

Table S1. Autodock Vina docking results against MEK1 binding pocket.

CID number	SMILES	Docking affinity (kcal/mol)
12969679 3	<chem>o1c(c(c(=O)c2C(=[C][C]=[C]c12)C(=O)/[C]=[C]/C1=[C][C]=C([C]=[C]1)O)O)C1=[C][C]=[C][C]=[C]1</chem>	-10.8
10813589	<chem>O(C1=[C][C]=C2C(=O)[C]=C(OC2=[C]1)C1=[C][C]=[C][C]=[C]1)[C][C@@]1(OC(=O)C(=[C])[C]1)C1=[C][C]=C([C]=[C]1)O[C]</chem>	-10.6
10991656	<chem>O1C2=[C][C]=C3C(=O)[C]=C(OC3=C2[C]=[C]C1([C])[C])C1=[C]C2=C([C]=[C]1)O[C]O2</chem>	-10.5
10981007	<chem>O1C2=C3C(=[C][C]=C2C(=O)[C][C]1C1=[C][C]=C2C(=[C]1)O[C]O2)OC([C])([C])[C]=[C]3</chem>	-10.5
10524567	<chem>O1C2=C([C]=C3C(=[C]2)O[C]([C]C3=O)C2=[C]C3=C([C]=[C]2)OC([C][C]3)([C])[C])[C][C]1([C])[C]</chem>	-10.5
11796528	<chem>C1(=[C][C]=C([C]=[C]1)O[C]C1=[C][C]=C2[C]=[C][C]=[C]C2=N1)C1=[C]C(=O)C2=C(O1)C(=[C][C]=[C]2)C(=O)O</chem>	-10.4
10575055	<chem>C1(=[C][C]=C([C]=[C]1)O[C]C1=[C][C]=C2[C]=[C][C]=[C]C2=N1)c1oc2c(c(=O)c1O)[C]=[C][C]=C2C(=O)O</chem>	-10.4
10094175 1	<chem>O1C2=C(C(=C(C(=[C]2)O)C2=[C][C]=C([C]=[C]2)O[C])O)C(=O)[C][C]1C1=[C][C]=C(C(=[C]1)O)O[C]</chem>	-10.3
10094174 8	<chem>O1C2=C(C(=C(C(=[C]2)O)C2=[C][C]=C([C]=[C]2)O[C])O)C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O</chem>	-10.3
23991884	<chem>o1c([C])c(c(=O)c2C(=[C]C(=[C]c12)O[C]C1=[C][C]=C(O1)C(=O)O)O)C1=[C][C]=[C][C]=[C]1</chem>	-10.3
180439	<chem>O1C(=[C]C(=O)C2=C1[C]=C(C(=[C]2)[C][C]=C([C])[C])O)C1=[C]C2=C([C]=[C]1)O[C]O2</chem>	-10.3
10094338 0	<chem>C1(=[C][C]=[C]C(=[C]1)C1=[C]C(=O)C2=[C][C]=[C][C]=C2O1)S(=O)(=O)NC1=[C][C]=C([C])[C]=[C]1</chem>	-10.2
53982668	<chem>O1C2=[C][C]=[C][C]=C2C(=O)/C(=[C]\N[C]C2=[C][C]=C([C]=[C]2)C(=O)O)/[C]1C1=[C][C]=[C][C]=[C]1</chem>	-10.2
11247668	<chem>O1C2=[C]C(=C(C(=C2C(=O)[C][C]1C1=[C][C]=C(C(=[C]1)O)O)O)[C]/[C]=C([C])/[C][C][C](C(=[C])[C])O)O</chem>	-10.2
10338671	<chem>C1(=[C][C]=C2C(=O)[C]=C(OC2=[C]1)C1=[C][C]=[C][C]=[C]1)O[C][C@]1(OC(=O)C(=[C])[C]1)[C]</chem>	-10.2
12985363 3	<chem>o1c(c(c(=O)c2C(=[C][C]=[C]c12)C(=O)/[C]=[C]/C1=[C][C]=C(C(=[C]1)O)O)O)C1=[C][C]=[C][C]=[C]1</chem>	-10.1
42608050	<chem>O1C([C])([C])[C]=[C]C2=C3C(=[C]C(=C12)[C]1[C]C(=O)C2=C([C]=C([C]=C2O1)O)O)[C]=[C]C([C])([C])O3</chem>	-10.1
42608003	<chem>O1c2c(c3c(C(=O)[C][C](O3)C3=[C][C]=C(C(=[C]3)O)O)c3OC([C])([C])[C][C]c23)[C][C]C1([C])[C]</chem>	-10.1
12019529	<chem>O1C(=[C]C(=O)C2=C([C]=C([C]=C12)OC(=O)[C]C1=[C][C]=[C][C]=[C]1)O)C1=[C][C]=[C][C]=[C]1</chem>	-10.1
10098646 3	<chem>O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O)OC(=O)[C]/[C]=[C]/C1=[C][C]=[C][C]=[C]1)C1=[C][C]=[C][C]=[C]1</chem>	-10

85823044	O1C(=[C]C(=O)C2=C([C]=[C][C]=C12)O[C]C1=[C][C]=[C][C]=[C]1)C1=[C][C]=C([C]=[C]1)[C]=O	-10
42607995	O1c2c(c(c(c2[C][C](C(=[C])[C])O)O)[C][C]=C([C])[C])O)C(=O)[C][C]1C1=[C][C]=C(C(=[C]1)O)O	-10
24133364	o1c([C])c(c(=O)c2[C]=[C]C(=[C]c12)O[C]C1=[C][C]=C(O1)C(=O)O)C1=[C][C]=[C][C]=[C]1	-10
907980	o1c([C])c(c(=O)c2=[C][C]=C([C]=c12)O[C]C1=[C][C]=[C][C]=[C]1)C1=[C][C]=[C][C]=[C]1	-10
10197413	O1C2=C(C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1)O)O)[C]c1c(=O)oc(c([C])c1O)[C][C]	-9.9
5		
73265448	O1[C]=C(C(=O)C2=C1[C]=C([C]=C2O)O[C]C1=[C][C]=[C][C]=[C]1)C1=[C][C]=C([C]=[C]1)N(=O)=O	-9.9
56649181	C1(=C([C]=C2C(=C1O)C(=O)[C]=C(O2)C1=[C][C]=[C][C]=[C]1)O)O[C]C1=[C][C]=C(F)[C]=[C]1	-9.9
54721824	O1C2=C(C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1)O)O)[C]c1c(=O)oc(c([C])c1O)[C][C]	-9.9
44382145	C1(=[C]C2=C(C(=[C]1)O)C(=O)[C]=C(O2)C1=[C][C]=[C][C]=[C]1)OC(=O)C1=[C][C]=C(F)[C]=[C]1	-9.9
23644952	c1(c(c(=O)c2[C]=[C]C(=[C]c2o1)O[C]C1=N[C]=[C][C]=[C]1)C1=[C][C]=[C][C]=[C]1)S[C]C1=[C][C]=N[C]=[C]1	-9.9
15469998	O(C1=[C][C]=C2C(=O)[C][C](OC2=[C]1)C1=[C][C]=[C][C]=[C]1)[C]1O[C]([C]([C]1O)O)O)C(=O)O	-9.8
5		
10168522	O1C2=[C]C=C(C(=C2C(=O)[C]([C]1C1=[C][C]=C([C]=[C]1)O)O)O)[C]C1=[C][C]=C([C]=[C]1)O)O	-9.8
2		
10124538	C1(=c2c(=C([C]=C1O)O)c(=O)c(c(o2)C1=[C][C]=C([C]=[C]1)O[C])O)O[C][C]1O[C]1C1=[C]C=C([C]=[C]1)O)O	-9.8
7		
10094174	O1C2=[C]C=C(C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O)C1=[C][C]=[C][C]=[C]1)O	-9.8
7		
44382144	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O)OC(=O)C1=[C][C]=C([C])[C]=[C]1)C1=[C][C]=[C][C]=[C]1	-9.8
10551087	O1C2=C3C(=[C]C(=C2[C][C](C1([C])[C])O)[C]1[C]C(=O)C2=C([C]=C([C]=C2O1)O)O)[C][C]C([C])([C])O3	-9.8
1522807	O1[C]=C(C(=O)C2=[C][C]=C([C]=C12)O[C]C1=[C][C]=C([C]=[C]1)N(=O)=O)C1=[C][C]=[C][C]=[C]1	-9.8
491718	O1c2c([C])c(c(c(c2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O)[C][C]=C([C])[C])O	-9.8
15469959	O([C]1O[C]([C]([C]([C]1O)O)O)C(=O)O)C1=[C][C]=[C][C]=C1C1=[C]C(=O)C2=[C][C]=[C][C]=C2O1	-9.7
8		
76333661	O(C1=[C][C]=C2C(=O)[C]=C(OC2=[C]1)C1=[C][C]=[C][C]=[C]1)[C]1O[C]([C]([C]([C]1O)O)O)[C]C(=O)[C]	-9.7
42607799	O1C2=C(C(=[C][C]=C2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1)O[C][C]=C([C])[C])/[C]=[C]/C([C])([C])O	-9.7
24861960	O1C2=[C]C=C(C(=C2C(=O)[C][C]1C1=[C][C]=C(C(=[C]1)O[C])O)O)[C]/[C]=C([C])/[C]/[C]=[C]/C([C])([C])O)O	-9.7
23644933	o1c2=[C]C(=[C][C]=c2c(=O)c(c1N1[C]=N[C]=[C]1)C1=[C][C]=[C][C]=[C]1)O[C]C1=[C][C]=[C][C]=[C]1	-9.7
19835337	O(C1=[C]C2=C([C]=[C]1)C(=O)[C]=C(O2)C1=[C][C]=[C][C]=[C]1)[C][C](O)[C]N[C][C][C][C]C1=[C]N[C][C]=[C]1	-9.7

