ccc(C)cc3)C2)cc1	7480	5.13
4390	COc1cc(/C=C2\CCC/C(=C\C3CCCCC3)C2=O)cc(OC)c1	7500	5.12
4391	C/C=C/C(=O)Nc1cc2c(Nc3ccc(F)c(Cl)c3)c(C#N)cnc2cc1OCC	7500	5.12
4392	CCOC(=O)CCCn1c(=O)oc2cc3ncnc(Nc4ccc(OC)cc4)c3cc21	7500	*
4393	CNc1ncc2cc(-c3c(Cl)cccc3Cl)c(=O)n(C)c2n1	7500	*
4394	Cc1cccc(CN(Cc2ccc(O)cc2)C(=O)Nc2ccccc2)c1O	7510	5.12
4395	CCCCOC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1C.Cl	7600	*
4396	CCCCOC(=O)Nc1ccc(Nc2ncnc3cc(OC)c(OC)cc23)cc1C	7600	*
4397	O=C1N=C(N2CCC[C@H]2C(=O)Nc2ccc3ncnc(Nc4cccc(Cl)c4)c3c2)S/C1=C/c1ccc(Cl)cc1	7600	*
4398	COc1ccc(C2=NN(c3nc(-c4ccc(Cl)cc4)cs3)C(c3ccc(O)cc3)C2)cc1	7660	5.12
4399	O=c1ccc2ccc(O)c(O)c2o1	7670	*
4400	COc1cc2ncc(C#N)c(Nc3cccc(C(N)=O)c3)c2cc1OC	7690	*
4401	COc1cccc(Nc2ccnc(Nc3cccc(OC)c3)n2)c1	7700	*
4402	COc1ccccc1/C=C/C(=O)Nc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	7710	5.11
4403	COc1cc2ncnc(Nc3ccc(NC(=O)Nc4cccc(Br)c4)cc3)c2cc1OC	7710	*
4404	COc1cc2ncnc(Oc3cccc(NC(=S)Nc4ccc(Cl)cc4Cl)c3)c2cc1OC	7710	*
4405	NC(=S)N1N=C(c2ccc(Cl)c(Cl)c2)CC1c1ccc([N+](=O)[O-])cc1	7780	5.11
4406	COc1ccc(C2=NN(c3nc(-c4ccc(Cl)cc4)cs3)C(c3ccc(Cl)cc3)C2)cc1	7780	5.11
4407	Cc1c(OCC(F)(F)F)ccnc1COc1ccc(Nc2ncnc3cc4oc(=O)n(CCCN5CCOCC5)c4cc23)cc1	7800	*
4408	CCOC(=O)CCCn1c(=O)oc2cc3ncnc(Nc4ccc(F)c(Cl)c4)c3cc21	7800	*
4409	Nc1cccc(-c2cc(=O)c3c(N)c(O)c(N)cc3o2)c1	7800	*
4410	O=C(Nc1ccccc1Br)c1ccc(N(CCCl)CCCl)cc1	7820	5.11
4411	Cc1ncc([N+](=O)[O-])n1CCOC(=O)/C=C/c1ccccc1	7830	5.11
4412	COc1ccc(C(/C=C/c2ccccc2Cl)=N\NC(N)=S)cc1	7830	5.11
4413	CCOC(=O)c1nn(-c2ccc(C)cc2)cc1C(=O)c1c(C)[nH]c(-c2ccccc2)c1-c1ccccc1	7880	*

4414	COC(=O)[C@@H](Nc1ncnc2oc(-c3ccccc3)c(-c3ccccc3)c12)c1ccccc1	7893	*
4415	COc1cc(/C=C/[N+](=O)[O-])ccc1O	7900	*
4416	Brc1cc2c(NCc3ccccn3)ncnc2s1	7904	*
4417	COc1cc(C=C(C#N)C#N)cc(CSc2ccccc2C(=O)O)c1O	7943.28	*
4418	COc1ccc(C2CC(c3ccc(Br)cc3)=NN2C2=NC(=O)CS2)cc1	7960	5.10
4419	COc1cc(/C=C2\CCC/C(=C\c3ccccc3Br)C2=O)cc(OC)c1	8000	*
4420	CCOC(=O)Nc1ccc(Nc2ncnc3cc(OCCN4CCOCC4)c(OC)cc23)cc1C.Cl	8000	*
4421	O=[N+]([O-])c1cccc2ncnc(NCc3ccccc3)c12	8000	*
4422	Nc1cc2ncnc(NCc3ccc(C(F)(F)F)cc3)c2cn1	8000	*
4423	CN=NNc1ccc2ncnc(N(C)c3ccccc3)c2c1	8000	*
4424	CCOc1cc(-c2nn(CCO)c3ncnc(N)c23)ccc1OC	8010	*
4425	Cc1ccc2nc(/C=C/c3ccc(N(C)C)cc3)cc(C(=O)O)c2c1	8010	*
4426	COc1cc(OC(C)C)c2c(Nc3ccc(F)c(Cl)c3)ncnc2c1	8068	*
4427	COc1cc(OC2CC2)c2c(Nc3ccc(F)c(Cl)c3)ncnc2c1	8068	*
4428	COc1ccc(C2CC(c3ccc(Br)c(Br)c3)=NN2C(N)=S)cc1	8090	5.09
4429	COC(=O)C1=C(N)N(c2cccnc2)C2=C(C(=O)CCC2)C1c1cc2cc(Cl)ccc2n2nnnc12	8100	5.09
4430	O=C1N=C(N2CCC[C@H]2C(=O)Nc2ccc3ncnc(Nc4cccc(Cl)c4)c3c2)S/C1=C/c1cccs1	8100	*
4431	Cc1ccc(/C=C/C(=O)OCCn2c([N+](=O)[O-])cnc2C)cc1	8110	5.09
4432	O=C1CSC(N2N=C(c3ccc(F)cc3)CC2c2ccccc2)=N1	8140	5.09
4433	NC(=S)N1N=C(c2ccc(Br)c(Br)c2)CC1c1ccc(Cl)cc1	8150	5.09
4434	O=C1CSC(N2N=C(c3ccc(Cl)cc3)CC2c2ccc(Cl)cc2)=N1	8160	5.09
4435	Cc1ncc([N+](=O)[O-])n1C/C(=N/NC(=O)c1ccncc1)c1ccc(Br)cc1	8190	5.09
4436	COc1cc2c(cc1OC)Sc1ncnc(Nc3ccc(F)c(Cl)c3)c1NC2	8200	5.09
4437	O=C(Nc1cccc(Cl)c1)c1ccc(Br)cc1OCc1ccccc1	8200	*
4438	NC(=S)N1N=C(c2ccc(F)cc2)CC1c1cccc2ccccc12	8250	5.08
4439	Cc1ccc(S(=O)(=O)NC(=O)Cc2ccc(F)cc2)cc1	8280	5.08
4440	Cn1c(SSc2c(CCCC(=O)O)c3ccccc3n2C)c(CCCC(=O)O)c2ccccc21	8300	*
4441	CC(C)(C)OC(=O)N1CCC(n2cc(-c3ccccc3)c3c(N)ncnc32)C1	8300	*
4442	CC(C)n1nc(-c2ccc3nonc3c2)c2c(N)ncnc21	8300	*
4443	O=[N+]([O-])c1ccc2ncnc(Nc3ccc(OCc4nccs4)c(Cl)c3)c2c1	8320	*
4444	Cc1ccc(C2CC(c3ccc(F)cc3)=NN2C2=NC(=O)CS2)cc1	8360	5.08
4445	CCOc1ccc(-c2cc(C(F)(F)F)c(C#N)c(SCC(=O)NCC(=O)O)n2)cc1	8400	5.08
4446	Cc1ccc2[nH]c(SSc3[nH]c4ccc(C)cc4c3CCC(=O)O)c(CCC(=O)O)c2c1	8400	*
4447	Cc1ccsc1C(=O)n1nc(Nc2ccc(S(N)(=O)=O)cc2)nc1N	8400	*
4448	CN(c1ccccc1)c1ncnc2ccc(N)cc12	8400	*
4449	COc1ccc(C2=NN(c3nc(-c4ccc(Cl)cc4)cs3)C(c3ccc([N+](=O)[O-])cc3)C2)cc1	8430	5.07
4450	O=C(Cc1c[nH]c2ccccc12)NNC(=S)Nc1ncccc1Br	8490	*
4451	O=C(Nc1ccc(Nc2ncnc3cc4oc(=O)n(CCOC(=O)CBr)c4cc23)cc1)NC1CCCCC1	8500	5.07
4452	CCOC(=O)Nc1ccc(Nc2ncnc3cc(OCCN4CCOCC4)c(OC)cc23)cc1Cl.Cl	8500	*
4453	O=C(CCc1c(SSc2[nH]c3ccccc3c2CCC(=O)NCc2ccc(C(=O)O)c(O)c2)[nH]c2ccccc12)NCc1ccc(C(=O)O)c(O)c1	8500	*
4454	Cc1cccc(CN(Cc2ccc(F)cc2)C(=S)Nc2ccccc2)c1O	8540	5.07
4455	COc1ccc(C2CC(c3ccc(Cl)cc3)=NN2C2=NC(=O)CS2)cc1	8580	5.07
4456	COc1cc(/C=C/C(=O)/C=C(O)/C=C/c2ccc(O)c(OC)c2)ccc1O	8600	5.07

4457	Cc1ccc(N2NC(=O)/C(=C/c3ccc(OCc4ccccc4)cc3)C2=O)cc1Cl	8600	5.07
4458	COc1ccc(C2=NN(c3nc(-c4ccccc4)cs3)C(c3ccc([N+](=O)[O-])cc3)C2)cc1	8630	5.06
4459	COc1cc(/C=C/C(=O)CC(=O)/C=C/c2ccc(O)c(OC)c2)ccc1O	8650	5.06
4460	Cc1ccc2nc(Oc3ccc(Cl)cc3)c(/C=N/NC(=O)Cn3c([N+](=O)[O-])cnc3C)cc2c1	8660	5.06
4461	COc1ccc(C(/C=C/c2ccccc2)=N\NC(N)=S)cc1	8660	5.06
4462	COc1cc2c(cc1OC)Oc1ncnc(Nc3ccc(Br)cc3)c1NC2	8700	5.06
4463	COc1cc(N2CCN(C)CC2)ccc1Nc1ncc(Cl)c(Oc2cccc(NC(=O)/C(C#N)=C/c3ccncc3)c2)n1	8700	5.06
4464	CN(c1ccccc1)c1cc2c(cc1Nc1ccccc1)C(=O)NC2=O	8700	*
4465	Nc1ccc(-c2cc(=O)c3cc(N)ccc3o2)cc1	8700	*
4466	CN1CCN(CCCNc2ncc3cc(-c4c(Cl)cccc4Cl)c(=O)n(C)c3n2)CC1	8700	*
4467	Nc1ncnc2c1c(-c1ccc(F)c(O)c1)nn2[C@H]1CCNC1	8700	*
4468	C=CC(=O)Nc1cc(Nc2ncc(Br)c(Nc3ccc4[nH]ccc4c3)n2)ccc1N(C)CCN(C)C	8700	*
4469	COc1cc(/C=C(\C#N)C(N)=O)cc(CSC2=NCCS2)c1O	8709.64	*
4470	CCCCCCNC(=O)COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1	8710	5.06
4471	COc1cc2ncc(C(=O)O)c(Nc3cccc(Br)c3)c2cc1OC	8719	5.06
4472	CN(C)c1ccc(/C=C/c2cc(-c3nnc(N)s3)c3cc(Br)ccc3n2)cc1	8780	*
4473	O=C(/C=C/c1cccs1)Nc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	8800	5.06
4474	O=[N+]([O-])/C=C/c1ccc(O)c(O)c1	8800	*
4475	COC(=O)c1ccccc1SCC(CN(C)C)C(=O)c1ccc(OCc2ccccc2)cc1.Cl	8800	*
4476	CN(C)CC(CSCCN)C(=O)c1ccc(OCc2ccccc2)cc1.Cl	8800	*
4477	COc1cccc(-c2ccc3c(c2)NC(=O)/C3=C\c2[nH]c3c(c2CCC(=O)O)CCCC3)c1	8880	*
4478	COc1ccc(C2=NN(C3=NC(=O)CS3)C(c3ccc(OC)cc3)C2)cc1	8890	5.05
4479	COc1ccc(C(=O)n2nc(-c3ccccc3)nc2N)cc1	8900	5.05
4480	CC(C)n1nc(-c2ccc(C#N)c(F)c2)c2c(N)ncnc21	8900	*
4481	NC(=S)N1N=C(c2ccc(Br)c(Br)c2)CC1c1ccc(F)cc1	8920	5.05
4482	Brc1ccc(C2=NN(c3nc(-c4ccccc4)cs3)C(c3ccc(Br)cc3)C2)cc1	8950	5.05
4483	O=C(/C=C/c1ccc2c(c1)OCCCCO2)Nc1ccccc1Cl	8970	*
4484	COC(=O)c1c(OCCN2CCCC2)c2ccccc2c2oc3c(c12)C(=O)c1ccccc1C3=O	9000	*
4485	COc1cc(C2=C(c3cn(COC(C)(C)C)c4ccccc34)CNC2=O)cc(OC)c1OC	9000	*
4486	CC(C)n1nc(-c2ccc(C=O)c(F)c2)c2c(N)ncnc21	9000	*
4487	CS(=O)CCCCN=C=S	9000	*
4488	COc1cc2ncc(C(=O)O)c(Nc3cccc(Cl)c3)c2cc1OC	9021	5.04
4489	COc1cc2ncc(C#N)c(Nc3ccc(O)c(Cl)c3)c2cc1OC	9040	*
4490	COc1ccc(NC(=O)/C=C/c2ccccc2)cc1	9050	*
4491	CCN(CC)CCOc1cc2c(Nc3ccc(Br)cc3F)ncnc2cc1OC	9100	*
4492	CCCCCCOC(=O)COc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1	9120	5.04
4493	C[C@@H](CN)n1nc(-c2ccc(Cl)c(O)c2)c2c(N)ncnc21	9140	*
4494	CCCCOc1cc2c(Nc3ccc(NC(=O)OCC)c(Cl)c3)ncnc2cc1OCCN(CC)CC	9150	*
4495	CC(=O)c1nn(-c2ccc(C)cc2)cc1C(=O)c1c(C)[nH]c(-c2ccccc2)c1-c1ccccc1	9190	*
4496	Cc1cc(C)c(O)c(CN(Cc2ccc(O)cc2)C(=O)Nc2ccccc2)c1	9260	5.03
4497	C=CC(=O)Nc1cc(Nc2n[nH]c3ccccc23)c(OC)cc1N(C)CCN(C)C	9272	*
4498	COc1cc2ncc(C(=O)O)c(Nc3ccc(F)c(Cl)c3)c2cc1OC	9284	5.03
4499	O=C(CBr)OCCn1c(=O)oc2cc3ncnc(Nc4ccc(NC(=O)N5CCCCC5)cc4)c3cc21	9300	5.03

4500	O=C(O)Cc1c(SSSc2[nH]c3ccccc3c2CC(=O)O)[nH]c2ccccc12	9300	*
4501	CN(c1ccccc1)c1ncnc2ccc(NN=NCc3ccccn3)cc12	9300	*
4502	CCOc1ccccc1NC(=O)/C=C/c1ccccc1	9350	*
4503	Clc1ccc(C2CC(c3ccc(Br)cc3)=NN2c2nc(-c3ccccc3)cs2)cc1	9370	5.03
4504	Nc1ncnc2c1c(-c1ccc(Cl)c(O)c1)nn2CC1CCCN1	9380	*
4505	COc1ccc(C(=O)n2nc(-c3cc(OC)c(OC)c(OC)c3)nc2N)cc1	9400	5.03
4506	C/C(=C\c1ccc(O)c(O)c1)[N+](=O)[O-]	9400	*
4507	CNC(=O)CCc1c(SSc2[nH]c3ccccc3c2CCC(=O)NC)[nH]c2ccccc12	9400	*
4508	CCN(CC)CCOc1cc2ncnc(Nc3ccc(C)c(Br)c3)c2cc1OC	9450	*
4509	O=C(Nc1ccccc1Cl)c1ccc(N(CCCl)CCCl)cc1	9460	5.02
4510	N=C(Nc1ccccc1)SCCCN1C(=O)C2=C(C1=O)n1ccc3cccc(c31)C1Cc3ccccc3N21	9500	*
4511	O=C(Cc1ccc(Cl)cc1)NS(=O)(=O)c1ccc(F)cc1	9590	5.02
4512	Nc1nccn2c1c(-c1ccc3ccc(-c4ccccc4)nc3c1)nc2[C@H]1C[C@@H](CN2CCC2)C1	9600	*
4513	COc1cc(OC2CCN(S(C)(=O)=O)CC2)c2c(Nc3ccc(F)c(Cl)c3)ncnc2c1	9601	*
4514	O=C(Nc1ccc(Cl)cc1Cl)c1cc(I)ccc1O	9660	*
4515	O=S(=O)(c1ccc(/N=C/c2cc(Br)ccc2O)cc1)N1CCCCC1	9700	5.01
4516	COc1cc2nc(Cl)nc(Nc3ccc(S(=O)(=O)Nc4nccs4)cc3)c2cc1OC	9700	*
4517	CNC(=O)c1cc(NCc2cc(O)ccc2O)ccc1O	9700	*
4518	NC(=S)N/N=C(/C=C/c1ccccc1)c1ccc(Cl)c(Cl)c1	9780	5.01
4519	c1ccc(-c2nc3sc(-c4ccccc4)cn3n2)cc1	9800	5.01
4520	CCCCOc1cc2c(Nc3ccc(NC(=O)OCC)c(Cl)c3)ncnc2cc1OCCN(CC)CC.Cl	9800	*
4521	O=C1N=C(N2CCC[C@H]2C(=O)Nc2ccc3ncnc(Nc4cccc(Cl)c4)c3c2)S/C1=C/c1ccncc1	9800	*
4522	Cc1ccc(C2CC(c3ccc(Br)c(Br)c3)=NN2C(N)=S)cc1	9830	5.01
4523	O=C(/C=C/c1ccccc1)Nc1ccccc1Cl	9860	*
4524	CCN(CC)CCOc1cc2ncnc(Nc3ccc(F)c(Cl)c3)c2cc1OC	9900	*
4525	CC(=O)Oc1cccc2c(C(=O)Nc3ccccc3)c(SSc3c(C(=O)Nc4ccccc4)c4cccc(OC(C)=O)c4n3C)n(C)c12	9900	*
4526	Cc1cc(-c2nn(C(C)C)c3ncnc(N)c23)sc1C=O	9900	*
4527	COC(=O)CNC(=O)c1ccc(Nc2ncnc3cc(OCCN4CCCCC4)c(OC)cc23)cc1	9941	*
4528	COc1cc(N2CCN(C)CC2)ccc1Nc1ncc(Cl)c(Oc2cccc(NC(=O)CCN3CCCCC3)c2)n1	10000	5.00
4529	Fc1cccc(COc2ccc(Nc3cc(Oc4ccccc4)ncn3)cc2Cl)c1	10000	5.00
4530	N#C/C(=C\c1cc(O)ccc1O)C(N)=O	10000	*
4531	Cn1c(SSc2c(C(=O)Nc3ccccc3)c3ccccc3n2C)c(C(=O)Nc2ccccc2)c2ccccc21	10000	*
4532	COc1ccc(CNc2ncnc3ccccc23)cc1	10000	*
4533	Nc1cc2ncnc(Nc3ccccc3C(F)(F)F)c2cn1	10000	*
4534	CN(C)c1cccc(CNc2ncnc3cc(N)ncc23)c1	10000	*
4535	Nc1cc2ncnc(NCc3ccccc3C(F)(F)F)c2cn1	10000	*
4536	N#C/C(=C\c1ccc(O)c(O)c1)C(=O)NCCN1CCN(C(=O)/C(C#N)=C/c2ccc(O)c(O)c2)CC1	10000	*
4537	Nc1ncnc2occ(-c3ccc(NC(=O)Nc4cc(C(F)(F)F)ccc4F)cc3)c12	10000	*
4538	COc1cc2ncnc(Nc3ccccc3C(F)(F)F)c2cc1OC	10000	*
4539	Cc1cccc(Cl)c1NC(=O)c1cnc(NC(=O)C2CC2)s1	10000	*
4540	NC[C@H](Cc1cccc(F)c1)NC(=O)c1cc(Br)c(-c2ccnc3[nH]ccc23)s1	10000	*
4541	Cn1nc(-c2ccc3occc(=O)c3c2)c2c(N)ncnc21	10000	*
4542	CC(C)n1nc(-c2cc(F)c(C=O)c(F)c2)c2c(N)ncnc21	10000	*

