

Table S1. Flavonoids docking affinity scores for MEK2 binding pocket.

Compound CID	SMILES	Docking affinity (kcal/mol)
129703940	<chem>oc1c(c(c(=O)c2c(cccc12)C(=O)c1cc(c(c(c1)O)O)O)O)c1ccccc1</chem>	-11.3
131751372	<chem>O1c2c3C=CC(C)(C)Oc3ccc2C(=O)[C@H]([C@@H]1c1ccc(c(c1)CC=C(C)C)O)O</chem>	-11.1
56649181	<chem>c1(c(cc2c(c(=O)cc(o2)c2ccccc2)c1O)O)OCc1ccc(F)cc1</chem>	-11.1
154699552	<chem>O([C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)C(=O)O)c1cccc(c1)c1cc(=O)c2ccccc2o1</chem>	-10.9
154699598	<chem>O([C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)C(=O)O)c1cccc1c1cc(=O)c2ccccc2o1</chem>	-10.9
44559902	<chem>O1c2cc(c(c(c2C(=O)[C@@H]([C@H]1c1ccc(cc1)O)O)O)Cc1ccc(cc1)O)O</chem>	-10.9
101685222	<chem>O1c2cc(c(c(c2C(=O)[C@H]([C@@H]1c1ccc(cc1)O)O)O)Cc1ccc(cc1)O)O</chem>	-10.8
11314387	<chem>oc1c(cc(=O)c2c(c(c(cc12)O)OCc1ccccc1)O)c1ccccc1</chem>	-10.8
100986463	<chem>oc1c(cc(=O)c2c(cc(cc12)OC(=O)C/C=C/c1ccccc1)O)c1ccccc1</chem>	-10.6
100986464	<chem>oc1c(cc(=O)c2c(cc(cc12)OC(=O)C/C=C/c1ccc(cc1)OC)O)c1ccccc1</chem>	-10.5
102577930	<chem>c1(cc(c2c(=O)cc(oc2c1)c1ccc(cc1)O)O)OS(O)(O)c1ccc(C)cc1</chem>	-10.5
12019529	<chem>oc1c(cc(=O)c2c(cc(cc12)OC(=O)Cc1ccccc1)O)c1ccccc1</chem>	-10.4
129696793	<chem>oc1c(c(c(=O)c2c(cccc12)C(=O)/C=C/c1ccc(cc1)O)O)c1ccccc1</chem>	-10.4
14304997	<chem>C(=O)(NCCCCN1CCN(CC1)c1ccccc1)c1c(=O)c2c(oc1c1ccccc1)cccc2</chem>	-10.4

14626316	<chem>O(c1ccc2c(=O)cc(oc2c1)c1ccccc1)C[C@H](O)CNCCc1ccc(cc1)O</chem>	-10.4
44382144	<chem>o1c(cc(=O)c2c(cc(cc12)OC(=O)c1ccc(C)cc1)O)c1ccccc1</chem>	-10.4
10575055	<chem>c1(ccc(cc1)OCc1ccc2ccccc2n1)c1oc2c(c(=O)c1O)cccc2C(=O)O</chem>	-10.3
14016776	<chem>c1(cc(c2c(=O)cc(oc2c1)c1ccc(cc1)O)O)OS(=O)(=O)O</chem>	-10.3
44382145	<chem>c1(cc(c2c(=O)cc(oc2c1)c1ccccc1)O)OC(=O)c1ccc(F)cc1</chem>	-10.3
73265448	<chem>o1cc(c(=O)c2c(cc(cc12)OCc1ccccc1)O)c1ccc(cc1)N(=O)=O</chem>	-10.3
10094175 1	<chem>O1c2cc(c(c(c2C(=O)C[C@H]1c1ccc(c(c1)O)OC)O)c1ccc(cc1)OC)O</chem>	-10.2
11395168	<chem>o1c(cc(=O)c2c(cc(cc12)OCc1ccccc1)O)c1ccc(c(c1)O)OC</chem>	-10.2
14408549	<chem>C(Oc1ccc2c(=O)cc(oc2c1)c1ccccc1)[C@H](O)CNCCc1ccc(c(c1)OC)OC</chem>	-10.2
25070110	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(cc1)O)O)OCc1ccccc1</chem>	-10.2
5471244	<chem>c1(cc(c2c(=O)cc(oc2c1)c1ccccc1)O)OS(=O)(=O)O</chem>	-10.2
69567244	<chem>o1c(cc(=O)c2c(cc(cc12)OCc1ccccc1)O)c1ccc(cc1)O</chem>	-10.2
85823044	<chem>o1c(cc(=O)c2c(cccc12)OCc1ccccc1)c1ccc(cc1)C=O</chem>	-10.2
10813589	<chem>O(c1ccc2c(=O)cc(oc2c1)c1ccccc1)C[C@@]1(OC(=O)C(=C)C1)c1ccc(cc1)OC</chem>	-10.1
12820520	<chem>O1c2c(cc3c(=O)c(c(oc3c2=CC1(C)C)c1ccc2c(OCO2)c1)OC)OC</chem>	-10.1
12985363 3	<chem>o1c(c(c(=O)c2c(cccc12)C(=O)/C=C/c1ccc(c(c1)O)O)O)c1ccccc1</chem>	-10.1
14735885	<chem>c1(cc(=O)c2ccccc2o1)c1ccc(cc1)C(F)(F)F</chem>	-10.1
180439	<chem>o1c(cc(=O)c2cc(c(cc12)O)CC=C(C)C)c1ccc2c(OCO2)c1</chem>	-10.1
19835337	<chem>O(c1ccc2c(=O)cc(oc2c1)c1ccccc1)C[C@H](O)CNCCCCc1cnccc1</chem>	-10.1
42608050	<chem>O1C(C)(C)C=Cc2c3c(C=CC(C)(C)O3)cc(c12)[C@@H]1CC(=O)c2c(cc(cc2O1)O)O</chem>	-10.1
10991656	<chem>O1c2ccc3c(=O)cc(oc3c2=CC1(C)C)c1ccc2c(OCO2)c1</chem>	-10.0
11582389	<chem>c1(ccc2c(=O)cc(oc2c1)c1ccccc1)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)OC)CO</chem>	-10.0
11790	<chem>o1c(cc(=O)c2ccc3ccccc3c12)c1ccccc1</chem>	-10.0
14626328	<chem>c1(ccc2c(=O)cc(oc2c1)c1ccccc1)OC[C@H](O)CCCO[C@H]1OCCCC1</chem>	-10.0

1522807	<chem>o1cc(c(=O)c2ccc(cc12)OCc1ccc(cc1)N(=O)=O)c1ccccc1</chem>	-10.0
563997	<chem>o1cc(c(=O)c2ccc(cc12)OCc1ccccc1)c1ccccc1</chem>	-10.0
56589538	<chem>c1(c(c(c2c(=O)cc(oc2c1)c1ccccc1)O)O)OCc1ccc(F)cc1</chem>	-10.0
67984060	<chem>o1c(c(c(=O)c2c(cc(cc12)OCc1ccccc1)O)O)c1ccc(c(c1)O)O</chem>	-10.0
100941748	<chem>O1c2cc(c(c(c2C(=O)C[C@H]1c1ccc(cc1)O)O)c1ccc(cc1)OC)O</chem>	-9.9
100941749	<chem>O1c2cc(c(c(c2C(=O)C[C@H]1c1ccc(c(c1)O)OC)O)c1ccccc1)O</chem>	-9.9
10338671	<chem>c1(ccc2c(=O)cc(oc2c1)c1ccccc1)OC[C@]1(OC(=O)C(=C)C1)C</chem>	-9.9
10981007	<chem>O1c2c(ccc3OC(C)(C)C=Cc23)C(=O)C[C@H]1c1ccc2c(OCO2)c1</chem>	-9.9
11247668	<chem>O1c2cc(c(c(c2C(=O)C[C@H]1c1ccc(c(c1)O)O)O)C/C=C(\C)/CC[C@@H](C(=C)C)O)O</chem>	-9.9
11358607	<chem>O1c2ccc3c(=O)cc(oc3c2C=CC1(C)C)c1ccccc1</chem>	-9.9
11796528	<chem>c1(ccc(cc1)OCc1ccc2ccccc2n1)c1oc2c(c(=O)c1)cccc2C(=O)O</chem>	-9.9
129834514	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(cc1)OC(=O)C)O)OCc1ccccc1</chem>	-9.9
154699985	<chem>O(c1ccc2C(=O)C[C@H](Oc2c1)c1ccccc1)[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)C(=O)O</chem>	-9.9
1760386	<chem>o1cc(c(=O)c2ccc(cc12)OCc1ccccc1)c1ccc(cc1)OC</chem>	-9.9
3070243	<chem>c1(c(C)c(=O)c2ccc(c(c2o1)CN1CCCCC1)OC)c1ccc(F)cc1</chem>	-9.9
3085261	<chem>c1(ccc2c(=O)c(coc2c1)c1ccc2c(OCO2)c1)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO</chem>	-9.9
52951514	<chem>c1(ccc(c(c1)OC)OC[C@H](C(C)(C)O)O)c1c(=O)c2c(cc3OC(C=Cc3c2)(C)C)oc1</chem>	-9.9
5469928	<chem>o1c(cc(=O)c2c(cc(c(c12)[C@H]1CCCCN1)O)O)c1ccccc1</chem>	-9.9
563887	<chem>c1(ccc(c(c1)OC)OCc1ccccc1)c1oc2ccccc2c(=O)c1OC</chem>	-9.9
101440521	<chem>o1c2cc(cc(c2c(=O)c(c1c1ccc(c(c1)C[C@@H](C(=C)C)O)O)O)O)O</chem>	-9.8
101999902	<chem>c1(coc2cc(c(c(c2c1=O)O)CCC(C)(C)O)O)c1ccc2OC(C=Cc2c1O)(C)C</chem>	-9.8

15108704	<chem>o1c(cc(=O)c2c(c(c(cc12)OCc1ccccc1)O)O)c1ccc(c(c1)O)O</chem>	-9.8
15342843	<chem>o1c(c(c(=O)c2c(cc(cc12)OC(=O)c1ccccc1)O)OC)c1ccccc1</chem>	-9.8
15383190	<chem>O1c2cc(c3c(=O)cc(oc3c2C=CC1(C)C)c1ccccc1)O</chem>	-9.8
44257869	<chem>O1c2cc3c(c(=O)cc(o3)c3ccc(cc3)O)c(c2C[C@H](C1(C)C)O)O</chem>	-9.8
49736	<chem>o1c(c(C)c(=O)c2ccc(c(c12)CN1CCCCC1)OC)c1ccccc1</chem>	-9.8
5315125	<chem>o1c2cc(cc(c2c(=O)cc1c1cc(c(c(c1)CC=C(C)C)O)O)O)O</chem>	-9.8
100943380	<chem>c1(cccc(c1)c1cc(=O)c2ccccc2o1)S(=O)(=O)Nc1ccc(C)cc1</chem>	-9.7
102321611	<chem>o1cc(c(=O)c2c(cc(cc12)[C@@H]1C=C([C@H]2C=CCOC2=C1)O)O)c1ccc(c(c1OC)OC)O</chem>	-9.7
10291777	<chem>O1c2ccc3C(=O)C[C@H](Oc3c2C[C@H]1C(C)(C)O)c1ccc(cc1O)O</chem>	-9.7
11597157	<chem>c1(ccc2c(=O)cc(oc2c1)c1ccc(cc1)O)O[C@@H]1O[C@H]([C@H]([C@@H]([C@H]1O)O)OC)CO</chem>	-9.7
12019528	<chem>o1c(cc(=O)c2c(cc(cc12)OC(=O)c1ccccc1OC(=O)C)O)c1ccccc1</chem>	-9.7
129791328	<chem>c1(ccc2c(=O)c(c(oc2c1)C(=O)O)c1ccccc1)OCc1sc2ccccc2n1</chem>	-9.7
129825556	<chem>o1c2cc(c(c(c2c(=O)c(c1c1ccc(c(c1)/C=C/C(=C)C)O)OC)O)OC)O</chem>	-9.7
15108702	<chem>o1c(cc(=O)c2c(c(c(cc12)OCc1ccccc1)O)O)c1ccccc1</chem>	-9.7
24861960	<chem>O1c2cc(c(c(c2C(=O)C[C@H]1c1ccc(c(c1)OC)O)O)C/C=C(\C)/C/C=C/C(C)(C)O)O</chem>	-9.7
24866261	<chem>c1(cc(c2c(=O)cc(oc2c1)c1ccccc1)O)O[C@@H]1O[C@H]([C@H]([C@@H]([C@H]1O)O)OC)CO</chem>	-9.7
3070242	<chem>c1(c(C)c(=O)c2ccc(c(c2o1)CN1CCCC1)OC)c1ccc(F)cc1</chem>	-9.7
440195	<chem>c1(ccc2C(=O)C[C@H](Oc2c1)c1ccccc1)O[C@@H]1O[C@H]([C@H]([C@@H]([C@H]1O)O)O)CO</chem>	-9.7
44259047	<chem>c1(c(cc2c(c(=O)c(c(o2)c2ccc(cc2)O)O)c1O)O)CCC(C)(C)O</chem>	-9.7
480763	<chem>O1c2cc(c(c(c2C(=O)C[C@@H]1c1ccccc1)O)CC=C(C)C)O</chem>	-9.7
49700	<chem>c1(c(ccc2c(=O)c(C)c(oc12)c1ccccc1)OC)CN1CCOCC1</chem>	-9.7
49788613	<chem>o1c(c(c(=O)c2c(cc(c(c12)OC)OCC=C(C)C)O)O)c1ccc2c(OCO2)c1</chem>	-9.7

629905	<chem>c1(ccc(c(c1)OCc1ccccc1)OC)c1oc2cc(ccc2c(=O)c1OC)OC</chem>	-9.7
74333987	<chem>O1c2cc(c(c(c2C(=O)[C@H]([C@H]1c1cc(c(c(c1)OC)O)O)O)O)CC=C(C)C)O</chem>	-9.7
10094174 7	<chem>O1c2cc(c(c(c2C(=O)C[C@H]1c1ccc(cc1)O)O)c1ccccc1)O</chem>	-9.6
11222065	<chem>o1c2ccccc2c(=O)c(c1c1ccccc1)[C@@H](c1ccc(cc1)OC)O</chem>	-9.6
12983453 9	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(cc1)O)OC)OCc1ccccc1</chem>	-9.6
14502737	<chem>O1c2cc(c3c(=O)c(coc3c2C=CC1(C)C)c1ccc2c(OCO2)c1)O</chem>	-9.6
15491286	<chem>o1c(c(c(=O)c2c(c(c(c12)O)OC)CC=C(C)C)O)c1ccc(c(c1)OC)O</chem>	-9.6
399491	<chem>o1c(cc(=O)c2c(c(c(cc12)O)CC=C(C)C)O)c1ccc(cc1O)O</chem>	-9.6
44342639	<chem>c1(c(cc(c2c(=O)cc(oc12)c1ccccc1)O)OC)C(F)(F)F</chem>	-9.6
69941512	<chem>c1(ccc2c(c(=O)cc(o2)c2ccccc2)c1)OCC[C@@H]1OC(=O)C(=C1O)O</chem>	-9.6
90300755	<chem>o1c(c(c(=O)c2cccc(c12)CC=C(C)C)O)c1ccccc1</chem>	-9.6
907980	<chem>o1c(C)c(c(=O)c2ccc(cc12)OCc1ccccc1)c1ccccc1</chem>	-9.6
9948081	<chem>c1(ccc2c(=O)cc(oc2c1)c1ccccc1)OC[C@H]1OC1</chem>	-9.6
10091405 2	<chem>c1(ccc(cc1)c1c(c(=O)c2ccccc2o1)O)N1CCOCCOCCOCCOCC1</chem>	-9.5
10149923 5	<chem>c1(cc(c(c(c1)OC)O[C@@H](CO)[C@@H](c1ccc(cc1)O)O)OC)[C@H]1Oc2cc(cc(c2C(=O)C1)O)O</chem>	-9.5
10206691 8	<chem>o1c(c(c(=O)c2c(c(c(cc12)OCc1ccccc1)OC)O)O)c1ccccc1</chem>	-9.5
10220349 6	<chem>o1c(cc(=O)c2c(cc(cc12)OCOC)OCOC)c1ccc(cc1)OCc1ccccc1</chem>	-9.5
10524567	<chem>O1c2cc3c(C(=O)C[C@@H](O3)c3ccc4c(CCC(C)(C)O4)c3)cc2CCC1(C)C</chem>	-9.5
11639597	<chem>c1(ccc2c(=O)cc(oc2c1)c1ccc(c(c1)O)O)OC[C@H](O)CNC(C)C</chem>	-9.5
11725803	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1cc(c(c(c1)CC=C(C)C)O)O)O)O</chem>	-9.5
12982116	<chem>c1(c(cc2c(C(=O)C[C@@H](O2)c2ccccc2)c1O)OC)C[C@H]1OC1(C)C</chem>	-9.5

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12983451 7	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(cc1)OC(=O)C)OC)OCc1cccc1</chem>	-9.5
15485967	<chem>O1c2cc(c(c(c2C(=O)C[C@H]1c1ccc(cc1)O)O)CC=C(C)C)OC</chem>	-9.5
29920547	<chem>o1c(cc(=O)c2c(C)cc(cc12)OC(=O)OCC)c1cccc1</chem>	-9.5
42608102	<chem>O1c2c3ccoc3c(c(c2C(=O)C[C@H]1c1ccc2c(OCO2)c1)O)OC</chem>	-9.5
467492	<chem>o1c(cc(=O)c2c(cc(cc12)OC(=O)C)OC(=O)C)c1cccc1</chem>	-9.5
46850208	<chem>c1(c(cc2c(c(=O)cc(o2)c2ccc(c(c2)OC)O)c1O)O)C/C=C(\C)/CC[C@@H](C(C)(C)O)O</chem>	-9.5
5316782	<chem>O1c2cc(c3C(=O)C[C@H](Oc3c2C[C@H]1C(C)(C)O)c1ccc(cc1)O)O</chem>	-9.5
56649091	<chem>c1(c(c(c2c(=O)cc(oc2c1)c1cccc1)O)O)OCCN1CCCCC1</chem>	-9.5
8395	<chem>o1c(cc(=O)c2ccc(cc12)OCC(=O)OCC)c1cccc1</chem>	-9.5
10193866 9	<chem>c1(ccc(cc1)c1c(c(=O)c2cccc2o1)O)N1OCCOCCOCCOCCOC1</chem>	-9.4
10449654	<chem>O1c2cc3c(c(=O)cc(o3)c3ccc(cc3)O)c(c2C=CC1(C)C)O</chem>	-9.4
10472357	<chem>o1c(cc(=O)c2c(c(c(cc12)O)NCCC(C)C)O)c1cccc1</chem>	-9.4
10814209	<chem>c1(c(cc2c(c(=O)c(c(o2)c2ccc(cc2)OC)O)c1O)O)OS(O)(O)c1ccc(C)cc1</chem>	-9.4
11552747	<chem>c1(ccc2c(=O)cc(oc2c1)c1cc(cc(c1)O)O)OC[C@H](O)CNC(C)C</chem>	-9.4
11661570	<chem>c1(ccc2c(=O)cc(oc2c1)c1cc(cc(c1)OC)OC)OC[C@H](O)CNC(C)C</chem>	-9.4
11954210	<chem>c1(ccc2c(=O)c(c(oc2c1)c1cccc1)O)O[C@@H]1O[C@H]([C@H]([C@@H]([C@H]1O)O)O)CO</chem>	-9.4
12918915	<chem>c1(ccc2c(=O)c(coc2c1)c1cccc1)O[C@@H](c1cccc1)CCNC</chem>	-9.4
129224	<chem>c1(ccc2c(=O)cc(oc2c1)c1ccc(C)cc1)OC[C@@H](O)CNC(C)C</chem>	-9.4
12982676 9	<chem>S=C1c2cccc2O[C@@H](C1)c1ccc(C)cc1</chem>	-9.4
14445197	<chem>c1(c(cc2c(c(=O)cc(o2)c2ccc(c(c2)O)OC)c1O)O)[C@@H]1O[C@H](C)[C@@H]([C@@H](C1)O)O</chem>	-9.4
14668157 4	<chem>o1c(c(c(=O)c2c(c3c(cc12)OCO3)O)OC(O)O)c1cccc1</chem>	-9.4

15118758	<chem>c1(ccc2c(=O)cc(oc2c1)c1ccccc1O)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO</chem>	-9.4
182342	<chem>O1c2ccc3c(=O)c(coc3c2C=CC1(C)C)c1ccc2c(OCO2)c1</chem>	-9.4
19358579	<chem>o1c(cc(=O)c2c(cc(cc12)OCc1ccccc1)OC)c1ccc(c(c1)OC)OC</chem>	-9.4
20301090	<chem>O1c2ccccc2C(=O)C(=C)[C@H]1c1ccc(cc1)N(=O)=O</chem>	-9.4
42607867	<chem>c1(cc(c2C(=O)C[C@H](Oc2c1)c1ccccc1)O)OC[C@H]1OC1(C)C</chem>	-9.4
42608112	<chem>O1c2c(c(c(c2C(=O)C[C@H]1c1ccccc1)O)Cc1cc(ccc1O)OC)OC)OC</chem>	-9.4
44258305	<chem>c1(cc(c2c(=O)cc(oc2c1)c1ccc(cc1)O)OC)OC[C@H]1OC1(C)C</chem>	-9.4
44258732	<chem>o1c(c(c(=O)c2c(c(C)c(c(C)c12)OC)O)O)c1ccccc1</chem>	-9.4
44259050	<chem>O1c2cc3c(c(=O)c(c(o3)c3ccc(cc3)O)O)c(c2C=CC1(C)C)O</chem>	-9.4
491718	<chem>O1c2c(C)c(c(c2C(=O)C[C@H]1c1ccc(cc1)O)O)CC=C(C)C)O</chem>	-9.4
5317480	<chem>o1cc(c(=O)c2c(cc(c(c12)CC=C(C)C)O)O)c1ccc(cc1)O</chem>	-9.4
5318267	<chem>c1(ccc2c(=O)c(coc2c1)c1ccc(c(c1)O)OC)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO</chem>	-9.4
53982668	<chem>O1c2ccccc2C(=O)/C(=C\NCC2ccc(cc2)C(=O)O)/[C@H]1c1ccccc1</chem>	-9.4
54410	<chem>c1(ccc2c(=O)cc(oc2c1)c1ccccc1)OC[C@H](O)CNCCC</chem>	-9.4
56649090	<chem>c1(c(c(c2c(=O)cc(oc2c1)c1ccccc1)O)O)OCCN1CCOCC1</chem>	-9.4
10149923 4	<chem>c1(cc(c(c(c1)OC)O[C@H](CO)[C@H](c1ccc(cc1)O)O)OC)[C@H]1Oc2cc(cc(c2C(=O)C1)O)O</chem>	-9.3
10168070 5	<chem>c1(ccc2c(=O)cc(oc2c1)c1ccccc1)C(=O)CBr</chem>	-9.3
10257793 2	<chem>c1(cc(c2c(=O)cc(oc2c1)c1ccc(cc1)O)O)OS(C)(O)O</chem>	-9.3
11077963	<chem>o1c2ccccc2c(=O)c(c1c1ccccc1)[C@@H](c1ccccc1)O</chem>	-9.3
11132477	<chem>o1c2ccccc2c(=O)c(c1c1ccccc1)[C@@H](c1ccc(cc1)N(=O)=O)O</chem>	-9.3
11611332	<chem>c1(ccc2c(=O)cc(oc2c1)c1ccc(c(c1)OC)OC)OC[C@H](O)CNC(C)C</chem>	-9.3
11618226	<chem>c1(ccc2c(=O)cc(oc2c1)c1ccc(c(c1)O)O)OC[C@H](O)CNC(C)(C)C</chem>	-9.3
11718263	<chem>c1(ccc2c(c(=O)cc(o2)c2ccc(c(c2)O)O)c1)OC[C@H](O)CNC(C)(C)C</chem>	-9.3