16737249	O1C2=C(C(=[C]C(=[C]2)O)O)C(=O)[C][C]1C1=[C]C2=C([C]=[C]1)OC([C]=[C]2)([C])[C]	-9.7
14304997	C(=O)(N[C][C][C][C]N1[C][C]N([C][C]1)C1=N[C]=[C][C]=[C]1)c1c(=O)c2c(oc1C1=[C][C]=[C][C]=[C]1)[C]=[C][C]=[C]2	-9.7
12109666	O1C2=C3C(=[C][C]=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O[C])OC([C])([C])[C]=[C]3	-9.7
11742974	c1(c2c([C]=[C]C([C])([C])O2)c(c2C(=O)[C][C](Oc12)C1=[C][C]=C([C]=[C]1)O)O)[C][C]1OC1([C])[C]	-9.7
11358607	O1C2=C(C3=C([C]=[C]2)C(=O)[C]=C(O3)C2=[C][C]=[C][C]=[C]2)[C]=[C]C1([C])[C]	-9.7
1760386	O1[C]=C(C(=O)C2=[C][C]=C([C]=C12)O[C]C1=[C][C]=[C][C]=[C]1)C1=[C][C]=C([C]=[C]1)O[C]	-9.7
10193866 9	C1(=[C][C]=C([C]=[C]1)c1c(c(=O)c2[C]=[C][C]=[C]c2o1)O)N1O[C][C]O[C][C]O[C][C]O[C]O[C]1	-9.6
10123824 1	C1(=[C]C2=C(C(=O)C(=[C]O2)C2=[C][C]=C([C]=[C]2)O)[C]=C1C(=O)[C])O[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-9.6
44559902	O1C2=[C]C=C(C(=C2C(=O)[C]([C]1C1=[C][C]=C([C]=[C]1)O)O)O)[C]C1=[C][C]=C([C]=[C]1)O)O	-9.6
15383190	O1C2=[C]C(=C3C(=O)[C]=C(OC3=C2[C]=[C]C1([C])[C])C1=[C][C]=[C][C]=[C]1)O	-9.6
11582389	C1(=[C]C2=C([C]=[C]1)C(=O)[C]=C(O2)C1=[C][C]=[C][C]=[C]1)O[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-9.6
11395168	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O)O[C]C1=[C][C]=[C][C]=[C]1)C1=[C]C(=C([C]=[C]1)O[C])O	-9.6
11314387	O1C(=[C]C(=O)C2=C(C(=C([C]=C12)O)O)[C]C1=[C][C]=[C][C]=[C]1)O)C1=[C][C]=[C][C]=[C]1	-9.6
10449654	O1C2=C(C(=C3C(=[C]2)OC(=[C]C3=O)C2=[C][C]=C([C]=[C]2)O)O)[C]=[C]C1([C])[C]	-9.6
563997	O1[C]=C(C(=O)C2=[C][C]=C([C]=C12)O[C]C1=[C][C]=[C][C]=[C]1)C1=[C][C]=[C][C]=[C]1	-9.6
440215	C1(=[C][C]=C2C(=O)C(=[C]OC2=[C]1)C1=[C][C]=[C][C]=[C]1)O[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-9.6
15469955 2	O([C]1O[C]([C]([C]([C]1O)O)O)C(=O)O)C1=[C][C]=[C]C(=[C]1)C1=[C]C(=O)C2=[C][C]=[C][C]=C2O1	-9.5
12988126 9	o1c2=[C][C]=C([C]=c2c(=O)c(c1C1=[C]C2=C([C]=[C]1)O[C]O2)O)C(=O)O	-9.5
12986727 7	O1C(=[C]C(=C2[C]=[C][C]=[C][C]12)[N]NC(=O)C1=[C][C]=[C][C]=[C]1)C1=[C][C]=[C][C]=[C]1	-9.5
12983451 4	O1C2=[C]C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)OC(=O)[C])O)O[C]C1=[C][C]=[C][C]=[C]1	-9.5
12979132 8	C1(=[C]c2c([C]=[C]1)c(=O)c(c(o2)C(=O)O)C1=[C][C]=[C][C]=[C]1)O[C]c1sc2[C]=[C][C]=[C]c2n1	-9.5
12236641 1	C1(=[C][C]=C([C]=[C]1)C1=[C]C(=O)C2=[C][C]=[C][C]=C2O1)OS([O])([O])C(F)(F)F	-9.5

10257793 0	C1(=[C]C(=C2C(=O)[C]=C(OC2=[C]1)C1=[C][C]=C([C]=[C]1)O)O)OS([O])([O])C1=[C][C]=C([C])C=[C]1	-9.5
54490901	O1C2=[C][C]=[C][C]=C2C(=O)/C(=[C]\C2=[C][C]=[C]C(=[C]2)NC(=O)[C])/[C]1C1=[C][C]=[C][C]=[C]1	-9.5
53249095	O1C2=[C]C3=C([C]=[C]C([C])([C])O3)C(=C2C(=O)[C][C]1C1=C([C]=C([C]=[C]1)O)O)O	-9.5
44584124	O1C2=[C]C3=C([C]=[C]C([C])([C])O3)C(=C2C(=O)[C][C]1C1=C([C]=[C][C]=[C]1)O)O	-9.5
25070110	O1C2=[C]C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O)O[C]C1=[C][C]=[C][C]=[C]1	-9.5
23644934	o1c2=[C]C(=[C][C]=c2c(=O)c(c1N1[C]=N[C]=[C]1)C1=[C][C]=C([C]=[C]1)O[C])O[C]C1=[C][C]=[C][C]=[C]1	-9.5
15939984	o1c2=[C][C]=C([C])[C]=c2c(=O)c(c1C1=[C][C]=C2C(=[C]1)O[C]O2)O	-9.5
15342845	o1c(c(c(=O)c2=C([C]=C([C]=c12)O)OC(=O)C1=[C][C]=[C][C]=[C]1)O[C])C1=[C][C]=[C][C]=[C]1	-9.5
14626316	O(C1=[C][C]=C2C(=O)[C]=C(OC2=[C]1)C1=[C][C]=[C][C]=[C]1)[C][C](O)[C]N[C][C]C1=[C][C]=C([C]=[C]1)O	-9.5
14408549	[C](OC1=[C][C]=C2C(=O)[C]=C(OC2=[C]1)C1=[C][C]=[C][C]=[C]1)[C](O)[C]N[C][C]C1=[C][C]=C(C(=[C]1)O[C])O[C]	-9.5
12071400	C1(=[C]C(=[C]c2oc(c(c(=O)c12)O)C1=[C]C(=C([C]=[C]1)O[C])O[C])O[C])OS([O])([O])C1=[C][C]=C([C]=[C]1)[C]	-9.5
11718263	C1(=[C][C]=C2C(=[C]1)C(=O)[C]=C(O2)C1=[C]C(=C([C]=[C]1)O)O)O[C][C](O)[C]NC([C])([C])[C]	-9.5
625630	O1C(=[C]C(=O)C2=C1C(=[C]C1=C2[C]=[C][C]=[C]1)O)C1=[C][C]=[C][C]=[C]1	-9.5
440195	C1(=[C]C2=C([C]=[C]1)C(=O)[C][C](O2)C1=[C][C]=[C][C]=[C]1)O[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-9.5
10220349 6	O1C(=[C]C(=O)C2=C([C]=C([C]=C12)O[C]O[C])O[C]O[C])C1=[C][C]=C([C]=[C]1)O[C]C1=[C][C]=[C][C]=[C]1	-9.4
10188772 1	C1(=C([C]=C(C2=C1OC(=[C]C2=O)C1=[C][C]=C([C]=[C]1)O)O)O[C])([C]1O[C]([C])[C](C(=O)[C]1)O	-9.4
10139688 8	O1c2c3C(=O)C(=[C]Oc3c(c(c2[C]=[C]C1([C])([C])O)[C][C](C([C])([C])O)O)C1=[C][C]=C([C]=[C]1)O	-9.4
69941512	C1(=[C]C2=C([C]=[C]1)OC(=[C]C2=O)C1=[C][C]=[C][C]=[C]1)O[C][C][C]1OC(=O)C(=C1O)O	-9.4
56589538	C1(=C(C(=C2C(=O)[C]=C(OC2=[C]1)C1=[C][C]=[C][C]=[C]1)O)O)O[C]C1=[C][C]=C(F)[C]=[C]1	-9.4
42607962	O1C2=C(C(=[C]C3=C2[C]=[C]C(O3)([C])([C])O)C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O[C]	-9.4
15342843	o1c(c(c(=O)c2C(=[C]C(=[C]c12)OC(=O)C1=[C][C]=[C][C]=[C]1)O)O[C])C1=[C][C]=[C][C]=[C]1	-9.4
15108704	O1C(=[C]C(=O)C2=C(C(=C([C]=C12)O[C]C1=[C][C]=[C][C]=[C]1)O)O)C1=[C][C]=C(C(=[C]1)O)O	-9.4
14187087	O1C2=C(C(=C3C(=[C]2)OC([C]=[C]3)([C])([C])O)C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O	-9.4
11247278	O1C2=C(C(=[C]C(=C2[C][C]=C([C])([C])OC(=O)[C])O)C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)OC(=O)[C]	-9.4
5466794	C1(=[C]C(=O)C2=C(C(=C([C]=C2O)O)[C]2[C][C]N([C])[C][C]2O)O1)C1=C(Cl)[C]=[C][C]=[C]1	-9.4