4543	CN(C)CCNc1ncnc2[nH]c3ccccc3c12	10000	*
4544	CCOC(C)=O.CN(C)CCNc1ncnc2[nH]c3ccccc3c12	10000	*
4545	Cc1nc(Nc2cccc(Br)c2)c2c(n1)[nH]c1ccccc12.Cl	10000	*
4546	COc1ccc(Oc2ccnc3cc(OC)c(OC)cc23)cc1OC	10000	*
4547	O=C(Nc1cccc(Cl)c1)c1cc2ccccc2cc1O	10000	*
4548	Cc1ccc(C(=O)Nc2cccc(Cl)c2)c(O)c1	10000	*
4549	O=C(Nc1cccc(Cl)c1)c1ccc(OS(=O)(=O)C(F)(F)F)cc1O	10000	*
4550	CCN(CC)c1ccc(C(=O)Nc2cccc(Cl)c2)c(O)c1	10000	*
4551	COc1ccc(-c2cc3c(NC(C)c4ccc(C(C)(C)C)cc4)ncnc3[nH]2)cc1	10000	*
4552	COc1cc2c(Oc3ccc(NC(=O)c4nnn(-c5ccc(F)cc5)c4C(F)(F)F)cc3F)ccnc2cc1OCCCN1CCCC1	10000	*
4553	COc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(Cl)c(Oc2ccc3ccccc3c2)n1	10000	*
4554	COc1ccc(NC(=O)/C=C/CN(C)C)cc1Nc1ncc(Cl)c(Sc2ccc3ccccc3c2)n1	10000	*
4555	O=C(O)C1CCC2(CC1)OOC1(OO2)C2CC3CC(C2)CC1C3	10000	*
4556	C=CC(=O)Nc1cc(Nc2n[nH]c3ccccc23)ccc1N(C)CCN(C)C	10000	*
4557	CCC(=O)Nc1cc(Nc2n[nH]c3ccccc23)ccc1N(C)CCN(C)C	10000	*
4558	CCC(=O)Nc1cc(Nc2n[nH]c3ccccc23)c(OC)cc1N(C)CCN(C)C	10000	*
4559	CN1CCN(c2ccc(Nc3ncc(Br)c(Nc4ccc5ncccc5c4)n3)cc2)CC1	10000	*
4560	COc1cccc(Nc2cc(Nc3ccc(S(N)(=O)=O)cc3)ncn2)c1	10000	*
4561	CCOc1ccc(Nc2cc(NC(=O)c3ccccc3)ncn2)cc1	10000	*
4562	O=C(O)CCC(=O)Nc1cc(Nc2ccc(Cl)cc2)ncn1	10000	*
4563	COc1cccc(Nc2cc(Nc3cccc(Cl)c3)ncn2)c1	10000	*
4564	O=C(O)CCCC(=O)Nc1cc(Nc2ccc(Cl)cc2)ncn1	10000	*
4565	CCOC(=O)CCC(=O)Nc1cc(Nc2cccc(Br)c2)ncn1	10000	*
4566	O=C(O)CCCC(=O)Nc1cc(Nc2ccccc2)ncn1	10000	*
4567	CCOC(=O)c1ccc(Nc2cc(Nc3cccc(OC)c3)ncn2)cc1	10000	*
4568	O=C(Nc1cc(Nc2ccc(Cl)cc2)ncn1)c1ccc(F)cc1	10000	*
4569	Cc1ncc([N+](=O)[O-])n1C/C(=N/NC(=O)c1ccccc1)c1ccc(Br)cc1	10020	5.00
4570	O=C(/C=C/c1ccccc1)Nc1ccc(F)cc1	10020	*
4571	NC(=S)N1N=C(c2ccc(Br)c(Br)c2)CC1c1ccc(Br)cc1	10060	5.00
4572	O=[N+]([O-])/C=C/c1ccc(O)cc1	10100	*
4573	Nc1cc2ncnc(NCc3cccc([N+](=O)[O-])c3)c2cn1	10100	*
4574	Cc1cccc(Nc2c(C#N)cnc3ccc(C(=O)/C=C/c4ccc(-c5ccc(S(N)(=O)=O)cc5)o4)cc23)c1	10110	*
4575	Cc1ccc(-n2nc(C)c(C3C(C#N)=C(N)N(c4cccnc4)C4=C3C(=O)CCC4)c2Cl)cc1	10120	4.99
4576	CN(c1ccc2c(ccn2C)c1)c1ccnc(Nc2ccc(N3CCOCC3)cc2)n1	10120	*
4577	COc1ccc(C2CC(c3ccc(Br)cc3)=NN2c2nc(-c3ccccc3)cs2)cc1	10170	4.99
4578	O=C(O)Cc1c(SSc2[nH]c3ccccc3c2CC(=O)O)[nH]c2ccccc12	10200	*
4579	COc1cc(F)c(-c2nn(C(C)C)c3ncnc(N)c23)cc1F	10200	*
4580	CCOc1ccc(NC(=O)/C=C/c2ccccc2)cc1	10230	*
4581	N#C/C(=C\c1ccc(O)c(O)c1)C(=O)NCc1cccc(CNC(=O)/C(C#N)=C/c2ccc(O)c(O)c2)c1	10300	*
4582	O=S(=O)(O)c1cc(NCc2cc(O)ccc2O)ccc1O	10300	*
4583	CCOc1cc2ncc(C#N)c(Nc3cccc(Br)c3)c2cc1NC(=O)/C=C/CN1CCOCC1	10320	4.99
4584	O=C(Cc1ccc(Cl)cc1)NS(=O)(=O)c1ccc(Cl)cc1	10340	4.99
4585	Cc1ncc([N+](=O)[O-])n1CC(=O)N/N=C/c1cc2ccccc2nc1Oc1ccccc1	10350	4.99

4586	Cc1ccc2c(c1)cc(C1C(C#N)=C(N)N(c3cccnc3)C3=C1C(=O)CCC3)c1nnnn12	10400	4.98
4587	COc1ccc(C2=NN(C(=O)c3ccc(Cl)cc3O)C(c3ccc(Cl)cc3)C2)cc1	10490	*
4588	CCC(C)[C@H]1[C@](C)(O)C(=O)[C@@]2(O)C[C@](C)(O)C[C@@H](C)[C@@H]2[C@]1(C)C(=O)/C=C/OC	10500	*
4589	COc1cc2ncc(C#N)c(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/C(C)N1CCOCC1	10590	4.97
4590	NC(=S)N1N=C(c2ccc(Br)c(Br)c2)CC1c1ccc([N+](=O)[O-])cc1	10640	4.97
4591	CN(C)C/C=C/C(=O)Nc1cccc(Nc2nc(N/N=C/c3ccc(F)cc3)ncc2Cl)c1	10650	*
4592	COc1ccc(C2CC(c3ccc(F)cc3)=NN2C2=NC(=O)CS2)cc1	10690	4.97
4593	Cc1cc(C)c(C(=O)/C(C#N)=C/c2ccc(O)c(O)c2)c(C)c1	10700	*
4594	O=C1CSC(N/N=C/c2cccc(Cl)c2)=N1	10780	4.97
4595	COc1cc2c(cc1OC)Oc1ncnc(Oc3ccc(F)c(Cl)c3)c1N(C)C2	10800	4.97
4596	COc1ccc(/C=C/C(=O)OCCn2c([N+](=O)[O-])cnc2C)cc1	10850	4.96
4597	N#Cc1ccc2c(c1)C(c1ccccc1F)=Nc1c[nH]nc1N2	10900	*
4598	O=C1CSC(N2N=C(c3ccc(F)cc3)CC2c2ccc(Cl)cc2)=N1	10920	4.96
4599	COc1cccc(/C=C/C(=N/NC(N)=S)c2ccccc2)c1	10950	4.96
4600	NC(=S)N1N=C(c2ccc(Br)c(Br)c2)CC1c1ccccc1Br	10970	4.96
4601	COc1cc2ncnc(Nc3cc(NC(=O)c4ccccc4)ccc3Cl)c2cc1OC	11000	*
4602	Cc1cccc(Nc2ccnc(Nc3ccc(N4CCN(C)CC4)cc3)n2)c1	11000	*
4603	N#CCCCCn1nc(-c2ccc(F)c(O)c2)c2c(N)ncnc21	11000	*
4604	COc1cc(Br)cc(-c2nn(C(C)C)c3ncnc(N)c23)c1	11000	*
4605	CCOC(=O)C1=C(N)N(c2cccnc2)C2=C(C(=O)CC(C)(C)C2)C1c1c(C)nn(-c2ccccc2)c1Cl	11180	4.95
4606	COc1ccccc1CNc1ccc2ncnc(Nc3cccc(Br)c3)c2c1	11220	4.95
4607	Fc1ccc(C2CC(c3ccc(Br)cc3)=NN2c2nc(-c3ccccc3)cs2)cc1	11240	4.95
4608	NC(=S)N1N=C(c2ccc(Br)c(Br)c2)CC1c1ccc(O)cc1	11270	4.95
4609	O=C(Cc1ccc(Cl)cc1)NS(=O)(=O)c1ccc(Br)cc1	11290	4.95
4610	Cn1c(SSc2c(C(=O)Nc3ccccc3)c3cc(Br)ccc3n2C)c(C(=O)Nc2ccccc2)c2cc(Br)ccc21	11400	*
4611	O=C(Nc1ccccc1F)c1ccc(N(CCCl)CCCl)cc1	11570	4.94
4612	O=C(/C=C/c1ccccc1)Nc1ccc(F)cc1F	11690	*
4613	C=CC(=O)Nc1cccc(Nc2nc(N/N=C(\C)c3ccc(F)cc3F)ncc2Cl)c1	11750	*
4614	O=C(Cc1ccc(Cl)cc1)NS(=O)(=O)c1ccccc1	11910	4.92
4615	CCOc1cc2ncnc(Nc3cccc(-c4csc(C)n4)c3)c2cc1OCC	11920	*
4616	CN(C)C(=O)CCc1c(SSc2[nH]c3ccccc3c2CCC(=O)N(C)C)[nH]c2ccccc12	12000	*
4617	O=[N+]([O-])c1ccc2c(Nc3cccc3)ncnc2c1	12000	*
4618	COc1cc2ncnc(N(C)c3cccc(C)c3)c2cc1OC.Cl	12000	*
4619	CC(=O)c1ccc(-c2nn(C(C)C)c3ncnc(N)c23)cc1	12000	*
4620	Nc1ncnc2c1c(-c1ccn3ccnc3c1)nn2C1CCCC1	12000	*
4621	CC(C)n1nc(-c2ccc3nc(N)ccc3c2)c2c(N)ncnc21	12000	*
4622	COc1ccc(-c2nn(C[C@H](C)CO)c3ncnc(N)c23)cc1OC	12000	*
4623	Cc1cccc(NC(=O)/C=C/c2ccc3c(c2)OCCCCO3)c1	12040	*
4624	Cn1cccc1-c1nc2cc(NC(=O)CCl)ccc2[nH]1	12070	*
4625	Cc1ccc(S(=O)(=O)NC(=O)c2cncc(Br)c2)cc1	12110	4.92
4626	O=C(Nc1ccc(Cl)cc1)c1cc(Br)cc(Br)c1O	12190	*
4627	NC(=S)N/N=C(/C=C/c1ccccc1)c1ccc(Br)cc1	12240	4.91

4628	NC(=S)N1N=C(c2ccc(Br)c(Br)c2)CC1c1ccccc1Cl	12260	4.91
4629	Cc1ccccc1NC(=O)/C=C/c1ccccc1	12290	*
4630	COc1ccccc1-c1nnc(SCc2ccccc2)o1	12320	4.91
4631	Nc1ncnc2c1c(-c1ccc(Cl)c(O)c1)nn2[C@@H]1CCNC1	12400	*
4632	Cc1ccc(-c2n[nH]c3ncnc(N)c23)cc1O	12400	*
4633	Cc1ncc([N+](=O)[O-])n1CCOC(=O)/C=C/c1cccc(F)c1	12420	4.91
4634	O=C(/C=C/c1ccc2c(c1)OCCCCO2)Nc1cccc(Cl)c1	12420	*
4635	Cc1ncc([N+](=O)[O-])n1C/C(=N/NC(=O)c1ccc(Cl)cc1)c1ccc(Br)cc1	12450	4.90
4636	N#CC(C#N)=C1C(=O)Nc2ccc(O)cc21	12500	*
4637	COC(=O)c1c(OC)c2ccccc2c2oc3c(c12)C(=O)c1ccccc1C3=O	12600	*
4638	COc1ccc(-c2nn([C@@H]3CCNC3)c3ncnc(N)c23)cc1O	12600	*
4639	Cc1ccc(NC(=O)/C=C/c2ccccc2)cc1	12690	*
4640	CCOc1cc2ncc(C#N)c(Nc3ccc(N4CCOCC4)c(Cl)c3)c2cc1NC(=O)/C=C/CN(C)C	12700	4.90
4641	C=CCNC(=S)Nc1scc(-c2ccc3ncc(C#N)c(Nc4cccc(Br)c4)c3c2)c1C#N	12770	*
4642	CC(C)n1nc(-c2ccc(NS(C)(=O)=O)cc2)c2c(N)ncnc21	12800	*
4643	CCOC(=O)Nc1ccc2c(C#N)cnc(Nc3cccc(Br)c3)c2c1	12800	*
4644	O=C(/C=C/c1ccccc1)Nc1cc(F)c(F)c(F)c1	12880	*
4645	CCOc1cc2ncc(C#N)c(Nc3cccc(OCc4ccccc4)c3)c2cc1NC(=O)/C=C/CN(C)C	13000	4.89
4646	CNC(=O)c1c([Se][Se]c2[nH]c3ccccc3c2C(=O)NC)[nH]c2ccccc12	13000	*
4647	CC(C)n1nc(-c2ccc(CC#N)cc2)c2c(N)ncnc21	13000	*
4648	O=C(Nc1ccc(Cl)cc1)c1cc(I)ccc1O	13040	*
4649	O=C1N=C(N2CCC[C@H]2C(=O)Nc2ccc3ncnc(Nc4cccc(Cl)c4)c3c2)S/C1=C/c1ccc(-c2ccccc2)cc1	13200	*
4650	O=C(/C=C/c1ccccc1)Nc1cc(F)cc(F)c1	13230	*
4651	CN(C)N=Nc1ccc2ncnc(N(C)c3ccccc3)c2c1	13350	*
4652	NC(=S)N1N=C(c2ccc(Br)c(Br)c2)CC1c1ccccc1F	13370	4.87
4653	CCCCC(Cc1coc2nc(N)nc(N)c12)c1ccccc1OC	13400	*
4654	Nc1ncnc2c1c(-c1ccccc1)cn2C1CCNC1	13400	*
4655	N#CC(C#N)=C(O)c1cc(O)c(O)c(O)c1	13500	*
4656	N#C/C(=C\c1ccc(O)c(O)c1)C(=O)NC1CCCC[C@@H]1NC(=O)/C(C#N)=C/c1ccc(O)c(O)c1	13500	*
4657	O=C1CSC(N/N=C/c2cccc(F)c2)=N1	13530	4.87
4658	COc1cc2ncc(C#N)c(Nc3ccc(F)c(Cl)c3)c2cc1NC(=O)/C=C/CN1CCOCC1	13570	4.87
4659	COC(=O)c1c(OCCCN(C)C)c2ccccc2c2oc3c(c12)C(=O)c1ccccc1C3=O	13600	*
4660	O=C(Nc1ccc(Br)cc1)c1cc(I)ccc1O	13700	*
4661	O=C(/C=C/c1ccccc1)Nc1ccc(Cl)cc1	13710	*
4662	Cc1ccc(S(=O)(=O)NC(=O)Cc2ccc(Cl)cc2)cc1	13730	4.86
4663	COc1cc2ncc(C#N)c(Nc3ccc(Cl)cc3F)c2cc1OC	13850	*
4664	COc1cccc(/C=C/C(=O)OCCn2c([N+](=O)[O-])cnc2C)c1	13870	4.86
4665	COc1ccccc1CNc1ccc2ncnc(Nc3cccc(Cl)c3)c2c1	13880	4.86
4666	O=C(/C=C/c1ccccc1)Nc1cc(Cl)cc(Cl)c1	13930	*
4667	O=C(NCc1ccccc1)C(O)Cc1c(SSc2[nH]c3ccccc3c2CC(O)C(=O)NCc2ccccc2)[nH]c2ccccc12	14000	*
4668	COc1cc(C2=C(c3cn(COCc4ccccc4)c4ccccc34)CNC2=O)cc(OC)c1OC	14000	*
4669	COc1cc2nccc(Oc3ccccc3C(=O)c3ccccc3)c2cc1OC	14000	*
4670	COc1cc2nccc(Oc3cccc(C)c3)c2cc1OC	14000	*