11912	<chem>c1(ccc2c(=O)cc(oc2c1)c1ccccc1)OCCCN(C)C</chem>	-9.3
12973022 2	<chem>o1c(cc(=O)c2cc(C)cc(c12)C(=O)CC)c1ccccc1</chem>	-9.3
12982170 5	<chem>o1c(c(C)c(=O)c2cc(c(c12)N(C)C)O)O)c1ccc(cc1)O</chem>	-9.3
12982447 9	<chem>O1C2=CC=CCC2=C(C=C1C1=CCC(=CC1)C=O)NO</chem>	-9.3
12982594 3	<chem>o1c2cc(cc(c2c(=O)cc1c1ccccc1C(=O)CCCC)O)OC</chem>	-9.3
13432335	<chem>o1c(cc(=O)c2c(C)cc(C)cc12)c1ccccc1</chem>	-9.3
14033984	<chem>O1c2c(cc3c(=O)c(c(oc3c2C=CC1(C)C)c1ccccc1)OC)OC</chem>	-9.3
15469991 9	<chem>O([C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)C(=O)O)c1ccc(cc1)c1cc(=O)c2ccccc2o1</chem>	-9.3
16737249	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc2c(C=CC(C)(C)O2)c1)O)O</chem>	-9.3
21325016	<chem>c1(cc(=O)c2cc(ccc2o1)C(=O)O)c1c(cccc1)OC[C@@H](CC)O</chem>	-9.3
2361	<chem>o1c(cc(=O)c2c3ccccc3ccc12)c1ccccc1</chem>	-9.3
23991884	<chem>o1c(C)c(c(=O)c2c(cc(cc12)OCc1ccc(o1)C(=O)O)O)c1ccccc1</chem>	-9.3
44258526	<chem>o1c(cc(=O)c2c3c(c(cc12)OC)OCO3)c1ccc2c(OCO2)c1</chem>	-9.3
44578052	<chem>o1c(cc(=O)c2c(c(c(c12)CN1CCCCC1)O)O)O)c1ccccc1</chem>	-9.3
53904139	<chem>c1(cccc(c1)c1cc(=O)c2ccccc2o1)S(=O)(=O)N</chem>	-9.3
5393156	<chem>o1c(cc(=O)c2c(C)cc(cc12)O)c1ccccc1</chem>	-9.3
66728267	<chem>c1(c(ccc(c1)c1coc2cc(cc(c2c1=O)O)O)O)CCC(C)(C)O</chem>	-9.3
10149923 6	<chem>c1(c(cc(cc1OC)c1cc(=O)c2c(cc(cc2o1)O)O)OC)O[C@H](CO)[C@@H](c1ccc(cc1)O)O</chem>	-9.2
10151666 5	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(cc1)OC(=O)C)O)OCC=C(C)C</chem>	-9.2
10184348 6	<chem>c1(ccc2c(C(=O)C[C@H](O2)c2ccccc2)c1)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)OC)CO</chem>	-9.2

10543665	<chem>c1(cc(=O)c2c(cccc2o1)OC)c1cccc(c1)C(F)(F)F</chem>	-9.2
10970624	<chem>O1c2c(c3c(C=CC(C)(C)O3)c(c2C(=O)C[C@H]1c1ccc(cc1)O)O)CO</chem>	-9.2
11149874	<chem>O1c2ccccc2C(=O)C[C@H]1c1ccc(cc1)N(=O)=O</chem>	-9.2
11545770	<chem>c1(ccc2c(=O)cc(oc2c1)c1cc(cc(c1)O)O)OC[C@H](O)CNC(C)(C)C</chem>	-9.2
11683340	<chem>c1(ccc2c(=O)cc(oc2c1)c1cc(cc(c1)OC)OC)OC[C@H](O)CNC(C)(C)C</chem>	-9.2
11847316	<chem>o1c2ccccc2c(=O)c(c1c1ccccc1)Cn1cncc1</chem>	-9.2
12984781 7	<chem>o1c(cc(=O)c2c(c(c(cc12)O)CCC(=C)C)O)c1ccc(cc1O)O</chem>	-9.2
14033976	<chem>O1c2cc(c3c(=O)cc(oc3c2C=CC1(C)C)c1ccc2c(OCO2)c1)OC</chem>	-9.2
15308126	<chem>c1(c(c(cc2oc(c(c(=O)c12)O)c1ccc(cc1)OC)OC)O)OS(O)(O)c1ccc(C)cc1</chem>	-9.2
15389725	<chem>c1(cc(=O)c2ccccc2o1)c1cccc(c1)S(=O)(=O)Cl</chem>	-9.2
15731439	<chem>o1c(cc(=O)c2ccc(c(c12)OC(=O)C)OC(=O)C)c1ccccc1</chem>	-9.2
24133364	<chem>o1c(C)c(c(=O)c2ccc(cc12)OCc1ccc(o1)C(=O)O)c1ccccc1</chem>	-9.2
3033107	<chem>c1(ccc(cc1)c1c(C)c(=O)c2ccccc2o1)OC[C@@H](O)CNC(C)(C)C</chem>	-9.2
41451	<chem>c1(ccc(cc1)c1c(C)c(=O)c2ccccc2o1)OC[C@@H](O)CNC(C)C</chem>	-9.2
42608049	<chem>O1c2cc(c3C(=O)C[C@H](Oc3c2CCC1(C)C)c1ccc(cc1O)O)O</chem>	-9.2
440215	<chem>c1(ccc2c(=O)c(coc2c1)c1ccccc1)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO</chem>	-9.2
44258693	<chem>O1c2c(cc3c(=O)c(c(oc3c2C=CC1(C)C)c1ccc(cc1)O)OC)OC</chem>	-9.2
44259326	<chem>O1c2cc(c3c(=O)c(c(oc3c2[C@@H](C)CC1(C)C)c1ccc(c(c1)O)O)O)O</chem>	-9.2
466268	<chem>o1c(cc(=O)c2ccc(cc12)OC)c1ccccc1</chem>	-9.2
46881227	<chem>c1(cc(c2C(=O)C[C@H](Oc2c1)c1ccccc1)O)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO</chem>	-9.2
49788612	<chem>o1c2cc(cc(c2c(=O)c(c1c1ccc2c(OCO2)c1)O)O)OC</chem>	-9.2
5272796	<chem>o1c2ccccc2c(=O)cc1c1ccc(cc1)C(=O)O</chem>	-9.2
5317478	<chem>o1cc(c(=O)c2c(c(c(cc12)O)CC=C(C)C)O)c1ccc(cc1)OC</chem>	-9.2
5317765	<chem>c1(c(c(=O)c2c(cc(cc2o1)O)O)O)c1ccc2OC([C@@H](Cc2c1)O)(C)C</chem>	-9.2
5378307	<chem>o1c(cc(=O)c2c3cc(ccc3ccc12)O)c1ccccc1</chem>	-9.2

564150	<chem>o1c(c(c(=O)c2ccc(cc12)OCc1cccc1)OC)c1ccc(c(c1)OC)OC</chem>	-9.2
625630	<chem>o1c(cc(=O)c2c3cccc3cc(c12)O)c1cccc1</chem>	-9.2
625631	<chem>o1c(cc(=O)c2c3ccc(cc3ccc12)O)c1cccc1</chem>	-9.2
66561376	<chem>o1c(c(c(=O)c2c(c3c(c(c12)OC)OCO3)O)OC)c1ccc2c(OCO2)c1</chem>	-9.2
676295	<chem>o1c2cccc2c(=O)c(c1c1cccc(c1)O)O</chem>	-9.2
74819425	<chem>O1c2cc3c(c(c2C(=O)C[C@H]1c1cccc1O)O)OCO3</chem>	-9.2
76333661	<chem>O(c1ccc2c(=O)cc(oc2c1)c1cccc1)[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CC(=O)C</chem>	-9.2
88881	<chem>o1c(cc(=O)c2c(cc(cc12)OC)OC)c1cccc1</chem>	-9.2
9883305	<chem>o1c(c(c(=O)c2c(c3c(cc12)OCO3)O)O)c1ccc(cc1)O</chem>	-9.2
100633	<chem>o1c(c(c(=O)c2ccc3c(cco3)c12)OC)c1cccc1</chem>	-9.1
10102840 2	<chem>o1c(cc(=O)c2c(c(c(cc12)O)NCC(C)C)O)c1cccc1</chem>	-9.1
10123824 1	<chem>c1(cc2c(c(=O)c(co2)c2ccc(cc2)O)cc1C(=O)C)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO</chem>	-9.1
10184348 4	<chem>c1(cccc2oc(cc(=O)c12)c1ccc(cc1)O)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)OC)CO</chem>	-9.1
10201716 5	<chem>o1c(cc(=O)c2c(cc(c(c12)CCC(=C)C)O)O)c1cccc1</chem>	-9.1
10206428 8	<chem>o1c(cc(=O)c2cccc(c12)/C=C/C)c1cccc1</chem>	-9.1
10209126 7	<chem>O1c2cccc2[C@H](C[C@H]1c1cccc1)NOC(=O)C</chem>	-9.1
10236976 3	<chem>O1c2ccc3CC[C@H](Oc3c2C[C@@H]1C(C)(C)O)c1ccc(cc1)O</chem>	-9.1
10337211	<chem>O1c2cc(c(cc2C(=O)C[C@H]1c1ccc(cc1)O)CC=C(C)C)OC</chem>	-9.1
10546844	<chem>c1(coc2cc(cc(c2c1=O)OC)O)c1cc(c2OC(C=Cc2c1)(C)C)O</chem>	-9.1
10708855	<chem>c1(cc(=O)c2cccc2o1)c1cccc(c1)CN=C=S</chem>	-9.1

11583077	<chem>c1(ccc2c(=O)cc(oc2c1)c1cc(c(c(c1)OC)OC)OC)OC[C@@H](O)CNC(C)C</chem>	-9.1
11612258	<chem>c1(ccc2c(=O)cc(oc2c1)c1cc(c(c(c1)OC)OC)OC)OC[C@@H](O)CNC(C)(C)C</chem>	-9.1
11834	<chem>c1(ccc2c(=O)cc(oc2c1)c1cccc1)OC[C@@H](C)CN(C)C</chem>	-9.1
12043065	<chem>c1(cc(=O)c2c(cc(c(c2o1)[C@@H]1CN(C)CC[C@@H]1O)O)O)c1c(Cl)cccc1</chem>	-9.1
12043069	<chem>c1(cc(=O)c2c(cc(c(c2o1)c1cnenc1)O)O)c1c(Cl)cccc1</chem>	-9.1
12146121	<chem>o1c(cc(=O)c2c(cc(cc12)OCOC)OCC=C(C)C)c1cccc1</chem>	-9.1
122835	<chem>O1c2cc(c(cc2C(=O)C[C@H]1c1ccc(cc1)O)CC=C(C)C)OC</chem>	-9.1
12968466 8	<chem>o1c(c(c(=O)c2c(c(c(c12)O)O)/C=C/C(=C)C)O)O)c1cccc1</chem>	-9.1
12970411 8	<chem>o1c(cc(=O)c2c(cc(cc12)OCO)OCO)c1cccc1</chem>	-9.1
12971614 9	<chem>c1(c(cc2c(c(=O)c(co2)c2ccc(cc2)O)c1O)O)[C@H]([C@@H]1OC1)CC=C(C)C</chem>	-9.1
12982075 5	<chem>c1(ccc2c(c(=O)c(c(o2)c2cccc2)O)c1)[C@@H](O)CCCC</chem>	-9.1
12988148 7	<chem>o1c2ccc(cc2c(=O)cc1c1cccc1C(=O)O)C(=O)O</chem>	-9.1
13253349 0	<chem>o1cc(c(=O)c2c(c(c(cc12)O)C[C@@H](C(=C)C)O)O)c1ccc2c(OCO2)c1</chem>	-9.1
13512149 8	<chem>c1(c(c(=O)c2c(cccc2o1)O)O)c1cc(c2c(c1)C2)OC</chem>	-9.1
13602334 3	<chem>c1(cc(=O)c2c(cc(c(c2o1)c1cncc1)O)O)c1c(Cl)cccc1</chem>	-9.1
14187087	<chem>O1c2cc3c(C=CC(C)(C)O3)c(c2C(=O)C[C@H]1c1ccc(cc1)O)O</chem>	-9.1
14237660	<chem>c1(coc2cc(cc(c2c1=O)O)O)c1ccc2OC(C=Cc2c1)(C)C</chem>	-9.1
14570642 7	<chem>O1c2cccc2C(=O)C[C@H]1c1cc(cc(c1)OC)O</chem>	-9.1
15160702	<chem>O1c2c(ccc3OC(C)(C)C=Cc23)C(=O)C[C@H]1c1ccc(c(c1)OC)OC</chem>	-9.1

1889	<chem>O1c2cc(ccc2C(=O)C[C@H]1c1ccc(cc1)O)O</chem>	-9.1
1890	<chem>O1c2cc(ccc2C(=O)C[C@H]1c1ccccc1)O</chem>	-9.1
21673114	<chem>o1c(cc(=O)c2c(cc(cc12)OCOC)O)c1ccccc1</chem>	-9.1
23286063	<chem>o1c(c(c(=O)c2cc(ccc12)C(=O)O)O)c1ccccc1</chem>	-9.1
238782	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccccc1)O)O</chem>	-9.1
25030431	<chem>o1c(c(c(=O)c2cc(ccc12)NC(=O)CCC(=O)O)O)c1ccc(c(c1)O)O</chem>	-9.1
25128870	<chem>o1c(cc(=O)c2c(cc(cc12)OCC1=NNNN1)OC)c1ccc(c(c1)OC)OC</chem>	-9.1
42607869	<chem>O1c2c(c(cc(c2C(=O)C[C@H]1c1ccccc1)O)O)C/C=C(\C)/CO</chem>	-9.1
42607870	<chem>O1c2c(c(cc(c2C(=O)C[C@H]1c1ccccc1)O)O)C/C=C(\C)/C=O</chem>	-9.1
42607962	<chem>O1c2c(c(cc3OC(C)(C)C=Cc23)O)C(=O)C[C@H]1c1ccc(cc1)OC</chem>	-9.1
44481784	<chem>o1cc(c(=O)c2c(cc(cc12)OC)O)c1ccc(c(c1)C[C@@H](C(=C)C)O)O</chem>	-9.1
5317300	<chem>c1(ccc(c(c1O)CC=C(C)C)O)c1coc2c(c1=O)ccc(c2)O</chem>	-9.1
5494866	<chem>o1cc(c(=O)c2c(cc(cc12)O)O)c1ccc(c(c1)CC=C(C)C)O</chem>	-9.1
58089059	<chem>o1c(c(c(=O)c2cc(ccc12)NC(=O)CCC(=O)O)O)c1ccc(cc1)O</chem>	-9.1
636525	<chem>O1c2c(c(cc3OC(C)(C)C=Cc23)O)C(=O)C[C@H]1c1ccc(c(c1)O)OC</chem>	-9.1
637111	<chem>O1c2c(c(c3C=CC(C)(C)Oc3c2CC=C(C)C)O)C(=O)[C@@H]([C@H]1c1ccccc1O)O</chem>	-9.1
6450959	<chem>o1cc(c(=O)c2c(cc(c(c12)C/C=C(\C)/CO)O)O)c1ccc(cc1)O</chem>	-9.1
676290	<chem>o1c2ccccc2c(=O)cc1c1ccc(cc1O)O</chem>	-9.1
688857	<chem>O1c2cc(ccc2C(=O)C[C@H]1c1ccccc1)O</chem>	-9.1
86083806	<chem>O1C2=C(CC=CC2)C=C/C/1=C\1/C=CC(=CC1)NC(=O)C</chem>	-9.1
10094338 2	<chem>Clc1cc(cc(c1OC)S(=O)(=O)NC(C)C)c1cc(=O)c2ccccc2o1</chem>	-9.0
10102840 4	<chem>o1c(cc(=O)c2c(cc(c(c12)NC(C)C)O)O)c1ccccc1</chem>	-9.0
10121493 9	<chem>c1(ccc(cc1)c1c(c(=O)c2ccccc2o1)O)N1CCN(CC1)[C@@H]1C(=CNC=C1)S(O)(O)O</chem>	-9.0

10335613	<chem>o1c(cc(=O)c2c(c(c(cc12)O)NC(C)C)O)c1ccccc1</chem>	-9.0
10357090	<chem>c1(cccc2c(=O)c(coc12)c1ccccc1)OC[C@H]1OC1</chem>	-9.0
10450773	<chem>o1c(cc(=O)c2c(c(c(cc12)O)/C=C/C(C)C)O)c1ccc(cc1O)O</chem>	-9.0
10659060	<chem>o1c2ccccc2c(=O)cc1c1cccc(c1)CC#N</chem>	-9.0
10736576	<chem>O1c2cc3c(c(=O)c(co3)c3ccc(cc3)O)c(c2C=CC1(C)C)OC</chem>	-9.0
10761522	<chem>[C@H]1(CC(=O)c2c(cc(cc2O1)O)O)c1cc(c2OC(C=Cc2c1)(C)C)OC</chem>	-9.0
11142360	<chem>o1cc(c(=O)c2CC3=C(Cc12)OCO3)c1cc(c2c(OCO2)c1)OC</chem>	-9.0
11177340	<chem>o1c(cc(=O)c2c(cc(cc12)OCOCCOC)OCC=C(C)C)c1ccccc1</chem>	-9.0
11186717	<chem>O1c2c(cc(cc2C=CC1(C)C)c1coc2cc(ccc2c1=O)O)O</chem>	-9.0
11742974	<chem>c1(c2c(C=CC(C)(C)O2)c(c2C(=O)C[C@H](Oc12)c1ccc(cc1)O)O)C[C@H]1OC1(C)C</chem>	-9.0
11810763	<chem>o1cc(c(=O)c2c(c3c(cc12)OCO3)OC)c1cc(c2c(OCO2)c1)OC</chem>	-9.0
118907	<chem>o1c(cc(=O)c2c(cc(cc12)OCC(=O)OCC)OCC(=O)OCC)c1ccccc1</chem>	-9.0
12988126 9	<chem>o1c2ccc(cc2c(=O)c(c1c1ccc2c(OCO2)c1)O)C(=O)O</chem>	-9.0
13393782	<chem>[C@H]1(CC(=O)c2ccccc2O1)c1cccc(F)c1</chem>	-9.0
13908069 7	<chem>o1c(c(c(=O)c2c(cc(cc12)OCC=C(C)C)O)O)c1ccc(c(c1)O)OC</chem>	-9.0
15160703	<chem>O1c2c(cc(c3OC(C)(C)C=Cc23)OC)C(=O)C[C@H]1c1ccc(c(c1)OC)OC</chem>	-9.0
242065	<chem>[C@H]1(CC(=O)c2ccccc2O1)c1ccc(Cl)cc1</chem>	-9.0
24960482	<chem>c1(ccc2c(=O)cc(oc2c1)c1cc(cc(c1)O)O)OC[C@@H](O)CNC(C)C</chem>	-9.0
3070240	<chem>c1(c(C)c(=O)c2ccc(c(c2o1)CN(C)C)OC)c1ccc(F)cc1</chem>	-9.0
44380969	<chem>o1c(cc(=O)c2c(cc(c(c12)NCCC(C)C)O)O)c1ccccc1</chem>	-9.0
44584124	<chem>O1c2cc3c(C=CC(C)(C)O3)c(c2C(=O)C[C@H]1c1ccccc1O)O</chem>	-9.0
462691	<chem>O1c2c(cccc2C(=O)C[C@H]1c1ccccc1)CC(=O)O</chem>	-9.0
466277	<chem>Br1ccc2c(=O)cc(oc2c1)c1ccccc1</chem>	-9.0
5270553	<chem>O1c2ccc(cc2C(=O)C[C@H]1c1ccccc1)C(=O)O</chem>	-9.0

5271991	<chem>o1c(cc(=O)c2c(cc(c(c12)OC)O)O)c1c(ccc(c1OC)O)O</chem>	-9.0
5281611	<chem>o1c2cc(ccc2c(=O)c(c1c1ccc(cc1)O)O)O</chem>	-9.0
5281617	<chem>o1c(cc(=O)c2c(cc(cc12)OC)O)c1ccc(cc1)O</chem>	-9.0
5281894	<chem>o1c(cc(=O)c2ccc(cc12)O)c1ccccc1</chem>	-9.0
5282073	<chem>o1c(cc(=O)c2ccc(cc12)O)c1ccc(cc1)O</chem>	-9.0
5320053	<chem>o1cc(c(=O)c2ccc(cc12)O)c1ccc(c(c1)CC=C(C)C)O</chem>	-9.0
53747690	<chem>c1(cc(c2c(=O)cc(oc2c1)c1ccccc1)O)C(=O)CBr</chem>	-9.0
57340186	<chem>o1c2cc(ccc2c(=O)cc1c1ccc(cc1)/C=C/C(=O)OCC)O</chem>	-9.0
624794	<chem>o1c2ccccc2c(=O)c(c1c1ccc2c(OCO2)c1)O</chem>	-9.0
637879	<chem>o1cc(c(=O)c2c(c3c(cc12)OCO3)OC)c1ccc2c(OCO2)c1</chem>	-9.0
85751070	<chem>N(C1=C[C@H](Oc2ccccc12)c1ccccc1)NC(=S)N</chem>	-9.0
90753092	<chem>o1c(c(c(=O)c2c(C)c(C)c(C)cc12)O)c1ccccc1</chem>	-9.0
91557562	<chem>O1c2cc(ccc2C(=O)C[C@H]1c1ccc(cc1O)O)O</chem>	-9.0
95400994	<chem>O1c2ccc3ccccc3c2C(=O)C[C@H]1c1ccccc1</chem>	-9.0
9973510	<chem>o1c2ccc(cc2c(=O)cc1c1ccccc1OC(C)C)C(=O)O</chem>	-9.0
10184348 5	<chem>c1(ccc2c(C(=O)C[C@@H](O2)c2ccccc2)c1)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)OC)CO</chem>	-8.9
10197413 5	<chem>O1c2c(c(cc(c2Cc2c(=O)oc(c(C)c2O)CC)O)O)C(=O)C[C@H]1c1ccccc1</chem>	-8.9
10230725 5	<chem>c1(c(=O)c2ccccc2oc1c1ccccc1)C(F)(F)F</chem>	-8.9
10244935	<chem>o1c(cc(=O)c2c(c(c(cc12)O)NCCC)O)c1ccccc1</chem>	-8.9
102674	<chem>O1c2ccccc2[C@H](C[C@H]1c1ccccc1)NN</chem>	-8.9
10543327	<chem>c1(cc(=O)c2ccccc2o1)c1cccc(c1)CBr</chem>	-8.9
10680	<chem>o1c2ccccc2c(=O)cc1c1ccccc1</chem>	-8.9
10889522	<chem>O=C1c2ccccc2N[C@@H](C1)c1ccccc1</chem>	-8.9