629905	C1(=[C][C]=C(C(=[C]1)O[C]C1=[C][C]=[C][C]=[C]1)O[C])c1oc2=[C]C(=[C][C]=c2c(=O)c1O[C])O[C]	-9.4
15469991 9	O([C]1O[C]([C]([C]([C]1O)O)O)C(=O)O)C1=[C][C]=C([C]=[C]1)C1=[C]C(=O)C2=C([C]=[C][C]=[C]2)O1	-9.3
13175137 2	O1C2=C3[C]=[C]C([C])([C])OC3=[C][C]=C2C(=O)[C]([C]1C1=[C][C]=C(C(=[C]1)[C][C]=C([C])([C])O)O	-9.3
10098646 4	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O)OC(=O)[C]/[C]=[C]/C1=[C][C]=C([C]=[C]1)O[C])C1=[C][C]=[C][C]=[C]1	-9.3
69567244	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O)O[C]C1=[C][C]=[C][C]=[C]1)C1=[C][C]=C([C]=[C]1)O	-9.3
14626328	C1(=[C][C]=C2C(=O)[C]=C(OC2=[C]1)C1=[C][C]=[C][C]=[C]1)O[C][C](O)[C][C][C]O[C]1O[C][C][C]1	-9.3
14304994	c1(c(=O)c2[C]=[C][C]=[C]c2oc1C1=[C][C]=[C][C]=[C]1)C(=O)N1[C][C]N([C][C]1)[C]C1=[C][C]=[C][C]=[C]1	-9.3
12019528	O1C(=[C]C(=O)C2=C([C]=C([C]=C12)OC(=O)C1=C([C]=[C][C]=[C]1)OC(=O)[C])O)C1=[C][C]=[C][C]=[C]1	-9.3
11995581	C1(=[C]C=C(C(=[C]1)[C][C]=C([C])([C])O[C])/[C]=[C]/C([C])([C])O)[C]1OC2=[C]C(=[C][C]=C2C(=O)[C]1)O	-9.3
11132477	o1c2=[C][C]=[C][C]=c2c(=O)c(c1C1=[C][C]=[C][C]=[C]1)[C](C1=[C][C]=C([C]=[C]1)N(=O)=O)O	-9.3
637111	O1c2c(c(c3[C]=[C]C([C])([C])Oc3c2[C][C]=C([C])([C])O)C(=O)[C]([C]1C1=C([C]=[C][C]=[C]1)O)O	-9.3
636525	O1C2=C(C(=[C]C3=C2[C]=[C]C(O3)([C])([C])O)C(=O)[C][C]1C1=[C]C(=C([C]=[C]1)O[C])O	-9.3
563887	C1(=[C][C]=C(C(=[C]1)O[C])O[C]C1=[C][C]=[C][C]=[C]1)c1oc2[C]=[C][C]=[C]c2c(=O)c1O[C]	-9.3
49700	C1(=c2c(=[C][C]=C1O[C])c(=O)c([C])c(o2)C1=[C][C]=[C][C]=[C]1)[C]N1[C][C]O[C][C]1	-9.3
13735036 9	C1=[C][C]=[C]C2=C1O[C]=C(C2=O)C1=[C][C]=[C][C]=[C]1)[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-9.2
12985615 1	O(c1c(=O)c2=[C][C]=[C][C]=c2oc1C1=[C][C]=[C][C]=[C]1)C(=O)[C]1O[C]([C]([C]([C]1O)O)O)O	-9.2
10188772 0	C1(=C([C]=C(C2=C1OC(=[C]C2=O)C1=[C][C]=C([C]=[C]1)O)O)O)[C]1O[C]([C])([C])([C]1)O)O	-9.2
10188771 9	C1(=C([C]=C(C2=C1OC(=[C]C2=O)C1=[C][C]=C([C]=[C]1)O)O)O)[C]1O[C]([C])([C])([C]1)O)O	-9.2
10142913 2	C1(=[C]C=C(C(=[C]1)/[C]=[C]/C([C])([C])O)O[C])([C][C]=C([C])([C]))[C]1OC2=C([C]=[C]C(=[C]2)O)C(=O)[C]1	-9.2
10121493 9	C1(=[C][C]=C([C]=[C]1)c1c(c(=O)c2[C]=[C][C]=[C]c2o1)O)N1[C][C]N([C][C]1)C1=C([C]N[C]=[C]1)S([O])([O])O	-9.2
52951514	C1(=[C]C=C(C([C]=[C]1)O[C][C](C([C])([C])O)O)O)[C]C1=[C]OC2=[C]C3=C([C]=C2C1=O)[C]=[C]C(O3)([C])[C]	-9.2

52951513	O1C2=[C]C3=C(C(=O)C(=[C]O3)C3=[C][C]=C(C(=[C]3)O[C])O[C][C](C([C])([C])O)O)C(=C2[C]=[C]C1([C])([C])O[C])	-9.2
42607996	O1C2=C(C(=[C]C(=C2C(=O)[C][C]1C1=[C]C(=C([C]=[C]1)O)O)O)O)[C]/[C]=C(\[C])/[C]OC(=O)[C]	-9.2
25030431	o1c(c(c(=O)c2=[C]C(=[C][C]=c12)NC(=O)[C][C]C(=O)O)O)C1=[C]C(=C([C]=[C]1)O)O	-9.2
24960482	C1(=[C]C2=C([C]=[C]1)C(=O)[C]=C(O2)C1=[C]C(=[C]C(=[C]1)O)O)O[C][C](O)[C]N[C]([C])[C]	-9.2
15308126	C1(=c2c(=[C]C(=C1O)O[C])oc(c(c2=O)O)C1=[C][C]=C([C]=[C]1)O[C])OS([O])([O])C1=[C][C]=C([C])([C]=[C]1	-9.2
14445197	C1(=C([C]=C2C(=C1O)C(=O)[C]=C(O2)C1=[C][C]=C(C(=[C]1)O)O[C])O)[C]1O[C]([C])([C]([C]1)O)O	-9.2
12043067	C1(=[C]C(=O)C2=C([C]=C(C(=C2O1)[C]1C(=O)[C]N([C])[C][C]1)O)O)C1=[C][C]=[C][C]=C1Cl	-9.2
11597157	C1(=[C]C2=C([C]=[C]1)C(=O)[C]=C(O2)C1=[C][C]=C([C]=[C]1)O)O[C]1O[C]([C]([C]([C]1O)O)O[C])[C]O	-9.2
11545770	C1(=[C][C]=C2C(=O)[C]=C(OC2=[C]1)C1=[C]C(=[C]C(=[C]1)O)O)O[C][C](O)[C]NC([C])([C])[C]	-9.2
10741771	O1C2=C(C(=C([C]=C2[C][C](C1([C])([C])O)[C]1[C]C(=O)C2=C([C]=C([C]=C2O)O)O1)[C][C]=C([C])([C])O	-9.2
10291777	O1C2=C(C3=C([C]=[C]2)C(=O)[C][C](O3)C2=C([C]=C([C]=[C]2)O)O)[C][C]1C([C])([C])O	-9.2
5481228	O1[C]=C(C(=O)C2=C([C]=C([C]=C12)O)O)C1=C([C]=C(C(=[C]1)[C][C]=C([C])([C])O)O	-9.2
5378307	O1C(=[C]C(=O)C2=C1[C]=[C]C1=C2[C]=C([C]=[C]1)O)C1=[C][C]=[C][C]=[C]1	-9.2
564150	o1c(c(c(=O)c2=[C][C]=C([C]=c12)O[C]C1=[C][C]=[C][C]=[C]1)O[C])C1=[C]C(=C([C]=[C]1)O[C])O[C]	-9.2
511789	O1C2=C(C(=[C][C]=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O[C])[C][C]=C([C])([C]	-9.2
177731	O1[C]=C(C(=O)C2=C1[C]=C([C]=[C]2)O[C][C]=C([C])([C])C1=[C][C]=C([C]=[C]1)O[C]	-9.2
11790	O1C(=[C]C(=O)C2=[C][C]=C3[C]=[C][C]=[C]C3=C12)C1=[C][C]=[C][C]=[C]1	-9.2
12983451	O1C2=C(C(=[C]C(=[C]2)O[C]C2=[C][C]=[C][C]=[C]2)O[C])C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)OC(=O)[C]	-9.1
7		
12982241	O1C(=[C]C(=O)C2=C1C(=[C]C(=[C]2)OC(=O)[C])N)C1=[C][C]=C([C]=[C]1)OC(=O)[C]	-9.1
3		
12971612	c1(c(=O)c2=[C][C]=[C][C]=c2oc1C1=[C][C]=[C][C]=[C]1)C(=O)[C]1O[C]([C]([C]([C]1O)O)O)O	-9.1
0		
12970394	o1c(c(c(=O)c2C(=[C][C]=[C]c12)C(=O)C1=[C]C(=C(C(=[C]1)O)O)O)O)C1=[C][C]=[C][C]=[C]1	-9.1
0		
10149923	C1(=[C]C(=C(C(=[C]1)O[C])O[C]([C]O)[C](C1=[C][C]=C([C]=[C]1)O)O)O[C])[C]1OC2=[C]C(=[C]C(=C2C(=O)[C]1)O)O	-9.1
4		
10139688	O1c2c3C(=O)C(=[C]Oc3c(c(c2[C][C]1C([C])([C])O)O)[C][C]=C([C])([C])C1=[C][C]=C([C]=[C]1)O	-9.1
7		
95400994	O1C2=[C][C]=C3[C]=[C][C]=[C]C3=C2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1	-9.1

67984060	o1c(c(c(=O)c2C(=[C]C(=[C]c12)O[C]C1=[C][C]=[C][C]=[C]1)O)O)C1=[C][C]=C(C(=[C]1)O)O	-9.1
46881227	C1(=[C]C2=C(C(=[C]1)O)C(=O)[C][C](O2)C1=[C][C]=[C][C]=[C]1)O[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-9.1
42608102	O1c2c3[C]=[C]Oc3c(c(c2C(=O)[C][C]1C1=[C][C]=C2C(=[C]1)O[C]O2)O)O[C]	-9.1
42608049	O1C2=[C]C(=C3C(=O)[C][C](OC3=C2[C][C]C1([C])[C])C1=C([C]=C([C]=[C]1)O)O)O	-9.1
24866261	C1(=[C]C(=C2C(=O)[C]=C(OC2=[C]1)C1=[C][C]=[C][C]=[C]1)O)O[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-9.1
21576252	O1[C]=C(C(=O)C2=C([C]=C([C]=C12)O[C][C]=C([C])[C])O)C1=[C][C]=C([C]=C1O)O	-9.1
15118758	C1(=[C][C]=C2C(=O)[C]=C(OC2=[C]1)C1=C([C]=[C][C]=[C]1)O)O[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-9.1
15108702	O1C(=[C]C(=O)C2=C(C(=C([C]=C12)O[C]C1=[C][C]=[C][C]=[C]1)O)O)C1=[C][C]=[C][C]=[C]1	-9.1
12428921	O1C2=[C][C]=[C][C]=C2C(=O)/C(=[C]\C2=[C][C]=[C]C(=[C]2)O)/[C]1C1=[C][C]=[C][C]=[C]1	-9.1
11618226	C1(=[C][C]=C2C(=O)[C]=C(OC2=[C]1)C1=[C][C]=C(C(=[C]1)O)O)O[C][C](O)[C]NC([C])([C])[C]	-9.1
11222065	o1c2=[C][C]=[C][C]=c2c(=O)c(c1C1=[C][C]=[C][C]=[C]1)[C](C1=[C][C]=C([C]=[C]1)O[C])O	-9.1
11077963	o1c2=[C][C]=[C][C]=c2c(=O)c(c1C1=[C][C]=[C][C]=[C]1)[C](C1=[C][C]=[C][C]=[C]1)O	-9.1
11048450	O1C([C])([C])[C]=[C]c2c(c3C(=O)[C][C](Oc3c(c12)[C][C](C([C])([C])O)O)C1=[C][C]=C([C]=[C]1)O)O	-9.1
10970624	O1c2c(c3c([C]=[C]C([C])([C])O3)c(c2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O)[C]O	-9.1
5494866	O1[C]=C(C(=O)C2=C([C]=C([C]=C12)O)O)C1=[C][C]=C(C(=[C]1)[C][C]=C([C])[C])O	-9.1
5316782	O1C2=C(C3=C(C(=[C]2)O)C(=O)[C][C](O3)C2=[C][C]=C([C]=[C]2)O)[C][C]1C([C])([C])O	-9.1
3085261	C1(=[C]C2=C([C]=[C]1)C(=O)C(=[C]O2)C1=[C]C2=C([C]=[C]1)O[C]O2)O[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-9.1
13959387	O1C(=[C]C(=O)C2=C1C(=[C]C(=[C]2)[C]C(=O)[C])O[C])C1=[C][C]=C([C]=[C]1)O[C]	-9
7		
12984781	O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O)[C][C]C(=[C])([C])O)C1=C([C]=C([C]=[C]1)O)O	-9
7		
12973586	O1C2=C([C]=[C][C]=C2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1)/[C]=[C]/C(=[C])[C]	-9
9		
10200538	C1(=[C]C(=O)C2=C(C(=C([C]=C2O[C])O[C])C2=[C][C]N([C])[C][C]2)O1)C1=C(Cl)[C]=C([C]=[C]1)Cl	-9
2		
10199990	C1(=[C]OC2=[C]C(=C(C(=C2C1=O)O)[C][C]C([C])([C])O)O)C1=[C][C]=C2OC([C]=[C]C2=C1O)([C])[C]	-9
2		
10165084	O1C2=[C][C]=[C][C]=C2C(=O)/C(=[C]\C2=[C][C]=[C]C(=[C]2)N(=O)=O)/[C]1C1=[C][C]=[C][C]=[C]1	-9
3		