4671	COc1cc2c(cc1OC)Sc1ncnc(Nc3ccc4c[nH]nc4c3)c1NC2	14100	4.85
4672	Nc1ccc(-c2cc(=O)c3cc(N)c(O)cc3o2)cc1	14100	*
4673	COc1cc2ncc(C#N)c(Nc3cccc(C#N)c3)c2cc1OC	14180	*
4674	O=C(Nc1ccccc1Cl)c1ccccc1O	14180	*
4675	O=C1CSC(N2N=C(c3ccc(Cl)cc3)CC2c2ccc(F)cc2)=N1	14210	4.85
4676	CC(=O)N1CCc2cc(Nc3nc(Nc4ccc(N5CCN(C)CC5)cc4)ncc3Br)ccc21	14300	*
4677	COc1cc(/C=C(\C#N)C(N)=O)cc(CSc2nc3ccccc3[nH]2)c1O	14454.4	*
4678	COc1cc2c(cc1OC)Sc1nc(C)nc(Nc3ccc4[nH]cnc4c3)c1NC2	14500	4.84
4679	Cc1ncc([N+](=O)[O-])n1CCOC(=O)/C=C/c1cccc([N+](=O)[O-])c1	14530	4.84
4680	O=C(Cc1ccc(Br)cc1)NS(=O)(=O)c1ccc(F)cc1	14530	4.84
4681	CC(C)c1ccc(NC(=O)/C=C/c2ccccc2)cc1	14580	*
4682	O=C(/C=C/c1ccccc1)Nc1cccc(Cl)c1	14590	*
4683	Cc1ccc(-n2nc(C)c(C3C(C#N)=C(N)N(c4cccnc4)C4=C3C(=O)CC(C)(C)C4)c2Cl)cc1	14700	4.83
4684	CN(C(=O)c1ccc(N(CCCl)CCCl)cc1)c1ccccc1	14720	4.83
4685	COc1ccc(/C=C/C(=N/NC(N)=S)c2ccccc2)cc1	14830	4.83
4686	O=C(O)CC1C(S)=Nc2ccccc21	14900	*
4687	Cc1cccc(-n2ncc3c(NCc4ccc5c(c4)OCO5)ncnc32)c1	15000	*
4688	Cn1nc(-c2cnc3[nH]ccc3c2)c2c(N)ncnc21	15000	*
4689	CC(C)n1nc(-c2ccc3c(c2)OCCO3)c2c(N)ncnc21	15000	*
4690	COc1cc(N(C)CCN(C)C)c(N)cc1Nc1nccc(-c2cn(C)c3ccccc23)n1	15000	*
4691	Cc1ccc(S(=O)(=O)NC(=O)c2ccc(C)nc2Cl)cc1	15020	4.82
4692	COc1cc2ncc(C(N)=O)c(Nc3cccc(Br)c3)c2cc1OC	15170	*
4693	COc1cc2c(cc1OC)Sc1nc(C)nc(Nc3ccc4ncsc4c3)c1NC2	15200	4.82
4694	COc1ccc(C2CC(c3ccc(C)c(C)c3)=NN2C(C)=O)cc1	15240	4.82
4695	COc1cc(/C=C2\CCC/C(=C\c3ccc(Cl)cc3)C2=O)cc(OC)c1	15300	4.82
4696	C/C(=N\Nc1ncc(Cl)c(Nc2cccc(NC(=O)/C=C/CN(C)C)c2)n1)c1ccc(F)cc1	15320	*
4697	CC(=O)N1N=C(c2ccc(C)c(C)c2)CC1c1ccc(F)cc1	15560	4.81
4698	Nc1ncnc2c1c(-c1ccc(F)c(O)c1)nn2[C@@H]1CCNC1	15600	*
4699	O=C(NS(=O)(=O)c1ccc(Br)cc1)c1ccncc1Cl	15680	4.80
4700	O=[N+]([O-])c1ccc(C2CC(c3ccc(Br)cc3)=NN2c2nc(-c3ccccc3)cs2)cc1	15720	4.80
4701	O=C(/C=C/c1ccccc1)Nc1ccccc1Br	15740	*
4702	COc1cc(/C=C(/C#N)C(N)=O)cc(CSCc2ccc(Cl)cc2)c1O	15848.93	*
4703	O=C(Cc1ccc(Br)cc1)NS(=O)(=O)c1ccc(Cl)cc1	15920	4.80
4704	NC(=O)CCc1c(SSc2[nH]c3ccccc3c2CCC(N)=O)[nH]c2ccccc12	16000	*
4705	O=C(/C=C/c1ccc(O)c(O)c1)c1ccc(O)cc1O	16000	*
4706	COc1cc2nccc(Oc3ccc(O)cc3)c2cc1OC	16000	*
4707	COc1cc2nccc(Oc3ccc(C(=O)c4cccs4)cc3)c2cc1OC	16000	*
4708	COc1cc2nccc(Oc3cccc(C(=O)c4cccs4)c3)c2cc1OC	16000	*
4709	CCOC(=O)C(C#N)C(=O)c1cc(/C=C/c2ccc(N(C)C)cc2)nc2ccc(Br)cc12	16010	*
4710	CC(=O)N1N=C(c2ccc(Cl)c(Cl)c2)CC1c1ccc(Cl)cc1	16140	4.79
4711	O=C(/C=C/c1ccccc1)Nc1ccc(Cl)cc1Cl	16170	*
4712	COc1cc2c(cc1OC)Sc1nc(C)nc(Nc3ccc4c(c3)CN=N4)c1NC2	16200	4.79
4713	Cc1[nH]c2ncnc(Nc3cccc(C(=O)O)c3)c2c1C	16300	*

4714	C=CC(=O)Nc1ccc(-n2c(=O)c(C)nc3cnc(Nc4ccc(OC)cc4)nc32)cc1	16338	4.79
4715	c1ccc(CSc2nnc(-c3ccccc3)o2)cc1	16630	4.78
4716	CCOC(=O)C1=C(N)N(c2cccnc2)C2=C(C(=O)CCC2)C1c1cc2cc(Cl)ccc2n2nnnc12	16700	4.78
4717	O=C1CSC(N2N=C(c3ccc(F)cc3)CC2c2ccc(F)cc2)=N1	16920	4.77
4718	COc1cc2c(cc1OC)Sc1nc(C)nc(Nc3ccc4ccccc4c3)c1NC2	17000	4.77
4719	C[C@@H](NC(=O)c1ccc(S(=O)(=O)Oc2ccc(/C=C/[N+](=O)[O-])cc2)cc1)C(=O)N[C@H](C)C(=O)NCCN	17000	*
4720	CC(C)n1nc(-c2cccc(CC#N)c2)c2c(N)ncnc21	17000	*
4721	COc1ccc(-c2nn(C3CNC3)c3ncnc(N)c23)cc1O	17000	*
4722	COc1cc2ncc(C#N)c(Nc3cc(Cl)ccc3O)c2cc1OC.Cl	17020	*
4723	COc1ccc(C2CC(c3ccc(Cl)c(Cl)c3)=NN2C(C)=O)cc1	17190	4.76
4724	O=C(Cc1ccc(Br)cc1)NS(=O)(=O)c1ccc(Br)cc1	17260	4.76
4725	COc1cc(OC)cc(C2CC(c3ccc(C)c(C)c3)=NN2C(C)=O)c1	17310	4.76
4726	Cc1ccc(/C=C/C(=N/NC(N)=S)c2ccccc2)cc1	17390	4.76
4727	CC(=O)N1N=C(c2ccc(C)c(C)c2)CC1c1ccc(C)cc1	17490	4.76
4728	O=C(NCc1ccccc1)c1ccc(N(CCCl)CCCl)cc1	17510	4.76
4729	O=C(Cc1ccc(Br)cc1)NS(=O)(=O)c1ccccc1	17810	4.75
4730	Clc1ccc(-c2csc(N3N=C(c4ccc(Br)cc4)CC3c3ccc(Cl)cc3)n2)cc1	17840	4.75
4731	O=C(O)CCCc1c(SSc2[nH]c3ccccc3c2CCCC(=O)O)[nH]c2ccccc12	18000	*
4732	COC(=O)Cc1c(SSc2[nH]c3ccccc3c2CC(=O)OC)[nH]c2ccccc12	18000	*
4733	COc1cc2cc3ncc(C#N)c(Nc4ccc(F)c(Cl)c4)c3cc2cc1OC	18000	*
4734	Cc1ccc2ccc(-c3nn(C(C)C)c4ncnc(N)c34)cc2n1	18000	*
4735	COc1ccc(-c2nn(C[C@@H](C)CO)c3ncnc(N)c23)cc1OC	18000	*
4736	CC(C)n1nc(-c2ccc3nccnc3c2)c2c(N)ncnc21	18000	*
4737	N#CCCCn1nc(-c2ccc(F)c(O)c2)c2c(N)ncnc21	18000	*
4738	COc1cccc(Oc2ccnc3cc(OC)c(OC)cc23)c1	18000	*
4739	Nc1ccc(-c2nc3c(Nc4ccc(Cl)cc4)ncnc3o2)cc1	18000	*
4740	Cc1nn(-c2ccccc2)c(Cl)c1C1C(C#N)=C(N)N(c2cccnc2)C2=C1C(=O)CCC2	18020	4.74
4741	CCCCN(Cc1cccc(Cl)c1O)C(=S)Nc1ccccc1	18120	4.74
4742	O=C(NS(=O)(=O)c1ccc(Cl)cc1)c1ccc(Cl)nc1	18150	4.74
4743	COc1ccccc1C(Cc1coc2nc(N)nc(N)c12)C(C)C	18200	*
4744	COc1ccc(-n2c(=O)cnc3cnc(Nc4cccc(N)c4)nc32)cc1	18280	4.74
4745	N#CC1=C(N)N(c2cccnc2)C2=C(C(=O)CCC2)C1c1cc2cc(Cl)ccc2n2nnnc12	18300	4.74
4746	CN(C)S(=O)(=O)c1ccc(Nc2nc(Cl)nc3cc4c(cc23)OCO4)cc1	18300	*
4747	Cc1ccc(S(=O)(=O)NC(=O)Cc2ccc(Br)cc2)cc1	18350	4.74
4748	CC(=O)N1N=C(c2ccc(Cl)c(Cl)c2)CC1c1ccc(F)cc1	18350	4.74
4749	CC(C)(C)c1ccc(OC[C@H](Cn2ccnc2[N+](=O)[O-])OC(=O)c2ccc(NC=C3C(=O)C=CC3=O)cc2)cc1	18400	*
4750	CC(=O)N1N=C(c2ccc(Cl)c(Cl)c2)CC1c1ccc(Br)cc1	18450	4.73
4751	COc1ccc(/C=C2\CCC/C(=C\c3cc(OC)cc(OC)c3)C2=O)cc1	18600	4.73
4752	COc1cc(/C=C2\CCCCC2=O)cc(OC)c1	18670	4.73
4753	O=C(Cc1cccc(Br)c1)NS(=O)(=O)c1ccc(F)cc1	18720	4.73
4754	COc1cc(/C=C(\C#N)C(=O)NCCCCNC(=O)/C(C#N)=C/c2cc(OC)c(O)c([N+](=O)[O-])c2)cc([N+](=O)[O-])c1O	19000	*
4755	Cc1ccc(-c2nn(C)c3ncnc(N)c23)cc1O	19000	*
4756	COc1cc2nccc(Oc3cccc(O)c3)c2cc1OC	19000	*

4757	COc1cc(/C=C(\C#N)C(N)=O)cc(CSc2nc3ccccc3s2)c1O	19054.61	*
4758	Cc1cc(C)c(NC(=O)/C(C#N)=C/c2ccc(O)c(O)c2)c(C)c1	19054.61	*
4759	NC(=S)N/N=C(/C=C/c1ccc(F)cc1)c1ccccc1	19120	4.72
4760	O=C(Nc1ccc([N+](=O)[O-])cc1)c1ccc(N(CCCl)CCCl)cc1	19260	4.72
4761	COc1cc2c(cc1OC)Sc1ncnc(Oc3cccc(Cl)c3F)c1NC2	19300	4.71
4762	O=C1CSC(N/N=C/c2cccc(O)c2)=N1	19320	4.71
4763	CC(=O)N1N=C(c2ccc(Cl)c(Cl)c2)CC1c1ccc(C)cc1	19320	4.71
4764	Cc1cc(C)c(O)c(CN(Cc2ccc(F)cc2)C(=S)Nc2ccccc2)c1	19410	4.71
4765	Cc1ccc(C2CC(c3ccc(Br)cc3)=NN2c2nc(-c3ccccc3)cs2)cc1	19640	4.71
4766	Cc1cccc(NC(=O)/C=C/c2ccccc2)c1	19690	*
4767	CC(=O)N1N=C(c2ccc(C)c(C)c2)CC1c1ccc(Cl)cc1	19730	4.70
4768	CCOc1cc2nc3c(c(Nc4cccc(-c5csc(C)n5)c4)c2cc1OCC)CCC3	19740	*
4769	COc1ccc(C2CC(c3ccc(Br)cc3)=NN2c2nc(-c3ccc(Cl)cc3)cs2)cc1	19830	4.70
4770	O=C(NS(=O)(=O)c1ccc(Cl)cc1)c1cccnc1Cl	19830	4.70
4771	Cc1c(Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)ncnc1-c1ccccc1	20000	4.70
4772	CC(=O)Oc1cccc2c1c(C(=O)Nc1ccccc1)c(SSc1c(C(=O)Nc3ccccc3)c3c(OC(C)=O)cccc3n1C)n2C	20000	*
4773	COc1cc2nccc(Oc3ccc(Br)cc3)c2cc1OC	20000	*
4774	CC(=O)N1N=C(c2ccc(C)c(C)c2)CC1c1ccccc1	20040	4.70
4775	O=C(NS(=O)(=O)c1ccccc1)c1cncc(Br)c1	20190	4.69
4776	C=CCNC(=S)Nc1scc(-c2ccc3ncc(C(N)=O)c(Nc4cccc(Br)c4)c3c2)c1C#N	20450	*
4777	NC(=S)N/N=C(/C=C/c1ccc(Cl)cc1)c1ccccc1	20480	4.69
4778	Nc1ncnc2c1c(-c1ccc(Cl)c(O)c1)nn2CCC1CCCNC1	20500	*
4779	CC(=O)N1N=C(c2ccc(C)c(C)c2)CC1c1ccc(Br)cc1	20610	4.69
4780	COc1cc(/C=C2\CCC/C(=C\c3ccccc3OC)C2=O)cc(OC)c1	20800	4.68
4781	CCC(=O)Nc1ccc2c(C#N)cnc(Nc3cccc(Br)c3)c2c1	20800	*
4782	Cc1ncc([N+](=O)[O-])n1CCOC(=O)/C=C/c1ccccc1Cl	20810	4.68
4783	COC(=O)CCc1c(SSc2[nH]c3ccccc3c2CCC(=O)OC)[nH]c2ccccc12	21000	*
4784	N#C/C(=C\c1ccc(O)c(O)c1)C(=O)NCCCCCCCCCNC(=O)/C(C#N)=C/c1ccc(O)c(O)c1	21000	*
4785	Cc1cc(C2CCN(CCCF)CC2)cc2[nH]c(-c3c(NCCn4cc(Cl)cn4)cc[nH]c3=O)nc12	21000	*
4786	CCOc1ccc2cc(-c3nn(C)c4ncnc(N)c34)ccc2c1	21000	*
4787	COc1cc2nccc(Oc3ccc(C(=O)c4ccccc4C(F)(F)F)cc3)c2cc1OC	21000	*
4788	Cc1ncc([N+](=O)[O-])n1CC(=O)N/N=C/c1cc2ccccc2nc1Oc1ccc(F)cc1	21020	4.68
4789	Clc1ccc2c(c1)SCc1cnc(Nc3ccccc3)nc1-2	21180	4.67
4790	CCOc1cc2c(Nc3ccc(C)c(O)c3)c(C#N)cnc2cc1OC	21190	*
4791	O=C(Cc1cccc(Br)c1)NS(=O)(=O)c1ccc(Cl)cc1	21280	4.67
4792	CC(C)(C)OC[C@@H](Cn1ccnc1[N+](=O)[O-])OC(=O)c1ccc(NC=C2C(=O)C=CC2=O)cc1	21300	*
4793	CC(=O)N1N=C(c2ccc(C)c(C)c2)CC1c1ccccc1Cl	21480	4.67
4794	Oc1ccc(C2CC(c3ccc(Br)cc3)=NN2c2nc(-c3ccc(Cl)cc3)cs2)cc1	21520	4.67
4795	COc1ccc(Nc2ncc3c(n2)-c2ccc(Cl)cc2SC3)cc1	21560	4.67
4796	Cc1ccc(C(=O)NS(=O)(=O)c2ccccc2)c(Cl)n1	21560	4.67
4797	COc1cc2c(cc1OC)Sc1ncnc(Oc3cccc(Br)c3)c1NC2	21700	4.66
4798	Cc1cccc(CN(Cc2ccc(F)cc2)C(=O)Nc2ccccc2)c1O	21710	4.66
4799	COc1ccc(CC(=O)NS(=O)(=O)c2ccc(F)cc2)cc1	21840	4.66