11247278	<chem>O1c2c(c(cc(c2C(=O)C[C@H]1c1ccc(cc1)OC(=O)C)O)OC(=O)C)CC=C(C)C</chem>	-8.9
11289628	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1cc(cc(c1)O)O)O)OC</chem>	-8.9
11382659	<chem>c1(cc(c(c(c1)CC=C(C)C)OC)O)[C@H]1Oc2cc(ccc2C(=O)C1)O</chem>	-8.9
11772232	<chem>o1c(cc(=O)c2c(cc(cc12)OCOCCOC)O)c1cccc1</chem>	-8.9
12136839	<chem>O1c2ccccc2C(=O)C[C@@H]1c1cccc1</chem>	-8.9
12148792 9	<chem>O1c2ccccc2C(=O)C[C@@H]1c1cccc1</chem>	-8.9
12985834 1	<chem>O1c2c(c(ccc2C(=O)C([C@@]1(c1cccc1)O)(O)O)OC)OC</chem>	-8.9
13227966 3	<chem>o1cc(c(=O)c2c(c(c(cc12)O)OC)OC)c1cccc2OCOc12</chem>	-8.9
14791391	<chem>o1c2cc(ccc2c(=O)cc1c1ccc(cc1)N(=O)=O)O</chem>	-8.9
14791392	<chem>o1c2cc(ccc2c(=O)cc1c1ccc(cc1)N)O</chem>	-8.9
15342845	<chem>o1c(c(c(=O)c2c(cc(cc12)O)OC(=O)c1cccc1)OC)c1cccc1</chem>	-8.9
15389441	<chem>O1c2cc3c(c(=O)c(co3)c3cc(c(cc3OC)OC)OC)cc2C=CC1(C)C</chem>	-8.9
15817847	<chem>o1c2cc(c(cc2c(=O)c(c1c1ccc(c(c1)OC)O)O)O)O</chem>	-8.9
176925	<chem>O1c2ccccc2C(=O)C[C@H]1c1cccc1O</chem>	-8.9
188308	<chem>O1c2cc(c(c(c2C(=O)C[C@H]1c1ccc(cc1)O)O)O)O</chem>	-8.9
188424	<chem>O1c2cc(cc(c2C(=O)C[C@@H]1c1ccc(cc1)O)OC)O</chem>	-8.9
19835350	<chem>c1(cccc2c(=O)cc(oc12)c1cccc1)OC[C@@H]1OC1</chem>	-8.9
20399	<chem>O1c2cc(ccc2C(=O)[C@H]([C@@H]1c1cc(c(c(c1)O)O)O)O)O</chem>	-8.9
21315742	<chem>c1(cc(=O)c2cc(ccc2o1)C(=O)O)c1c(ccc(C)c1)OC(C)C</chem>	-8.9
23644933	<chem>o1c2cc(ccc2c(=O)c(c1n1cncc1)c1cccc1)OCc1cccc1</chem>	-8.9
23644934	<chem>o1c2cc(ccc2c(=O)c(c1n1cncc1)c1ccc(cc1)OC)OCc1cccc1</chem>	-8.9
23644952	<chem>c1(c(c(=O)c2ccc(cc2o1)OCc1cccn1)c1cccc1)SCc1cncc1</chem>	-8.9
250312	<chem>O1C(=CC(=C2CC=CC=C12)NO)c1cccc1</chem>	-8.9

25073757	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1cc(ccc1O)O)O)O</chem>	-8.9
3078	<chem>o1c(c(C)c(=O)c2ccc(c(c12)CN(C)C)OC)c1cccc1</chem>	-8.9
343080	<chem>o1cc(c(=O)c2ccc(cc12)OCC=C(C)C)c1cc2c(cc1OC)OCO2</chem>	-8.9
3534982	<chem>O1c2ccccc2C(=O)C[C@H]1c1cccc(c1)O</chem>	-8.9
369599	<chem>o1c(cc(=O)c2c(c(C)c(cc12)OC)O)c1cccc1</chem>	-8.9
42607959	<chem>c1(cc(c(c(c1)CC=C(C)C)OC)/C=C/C(C)(C)O)[C@H]1Oc2cc(cc(c2C(=O)C1)O)O</chem>	-8.9
439246	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(cc1)O)O)O</chem>	-8.9
44380895	<chem>o1c(cc(=O)c2c(cc(c(c12)NCC(C)C)O)O)c1cccc1</chem>	-8.9
45933941	<chem>o1c2ccccc2c(=O)cc1c1cc(cc(c1)O)O</chem>	-8.9
511789	<chem>O1c2c(c(ccc2C(=O)C[C@H]1c1ccc(cc1)O)OC)CC=C(C)C</chem>	-8.9
5270543	<chem>Fc1ccc2c(O[C@@H](CC2=O)c2ccccc2)c1</chem>	-8.9
5280863	<chem>o1c(c(c(=O)c2c(cc(cc12)O)O)O)c1ccc(cc1)O</chem>	-8.9
5281616	<chem>o1c(c(c(=O)c2c(cc(cc12)O)O)O)c1cccc1</chem>	-8.9
5281954	<chem>o1c(cc(=O)c2c(cc(cc12)OC)O)c1cccc1</chem>	-8.9
5317287	<chem>o1c(c(c(=O)c2c(c(c(cc12)OC)OC)O)O)c1ccc(c(c1)O)OC</chem>	-8.9
53247947	<chem>c1(ccc(cc1)[C@H]1CC(=O)c2ccccc2O1)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO</chem>	-8.9
5391140	<chem>o1c(cc(=O)c2ccc(cc12)O)c1cccc(c1)O</chem>	-8.9
5393152	<chem>o1c(c(c(=O)c2ccc(cc12)O)O)c1cccc1</chem>	-8.9
5465885	<chem>O1c2ccccc2[C@H](C[C@H]1c1cccc1)NN</chem>	-8.9
54721824	<chem>O1c2c(c(cc(c2Cc2c(=O)oc(c(C)c2O)CC)O)O)C(=O)C[C@H]1c1cccc1</chem>	-8.9
5491798	<chem>o1c(c(c(=O)c2c(cc(c(c12)OC)OC)O)O)c1cccc1</chem>	-8.9
6077518	<chem>O1c2ccccc2[C@H](C[C@H]1c1cccc1)NOCCN(CC)CC</chem>	-8.9
676310	<chem>o1c(cc(=O)c2ccc(c(c12)O)O)c1cccc(c1)O</chem>	-8.9
688659	<chem>o1c(c(c(=O)c2cc(ccc12)O)O)c1cccc1</chem>	-8.9
688861	<chem>O1c2ccccc2C(=O)C[C@H]1c1cccc(c1)O</chem>	-8.9

689010	O1c2ccccc2C(=O)C[C@@H]1c1ccccc1	-8.9
70696494	O1c2cc(cc(c2C(=O)C[C@H]1c1cc(cc(c1)O)O)O)OC	-8.9
71777365	O1c2ccccc2C(=O)C[C@@H]1c1ccccc1	-8.9
932	O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(cc1)O)O)O	-8.9
101028403	o1c(cc(=O)c2c(c(c(cc12)O)NCC=C)O)c1ccccc1	-8.8
101624373	O1c2cc(ccc2[C@H](C[C@@H]1c1ccccc1)O)OC	-8.8
101643010	O1c2c(c(cc(c2C(=O)[C@@H]([C@H]1c1ccc(cc1)O)O)O)O)CC=C(C)C	-8.8
101932121	c1(cc2c(c(=O)cc(o2)c2ccc(cc2)O)c(c1OC)O)O[C@@H]1O[C@H]([C@@H]([C@H]([C@H]1O)O)O)C	-8.8
102017163	o1c(c(c(=O)c2c(cc(c(c12)CCC(=C)C)O)O)O)c1ccccc1	-8.8
102154220	O1c2cc3c(c(=O)cc(o3)c3ccc(cc3)O)c(c2[C@@H](CC1(C)C)O)O	-8.8
10491973	o1c(cc(=O)c2c(cccc12)OCC)c1ccccc1	-8.8
10612616	o1c(cc(=O)c2c(cccc12)OCC=C)c1ccccc1	-8.8
10848398	o1c2cc(ccc2c(=O)cc1c1ccc(C)cc1)O	-8.8
12071400	c1(cc(cc2oc(c(c(=O)c12)O)c1ccc(c(c1)OC)OC)OC)OS(O)(O)c1ccc(C)cc1	-8.8
12109666	O1c2c(ccc3OC(C)(C)C=Cc23)C(=O)C[C@H]1c1ccc(cc1)OC	-8.8
122366411	c1(ccc(cc1)c1cc(=O)c2ccccc2o1)OS(O)(O)C(F)(F)F	-8.8
122383344	O1c2cc(c(cc2C(=O)C[C@H]1c1ccc(cc1)O)C[C@@H](C(=C)C)O)O	-8.8
12261178	o1c2ccccc2c(=O)cc1c1ccc(cc1)C=O	-8.8
12813780	O1c2ccccc2C(=O)C[C@H]1c1cccc(C)c1	-8.8
12813783	o1c2ccccc2c(=O)cc1c1cccc(C)c1	-8.8

129633578	<chem>o1c(c(c(=O)c2ccc(c(c12)OC)OC)O)c1ccc(c(c1)OC)OC</chem>	-8.8
129813354	<chem>O1c2cc(ccc2C(=O)C[C@H]1c1cc(c(c(c1)O)O)O)OC</chem>	-8.8
129824490	<chem>O1C2=CC=CCC2=C(C=C1c1ccc(cc1)C=O)NOCC</chem>	-8.8
129834540	<chem>c1(c(cc2c(c(=O)cc(o2)c2ccc(C)cc2)c1O)O)S(O)(O)O</chem>	-8.8
132540297	<chem>o1c2cc(cc(c2c(=O)c(c1c1ccc(c(c1)OC(=O)C)OC(=O)C)O)O)O</chem>	-8.8
133611769	<chem>c1(ccc2c(=O)c(coc2c1)c1cc(cc(c1)OC)O)O[C@H]1O[C@H]([C@@H]([C@H]([C@H]1O)O)O)CO</chem>	-8.8
137327	<chem>o1c(cc(=O)c2cc(C)cc(c12)CC(=O)O)c1cccc1</chem>	-8.8
13908971	<chem>O1c2cc(c3c(=O)c(coc3c2C[C@H]1C(=C)C)c1ccc(cc1O)O)O</chem>	-8.8
13942547	<chem>o1c(c(c(=O)c2c(cc(c(c12)OC)OCC=C(C)C)OC)OC)c1ccc2c(OCO2)c1</chem>	-8.8
15939984	<chem>o1c2ccc(C)cc2c(=O)c(c1c1ccc2c(OCO2)c1)O</chem>	-8.8
161860	<chem>o1c2cccc2c(=O)cc1c1cccc1O</chem>	-8.8
165506	<chem>O1c2cccc2C(=O)C[C@H]1c1ccc(cc1)O</chem>	-8.8
19972541	<chem>o1c(c(C)c(=O)c2cccc(c12)C(=O)OCC)c1cccc1</chem>	-8.8
20522556	<chem>c1(c(c(=O)c2c(cc(cc2o1)OC)O)OC)c1ccc(c(c1)OC)OC(=O)C(C)(C)C</chem>	-8.8
229016	<chem>o1c2cccc2c(=O)cc1c1ccc(cc1)O</chem>	-8.8
3070241	<chem>c1(c(C)c(=O)c2ccc(c(c2o1)CN(CC)CC)OC)c1ccc(F)cc1</chem>	-8.8
343079	<chem>o1cc(c(=O)c2ccc3c(OCO3)c12)c1ccc2c(OCO2)c1</chem>	-8.8
41449	<chem>c1(ccc(cc1)c1cc(=O)c2cccc2o1)OC[C@@H](O)CNC(C)C</chem>	-8.8
41450	<chem>c1(ccc(cc1)c1cc(=O)c2cccc2o1)OC[C@@H](O)CNC(C)(C)C</chem>	-8.8
42607995	<chem>O1c2c(c(c(c2C[C@@H](C(=C)C)O)O)CC=C(C)C)O)C(=O)C[C@H]1c1ccc(c(c1)O)O</chem>	-8.8
44257318	<chem>o1cc(c(=O)c2c(cc(c(c12)C/C=C(\C)/CO)O)O)c1ccc(cc1O)O</chem>	-8.8

44380894	<chem>o1c(cc(=O)c2c(cc(c(c12)NCCC)O)O)c1cccc1</chem>	-8.8
44380950	<chem>o1c(cc(=O)c2c(cc(c(c12)NCC=C)O)O)c1cccc1</chem>	-8.8
462697	<chem>O1c2cc(cc(c2C(=O)[C@H]([C@H]1c1ccc(c(c1)OCc1cccc1)OC)OC)O)O</chem>	-8.8
5280362	<chem>c1(c(=O)c2c(cc(cc2oc1c1ccc(c(c1)O)O)O)O)OS(=O)(=O)O</chem>	-8.8
5280443	<chem>o1c(cc(=O)c2c(cc(cc12)O)O)c1ccc(cc1)O</chem>	-8.8
5281607	<chem>o1c(cc(=O)c2c(cc(cc12)O)O)c1cccc1</chem>	-8.8
5281691	<chem>o1c(c(c(=O)c2c(cc(cc12)OC)O)O)c1ccc(c(c1)O)O</chem>	-8.8
5281692	<chem>o1c2cc(ccc2c(=O)c(c1c1cc(c(c(c1)O)O)O)O)O</chem>	-8.8
5281814	<chem>o1cc(c(=O)c2c(c(c(cc12)O)CC=C(C)C)O)c1ccc(cc1)O</chem>	-8.8
5282154	<chem>o1c2cc(cc(c2c(=O)c(c1c1cc(c(c(c1)OC)O)O)O)O)O</chem>	-8.8
5315202	<chem>o1c(cc(=O)c2c(cc(cc12)O)OC)c1ccc(cc1)O</chem>	-8.8
5320287	<chem>o1c(c(c(=O)c2c(cc(cc12)OC)O)O)c1ccc(c(c1)O)OC</chem>	-8.8
5321435	<chem>o1c(c(c(=O)c2c(c(c(cc12)O)OC)O)O)c1ccc(c(c1)OC)O</chem>	-8.8
5326329	<chem>o1cc(c(=O)c2ccc(c(c12)CC=C(C)C)O)c1ccc(c(c1)O)OC</chem>	-8.8
5353357	<chem>o1c(cc(=O)c2cc(c(cc12)O)O)c1cccc1</chem>	-8.8
5356690	<chem>O1c2cccc2[C@H](C[C@H]1c1cccc1)NO</chem>	-8.8
5362017	<chem>o1c(c(c(=O)c2c(cc(c(c12)O)O)O)O)c1cccc1</chem>	-8.8
5378945	<chem>o1cc(c(=O)c2c(c(c(cc12)O)C/C=C(\C)/CO)O)c1ccc(cc1)O</chem>	-8.8
5490139	<chem>O1c2cc3c(c(=O)c(co3)c3ccc(cc3)O)c(c2C=CC1(C)C)O</chem>	-8.8
56649088	<chem>o1c(cc(=O)c2c(c(c(cc12)OCC=C)O)O)c1cccc1</chem>	-8.8
57340184	<chem>c1(cc(=O)c2ccc(cc2o1)O)c1ccc(F)cc1</chem>	-8.8
57368437	<chem>o1c(c(c(=O)c2cc(cc(c12)O)O)O)c1ccc(cc1)O</chem>	-8.8
602425	<chem>O1c2c(c(ccc2C(=O)[C@H]([C@@H]1c1ccc(c(c1)OC)OC)O)OC)OC</chem>	-8.8
6453535	<chem>o1c(c(c(=O)c2c(c(c(cc12)OC)OC)O)O)c1ccc(c(c1)OC)O</chem>	-8.8
676309	<chem>o1c(cc(=O)c2ccc(c(c12)O)O)c1cccc1O</chem>	-8.8

688859	<chem>O1c2ccccc2C(=O)C[C@H]1c1ccc(cc1)O</chem>	-8.8
71588424	<chem>O1C2=CC(=O)[C@H]3C(=O)C=C(O[C@H]3C2=C([C@H](C1(C)C)O)O)c1ccc(cc1)O</chem>	-8.8
71621984	<chem>c1(cc(c2c(=O)c(coc2c1)c1ccc(cc1)O)O)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)OC)CO</chem>	-8.8
71621987	<chem>c1(ccc2c(=O)c(coc2c1)c1ccc(cc1)O)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)OC)CO</chem>	-8.8
86236608	<chem>c1(ccc2c(=O)cc(oc2c1)c1cc(cc(c1)OC)OC)OC[C@@H]1OC1</chem>	-8.8
9950264	<chem>c1(c(cc2c(c(=O)cc(o2)c2ccccc2)c1O)O)OS(=O)(=O)O</chem>	-8.8
10094338 5	<chem>Clc1cc(cc(c1OC)S(=O)(=O)Cl)c1cc(=O)c2ccccc2o1</chem>	-8.7
10159128 0	<chem>c1(ccc2c(c(=O)cc(o2)c2ccc(c(c2)OC)O)c1OC)OCCCCC</chem>	-8.7
10168070 6	<chem>c1(c(ccc2c(=O)cc(oc12)c1ccccc1)C(=O)CBr)C(=O)CBr</chem>	-8.7
10189069 3	<chem>O1c2c(C)c(c(C)c(c2C(=O)C[C@H]1c1ccccc1)OC)O</chem>	-8.7
10193061 3	<chem>O1c2ccccc2C=C/C/1=C\1/CC=C(C=C1)NC(C)(C)C</chem>	-8.7
10251	<chem>O1c2ccccc2C(=O)C[C@H]1c1ccccc1</chem>	-8.7
10498462	<chem>O1c2cc(c(c(c2C(=O)C[C@H]1c1ccc(c(c1)O)O)O)C(C)(C)C=C)O</chem>	-8.7
10761665	<chem>O1c2cc(c(c(c2C(=O)C[C@H]1c1ccc(c(c1)OC)O)O)C(C)(C)C=C)O</chem>	-8.7
11032058	<chem>[C@@H]1(CC(=O)c2ccccc2O1)c1ccc(F)cc1</chem>	-8.7
11095	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(c(c1)O)O)O)O</chem>	-8.7
12049385	<chem>O1/C(=C\2/C=CC(=CC2)N(C)C)/C=Cc2ccc(cc12)N(CC)CC</chem>	-8.7
12114693	<chem>O1[C@@H](CC(=O)c2c(cc(c(c12)C(C)(C)C=C)O)O)c1ccc(cc1)O</chem>	-8.7
12132943	<chem>O1c2c(c(c(C)c(c2C(=O)C[C@H]1c1ccccc1)O)OC)C=O</chem>	-8.7
12310641	<chem>O1c2cc(ccc2C(=O)[C@H]([C@@H]1c1ccc(c(c1)O)O)O)O</chem>	-8.7
1232440	<chem>O1c2ccccc2CC[C@@H]1c1ccccc1</chem>	-8.7
12753173	<chem>[C@H]1(CC(=O)c2ccccc2O1)c1c(Cl)cc(cc1)Cl</chem>	-8.7

12968987 5	<chem>o1c(cc(=O)c2c(cccc12)OC(O)(O)O)c1ccccc1</chem>	-8.7
12976274 2	<chem>O1c2cc(cc(c2C(=O)C([C@@H]1c1ccc(cc1)OC)(O)O)O)OC</chem>	-8.7
12978776 5	<chem>O1C(=CC(=C2CC=CC=C12)NN)c1ccccc1</chem>	-8.7
12982445 6	<chem>O1[C@H](C=C(c2cc(ccc12)C=O)NO)c1ccccc1</chem>	-8.7
12983023 9	<chem>c1(cc(c(cc1c1c(c(=O)c2c(cc(cc2o1)O)O)O)O)O)S(=O)(=O)c1ccc(C)cc1</chem>	-8.7
12984791 0	<chem>O1c2cc(cc(c2[C@H](C(=O)[C@H]1c1cccc(c1)OC)O)O)O</chem>	-8.7
12986426 5	<chem>O1c2c(cccc2C(=O)C[C@@]1(c1ccccc1)O)OC</chem>	-8.7
13291608	<chem>o1c(c(c(=O)c2c(c(c(cc12)OC)OC)O)O)c1ccccc1</chem>	-8.7
13306495 3	<chem>o1c(c(c(=O)c2c(cccc12)CC#C)N)c1ccccc1</chem>	-8.7
13735036 9	<chem>c1(cccc2c(=O)c(coc12)c1ccccc1)[C@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO</chem>	-8.7
13958412 4	<chem>o1cc(c(=O)c2c(cc(cc12)OC)O)c1ccc(cc1)OCC=C(C)C</chem>	-8.7
14034288	<chem>O1c2c(c(cc(c2C(=O)C[C@H]1c1ccccc1O)O)OC)O</chem>	-8.7
14057034	<chem>O1c2cc(c3c(=O)c(coc3c2C=CC1(C)C)c1cc(c(cc1OC)O)OC)O</chem>	-8.7
14704648	<chem>o1c(c(c(=O)c2c(c3c(cc12)OCO3)OC)OC)c1cc(c2c(OCO2)c1)OC</chem>	-8.7
14730798	<chem>O1c2cc(ccc2C(=O)[C@H]([C@@H]1c1ccccc1)O)O</chem>	-8.7
1686	<chem>c1(cc(=O)c2ccccc2o1)c1ccc(Br)cc1</chem>	-8.7
177731	<chem>o1cc(c(=O)c2ccc(cc12)OCC=C(C)C)c1ccc(cc1)OC</chem>	-8.7
21325023	<chem>o1c2cc(ccc2c(=O)cc1c1ccccc1OC(C)C)C(=O)O</chem>	-8.7

21576252	<chem>o1cc(c(=O)c2c(cc(cc12)OCC=C(C)C)O)c1ccc(cc1O)O</chem>	-8.7
21636237	<chem>O1c2c(c(cc(c2C(=O)C[C@H]1c1cccc1OC)O)OC)OC</chem>	-8.7
2734580	<chem>O1c2ccc(cc2C(=O)C[C@H]1c1cccc1)O</chem>	-8.7
3070247	<chem>c1(c(C)c(=O)c2ccc(c(c2o1)CN1CCCC1)OC)c1ccc(Cl)cc1</chem>	-8.7
378567	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1cccc1)OC)OC</chem>	-8.7
3870517	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(cc1)OC(=O)C)O)OC(=O)C</chem>	-8.7
42607996	<chem>O1c2c(c(cc(c2C(=O)C[C@H]1c1ccc(c(c1)O)O)O)O)C/C=C(\C)/COC(=O)C</chem>	-8.7
439652	<chem>O1c2cccc2C(=O)C[C@H]1c1cccc1</chem>	-8.7
441251	<chem>o1cc(c(=O)c2c(c(c(cc12)OC)CC=C(C)C)O)c1ccc(cc1O)O</chem>	-8.7
44258533	<chem>o1c(cc(=O)c2c(c(c(cc12)OC)OC)OC)c1cc(c(c(c1)OC)OCC=C(C)C)OC</chem>	-8.7
44259869	<chem>o1c(c(c(=O)c2c(c(c(cc12)O)OC)O)O)c1ccc(c(c1)OC)OC</chem>	-8.7
50909808	<chem>o1cc(c(=O)c2c(cc(cc12)O)O)c1ccc2c(OCO2)c1</chem>	-8.7
5281606	<chem>c1(c(c(=O)c2c(cc(c(c2o1)OC)OC)O)OC)c1cccc(Cl)c1O</chem>	-8.7
5281654	<chem>o1c2cc(cc(c2c(=O)c(c1c1ccc(c(c1)OC)O)O)O)O</chem>	-8.7
5281697	<chem>o1c(cc(=O)c2c(c(c(cc12)O)O)O)c1ccc(cc1)O</chem>	-8.7
5281703	<chem>o1c(cc(=O)c2c(cc(c(c12)OC)O)O)c1cccc1</chem>	-8.7
5281789	<chem>o1cc(c(=O)c2c(cc(cc12)O)O)c1ccc(c(c1O)CC=C(C)C)O</chem>	-8.7
5317481	<chem>o1cc(c(=O)c2c(cc(c(c12)C/C=C(\C)/CO)O)O)c1ccc(c(c1)O)OC</chem>	-8.7
5317756	<chem>o1c(=O)c(cc2c(c(c(cc12)O)CC=C(C)C)OC)c1ccc(cc1O)O</chem>	-8.7
5320945	<chem>o1c(c(c(=O)c2c(cc(cc12)OC)O)O)c1ccc(c(c1)OC)O</chem>	-8.7
53247945	<chem>c1(ccc(cc1)[C@H]1CC(=O)c2cccc2O1)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)OC)CO</chem>	-8.7
53249095	<chem>O1c2cc3c(C=CC(C)(C)O3)c(c2C(=O)C[C@H]1c1ccc(cc1O)O)O</chem>	-8.7
5360930	<chem>o1c(c(c(=O)c2c(cc(c(c12)O)O)O)OC)c1cccc1</chem>	-8.7
5377945	<chem>o1c(c(c(=O)c2c(c(c(cc12)O)OC)O)O)c1ccc(cc1)O</chem>	-8.7
54073202	<chem>c1(cc(c2c(O[C@@H](CC2=O)c2ccc(c(c2)O)OC)c1)O)OCCBr</chem>	-8.7