10151666 5	O1C2=[C]C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)OC(=O)[C])O)O[C][C]=C([C])[C]	-9
74333987	O1C2=C(C(=C(C(=[C]2)O)[C][C]=C([C])[C])O)C(=O)[C]([C]1C1=[C]C(=C(C(=[C]1)O[C])O)O)O	-9
58089059	o1c(c(c(=O)c2[C]=C([C]=[C]c12)NC(=O)[C][C]C(=O)O)O)C1=[C][C]=C([C]=[C]1)O	-9
54450648	O1C2=[C][C]=[C][C]=C2C(=O)/C(=[C]\NC2=C([C]=[C][C]=[C]2)O)/[C]1C1=[C][C]=[C][C]=[C]1	-9
53904139	C1(=[C][C]=[C]C(=[C]1)C1=[C]C(=O)C2=C([C]=[C][C]=[C]2)O1)S(=O)(=O)N	-9
49788613	o1c(c(c(=O)c2=C([C]=C(C(=c12)O[C])O[C][C]=C([C])[C])O)O)C1=[C]C2=C([C]=[C]1)O[C]O2	-9
46850208	C1(=C([C]=C2C(=C1O)C(=O)[C]=C(O2)C1=[C]C(=C([C]=[C]1)O)O[C])O)[C]/[C]=C(\[C])/[C][C][C](C([C])([C])O)O	-9
44257869	O1C2=[C]C3=C(C(=O)[C]=C(O3)C3=[C][C]=C([C]=[C]3)O)C(=C2[C][C](C1([C])[C])O)O	-9
42607867	C1(=[C]C2=C(C(=[C]1)O)C(=O)[C][C](O2)C1=[C][C]=[C][C]=[C]1)O[C][C]1OC1([C])[C]	-9
19358579	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O[C])O[C]C1=[C][C]=[C][C]=[C]1)C1=[C][C]=C(C(=[C]1)O[C])O[C]	-9
15389725	C1(=[C]C(=O)C2=[C][C]=[C][C]=C2O1)C1=[C][C]=[C]C(=[C]1)S(=O)(=O)Cl	-9
14735885	C1(=[C]C(=O)C2=[C][C]=[C][C]=C2O1)C1=[C][C]=C([C]=[C]1)C(F)(F)F	-9
12753176	[C]1(C(=[C])C(=O)C2=[C][C]=[C][C]=C2O1)C1=C(Cl)[C]=C([C]=[C]1)Cl	-9
12043064	C1(=[C]C(=O)C2=C([C]=C(C(=C2O1)[C]1[C]N([C])[C][C][C]1O)O)O)C1=[C][C]=[C][C]=C1Cl	-9
12043063	C1(=[C]C(=O)C2=C([C]=C(C(=C2O1)[C]1[C]N([C])[C][C][C]1O)O[C])O[C])C1=[C][C]=[C][C]=C1Cl	-9
10814209	C1(=C([C]=c2c(=C1O)c(=O)c(c(o2)C1=[C][C]=C([C]=[C]1)O[C])O)O)OS([O])([O])C1=[C][C]=C([C]=[C]1)[C]	-9
5320053	O1[C]=C(C(=O)C2=[C][C]=C([C]=C12)O)C1=[C][C]=C(C(=[C]1)[C][C]=C([C])[C])O	-9
3870517	O1C2=C(C(=[C]C(=[C]2)OC(=O)[C])O)C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)OC(=O)[C]	-9
3070243	c1(c([C])c(=O)c2[C]=[C]C(=C(c2o1)[C]N1[C][C][C][C]1)O[C])C1=[C][C]=C(F)[C]=[C]1	-9
3070242	c1(c([C])c(=O)c2[C]=[C]C(=C(c2o1)[C]N1[C][C][C][C]1)O[C])C1=[C][C]=C(F)[C]=[C]1	-9
491719	O1c2c(c(c([C])c(c2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O)O)[C][C]=C([C])[C]	-9
480763	O1C2=[C]C(=C(C(=C2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1)O)[C][C]=C([C])[C])O	-9
399491	O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O)[C][C]=C([C])[C])O)C1=C([C]=C([C]=[C]1)O)O	-9
2361	O1C(=[C]C(=O)C2=C1[C]=[C]C1=C2[C]=[C][C]=[C]1)C1=[C][C]=[C][C]=[C]1	-9
14594569 3	O1[C]([C]([C]([C]([C]([C@]1(c1c(=O)c2=[C][C]=[C][C]=c2oc1C1=[C][C]=[C][C]=[C]1)O)O)O)[C]O	-8.9
12988148 7	O1C2=[C][C]=C([C]=C2C(=O)[C]=C1C1=[C][C]=[C][C]=C1C(=O)O)C(=O)O	-8.9

12983453 9	O1C2=C(C(=[C]C(=[C]2)O[C]C2=[C][C]=[C][C]=[C]2)O[C])C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O	-8.9
12971430 2	O1C2=[C][C]=[C][C]=C2C(=O)[C]([C@@]1(C1=[C][C]=[C][C]=[C]1)[C]C1=[C][C]=[C][C]=[C]1)O	-8.9
10232161 1	O1[C]=C(C(=O)C2=C1[C]=C([C]=C2O)C1=[C][C]2C(=[C][C]=[C]O2)C(=[C]1)O)C1=[C][C]=C(C(=C1O[C])O[C])O	-8.9
10193212 1	C1(=C(C(=C2C(=[C]1)OC(=[C]C2=O)C1=[C][C]=C([C]=[C]1)O)O)O[C])O[C]1O[C]([C]([C]([C]1O)O)O)[C]	-8.9
10188771 8	C1(=C([C]=C(C2=C1OC(=[C]C2=O)C1=[C][C]=C([C]=[C]1)O)O)O)[C]1O[C]([C])([C])([C]1)O)O	-8.9
10136776 7	O1C2=C(C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O)O)[C]/[C]=C([C])/[C]=O	-8.9
10106405 5	C1(=[C]OC2=[C][C]=[C][C]=C2C1=O)C1=[C][C]=C([C]=[C]1)C(F)(F)F	-8.9
10102840 2	O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O)N[C][C]([C])([C])O)C1=[C][C]=[C][C]=[C]1	-8.9
10094174 9	O1C2=[C]C(=C(C(=C2C(=O)[C][C]1C1=[C]C(=[C]=[C]1)O[C])O)O)C1=[C][C]=[C][C]=[C]1O	-8.9
71588424	O1C2=[C]C(=O)[C]3C(=O)[C]=C(O[C]3C2=C([C](C1([C])([C])O)O)C1=[C][C]=C([C]=[C]1)O	-8.9
66783913	O1C(=[C]C(=O)C2=C(C3=C([C]=C12)O[C]O3)O)C1=[C][C]=C([C]=[C]1)O[C]	-8.9
66728267	C1(=[C]C(=[C][C]=C1O)C1=[C]OC2=[C]C(=[C]C(=C2C1=O)O)O)[C][C]C([C])([C])O	-8.9
54505099	O1C2=C([C]=[C][C]=[C]2)C(=O)/C(=[C]\N2[C]=N[C]=[C]2)/[C]1C1=[C][C]=[C][C]=[C]1	-8.9
49788614	o1c2[C]=C([C]=C(c2c(=O)c(c1C1=[C]C2=C([C]=[C]1)O[C]O2)O[C][C]=C([C])([C])O)O)[C]	-8.9
44578052	O1C(=[C]C(=O)c2c(c(c(c12)[C]N1[C][C][C][C]1)O)O)O)C1=[C][C]=[C][C]=[C]1	-8.9
44265534	C1(=[C]C(=O)C2=C(C(=[C]=C2O)O)C2=[C][C]N([C])([C][C]2)O1)C1=C(F)[C]=[C][C]=[C]1	-8.9
44259326	O1C2=[C]C(=c3c(=O)c(c(oc3=C2[C]([C])([C])C1([C])([C])C1=[C]C(=[C]=[C]1)O)O)O)O	-8.9
44258305	C1(=[C]C(=C2C(=O)[C]=C(OC2=[C]1)C1=[C][C]=C([C]=[C]1)O)O[C])O[C][C]1OC1([C])([C]	-8.9
42607940	c1(c2c([C]=[C]C([C])([C])O2)c(c2C(=O)[C][C](Oc12)C1=[C][C]=C([C]=[C]1)O)O)[C]([C]1OC1([C])([C])O	-8.9
24205532	C1(=[C]c2c(C(=[C]1)O[C])c(=O)c(c(o2)C1=[C][C]=C([C]=[C]1)O)[C][C]=C([C])([C])O[C]1O[C]([C]([C]([C]1O)O)O)[C]	-8.9
21315742	C1(=[C]C(=O)C2=C([C]=[C]C(=[C]2)C(=O)O)O1)C1=[C]C(=[C][C]=C1O[C]([C])([C])([C])	-8.9