4800	COc1cc(/C=C(\C#N)C(N)=O)cc(CSc2ccccc2NC(C)=O)c1O	21877.62	*
4801	O=C(Nc1ccccc1Br)c1ccccc1O	21920	*
4802	Fc1cccc(COc2ccc(Nc3cc(-c4ccsc4)ncn3)cc2Cl)c1	22000	4.66
4803	NC(=O)CCC1C(S)=Nc2ccccc21	22000	*
4804	COc1cc(C2=C(c3cn(COCC[Si](C)(C)C)c4ccccc34)CNC2=O)cc(OC)c1OC	22000	*
4805	CN1CC[C@H](c2c(O)cc(O)c3c(=O)cc(-c4ccccc4Cl)oc23)[C@H](O)C1	22000	*
4806	CCCCN(Cc1cccc(Br)c1O)C(=S)Nc1ccccc1	22040	4.66
4807	Cc1ccc(C(=O)Nc2ccccc2Br)c(O)c1	22190	*
4808	Cn1c(SSc2c(C(=O)Nc3ccccc3)c3cccnc3n2C)c(C(=O)Nc2ccccc2)c2cccnc21	22300	*
4809	Oc1ccc(C2CC(c3ccc(Br)cc3)=NN2c2nc(-c3ccccc3)cs2)cc1	22360	4.65
4810	NC(=S)N/N=C(/C=C/c1ccccc1F)c1ccccc1	22360	4.65
4811	COc1ccc(NC(=O)c2cc(Br)cc(Br)c2O)cc1	22390	*
4812	CCCCNC(=O)c1ccc(N(CCCl)CCCl)cc1	22810	4.64
4813	COc1cc(C=C(C#N)C#N)cc(CS(=O)(=O)c2ccc(C)cc2)c1O	22908.68	*
4814	COC[C@H](Cn1ccnc1[N+](=O)[O-])OC(=O)c1ccc(NC=C2C(=O)C=CC2=O)cc1	23000	*
4815	COc1cc(C2=C(c3c[nH]c4ccccc34)CNC2=O)cc(OC)c1OC	23000	*
4816	Cc1cccc(N2NC(=O)/C(=C/c3ccc(-c4ccccc4F)o3)C2=O)c1	23100	4.64
4817	Cc1ccc(Oc2nc3ccccc3cc2/C=N/NC(=O)Cn2c([N+](=O)[O-])cnc2C)cc1	23130	4.64
4818	O=C(/C=C/c1ccccc1)Nc1ccccc1	23160	*
4819	NC(=S)N/N=C(/C=C/c1ccccc1Cl)c1ccccc1	23270	4.63
4820	Cc1cccc(/C=N/NC2=NC(=O)CS2)c1	23490	4.63
4821	CC1=C(C(=O)Nc2ccc(C)cc2)C(c2ccc(O)cc2O)NC(NCc2ccccc2)=N1	23500	*
4822	O=C(CCc1c(SSc2[nH]c3ccccc3c2CCC(=O)NCCc2ccccc2)[nH]c2ccccc12)NCCc1ccccc1	24000	*
4823	COc1cc2nccc(Oc3cccc(F)c3)c2cc1OC	24000	*
4824	Cc1nn(-c2ccc(Cl)cc2)c(Cl)c1C1C(C#N)=C(N)N(c2cccnc2)C2=C1C(=O)CC(C)(C)C2	24050	4.62
4825	COc1ccc(CC(=O)NS(=O)(=O)c2ccc(Br)cc2)cc1	24150	4.62
4826	CC(=O)N1N=C(c2ccc(Cl)c(Cl)c2)CC1c1ccccc1Cl	24150	4.62
4827	Fc1ccc(C2CC(c3ccc(Br)cc3)=NN2c2nc(-c3ccc(Cl)cc3)cs2)cc1	24160	4.62
4828	Clc1cccc(Nc2[nH]nc3ncnc(Oc4cccc(Cl)c4)c23)c1	24200	*
4829	Cc1ncc([N+](=O)[O-])n1CCOC(=O)/C=C/c1ccccc1Br	24320	4.61
4830	O=C(Cc1cccc(Br)c1)NS(=O)(=O)c1ccc(Br)cc1	24330	4.61
4831	O=[N+]([O-])c1ccc(C2CC(c3ccc(Br)cc3)=NN2c2nc(-c3ccc(Cl)cc3)cs2)cc1	24370	4.61
4832	COc1cc2c(cc1OC)Sc1nc(C)nc(Nc3ccc4c[nH]nc4c3)c1NC2	24600	4.61
4833	CCCCN(Cc1cc(Cl)cc(Cl)c1O)C(=S)Nc1ccccc1	24650	4.61
4834	O=C(Cc1cccc(Br)c1)NS(=O)(=O)c1ccccc1	24680	4.61
4835	Cc1ccc(S(=O)(=O)NC(=O)c2cccnc2)cc1	24830	4.61
4836	O=C(Nc1ccccc1F)c1ccccc1O	24830	*
4837	Cc1ncc([N+](=O)[O-])n1CCOC(=O)/C=C/c1ccccc1[N+](=O)[O-]	25000	4.60
4838	N#C/C(=C\c1ccc(O)c(O)c1)C(=O)O	25000	*
4839	O=C(CCc1c(SSc2[nH]c3ccccc3c2CCC(=O)Nc2ccccc2)[nH]c2ccccc12)Nc1ccccc1	25000	*
4840	N#C/C(=C\c1ccc(O)c(O)c1)C(=O)N1CCN(C(=O)/C(C#N)=C/c2ccc(O)c(O)c2)CC1	25000	*
4841	CNc1ncnc(-c2cccnc2Oc2ccc(F)c(C(=O)Nc3cc(C(F)(F)F)ccc3N(C)CCCN(C)C)c2)n1	25000	*
4842	CNc1ncnc(-c2cccnc2Oc2cc(NC(=O)c3cccc(OC(F)(F)C(F)F)c3)ccc2C)n1	25000	*

4843	CC(C)n1nc(-c2ccc3cnccc3c2)c2c(N)ncnc21	25000	*
4844	Nc1ccc2ncnc(Nc3ccc(OCc4nccs4)c(Cl)c3)c2c1	25000	*
4845	CC(=O)Nc1ccc(C#Cc2cncnc2Nc2ccc(OCc3cccc(F)c3)c(Cl)c2)cc1	25100	*
4846	O=C(Cc1nc2ccccc2[nH]1)N1N=C(c2ccc(Cl)cc2)CC1c1ccc(Br)cc1	25200	*
4847	O=C(NS(=O)(=O)c1ccc(Cl)cc1)c1cccnc1	25360	4.60
4848	COc1cc(OC)cc(C2CC(c3ccc(Cl)c(Cl)c3)=NN2C(C)=O)c1	25470	4.59
4849	O=C(O)c1cccc(Nc2[nH]cnc3nc4c(c2-3)CCCC4)c1	25700	*
4850	Clc1ccc(-c2csc(N3N=C(c4ccc(Br)cc4)CC3c3ccc(Br)cc3)n2)cc1	25740	4.59
4851	Cc1ccc(NC(=O)c2ccccc2O)cc1	25740	*
4852	COc1ccc(-n2c(=O)cnc3cnc(Nc4ccc(N)cc4)nc32)cc1	25825	4.59
4853	CN(C)c1nc(N/N=C/c2cc(Br)c(O)c(Br)c2O)nc(Nc2ccc(F)cc2)n1	25900	*
4854	NC(=S)N/N=C(/C=C/c1ccccc1Br)c1ccccc1	26000	4.59
4855	CN1C(=O)C(=C(C#N)C#N)c2cc(O)ccc21	26000	*
4856	C[C@@H](CN)n1nc(-c2ccc(F)c(O)c2)c2c(N)ncnc21	26000	*
4857	C/C1=C/CC[C@]23O[C@H]2[C@@H](OC3=O)c2c(O)ccc(O)c2C1	26000	*
4858	COc1cc(OC)cc(-c2nnc(SCc3ccccc3)o2)c1	26060	4.58
4859	Cc1ccc(S(=O)(=O)NC(=O)Cc2cccc(Br)c2)cc1	26170	4.58
4860	COc1ccc(CC(=O)NS(=O)(=O)c2ccccc2)cc1	26200	4.58
4861	C=CC(=O)Nc1cc(Nc2ncc(Br)c(Nc3ccc4c(c3)CCC4)n2)ccc1N(C)CCN(C)C	26200	*
4862	COc1ccc(Nc2ncc3ncc(=O)n(-c4cccc(NC(=O)/C=C/CN(C)C)c4)c3n2)cc1	26283	4.58
4863	NC(=S)N/N=C(/C=C/c1ccc(Br)cc1)c1ccccc1	26560	4.58
4864	C=C(N/N=C/c1cn[nH]c1-c1ccccc1)[C@H](C)Cc1ccccc1	26600	4.58
4865	Cc1nc(Nc2ncc(C(=O)Nc3c(C)cccc3Cl)s2)cc(N2CCN(CCOC(=O)c3ccc(C(=O)Nc4ccc5ncnc(Nc6cccc(Cl)c6)c5c4)cn3)CC2)n1	26600	*
4866	O=C1CSC(N/N=C/c2cccc([N+](=O)[O-])c2)=N1	26610	4.57
4867	Cc1ncc([N+](=O)[O-])n1CCOC(=O)/C=C/c1ccccc1F	26740	4.57
4868	C=CC(=O)Nc1cc(Nc2nccc(Nc3ccc4c(ccn4C)c3)n2)c(OC)cc1N1CCN(C)CC1	26900	*
4869	O=C1CSC(NN=C2CCCCCCC2)=N1	27000	4.57
4870	COc1cc2c(cc1OC)Sc1ncnc(N(C)c3cccc(Cl)c3)c1NC2	27000	4.57
4871	CONC(=O)c1cc(/N=C/c2cc(O)ccc2O)ccc1O	27000	*
4872	C/C1=C/CC[C@]23O[C@H]2[C@@H](OC3=O)C2=C(C1)C(=O)C=CC2=O	27000	*
4873	Cc1ccc(S(=O)(=O)NC(=O)c2cccnc2Cl)cc1	27050	4.57
4874	CCCCCCCCCCCCCCNC(=O)c1cc(NCc2cc(O)ccc2O)ccc1O	27200	*
4875	Cc1cc(C)c(O)c(CN(Cc2ccc(F)cc2)C(=O)Nc2ccccc2)c1	27350	4.56
4876	CO[C@H](C)c1c(O)cc2c(c1O)C(=O)c1c(O)cc(O)cc1C2=O	27500	*
4877	CC(=O)OC(Cc1c(SSc2[nH]c3ccccc3c2CC(OC(C)=O)C(=O)NCc2ccccc2)[nH]c2ccccc12)C(=O)NCc1ccccc1	28000	*
4878	N#Cc1cnc(Nc2cccc(Br)c2)c2cc(NC(=O)CCc3cc4ccccc4[nH]3)ccc12	28000	*
4879	COc1cc2nccc(Oc3ccc(C(=O)c4cccc(F)c4)cc3)c2cc1OC	28000	*
4880	Cc1ccc(C2CC(c3ccc(Br)cc3)=NN2c2nc(-c3ccc(Cl)cc3)cs2)cc1	28170	4.55
4881	O=C(Nc1ccc(Br)cc1)c1cc(Br)cc(Br)c1O	28530	*
4882	O=C(NS(=O)(=O)c1ccc(F)cc1)c1cccnc1Cl	28660	4.54
4883	CC(=O)N1N=C(c2ccc(Cl)c(Cl)c2)CC1c1ccccc1	28690	4.54
4884	O=C1NC(=O)c2c1c1c3cccc(O)c3[nH]c1c1[nH]c3c(O)cccc3c21	29000	*

4885	COc1cc2ncnc(Nc3cc(NC(=O)c4cccc(N(C)C)c4)ccc3Cl)c2cc1OC	29000	*
4886	CC(C)n1nc(-c2ccc3occc(=O)c3c2)c2c(N)ncnc21	29000	*
4887	O=C(NS(=O)(=O)c1ccc(Br)cc1)c1ccc(Cl)nc1	29070	4.54
4888	NS(=O)(=O)c1ccc2c(c1)/C(=C/c1[nH]c3c(c1CCC(=O)O)CCCC3)C(=O)N2	29100	*
4889	Cc1ccc(Nc2ncnn3c(C)ccc23)cc1O	29400	*
4890	O=C(Cc1nc2ccccc2[nH]1)N1N=C(c2ccc(Cl)cc2)CC1c1ccc(F)cc1	29400	*
4891	Nc1scc2c1c(Nc1ccc(S(N)(=O)=O)cc1)nc1ncnc(N)c12	29500	*
4892	CC(C)n1ncc2c(NCc3ccc(N)cc3)nc(NCCO)nc21	29500	*
4893	CC(C)n1ncc2c(NCc3cccc(F)c3)nc(NCCO)nc21	29500	*
4894	CC(C)c1ccc(NC(=O)c2ccccc2O)cc1	29620	*
4895	CCCN(CCC)C(=O)c1ccc(N(CCCl)CCCl)cc1	29830	4.53
4896	CC(C)(C)NC(=O)/C=C/c1ccccc1	29850	*
4897	O=c1oc2cc3ncnc(Nc4ccccc4O)c3cc2n1CCCN1CCOCC1	30000	*
4898	COc1cc2ncnc(N(C)c3cccc(C(F)(F)F)c3)c2cc1OC.Cl	30000	*
4899	CN1CCC(NC(=O)c2cnc(NCc3cc(Cl)ccc3Cl)nc2NC2CCCC2)CC1	30000	*
4900	CN1CCC(NC(=O)c2cnc(Nc3cc(Cl)cc(Cl)c3)nc2N[C@@H]2COC[C@H]2O)CC1	30000	*
4901	COc1ccccc1CNc1ncc(C(=O)NC2CCN(C)CC2)c(NC2CCCC2)n1	30000	*
4902	CN1CCC(NC(=O)c2cnc(Nc3cc(Cl)cc(Cl)c3)nc2NC2CCC(N(C)C)CC2)CC1	30000	*
4903	COc1cc2nccc(Oc3ccc(C(=O)Nc4ccc(C(C)(C)C)cc4)cc3)c2cc1OC	30000	*
4904	COc1ccc(OC)c(Nc2cc(Nc3cc(OC)ccc3OC)ncn2)c1	30000	*
4905	Clc1cccc(Nc2cc(Nc3cccc(Cl)c3)ncn2)c1	30000	*
4906	Clc1cccc(Nc2cc(Nc3cccc(Br)c3)ncn2)c1	30000	*
4907	Fc1ccc(Nc2cc(Nc3ccc(F)cc3)ncn2)cc1	30000	*
4908	COc1cccc(Nc2cc(NC(=O)c3ccc(F)cc3)ncn2)c1	30000	*
4909	COc1cccc(Nc2cc(Nc3ccc(Cl)cc3)ncn2)c1	30000	*
4910	O=C(/C=C/c1ccc(F)cc1)Nc1cc(Nc2ccc(Cl)cc2)ncn1	30000	*
4911	CCOC(=O)CCC(=O)Nc1cc(Nc2ccc(S(N)(=O)=O)cc2)ncn1	30000	*
4912	CN1CCN(c2cc(NC(=O)/C=C/c3ccc(F)cc3)ncn2)CC1	30000	*
4913	Fc1ccc(Nc2cc(Nc3ccc(Cl)cc3)ncn2)cc1	30000	*
4914	COc1ccc(Nc2cc(NC(=O)c3ccc(F)cc3)ncn2)cc1	30000	*
4915	CCOC(=O)CC(=O)Nc1cc(Nc2ccc(F)cc2)ncn1	30000	*
4916	O=C(C=Cc1ccccc1)Nc1cc(Nc2ccc(N3CCOCC3)cc2)ncn1	30000	*
4917	O=C(Nc1cc(Nc2cccc(Cl)c2)ncn1)c1ccccc1	30000	*
4918	COc1ccc(Nc2cc(NC(=O)c3ccccc3)ncn2)c([N+](=O)[O-])c1	30000	*
4919	O=C(/C=C/c1ccc(F)cc1)Nc1cc(Nc2ccc(N3CCOCC3)cc2)ncn1	30000	*
4920	CCOC(=O)CCC(=O)Nc1cc(Nc2ccc(Cl)cc2)ncn1	30000	*
4921	CCOC(=O)CCC(=O)Nc1cc(Nc2ccc(C(=O)OCC)cc2)ncn1	30000	*
4922	CCOC(=O)CCC(=O)Nc1cc(Nc2cccc(C(=O)OCC)c2)ncn1	30000	*
4923	COc1cccc(Nc2cc(Nc3cccc(Br)c3)ncn2)c1	30000	*
4924	COc1ccc(OC)c(Nc2cc(Nc3ccc(Cl)cc3)ncn2)c1	30000	*
4925	COc1cccc(Nc2cc(NC(=O)c3ccccc3)ncn2)c1	30000	*
4926	COc1ccc(Nc2cc(NC(=O)C=Cc3ccccc3)ncn2)cc1	30000	*
4927	CCOC(=O)c1c(Nc2cc(NC(=O)CCC(=O)OC(C)C)ncn2)sc2c1CCCC2	30000	*