5466136	<chem>o1c2cc(c(c2c(=O)c(c1c1ccc2c(OCO2)c1)OC)O)OC)OC</chem>	-8.7
5466137	<chem>o1c2cc(cc2c(=O)c(c1c1ccc2c(OCO2)c1)OC)O)OC</chem>	-8.7
5468257	<chem>O1c2ccccc2[C@H](C[C@H]1c1ccccc1)NN</chem>	-8.7
5481228	<chem>o1cc(c(=O)c2c(cc(cc12)O)O)c1c(cc(c(c1)CC=C(C)C)O)O</chem>	-8.7
5487855	<chem>o1c2cc(cc2c(=O)c(c1c1ccc(c(c1)OC)OC)O)O)O</chem>	-8.7
555407	<chem>o1c(nc(=O)c2ccccc12)c1ccccc1</chem>	-8.7
56658060	<chem>O1c2cc(cc2C(=O)[C@H]([C@@H]1c1ccc(c(c1)OC)O)O)O)O</chem>	-8.7
57340187	<chem>o1c2cc(ccc2c(=O)cc1c1ccc(cc1)/C=C/C(=O)O)O</chem>	-8.7
636496	<chem>O1c2cc3c(c(=O)c(co3)c3ccc(cc3O)OC)c(c2C=CC1(C)C)OC</chem>	-8.7
66783912	<chem>c1(cc(=O)c2c(c3c(cc2o1)OCO3)O)c1ccc(cc1)OCCN(CC)CC</chem>	-8.7
66783913	<chem>o1c(cc(=O)c2c(c3c(cc12)OCO3)O)C1=CCC(=CC1)OC</chem>	-8.7
676034	<chem>o1c2ccc(cc2c(=O)cc1c1ccccc1OC)O</chem>	-8.7
676289	<chem>o1c2ccccc2c(=O)cc1c1cccc(c1O)O</chem>	-8.7
688835	<chem>o1c2ccc(cc2c(=O)c(c1c1cccc(c1)OC)O)OC</chem>	-8.7
688836	<chem>o1c(c(c(=O)c2ccc(cc12)OC)O)c1cccc(c1)OC</chem>	-8.7
69030367	<chem>o1c2cc(ccc2c(=O)cc1c1cc(cc(c1)OC)OC)O</chem>	-8.7
69234627	<chem>O([C@@]1(CCc2ccccc2O1)c1ccccc1)[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO</chem>	-8.7
72279	<chem>o1c(cc(=O)c2cc(ccc12)O)c1ccccc1</chem>	-8.7
73202	<chem>O1c2cc(cc2C(=O)[C@@H]([C@H]1c1ccccc1)O)O)O</chem>	-8.7
73829901	<chem>O1c2cc3c(c2C(=O)[C@@H]([C@H]1c1ccccc1)O)OC)OCO3</chem>	-8.7
76573	<chem>o1c(cc(=O)c2c(c(C)c(c(C)c12)OC)O)c1ccc(cc1)OC</chem>	-8.7
94156	<chem>O1c2ccccc2CC[C@@H]1c1ccccc1</chem>	-8.7
101101153	<chem>c1(cc2c(c(=O)cc(o2)c2ccccc2)c(c1OC)O)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO</chem>	-8.6
101214938	<chem>c1(ccc(cc1)N1CCN(CC1)c1ccncc1)c1oc2ccccc2c(=O)c1O</chem>	-8.6

10142913 2	<chem>c1(cc(c(c1)CC=C(C)C)OC)/C=C/C(C)(C)O[C@H]1Oc2cc(ccc2C(=O)C1)O</chem>	-8.6
10234148 7	<chem>c1(cc(c2c(=O)cc(oc2c1)c1ccc(c1)OC)OC)O)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@@H]1O)O)O)C</chem>	-8.6
10901472	<chem>o1c2ccccc2c(=O)c(c1c1ccc(cc1)C=C)O</chem>	-8.6
11995581	<chem>c1(cc(c(c1)CC=C(C)C)OC)/C=C/C(C)(C)O[C@H]1Oc2cc(ccc2C(=O)C1)O</chem>	-8.6
1232441	<chem>O1c2ccccc2CC[C@H]1c1ccccc1</chem>	-8.6
12753176	<chem>[C@H]1(C(=C)C(=O)c2ccccc2O1)c1c(Cl)cc(cc1)Cl</chem>	-8.6
12971127 8	<chem>c1(cccc2oc(cc(=O)c12)c1ccccc1)C(O)(O)[C@@H](C(C)C)O</chem>	-8.6
13247200 6	<chem>o1c2cc(C)cc(c2c(=O)c(C)c1c1ccc(C)cc1)O</chem>	-8.6
13959387 7	<chem>o1c(cc(=O)c2cc(cc(c12)OC)CC(=O)C)c1ccc(cc1)OC</chem>	-8.6
14134114	<chem>o1c(c(c(=O)c2c(cc(c12)C(=O)C[C@@H](C)C(=O)O)O)O)c1ccc(cc1)O</chem>	-8.6
14254494	<chem>o1cc(c(=O)c2c(C)cc(cc12)O)c1ccccc1</chem>	-8.6
145726	<chem>o1c2ccccc2c(=O)cc1c1ccc(c1)O)O</chem>	-8.6
160237	<chem>o1c(cc(=O)c2c(c(c12)OC)OC)O)c1ccc(c1)O)O</chem>	-8.6
20489	<chem>o1c(cc(=O)c2c(cc(c12)O)OC)O)c1ccccc1</chem>	-8.6
21325037	<chem>c1(ccc2c(c(=O)cc(o2)c2ccccc2OC(C)C)c1)C(=O)Cl</chem>	-8.6
21604819	<chem>O1c2c(c(ccc2CC[C@H]1c1ccc(cc1)O)O)CC=C(C)C</chem>	-8.6
246330	<chem>O1c2cc(ccc2C(=O)[C@@H]([C@@H]1c1ccc(c1)O)O)O)O</chem>	-8.6
25022738	<chem>O1c2cc(c(cc2C(=O)C[C@H]1c1ccccc1)OC)O</chem>	-8.6
25058575	<chem>c1(cc(c(cc1OC)OCC=C(C)C)OC)c1coc2c(c1=O)c(cc(c2)OC)OC</chem>	-8.6
25201487	<chem>O1[C@@H](C(=O)C(=O)c2ccccc12)c1ccccc1</chem>	-8.6
368925	<chem>O1c2c(c(cc(c2C(=O)[C@@H]([C@@H]1c1ccc(cc1)O)O)O)O)CC=C(C)C</chem>	-8.6
373261	<chem>O1c2cc(cc(c2C(=O)C[C@@H]1c1ccc(c1)O)O)O)O</chem>	-8.6

4169706	<chem>Fc1ccc2c(C(=O)C[C@@H](O2)c2ccccc2)c1</chem>	-8.6
42608069	<chem>O1c2c(c(cc3OC(C)(C)C=Cc23)OC)C(=O)C[C@H]1c1ccc(c(c1)OC)OC</chem>	-8.6
42608071	<chem>O1c2c(c(cc(c2C(=O)C[C@H]1c1ccc(cc1)O)O)OC)CC=C(C)C</chem>	-8.6
44257359	<chem>o1cc(c(=O)c2c(c3c(cc12)OCO3)OC)c1ccc(c(c1)O)OC</chem>	-8.6
44258651	<chem>o1c(cc(=O)c2c(c(c(c12)OC)O)OC)O)c1ccc2c(OCO2)c1</chem>	-8.6
44259965	<chem>o1c(c(c(=O)c2c(cc(c(c12)O)OC)O)O)c1ccc(cc1)O</chem>	-8.6
44260022	<chem>o1c(c(c(=O)c2c(cc(c(c12)OC)OCC=C(C)C)O)OC)c1ccc(c(c1)OC)O</chem>	-8.6
44260056	<chem>o1c(cc(=O)c2c(c(c(c12)OC)OC)OC(=O)C(C)C)O)c1ccc(cc1)O</chem>	-8.6
455313	<chem>o1c2ccccc2c(=O)c(c1c1ccccc1O)O</chem>	-8.6
462699	<chem>O1c2ccc(cc2C(=O)C[C@H]1c1ccc(cc1)O)O</chem>	-8.6
468911	<chem>O1c2c(c(cc(c2C(=O)[C@@H]([C@H]1c1ccc(cc1)O)O)O)O)O</chem>	-8.6
49676	<chem>o1c(c(C)c(=O)c2ccc(c(c12)CN(CC)CC)OC)c1ccccc1</chem>	-8.6
509245	<chem>O1c2c(c(cc(c2C(=O)C[C@H]1c1ccc(cc1)O)O)O)CC=C(C)C</chem>	-8.6
5272801	<chem>o1c2ccccc2c(=O)cc1c1ccc(cc1)C1=NCCO1</chem>	-8.6
5280681	<chem>o1c2cc(cc(c2c(=O)c(c1c1ccc(c(c1)O)O)OC)O)O</chem>	-8.6
5280699	<chem>o1c(c(c(=O)c2c(c(c(cc12)OC)OC)O)OC)c1ccc(c(c1)O)O</chem>	-8.6
5281603	<chem>o1c(c(c(=O)c2c(c(c(cc12)O)OC)O)OC)c1ccc(c(c1)O)O</chem>	-8.6
5281614	<chem>o1c2cc(ccc2c(=O)c(c1c1ccc(c(c1)O)O)O)O</chem>	-8.6
5281670	<chem>o1c2cc(cc(c2c(=O)c(c1c1ccc(cc1O)O)O)O)O</chem>	-8.6
5281674	<chem>o1c(cc(=O)c2c(cc(c(c12)O)O)O)c1ccccc1</chem>	-8.6
5316653	<chem>o1cc(c(=O)c2c(c3c(cc12)OCO3)O)c1cc(c(c(c1)OC)OC)O</chem>	-8.6
5316900	<chem>o1c2cc(cc(c2c(=O)c(c1c1ccc(c(c1)OC)O)OC)O)O</chem>	-8.6
5322065	<chem>o1c2cc(ccc2c(=O)cc1c1ccc(c(c1)O)O)O</chem>	-8.6
5378171	<chem>o1c(cc(=O)c2c(cc(C)cc12)O)c1ccc(cc1)OC</chem>	-8.6
5378210	<chem>o1c(cc(=O)c2c(cc(cc12)O)O)c1ccccc1OC</chem>	-8.6

54553686	<chem>O1c2ccccc2C(=O)C[C@H]1c1cccc(c1)C#N</chem>	-8.6
5487268	<chem>c1(cc(c(cc1C(C)(C)C=C)c1coc2cc(cc(c2c1=O)O)O)O)O</chem>	-8.6
55748	<chem>o1c(cc(=O)c2cccc(c12)CC(=O)O)c1cccc1</chem>	-8.6
57340185	<chem>c1(cc(=O)c2ccc(cc2o1)O)c1ccc(I)cc1</chem>	-8.6
578729	<chem>o1c2ccccc2c(=O)c(c1c1ccccc1OC)O</chem>	-8.6
6028923	<chem>c1(cc(=O)c2ccc(cc2o1)O)c1ccc(Br)cc1</chem>	-8.6
66650373	<chem>c1(cccc2oc(cc(=O)c12)c1cccc1)CBr</chem>	-8.6
676033	<chem>o1c2ccccc2c(=O)cc1c1cccc(c1OC)OC</chem>	-8.6
676299	<chem>o1c(cc(=O)c2ccc(c(c12)O)OC)c1cccc1</chem>	-8.6
68112	<chem>o1c(cc(=O)c2c(cccc12)O)c1cccc1</chem>	-8.6
688672	<chem>o1c(cc(=O)c2ccc(cc12)OC)c1cccc(c1)OC</chem>	-8.6
69029207	<chem>c1(ccc2c(=O)cc(oc2c1)c1ccc(c(c1)OC)OC)OCCCB</chem>	-8.6
69279473	<chem>O1c2ccc(cc2C(=O)[C@H]([C@H]1c1cccc1)O)CCCC</chem>	-8.6
70350763	<chem>O1c2ccccc2C(=O)/C(=C\O)/[C@H]1c1cccc1</chem>	-8.6
71588336	<chem>O1c2cc(c3c(=O)cc(oc3c2[C@H]([C@@H](C1(C)C)O)O)c1ccc(cc1)O)O</chem>	-8.6
71621986	<chem>c1(cc2c(c(=O)c(co2)c2ccc(cc2)O)cc1OC)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)OC)CO</chem>	-8.6
73829902	<chem>O1c2c(c(ccc2C(=O)[C@H]([C@@H]1c1ccc(c(c1)O)O)O)O)O</chem>	-8.6
86236611	<chem>c1(ccc2c(=O)cc(oc2c1)c1ccc(c(c1)OC)OC)OC[C@@H]1OC1</chem>	-8.6
89858365	<chem>o1c(c(c(=O)c2c(cccc12)C(=O)C)O)c1cccc1</chem>	-8.6
9972910	<chem>o1c(c(c(=O)c2c(cc(c(c12)OC)O)O)OC)c1cccc1</chem>	-8.6
10022760	<chem>c1(cc(c2c(=O)c(c(oc2c1)c1ccc(c(c1)O)O)O)O)OS(=O)(=O)O</chem>	-8.5
10124538 7	<chem>c1(c(cc(c2c(=O)c(c(oc12)c1ccc(cc1)OC)O)O)O)OC[C@H]1O[C@@H]1c1ccc(c(c1)O)O</chem>	-8.5
10168525 1	<chem>c1(ccc(cc1)C(=O)NCCO)c1oc2ccccc2c(=O)c1</chem>	-8.5
10174053	<chem>c1(cc2c(c(=O)cc(o2)c2ccccc2)c(c1OC)O)OS(=O)(=O)O</chem>	-8.5

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10214569 8	<chem>O1c2cc(c(cc2C(=O)C[C@@H]1c1ccc(c(c1)O)O)O)OC</chem>	-8.5
102928	<chem>O1c2ccccc2C(=O)C[C@H]1c1ccc(cc1)OC</chem>	-8.5
10598514	<chem>O1[C@@H](CC(=O)c2c(cc(c(c12)C[C@H](C(=C)C)CCC(C)(C)O)O)O)c1cccc1O</chem>	-8.5
10685123	<chem>c1(ccc2c(c(=O)cc(o2)c2ccccc2)c1)CN=C=S</chem>	-8.5
10902653	<chem>c1(cc(=O)c2ccccc2o1)c1ccc(cc1)S(=O)(=O)C</chem>	-8.5
11382711	<chem>c1(c(cc2c(c(=O)c(co2)c2ccc(cc2)O)c1O)O)CCC(C)(C)O</chem>	-8.5
12088189	<chem>o1c2ccccc2c(=O)c(c1c1ccc(cc1)N(CC)CC)O</chem>	-8.5
12098358	<chem>O1c2c(c(cc(c2C(=O)C[C@H]1c1ccccc1O)O)OC)OC</chem>	-8.5
126392	<chem>o1c(cc(=O)c2cccc(c12)CC(=O)OCCN(C)C)c1ccccc1</chem>	-8.5
12674946	<chem>o1c2ccccc2c(=O)c(c1c1ccccc1)C(=O)O</chem>	-8.5
12735893	<chem>o1c(c(c(=O)c2ccc3c(cco3)c12)OC)c1ccc(cc1)OC</chem>	-8.5
12753167	<chem>[C@H]1(C(=C)C(=O)c2ccccc2O1)c1ccc(Cl)cc1</chem>	-8.5
129394	<chem>O1c2c(c(c(C)c(c2[C@@H](C[C@H]1c1ccccc1)O)OC)O)C=O</chem>	-8.5
12967047 6	<chem>O1c2c(C)ccc(c2C(=O)C[C@H]1c1ccccc1)CO</chem>	-8.5
12982236 1	<chem>o1c(cc(=O)c2cc(c(c(c12)N)OC(=O)C)OC(=O)C)c1ccccc1</chem>	-8.5
12982241 3	<chem>o1c(cc(=O)c2cc(cc(c12)N)OC(=O)C)c1ccc(cc1)OC(=O)C</chem>	-8.5
12986463 5	<chem>o1c(cc(=O)c2c(cccc12)OCO)c1ccccc1</chem>	-8.5
12988090	<chem>c1(ccc2c(=O)cc(oc2c1)c1ccccc1)OP(=O)(OCC)OCC</chem>	-8.5
13889022	<chem>o1c(cc(=O)c2c(cc(c(c12)OC)OC)O)c1c(cccc1OC)O</chem>	-8.5
13959387 8	<chem>o1c(cc(=O)c2cc(cc(c12)OC)CCCO)c1ccc(cc1)OC</chem>	-8.5

14885875	<chem>O1c2cc(cc(c2CC[C@H]1c1cccc1)OC)O</chem>	-8.5
16681753	<chem>o1c(cc(=O)c2c(c(c(cc12)OC)OC)O)c1cc(c(c(c1)OC)O)OC</chem>	-8.5
177032	<chem>O1c2cc(c(c(c2C(=O)C[C@H]1c1cccc1)O)OC)O</chem>	-8.5
182026	<chem>O1c2cc(c(C)c(c2C(=O)[C@@H]([C@H]1c1ccc(c(c1)O)O)O)O)O</chem>	-8.5
195603	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1c(cccc1O)O)O)OC</chem>	-8.5
21325058	<chem>O1c2ccc(cc2C(=O)C[C@@H]1c1cccc1N(=O)=O)C(=O)OC</chem>	-8.5
227445	<chem>o1c(c(c(=O)c2cc(C)ccc12)O)c1cccc1</chem>	-8.5
265699	<chem>o1c(c(c(=O)c2ccc(cc12)OC)O)c1ccc(cc1)OC</chem>	-8.5
342294	<chem>O1c2cc(cc(c2CC[C@H]1c1cccc1)OC)O</chem>	-8.5
344546	<chem>o1c(c(c(=O)c2ccc(cc12)OC)O)c1cccc1</chem>	-8.5
348130	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(cc1)O)O)OC</chem>	-8.5
369608	<chem>O1c2c(cc(cc2[C@H](C[C@@H]1c1cccc1)O)CC=C)OC</chem>	-8.5
4231835	<chem>o1c2cccc2c(=O)cc1c1cc(ccc1OC)OC</chem>	-8.5
42608063	<chem>O1c2c(c(cc3OC(C)(C)C=Cc23)OC)C(=O)C[C@H]1c1ccc(cc1)OC</chem>	-8.5
4303567	<chem>o1c(cc(=O)c2c(cc(cc12)OC(=O)C)OC(=O)C)c1ccc(cc1)OC</chem>	-8.5
439712	<chem>O1c2ccccc2[C@H](C[C@H]1c1cccc1)O</chem>	-8.5
44258621	<chem>O1c2c3c(=O)cc(oc3c(c(c2C=CC1(C)C)OC)OC)c1cc(c(c(c1)OC)OC)OC</chem>	-8.5
462700	<chem>O1c2ccccc2C(=O)C[C@H]1c1ccc(c(c1)O)O</chem>	-8.5
4872981	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(c(c1)O)O)O)OC</chem>	-8.5
491719	<chem>O1c2c(c(c(C)c(c2C(=O)C[C@H]1c1ccc(cc1)O)O)O)CC=C(C)C</chem>	-8.5
49788611	<chem>o1c(c(c(=O)c2c(cc(c(c12)OC)OC)O)O)c1ccc2c(OCO2)c1</chem>	-8.5
51459	<chem>o1c2cccc2c(=O)c(C)c1c1cccc1</chem>	-8.5
5271551	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(cc1)O)OC)OC</chem>	-8.5
5281666	<chem>o1c(c(c(=O)c2c(cc(cc12)O)O)O)c1ccc(cc1)OC</chem>	-8.5
5281797	<chem>o1cc(c(=O)c2c(c(c(cc12)O)CC=C(C)C)O)c1ccc(cc1O)O</chem>	-8.5

5317284	<chem>o1c(cc(=O)c2c(c(c(cc12)O)OC)O)c1ccc(c(c1)O)O</chem>	-8.5
5317747	<chem>O1c2cc(cc(c2C(=O)[C@H]([C@@H]1c1ccccc1)O)O)OC</chem>	-8.5
5321861	<chem>o1c(c(c(=O)c2c(cc(c(c12)O)O)O)OC)c1ccc(c(c1)O)OC</chem>	-8.5
5378202	<chem>c1(c(cc(c2c(=O)c(coc12)c1ccc(cc1)O)O)O)CCC(C)(C)O</chem>	-8.5
53947837	<chem>O1c2ccc(C)cc2CC[C@H]1c1ccc(cc1)OC</chem>	-8.5
5469524	<chem>o1c(cc(=O)c2c(c(c(cc12)O)OC)O)c1ccc(c(c1)O)OC</chem>	-8.5
57363368	<chem>o1c(c(c(=O)c2cc(cc(c12)O)O)O)c1ccc(cc1)OC</chem>	-8.5
619834	<chem>o1c2ccccc2c(=O)cc1c1cccc(c1)OC</chem>	-8.5
6253276	<chem>c1(c(c(cc(c1C(=O)/C=C/c1ccc(cc1)OC)O)OC)OC)OC</chem>	-8.5
66916672	<chem>o1c2ccccc2c(=O)c(c1C(=O)C)c1ccccc1</chem>	-8.5
67424417	<chem>c1(ccc(cc1)[C@@H]1CC(=O)c2ccccc2O1)S(=O)(=O)C(F)(F)F</chem>	-8.5
688671	<chem>o1c(cc(=O)c2ccc(cc12)OC)c1ccccc1OC</chem>	-8.5
688715	<chem>o1c2ccccc2c(=O)c(c1c1ccc(cc1)O)O</chem>	-8.5
688853	<chem>o1c(cc(=O)c2ccc(c(c12)O)O)c1ccc(cc1)O</chem>	-8.5
689014	<chem>o1c(cc(=O)c2ccc(c(c12)OC)OC)c1ccccc1</chem>	-8.5
69030155	<chem>c1(ccc2c(=O)cc(oc2c1)c1cc(cc(c1)OC)OC)OCCBr</chem>	-8.5
71588337	<chem>O1c2cc(c3c(=O)cc(oc3c2[C@@H]([C@H](C1(C)C)O)OCC)c1ccc(cc1)O)O</chem>	-8.5
72304	<chem>o1cc(c(=O)c2ccccc12)c1ccccc1</chem>	-8.5
7330537	<chem>O1c2ccc3c(=O)c(coc3c2C=CC1(C)C)c1cc(c2c(OCO2)c1)OC</chem>	-8.5
73571	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(cc1)O)O)OC</chem>	-8.5
76852307	<chem>o1c(cc(=O)c2ccc(c(c12)C=O)O)c1ccccc1</chem>	-8.5
97214	<chem>o1c(cc(=O)c2c(c(c(cc12)OC)OC)O)c1ccc(c(c1)O)OC</chem>	-8.5
10018499	<chem>O1c2c(c(c(C)c(c2C(=O)C[C@]1(c1ccccc1)O)O)O)C=O</chem>	-8.4
10106405 5	<chem>c1(coc2ccccc2c1=O)c1ccc(cc1)C(F)(F)F</chem>	-8.4
10113705	<chem>c1(c(cc(c2c(=O)c(coc12)c1ccc(cc1)O)O)O)O)CC(C)(C)O</chem>	-8.4