15160702	O1C2=C([C]=[C]C3=C2[C]=[C]C(O3)([C])([C])C(=O)[C][C]1C1=[C][C]=C(C(=[C]1)O[C])O[C]	-8.9
14237660	C1(=[C]OC2=C(C(=[C]C(=[C]2)O)O)C1=O)C1=[C][C]=C2OC([C]=[C]C2=[C]1)([C])[C]	-8.9
12918915	C1(=[C][C]=C2C(=O)C(=[C]OC2=[C]1)C1=[C][C]=[C][C]=[C]1)O[C](C1=[C][C]=[C][C]=[C]1)[C][C]N[C]	-8.9
12093281	O1C2=[C][C]=[C][C]=C2C(=O)/C(=[C]\C2=[C][C]=C([C]=[C]2)N(=O)=O)/[C]1C1=[C][C]=[C][C]=[C]1	-8.9
11639597	C1(=[C][C]=C2C(=O)[C]=C(OC2=[C]1)C1=[C][C]=C(C(=[C]1)O)O)O[C][C](O)[C]N[C]([C])[C]	-8.9
11024735	O1C2=C([C]=[C][C]=[C]2)C(=O)/C(=[C]/C2=[C][C]=C([C]=[C]2)N(=O)=O)/[C]1C1=[C][C]=[C][C]=[C]1	-8.9
10472357	O1C(=[C]C(=O)C2=C(C(=C([C]=C12)O)N[C][C][C]([C])([C])O)C1=[C][C]=[C][C]=[C]1	-8.9
10337211	O1C2=[C]C=C([C]=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)[C][C]=C([C])([C])O[C]	-8.9
9951997	C1(=[C]C(=O)C2=C([C]=C(C(=C2O1)C1=[C][C]N([C])[C][C]1)O)O)C1=[C][C]=[C][C]=C1Cl	-8.9
7330537	O1C2=[C][C]=C3C(=O)C(=[C]OC3=C2[C]=[C]C1([C])([C])C1=[C]C2=C(C(=[C]1)O[C])O[C]O2	-8.9
5317765	c1(c(c(=O)c2=C([C]=C([C]=c2o1)O)O)O)C1=[C]C2=C(OC([C]([C]2)O)([C])([C])[C]=[C]1	-8.9
5281814	O1[C]=C(C(=O)C2=C1[C]=C(C(=C2O)[C][C]=C([C])([C])O)C1=[C][C]=C([C]=[C]1)O	-8.9
509245	O1C2=C(C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O)O)[C][C]=C([C])([C])	-8.9
343080	O1[C]=C(C(=O)C2=C1[C]=C([C]=[C]2)O[C][C]=C([C])([C])C1=C([C]=C2C(=[C]1)O[C]O2)O[C]	-8.9
129224	C1(=[C]C2=C([C]=[C]1)C(=O)[C]=C(O2)C1=[C][C]=C([C])([C]=[C]1)O[C][C](O)[C]N[C]([C])[C]	-8.9
122835	O1C2=[C]C=C([C]=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)[C][C]=C([C])([C])O[C]	-8.9
13602334	C1(=[C]C(=O)C2=C([C]=C(C(=C2O1)C1=[C][C]=N[C]=[C]1)O)O)C1=[C][C]=[C][C]=C1Cl	-8.8
3		
13254029	o1c2[C]=C([C]=C(c2c(=O)c(c1C1=[C][C]=C(C(=[C]1)OC(=O)[C])OC(=O)[C])O)O)O	-8.8
7		
10206691	o1c(c(c(=O)c2=C(C(=C([C]=c12)O[C]C1=[C][C]=[C][C]=[C]1)O[C])O)O)C1=[C][C]=[C][C]=[C]1	-8.8
8		
10200537	C1(=[C]C(=O)C2=C([C]=C(C(=C2O1)C1=[C][C]N([C])[C][C]1)O[C])O[C])C1=[C][C]=[C]C(=[C]1)Cl	-8.8
7		
10184348	C1(=[C]C2=C([C]=[C]1)O[C]([C]C2=O)C1=[C][C]=[C][C]=[C]1)O[C]1O[C]([C]([C]([C]1O)O)O[C])[C]O	-8.8
5		
10121493	C1(=[C][C]=C([C]=[C]1)N1[C][C]N([C][C]1)C1=[C][C]=N[C]=[C]1)c1oc2=[C][C]=[C][C]=c2c(=O)c1O	-8.8
8		
91724402	O1C2=[C]C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)OC(=O)[C])O)O[C]	-8.8
71588336	O1C2=[C]C(=C3C(=O)[C]=C(OC3=C2[C]([C](C1([C])([C])O)O)C1=[C][C]=C([C]=[C]1)O)O	-8.8

57253387	<chem>O1C2=C([C]=[C][C]=[C]2)[C]([C][C]1C1=[C][C]=[C][C]=[C]1)[N]NC(=O)N</chem>	-8.8
56648913	<chem>C1(=C(C(=C2C(=[C]1)OC(=[C]C2=O)C1=[C][C]=[C][C]=[C]1)OC(=O)[C])OC(=O)[C])O[C]C1=[C][C]=C(F)[C]=[C]1</chem>	-8.8
54488609	<chem>c1(c(=O)c2[C]=[C][C]=[C]c2oc1C1=[C][C]=[C][C]=[C]1)O[C]1O[C]([C]([C]([C]1O)O)O)[C]O</chem>	-8.8
53247947	<chem>C1(=[C][C]=C([C]=[C]1)[C]1[C]C(=O)C2=C([C]=[C][C]=[C]2)O1)O[C]1O[C]([C]([C]([C]1O)O)O)[C]O</chem>	-8.8
46173806	<chem>c1(c(=O)c2[C]=[C][C]=[C]c2oc1C1=[C][C]=[C][C]=[C]1)O[C]1O[C]([C]([C]([C]1O)O)O)[C]O</chem>	-8.8
44258651	<chem>O1C(=[C]C(=O)c2c(c(c(c12)O[C])O)O[C])O)C1=[C]C2=C([C]=[C]1)O[C]O2</chem>	-8.8
42608112	<chem>O1c2c(c(c(c2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1)O)[C]C1=[C]C(=[C][C]=C1O)O[C])O[C])O[C]</chem>	-8.8
42608036	<chem>O1[C]([C]C(=O)C2=C1C(=C([C]=C2O)O)[C][C]([C]([C])O)[C]C(=[C])O)[C]C1=[C][C]=C([C]=C1O[C])O</chem>	-8.8
42607957	<chem>O1C2=C(C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O[C])O)O)[C]C(=[C])O</chem>	-8.8
42607939	<chem>O1C([C])([C])[C]=[C]c2c(c3C(=O)[C][C](O)c3c(c12)[C][C](C(=[C])[C])O)C1=[C][C]=C([C]=[C]1)O)O</chem>	-8.8
23724473	<chem>c1(c(=O)c2[C]=[C][C]=[C]c2oc1C1=[C][C]=[C][C]=[C]1)O[C]1O[C]([C]([C]([C]1O)O)O)[C]O</chem>	-8.8
21604819	<chem>O1C2=C(C(=[C][C]=C2[C][C]1C1=[C][C]=C([C]=[C]1)O)O)[C][C]=C([C])[C]</chem>	-8.8
20301090	<chem>O1C2=C([C]=[C][C]=[C]2)C(=O)C(=[C])[C]1C1=[C][C]=C([C]=[C]1)N(=O)=O</chem>	-8.8
16126803	<chem>c1(c(=O)c2[C]=[C][C]=[C]c2oc1C1=[C][C]=[C][C]=[C]1)O[C]1O[C]([C]([C]([C]1O)O)O)[C]O</chem>	-8.8
16072086	<chem>C1(=[C]C(=O)C2=C([C]=C(C(=C2O1)C1=[C][C]N([C])[C][C]1)O)O)C1=[C][C]=[C]C(=[C]1)Cl</chem>	-8.8
12820520	<chem>O1C2=C([C]=c3c(=O)c(c(oc3=C2[C]=[C]C1([C])[C])C1=[C]C2=C([C]=[C]1)O[C]O2)O[C])O[C]</chem>	-8.8
12428924	<chem>O1C2=[C][C]=[C][C]=C2C(=O)/C(=[C]\C2=[C][C]=C([C]=[C]2)O)/[C]1C1=[C][C]=[C][C]=[C]1</chem>	-8.8
12146121	<chem>O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O[C][C]=C([C])[C])O[C]O[C])C1=[C][C]=[C][C]=[C]1</chem>	-8.8
12043069	<chem>C1(=[C]C(=O)C2=C(C(=C([C]=C2O)O)C2=[C]N=[C]N=[C]2)O1)C1=C(Cl)[C]=[C][C]=[C]1</chem>	-8.8
11953828	<chem>c1(c(=O)c2=[C][C]=[C][C]=c2oc1C1=[C][C]=[C][C]=[C]1)O[C]1O[C]([C]([C]([C]1O)O)O)[C]O</chem>	-8.8
11552747	<chem>C1(=[C][C]=C2C(=O)[C]=C(OC2=[C]1)C1=[C]C(=[C]C(=[C]1)O)O)O[C][C](O)[C]N([C])([C])[C]</chem>	-8.8
11382659	<chem>C1(=[C]C(=C(C(=[C]1)O)O[C])[C][C]=C([C])[C])[C]1OC2=[C]C(=[C][C]=C2C(=O)[C]1)O</chem>	-8.8
11244593	<chem>O1C2=[C]C(=C([C]=C2[C]=[C]C1([C])[C])C1=[C]OC2=C([C]=[C]C(=[C]2)O)C1=O)O</chem>	-8.8
11111496	<chem>O1C2=C(C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C(C(=[C]1)O)O)O)O)[C]/[C]=C([C])/[C]O</chem>	-8.8
10598514	<chem>O1[C]([C]C(=O)C2=C1C(=C([C]=C2O)O)[C][C](C(=[C])[C])[C][C]C([C])([C])O)C1=C([C]=[C][C]=[C]1)O</chem>	-8.8
10546844	<chem>C1(=[C]OC2=C(C(=[C]C(=[C]2)O)O[C])C1=O)C1=[C]C(=C2OC([C]=[C]C2=[C]1)([C])[C])O</chem>	-8.8
10543665	<chem>C1(=[C]C(=O)C2=C([C]=[C][C]=C2O[C])O1)C1=[C]C(=[C][C]=[C]1)C(F)(F)F</chem>	-8.8
10050660	<chem>O1C2=C(C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O[C])O[C])O[C])[C]1C(=O)C2=[C][C]=C([C]=C2O1)O[C]</chem>	-8.8
5372237	<chem>o1c2[C]=[C][C]=C(c2c(=O)c(c1C1=[C][C]=C([C]=[C]1)O[C])C(=O)C1=[C][C]=C([C]=[C]1)O[C])O</chem>	-8.8