4928	CCOC(=O)CCC(=O)Nc1cc(Nc2cccc(OC)c2)ncn1	30000	*
4929	CCCC(C)OC(=O)CCC(=O)Nc1cc(Nc2cccc(C(=O)OC(C)CCC)c2)ncn1	30000	*
4930	CCOc1ccc(Nc2cc(NC(=O)c3ccc(F)cc3)ncn2)cc1	30000	*
4931	O=C(Nc1cc(N2CCOCC2)ncn1)c1ccccc1	30000	*
4932	O=C(O)CCC(=O)Nc1cc(Nc2cccc(Br)c2)ncn1	30000	*
4933	O=C(Nc1cc(Nc2cccc(Cl)c2)ncn1)c1ccc(F)cc1	30000	*
4934	CC(C)OC(=O)CCC(=O)Nc1cc(Nc2ccc(C(=O)OC(C)C)cc2)ncn1	30000	*
4935	CCNc1cc(Nc2cc(OC)ccc2OC)ncn1	30000	*
4936	CN1CCN(c2cc(NC(=O)CCCC(=O)O)ncn2)CC1	30000	*
4937	CCOC(=O)CCC(=O)Nc1cc(NCCc2cccs2)ncn1	30000	*
4938	COc1ccc(/C=C/C(=O)Nc2cc(Nc3ccc(Cl)cc3Cl)ncn2)cc1	30000	*
4939	COc1cccc(Nc2cc(NC(=O)CCC(=O)O)ncn2)c1	30000	*
4940	O=C(O)CCC(=O)Nc1cc(Nc2cccc(C(=O)O)c2)ncn1	30000	*
4941	COc1ccc(/C=C/C(=O)Nc2cc(N3CCN(C)CC3)ncn2)cc1	30000	*
4942	O=C(Nc1cc(Nc2ccc(N3CCOCC3)cc2)ncn1)c1ccc(F)cc1	30000	*
4943	CC(C)OC(=O)CCC(=O)Nc1cc(Nc2ccc(F)cc2)ncn1	30000	*
4944	O=C(O)CCC(=O)Nc1cc(Nc2cccc(Cl)c2)ncn1	30000	*
4945	O=C(/C=C/c1ccc(F)cc1Br)Nc1cc(N2CCOCC2)ncn1	30000	*
4946	Cc1ccc(Nc2cc(NC(=O)c3ccc(F)cc3)ncn2)cc1	30000	*
4947	CCCC(C)OC(=O)CCC(=O)Nc1cc(Nc2cccc(Br)c2)ncn1	30000	*
4948	O=C(/C=C/c1ccc(F)cc1)Nc1cc(Nc2ccc(Cl)cc2Cl)ncn1	30000	*
4949	CCOC(=O)CCCC(=O)Nc1cc(Nc2cc(OC)ccc2OC)ncn1	30000	*
4950	CCOc1cccc(Nc2cc(NC(=O)c3ccc(F)cc3)ncn2)c1	30000	*
4951	COc1ccc(/C=C/C(=O)Nc2cc(Nc3ccc(Cl)cc3)ncn2)cc1	30000	*
4952	CN1CCN(c2ccc(Nc3cc(NC(=O)CCC(=O)O)ncn3)cc2)CC1	30000	*
4953	CCOC(=O)CCC(=O)Nc1cc(Nc2cc(OC)ccc2OC)ncn1	30000	*
4954	CCOC(=O)c1ccc(Nc2cc(NC(=O)CCC(=O)O)ncn2)cc1	30000	*
4955	O=C(O)CCCC(=O)Nc1cc(Nc2ccccc2Br)ncn1	30000	*
4956	Clc1ccc(Nc2cc(Nc3ccc(Cl)cc3)ncn2)cc1	30000	*
4957	Clc1ccc(Nc2cc(Nc3ccc4cn[nH]c4c3)ncn2)cc1	30000	*
4958	O=C(Nc1cc(Nc2ccc(Cl)cc2)ncn1)c1ccccc1	30000	*
4959	CCOc1ccc(Nc2cc(NC(=O)C=Cc3ccccc3)ncn2)cc1	30000	*
4960	COc1cccc(Nc2cc(NC(=O)C=Cc3ccccc3)ncn2)c1	30000	*
4961	COc1ccc(Nc2cc(NC(=O)C=Cc3ccccc3)ncn2)c([N+](=O)[O-])c1	30000	*
4962	O=C(C=Cc1ccccc1)Nc1cc(Nc2ccc(O)cc2)ncn1	30000	*
4963	O=C(/C=C/c1ccc(F)cc1Br)Nc1cc(Nc2ccc(Cl)cc2Cl)ncn1	30000	*
4964	COc1ccc(Nc2cc(NC(=O)/C=C/c3ccc(F)cc3Br)ncn2)c([N+](=O)[O-])c1	30000	*
4965	O=C(/C=C/c1ccc(F)cc1Br)Nc1cc(Nc2ccc(N3CCOCC3)cc2)ncn1	30000	*
4966	CN1CCN(c2ccc(Nc3cc(NC(=O)/C=C/c4ccc(F)cc4)ncn3)cc2)CC1	30000	*
4967	COc1ccc(/C=C/C(=O)Nc2cc(Nc3cccc(Br)c3)ncn2)cc1	30000	*
4968	CCOc1ccc(Nc2cc(NC(=O)/C=C/c3ccc(OC)cc3)ncn2)cc1	30000	*
4969	COc1ccc(/C=C/C(=O)Nc2cc(N3CCOCC3)ncn2)cc1	30000	*
4970	Clc1ccc(Nc2cc(Nc3cccc(Cl)c3)ncn2)cc1	30000	*

4971	CCOC(=O)c1ccc(Nc2cc(Nc3ccc(C(=O)OCC)cc3)ncn2)cc1	30000	*
4972	CCOC(=O)CCC(=O)Nc1cc(Nc2ccc(N3CCN(C)CC3)cc2)ncn1	30000	*
4973	COc1cc2c(cc1OC)Sc1nc(C)nc(Nc3cccc(Br)c3)c1NC2	30700	4.51
4974	CC(C)(C)ONC(=O)Cc1cc(/N=C/c2cc(O)ccc2O)ccc1O	31000	*
4975	COC(=O)c1c(OCCN(C)C)c2ccccc2c2oc3c(c12)C(=O)c1ccccc1C3=O	31000	*
4976	COc1cc2nccc(Oc3ccc(C(=O)c4ccc(Cl)c(Cl)c4)cc3)c2cc1OC	31000	*
4977	Cc1ccc(C(=O)Nc2ccc(Cl)cc2Cl)c(O)c1	31090	*
4978	CCCCN(CCCC)C(=O)c1ccc(N(CCCl)CCCl)cc1	31180	4.51
4979	COc1cccc(/C=N/NC2=NC(=O)CS2)c1	31250	4.51
4980	O=C1N=C(N2CCC[C@H]2C(=O)Nc2ccc3ncnc(Nc4cccc(Cl)c4)c3c2)S/C1=C/c1ccc(Br)s1	31400	*
4981	CC(C)(C)NC(=O)c1ccc(N(CCCl)CCCl)cc1	31430	4.50
4982	CCCCN(Cc1cc(Br)cc(Br)c1O)C(=S)Nc1ccccc1	31940	4.50
4983	COc1ccccc1/C=C/C(=O)OCCn1c([N+](=O)[O-])cnc1C	32000	4.49
4984	N#CCc1c(SSc2[nH]c3ccccc3c2CC#N)[nH]c2ccccc12	32000	*
4985	COc1cc(C2=C(c3c[nH]c4ccccc34)C(=O)NC2=O)cc(OC)c1OC	32000	*
4986	CCCCN(Cc1cccc(Cl)c1O)C(=O)Nc1ccccc1	32120	4.49
4987	Cc1nn(-c2ccccc2)c(Cl)c1C1C(C#N)=C(N)N(c2cccnc2)C2=C1C(=O)CC(C)(C)C2	32130	4.49
4988	COc1ccc(CC(=O)NS(=O)(=O)c2ccc(Cl)cc2)cc1	32850	4.48
4989	COc1ccccc1/C=C/C(=N/NC(N)=S)c1ccccc1	33000	4.48
4990	COC(=O)Cc1c(SSc2c(CC(=O)OC)c3ccccc3n2C)n(C)c2ccccc12	33000	*
4991	CCOc1cc2ncc(C#N)c(Nc3cccc(Br)c3)c2cc1OC	33020	*
4992	C=CC(=O)Nc1ccc(Nc2ncc3ncc(=O)n(-c4ccc(OC)cc4)c3n2)cc1	33885	4.47
4993	Cn1nc(-c2ccc3ncccc3c2)c2c(N)ncnc21	34000	*
4994	Cc1ccc(-c2nnc(SCc3ccccc3)o2)c(O)c1	34250	4.47
4995	CC(=O)c1ccccc1C(=O)Nn1c(-c2ccccc2)nc2cc(Cl)ccc2c1=O	34320	4.46
4996	NS(=O)(=O)c1ccc(Nc2nc(Cl)nc3cc4c(cc23)OCO4)cc1	34600	*
4997	Cc1ccc(NC(=O)c2ccc(C)cc2O)cc1	34670	*
4998	O=C(O)Cc1cc(/N=C/c2cc(O)ccc2O)ccc1O	35000	*
4999	COC(=O)Cc1c(SSSc2[nH]c3ccccc3c2CC(=O)OC)[nH]c2ccccc12	35000	*
5000	Nc1ncnc2c1ncn2CC(=O)c1c[nH]c2ccccc12	35000	*
5001	COc1cc2nccc(Oc3cccc([N+](=O)[O-])c3)c2cc1OC	35000	*
5002	O=C(NC1CCCC1)c1ccc(N(CCCl)CCCl)cc1	35290	4.45
5003	CC(=O)Nc1ccc(S(=O)(=O)Nc2nc3ccccc3nc2Nc2ccc(C(=O)O)cc2)cc1	35800	*
5004	O=C1CSC(NN=C2CCCCCC2)=N1	36000	4.44
5005	COc1cc2nc(Cl)nc(Nc3ccc(N(C)C)cc3)c2cc1OC	36000	*
5006	Cn1ncc2c(Nc3cccc(F)c3)nc(N(CCO)CCO)nc21	36300	*
5007	Cn1ncc2c(NCc3cccc(Br)c3)nc(NCCO)nc21	36300	*
5008	CCCCN(Cc1cccc(Br)c1O)C(=O)Nc1ccccc1	36880	4.43
5009	N#CC(C#N)=Cc1cc(O)cc(O)c1	37000	*
5010	C[C@@H](O)c1c(O)cc2c(c1O)C(=O)c1c(O)cc(O)cc1C2=O	37500	*
5011	COc1cc2nc(Cl)nc(Nc3ccc(NC(C)=O)cc3)c2cc1OC	37600	*
5012	O=C(Cc1c(SSc2[nH]c3ccccc3c2CC(=O)NCc2ccccc2)[nH]c2ccccc12)NCc1ccccc1	38000	*
5013	O=[N+]([O-])c1ccccc1-c1nnc(SCc2ccccc2)o1	38320	4.42

5014	CCOc1ccccc1-c1nnc(SCc2ccccc2)o1	38430	4.42
5015	CCCCCCCCCCCCCNC(=O)/C=C/c1ccccc1	38460	*
5016	COc1ccc(CC(=O)NS(=O)(=O)c2ccc(C)cc2)cc1	38520	4.41
5017	Cc1ccc(C2=NN(C(=O)Cc3nc4ccccc4[nH]3)C(c3ccc(Br)cc3)C2)cc1	39700	*
5018	COc1ccc(NC(=O)c2ccccc2O)cc1	39980	*
5019	N#CC(C#N)=Cc1ccc(O)c(O)c1	40000	*
5020	N#CC(C#N)=C1C(=O)Nc2ccc([N+](=O)[O-])cc21	40000	*
5021	C[C@@H](NC(=O)c1ccc(S(=O)(=O)Oc2ccc(/C=C/[N+](=O)[O-])cc2)cc1)C(=O)N[C@H](C)C(=O)OC(C)(C)C	40000	*
5022	COc1cc2nccc(Oc3cccc(N)c3)c2cc1OC	40000	*
5023	Cc1ccc(C(=O)Nc2ccc(F)cc2)c(O)c1	40170	*
5024	Cn1c(SSc2c(C(=O)Nc3ccccc3)c3cc(O)ccc3n2C)c(C(=O)Nc2ccccc2)c2cc(O)ccc21	40500	*
5025	O=C1CSC(NN=C2CCCCC2)=N1	41000	4.39
5026	CO[C@H](C)c1c(O)cc2c(c1O)C(=O)c1c(cc(O)c(O)c1O)C2=O	41000	*
5027	O=C(Cc1nc2ccccc2[nH]1)N1N=C(c2ccc(O)cc2)CC1c1ccc(Cl)cc1	41000	*
5028	O=C(Nc1ccc(Cl)cc1)c1ccccc1O	41760	*
5029	Oc1ccc(NCc2cc(O)ccc2O)cc1	41900	*
5030	COc1cc2nccc(Oc3ccc(C(=O)c4ccccc4C)cc3)c2cc1OC	43000	*
5031	CCCCN(Cc1cccc(C)c1O)C(=S)Nc1ccccc1	43210	4.36
5032	Cn1c(SSc2c(C(=O)Nc3ccccc3)c3ccc(O)cc3n2C)c(C(=O)Nc2ccccc2)c2ccc(O)cc21	44000	*
5033	COC(=O)c1ccc(CNC(=O)CCc2c(SSc3[nH]c4ccccc4c3CCC(=O)NCc3ccc(C(=O)OC)cc3)[nH]c3ccccc23)cc1	44000	*
5034	CC(O)C(/N=C1/C=C(O)/C(=N\C(C(=O)O)C(C)O)C=C1O)C(=O)O	44000	*
5035	COc1ccc(Oc2ccnc3cc(OC)c(OC)cc23)cc1	44000	*
5036	NCCCNC(=O)c1cccc(Nc2nccc(-c3cccnc3)n2)c1	45000	*
5037	CC(C)n1nc(-c2ccn3ccnc3c2)c2c(N)ncnc21	45000	*
5038	O=C(N/N=C/c1cccn1CCCN1CCCC1)Nc1ccc(Oc2ccnc3[nH]ccc23)cc1	45000	*
5039	N#Cc1cnc(Nc2cccc(Br)c2)c2cc(NC(=O)c3ccoc3)ccc12	45200	*
5040	O=C(Nc1ccc(Cl)cc1Cl)c1ccccc1O	45290	*
5041	Clc1ccc(Nc2ncc3c(n2)-c2ccc(Cl)cc2SC3)cc1	45700	4.34
5042	Cc1ccc(F)c(C(=O)n2nc(Nc3ccc(S(N)(=O)=O)cc3)nc2C)c1F	45800	*
5043	COc1cc2c(cc1OC)Sc1nc(C)nc(Nc3ccc(F)c(Cl)c3)c1NC2	45900	4.34
5044	Fc1cccc(COc2ccc(Nc3cc(-c4cccnc4)ncn3)cc2Cl)c1	47000	4.33
5045	N#C/C(=C\c1ccc(C=O)cc1)C(=O)O	47000	*
5046	N#CCCc1c(SSc2[nH]c3ccccc3c2CCC#N)[nH]c2ccccc12	47000	*
5047	COc1cc(/C=C(\C#N)C(N)=O)cc(SCCCC(=O)O)c1O	47863.01	*
5048	Cc1c(C#N)c(NCCO)nc2nc(NCCO)nc(N)c12	47900	*
5049	CC1=C(C(=O)Nc2cccc([N+](=O)[O-])c2)C(c2ccc(O)cc2O)NC(NN)=N1	47900	*
5050	CC(C)n1ncc2c(NCc3ccccc3)nc(NCCO)nc21	47900	*
5051	Cn1ncc2c(NCc3cccc(Br)c3)nc(N(CCO)CCO)nc21	47900	*
5052	COc1cc2ncc(C#N)c(Nc3ccc(F)cc3)c2cc1OC	47940	*
5053	COc1cc2nccc(Oc3ccc(NC(=O)c4ccc(Br)cc4)cc3)c2cc1OC	48000	*
5054	O=C(Cc1ccc(F)cc1)Nc1cc(SC[C@@H](O)CO)cc([N+](=O)[O-])c1	48600	4.31
5055	COc1cc(OC)cc(Oc2ccnc3cc(OC)c(OC)cc23)c1	49000	*
5056	CCOC(=O)c1cc(/N=C/c2cc(O)ccc2O)ccc1O	50000	*

5057	O=C(Cc1cc(/N=C/c2cc(O)ccc2O)ccc1O)NOCc1ccccc1	50000	*
5058	CCN(CC)c1ccc(Nc2cc3c(cc2Nc2ccc(N(CC)CC)cc2)C(=O)NC3=O)cc1	50000	*
5059	COc1cc(OC)cc(-c2cc3cnc(N)nc3nc2NC(=O)NC(C)(C)C)c1	50000	*
5060	Nc1cccc(Nc2nccc(-c3cccnc3)n2)c1	50000	*
5061	O=C(Nc1cccc(-c2cn3ccnc3c(NCc3ccncc3)n2)c1)Nc1cccc(C(F)(F)F)c1	50000	*
5062	COc1cc2nccc(Oc3ccccc3)c2cc1OC	50000	*
5063	COc1cc2nccc(Oc3ccc(C(=O)c4ccccc4)cc3)c2cc1OC	50000	*
5064	O=C(Nc1ccccc1)c1ccccc1O	50000	*
5065	O=C(Nc1ccc(Br)cc1)c1ccccc1O	50000	*
5066	O=C(Nc1ccc(F)cc1)c1ccccc1O	50000	*
5067	Cc1ccc(C(=O)Nc2ccccc2)c(O)c1	50000	*
5068	O=C(Nc1ccc(F)cc1)c1cc(Br)cc(Br)c1O	50000	*
5069	O=C(Nc1ccc(F)cc1F)c1ccccc1O	50000	*
5070	Cc1ccc(C(=O)Nc2ccc(Cl)cc2)c(O)c1	50000	*
5071	O=C(Nc1ccc(F)cc1)c1cc(I)ccc1O	50000	*
5072	Cc1ccc(C(=O)Nc2ccc(C(C)C)cc2)c(O)c1	50000	*
5073	Cc1ccc(C(=O)Nc2ccc(F)cc2F)c(O)c1	50000	*
5074	COc1ccc(Nc2c(C#N)cnc3cc(OC)c(OC)cc23)cc1OC	50490	*
5075	CC(=O)NC(Cc1c(SSc2[nH]c3ccccc3c2CC(NC(C)=O)C(=O)NCc2ccccc2)[nH]c2ccccc12)C(=O)NCc1ccccc1	51000	*
5076	Cn1c(SSc2c(CC(=O)O)c3ccccc3n2C)c(CC(=O)O)c2ccccc21	53000	*
5077	COc1cc(C=C(C#N)C#N)cc(SCC(=O)O)c1O	53703.18	*
5078	Cn1c(SSc2c(C(=O)Nc3ccccc3)c3cc(C#N)ccc3n2C)c(C(=O)Nc2ccccc2)c2cc(C#N)ccc21	54100	*
5079	CCOc1cc(-c2nn(C(C)C)c3ncnc(N)c23)ccc1OC	54200	*
5080	CCCCc1cc(/C=C(\C#N)C(N)=O)cc(CCCC)c1O	55000	*
5081	Cn1ncc2c(NCc3ccccc3)nc(N(CCO)CCO)nc21	55000	*
5082	CC1=C(C(=O)Nc2cccc([N+](=O)[O-])c2)C(c2ccc(O)cc2O)NC(SCc2ccccc2)=N1	55600	*
5083	N#Cc1cnc(Nc2cccc(Br)c2)c2cc(NC(=O)c3ccco3)ccc12	55600	*
5084	COc1cc(/C=C2\SC(=N)NC2=O)ccc1OCCCOc1cc(C)cc(C)c1	56000	*
5085	COc1ccccc1C(Cc1coc2nc(N)nc(N)c12)C1CC1	56500	*
5086	O=C(O)CCc1c(/C=C2\C(=O)Nc3ccc(C(=O)O)cc32)[nH]c2c1CCCC2	56500	*
5087	O=c1c(-c2cccc(Cl)c2)coc2cc(O)ccc12	58800	*
5088	CCCNN1C(=O)c2c(c3c4cccc(O)c4n(C4OC(CO)C(O)C(O)C4O)c3c3[nH]c4c(O)cccc4c23)C1=O	59000	*
5089	COc1cc2c(cc1O)NC(=O)C2=C(C#N)C#N	60000	*
5090	N#CC(C#N)=Cc1ccc(C=O)cc1	60000	*
5091	N#CC(C#N)=C(N)/C(C#N)=C/c1ccc(O)c([N+](=O)[O-])c1	60000	*
5092	CC1=C(C(=O)Nc2ccc(C)cc2)C(c2ccc(O)cc2O)NC(Nc2ccc([N+](=O)[O-])cc2Cl)=N1	60900	*
5093	COc1cc2nc(Cl)nc(Nc3ccc(S(C)(=O)=O)cc3)c2cc1OC	61500	*
5094	Cc1cc(C=C(C#N)C#N)cc(O)c1O	61659.5	*
5095	COc1cc2ncc(C#N)c(Nc3cccc(C(C)C)c3)c2cc1OC	62320	*
5096	COc1cc2c(cc1OC)Sc1ncnc(Nc3cccc(Cl)c3F)c1NC2	62900	4.20
5097	C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4ccccc34)n2)c(OC)cc1N(C)CCN(C)C	63000	*
5098	O=c1oc2cc3ncnc(NCc4ccccc4)c3cc2n1CCCN1CCOCC1	65000	*
5099	Nc1cc2ncnc(Nc3ccc([N+](=O)[O-])cc3)c2cn1	65000	*