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10136776 7	<chem>O1c2c(c(cc(c2C(=O)C[C@H]1c1ccc(cc1)O)O)O)C/C=C(\C)/C=O</chem>	-8.4
10185	<chem>O1c2cc(cc(c2C(=O)[C@H]([C@H]1c1ccc(c(c1)O)O)O)O)O</chem>	-8.4
10832934	<chem>O1c2ccc(cc2[C@H]([C@@H](C1(C)C)O)O)c1coc2cc(cc(c2c1=O)O)O</chem>	-8.4
11033582	<chem>O1c2c(c(ccc2C[C@@H]([C@H]1c1ccc(c(c1)O)O)O)O)O</chem>	-8.4
11055	<chem>o1c(cc(=O)c2c(ccc(c12)O)O)c1cccc1</chem>	-8.4
11810419	<chem>O1c2c(c(cc(c2C(=O)C[C@@H]1c1ccc(cc1O)O)O)O)CC=C(C)C</chem>	-8.4
12052874	<chem>O1c2cc(ccc2CC[C@H]1c1ccc2c(OCO2)c1)O</chem>	-8.4
12318031	<chem>O1c2ccccc2C[C@H]([C@H]1c1ccccc1)O</chem>	-8.4
12360936	<chem>O1c2cc(ccc2[C@@H](C[C@H]1c1ccccc1)O)OC</chem>	-8.4
125526	<chem>O1c2cc(cc(c2C(=O)[C@@H](C)[C@H]1c1ccc(cc1)O)O)O</chem>	-8.4
12968443 5	<chem>O1c2ccccc2C[C@H]([C@H]1c1ccccc1)O</chem>	-8.4
12981955 7	<chem>O1c2ccccc2C(=O)[C@H]([C@H]1c1ccccc1)O</chem>	-8.4
12984795 9	<chem>O1c2c(c(ccc2[C@H]([C@@H]([C@H]1c1ccc(cc1)O)O)O)O)O</chem>	-8.4
12985837 0	<chem>o1c2cc(ccc2c(=O)cc1c1cc(c(c(c1)OC)OC)OC)OCC(=O)O</chem>	-8.4
12988102 7	<chem>o1cc(c(=O)c2ccc(c(c12)CO)O)c1cc(c(c(c1)CO)O)CO</chem>	-8.4
14034216	<chem>o1c(c(c(=O)c2c(cc(c(c12)OC)OC)O)O)c1ccc(c(c1)OC)OC</chem>	-8.4
15301053	<chem>o1cc(c(=O)c2c(cc(cc12)O)O)c1ccc2c(OCO2)c1</chem>	-8.4
153441	<chem>o1c(cc(=O)c2c(c(c(c12)O)OC)OC)O)c1cccc1</chem>	-8.4
15389726	<chem>c1(cc(=O)c2ccccc2o1)c1ccc(cc1)S(=O)(=O)Cl</chem>	-8.4
15389730	<chem>c1(cccc(c1)c1cc(=O)c2ccccc2o1)S(=O)(=O)N(CC)CC</chem>	-8.4

15458309	<chem>O1c2c(c(ccc2C(=O)C[C@H]1c1ccc(cc1)OC)OC)OC</chem>	-8.4
158311	<chem>o1c(cc(=O)c2c(c(c(cc12)OC)OC)O)c1cc(c(cc1O)O)OC</chem>	-8.4
161271	<chem>o1c(cc(=O)c2c(c(c(cc12)OC)OC)O)c1ccc(cc1)OC</chem>	-8.4
162464	<chem>o1c(cc(=O)c2c(c(c(cc12)OC)OC)O)c1ccc(c(c1)OC)O</chem>	-8.4
1666397	<chem>o1c2ccccc2c(=O)c(c1c1ccccc1)OC(=O)C</chem>	-8.4
1880	<chem>o1c(cc(=O)c2ccc(c(c12)O)O)c1ccccc1</chem>	-8.4
194690	<chem>o1c(cc(=O)c2cc(cc(c12)OC)OC)c1ccccc1</chem>	-8.4
20301086	<chem>O1c2ccccc2C(=O)C(=C)[C@@H]1c1ccc(c1)N(=O)=O</chem>	-8.4
20394006	<chem>o1c(C)c(c(=O)c2c(cc(cc12)OC(=O)C)OC(=O)C)c1ccccc1</chem>	-8.4
21270134	<chem>c1(coc2cc(c(cc2c1=O)O)O)c1cccc(Cl)c1</chem>	-8.4
21270152	<chem>o1cc(c(=O)c2ccc(c(C)c12)O)c1ccc(cc1)N(=O)=O</chem>	-8.4
213728	<chem>o1c(cc(=O)c2cccc(c12)OC)c1ccccc1</chem>	-8.4
226342	<chem>O1c2ccccc2C(=O)C[C@H]1c1ccc(c(c1)OC)O</chem>	-8.4
227443	<chem>o1c(c(c(=O)c2cc(C)ccc12)O)c1ccc(cc1)OC</chem>	-8.4
24205532	<chem>c1(cc(c2c(=O)c(c(oc2c1)c1ccc(cc1)O)CC=C(C)C)OC)O[C@H]1O[C@H]([C@@H]([C@H]([C@H]1O)O)O)C</chem>	-8.4
26034	<chem>o1c(c(c(=O)c2c(cc(cc12)OC)OC)O)c1ccc(c(c1)O)O</chem>	-8.4
3082330	<chem>O1c2cc(cc(c2C(=O)[C@@H]([C@H]1c1ccccc1O)O)O)O</chem>	-8.4
31161	<chem>o1c(cc(=O)c2c(c(c(cc12)OC)O)O)c1ccc(c(c1)O)O</chem>	-8.4
321347	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(c(c1)OC)O)O)OC</chem>	-8.4
3707243	<chem>O1c2ccccc2C[C@H]([C@H]1c1ccccc1)O</chem>	-8.4
373260	<chem>o1c(cc(=O)c2c(c(c(cc12)OC)O)O)c1ccc(c(c1)O)OC</chem>	-8.4
3826106	<chem>O1c2ccccc2[C@H](CC1)c1ccccc1</chem>	-8.4
42607939	<chem>O1C(C)(C)C=Cc2c(c3C(=O)C[C@H](Oc3c(c12)C[C@@H](C(=C)C)O)c1ccc(cc1)O)O</chem>	-8.4
439533	<chem>O1c2cc(cc(c2C(=O)[C@@H]([C@H]1c1ccc(c(c1)O)O)O)O)O</chem>	-8.4
44258614	<chem>O1c2c3c(=O)cc(oc3c(c(c2C=CC1(C)C)OC)OC)c1ccc(c(c1)OC)OC</chem>	-8.4

442621	<chem>o1c(c(c(=O)c2c(c(c(cc12)OC)O)O)OC)c1ccc(c(c1)O)OC</chem>	-8.4
443638	<chem>O1c2cc(cc(c2[C@H](C[C@H]1c1ccc(cc1)O)O)O)O</chem>	-8.4
466078	<chem>O1c2cc(ccc2CC[C@H]1c1ccc2c(OCO2)c1)O</chem>	-8.4
466293	<chem>Clc1ccc2c(c(=O)c(c(o2)c2ccc(cc2)OC)O)c1</chem>	-8.4
5106787	<chem>O1c2ccc(cc2C(=O)C[C@H]1c1ccccc1O)O</chem>	-8.4
513103	<chem>O1c2ccccc2C(=O)[C@H](C1)Cc1ccccc1</chem>	-8.4
5272799	<chem>O1c2ccccc2C(=O)C[C@H]1c1ccc(cc1)C1=NCCO1</chem>	-8.4
5273755	<chem>o1c(cc(=O)c2c(c(c(cc12)O)OC)O)c1ccc(c(c1)OC)OC</chem>	-8.4
5280417	<chem>o1c(c(c(=O)c2c(cc(cc12)OC)O)OC)c1ccc(c(c1)O)O</chem>	-8.4
5280445	<chem>o1c(cc(=O)c2c(cc(cc12)O)O)c1ccc(c(c1)O)O</chem>	-8.4
5281612	<chem>o1c2cc(cc(c2c(=O)cc1c1ccc(c(c1)O)OC)O)O</chem>	-8.4
52951513	<chem>O1c2cc3c(c(=O)c(co3)c3ccc(c(c3)OC)OC[C@H](C(C)(C)O)O)c(c2C=CC1(C)C)OC</chem>	-8.4
5317435	<chem>O1c2cc(ccc2C(=O)[C@@H]([C@H]1c1ccc(c(c1)O)O)O)O</chem>	-8.4
5318869	<chem>o1c(c(c(=O)c2c(cc(cc12)OC)O)OC)c1ccc(cc1)O</chem>	-8.4
5320181	<chem>o1c(cc(=O)c2c(c(c(cc12)O)O)O)c1ccc(c(c1)OC)O</chem>	-8.4
5320693	<chem>o1c2cc(ccc2c(=O)cc1c1ccc(cc1)OC)O</chem>	-8.4
53247999	<chem>c1(ccc(cc1)[C@H]1CC(=O)c2ccccc2O1)O[C@H]1O[C@@H]([C@H]([C@H]([C@H]1O)O)O)C</chem>	-8.4
53398699	<chem>c1(ccc2c(=O)c(coc2c1)c1ccc(cc1)O)O[C@@H]1O[C@H]([C@@H]([C@H]([C@H]1O)O)O)COC(=O)C</chem>	-8.4
53645	<chem>o1c(cc(=O)c2cccc(c12)O)c1ccccc1</chem>	-8.4
5377381	<chem>o1cc(c(=O)c2c(cc(cc12)O)O)c1ccccc1</chem>	-8.4
5378518	<chem>o1c2cc(ccc2c(=O)cc1c1ccc(c(c1)OC)OC)O</chem>	-8.4
5383438	<chem>o1c2cc(cc(c2c(=O)c(c1c1ccc(c(c1)OC)OC)OC)O)O</chem>	-8.4
5407860	<chem>o1cc(c(=O)c2ccc(c(c12)O)O)c1ccccc1</chem>	-8.4
54512651	<chem>O1c2ccccc2C(=O)/C(=C\N)/[C@H]1c1ccccc1</chem>	-8.4
55750	<chem>c1(cccc2c(=O)cc(oc12)c1ccccc1)CC(=O)OCCN(CC)CC</chem>	-8.4

5748553	<chem>o1c(c(c(=O)c2c(cc(c(c12)OC)O)O)OC)c1ccc(c(c1)O)O</chem>	-8.4
57679080	<chem>O1c2ccccc2CC[C@H]1c1ccc(c(c1)O)O</chem>	-8.4
586090	<chem>O1c2cccc(c2C(=O)C[C@H]1c1cccc1)O</chem>	-8.4
59059924	<chem>o1cc(c(=O)c2ccc(cc12)OC(=O)C(=C)C)c1cccc1</chem>	-8.4
631171	<chem>o1c2cc(ccc2c(=O)c(c1c1ccc(c(c1)OC)OC)OC)OC</chem>	-8.4
66968868	<chem>c1(ccc2c(c(=O)c(c(o2)c2ccc(cc2)N(CC)CC)O)c1)CBr</chem>	-8.4
67425485	<chem>c1(cc(c2c(=O)cc(oc2c1)c1ccc(c(c1)OC)OC)OC)OCP(=O)(C(C)C)C(C)C</chem>	-8.4
69030799	<chem>c1(ccc2c(=O)cc(oc2c1)c1cc(c(c(c1)OC)OC)OC)OCCCB</chem>	-8.4
70018578	<chem>O1c2cc(ccc2C(=O)C[C@@H]1c1ccc(cc1)OC)O</chem>	-8.4
70253991	<chem>o1c(c(c(=O)c2c(c(c(c12)O)OC)OC)O)O)c1cccc1</chem>	-8.4
73265447	<chem>c1(coc2c(C)c(ccc2c1=O)O)c1ccc(cc1)C(F)(F)F</chem>	-8.4
10108482	<chem>c1(ccc2c(=O)c(coc2c1)c1cccc1)OC[C@H]1OC1</chem>	-8.3
10136776 6	<chem>O1c2c(c(cc(c2C(=O)C[C@H]1c1ccc(cc1)O)O)O)C/C=C(\C)/CO</chem>	-8.3
10159199 8	<chem>c1(cc(c2c(=O)cc(oc2c1OC)c1cccc1)OC)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO</chem>	-8.3
10168524 9	<chem>c1(ccc(cc1)C(=O)NCCO)[C@H]1Oc2ccccc2C(=O)C1</chem>	-8.3
10422310	<chem>o1c(cc(=O)c2c(cccc12)N)c1ccc(cc1)N</chem>	-8.3
10904774	<chem>c1(c(cc(c2c(=O)c(coc12)c1ccc(cc1O)O)O)O)CCC(C)(C)O</chem>	-8.3
11111496	<chem>O1c2c(c(cc(c2C(=O)C[C@H]1c1ccc(c(c1)O)O)O)O)C/C=C(\C)/CO</chem>	-8.3
11244593	<chem>O1c2cc(c(cc2C=CC1(C)C)c1coc2cc(ccc2c1=O)O)O</chem>	-8.3
11349	<chem>o1c2ccccc2c(=O)c(c1c1cccc1)O</chem>	-8.3
11507421	<chem>o1c2ccccc2c(=O)cc1c1ccc(cc1)OC(=O)C</chem>	-8.3
11723752	<chem>o1cc(c(=O)c2c(C)cc(cc12)OC(=O)OCC)c1cccc1</chem>	-8.3
11739635	<chem>c1(cc(c(c(c1)CC=C(C)C)OC)O)c1coc2c(c1=O)ccc(c2)O</chem>	-8.3

117900	<chem>o1c(c(c(=O)c2c(cc(cc12)OC)OC)OC)c1ccccc1</chem>	-8.3
12444947	<chem>c1(cc2c(c(=O)c(co2)c2ccc(cc2)OC)cc1OC)O[C@@H]1O[C@H]([C@@H]([C@H]([C@H]1O)O)O)CO</chem>	-8.3
12578908	<chem>O1c2cc(cc(c2C(=O)[C@H](C1)c1ccccc1)O)O</chem>	-8.3
12971122 2	<chem>O1C2=C(CC(=O)C=C2)CC[C@@H]1c1ccccc1</chem>	-8.3
12984790 9	<chem>o1c(c(c(=O)c2ccc(cc12)OC(O)O)OCO)c1ccccc1</chem>	-8.3
12986429 4	<chem>O1c2c(cccc2C(=O)C[C@H]1c1ccc(cc1)O)OC</chem>	-8.3
12988240 4	<chem>o1cc(c(=O)c2ccccc12)c1ccc(cc1)CN</chem>	-8.3
13250353	<chem>O1c2cccc(c2CC[C@H]1c1ccccc1)O</chem>	-8.3
13253615 8	<chem>o1c(cc(=O)c2c(cc(cc12)OC(=O)C=C)OC(=O)C=C)c1ccc(cc1)OC(=O)C=C</chem>	-8.3
13482227 8	<chem>o1cc(c(=O)c2c(c3c(cc12)OCO3)O)C1=CCC(=CC1)OC</chem>	-8.3
13942548	<chem>o1c(c(c(=O)c2c(c3c(c(c12)OC)OCO3)OC)OC)c1ccc2c(OCO2)c1</chem>	-8.3
13964544	<chem>o1c(cc(=O)c2c(cc(cc12)O)OC)c1ccc(c(c1)OC)OC</chem>	-8.3
147157	<chem>o1c(cc(=O)c2cc(ccc12)OC)c1ccccc1</chem>	-8.3
15385487	<chem>O1c2cc(ccc2C(=O)C[C@H]1c1ccc(c(c1)OC)O)O</chem>	-8.3
154227	<chem>o1c2cc(ccc2c(=O)cc1c1ccc(c(c1)OC)OC)OC</chem>	-8.3
1546800	<chem>O1c2ccccc2C(=O)[C@@H]([C@@H]1c1ccccc1)O</chem>	-8.3
15896301	<chem>o1c(cc(=O)c2c(c(c(c12)OC)OC)OC)O)c1cccc(c1O)OC</chem>	-8.3
177000	<chem>o1c2cc(ccc2c(=O)c(C)c1c1cc(c(c(c1)OC)OC)OC)OC</chem>	-8.3
18702583	<chem>o1c(cc(=O)c2c(c(ccc12)OC)O)c1ccc(c(c1)O)O</chem>	-8.3
188323	<chem>o1c(cc(=O)c2c(c(c(cc12)OC)OC)O)c1ccc(cc1)O</chem>	-8.3
21315732	<chem>o1c2ccc(cc2c(=O)cc1c1cc(C)ccc1OC(C)C)C(=O)OCC</chem>	-8.3

21576250	<chem>o1cc(c(=O)c2c(cc(c(c12)C(C)(C)C=C)O)O)c1ccc(cc1O)O</chem>	-8.3
23644935	<chem>o1c2cc(ccc2c(=O)c(c1n1ncn1)c1cccc1)OC</chem>	-8.3
242486	<chem>O1c2cc(c(c(c2C(=O)C[C@H]1c1ccc(cc1)OC)OC)OC)OC</chem>	-8.3
24866262	<chem>c1(ccc(cc1OC)c1cc(=O)c2c(cc(cc2o1)O)O)O[C@H]1O[C@@H]([C@H]([C@H]([C@H]1O)O)O)C</chem>	-8.3
24866263	<chem>c1(ccc(cc1)c1cc(=O)c2c(cc(cc2o1)O)O)O[C@H]1O[C@@H]([C@H]([C@H]([C@H]1O)O)O)C</chem>	-8.3
253959	<chem>O1c2ccccc2[C@H](C[C@@H]1c1cccc1)O</chem>	-8.3
2734290	<chem>o1cc(c(=O)c2c(C)cc(cc12)OC)c1cccc1</chem>	-8.3
27443	<chem>o1c(c(C)c(=O)c2cc(ccc12)CN(CC)CC)c1cccc1</chem>	-8.3
3062797	<chem>o1cc(c(=O)c2ccc(cc12)O[C@@H](C)C(=O)O)c1cccc1</chem>	-8.3
3593	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(c(c1)O)OC)O)O</chem>	-8.3
3890073	<chem>N([C@@H]1c2ccccc2O[C@@H](C1)c1cccc1)NC(=S)N</chem>	-8.3
462695	<chem>O1c2cc(cc(c2C(=O)[C@H]([C@@H]1c1ccc(c(c1)OC)OC)O)OC)OC</chem>	-8.3
471	<chem>O1c2cc(cc(c2C(=O)[C@@H]([C@@H]1c1ccc(c(c1)O)O)O)O)O</chem>	-8.3
5049148	<chem>O1c2c(c(c3c(=O)c(coc3c2C=CC1(C)C)c1ccc2c(OCO2)c1)OC)OC</chem>	-8.3
5280343	<chem>o1c(c(c(=O)c2c(cc(cc12)O)O)O)c1ccc(c(c1)O)O</chem>	-8.3
5280666	<chem>o1c2cc(cc(c2c(=O)cc1c1ccc(c(c1)OC)O)O)O</chem>	-8.3
5281628	<chem>o1c(cc(=O)c2c(c(c(cc12)O)OC)O)c1ccc(cc1)O</chem>	-8.3
5281702	<chem>o1c2cc(cc(c2c(=O)cc1c1cc(c(c(c1)OC)O)OC)O)O</chem>	-8.3
5281805	<chem>c1(coc2cc(ccc2c1=O)O)c1ccc2OCOc2c1</chem>	-8.3
5316733	<chem>O1c2cc(c(c(c2C(=O)C[C@H]1c1cccc1)O)OC)O</chem>	-8.3
5320351	<chem>o1c(c(c(=O)c2c(c(c(cc12)OC)OC)O)OC)c1ccc(c(c1)OC)OC</chem>	-8.3
5320438	<chem>o1c(cc(=O)c2c(c(c(cc12)O)OC)O)c1ccc(cc1)OC</chem>	-8.3
5321538	<chem>O1c2cc(c(cc2C(=O)C[C@@H]1c1ccc(c(c1)O)O)OC)O</chem>	-8.3
5321987	<chem>[C@@H]1(c2cc(ccc2OC[C@@H]1c1cc(cc(c1O)OC)/C=C/C(=O)O)OC)OS(=O)(=O)O</chem>	-8.3
53247946	<chem>c1(ccc2c(C(=O)C[C@H](O2)c2ccc(cc2)O)c1)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)OC)CO</chem>	-8.3

5352005	<chem>o1c2cc(cc(c2c(=O)c(c1c1ccc(c(c1)OC)OC)OC)O)OC</chem>	-8.3
5352032	<chem>o1c(c(c(=O)c2c(c(c(cc12)O)OC)O)OC)c1ccc(cc1)O</chem>	-8.3
5380976	<chem>o1c2cc(ccc2c(=O)c(c1C)c1cccc1)O</chem>	-8.3
5381919	<chem>o1c(cc(=O)c2c(cc(C)cc12)O)c1cc(c(c(c1)OC)OC)OC</chem>	-8.3
5384810	<chem>o1c(c(c(=O)c2c(cc(c(c12)OC(=O)CCC)OC)O)O)c1ccc(cc1)OC</chem>	-8.3
5395695	<chem>o1c(C)c(c(=O)c2c(cc(cc12)O)O)c1cccc1</chem>	-8.3
5459184	<chem>o1c(c(c(=O)c2c(cc(c(c12)OC)OC)O)OC)c1ccc(c(c1)OC)O</chem>	-8.3
54799	<chem>o1c(c(c(=O)c2c(c(c(c12)OC)OC)OC)O)OC)c1ccc(c(c1)O)O</chem>	-8.3
56648913	<chem>c1(cc2c(c(=O)cc(o2)c2cccc2)c(c1OC(=O)C)OC(=O)C)OCc1ccc(F)cc1</chem>	-8.3
57253387	<chem>O1c2cccc2[C@H](C[C@H]1c1cccc1)NNC(=O)N</chem>	-8.3
624831	<chem>o1c(c(c(=O)c2c(cc(cc12)OC)OC)O)c1ccc(cc1)OC</chem>	-8.3
636642	<chem>Clc1c(cc2c(C[C@@H]([C@H](O2)c2ccc(c(c2)O)O)O)c1O)O</chem>	-8.3
6399103	<chem>O1c2cccc2C(=O)[C@@H](NO)[C@H]1c1cccc1</chem>	-8.3
67114276	<chem>o1c(c(c(=O)c2c(cccc12)C(=O)C)C(=O)C)c1cccc1</chem>	-8.3
71762131	<chem>o1c(cc(=O)c2ccc(c(c12)OC)O)c1cccc1</chem>	-8.3
72281	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(c(c1)O)OC)O)O</chem>	-8.3
77793	<chem>o1c2cccc2c(=O)cc1c1ccc(cc1)OC</chem>	-8.3
86606987	<chem>c1(ccc2c(=O)cc(oc2c1)c1cc(c(c(c1)OC)OC)OC)OC[C@@H]1OC1</chem>	-8.3
86641845	<chem>o1c(cc(=O)c2c(cc(cc12)OCC#C)O)c1ccc(c(c1)OC)OC</chem>	-8.3
91724402	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(cc1)OC(=O)C)O)OC</chem>	-8.3
97142	<chem>o1c(c(c(=O)c2c(cc(cc12)OC)OC)O)c1ccc(c(c1)OC)OC</chem>	-8.3
9798295	<chem>O1c2cc(c(c(c2C(=O)C[C@H]1c1ccc(c(c1)O)O)OC)OC)OC</chem>	-8.3
10193217 3	<chem>c1(c(c(c2C(=O)C[C@H](Oc2c1)c1cccc1)O)OC)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO</chem>	-8.2
10257792 6	<chem>o1c(cc(=O)c2c(cc(cc12)O)O)c1ccc(cc1)OCOC</chem>	-8.2

10613051	<chem>c1(cc(=O)c2ccccc2o1)c1ccc(cc1)[S@](=O)C</chem>	-8.2
11316719	<chem>o1c(cc(=O)c2c(c(c(cc12)OCc1ccccc1)OC(=O)C)OC(=O)C)c1ccccc1</chem>	-8.2
11609345	<chem>o1c(cc(=O)c2c(c(c(c12)OC)O)OC)O)c1ccccc1</chem>	-8.2
12000157	<chem>O1c2cc(cc(c2C(=O)C[C@@H]1c1ccc(cc1O)O)O)OC</chem>	-8.2
12043066	<chem>c1(cc(=O)c2c(cc(c(c2o1)[C@@H]1CCCC[C@@H]1O)O)O)c1c(Cl)cccc1</chem>	-8.2
12241083	<chem>o1cc(c(=O)c2c(cc(cc12)O)O)c1ccc(cc1)N(=O)=O</chem>	-8.2
12407866	<chem>o1c(cc(=O)c2cc(ccc12)C(=O)OC)c1ccccc1O</chem>	-8.2
1241435	<chem>o1c2ccccc2c(=O)cc1c1ccc(cc1)N(C)C</chem>	-8.2
12971430 2	<chem>O1c2ccccc2C(=O)[C@H]([C@@]1(c1ccccc1)Cc1ccccc1)O</chem>	-8.2
12973227 0	<chem>o1c2ccccc2c(=O)c(c1c1ccccc1)OO</chem>	-8.2
12981827 7	<chem>O1c2cc(ccc2[C@H](C(=O)[C@@H]1c1ccccc1)OC)O</chem>	-8.2
12984453 1	<chem>O1c2cc(cc(c2C(=O)[C@@](C)([C@H]1c1ccc(c(C)c1)O)O)O)O</chem>	-8.2
12985870 7	<chem>O1c2cc(cc(c2C(=O)[C@@]([C@@H]1c1ccc(c(c1)O)O)(OC)O)O)O</chem>	-8.2
12988780 1	<chem>o1c2ccc(c(c2c(=O)c(c1c1ccc(c(c1)OC)OC)OC)O)O</chem>	-8.2
13482072 6	<chem>o1c(cc(=O)c2cc(cc(c12)OC)OC)c1ccc(cc1)OC</chem>	-8.2
13482126 8	<chem>O1[C@@H]2Cc3ccccc3O[C@]12c1ccccc1</chem>	-8.2
13568446	<chem>o1c2ccccc2c(=O)c(c1c1ccccc1)C(=O)C</chem>	-8.2
14130926	<chem>o1c(c(c(=O)c2c(cc(cc12)OC(=O)C)OC(=O)C)OC(=O)C)c1ccc(cc1)OC(=O)C</chem>	-8.2
14606539	<chem>o1c(c(c(=O)c2c(c(c(cc12)OC)OC)OC)O)c1ccccc1</chem>	-8.2
18324985	<chem>Ic1c(=O)c2ccccc2oc1c1ccc(cc1)S(=O)(=O)C</chem>	-8.2