5317756	O1C(=O)C(=[C]C2=C(C(=C([C]=C12)O)[C][C]=C([C])[C])O[C])C1=[C][C]=C([C]=C1O)O	-8.8
5317478	O1[C]=C(C(=O)C2=C(C(=C([C]=C12)O)[C][C]=C([C])[C])O)C1=[C][C]=C([C]=[C]1)O[C]	-8.8
5315125	O1C2=C(C(=[C]C(=[C]2)O)O)C(=O)[C]=C1C1=[C]C(=C(C(=[C]1)O)O)[C][C]=C([C])[C]	-8.8
5281797	O1[C]=C(C(=O)C2=C1[C]=C(C(=C2O)[C][C]=C([C])[C])O)C1=[C][C]=C([C]=C1O)O	-8.8
5281789	O1[C]=C(C(=O)C2=C1[C]=C([C]=C2O)O)C1=C(C(=C([C]=[C]1)O)[C][C]=C([C])[C])O	-8.8
624794	o1c2=[C][C]=[C][C]=c2c(=O)c(c1C1=[C][C]=C2C(=[C]1)O[C]O2)O	-8.8
462700	O1C2=[C][C]=[C][C]=C2C(=O)[C][C]1C1=[C]C(=C([C]=[C]1)O)O	-8.8
343079	O1[C]=C(C(=O)C2=C1C1=C([C]=[C]2)O[C]O1)C1=[C][C]=C2C(=[C]1)O[C]O2	-8.8
227443	o1c(c(=O)c2=[C]C(=[C][C]=c12)[C])O)C1=[C][C]=C([C]=[C]1)O[C]	-8.8
49736	o1c(c([C])c(=O)c2[C]=[C]C(=C(c12)[C]N1[C][C][C][C]1)O[C])C1=[C][C]=[C][C]=[C]1	-8.8
14570642 7	O1C2=C([C]=[C][C]=[C]2)C(=O)[C][C]1C1=[C]C(=[C]C(=[C]1)O)O[C]	-8.7
13959387 8	O1C(=[C]C(=O)C2=C1C(=[C]C(=[C]2)[C][C][C]O)O[C])C1=[C][C]=C([C]=[C]1)O[C]	-8.7
13361176 9	C1(=[C]C2=C([C]=[C]1)C(=O)C(=[C]O2)C1=[C]C(=[C]C(=[C]1)O[C])O)O[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-8.7
13253349 0	O1[C]=C(C(=O)C2=C1[C]=C(C(=C2O)[C][C](C(=[C])[C])O)O)C1=[C][C]=C2C(=[C]1)O[C]O2	-8.7
12982116 5	C1(=C([C]=C2C(=C1O)C(=O)[C][C](O2)C1=[C][C]=[C][C]=[C]1)O[C])[C][C]1OC1([C])[C]	-8.7
12971674 8	[P@]12(=O)O[C]3[C]4C5=C([C]=[C][C]=[C]5)O[P@]5(=O)O[C]6[C]([C]([C]([C]([C]6O1)O2)C3=O)O4)O5	-8.7
12968443 5	O1C2=C([C]=[C][C]=[C]2)[C][C]([C]1C1=[C][C]=[C][C]=[C]1)O	-8.7
12238334 4	O1C2=[C]C(=C([C]=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)[C][C](C(=[C])[C])O)O	-8.7
10234148 7	C1(=[C]C(=C2C(=O)[C]=C(OC2=[C]1)C1=[C][C]=C(C(=[C]1)O[C])O[C])O)O[C]1O[C]([C]([C]([C]1O)O)O)[C]	-8.7
10230725 5	c1(c(=O)c2[C]=[C][C]=[C]c2oc1C1=[C][C]=[C][C]=[C]1)C(F)(F)F	-8.7

10200538 0	C1(=[C]C(=O)C2=C(C(=C([C]=C2O[C])O[C])C2=[C][C]N([C])[C][C]2)O1)C1=C(Br)[C]=[C][C]=[C]1	-8.7
10200537 3	C1(=[C]C(=O)C2=C(C(=C([C]=C2O[C])O[C])[C]2[C]N([C])[C][C][C]2)O1)C1=C(Cl)[C]=[C][C]=[C]1	-8.7
10193217 3	C1(=C(C(=C2C(=O)[C][C](OC2=[C]1)C1=[C][C]=[C][C]=[C]1)O)O[C])O[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-8.7
10184348 6	C1(=[C]C2=C([C]=[C]1)O[C]([C]C2=O)C1=[C][C]=[C][C]=[C]1)O[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-8.7
90300755	o1c(c(c(=O)c2[C]=[C][C]=C(c12)[C][C]=C([C])[C])O)C1=[C][C]=[C][C]=[C]1	-8.7
71588337	O1C2=C(C3=C(C(=[C]2)O)C(=O)[C]=C(O3)C2=[C][C]=C([C]=[C]2)O)[C]([C](C1([C])[C])O)O[C][C]	-8.7
67424417	C1(=[C][C]=C([C]=[C]1)[C]1[C]C(=O)C2=C([C]=[C][C]=[C]2)O1)S(=O)(=O)C(F)(F)F	-8.7
56649091	C1(=[C]C2=C(C(=C1O)O)C(=O)[C]=C(O2)C1=[C][C]=[C][C]=[C]1)O[C][C]N1[C][C][C][C][C]1	-8.7
56649090	C1(=C(C(=C2C(=O)[C]=C(OC2=[C]1)C1=[C][C]=[C][C]=[C]1)O)O)O[C][C]N1[C][C]O[C][C]1	-8.7
44481784	O1[C]=C(C(=O)C2=C([C]=C([C]=C12)O[C])O)C1=[C]C(=C([C]=[C]1)O)[C][C](C(=[C])[C])O	-8.7
44342639	C1(=C([C]=C(C2=C1OC(=[C]C2=O)C1=[C][C]=[C][C]=[C]1)O)O[C])C(F)(F)F	-8.7
44265521	C1(=[C]C(=O)C2=C([C]=C(C(=C2O1)C1=[C][C]N([C])[C][C]1)O)O)C1=[C][C]=C([C]=C1Cl)Cl	-8.7
44259050	O1C2=[C]c3c(c(=O)c(c(o3)C3=[C][C]=C([C]=[C]3)O)O)C(=C2[C]=[C]C1([C])[C])O	-8.7
42607959	C1(=[C]C(=C(C(=[C]1)[C][C]=C([C])[C])O[C])/[C]=[C]/C([C])([C])O)[C]1OC2=[C]C(=[C]C(=C2C(=O)[C]1)O)O	-8.7
42607870	O1C2=C(C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1)O)O)[C]/[C]=C([C])/[C]=O	-8.7
25067674	C1(=[C]C(=O)C2=C([C]=C(C(=C2O1)[C]1[C][C]N([C])[C][C]1O)O[C])O[C])C1=[C][C]=[C][C]=C1Cl	-8.7
22737159	O1C2=[C][C]=[C][C]=C2[C][C]([C]1C1=[C][C]=[C][C]=[C]1)OC(=O)C1=[C]C(=C(C(=[C]1)O)O)O	-8.7
21325023	O1C2=C([C]=[C]C(=[C]2)C(=O)O)C(=O)[C]=C1C1=C([C]=[C][C]=[C]1)O[C]([C])[C]	-8.7
21325016	C1(=[C]C(=O)C2=[C]C(=[C][C]=C2O1)C(=O)O)C1=C([C]=[C][C]=[C]1)O[C][C]([C][C])O	-8.7
15389730	C1(=[C][C]=[C]C(=[C]1)C1=[C]C(=O)C2=C([C]=[C][C]=[C]2)O1)S(=O)(=O)N([C][C])[C][C]	-8.7
14033976	O1C2=C(C3=C(C(=[C]2)O[C])C(=O)[C]=C(O3)C2=[C][C]=C3C(=[C]2)O[C]O3)[C]=[C]C1([C])[C]	-8.7
12753167	[C]1(C(=[C])C(=O)C2=C([C]=[C][C]=[C]2)O1)C1=[C][C]=C(Cl)[C]=[C]1	-8.7
12318031	O1C2=C([C]=[C][C]=[C]2)[C][C]([C]1C1=[C][C]=[C][C]=[C]1)O	-8.7
12052874	O1C2=C([C]=[C]C(=[C]2)O)[C][C][C]1C1=[C]C2=C([C]=[C]1)O[C]O2	-8.7
12043065	C1(=[C]C(=O)C2=C([C]=C(C(=C2O1)[C]1[C]N([C])[C][C][C]1O)O)O)C1=[C][C]=[C][C]=C1Cl	-8.7