5100	Cc1ccc(NC(=O)c2ccccc2)cc1Nc1nccc(-c2cccnc2)n1	65000	*
5101	Nc1scc2c1c(NCCO)nc1nc(NCCO)nc(N)c12	66100	*
5102	Cn1ncc2c(Nc3cccc(F)c3)nc(NCCO)nc21	66100	*
5103	OCCN(CCO)c1nc(NCc2cccc(F)c2)c2cn[nH]c2n1	66100	*
5104	COc1cc2nc(Cl)nc(Nc3ccc(S(=O)(=O)N(C)C)cc3)c2cc1OC	67200	*
5105	CONC(=O)CCc1c(SSc2[nH]c3ccccc3c2CCC(=O)NOC)[nH]c2ccccc12	68000	*
5106	CN(C)c1ccccc1Nc1ncnc2cc(N)ncc12	69000	*
5107	COc1cc2ncc(C#N)c(Nc3cccc(NC(C)=O)c3)c2cc1OC	69400	*
5108	N#CC(Cc1ccc(O)c(O)c1)C(=N)S	70000	*
5109	CC(C)n1nc(-c2cnc3nccnc3c2)c2c(N)ncnc21	70000	*
5110	COc1cc2c(C#N)cnc(Nc3cccc(Br)c3)c2cc1OC.Cl	70840	*
5111	Cc1nn(C)cc1C(=O)Nc1ccn(Cc2c(F)cccc2Cl)n1	72400	4.14
5112	Cc1ccc(N2NC(=O)/C(=C\c3ccc(-c4cc([N+](=O)[O-])ccc4O)o3)C2=O)cc1C	74300	4.13
5113	Cc1cc(C)cc(Nc2ncnc3cc4oc(=O)n(CCCN5CCOCC5)c4cc23)c1	75000	*
5114	N#C/C(=C/c1cc(O)ccc1O)C(=O)O	75000	*
5115	COc1cc2c(cc1OC)Nc1ncnc(O)c1C2	75000	*
5116	Nc1ncnc2c1ncn2CC(=O)c1ccccc1	75000	*
5117	COc1cc2nccc(Oc3ccc(C(=O)c4ccc(F)cc4)cc3)c2cc1OC	75000	*
5118	Cc1[nH]c2ncnc(Nc3ccccc3Cl)c2c1C	75100	*
5119	COc1ccc2c3oc(=O)cc(O)c3c(=O)n(C)c2c1	76400	*
5120	C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4cccnc34)n2)c(OC)cc1NCCN(C)C.Cl	77000	*
5121	CCc1ccc(Nc2[nH]cnc3nc(C)c(C)c2-3)cc1	77500	*
5122	Cn1ncc2c(NCc3ccc([N+](=O)[O-])cc3)nc(NCCO)nc21	77600	*
5123	O=c1c2ccccc2nc(-c2ccccc2)n1-c1nnc(-c2ccccc2Cl)s1	78230	4.11
5124	CC(C)(C)c1ccc(Nc2ncnc3cc4oc(=O)n(CCCN5CCOCC5)c4cc23)cc1	79000	*
5125	CC1=C(C(=O)Nc2cccc([N+](=O)[O-])c2)C(c2ccc(O)cc2O)NC(Nc2ccc(S(=O)(=O)Nc3nc(C)cc(C)n3)cc2)=N1	79800	*
5126	COc1ccc(Nc2ccnc3cc(OC)c(OC)cc23)cc1OC	80500	*
5127	CC1=C(C(=O)Nc2cccc([N+](=O)[O-])c2)C(c2ccc(O)cc2O)NC(NN2C(=O)/C(=C\c3cccs3)SC2=S)=N1	80600	*
5128	COc1cc2nccc(Oc3c(OC)cccc3OC)c2cc1OC	81000	*
5129	Cc1ccc(-n2c(SCC(=O)Nc3ccccc3Cl)nc3sc(C)c(C)c3c2=O)cc1	81600	*
5130	CCOC(=O)c1cnc2cc(OC)c(OC)cc2c1Nc1cccc(Br)c1	81800	*
5131	Nc1ncnc2ncn(CC(=O)c3c[nH]c4ccccc34)c12	82000	*
5132	COc1cc(/C=C(\C#N)C(N)=O)cc(CSc2nc3cc(Cl)ccc3s2)c1O	83176.38	*
5133	Cn1c(NCc2cccc(C(F)(F)F)c2)cc(=O)n(C)c1=O	83900	4.08
5134	Cc1[nH]c(/C=C2\C(=O)Nc3ccc(S(N)(=O)=O)cc32)c(C)c1CCC(=O)O	84800	*
5135	O=c1c2c(-c3ccccc3)c3c(nc2nc2[nH]nc(S)n12)-c1ccccc1CC3	85600	*
5136	COc1cc(C=C(C#N)C#N)cc(C)c1O	87096.36	*
5137	COc1cc2c(C#N)cnc(Nc3cccc(Cl)c3)c2cc1OC	88290	*
5138	CC1=C(C(=O)Nc2cccc([N+](=O)[O-])c2)C(c2ccc(O)cc2O)NC(Nc2ccc(S(=O)(=O)Nc3ncccn3)cc2)=N1	88300	*
5139	O=[N+]([O-])CCc1c(SSc2[nH]c3ccccc3c2CC[N+](=O)[O-])[nH]c2ccccc12	89000	*
5140	Nc1ncnc2c1ncn2CC(=O)c1ccccn1	89000	*
5141	COc1cc2nccc(Oc3cccc(C(=O)c4ccccc4)c3)c2cc1OC	89000	*
5142	O=C(O)c1ccc(NN2C(=O)c3c(c4c5cccc(O)c5n(C5OC(CO)C(O)C(O)C5O)c4c4[nH]c5c(O)cccc5c34)C2=O)cc1	90000	*

5143	O=C1NC(=O)c2c1c1c3cccc(O)c3[nH]c1c1c2c2cccc(O)c2n1C1OC(CO)C(O)C(O)C1O	90000	*
5144	COc1ccccc1Nc1ccnc(Nc2ccccc2OC)n1	90400	*
5145	COc1cc2ncc(C#N)c(Nc3ccc(Br)cc3F)c2cc1OC.Cl	91200	*
5146	COc1cc2nccc(Oc3ccccc3OC)c2cc1OC	92000	*
5147	C=CC(=O)Nc1cc(Nc2ncc(Br)c(Nc3ccc4[nH]ccc4c3)n2)c(OC)cc1N1CCN(C)CC1	92100	*
5148	CCOC(=O)c1ccc(NC(=O)CSc2nnc(CNc3ccc(OC)cc3)n2-c2ccccc2)cc1	92400	*
5149	Nc1ncnc2c1ncn2CC(=O)c1cccnc1	93000	*
5150	COc1cc2nccc(Oc3ccc(NC(=O)c4ccc(C(F)(F)F)cc4)cc3)c2cc1OC	93000	*
5151	N#Cc1cc2c(N)ncnc2nc1NCCO	93300	*
5152	Cn1ncc2c(NCc3ccccc3)nc(NCCO)nc21	93300	*
5153	CC1=C(C(=O)Nc2ccc(C)cc2)C(c2ccc(O)cc2O)NC(SCc2ccccc2)=N1	93500	*
5154	O=C(Nc1ccccc1)NN1C(=O)c2c(c3c4cccc(O)c4n(C4OC(CO)C(O)C(O)C4O)c3c3[nH]c4c(O)cccc4c23)C1=O	95000	*
5155	COc1cc2nccc(Oc3ccc(C(=O)c4cccc(C)c4)cc3)c2cc1OC	95000	*
5156	N#CC(C#N)=Cc1cc(O)ccc1[N+](=O)[O-]	96000	*
5157	C[S+]([O-])c1ccc(-c2nc(-c3ccc(F)cc3)c(-c3ccncc3)[nH]2)cc1	96000	*
5158	COC(=O)C1CCN(c2ncnc3cc(OC)c(OC)cc23)CC1	97600	*
5159	COc1cc2ncnc(Nc3cc(=O)[nH]c(SC)n3)c2cc1OC	99100	*
5160	CC1=C(C(=O)Nc2cccc([N+](=O)[O-])c2)C(c2ccc(O)cc2O)NC(NN2C(=O)/C(=C\c3ccco3)SC2=S)=N1	99300	*
5161	O=C1/C(=C\c2ccc(O)c(O)c2)Oc2ccccc21	100000	4.00
5162	Cn1c(SSc2c(C(=O)Nc3ccccc3)c3cccc(O)c3n2C)c(C(=O)Nc2ccccc2)c2cccc(O)c21	100000	*
5163	Cn1c(SSc2c(C(=O)Nc3ccccc3)c3c(Cl)cccc3n2C)c(C(=O)Nc2ccccc2)c2c(Cl)cccc21	100000	*
5164	CCOC(=O)Cc1cc(/N=C/c2cc(O)ccc2O)ccc1O	100000	*
5165	COC(=O)Cc1cc(/N=C/c2cc(O)ccc2O)ccc1O	100000	*
5166	CN(c1ccccc1)c1ncnc2ccccc12	100000	*
5167	COC(=O)CC1C(S)=Nc2ccccc21	100000	*
5168	O=C(CCCc1c(SSc2[nH]c3ccccc3c2CCCC(=O)NCc2ccccc2)[nH]c2ccccc12)NCc1ccccc1	100000	*
5169	O=C(CCC1C(S)=Nc2ccccc21)NCc1ccccc1	100000	*
5170	COC(=O)c1ccc(CNC(=O)CCc2c(SSc3[nH]c4ccccc4c3CCC(=O)NCc3ccc(C(=O)OC)c(O)c3)[nH]c3ccccc23)cc1O	100000	*
5171	O=C(CC1C(S)=Nc2ccccc21)NCc1ccccc1	100000	*
5172	COc1ccccc1CNc1ncnc2cc(N)ncc12	100000	*
5173	CC(CN(C)C)C(=O)c1ccc(OS(=O)(=O)c2ccc(C(=O)O)cc2)cc1.Cl	100000	*
5174	COc1ccccc1C(=O)Nc1cccc(Nc2nccc(-c3cccnc3)n2)c1	100000	*
5175	O=[N+]([O-])c1cccc(Nc2nccc(-c3cccnc3)n2)c1	100000	*
5176	c1ccc(Nc2nccc(-c3cccnc3)n2)cc1	100000	*
5177	CNN1C(=O)c2c(c3c4cccc(O)c4n(C4OC(CO)C(O)C(O)C4O)c3c3[nH]c4c(O)cccc4c23)C1=O	100000	*
5178	Cc1nc(O)c2c(ccc3[nH]c(Nc4c(Cl)cccc4Cl)nc32)c1C	100000	*
5179	CC(C)n1nc(-c2cncnc2)c2c(N)ncnc21	100000	*
5180	CC(C)n1nc(-c2ccc3nccc(N)c3c2)c2c(N)ncnc21	100000	*
5181	CC(C)n1nc(-c2ccc(C#N)nc2)c2c(N)ncnc21	100000	*
5182	Nc1ncnc2c1c(-c1ccc(F)c(O)c1)nn2CC1CCNCC1	100000	*
5183	COc1ccc(-c2n[nH]c3ncnc(N)c23)cc1O	100000	*
5184	CC(C)n1nc(-c2cccnc2)c2c(N)ncnc21	100000	*

5185	CCOc1ccc(-c2n[nH]c3ncnc(N)c23)cc1OC	100000	*
5186	CC(C)n1nc(-c2cccc(C#N)c2)c2c(N)ncnc21	100000	*
5187	Cc1ccc2cc(-c3nn(C(C)C)c4ncnc(N)c34)ccc2n1	100000	*
5188	Cn1nc(-c2ccc(Br)c(O)c2)c2c(N)ncnc21	100000	*
5189	CC(C)n1nc(-c2cccc(NS(C)(=O)=O)c2)c2c(N)ncnc21	100000	*
5190	CC(C)n1nc(-c2ccc3ccncc3c2)c2c(N)ncnc21	100000	*
5191	CC(C)n1nc(-c2cccc(CO)c2)c2c(N)ncnc21	100000	*
5192	Nc1ncnc2c1c(-c1ccc(Cl)c(O)c1)nn2CC1CCNCC1	100000	*
5193	Cc1nn(-c2ccccc2)nc1Cn1nc(-c2ccc(F)c(O)c2)c2c(N)ncnc21	100000	*
5194	CC(C)n1nc(-c2cccc(S(N)(=O)=O)c2)c2c(N)ncnc21	100000	*
5195	COc1ccc(-c2nn(C)c3ncnc(N)c23)cc1O	100000	*
5196	CC(C)n1nc(-c2ccc3nc(Cl)ccc3c2)c2c(N)ncnc21	100000	*
5197	CC(C)n1nc(-c2cc3cc(C=O)ccc3s2)c2c(N)ncnc21	100000	*
5198	CC(C)n1nc(-c2ccc3nccc(NC(=O)OC(C)(C)C)c3c2)c2c(N)ncnc21	100000	*
5199	Nc1ncnc2c1c(-c1ccc(F)c(O)c1)nn2Cc1ocnc1-c1ccccc1	100000	*
5200	CC(C)n1nc(-c2ccc(F)c(C#N)c2)c2c(N)ncnc21	100000	*
5201	C[C@H](CN)n1nc(-c2ccc(F)c(O)c2)c2c(N)ncnc21	100000	*
5202	CC(C)n1nc(-c2cc3ccccc3nc2Cl)c2c(N)ncnc21	100000	*
5203	COc1ncc(-c2nn(C(C)C)c3ncnc(N)c23)c(OC)n1	100000	*
5204	CC(C)n1nc(-c2ccc(C(N)=O)c(Cl)c2)c2c(N)ncnc21	100000	*
5205	CC(C)n1nc(-c2ccc(S(N)(=O)=O)cc2)c2c(N)ncnc21	100000	*
5206	Nc1ncnc2c1c(-c1ccc3occc(=O)c3c1)nn2C1CCCC1	100000	*
5207	C[C@H](Nc1ncnc2c1[nH]c1ccccc12)c1ccccc1	100000	*
5208	c1ccc2c(c1)[nH]c1c(NC3CCCCC3)ncnc12	100000	*
5209	Cc1nc(Nc2cccc(Br)c2)c2c(n1)[nH]c1ccccc12	100000	*
5210	C[C@H](Nc1ncnc2c1[nH]c1ccccc12)c1ccccc1.Cl	100000	*
5211	CN(C)CCNc1ncnc2c1[nH]c1ccccc12.Cl	100000	*
5212	OCCNc1nc(Nc2cccc(F)c2)c2cn[nH]c2n1	100000	*
5213	COc1cccc(Nc2nc(NCCO)nc3[nH]ncc23)c1	100000	*
5214	COc1cccc(Nc2nc(NCCO)nc3c2cnn3C)c1	100000	*
5215	OCCNc1nc(Nc2cccc(Br)c2)c2cn[nH]c2n1	100000	*
5216	Cn1ncc2c(Nc3cccc(Br)c3)nc(NCCO)nc21	100000	*
5217	Cn1ncc2c(NCc3ccc(N)cc3)nc(NCCO)nc21	100000	*
5218	CC(C)n1ncc2c(Nc3cccc(F)c3)nc(NCCO)nc21	100000	*
5219	CC(C)n1ncc2c(Nc3cccc(Br)c3)nc(NCCO)nc21	100000	*
5220	COc1cccc(Nc2nc(NCCO)nc3c2cnn3C(C)C)c1	100000	*
5221	OCCN(CCO)c1nc(NCc2ccccc2)c2cn[nH]c2n1	100000	*
5222	OCCN(CCO)c1nc(Nc2cccc(Br)c2)c2cn[nH]c2n1	100000	*
5223	COc1cccc(Nc2nc(N(CCO)CCO)nc3[nH]ncc23)c1	100000	*
5224	OCCN(CCO)c1nc(Nc2cccc(F)c2)c2cn[nH]c2n1	100000	*
5225	COc1cccc(Nc2nc(N(CCO)CCO)nc3c2cnn3C)c1	100000	*
5226	CC(C)n1ncc2c(NCc3ccc([N+](=O)[O-])cc3)nc(NCCO)nc21	100000	*
5227	CC(C)n1ncc2c(NCc3ccccc3)nc(N(CCO)CCO)nc21	100000	*