187093	<chem>O1c2cc(ccc2C(=O)C[C@H]1c1ccc(c(c1)O)OC)O</chem>	-8.2
19358638	<chem>o1c(cc(=O)c2c(cc(cc12)OCCO)OC)c1ccc(c(c1)OC)OC</chem>	-8.2
2017481	<chem>c1(ccc2c(=O)c(coc2c1)c1ccccc1)OS(C)(O)O</chem>	-8.2
20394007	<chem>c1(ccc2c(=O)c(coc2c1)c1ccccc1)O[C@H](C)CC</chem>	-8.2
2064449	<chem>O1c2cc(cc(c2C(=O)[C@@H]([C@H]1c1ccc(c(c1)OC)OC)O)OC)OC</chem>	-8.2
3070245	<chem>c1(c(C)c(=O)c2ccc(c(c2o1)CN(C)C)OC)c1ccc(Cl)cc1</chem>	-8.2
315709	<chem>o1c(cc(=O)c2cc(c(cc12)OC)OC)c1ccc(c(c1)OC)OC</chem>	-8.2
321346	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(cc1)OC)O)OC</chem>	-8.2
343081	<chem>o1cc(c(=O)c2ccc3c(OCO3)c12)c1ccc(c(c1)OC)OC</chem>	-8.2
369609	<chem>O1c2c(cc(cc2[C@H](C[C@H]1c1ccc(c(c1)OC)OC)O)CC=C)OC</chem>	-8.2
3825918	<chem>o1c2ccccc2c(=O)c(c1c1ccccc1)n1cnnn1</chem>	-8.2
42608036	<chem>O1[C@@H](CC(=O)c2c(cc(c(c12)C[C@H]([C@H](C)CO)CC=C(C)C)O)O)c1ccc(cc1OC)O</chem>	-8.2
44382543	<chem>c1(c(cc(c2c(=O)cc(oc12)c1ccccc1)OC)OC)C(F)(F)F</chem>	-8.2
471706	<chem>o1cc(c(=O)c2cc(c(cc12)OC(=O)C)OC(=O)C)c1ccc(cc1)OC(=O)C</chem>	-8.2
5272653	<chem>o1c(cc(=O)c2c(cc(cc12)OC)O)c1ccc(c(c1)OC)OC</chem>	-8.2
5280442	<chem>o1c(cc(=O)c2c(cc(cc12)O)O)c1ccc(cc1)OC</chem>	-8.2
5281601	<chem>o1c(cc(=O)c2c(cc(cc12)OC)O)c1ccc(cc1)OC</chem>	-8.2
5281779	<chem>o1cc(c(=O)c2c(c3c(cc12)OCO3)O)c1ccc(cc1)O</chem>	-8.2
5351234	<chem>o1c2cc(cc(c2c(=O)cc1c1ccc(c(c1)OC)OC)O)O</chem>	-8.2
5379262	<chem>o1c(c(c(=O)c2c(c(c(c12)OC)OC)OC)O)O)c1ccccc1</chem>	-8.2
5386961	<chem>o1c(c(c(=O)c2c(cc(c(c12)OC)O)O)OC)c1ccc(c(c1)OC)O</chem>	-8.2
5492944	<chem>o1cc(c(=O)c2c(cc(c(c12)O)O)O)c1ccc(cc1)O</chem>	-8.2
624789	<chem>o1cc(c(=O)c2cc(c(cc12)OC)OC)c1ccccc1</chem>	-8.2
632255	<chem>o1c(cc(=O)c2c(c(c(c12)OC)OC)O)O)c1ccc(c(c1)OC)OC</chem>	-8.2
69033169	<chem>c1(ccc2c(=O)cc(oc2c1)c1cc(c(c(c1)OC)OC)OC)OCCBr</chem>	-8.2

725376	<chem>o1c(cc(=O)c2cc(ccc12)OC(=O)C)c1ccc(cc1)OC</chem>	-8.2
746742	<chem>c1(coc2cc(ccc2c1=O)OC(C)C)c1ccc(F)cc1</chem>	-8.2
9562299	<chem>N([C@@H]1c2ccccc2O[C@@H](C1)c1ccccc1)NC(=S)N</chem>	-8.2
96118	<chem>o1c(cc(=O)c2c(c(cc12)OC)OC)OC)c1ccc(cc1)OC</chem>	-8.2
97332	<chem>o1c(c(c(=O)c2c(cc(cc12)OC)OC)OC)c1ccc(c(c1)OC)OC</chem>	-8.2
10162120 6	<chem>O1c2ccc(C)cc2C(=O)C[C@H]1c1ccc(cc1)N(C)C</chem>	-8.1
10176363 2	<chem>c1(c(cc2c(c(=O)c(co2)c2ccc(cc2)O)c1O)O)CC(C)(C)O</chem>	-8.1
10200304 5	<chem>O1c2cc(ccc2C=C(C1)c1cc2c(cc1OC)OCO2)O</chem>	-8.1
10232003 9	<chem>o1cc(c(=O)c2c(c(c(c12)O)O)OC)O)c1ccc(c(c1)OC)O</chem>	-8.1
10475482	<chem>o1c(c(c(=O)c2c(c(c(c12)OC)OC)OC)O)O)c1ccc(c(c1)OC)O</chem>	-8.1
10542374	<chem>o1cc(c(=O)c2c(cc(c(c12)O)O)O)c1ccc(c(c1)O)O</chem>	-8.1
10643413	<chem>Brclc(=O)c2ccccc2oc1c1ccc(cc1)S(=O)(=O)C</chem>	-8.1
10665235	<chem>o1c(c(c(=O)c2c(cc(c(c12)OC)OC)O)O)c1ccc(c(c1)O)O</chem>	-8.1
10708856	<chem>c1(cc(=O)c2ccccc2o1)c1ccc(cc1)CN=C=S</chem>	-8.1
10741771	<chem>O1c2c(c(c(cc2C[C@@H](C1(C)C)O)[C@@H]1CC(=O)c2c(cc(cc2O1)O)O)CC=C(C)C)O</chem>	-8.1
10777811	<chem>o1c2ccccc2c(=O)cc1c1ccc(cc1)CC#N</chem>	-8.1
10937632	<chem>O1c2cc(c(c(c2C(=O)C[C@H]1c1ccc(c(c1)OC)OC)OC)OC)OC</chem>	-8.1
11494111	<chem>c1(coc2cc(cc(c2c1=O)O)O)c1ccc(c2OC(CCc12)(C)C)O</chem>	-8.1
11499970	<chem>O1c2ccccc2C(=O)C[C@H]1c1ccc(cc1)N(C)C</chem>	-8.1
11709692	<chem>o1c(c(c(=O)c2c(cc(cc12)O)OC)O)c1ccc(cc1OC)O</chem>	-8.1
11726019	<chem>o1c(cc(=O)c2c(c(c(c12)O)OC)OC)O)c1ccc(c(c1)OC)O</chem>	-8.1
11777425	<chem>o1c(cc(=O)c2cc(ccc12)CC#N)c1ccccc1</chem>	-8.1

12318033	<chem>O1c2ccccc2CC(=O)[C@H]1c1ccccc1</chem>	-8.1
124211	<chem>o1c(cc(=O)c2c(c(c(c12)OC)OC)OC)O)c1c(cccc1OC)O</chem>	-8.1
125540	<chem>Clc1c(cc(c2C(=O)[C@@H](C)[C@H](Oc12)c1ccc(cc1)O)O)O</chem>	-8.1
12973586 9	<chem>O1c2c(cccc2C(=O)C[C@H]1c1ccccc1)/C=C/C(=C)C</chem>	-8.1
12978128 8	<chem>O1CC(=C(c2ccccc12)NO)c1ccccc1</chem>	-8.1
12982959 8	<chem>o1c(c(c(=O)c2c(c(c(c12)O)O)O)OC)O)c1ccccc1</chem>	-8.1
12988748 1	<chem>o1c(c(c(=O)c2c(c(ccc12)O)OC)c1ccccc1)OC</chem>	-8.1
12988767 6	<chem>O1c2cc(c(cc2C(=O)[C@@H]([C@@H]1c1ccccc1)O)OC)O</chem>	-8.1
13840297 3	<chem>o1cc(c(=O)c2cc(c(cc12)CCCO)O)c1ccc(cc1)O</chem>	-8.1
13886894	<chem>O1c2cc(ccc2[C@H]([C@H]([C@H]1c1ccc(cc1)O)O)O)O</chem>	-8.1
14055876	<chem>o1c(cc(=O)c2c(c(ccc12)OC)OC)c1ccc(c(c1)OC)OC</chem>	-8.1
14440496	<chem>o1c2cc(ccc2c(=O)c(c1c1ccccc1OC)O)OC</chem>	-8.1
14504257	<chem>c1(c(c(cc(c1c1coc2cc(ccc2c1=O)O)O)O)OC)CCC(C)(C)O</chem>	-8.1
145659	<chem>o1c(cc(=O)c2c(c(c(cc12)OC)OC)OC)c1ccc(c(c1)OC)OC</chem>	-8.1
14756305	<chem>O1c2cc(cc(c2C(=O)[C@H](C)[C@@H]1c1ccc(cc1)O)O)O</chem>	-8.1
1560918	<chem>c1(ccc2c(=O)c(coc2c1)c1ccccc1OC)OS(C)(O)O</chem>	-8.1
15761521	<chem>o1c2ccccc2c(=O)c(c1c1ccccc1)[C@@H](C)C#N</chem>	-8.1
160921	<chem>o1c(cc(=O)c2c(c(c(c12)OC)O)OC)O)c1ccc(cc1)OC</chem>	-8.1
185670	<chem>o1c(cc(=O)c2c(c(c(cc12)OC)OC)OC)c1cc(c(c(c1)OC)OC)OC</chem>	-8.1
18721	<chem>o1c(cc(=O)c2c(cc(cc12)OC(=O)C)OC(=O)C)c1ccc(cc1)OC(=O)C</chem>	-8.1
20452436	<chem>O1c2ccccc2CC[C@H]1c1ccc(cc1)O</chem>	-8.1

21270160	<chem>o1cc(c(=O)c2ccc(c(C)c12)O)c1ccc(C)cc1</chem>	-8.1
21291576	<chem>o1cc(c(=O)c2c(cc(C)cc12)O)c1ccc(cc1)O</chem>	-8.1
23644623	<chem>o1c2cc(ccc2c(=O)c(c1n1cncc1)c1ccccc1)OC</chem>	-8.1
23786424	<chem>O1c2c(c(cc(c2C(=O)C[C@@H]1c1ccccc1)OC)O)OC</chem>	-8.1
245874	<chem>O1c2cc(c(c(c2C(=O)C[C@H]1c1ccc(cc1)OC)OC)O)OC</chem>	-8.1
25058047	<chem>o1c(c(c(=O)c2c(cc(c(c12)CC=C(C)C)OCCO)O)OCCO)c1ccc(cc1)OC</chem>	-8.1
25201019	<chem>O1c2cc(cc(O)c2C(=O)C[C@H]1c1ccc(cc1)OC)O</chem>	-8.1
3083783	<chem>o1c(cc(=O)c2c(c(c(c12)O)OC)OC)O)c1ccc(cc1)OC</chem>	-8.1
4183640	<chem>c1(ccc2c(=O)c(coc2c1)c1ccc(cc1)O)O[C@H]1O[C@@H]([C@H]([C@H]([C@@H]1O)O)O)CO</chem>	-8.1
44260080	<chem>o1c(c(c(=O)c2c(c3c(c(c12)OC)OCO3)OC)OC)c1cc(c2c(OCO2)c1)OC</chem>	-8.1
44566483	<chem>O1c2cc(c(c(c2C(=O)C[C@H]1c1ccc(cc1)OC)OC)O)OC</chem>	-8.1
5281949	<chem>o1c(c(c(=O)c2c(cc(c(c12)C(C)(C)C=C)O)O)O)c1ccc(cc1)OC</chem>	-8.1
5310669	<chem>c1(coc2cc(ccc2c1=O)O)c1ccc(F)cc1</chem>	-8.1
5317652	<chem>O1c2ccc(c(c2C=CC1(C)C)O)c1coc2cc(ccc2c1=O)O</chem>	-8.1
5321859	<chem>o1c(cc(=O)c2c(c(c(c12)OC)O)OC)O)c1ccc(c(c1)O)O</chem>	-8.1
5379265	<chem>o1c2cc(cc(c2c(=O)cc1c1cc(c(c1)OC)OC)OC)O)O</chem>	-8.1
5386963	<chem>o1c(c(c(=O)c2c(c(c(c12)OC)O)OC)O)OC)c1cc(c(c1)OC)OC)OC</chem>	-8.1
54140747	<chem>c1(c(=O)c2ccccc2oc1c1ccccc1)OS(=O)(=O)O</chem>	-8.1
54450648	<chem>O1c2ccccc2C(=O)/C(=C\Ne2ccccc2O)/[C@H]1c1ccccc1</chem>	-8.1
5488781	<chem>o1cc(c(=O)c2c(c(c12)O)OC)O)c1ccc(c(c1)O)OC</chem>	-8.1
5490001	<chem>o1c2cc(ccc2c(=O)c(c1c1cc(c(c1)OC)OC)OC)O</chem>	-8.1
5491643	<chem>o1c(cc(=O)c2c(c(c12)O)OC)OC)c1ccc(c(c1)OC)OC</chem>	-8.1
59331779	<chem>o1c(cc(=O)c2c(cc(cc12)OCC#N)OC)c1ccc(c(c1)OC)OC</chem>	-8.1
631170	<chem>o1c(cc(=O)c2c(cc(cc12)OC)OC)c1ccc(c(c1)OC)OC</chem>	-8.1
688827	<chem>o1c2ccccc2c(=O)c(c1c1cc(c(c1)OC)OC)OC)O</chem>	-8.1

736738	<chem>O1c2ccccc2C(=O)[C@@H]([C@H]1c1ccccc1)O</chem>	-8.1
79730	<chem>o1c(cc(=O)c2c(cc(cc12)OC)OC)c1ccc(cc1)OC</chem>	-8.1
847733	<chem>O1c2ccccc2C[C@@H]([C@H]1c1ccccc1)O</chem>	-8.1
9064	<chem>O1c2cc(cc(c2C[C@@H]([C@H]1c1ccc(c(c1)O)O)O)O)O</chem>	-8.1
97860	<chem>O1c2ccc(cc2C(=O)C[C@H]1c1ccccc1)OC</chem>	-8.1
10050660	<chem>O1c2c(c(cc(c2[C@@H]2C(=O)c3ccc(cc3O2)OC)OC)OC)C(=O)C[C@H]1c1ccc(cc1)OC</chem>	-8.0
100943379	<chem>c1(ccc(cc1)c1cc(=O)c2ccccc2o1)S(=O)(=O)N(CC)CC</chem>	-8.0
101028405	<chem>o1c(cc(=O)c2c(cc(c(c12)NC(C)C)OC)OC)c1ccccc1</chem>	-8.0
101591281	<chem>c1(cc(c2c(=O)c(c(oc2c1OC)c1ccc(c(c1)OC)O)OC)OC)OCCCCC</chem>	-8.0
102320040	<chem>o1cc(c(=O)c2c(c(c(c12)O)O)OC)O)c1ccc(cc1)O</chem>	-8.0
102330217	<chem>O1c2cc(ccc2C(=O)[C@@H]([C@@H]1c1ccc(cc1)OC)O)OC</chem>	-8.0
10742453	<chem>O1[C@@H](CC(=O)c2c(cc(c(c12)C[C@@H](C(=C)C)CCC(C)(C)O)O)O)c1ccc(cc1OC)O</chem>	-8.0
10755200	<chem>o1c2ccc(cc2c(=O)cc1c1ccc(cc1)N(C)C)N</chem>	-8.0
12093281	<chem>O1c2ccccc2C(=O)/C(=C\c2ccc(cc2)N(=O)=O)/[C@H]1c1ccccc1</chem>	-8.0
12132870	<chem>o1cc(c(=O)c2cc(c(cc12)OC)O)c1ccc(cc1)OC</chem>	-8.0
12405140	<chem>O1c2cc(c(c(c2C(=O)C[C@@H]1c1ccc(c(c1)OC)OC)OC)OC)OC</chem>	-8.0
129661517	<chem>O1c2cc(cc(c2[C@H](C(=O)[C@@H]1c1ccccc1)O)O)O</chem>	-8.0
129661527	<chem>O1c2cc(cc(c2[C@H](C(=O)[C@@]1(c1ccccc1)O)O)O)O</chem>	-8.0
129680256	<chem>O1c2ccccc2CC([C@H]1c1ccccc1)(O)O</chem>	-8.0
12971122	<chem>O1C2=C(C=CCC2=O)CC[C@@H]1c1ccccc1</chem>	-8.0

0		
12973362 2	<chem>O1c2ccc(c(c2C(=O)C([C@@]1(c1cccc1)O)(O)O)O)OC</chem>	-8.0
12985216 0	<chem>c1(cccc2oc(c(c(=O)c12)O)c1cccc1)[C@@H]1O[C@@H]([C@@H]([C@@H]([C@H]1O)O)O)CO</chem>	-8.0
12985615 1	<chem>O(c1c(=O)c2ccccc2oc1c1cccc1)C(=O)[C@H]1O[C@@H]([C@@H]([C@@H]([C@@H]1O)O)O)O</chem>	-8.0
14057036	<chem>O1c2cc(c3c(=O)c(coc3c2C=CC1(C)C)c1cc(c(cc1OC)OC)OC)O</chem>	-8.0
147806	<chem>O1c2ccccc2C(=O)[C@H]([C@@H]1c1cccc1)O</chem>	-8.0
167616	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(c(c1)OC)OC)OC)OC</chem>	-8.0
21270125	<chem>c1(coc2cc(c(cc2c1=O)O)O)c1ccc(Cl)cc1</chem>	-8.0
21626042	<chem>o1cc(c(=O)c2c(c3c(cc12)OCO3)OC)c1cc2c(cc1OC)OCO2</chem>	-8.0
23724666	<chem>c1(coc2cc(ccc2c1=O)O)c1c(cc2OCOc2c1)O</chem>	-8.0
25068463	<chem>O1c2cc(cc(c2CC(=O)[C@H]1c1ccc(c(c1)OC)OC)OC)OC</chem>	-8.0
261859	<chem>o1c(cc(=O)c2c(c(c(c12)OC)OC)OC)O)c1cc(c(c(c1)OC)OC)OC</chem>	-8.0
3070246	<chem>c1(c(C)c(=O)c2ccc(c(c2o1)CN(CC)CC)OC)c1ccc(Cl)cc1</chem>	-8.0
3245800	<chem>c1(cc(=O)c2ccccc2o1)c1ccc(cc1)SC</chem>	-8.0
35028119	<chem>o1c(cc(=O)c2c(c(c(c12)OC)OC)OC)OC)c1cccc(c1)OC</chem>	-8.0
3747	<chem>c1(ccc2c(=O)c(coc2c1)c1cccc1)OC(C)C</chem>	-8.0
44257042	<chem>O1[C@H](C=C[C@H]2C(=C([C@H](C=C12)O)O)OC)c1ccc(c(c1)O)O</chem>	-8.0
44258304	<chem>o1c(cc(=O)c2c(cc(cc12)OC)OC)c1cc(c(cc1O)O)O</chem>	-8.0
442583	<chem>o1c(cc(=O)c2c(c(c(cc12)OC)OC)OC)c1cccc1</chem>	-8.0
44259864	<chem>o1c(c(c(=O)c2c(c(c3c(cco3)c12)OC)OC)OC)c1ccc2c(OCO2)c1</chem>	-8.0
5003667	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(cc1)OC)OC)OC</chem>	-8.0
5353911	<chem>o1cc(c(=O)c2c(cc(c(c12)OC)O)O)c1ccc(cc1)O</chem>	-8.0
5372237	<chem>o1c2cccc(c2c(=O)c(c1c1ccc(cc1)OC)C(=O)c1ccc(cc1)OC)O</chem>	-8.0

5380905	<chem>o1c2cc(cc(c2c(=O)c(c1c1ccc(c(c1)O)OC)OC)O)O</chem>	-8.0
5381920	<chem>o1c2cc(ccc2c(=O)cc1c1cc(c(c1)OC)OC)OC)O</chem>	-8.0
54490901	<chem>O1c2ccccc2C(=O)/C(=C\c2cccc(c2)NC(=O)C)/[C@H]1c1ccccc1</chem>	-8.0
5491929	<chem>o1cc(c(=O)c2c(c3c(cc12)OCO3)O)c1ccccc1OC</chem>	-8.0
586387	<chem>O1c2cc(cc(c2C(=O)[C@@H]([C@@H]1c1ccc(cc1)OC)O)O)O</chem>	-8.0
629965	<chem>o1c(cc(=O)c2c(c(ccc12)OC)OC)c1c(cccc1OC)OC</chem>	-8.0
631095	<chem>o1c(c(c(=O)c2c(cc(cc12)OC)OC)OC)c1ccc(cc1)OC</chem>	-8.0
633124	<chem>o1c(cc(=O)c2c(c(c(c12)OC)O)OC)O)c1cc(c(c1)OC)OC)O</chem>	-8.0
6710704	<chem>o1cc(c(=O)c2c(cc(cc12)OC)OC)c1ccccc1</chem>	-8.0
67743168	<chem>O1c2cc(cc(c2[C@H]([C@@H]([C@@H]1c1cccc(c1)O)O)O)O)O</chem>	-8.0
740761	<chem>c1(coc2cc(ccc2c1=O)OC(C)C)c1c(F)cccc1</chem>	-8.0
86641846	<chem>o1c(cc(=O)c2c(cc(cc12)OCC#C)OC)c1ccc(c(c1)OC)OC</chem>	-8.0
9813808	<chem>O1c2ccccc2C[C@H]([C@H]1c1ccc(c(c1)O)O)O</chem>	-8.0
10121375 9	<chem>o1cc(c(=O)c2c(cc(cc12)O)O)c1c(cc(c(c1)CC=C(C)C)OC)O</chem>	-7.9
10121493 7	<chem>o1c(c(c(=O)c2cc(ccc12)CN(CC)CC)O)c1ccc(cc1)N(CC)CC</chem>	-7.9
10139688 7	<chem>O1c2c3c(=O)c(coc3c(c(c2C[C@@H]1C(C)(C)O)O)CC=C(C)C)c1ccc(cc1)O</chem>	-7.9
10159128 2	<chem>c1(cc(c2c(=O)c(c(oc2c1OC)c1ccc(c(c1)OC)OC)OC)OC)OCCCCC</chem>	-7.9
10188771 8	<chem>c1(c(cc(c2c(=O)cc(oc12)c1ccc(cc1)O)O)O)[C@@H]1O[C@@H](C)[C@@H]([C@@H](C1)O)O</chem>	-7.9
10386481	<chem>o1c(cc(=O)c2c(c(c(c12)OC)OC)OC)O)c1cc(c(c(c1)OC)O)OC</chem>	-7.9
10468234	<chem>O1c2ccccc2C(=O)[C@@](C)([C@H]1c1ccc(C)cc1)O</chem>	-7.9
10594862	<chem>Br1c(=O)c2ccccc2oc1c1ccc(cc1)[S@@](=O)C</chem>	-7.9
10759582	<chem>O1c2cc(c(c(c2C(=O)C[C@H]1c1ccc(cc1)O)O)C(C)(C)C=C)O</chem>	-7.9