11810419	O1C2=C(C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=C1O)O)O)[C][C]=C([C])[C]	-8.7
11723752	O1[C]=C(C(=O)C2=C1[C]=C([C]=C2[C])OC(=O)O[C][C])C1=[C][C]=[C][C]=[C]1	-8.7
11711336	c1(c(=O)c2=[C][C]=[C][C]=c2oc1C1=[C][C]=[C][C]=[C]1)O[C]1O[C]([C]([C]([C]1O)O)O[C])[C]O	-8.7
11611332	C1(=[C]C2=C([C]=[C]1)C(=O)[C]=C(O2)C1=[C][C]=C(C(=[C]1)O[C])O[C])O[C][C](O)[C]N[C]([C])[C]	-8.7
11507421	O1C2=[C][C]=[C][C]=C2C(=O)[C]=C1C1=[C][C]=C([C]=[C]1)OC(=O)[C]	-8.7
11177340	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O[C][C]=C([C])[C])O[C]O[C][C]O[C])C1=[C][C]=[C][C]=[C]1	-8.7
11164320	c1(c(c(=O)c2[C]=[C]C(=[C]c2o1)O)C1=[C][C]=[C][C]=[C]1)S[C]C1=[C][C]=N[C]=[C]1	-8.7
10889522	O=C1C2=C([C]=[C][C]=[C]2)N[C]([C]1)C1=[C][C]=[C][C]=[C]1	-8.7
10832934	O1C2=[C][C]=C([C]=C2[C]([C](C1([C])[C])O)O)C1=[C]OC2=C(C(=[C]C(=[C]2)O)O)C1=O	-8.7
10317448	c1(c(c(=O)c2[C]=[C]C(=[C]c2o1)O)C1=[C][C]=C([C]=[C]1)O)S[C]C1=[C][C]=N[C]=[C]1	-8.7
9948081	C1(=[C]C2=C([C]=[C]1)C(=O)[C]=C(O2)C1=[C][C]=[C][C]=[C]1)O[C][C]1O[C]1	-8.7
5469928	O1C(=[C]C(=O)C2=C1C(=C([C]=C2O)O)[C]1[C][C][C][C]N1)C1=[C][C]=[C][C]=[C]1	-8.7
5326329	O1[C]=C(C(=O)C2=[C][C]=C(C(=C12)[C][C]=C([C])[C])O)C1=[C]C(=C([C]=[C]1)O[C])O	-8.7
3707243	O1C2=C([C]=[C][C]=[C]2)[C][C]([C]1C1=[C][C]=[C][C]=[C]1)O	-8.7
3534982	O1C2=C([C]=[C][C]=[C]2)C(=O)[C][C]1C1=[C]C(=[C][C]=[C]1)O	-8.7
3070247	c1(c([C])c(=O)c2[C]=[C]C(=C(c2o1)[C]N1[C][C][C][C]1)O[C])C1=[C][C]=C(Cl)[C]=[C]1	-8.7
3033107	C1(=[C][C]=C([C]=[C]1)c1c([C])c(=O)c2=[C][C]=[C][C]=c2o1)O[C][C](O)[C]N(C([C])([C])[C])	-8.7
688861	O1C2=C([C]=[C][C]=[C]2)C(=O)[C][C]1C1=[C]C(=[C][C]=[C]1)O	-8.7
637879	O1[C]=C(C(=O)C2=C(C3=C([C]=C12)O[C]O3)O[C])C1=[C][C]=C2C(=[C]1)O[C]O2	-8.7
635396	C1(=C([C]=C(C2=C1OC(=[C]C2=O)C1=[C][C]=C([C]=[C]1)O[C])O[C])O[C])[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-8.7
625631	O1C(=[C]C(=O)C2=C1[C]=[C]C1=C2[C]=[C]C(=[C]1)O)C1=[C][C]=[C][C]=[C]1	-8.7
466078	O1C2=C([C]=[C]C(=[C]2)O)[C][C][C]1C1=[C]C2=C([C]=[C]1)O[C]O2	-8.7
54410	C1(=[C]C2=C([C]=[C]1)C(=O)[C]=C(O2)C1=[C][C]=[C][C]=[C]1)O[C][C](O)[C]N[C][C][C]	-8.7
41450	C1(=[C][C]=C([C]=[C]1)C1=[C]C(=O)C2=[C][C]=[C][C]=C2O1)O[C][C](O)[C]N(C([C])([C])[C])	-8.7
11834	C1(=[C]C2=C([C]=[C]1)C(=O)[C]=C(O2)C1=[C][C]=[C][C]=[C]1)O[C][C]([C])[C]N([C])[C]	-8.7
13958412	O1[C]=C(C(=O)C2=C([C]=C([C]=C12)O[C])O)C1=[C][C]=C([C]=[C]1)O[C][C]=C([C])[C]	-8.6
4		
12988194	c1(c(=O)c2=[C][C]=[C][C]=c2oc1C1=[C][C]=[C][C]=[C]1)[C]1O[C]([C])[C]([C]([C]1)O)O	-8.6
0		

12982449 8	O1C(=[C]C(=O)C2=C1C(=C([C]=C2O[C])O[C])C1=[C][C]=C(C(=[C]1)O[C])O[C])C1=[C][C]=[C][C]=[C]1	-8.6
12967509 9	o1c2=[C][C]=[C][C]=c2c(=O)c(c1c1=[C][C]=[C][C]=[C]1)OC(=O)C1=[C]C=C(C(=[C]1)O)O)O	-8.6
10236976 3	O1C2=[C][C]=C3[C][C][C](OC3=C2[C][C]1C([C])([C])O)C1=[C][C]=C([C]=[C]1)O	-8.6
10200537 8	C1(=[C]C(=O)C2=C(C(=C([C]=C2O[C])O[C])C2=[C][C]N([C])[C][C]2)O1)C1=[C][C]=C(Cl)[C]=[C]1	-8.6
10094338 2	ClC1=[C]C(=[C]C(=C1O[C])S(=O)(=O)N[C]([C])([C])C1=[C]C(=O)C2=C([C]=[C][C]=[C]2)O1	-8.6
91557562	O1C2=C([C]=[C]C(=[C]2)O)C(=O)[C][C]1C1=[C][C]=C([C]=C1O)O	-8.6
76852307	O1C(=[C]C(=O)C2=C1C(=C([C]=[C]2)O)[C]=O)C1=[C][C]=[C][C]=[C]1	-8.6
74819425	O1C2=[C]C3=C(C(=C2C(=O)[C][C]1C1=C([C]=[C][C]=[C]1)O)O)O[C]O3	-8.6
59059924	O1[C]=C(C(=O)C2=[C][C]=C([C]=C12)OC(=O)C(=[C])([C])C1=[C][C]=[C][C]=[C]1	-8.6
57679080	O1C2=[C][C]=[C][C]=C2[C][C][C]1C1=[C][C]=C(C(=[C]1)O)O	-8.6
53947837	O1C2=[C][C]=C([C])[C]=C2[C][C][C]1C1=[C][C]=C([C]=[C]1)O[C]	-8.6
50909808	O1[C]=C(C(=O)C2=C([C]=C([C]=C12)O)[O])C1=[C][C]=C2C(=[C]1)O[C]O2	-8.6
44259047	C1(=C(c2c([C]=C1O)oc(c2=O)O)C1=[C][C]=C([C]=[C]1)O)O)[C][C]C([C])([C])O	-8.6
42607933	O1C2=C(C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O)O)[C][C](C(=[C])([C])O	-8.6
25128870	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O[C])O[C]C1=N[N]N[N]1)C1=[C][C]=C(C(=[C]1)O[C])O[C]	-8.6
23286063	o1c(c(c(=O)c2=[C]C(=[C][C]=c12)C(=O)O)O)C1=[C][C]=[C][C]=[C]1	-8.6
18324937	c1(c(c(=O)c2=[C][C]=[C][C]=c2o1)C1=[C][C]=C([C]=[C]1)F)C1=[C][C]=C([C]=[C]1)S(=O)(=O)N	-8.6
15731439	O1C(=[C]C(=O)C2=[C][C]=C(C(=C12)OC(=O)[C])OC(=O)[C])C1=[C][C]=[C][C]=[C]1	-8.6
15389726	C1(=[C]C(=O)C2=[C][C]=[C][C]=C2O1)C1=[C][C]=C([C]=[C]1)S(=O)(=O)Cl	-8.6
14630497	o1c(c(c(=O)c2=C([C]=C3C(=c12)[C]=[C]C([C])([C])O3)O)[C][C]C([C])([C])O)C1=C([C]=C(C(=[C]1)O)O)O	-8.6
14502737	O1C2=C(C3=C(C(=[C]2)O)C(=O)C(=[C]O3)C2=[C][C]=C3C(=[C]2)O[C]O3)[C]=[C]C1([C])[C]	-8.6
14134114	o1c(c(c(=O)c2C(=[C]C(=C(c12)C(=O)[C][C]([C])C(=O)O)O)O)O)C1=[C][C]=C([C]=[C]1)O	-8.6
14130926	o1c(c(c(=O)c2=C([C]=C([C]=C12)OC(=O)[C])OC(=O)[C])OC(=O)[C])C1=[C][C]=C([C]=[C]1)OC(=O)[C]	-8.6
14016776	C1(=[C]C(=C2C(=O)[C]=C(OC2=[C]1)C1=[C][C]=C([C]=[C]1)O)O)OS([O])([O])O	-8.6

12988090	C1(=[C]C2=C([C]=[C]1)C(=O)[C]=C(O2)C1=[C][C]=[C][C]=[C]1)OP(=O)(O[C][C])O[C][C]	-8.6
11954210	C1(=[C][C]=c2c(=O)c(c(oc2=[C]1)C1=[C][C]=[C][C]=[C]1)O)O[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-8.6
11725803	O1C2=C(C(=[C]C(=[C]2)O)O)C(=O)[C][C]1C1=[C]C=C(C(=[C]1)O)O)[C][C]=C([C])[C]	-8.6
11612258	C1(=[C]C2=C([C]=[C]1)C(=O)[C]=C(O2)C1=[C]C=C(C(=[C]1)O[C])O[C])O[C]O[C][C](O)[C]NC([C])([C])[C]	-8.6
10708855	C1(=[C]C(=O)C2=C([C]=[C][C]=[C]2)O1)C1=[C]C(=[C][C]=[C]1)[C]N=C=S	-8.6
10543327	C1(=[C]C(=O)C2=[C][C]=[C][C]=C2O1)C1=[C][C]=[C]C(=[C]1)[C]Br	-8.6
10450773	O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O)/[C]=[C]/[C]([C])([C])O)C1=C([C]=C([C]=[C]1)O)O	-8.6
9973510	O1C2=C([C]=C([C]=[C]2)C(=O)O)C(=O)[C]=C1C1=C([C]=[C][C]=[C]1)O[C]([C])[C]	-8.6
9950264	C1(=C(C2=C([C]=C1O)OC(=[C]C2=O)C1=[C][C]=[C][C]=[C]1)O)OS([O])([O])O	-8.6
9928523	O1C2=C(C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O[C])O)[C][C]=C([C])[C]	-8.6
5481229	O1C2=C(C(=[C]C(=C2O)O[C])C2=[C]OC3=[C]C(=[C]C(=C3C2=O)O)O)[C]=[C]C1([C])[C]	-8.6
5471244	C1(=[C]C(=C2C(=O)[C]=C(OC2=[C]1)C1=[C][C]=[C][C]=[C]1)O)OS([O])([O])O	-8.6
5318267	C1(=[C][C]=C2C(=O)C(=[C]OC2=[C]1)C1=[C][C]=C(C(=[C]1)O)O[C])O[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-8.6
5270553	O1C2=C([C]=C([C]=[C]2)C(=O)O)C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1	-8.6
3062797	O1[C]=C(C(=O)C2=C1[C]=C([C]=[C]2)O[C]([C])C(=O)O)C1=[C][C]=[C][C]=[C]1	-8.6
725376	O1C(=[C]C(=O)C2=C1[C]=[C]C(=[C]2)OC(=O)[C])C1=[C][C]=C([C]=[C]1)O[C]	-8.6
467492	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2OC(=O)[C])OC(=O)[C])C1=[C][C]=[C][C]=[C]1	-8.6
466293	ClC1=[C]c2c([C]=[C]1)oc(c(c2=O)O)C1=[C][C]=C([C]=[C]1)O[C]	-8.6
462699	O1C2=[C][C]=C([C]=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O	-8.6
368925	O1C2=C(C(=[C]C(=C2[C][C]=C([C])([C])O)O)C(=O)[C]([C]1C1=[C][C]=C([C]=[C]1)O)O	-8.6
227445	o1c(c(c(=O)c2[C]=C([C])[C]=[C]c12)O)C1=[C][C]=[C][C]=[C]1	-8.6
182342	O1C2=[C][C]=C3C(=O)C(=[C]OC3=C2[C]=[C]C1([C])([C])C1=[C]C2=C([C]=[C]1)O[C]O2	-8.6
118907	O1C(=[C]C(=O)C2=C([C]=C([C]=C12)O[C]C(=O)O[C][C])O[C]C(=O)O[C][C])C1=[C][C]=[C][C]=[C]1	-8.6
11912	C1(=[C][C]=C2C(=O)[C]=C(OC2=[C]1)C1=[C][C]=[C][C]=[C]1)O[C][C][C]N([C])[C]	-8.6
13908069	o1c(c(c(=O)c2C(=[C]C(=[C]c12)O[C][C]=C([C])([C])O)O)C1=[C][C]=C(C(=[C]1)O)O)[C]	-8.5
7		
13482126	O1[C]2[C]C3=[C][C]=[C][C]=C3O[C@]12C1=[C][C]=[C][C]=[C]1	-8.5
8		