5228	Cn1ncc2c(Nc3cccc(Br)c3)nc(N(CCO)CCO)nc21	100000	*
5229	CC(C)n1ncc2c(Nc3cccc(F)c3)nc(N(CCO)CCO)nc21	100000	*
5230	CC(C)n1ncc2c(Nc3cccc(Br)c3)nc(N(CCO)CCO)nc21	100000	*
5231	COc1cccc(Nc2nc(N(CCO)CCO)nc3c2cnn3C(C)C)c1	100000	*
5232	OCCNc1nc(NCc2cccc(Br)c2)c2cn[nH]c2n1	100000	*
5233	OCCN(CCO)c1nc(NCc2cccc(Br)c2)c2cn[nH]c2n1	100000	*
5234	CC(C)n1ncc2c(NCc3cccc(Br)c3)nc(NCCO)nc21	100000	*
5235	CC(C)n1ncc2c(NCc3cccc(Br)c3)nc(N(CCO)CCO)nc21	100000	*
5236	OCCNc1nc(NCc2cccc(F)c2)c2cn[nH]c2n1	100000	*
5237	Cn1ncc2c(NCc3cccc(F)c3)nc(NCCO)nc21	100000	*
5238	Cn1ncc2c(NCc3cccc(F)c3)nc(N(CCO)CCO)nc21	100000	*
5239	CC(C)n1ncc2c(NCc3cccc(F)c3)nc(N(CCO)CCO)nc21	100000	*
5240	COc1cccc(CNc2nc(NCCO)nc3[nH]ncc23)c1	100000	*
5241	COc1cccc(CNc2nc(N(CCO)CCO)nc3[nH]ncc23)c1	100000	*
5242	COc1cccc(CNc2nc(NCCO)nc3c2cnn3C)c1	100000	*
5243	COc1cccc(CNc2nc(N(CCO)CCO)nc3c2cnn3C)c1	100000	*
5244	COc1cccc(CNc2nc(NCCO)nc3c2cnn3C(C)C)c1	100000	*
5245	COc1cccc(CNc2nc(N(CCO)CCO)nc3c2cnn3C(C)C)c1	100000	*
5246	COc1cc2nccc(Oc3ccc(N)cc3)c2cc1OC	100000	*
5247	COc1cc2nccc(Oc3ccc(C(=O)c4ccc(C(C)(C)C)cc4)cc3)c2cc1OC	100000	*
5248	COc1cc2nccc(Oc3ccc(NC(=O)c4cccs4)cc3)c2cc1OC	100000	*
5249	COc1cc2nccc(Oc3ccc(NC(=O)c4ccco4)cc3)c2cc1OC	100000	*
5250	COc1cc2nccc(Oc3cccc(OC)c3OC)c2cc1OC	100000	*
5251	COc1cc2nccc(Oc3cccc(C(C)=O)c3)c2cc1OC	100000	*
5252	COc1cc2nccc(Oc3ccc(C(=O)c4ccc(C)cc4)cc3)c2cc1OC	100000	*
5253	COc1cc2nccc(Oc3ccc(C(=O)c4ccc(Br)cc4)cc3)c2cc1OC	100000	*
5254	COc1cc2nccc(Oc3ccc(C(=O)c4ccc(Cl)cc4)cc3)c2cc1OC	100000	*
5255	COc1cc2nccc(Oc3ccc(NC(=O)C4CCCC4)cc3)c2cc1OC	100000	*
5256	COc1cc2nccc(Oc3ccc(C(=O)c4ccc(I)cc4)cc3)c2cc1OC	100000	*
5257	COc1cc2nccc(Oc3ccc(C(=O)C4CCCCC4)cc3)c2cc1OC	100000	*
5258	COc1cc2nccc(Oc3ccc(C(=O)c4ccc([N+](=O)[O-])cc4)cc3)c2cc1OC	100000	*
5259	COc1cc2nccc(Oc3ccc(C(=O)c4ccc(C#N)cc4)cc3)c2cc1OC	100000	*
5260	COc1cc2nccc(Oc3ccc(NC(=O)c4ccc(C(C)=O)cc4)cc3)c2cc1OC	100000	*
5261	COc1cc2nccc(Oc3ccc(NC(=O)c4ccc(C(C)(C)C)cc4)cc3)c2cc1OC	100000	*
5262	COc1cc2nccc(Oc3ccc(NC(=O)c4ccc([N+](=O)[O-])cc4)cc3)c2cc1OC	100000	*
5263	CCCCc1ccc(C(=O)c2ccc(Oc3ccnc4cc(OC)c(OC)cc34)cc2)cc1	100000	*
5264	COc1cc2nccc(Oc3ccc(C(=O)c4ccc(C(F)(F)F)cc4)cc3)c2cc1OC	100000	*
5265	COc1cc2nccc(Oc3ccc(C(=O)c4cccc(C(F)(F)F)c4)cc3)c2cc1OC	100000	*
5266	COc1cc2nccc(Oc3ccc(NC(=O)C4CCCCC4)cc3)c2cc1OC	100000	*
5267	COc1cc2nccc(Oc3ccc(C(=O)c4ccc(OC(F)(F)F)cc4)cc3)c2cc1OC	100000	*
5268	COc1ccc(C(=O)Nc2ccc(Oc3ccnc4cc(OC)c(OC)cc34)cc2)cc1OC	100000	*
5269	CCCCc1ccc(C(=O)Nc2ccc(Oc3ccnc4cc(OC)c(OC)cc34)cc2)cc1	100000	*
5270	COc1cc2nccc(Oc3ccc(NC(=O)c4ccc(-c5ccccc5)cc4)cc3)c2cc1OC	100000	*

5271	CCCCOc1ccc(C(=O)Nc2ccc(Oc3ccnc4cc(OC)c(OC)cc34)cc2)cc1	100000	*
5272	COc1cc2nccc(Oc3ccc(C(C)=O)cc3)c2cc1OC	100000	*
5273	COC(=O)c1cccc(Oc2ccnc3cc(OC)c(OC)cc23)c1	100000	*
5274	COc1cc2nccc(Oc3ccc(NC(C)=O)cc3)c2cc1OC	100000	*
5275	COc1cc2nccc(Oc3ccc(C(=O)c4ccco4)cc3)c2cc1OC	100000	*
5276	COc1cc2nccc(Oc3ccc(C(=O)c4ccc(-c5ccccc5)cc4)cc3)c2cc1OC	100000	*
5277	CCCc1ccc(C(=O)c2ccc(Oc3ccnc4cc(OC)c(OC)cc34)cc2)cc1	100000	*
5278	CCOc1cc2nc3c(c(Nc4cccc(-c5csc(C)n5)c4)c2cc1OCC)CC(CN)C3	100000	*
5279	CCOc1cc2nc3c(c(Nc4cccc(-c5csc(C)n5)c4)c2cc1OCC)C(CNC(C)=O)CC3	100000	*
5280	COc1cc2c(Oc3ccc(NC=C4C(=O)NC(=O)N(c5ccc(C)cc5)C4=O)cc3F)ccnc2cc1OCCCN1CCCC1	100000	*
5281	COc1cc2c(Oc3ccc(NC(=O)c4c(Cl)c5ccccc5n(-c5ccc(F)cc5)c4=O)cc3F)ccnc2cc1OCCCN1CCN(C)CC1	100000	*
5282	O=C(N/N=C/c1ccc(O)cc1)Nc1ccc(Oc2ccnc3[nH]ccc23)c(F)c1	100000	*
5283	CCOc1cc2nc3c(c(NCCCCCNc4c5c(nc6cc(OCC)c(OCC)cc46)CCC5)c2cc1OCC)CCC3	101620	*
5284	COc1cc(/C=C(\C#N)C(=O)NCCCCNC(=O)/C(C#N)=C/c2cc(Br)c(O)c(OC)c2)cc(Br)c1O	102000	*
5285	COc1cc2ncc(CO)c(Nc3cccc(Br)c3)c2cc1OC	102200	*
5286	N#Cc1cnc2cc3c(cc2c1Nc1cccc(Br)c1)OCCO3	104700	*
5287	CCOC(=O)c1c(Nc2ncnc3cc(OC)c(OC)cc23)sc2c1CCCC2	108200	*
5288	COc1ccccc1C(=Cc1coc2nc(=N)[nH]c(N)c12)C(C)C	111400	*
5289	COc1cc2ncnc(Sc3nnc(NC(=O)c4ccccc4F)s3)c2cc1OC	115800	*
5290	N#CC(C#N)=Cc1ccc(O)c([N+](=O)[O-])c1	125000	*
5291	COc1cc2ncnc(Nc3nc4ccccc4[nH]3)c2cc1OC	127400	*
5292	COc1cc2ncnc(Nc3nnc(S)s3)c2cc1OC	139200	*
5293	COc1cc(C=C(C#N)C#N)cc(Br)c1O	153000	*
5294	COc1cc2ncnc(Sc3nnc(NC(=O)c4ccccc4)s3)c2cc1OC	154300	*
5295	COc1cc(C=C(C#N)C#N)cc([N+](=O)[O-])c1O	160000	*
5296	COc1cc2c(cc1OC)Nc1ncn(C)c(=O)c1C2	160000	*
5297	CCCC(=Cc1coc2nc(=N)[nH]c(N)c12)c1ccccc1OC	160300	*
5298	N#C/C(=C\c1ccc(O)cc1)C(=O)O	165000	*
5299	CCOc1ccc2sc(SCc3cc(/C=C(\C#N)C(N)=O)cc(OC)c3O)nc2c1	165958.7	*
5300	COc1cc2ncnc(Nc3cc(=O)[nH]c(S)n3)c2cc1OC	169500	*
5301	CCOC(=O)c1c(Nc2ncnc3cc(OC)c(OC)cc23)sc2c1CCCCC2	173000	*
5302	COc1cc2ncnc(Sc3nnc(NC(=O)c4ccccc4C)s3)c2cc1OC	175200	*
5303	O=C1c2c(c3c4cccc(O)c4n(C4OC(CO)C(O)C(O)C4O)c3c3[nH]c4c(O)cccc4c23)C(=O)N1NCC(O)CO	180000	*
5304	Nc1ncnc2c1ncn2[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O	195000	*
5305	COc1cc(C=C(C#N)C#N)ccc1O	200000	*
5306	C=CC(=O)Nc1cc(Nc2ncc(Br)c(Nc3ccc4c(c3)CCC4)n2)c(OC)cc1N1CCN(C)CC1	202500	*
5307	COc1cc2ncnc(Sc3nc4ccccc4[nH]3)c2cc1OC	207900	*
5308	CC(C)(C)OC[C@H](Cn1ccnc1[N+](=O)[O-])OC(=O)c1ccc(NC=C2C(=O)C=CC2=O)cc1	213000	*
5309	N#CC(C#N)=Cc1cccnc1	225000	*
5310	N#CC(C#N)=NNc1ccc(O)cc1	225000	*
5311	C=CC(=O)Nc1cc(Nc2nccc(Nc3cc4ccccc4n3C)n2)c(OC)cc1N(C)CCN(C)C	228900	*
5312	N#CC(C#N)=C(O)c1ccc(O)cc1	230000	*
5313	C=CC(=O)Nc1cc(Nc2ncc(Br)c(Nc3ccc4[nH]ccc4c3)n2)ccc1N1CCN(C)CC1	233800	*

5314	O=P(O)(O)C(O)c1ccc2ccccc2c1	250000	*
5315	N#CC(C#N)=Cc1ccncc1	250000	*
5316	N#CC(C#N)=Cc1ccc[nH]1	260000	*
5317	COc1cc(/C=C(\C#N)C(=O)O)cc(OC)c1O	264000	*
5318	C=CC(=O)Nc1cc(Nc2nccc(-c3cn(C)c4cccnc34)n2)c(OC)cc1N(C)CCNC.Cl	277000	*
5319	C=CC(=O)Nc1cc(Nc2ncc(Br)c(Nc3ccc4c(ccn4C)c3)n2)c(OC)cc1N1CCN(C)CC1	280400	*
5320	COc1ccc(C(=O)c2ccc(=O)n(CCN(C)C)c2)c(O)c1	300000	*
5321	COc1cc2ncnc(NC3CCC(O)CC3)c2cc1OC	318500	*
5322	CC(C)(C)c1cc(C=C2C(=O)C=CC2=O)cc(C(C)(C)C)c1O	320000	*
5323	COc1cc(/C=C(\C#N)C(=O)O)ccc1O	325000	*
5324	N#CC(C#N)=Cc1ccc2c(c1)OCO2	350000	*
5325	N#CC(C#N)=CNc1ccc(O)cc1	350000	*
5326	N#CC(C#N)=Cc1cccc(O)c1	375000	*
5327	C=CC(=O)Nc1cc(Nc2ncc(Br)c(Nc3ccc4c(ccn4C)c3)n2)ccc1N1CCN(C)CC1	414100	*
5328	N#CC(C#N)=Cc1ccc(C(=O)O)cc1	430000	*
5329	Cc1cc(C=C2C(=O)C=CC2=O)cc(C)c1O	440000	*
5330	Cn1cnc2c(NCc3ccccc3)nc(NCCO)nc21	440000	*
5331	N#CC(C#N)=Cc1ccc([N+](=O)[O-])c(O)c1	450000	*
5332	COc1ccc(C(O)=C(C#N)C#N)cc1	450000	*
5333	N#CC(C#N)=Cc1ccc(/C=C/C(=O)O)cc1	450000	*
5334	CC(C)(C)c1cc(C=C(C#N)C#N)cc(C(C)(C)C)c1O	460000	*
5335	C=CC(=O)Nc1cc(Nc2ncc(Br)c(Nc3ccc4c(c3)CCC4)n2)ccc1N1CCN(C)CC1	465700	*
5336	CC(=C(C#N)C#N)c1ccc(NC(=O)CCC(=O)O)cc1	500000	*
5337	COc1cc(OC)c2c(=O)c(-c3cccc(Cl)c3)coc2c1	500000	*
5338	CC(C)(C)Oc1cc(/C=C(\C#N)C(=N)S)cc(C(C)(C)C)c1O	501187.2	*
5339	CCCCC(=Cc1coc2nc(=N)[nH]c(N)c12)c1ccccc1OC	529300	*
5340	N#CC(C#N)=Cc1ncc[nH]1	532000	*
5341	N#CC(C#N)=Cc1ccc(O)cc1	560000	*
5342	N#CC(C#N)=Cc1cc2c(cc1[N+](=O)[O-])OCO2	560000	*
5343	COC(=O)[C@@]1(Cc2ccc(O)c(CC=C(C)C)c2)OC(=O)C(O)=C1c1ccc(O)cc1	590000	*
5344	COc1ccc(NN=C(C#N)C#N)cc1	600000	*
5345	N#CCNC(=O)/C(C#N)=C/c1ccc(O)cc1	625000	*
5346	N#CC(C#N)=Cc1ccc(NC(=O)CCC(=O)O)cc1	640000	*
5347	COc1ccc(C=C(C#N)C#N)cc1F	800000	*
5348	N#C/C(=C\c1ccc(O)cc1)C(N)=O	800000	*
5349	N#CC(C#N)=C(N)/C(C#N)=C/c1ccc2[nH]ccc2c1	820000	*
5350	N#C/C(=C\c1ccc(F)cc1)C(=O)O	833000	*
5351	COc1ccc(/C=C(\C#N)C(=O)O)cc1	833000	*
5352	COc1cc(C=C(C#N)C#N)cc(OC)c1O	850000	*
5353	N#C/C(=C\c1ccccc1)C(=O)O	850000	*
5354	N[C@@H](Cc1ccc(O)c(O)c1)C(=O)O	900000	*
5355	CN(C)CCNc1ncnc2c1[nH]c1ccccc12	1000000	*
5356	COc1cc(/C(C)=C(\C#N)C(=O)O)ccc1O	1100000	*

5357	N#CC(C#N)=C1CCCc2c(O)cccc21	1200000	*
5358	O=C(O)/C=C/c1ccc(O)c(O)c1	1200000	*
5359	N#CC(C#N)=Cc1cc[n+]([O-])cc1	1300000	*
5360	N#C/C(=C\c1ccc([N+](=O)[O-])cc1)C(=O)O	1300000	*
5361	N#C/C(=C/c1ccc[nH]1)C(=O)O	1360000	*
5362	N#CC(C#N)=Cc1ccc(C#N)cc1	1400000	*
5363	N#CC(C#N)=C1C(=O)NC(=O)NC1=O	1400000	*
5364	N#CC(C#N)=Cc1cc[nH]n1	1480000	*
5365	O=C(O)C(=Cc1ccc(O)cc1)C(=O)O	1500000	*
5366	C[S+]([O-])c1ccc(C=C(C#N)C#N)cc1	1800000	*
5367	N#CC(C#N)=Cc1ccc2[nH]ccc2c1	2200000	*
5368	N#C/C=C/c1ccc(O)cc1	2400000	*
5369	O=C(O)/C=C/c1ccc(O)cc1	3000000	*
5370	CN(c1cccnc1)c1cc2c(Nc3ccc(F)c(Cl)c3)c(C#N)cnc2cn1	5000000	*
5371	N#CC(C#N)Cc1ccc(O)cc1	6500000	*

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77, 593–599. https://doi.org/10.1016/j.bioorg.2018.01.035.

Table S2. Dataset 2 for generating queries from crystal structures.

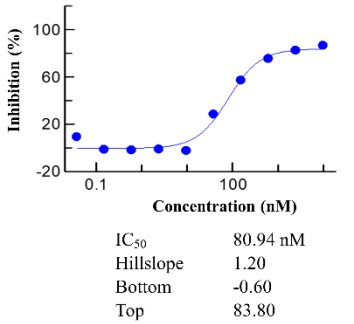
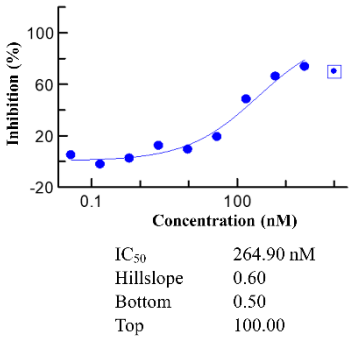
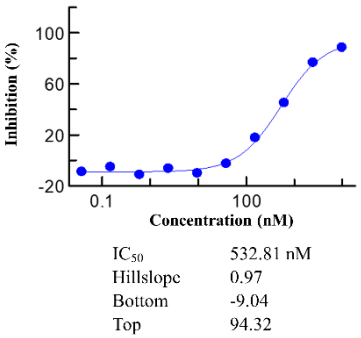
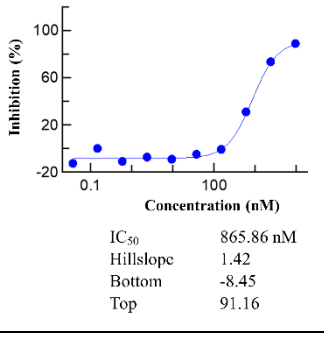
Num	Ligand name	PDB code	Num	Ligand name	PDB code
1	1c9	4I23	13	ire	4WKQ
2	1wy	4LI5	14	kj8	4JQ8
3	03p	3POZ	15	kjq	4JQ7
4	4zq	5CAV	16	kjr	4JR3

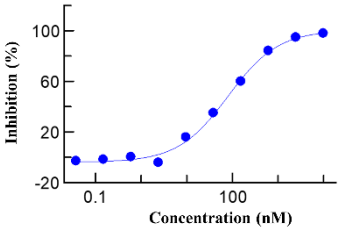
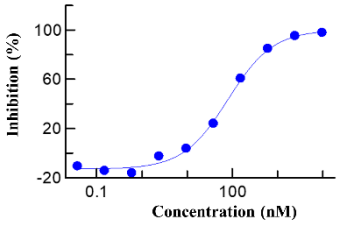
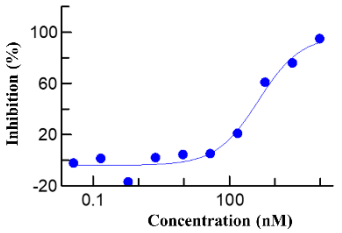
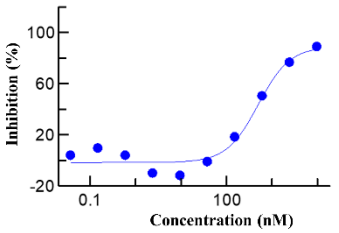
5	5q4	5EM8	17	kjv	4JRV
6	5x4	5FED	18	o44	5V8L
7	aee	2J6M	19	own	4G5J
8	aq4	1M17	20	pox	3BEL
9	cko	6JZO	21	w19	3W33
10	djk	2J5F	22	w32	3W32
11	fmm	1XKK	23	yun	4LRM
12	hyz	2RGP	24	yy3	4ZAU

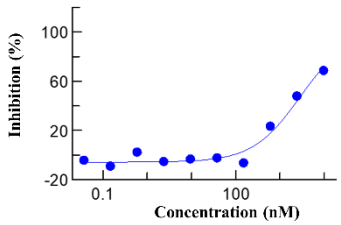
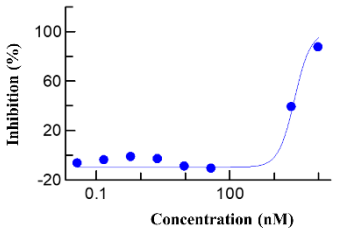
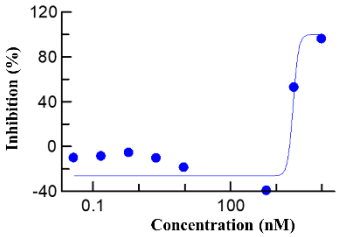
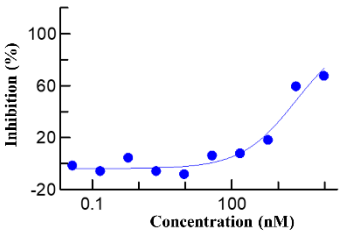
Table S3. The optimized parameters used in SAR and QSAR models.