12043067	<chem>c1(cc(=O)c2c(cc(c(c2o1)[C@@H]1C(=O)CN(C)CC1)O)O)c1c(Cl)cccc1</chem>	-7.9
12403736 3	<chem>O1c2ccccc2[C@@H]([C@@H]([C@H]1c1ccccc1)O)O</chem>	-7.9
12967509 9	<chem>o1c2ccccc2c(=O)c(c1c1ccccc1)OC(=O)c1cc(c(c(c1)O)O)O</chem>	-7.9
13916267	<chem>o1c(c(c(=O)c2c(cc(c(c12)OC)O)OC)OC)c1ccc(c(c1)OC)OC</chem>	-7.9
14372618	<chem>o1c(cc(=O)c2c(c(c(cc12)OC)O)OC)c1ccccc1</chem>	-7.9
14630497	<chem>o1c(c(c(=O)c2c(cc3c(C=CC(C)(C)O3)c12)O)CCC(C)(C)O)c1cc(c(cc1O)O)O</chem>	-7.9
15126657	<chem>o1cc(c(=O)c2ccc(c(C)c12)O)c1ccc(cc1)O</chem>	-7.9
15625549	<chem>O1c2c(c(c(c2C(=O)C[C@H]1c1ccc(c(c1)OC)OC)O)OC)OC)OC</chem>	-7.9
181092	<chem>o1c(cc(=O)c2c(c(c(c(c12)OC)OC)OC)O)c1ccc(c(c1)OC)O</chem>	-7.9
18324915	<chem>c1(c(c(=O)c2ccccc2o1)c1cccc(F)c1)c1ccc(cc1)S(=O)(=O)C</chem>	-7.9
25022469	<chem>o1c(cc(=O)c2c(c(cc(c12)OC)OC)OC)c1cc(ccc1OC)OC</chem>	-7.9
25585	<chem>o1c(C)c(c(=O)c2cccc(c12)OCCN(C)C)c1ccc(cc1)OC</chem>	-7.9
282014	<chem>O1c2cc(cc(c2C[C@H]([C@H]1c1ccc(cc1)O)O)O)O</chem>	-7.9
3080750	<chem>o1c(cc(=O)c2c(c(c(c(c12)OC)OC)OC)O)c1ccc(c(c1)O)OC</chem>	-7.9
3083840	<chem>o1cc(c(=O)c2cc(c(cc12)OC(=O)C)OC)c1ccc(cc1)OC</chem>	-7.9
3084507	<chem>o1c(cc(=O)c2c(c(c(c(c12)OC)OC)OC)O)c1cc(c(c(c1)OC)OC)O</chem>	-7.9
3084508	<chem>o1c(cc(=O)c2c(c(c(c(c12)OC)OC)OC)O)c1cc(c(c(c1)O)OC)O</chem>	-7.9
331149	<chem>o1c(cc(=O)c2c(c(c(c(c12)OC)OC)OC)OC)c1cc(c2c(OCO2)c1)OC</chem>	-7.9
369612	<chem>O1c2c(cc(cc2[C@H](C[C@H]1c1ccc(c(c1)OC)OC)OC)CC=C)OC</chem>	-7.9
462696	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1cc(c(c(c1)OC)OC)OC)O)O</chem>	-7.9
493376	<chem>o1c2cc(cc(c2c(=O)cc1c1cc(c(c(c1)OC)OC)OC)OC)OC</chem>	-7.9
49788614	<chem>o1c2cc(cc(c2c(=O)c(c1c1ccc2c(OCO2)c1)OCC=C(C)C)O)OC</chem>	-7.9
5280373	<chem>o1cc(c(=O)c2c(cc(cc12)O)O)c1ccc(cc1)OC</chem>	-7.9
5281695	<chem>o1c(c(c(=O)c2c(c(c(cc12)O)OC)O)OC)c1ccc(cc1)OC</chem>	-7.9

5281804	<chem>o1cc(c(=O)c2c(cc(cc12)OC)O)c1ccc(cc1)O</chem>	-7.9
5281811	<chem>o1cc(c(=O)c2c(c(c(cc12)O)OC)O)c1ccc(cc1)O</chem>	-7.9
5284649	<chem>o1cc(c(=O)c2cc(c(cc12)O)O)c1ccc(cc1)O</chem>	-7.9
53233892	<chem>c1(ccc2c(c(=O)cc(o2)c2ccccc2)c1)OP(=O)(OCC)OCC</chem>	-7.9
5385091	<chem>c1(coc2cc(ccc2c1=O)O)c1c(cc2OCOc2c1)OC</chem>	-7.9
54070148	<chem>c1(ccc(cc1)OCCO)[C@H]1Oc2ccccc2CC1</chem>	-7.9
5481647	<chem>o1c(cc(=O)c2c(c(c(cc12)O)OC)OC)c1ccccc1</chem>	-7.9
57409964	<chem>c1(cc(c(c(c1)C[C@@H](C(=C)C)O)O)C/C=C(/C)\CO)c1oc2cc(c(c(c2c(=O)c1OC)O)OC)O</chem>	-7.9
5748605	<chem>o1cc(c(=O)c2ccc(cc12)O)c1ccc(c(c1)OC)OC</chem>	-7.9
614295	<chem>[C@H]1(C(=O)c2ccccc2O[C@@H]1c1ccccc1)SCCC</chem>	-7.9
68077	<chem>o1c(cc(=O)c2c(c(c(c12)OC)OC)OC)OC)c1ccc(cc1)OC</chem>	-7.9
69047096	<chem>c1(ccc(cc1OCOC)OCOC)[C@@H]1Oc2ccccc2C(=O)C1</chem>	-7.9
72344	<chem>o1c(cc(=O)c2c(c(c(c12)OC)OC)OC)OC)c1ccc(c(c1)OC)OC</chem>	-7.9
7309334	<chem>O1c2ccccc2C[C@H]([C@@H]1c1ccccc1)O</chem>	-7.9
7454026	<chem>o1cc(c(=O)c2ccc(cc12)O)c1ccc(cc1)N(=O)=O</chem>	-7.9
91584129	<chem>o1c2cc(c(c(c2c(=O)cc1c1ccc(c(c1OC)OC)O)O)OC)O</chem>	-7.9
10102840 9	<chem>o1c(cc(=O)c2c(cc(c(c12)NCC=C)OC)OC)c1ccccc1</chem>	-7.8
10156189 8	<chem>o1c2ccccc2c(=O)c(c1c1ccccc1)OCC#C</chem>	-7.8
10814211	<chem>o1c(c(c(=O)c2c(c(c(c12)OC)OCC=C(C)C)OC)OC)c1ccc2c(OCO2)c1</chem>	-7.8
11048450	<chem>O1C(C)(C)C=Cc2c(c3C(=O)C[C@H](Oc3c(c12)C[C@@H](C(C)(C)O)O)c1ccc(cc1)O)O</chem>	-7.8
12407921	<chem>o1c2ccc(cc2c(=O)cc1c1ccc(cc1)OCCO)C(=O)O</chem>	-7.8
12967478 1	<chem>O1c2ccccc2C[C@@H]([C@@H]1c1ccccc1)OC</chem>	-7.8
12983450	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(cc1)OC(=O)C)OC)OC(=O)C</chem>	-7.8

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12984454 3	<chem>o1cc(c(=O)c2c(c(c(c12)O)O)OC)O)c1cc(c(c1)OC)OC)O</chem>	-7.8
13873818	<chem>o1c(cc(=O)c2c(c(c(cc12)OCc1cccc1)OC)OC)c1ccc(c(c1)OC)OC</chem>	-7.8
14304977	<chem>o1c2cccc2c(=O)c(c1c1cc(c(c1)OC)OC)OC)C(=O)O</chem>	-7.8
182659	<chem>O1c2cc(cc(c2C[C@@H]([C@H]1c1ccc(c(c1)OC)OC)O)OC)OC</chem>	-7.8
18324902	<chem>c1(c(c(=O)c2cccc2o1)c1ccc(cc1)F)c1ccc(cc1)S(=O)(=O)C</chem>	-7.8
358832	<chem>o1c(cc(=O)c2c(c(c(c12)OC)OC)OC)O)c1ccc(c(c1)OC)OC</chem>	-7.8
369615	<chem>O1c2c(cccc2C(=C)C[C@@H]1c1ccc(c(c1)OC)O)OC</chem>	-7.8
42607933	<chem>O1c2c(c(cc(c2C[C@@H](C(=C)C)O)O)O)C(=O)C[C@H]1c1ccc(cc1)O</chem>	-7.8
42607957	<chem>O1c2c(c(cc(c2C(=O)C[C@H]1c1ccc(cc1)OC)O)O)CC(=C(C)C)O</chem>	-7.8
42608126	<chem>O1c2c(c(c(c2C(=O)C[C@H]1c1cc(c2c(OCO2)c1)OC)OC)OC)OC</chem>	-7.8
44257043	<chem>O1[C@H](C=C[C@H]2C(=C([C@H](C=C12)O)O)OC)c1ccc(c(c1)O)OC</chem>	-7.8
44260053	<chem>o1c(c(c(=O)c2c(c(c(c12)OC(=O)CC(C)C)O)OC)O)OC)c1ccc(cc1)OC</chem>	-7.8
5280961	<chem>o1cc(c(=O)c2c(cc(cc12)O)O)c1ccc(cc1)O</chem>	-7.8
5281676	<chem>o1c2cc(cc(c2c(=O)c(c1c1cc(c(cc1O)OC)O)OC)O)OC</chem>	-7.8
5281781	<chem>o1cc(c(=O)c2c(c(c(cc12)O)OC)O)c1ccc(cc1)OC</chem>	-7.8
5281801	<chem>o1cc(c(=O)c2c(cc(cc12)O)O)c1ccc(c(c1)O)O</chem>	-7.8
5284648	<chem>o1cc(c(=O)c2ccc(cc12)O)c1ccc(c(c1)O)O</chem>	-7.8
5376891	<chem>o1cc(c(=O)c2ccc(cc12)O)c1cccc1</chem>	-7.8
5378391	<chem>o1c(C)c(c(=O)c2ccc(c(c12)CC=C)O)c1cccc1</chem>	-7.8
5385026	<chem>o1c(c(c(=O)c2c(c(c(cc12)O)OC)OC)O)c1cccc1</chem>	-7.8
5417907	<chem>o1c2cc(ccc2c(=O)c(c1C)c1ccc(cc1)N(=O)=O)O</chem>	-7.8
5487785	<chem>o1cc(c(=O)c2c(c(c(cc12)OC)OC)O)c1ccc(cc1)O</chem>	-7.8
5491412	<chem>o1c2cc(cc(c2c(=O)c(c1c1cc(c(c1)O)OC)O)OC)O)OC</chem>	-7.8
628412	<chem>o1c(c(c(=O)c2c(cc(cc12)OC)OC)OC)c1cccc1OC</chem>	-7.8

628555	<chem>o1c2cc(ccc2c(=O)c(c1c1ccc(cc1)OC)OC)OC</chem>	-7.8
638006	<chem>o1cc(c(=O)c2ccc(cc12)OC)c1ccccc1</chem>	-7.8
96539	<chem>o1c(cc(=O)c2c(c(c(c12)OC)OC)OC)O)c1ccc(cc1)OC</chem>	-7.8
10102840 6	<chem>o1c(cc(=O)c2c(cc(c12)NCCC)OC)OC)c1ccccc1</chem>	-7.7
10102840 7	<chem>o1c(cc(=O)c2c(cc(c12)NCC(C)C)OC)OC)c1ccccc1</chem>	-7.7
10117916 5	<chem>o1c(c(c(=O)c2c(cc(cc12)OC)OCCCO)OC)c1ccc(c(c1)OC)OC</chem>	-7.7
10165084 3	<chem>O1c2ccccc2C(=O)/C(=C\c2cccc(c2)N(=O)=O)/[C@H]1c1ccccc1</chem>	-7.7
10315196	<chem>O1c2cc(c(c(c2C(=O)C[C@@H]1c1ccc(cc1)O)O)C(C)(C)C=C)O</chem>	-7.7
10665307	<chem>Br1c(=O)c2ccccc2oc1c1ccc(cc1)SC</chem>	-7.7
12973375 0	<chem>Cl[C@H]1c2ccccc2O[C@@H]([C@@H]1O)c1ccccc1</chem>	-7.7
12988275 2	<chem>o1cc(c(=O)c2c(cc(c12)OC)OC)OC)c1ccc(cc1)O</chem>	-7.7
13045742	<chem>O1c2cc(cc(c2CC[C@H]1c1ccc(c(c1)OC)OC)OC)OC</chem>	-7.7
13045744	<chem>O1c2cc(cc(c2CC[C@H]1c1ccc(c(c1)OC)OC)OC)OC</chem>	-7.7
13250796 0	<chem>o1cc(c(=O)c2cc(c(cc12)CO)OC)c1ccc(cc1)O</chem>	-7.7
14732294	<chem>O1c2cc(cc(c2C[C@@H]([C@@H]1c1ccc(c(c1)O)O)O)OC)OC</chem>	-7.7
17585058	<chem>c1(ccc2c(=O)c(coc2c1)c1ccccc1)OCCBr</chem>	-7.7
18324974	<chem>c1(c(=O)c2ccccc2oc1c1ccc(cc1)S(=O)(=O)C)c1ccc(Cl)cc1</chem>	-7.7
185027	<chem>O1c2c(c(ccc2C(=O)C[C@@H]1c1ccccc1)OC)/C=C/C(=C)C</chem>	-7.7
189551	<chem>O1C(=C(C(=O)[C@]2(CC=CC(=C12)OC)O)OC)c1ccccc1</chem>	-7.7
20452422	<chem>O1c2ccccc2CC[C@H]1c1ccc(cc1)N(C)C</chem>	-7.7

21573556	<chem>O1c2cc(cc(c2C(=O)C[C@H]1c1ccc(c(c1OC)OC)OC)OC)OC</chem>	-7.7
25232840	<chem>O1c2cc(cc(c2CC[C@H]1c1ccc(cc1)OC)O)O</chem>	-7.7
343083	<chem>c1(coc2cc(ccc2c1=O)OC)c1c(cc2OCOc2c1)OC</chem>	-7.7
44133602	<chem>o1cc(c(=O)c2c(c(c(cc12)O)OC)O)c1cc(c(c(c1)OC)O)OC</chem>	-7.7
462698	<chem>O1c2c(c(c(c2C(=O)C[C@@H]1c1ccc(cc1)OC)OC)OC)OC)OC</chem>	-7.7
5280448	<chem>o1cc(c(=O)c2ccc(cc12)O)c1ccc(c(c1)O)OC</chem>	-7.7
5318041	<chem>o1c(cc(=O)c2c(c(c(c12)OC)OC)OC)OC)c1ccc(c(c1)O)O</chem>	-7.7
5318979	<chem>O1c2ccccc2[C@@H]([C@@H]([C@@H]1c1ccccc1)O)O</chem>	-7.7
5319422	<chem>o1cc(c(=O)c2ccc(cc12)O)c1ccc(c(c1)OC)O</chem>	-7.7
5481229	<chem>O1c2c(c(cc(c2C=CC1(C)C)c1coc2cc(cc(c2c1=O)O)O)OC)O</chem>	-7.7
56648912	<chem>o1c(cc(=O)c2c(c(c(cc12)OCC=C)OC(=O)C)OC(=O)C)c1ccccc1</chem>	-7.7
71346541	<chem>o1c2ccccc2c(=O)c(c1c1ccc(cc1)N(C)C)OC</chem>	-7.7
71428798	<chem>o1cc(c(=O)c2ccc(c(c12)OC)O)c1ccc(cc1)O</chem>	-7.7
74977227	<chem>O1c2cc(cc(c2CC[C@H]1c1ccc(c(c1)OC)OC)O)O</chem>	-7.7
911486	<chem>o1c2cc(ccc2c(=O)c(c1C)c1ccc(cc1)N(=O)=O)OC</chem>	-7.7
10069029	<chem>c1(c(c(=O)c2ccc(cc2o1)O)c1ccc(cc1)OC)SCc1ccncc1</chem>	-7.6
10317448	<chem>c1(c(c(=O)c2ccc(cc2o1)O)c1ccc(cc1)O)SCc1ccncc1</chem>	-7.6
10526049	<chem>o1c(c(c(=O)c2c(c(c(c12)OC)OC)OCOC)OC)O)c1ccc(cc1)OC</chem>	-7.6
11417114	<chem>c1(c(c(=O)c2ccc(cc2o1)O)c1ccccc1)SCc1enccc1</chem>	-7.6
11704980	<chem>o1c2ccccc2c(=O)c(c1c1cc(c(c(c1)OC)OC)OC)C(=O)c1ccc(cc1)OC</chem>	-7.6
12903597 6	<chem>O1c2ccccc2C[C@@H]([C@@H]1c1ccccc1)O</chem>	-7.6
12966237 4	<chem>o1c2ccccc2c(=O)c(c1C)c1ccc(cc1)N(=O)=O</chem>	-7.6
12967461 9	<chem>[C@H]1(c2ccccc2O[C@H](C1)c1ccccc1)S</chem>	-7.6

12973416 4	<chem>o1c(c(c(=O)c2c(c(c(c12)O)OC)OC)OC)O)c1cccc1O</chem>	-7.6
12986412 1	<chem>o1c2cc(cc(c2c(=O)c(c1c1ccc(cc1)O[C@H](C(=C)C)CO)OC)O)OC</chem>	-7.6
13251736 8	<chem>o1c(cc(=O)c2c(c(C)c(c(c12)C(C)(C)O)OC)O)c1ccc(cc1)OC</chem>	-7.6
136418	<chem>o1c(cc(=O)c2c(c(c(cc12)OC(=O)C)OC(=O)C)OC(=O)C)c1ccc(cc1)OC(=O)C</chem>	-7.6
13903075 7	<chem>o1cc(c(=O)c2ccc(c(c12)OC)CCCO)c1ccc(cc1)OC</chem>	-7.6
14304994	<chem>c1(c(=O)c2ccccc2oc1c1cccc1)C(=O)N1CCN(CC1)Cc1cccc1</chem>	-7.6
14630603	<chem>o1cc(c(=O)c2c(c3c(cc12)OCO3)OC)c1cccc(c1OC)OC</chem>	-7.6
14804713	<chem>o1c(c(c(=O)c2c(C)cc(cc12)OC)OC)c1ccc(cc1)O</chem>	-7.6
14886014	<chem>o1c2c(c(cc(c2c(=O)c(c1c1ccc2c(OCO2)c1)OC)OC)O)OC</chem>	-7.6
18325002	<chem>c1(c(c(=O)c2ccccc2o1)c1cccc1F)c1ccc(cc1)S(=O)(=O)C</chem>	-7.6
22134047	<chem>o1c(c(c(=O)c2c(c(ccc12)OC)OC)O)c1cccc1</chem>	-7.6
44257187	<chem>O1c2c(c(cc(c2CC[C@H]1c1cccc1)OC)OC)CCC(C)(C)O</chem>	-7.6
44412009	<chem>O1c2c(C)c(cc(c2C(=O)C[C@H]1c1cccc1)OC)OC</chem>	-7.6
5281704	<chem>o1cc(c(=O)c2cc(c(cc12)O)OC)c1ccc(cc1)OC</chem>	-7.6
631791	<chem>o1c(c(c(=O)c2c(c(c3c(cco3)c12)OC)OC)OC)c1cccc1</chem>	-7.6
632135	<chem>o1c(cc(=O)c2c(cc(c(c12)OC)OC)OC)c1ccc(c(c1)OC)OC</chem>	-7.6
66692593	<chem>O1c2ccccc2C[C@@H]([C@@H]1c1cccc1)O</chem>	-7.6
9821032	<chem>c1(c(c(=O)c2ccccc2o1)c1cccc1)c1ccc(cc1)S(=O)(=O)C</chem>	-7.6
9928523	<chem>O1c2c(c(cc(c2C(=O)C[C@H]1c1ccc(cc1)O)OC)O)CC=C(C)C</chem>	-7.6
10102840 8	<chem>o1c(cc(=O)c2c(cc(c(c12)NCCC(C)C)OC)OC)c1cccc1</chem>	-7.5
11244229	<chem>c1(c(c(=O)c2ccc(cc2o1)OC)c1cccc1)SCC=C</chem>	-7.5
11795367	<chem>o1c(c(c(=O)c2c(c(c(c12)OC)O)OC)OC)OC)c1ccc2c(OCO2)c1</chem>	-7.5

12428921	<chem>O1c2ccccc2C(=O)/C(=C\c2cccc(c2)O)/[C@H]1c1ccccc1</chem>	-7.5
13916278	<chem>o1c(c(c(=O)c2c(cc(c(c12)OC)O)O)OC)c1ccc(cc1)OC</chem>	-7.5
15761525	<chem>O1c2ccccc2C(=O)C([C@H]1c1ccccc1)(CO)CO</chem>	-7.5
16215025	<chem>c1(cc(c(c2O[C@H](CC(=O)c12)c1ccccc1)OC)OC)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO</chem>	-7.5
18324995	<chem>c1(c(c(=O)c2ccccc2o1)c1ccccc1F)c1ccc(cc1)S(=O)(=O)N</chem>	-7.5
369616	<chem>O1c2c(cc(cc2[C@H](C[C@H]1c1ccc(c(c1)OC)OC)OC(=O)C)CC=C)OC</chem>	-7.5
386331	<chem>o1c(c(c(=O)c2c(c(c(cc12)OC)OC)OC)OC)c1ccc(c(c1)OC)OC</chem>	-7.5
44257206	<chem>o1c(C)c(c(=O)c2ccc(c(c12)C(=O)C)O)c1ccccc1</chem>	-7.5
5282074	<chem>o1cc(c(=O)c2c(cc(cc12)O)O)c1ccc(cc1O)O</chem>	-7.5
5322009	<chem>o1c(cc(=O)c2c(c(c(cc12)OC(=O)C)OC)OC(=O)C)c1ccc(cc1)OC(=O)C</chem>	-7.5
54423602	<chem>c1(c(c(=O)c2ccccc2o1)c1ccccc1)OC(C)C</chem>	-7.5
626146	<chem>o1c(C)c(c(=O)c2ccc(cc12)OCC=C)c1ccccc1</chem>	-7.5
631176	<chem>o1cc(c(=O)c2cc(c(cc12)OC)OC)c1ccc(c(c1)OC)OC</chem>	-7.5
634440	<chem>o1c(c(c(=O)c2c(c(c(cc12)OC)OCC)OCC)OC)c1ccc(c(c1)OCC)OC</chem>	-7.5
71586772	<chem>o1c(cc(=O)c2c(c(c(cc12)OC(=O)C)OC)OC(=O)C)c1ccccc1</chem>	-7.5
97151	<chem>o1c(cc(=O)c2c(c(c(c12)OC)OC)OC)OC)c1ccc2c(OCO2)c1</chem>	-7.5
10166596 2	<chem>o1c2cc(ccc2c(=O)c(c1c1ccc(c(c1)OCCO)OCCO)OCCO)OCCO</chem>	-7.4
10219490 9	<chem>o1c(c(c(=O)c2c(c(c(c12)OC)OCC=C(C)C)OC)OC)OC)c1ccc(c(c1)OC)OC</chem>	-7.4
11610052	<chem>o1cc(c(=O)c2c(cc(cc12)O)O)c1ccc(c(c1CC=C(C)C)O)O</chem>	-7.4
12043064	<chem>c1(cc(=O)c2c(cc(c(c2o1)[C@@H]1CN(C)CC[C@H]1O)O)O)c1c(Cl)cccc1</chem>	-7.4
12982055 4	<chem>o1c(c(c(=O)c2c(cc(c(c12)OC)OC)OC)O)c1ccc(c(c1)OC)OC</chem>	-7.4
12983719 5	<chem>o1c(c(c(=O)c2c(c(c(c12)O)O)O)OC)OC)c1ccccc1O</chem>	-7.4