Model	Optimized parameters
Model 1A	C: {8}, gamma: {0.03125}
Model 1B	C: {4}, gamma: {64}, descriptors: {3DACorr:PiChg:Cor3D:ori1_1, 3DACorr:PiEN:Cor3D:ori1_2, 3DACorr:LpEN:Cor3D:ori1_5, ComplexRing, 3DACorr:PiChg:Cor3D:ori1_4, 3DACorr:Polariz:Cor3D:ori1_6,3DACorr:PiEN:Cor3D:ori1_10, 3DACorr:PiEN:Cor3D:ori1_3,HAccN, 3DACorr:PiChg:Cor3D:ori1_2, 3DACorr:LpEN:Cor3D:ori1_2, 3DACorr:Ident:Cor3D:ori1_11, 3DACorr:TotChg:Cor3D:ori1_2, 3DACorr:SigChg:Cor3D:ori1_5, TPSA}
Model 2A	C: {4}, gamma: {0.03125}
Model 2B	C: {4}, gamma: {32}, descriptors: {3DACorr:LpEN:Cor3D:ori1_5, HAccN, 3DACorr:Ident:Cor3D:ori1_3, 3DACorr:Ident:Cor3D:ori1_1, 3DACorr:PiChg:Cor3D:ori1_4, 3DACorr:SigChg:Cor3D:ori1_5, HAcc,3DACorr:PiEN:Cor3D:ori1_2, 3DACorr:PiEN:Cor3D:ori1_12, 3DACorr:Ident:Cor3D:ori1_11, 3DACorr:Polariz:Cor3D:ori1_12, 3DACorr:LpEN:Cor3D:ori1_8, 3DACorr:LpEN:Cor3D:ori1_10, 3DACorr:PiEN:Cor3D:ori1_6, 3DACorr:SigEN:Cor3D:ori1_9, 3DACorr:PiChg:Cor3D:ori1_5, 3DACorr:TotChg:Cor3D:ori1_2, 3DACorr:TotChg:Cor3D:ori1_1, 3DACorr:SigChg:Cor3D:ori1_1, 3DACorr:SigChg:Cor3D:ori1_2}
Model 3A	C: {4}, epsilon: {0.25}, gamma: {8}, descriptors: {HAccN, BondsRot, 3DACorr:PiChg:Cor3D:ori1_4, 3DACorr:SigEN:Cor3D:ori1_3, ComplexRing, 3DACorr:LpEN:Cor3D:ori1_8, 3DACorr:SigChg:Cor3D:ori1_1, 3DACorr:LpEN:Cor3D:ori1_2, 3DACorr:TotChg:Cor3D:ori1_8, 3DACorr:SigChg:Cor3D:ori1_8, 3DACorr:SigChg:Cor3D:ori1_6, 3DACorr:TotChg:Cor3D:ori1_5, 3DACorr:TotChg:Cor3D:ori1_4, 3DACorr:LpEN:Cor3D:ori1_10, 3DACorr:TotChg:Cor3D:ori1_7, 3DACorr:PiEN:Cor3D:ori1_8, 3DACorr:PiEN:Cor3D:ori1_4, 3DACorr:Polariz:Cor3D:ori1_4, 3DACorr:SigChg:Cor3D:ori1_3}
Model 3B	C: {8}, epsilon: {0.125}, gamma: {8}, descriptors: {3DACorr:Polariz:Cor3D:ori1_2, 3DACorr:Polariz:Cor3D:ori1_5, HAccN, 3DACorr:PiChg:Cor3D:ori1_4, BondsRot, 3DACorr:SigChg:Cor3D:ori1_6, 3DACorr:LpEN:Cor3D:ori1_8, 3DACorr:SigEN:Cor3D:ori1_8, Ro5ViolExt, 3DACorr:TotChg:Cor3D:ori1_8, 3DACorr:SigChg:Cor3D:ori1_8, 3DACorr:LpEN:Cor3D:ori1_2, 3DACorr:PiEN:Cor3D:ori1_6, 3DACorr:PiEN:Cor3D:ori1_4, 3DACorr:PiEN:Cor3D:ori1_8, ComplexRing, 3DACorr:SigChg:Cor3D:ori1_1, 3DACorr:SigChg:Cor3D:ori1_3, HAccO, 3DACorr:TotChg:Cor3D:ori1_5, HDon}
Model 3C	C: {4}, epsilon: {0.25}, gamma: {8}, descriptors: {3DACorr:SigEN:Cor3D:ori1_6, 3DACorr:SigEN:Cor3D:ori1_5, HAccN, ComplexRing, 3DACorr:PiChg:Cor3D:ori1_4, 3DACorr:SigChg:Cor3D:ori1_6, 3DACorr:TotChg:Cor3D:ori1_4, 3DACorr:TotChg:Cor3D:ori1_5, 3DACorr:PiEN:Cor3D:ori1_6, 3DACorr:LpEN:Cor3D:ori1_8, 3DACorr:SigChg:Cor3D:ori1_1, 3DACorr:LpEN:Cor3D:ori1_2, 3DACorr:TotChg:Cor3D:ori1_8, 3DACorr:SigChg:Cor3D:ori1_8, 3DACorr:TotChg:Cor3D:ori1_7, BondsRot, HAccO, 3DACorr:PiEN:Cor3D:ori1_8, 3DACorr:TotChg:Cor3D:ori1_1}

Table S4. IC_{50} curves for hit compounds experimented on EGFR and ErbB-2.

Compound	Compound concentration (nM)	Inhibition (%)	IC_{50} curve
Inhibitory activity against EGFR			
hit 1	10000	86.3	
	2500.0	82.2	
	625.0	75.2	
	156.3	56.9	
	39.1	28.1	
	9.8	-2.8	
	2.4	-1.5	
	0.6	-2.2	
	0.2	-1.7	
	0.0	8.9	
hit 2	10000	69.9	
	2500.0	73.5	
	625.0	65.8	
	156.3	48.2	
	39.1	19.0	
	9.8	9.1	
	2.4	12.1	
	0.6	2.2	
	0.2	-2.4	
	0.0	4.8	
hit 3	10000	88.3	
	2500.0	76.4	
	625.0	44.9	
	156.3	17.5	
	39.1	-2.7	
	9.8	-10.2	
	2.4	-6.5	
	0.6	-11.4	
	0.2	-5.3	
	0.0	-9.1	
hit 4	10000	88.3	
	2500.0	72.9	
	625.0	30.4	
	156.3	-1.4	
	39.1	-5.5	
	9.8	-9.7	
	2.4	-8.0	
	0.6	-11.6	

	0.2	-0.6	
	0.0	-13.3	
hit 5	10000	97.7	 IC_{50} 80.24 nM Hillslope 0.79 Bottom -4.02 Top 100.37
	2500.0	94.5	
	625.0	83.9	
	156.3	59.7	
	39.1	34.8	
	9.8	15.6	
	2.4	-4.5	
	0.6	0.0	
	0.2	-2.1	
	0.0	-3.2	
hit 6	10000	97.7	 IC_{50} 80.31 nM Hillslope 0.87 Bottom -13.06 Top 100.14
	2500.0	95.1	
	625.0	84.6	
	156.3	60.5	
	39.1	23.8	
	9.8	3.5	
	2.4	-2.8	
	0.6	-16.4	
	0.2	-14.5	
	0.0	-10.8	
hit 7	10000	94.5	 IC_{50} 433.43 nM Hillslope 0.93 Bottom -4.05 Top 97.27
	2500.0	75.5	
	625.0	60.5	
	156.3	20.5	
	39.1	4.6	
	9.8	3.9	
	2.4	1.5	
	0.6	-17.5	
	0.2	0.9	
	0.0	-2.8	
hit 8	10000	88.5	 IC_{50} 499.77 nM Hillslope 1.26 Bottom -1.72 Top 88.98
	2500.0	76.3	
	625.0	50.0	
	156.3	17.8	
	39.1	-1.5	
	9.8	-12.3	
	2.4	-10.4	
	0.6	3.5	
	0.2	9.1	
	0.0	3.5	
	10000	68.3	

hit 9	2500.0	47.4	 IC_{50} 2826.72 nM Hillslope 0.81 Bottom -5.76 Top 100.00
	625.0	22.9	
	156.3	-6.9	
	39.1	-2.8	
	9.8	-3.7	
	2.4	-5.8	
	0.6	1.8	
	0.2	-9.5	
	0.0	-4.7	
Inhibitory activity against ErbB-2			
hit 5	10000	87.2	 IC_{50} 2867.64 nM Hillslope 2.41 Bottom -9.66 Top 100.00
	2500.0	39.0	
	625.0	-20.4	
	156.3	-20.1	
	39.1	-10.9	
	9.8	-9.2	
	2.4	-3.2	
	0.6	-1.5	
	0.2	-4.1	
	0.0	-6.6	
hit 6	10000	95.8	 IC_{50} 2339.27 nM Hillslope 7.56 Bottom -26.08 Top 100.00
	2500.0	52.5	
	625.0	-39.6	
	156.3	-66.0	
	39.1	-48.2	
	9.8	-19.0	
	2.4	-10.7	
	0.6	-5.8	
	0.2	-8.9	
	0.0	-10.4	
hit 8	10000	67.1	 IC_{50} 2365.20 nM Hillslope 0.75 Bottom -3.90 Top 100.00
	2500.0	59.1	
	625.0	17.7	
	156.3	7.4	
	39.1	5.7	
	9.8	-8.7	
	2.4	-6.4	
	0.6	4.0	
	0.2	-6.4	
	0.0	-2.1	

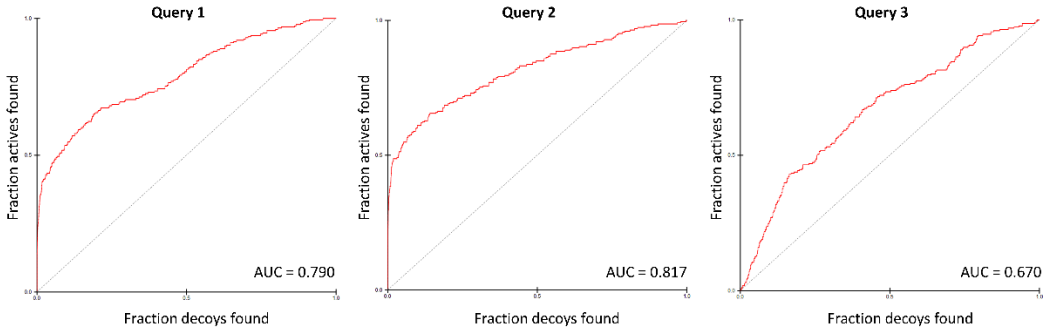


Figure S1. The ROC curves and AUC values of 3 queries. Query 1 was generated from crystal structure djk in 2J5F. Query 2 was generated from crystal structures ire and kj8 in 4WKQ and 4JQ8, respectively. Query 3 was generated from DGMG model.

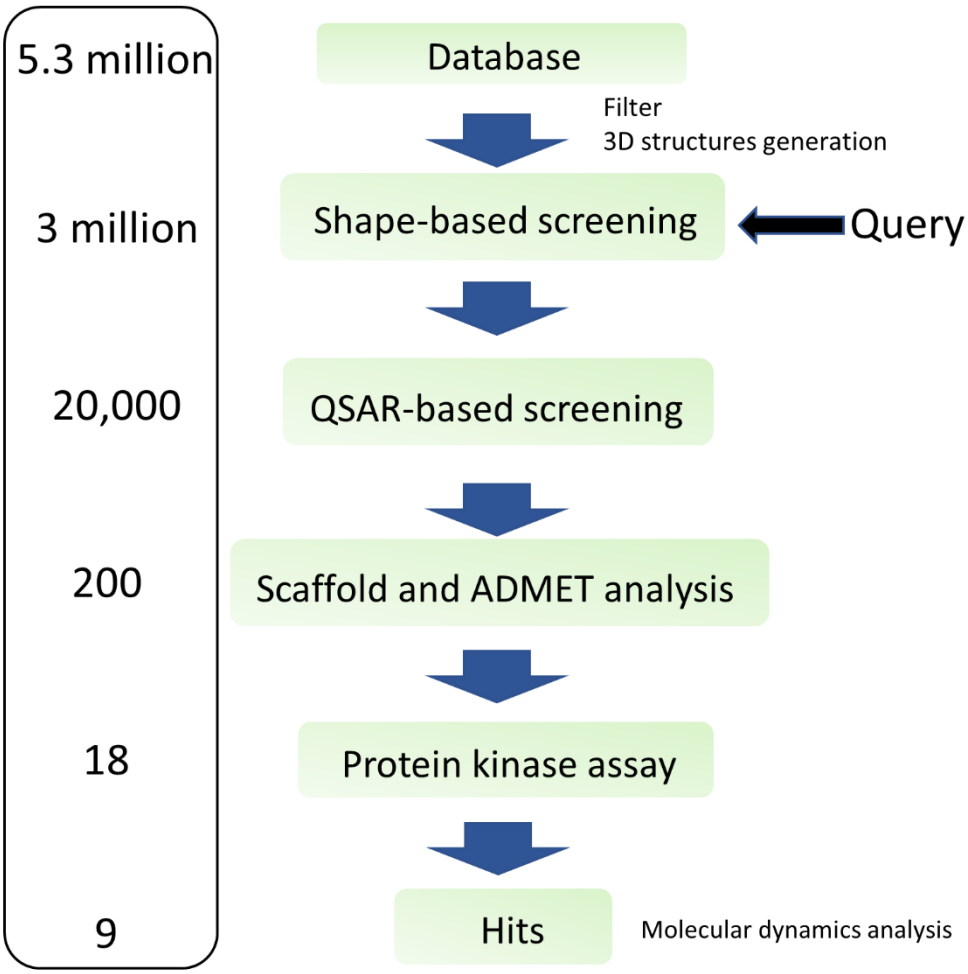


Figure S2. The cascade of the hierarchical ligand-based virtual screening of novel EGFR inhibitors. For shape-based similarity screening, two queries were from crystal structures and one query was generated from DGMG model.

Kinase assay method

We tested 20 compounds (18 selected compounds and 2 reference molecules) for the in vitro inhibitory activities against EGFR and ErbB-2 by using Mobility Shift Assay. The compounds were tested from 10μM for 10 concentrations, 4-fold, in single. The details of the experimental materials and process are as following:

Materials

EGFR (Eurofins, Cat.No 14-531, Lot. No WAB0528)
HER2 (Invitrogen, Cat.No. PV3590, Lot. No. 1689418B)
Peptide FAM-P22 (GL Biochem, Cat. No. 112393, Lot. No. P180116-MJ112393)
ATP (MCE, Cat. No. HY-15141, Lot. No.21226)
DMSO (Sigma, Cat. No. D2650, Lot. No. 474382)
EDTA (Sigma, Cat. No. E5134, CAS No. 60-00-4)
96-well plate (Corning, Cat. No. 3365, Lot. No. 22008026)
384-well plate (Corning, Cat. No. 3573, Lot. No. 12608008)

Kinases reaction condition

Kinase	Enzyme concentration (nM)	ATP concentration (μM)	Substrate	Substrate concentration (μM)
HER2	20	8.8	Peptide22	3
EGFR	6	1	Peptide22	3

Instrument information

Name	Model	Manufacturer	SN
Caliper EZ Reader (No.2)	EZ ReaderII	Perkin Elmer	DS1152N0107
Precision	PRC384U	BioTek	214145
Biochemical incubator	SPX-100B-Z	Boxun	/
Centrifuge	5810R	Eppendorf	5811L941179

In vitro kinase assays

All compounds were initially prepared as 10 mM stocks in DMSO and subsequently diluted in DMSO to 50 × their final concentrations. Ten μL of each DMSO dilution was transferred to a well in a fresh 96-well cluster plate containing 90 μL 1 × Kinase buffer (50 mM HEPES pH 7.5, 10 mM $MgCl_2$, 2 mM DTT and 0.0015% Brij-35) and then mixed for 10 min. Five μL of each compound dilution was subsequently added to 384-well plate in duplicate. To each well, 10 μL of enzyme solution containing either HER2(final concentrations 20 nM) or EGFR (final concentrations 6 nM) in 1 × Kinase buffer and the mix incubated at room temperature for 10 min. To initiate each reaction, 10 μL of peptide solution containing FAM-labelled peptide (final concentrations 3000 nM FAM-22 and ATP (final concentrations 8.8μM or 1μ M,

respectively) in 1 × Kinase buffer was added to each well. All reactions were incubated at 28°C for a period time and then terminated by the addition of 25 µL stop buffer (100 mM HEPES pH 7.5, 50 mM EDTA, 0.2% Coating Reagent #3 and 0.015% Brij-35). All samples were then subjected to analysis using Caliper EZ ReaderII (Down stream voltages:-500V, Up stream voltages:-2250V, Base pressure -0.5 PSI, Screen pressure -1.2 PSI)to read conversion values. Conversion values were transformed into % inhibition of kinase activity using the formula: % Inhibition = [(MA – X)/(MA - MI)] × 100% where MA = conversion value of DMSO only controls, MI = conversion value of no enzyme controls and X = conversion value at any given compound dose. IC50 values were then calculated by plotting dose-response curves and then using the XLfit application in Excel software.