12988194 0	<chem>c1(c(=O)c2ccccc2oc1c1ccccc1)[C@@H]1O[C@H](C)[C@@H]([C@H](C1)O)O</chem>	-7.4
13045799	<chem>O1c2ccccc2C[C@@H]([C@@H]1c1ccccc1)OC(=O)C</chem>	-7.4
13251736 6	<chem>o1c(cc(=O)c2cc(c(c(c12)/C=C(\C)/CO)OC)O)c1ccc(cc1)OC</chem>	-7.4
136420	<chem>o1cc(c(=O)c2c(cc(cc12)OC)OC)c1ccc(cc1)OC</chem>	-7.4
13903076 7	<chem>o1cc(c(=O)c2ccc(c(c12)OC)C(=O)CCO)c1ccc(cc1)OC</chem>	-7.4
18324937	<chem>c1(c(c(=O)c2ccccc2o1)c1ccc(cc1)F)c1ccc(cc1)S(=O)(=O)N</chem>	-7.4
44257040	<chem>O1[C@H](C=C[C@H]2C(=C([C@H](C=C12)O)O)OC)c1ccc(cc1)OC</chem>	-7.4
5281706	<chem>o1cc(c(=O)c2c(cc(cc12)OC)O)c1ccc(cc1O)O</chem>	-7.4
53796934	<chem>o1cc(c(=O)c2c(cc(cc12)OC)O)c1ccc(cc1O)OC</chem>	-7.4
5466794	<chem>c1(cc(=O)c2c(cc(c(c2o1)[C@@H]1CCN(C)C[C@H]1O)O)O)c1c(Cl)cccc1</chem>	-7.4
6116651	<chem>O1c2ccccc2C(=O)/C(=C\c2cnc2)/[C@H]1c1ccccc1</chem>	-7.4
633456	<chem>o1c2cc(ccc2c(=O)c(c1C)c1cc(c(cc1OC)OC)OC)OC(=O)C</chem>	-7.4
9864504	<chem>c1(c(c(=O)c2ccccc2o1)c1ccccc1)c1ccc(cc1)S(=O)(=O)N</chem>	-7.4
10232161 0	<chem>c1(coc2cc(cc(c2c1=O)O)O)c1ccc2OCOc2c1OC</chem>	-7.3
10957930	<chem>O1c2ccccc2C(=O)/C(=C/c2ccccc2)/[C@@H]1c1ccccc1</chem>	-7.3
11024735	<chem>O1c2ccccc2C(=O)/C(=C/c2ccc(cc2)N(=O)=O)/[C@@H]1c1ccccc1</chem>	-7.3
11176755	<chem>c1(c(c(=O)c2ccc(cc2o1)OC)c1ccc(C)cc1)SCc1cnc1</chem>	-7.3
11500888	<chem>O1c2cc(cc(c2C(=O)[C@@H]([C@H]1c1ccc(cc1OC)O)O)OC)O</chem>	-7.3
12043063	<chem>c1(cc(=O)c2c(cc(c(c2o1)[C@@H]1CN(C)CC[C@H]1O)OC)OC)c1c(Cl)cccc1</chem>	-7.3
12310757	<chem>c1(c(cc(c2c(=O)c(c(oc12)c1ccc(cc1)OC)O)O)O)CCC(C)(C)O</chem>	-7.3
12976293 0	<chem>O1c2cc(cc(c2C(=O)C[C@]1(c1ccc(cc1)O)OC)O)OC</chem>	-7.3
12983478	<chem>o1c(c(c(=O)c2c(c(c(cc12)OC)OC)OC)OCC)c1ccc(c(c1)OCC)OC</chem>	-7.3

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12986605 2	<chem>o1c2cccc2c(=O)c(c1c1cccc1)[C@H]1CNCCN1Cc1cccc1</chem>	-7.3
15761527	<chem>C1(C(=O)c2cccc2O[C@H]1c1cccc1)(CCl)CCl</chem>	-7.3
23644938	<chem>c1(c(c(=O)c2ccc(cc2o1)OC)c1cccc1)Sc1ncn[nH]1</chem>	-7.3
44257041	<chem>O1[C@H](C=C[C@H]2C(=C([C@H](C=C12)O)O)OC)C1=CCC(=CC1)O</chem>	-7.3
51041990	<chem>o1c2cc(cc(c2c(=O)c(c1c1cc(cc(c1CC=C(C)C)O)OC)OC)O)O</chem>	-7.3
54140898	<chem>o1c(c(c(=O)c2c(c(ccc12)OCC)OCC)OCC)c1cccc1</chem>	-7.3
54728923	<chem>o1c(=O)c(c(c2c(cc(cc12)O)O)O)c1ccc(cc1)O</chem>	-7.3
631782	<chem>o1c2cc(ccc2c(=O)c(c1C)c1ccc(cc1OC)OC)OCC=C</chem>	-7.3
634724	<chem>o1c(c(c(=O)c2c(c(c(cc12)OCC)OC)OCC)OC)c1ccc(c(c1)OC)OCC</chem>	-7.3
91727421	<chem>O1c2cc(cc(c2C(=O)[C@H]([C@@H]1c1ccc(c(c1)OC)OC)OC(=O)C)OC)OC</chem>	-7.3
10188772 1	<chem>c1(c(cc(c2c(=O)cc(oc12)c1ccc(cc1)O)O)OC)[C@@H]1O[C@@H](C)[C@@H](C(=O)C1)O</chem>	-7.2
10551087	<chem>O1c2c3c(cc(c2C[C@H](C1(C)C)O)[C@@H]1CC(=O)c2c(cc(cc2O1)O)O)CCC(C)(C)O3</chem>	-7.2
11471620	<chem>o1cc(c(=O)c2ccc(cc12)OC)c1ccc(cc1O)O</chem>	-7.2
11485667	<chem>c1(c(c(=O)c2ccc(cc2o1)OC)c1cccc1)SCc1cccn1</chem>	-7.2
12428924	<chem>O1c2cccc2C(=O)/C(=C\c2ccc(cc2)O)/[C@H]1c1cccc1</chem>	-7.2
12971674 8	<chem>[P@]12(=O)O[C@@H]3[C@@H]4c5cccc5O[P@]5(=O)O[C@H]6[C@H]([C@H]([C@H]([C@H]([C@H]6O1)O2)C3=O)O4)O5</chem>	-7.2
12981808 8	<chem>Br[C@]1(C(=O)c2cccc2O[C@H]1c1cccc1)N(=O)=O</chem>	-7.2
12984868 0	<chem>o1c(c(c(=O)c2c(c(cc(c12)OC)OC)OC)OC)c1ccc(c(c1)OC)OC</chem>	-7.2
150893	<chem>o1c(c(c(=O)c2c(c(c(c12)OC)OC)OC)OC)OC)c1ccc(c(c1)OC)OC</chem>	-7.2
16213663	<chem>O1/C(=C/2\C=CC(=CC2)N(C)C)/C=C(c2ccc(cc12)N(CC)CC)c1cccc1C(=O)O</chem>	-7.2
23644937	<chem>c1(c(c(=O)c2ccc(cc2o1)OC)c1cccc1)Sc1ncn1C</chem>	-7.2

42608003	<chem>O1c2c(c3c(C(=O)C[C@H](O3)c3ccc(c(c3)O)O)c3OC(C)(C)CCc23)CCC1(C)C</chem>	-7.2
462694	<chem>O1c2cc(ccc2C(=O)[C@H]([C@H]1c1ccc(cc1)OC)OC)O</chem>	-7.2
5378260	<chem>o1cc(c(=O)c2ccc(c(c12)O)O)c1ccc(cc1O)O</chem>	-7.2
90000191	<chem>o1c(c(c(=O)c2c(c(c(c12)OC)OC)OC)O)O)c1cccc(c1OC)OC</chem>	-7.2
10139688	<chem>O1c2c3c(=O)c(coc3c(c(c2C=CC1(C)C)O)C[C@H](C(C)(C)O)O)c1ccc(cc1)O</chem>	-7.1
10200537	<chem>c1(cc(=O)c2c(cc(c(c2o1)[C@@H]1CN(C)CC[C@@H]1O)OC)OC)c1c(Cl)cccc1</chem>	-7.1
11246736	<chem>c1(c(c(=O)c2ccc(cc2o1)OC)c1ccc(cc1)OC)SCc1ccncc1</chem>	-7.1
12972874	<chem>c1(c(c(=O)c2cccc(c2o1)c1cccc1)[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO</chem>	-7.1
12983569	<chem>O1c2cccc2C(=O)[C@@]([C@]1(c1cccc1)O)(c1c(=O)c2cccc2oc1c1cccc1)O</chem>	-7.1
12989197	<chem>o1cc(c(=O)c2ccc(c(c12)OC)O)c1ccc(cc1O)OC</chem>	-7.1
14594569	<chem>O1[C@H]([C@@H]([C@H]([C@H]([C@]1(c1c(=O)c2cccc2oc1c1cccc1)O)O)O)O)CO</chem>	-7.1
16072086	<chem>c1(cc(=O)c2c(cc(c(c2o1)C1=CCN(C)CC1)O)O)c1cccc(Cl)c1</chem>	-7.1
42607799	<chem>O1c2c(c(ccc2C(=O)C[C@H]1c1cccc1)OCC=C(C)C)/C=C/C(C)(C)O</chem>	-7.1
44265521	<chem>c1(cc(=O)c2c(cc(c(c2o1)C1=CCN(C)CC1)O)O)c1c(Cl)cc(cc1)Cl</chem>	-7.1
5280378	<chem>o1cc(c(=O)c2ccc(cc12)O)c1ccc(cc1)OC</chem>	-7.1
5281708	<chem>o1cc(c(=O)c2ccc(cc12)O)c1ccc(cc1)O</chem>	-7.1
5380187	<chem>o1c(c(c(=O)c2c(cc(cc12)O)O)c1ccc(cc1)OC)C(=O)OCC</chem>	-7.1
631156	<chem>o1cc(c(=O)c2ccc(c(c12)OC)OC)c1ccc(cc1OC)OC</chem>	-7.1
634113	<chem>o1c2cc(cc(c2c(=O)c(c1c1cc(c(c1)OC)OC)OC)OC)OC</chem>	-7.1
10158423	<chem>O1c2c(c(cc(c2C(=O)C[C@H]1c1cccc1)OC)OC)/C=C\C(C)(C)O</chem>	-7.0

10188772 0	<chem>c1(c(cc(c2c(=O)cc(oc12)c1ccc(cc1)O)O)O)[C@@H]1O[C@@H](C)[C@H]([C@@H](C1)O)O</chem>	-7.0
11164739	<chem>c1(c(c(=O)c2ccc(cc2o1)OC)c1cccc1)SCc1cnccc1</chem>	-7.0
11797078	<chem>o1c(c(c(=O)c2c(c(c(c12)OC)OC)OCOC)OC)O)c1ccc(c(c1)OC)O</chem>	-7.0
12982239 5	<chem>Clc1c(c(c(c2c(=O)cc(oc12)c1ccc(cc1)OC(=O)C)OC(=O)C)OC(=O)C)OC(=O)C</chem>	-7.0
12985288 2	<chem>[S]([C@H]1C(=O)c2c(c(c(c2O[C@H]1c1ccc(c(c1)OC)OC)OC)OC)OC)(O)O</chem>	-7.0
23270524	<chem>O1c2cc(cc(c2C(=O)[C@H]([C@@H]1c1ccc(cc1OC)OC)OC(=O)C)OC)OC</chem>	-7.0
23644932	<chem>o1c2cc(ccc2c(=O)c(c1n1cncc1)c1ccc(cc1)OC)OC</chem>	-7.0
23644936	<chem>c1(c(c(=O)c2ccc(cc2o1)OC)c1cccc1)Sc1ncc[nH]1</chem>	-7.0
44265534	<chem>c1(cc(=O)c2c(cc(c(c2o1)C1=CCN(C)CC1)O)O)c1c(F)cccc1</chem>	-7.0
44265561	<chem>c1(cc(=O)c2c(cc(c(c2o1)C1=CCN(C)CC1)O)O)c1ccc(Cl)cc1</chem>	-7.0
5386297	<chem>o1c(c(c(=O)c2c(c(c(cc12)O)OC)O)c1cc(c(cc1OC)OC)OC)C(=O)O</chem>	-7.0
54368735	<chem>c1(c(=O)c2cccc2oc1c1cc(c(c(c1)OC)OC)OC)C(=O)NCCBr</chem>	-7.0
632958	<chem>o1cc(c(=O)c2cc(c(cc12)OC)OC)c1cc(c(cc1OC)OC)OC</chem>	-7.0
11153057	<chem>c1(c(c(=O)c2ccc(cc2o1)OC)c1cccc1)SCc1cnccc1</chem>	-6.9
11164320	<chem>c1(c(c(=O)c2ccc(cc2o1)O)c1cccc1)SCc1cnccc1</chem>	-6.9
11711336	<chem>c1(c(=O)c2cccc2oc1c1cccc1)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)OC)CO</chem>	-6.9
12967470 6	<chem>O1c2cccc2C[C@@H]([C@]1(c1cccc1)C=O)O</chem>	-6.9
12967896 8	<chem>[C@H]1(c2cccc2O[C@](C1)(c1cccc1)OC)SOC(=O)C</chem>	-6.9
12971612 0	<chem>c1(c(=O)c2cccc2oc1c1cccc1)C(=O)[C@@H]1O[C@H]([C@@H]([C@H]([C@H]1O)O)O)O</chem>	-6.9
12982441 8	<chem>O1c2cccc2C[C@H]([C@]1(c1cccc1)CC(=O)O)O</chem>	-6.9

12982449 8	<chem>o1c(cc(=O)c2c(cc(c(c12)c1ccc(c(c1)OC)OC)OC)OC)c1cccc1</chem>	-6.9
12982451 0	<chem>o1c(cc(=O)c2c(cc(c(c12)c1cc(c(c(c1)OC)OC)OC)OC)OC)c1cccc1</chem>	-6.9
12986727 7	<chem>O1C(=CC(=C2CC=CC=C12)NNC(=O)c1cccc1)c1cccc1</chem>	-6.9
13415942 0	<chem>o1c2cccc2c(=O)c(c1c1cc(c(cc1C(=O)O)O)O)c1cccc1</chem>	-6.9
13959263 0	<chem>O1c2cc(ccc2[C@@H]2C[C@H]1[C@@H]1CC=C[C@H](OCO2)C1)O</chem>	-6.9
389000	<chem>o1c(c(c(=O)c2c(c(c(c12)OC)OC)OC)OC)OC)c1cc(c(c(c1)OC)OC)OC</chem>	-6.9
44265522	<chem>o1c(cc(=O)c2c(cc(c(c12)C1=CCN(C)CC1)O)O)c1cccc1</chem>	-6.9
44265523	<chem>c1(cc(=O)c2c(cc(c(c2o1)C1=CCN(C)CC1)O)O)c1c(I)cccc1</chem>	-6.9
44265528	<chem>c1(cc(=O)c2c(cc(c(c2o1)C1=CCN(C)CC1)O)O)c1c(Br)cccc1</chem>	-6.9
46173806	<chem>c1(c(=O)c2cccc2oc1c1cccc1)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO</chem>	-6.9
630804	<chem>o1cc(c(=O)c2c(cc(c(c12)CC=C(C)C)OC(=O)C)OC(=O)C)c1ccc(cc1)OC(=O)C</chem>	-6.9
9951997	<chem>c1(cc(=O)c2c(cc(c(c2o1)C1=CCN(C)CC1)O)O)c1c(Cl)cccc1</chem>	-6.9
10188771 9	<chem>c1(c(cc(c2c(=O)cc(oc12)c1ccc(cc1)O)O)OC)[C@@H]1O[C@@H](C)[C@@H]([C@@H](C1)O)O</chem>	-6.8
10200537 4	<chem>c1(cc(=O)c2c(cc(c(c2o1)[C@@H]1CCCC[C@@H]1O)OC)OC)c1c(Cl)cccc1</chem>	-6.8
10236007 9	<chem>O1c2cc(c3C(=O)C[C@H](Oc3c2[C@H]([C@H](C1(C)C)OC(=O)C)OC(=O)C)c1cccc1)OC</chem>	-6.8
10980660	<chem>O1c2c(c(cc(c2C(=O)C[C@H]1c1cccc1)O)OC)/C=C/C(=O)C</chem>	-6.8
11741814	<chem>o1c(c(c(=O)c2c(c(c(c12)OC)OC)OC)OC)OC)c1ccc(cc1)OC</chem>	-6.8
11847318	<chem>c1(c(c(=O)c2cccc2o1)Cn1ncc1)c1ccc(Br)cc1</chem>	-6.8
11847319	<chem>o1c2cccc2c(=O)c(c1c1ccc(cc1)C#N)Cn1ncc1</chem>	-6.8
11953828	<chem>c1(c(=O)c2cccc2oc1c1cccc1)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO</chem>	-6.8

12977612 2	<chem>O1c2cc(c(c(c2C(=O)C([C@@H]1c1cccc1)(OC)OC)O)O)OC</chem>	-6.8
165203	<chem>o1cc(c(=O)c2ccc(cc12)OC)c1cc(c(cc1OC)OC)OC</chem>	-6.8
24850296	<chem>O1c2cc(cc(c2C(=O)[C@@]([C@]1(c1ccc(c(c1)O)O)OC)(O)CC(=O)OC)O)O</chem>	-6.8
42607940	<chem>c1(c2c(C=CC(C)(C)O2)c(c2C(=O)C[C@H](Oc12)c1ccc(cc1)O)O)[C@H]([C@H]1OC1(C)C)O</chem>	-6.8
44266353	<chem>O1c2cccc2C(=O)/C(=C/c2cncc2)/[C@H]1c1cccc1</chem>	-6.8
54488609	<chem>c1(c(=O)c2cccc2oc1c1cccc1)O[C@@H]1O[C@@H]([C@H]([C@@H]([C@H]1O)O)O)CO</chem>	-6.8
5465888	<chem>O1c2cccc2/C(=N/N(C(=O)C)C(=O)C)/C[C@H]1c1cccc1</chem>	-6.8
631105	<chem>o1c2cc(cc(c2c(=O)c(c1c1ccc(cc1OC)OC)OC)OC)OC</chem>	-6.8
10158423 2	<chem>O1c2c(c(cc(c2C(=O)C[C@H]1c1cccc1)OC)OC)/C=C/C(=C)C</chem>	-6.7
16126803	<chem>c1(c(=O)c2cccc2oc1c1cccc1)O[C@@H]1O[C@@H]([C@@H]([C@@H]([C@H]1O)O)O)CO</chem>	-6.7
22737159	<chem>O1c2cccc2C[C@@H]([C@@H]1c1cccc1)OC(=O)c1cc(c(c(c1)O)O)O</chem>	-6.7
23724473	<chem>c1(c(=O)c2cccc2oc1c1cccc1)O[C@@H]1O[C@@H]([C@@H]([C@@H]([C@H]1O)O)O)CO</chem>	-6.7
44257169	<chem>O1c2c3ccoc3c(c(c2[C@H]([C@@H]([C@@H]1c1cccc1)OC)OC)OC)OC</chem>	-6.7
10200538 0	<chem>c1(cc(=O)c2c(cc(c(c2o1)C1=CCN(C)CC1)OC)OC)c1c(Br)cccc1</chem>	-6.6
10218073 9	<chem>o1c2cccc2c(=O)c(c1c1ccc(c(c1OC)OC)OC)c1ccc(cc1)OC</chem>	-6.6
54505099	<chem>O1c2cccc2C(=O)/C(=C\n2cncc2)/[C@@H]1c1cccc1</chem>	-6.6
635396	<chem>c1(c(cc(c2c(=O)cc(oc12)c1ccc(cc1)OC)OC)OC)[C@H]1O[C@@H]([C@H]([C@H]([C@@H]1O)O)O)CO</chem>	-6.6
67200543	<chem>O1c2cccc2C(=O)[C@@H]([C@@H]1c1cccc1)C(=O)OC(C)(C)C</chem>	-6.6
10195886 2	<chem>O1c2cccc2C(=O)C[C@]1(c1cccc1)C(=O)O</chem>	-6.5
10200537 6	<chem>c1(cc(=O)c2c(cc(c(c2o1)C1=CCN(C)CC1)OC)OC)c1c(Cl)cccc1</chem>	-6.5
10200537	<chem>c1(cc(=O)c2c(cc(c(c2o1)C1=CCN(C)CC1)OC)OC)c1cccc(Cl)c1</chem>	-6.5

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102005378	<chem>c1(cc(=O)c2c(cc(c(c2o1)C1=CCN(C)CC1)OC)OC)c1ccc(Cl)cc1</chem>	-6.5
102005379	<chem>c1(cc(=O)c2c(cc(c(c2o1)C1=CCN(C)CC1)OC)OC)c1c(F)cccc1</chem>	-6.5
129876105	<chem>O1c2ccccc2C(=O)C[C@]1(c1cn[nH]c1)c1ccccc1</chem>	-6.5
129882615	<chem>O1[C@H]([C@H]2C(=O)[C@H]3C=CC[C@@H]1[C@H]3C2=O)c1ccccc1</chem>	-6.5
238791	<chem>c1(c(cc(cc1c1cc(cc(c1OC)OC)C(=O)C)C(=O)C)OC)OC</chem>	-6.5
66780856	<chem>O1c2cccc(c2C(=O)C([C@]1(c1ccccc1)OC)(O)O)O</chem>	-6.5
102005382	<chem>c1(cc(=O)c2c(cc(c(c2o1)C1=CCN(C)CC1)OC)OC)c1c(Cl)cc(cc1)Cl</chem>	-6.4
129710808	<chem>O1c2ccccc2C(=O)C[C@@]1(c1ccccc1)/C=C/C(=C)C</chem>	-6.4
129822386	<chem>Br1c(c(c(c2c(=O)cc(oc12)c1ccccc1)OC(=O)C)OC(=O)C)OC(=O)C</chem>	-6.4
132281498	<chem>O1c2cc(c(c(c2C(=O)C([C@]1(c1ccccc1)OC)(OC)OC)OC)OC)OC</chem>	-6.4
25067674	<chem>c1(cc(=O)c2c(cc(c(c2o1)[C@@H]1CCN(C)C[C@@H]1O)OC)OC)c1c(Cl)cccc1</chem>	-6.4
49800274	<chem>o1c(cc(=O)c2c(cc(c(c12)C1=CCN(C)CC1)OC)OC)c1ccccc1</chem>	-6.4
90690372	<chem>O1c2ccccc2C(=O)C([C@@]1(c1ccccc1)OC)(OC)OC</chem>	-6.4
138454529	<chem>O1c2ccccc2C(=O)[C@H]([C@]1(c1ccccc1)OC(O)(O)O)O</chem>	-6.3
155365	<chem>O1c2cc(c3c(=O)cc(oc3c2[C@@@H](C1)[C@H](C(C)(C)OC(=O)C)OC(=O)C)c1ccccc1)OC</chem>	-6.3
44257645	<chem>O1c2cc(c3c(=O)cc(oc3c2[C@@@H](C1)[C@@H](C(C)(C)OC(=O)C)OC(=O)C)c1ccccc1)OC</chem>	-6.3
87771765	<chem>[C@H]1(C(=O)c2ccccc2O[C@]1(c1ccccc1)C(=O)c1cc(c(c(c1)O)O)O)OS(=O)(=O)O</chem>	-6.3
12971327	<chem>Cl[C@@]1(CC(=S)c2ccccc2O1)c1ccccc1</chem>	-6.2

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12988909 7	<chem>O1c2cccc(C)c2[C@](C)([C@@](C)([C@]1(C)c1cccc1)O)O</chem>	-6.2
12982239 0	<chem>o1c(cc(=O)c2c(c(c(c12)N(=O)=O)OC(=O)C)OC(=O)C)OC(=O)C)c1cccc1</chem>	-6.1
16092266	<chem>Clc1cc(ncn1)N1CCNCC1</chem>	-5.9
9262	<chem>n1cncnc1</chem>	-3.3