13306495 3	o1c(c(c(=O)c2C(=[C][C]=[C]c12)[C]C#[C])N)C1=[C][C]=[C][C]=[C]1	-8.5
13251736 6	O1C(=[C]C(=O)C2=C1C(=C(C(=[C]2)O)O[C]))/[C]=C(\[C])/[C]O)C1=[C][C]=C([C]=[C]1)O[C]	-8.5
12983450 7	O1C2=[C]C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)OC(=O)[C])O[C])OC(=O)[C]	-8.5
12982239 5	Clc1c(c(c2C(=O)[C]=C(Oc12)C1=[C][C]=C([C]=[C]1)OC(=O)[C])OC(=O)[C])OC(=O)[C])OC(=O)[C]	-8.5
12982236 1	O1C(=[C]C(=O)C2=C1C(=C(C(=[C]2)OC(=O)[C])OC(=O)[C])N)C1=[C][C]=[C][C]=[C]1	-8.5
10257793 2	C1(=[C]C2=C(C(=[C]1)O)C(=O)[C]=C(O2)C1=[C][C]=C([C]=[C]1)O)OS([C])([O])[O]	-8.5
10200537 9	C1(=[C]C(=O)C2=C(C(=C([C]=C2O[C])O[C])C2=[C][C]N([C])[C][C]2)O1)C1=[C][C]=[C][C]=C1F	-8.5
10200537 6	C1(=[C]C(=O)C2=C(C(=C([C]=C2O[C])O[C])C2=[C][C]N([C])[C][C]2)O1)C1=[C][C]=[C][C]=C1Cl	-8.5
10200304 5	O1C2=[C]C(=[C][C]C2=[C]C(=[C]1)C1=C([C]=C2C(=[C]1)O[C]O2)O[C])O	-8.5
10168070 5	C1(=[C]C2=C([C]=[C]1)C(=O)[C]=C(O2)C1=[C][C]=[C][C]=[C]1)C(=O)[C]Br	-8.5
10164301 0	O1C2=C(C(=[C]C(=C2[C][C]=C([C])[C])O)O)C(=O)[C]([C]1C1=[C][C]=C([C]=[C]1)O)O	-8.5
10144052 1	o1c2[C]=C([C]=C(c2c(=O)c(c1C1=[C][C]=C(C(=[C]1)[C][C](C(=[C])[C])O)O)O)O	-8.5
10136776 6	O1C2=C(C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O)[C]/[C]=C(\[C])/[C]O	-8.5
10121375 9	O1[C]=C(C(=O)C2=C1[C]=C([C]=C2O)O)C1=C([C]=C(C(=[C]1)[C][C]=C([C])[C])O[C])O	-8.5
10110115 3	C1(=C(C(=C2C(=[C]1)OC(=[C]C2=O)C1=[C][C]=[C][C]=[C]1)O)O[C])O[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-8.5
90753092	o1c(c(c(=O)c2=C([C])C(=C([C])[C]=c12)[C])O)C1=[C][C]=[C][C]=[C]1	-8.5

69279473	O1C2=C([C]=C([C]=[C]2)[C][C][C][C])C(=O)[C]([C]1C1=[C][C]=[C][C]=[C]1)O	-8.5
54512651	O1C2=[C][C]=[C][C]=C2C(=O)/C(=[C]\N)/[C]1C1=[C][C]=[C][C]=[C]1	-8.5
53747690	C1(=[C]C2=C(C(=[C]1)O)C(=O)[C]=C(O2)C1=[C][C]=[C][C]=[C]1)C(=O)[C]Br	-8.5
53247945	C1(=[C][C]=C([C]=[C]1)[C]1[C]C(=O)C2=C([C]=[C][C]=[C]2)O1)O[C]1O[C]([C]([C]([C]1O)O)O[C])[C]O	-8.5
49800274	O1C(=[C]C(=O)C2=C1C(=C([C]=C2O[C])O[C])C1=[C][C]N([C])[C][C]1)C1=[C][C]=[C][C]=[C]1	-8.5
44382543	C1(=C([C]=C(C2=C1OC(=[C]C2=O)C1=[C][C]=[C][C]=[C]1)O[C])O[C])C(F)(F)F	-8.5
44380969	O1C(=[C]C(=O)C2=C([C]=C(C(=C12)N[C][C][C]([C])O)O)C1=[C][C]=[C][C]=[C]1	-8.5
44380895	O1C(=[C]C(=O)C2=C([C]=C(C(=C12)N[C][C]([C])O)O)C1=[C][C]=[C][C]=[C]1	-8.5
44265561	C1(=[C]C(=O)C2=C(C(=C([C]=C2O)O)C2=[C][C]N([C])[C][C]2)O1)C1=[C][C]=C(Cl)[C]=[C]1	-8.5
44265528	C1(=[C]C(=O)C2=C([C]=C(C(=C2O1)C1=[C][C]N([C])[C][C]1)O)O)C1=[C][C]=[C][C]=C1Br	-8.5
44265522	O1C(=[C]C(=O)C2=C1C(=C([C]=C2O)O)C1=[C][C]N([C])[C][C]1)C1=[C][C]=[C][C]=[C]1	-8.5
44258693	O1C2=C(c3c([C]=C2O[C])c(=O)c(c(o3)C2=[C][C]=C([C]=[C]2)O)O[C])[C]=[C]C1([C])[C]	-8.5
42607869	O1C2=C(C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1)O)O)[C]/[C]=C(\[C])/[C]O	-8.5
25201019	O1C2=C(C(=[C]C(=[C]2)O)[O])C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O[C]	-8.5
25058575	C1(=C([C]=C(C(=[C]1)O[C])O[C][C]=C([C])O[C])C1=[C]OC2=C(C1=O)C(=[C]C(=[C]2)O[C])O[C]	-8.5
21325058	O1C2=C([C]=C([C]=[C]2)C(=O)O[C])C(=O)[C][C]1C1=[C][C]=[C][C]=C1N(=O)=O	-8.5
14791391	O1C2=C([C]=[C]C(=[C]2)O)C(=O)[C]=C1C1=[C][C]=C([C]=[C]1)N(=O)=O	-8.5
14033984	O1C2=C([C]=c3c(=O)c(c(oc3=C2[C]=[C]C1([C])[C])C1=[C][C]=[C][C]=[C]1)O[C])O[C]	-8.5
13432335	O1C(=[C]C(=O)C2=C([C])[C]=C([C])[C]=C12)C1=[C][C]=[C][C]=[C]1	-8.5
13393782	[C]1([C]C(=O)C2=[C][C]=[C][C]=C2O1)C1=[C][C]=[C]C(=[C]1)F	-8.5
12753173	[C]1([C]C(=O)C2=[C][C]=[C][C]=C2O1)C1=C(Cl)[C]=C([C]=[C]1)Cl	-8.5
12049385	O1C(=[C][C]=C2[C][C]=C([C]=C12)N([C][C])[C][C])C1=[C][C]=C([C]=[C]1)N([C])[C]	-8.5
12043066	C1(=[C]C(=O)C2=C([C]=C(C(=C2O1)[C]1[C][C][C][C]1O)O)O)C1=[C][C]=[C][C]=C1Cl	-8.5
11683340	C1(=[C]C2=C([C]=[C]1)C(=O)[C]=C(O2)C1=[C]C(=[C]C(=[C]1)O[C])O[C])O[C][C](O)[C]NC([C])([C])[C]	-8.5
11186717	O1C2=C([C]=C([C]=C2[C]=[C]C1([C])[C])C1=[C]OC2=C([C]=[C]C(=[C]2)O)C1=O)O	-8.5
10957930	O1C2=[C][C]=[C][C]=C2C(=O)/C(=[C]/C2=[C][C]=[C][C]=[C]2)/[C]1C1=[C][C]=[C][C]=[C]1	-8.5
10848398	O1C2=C([C]=[C]C(=[C]2)O)C(=O)[C]=C1C1=[C][C]=C([C])[C]=[C]1	-8.5
10761522	[C]1([C]C(=O)C2=C([C]=C([C]=C2O)O)O1)C1=[C]C(=C2OC([C]=[C]C2=[C]1)([C])[C])O[C]	-8.5
10708856	C1(=[C]C(=O)C2=C([C]=[C][C]=[C]2)O1)C1=[C][C]=C([C]=[C]1)[C]N=C=S	-8.5

10018499	O1c2c(c(c([C])c(c2C(=O)[C][C@]1(C1=[C][C]=[C][C]=[C]1)O)O)[C]=O	-8.5
6116651	O1C2=[C][C]=[C][C]=C2C(=O)/C(=[C]\C2=[C][C]=N[C]=[C]2)/[C]1C1=[C][C]=[C][C]=[C]1	-8.5
5378945	O1[C]=C(C(=O)C2=C(C(=C([C]=C12)O)[C]/[C]=C(\[C])/[C]O)O)C1=[C][C]=C([C]=[C]1)O	-8.5
5322065	O1C2=C([C]=[C]C(=[C]2)O)C(=O)[C]=C1C1=[C]C(=C([C]=[C]1)O)O	-8.5
5321987	[C]1(C2=C([C]=[C]C(=[C]2)O[C])O[C][C]1C1=[C]C(=[C]C(=C1O)O[C])/[C]=[C]/C(=O)O)OS([O])([O])O	-8.5
5317300	C1(=C(C(=C([C]=[C]1)O)[C][C]=C([C])[C])O)C1=[C]OC2=C(C1=O)[C]=[C]C(=[C]2)O	-8.5
5272799	O1C2=[C][C]=[C][C]=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)C1=N[C][C]O1	-8.5
5270543	FC1=[C]C2=C([C]=[C]1)C(=O)[C][C](O2)C1=[C][C]=[C][C]=[C]1	-8.5
5049148	O1c2c(c(c3C(=O)C(=[C]Oc3c2[C]=[C]C1([C])[C])C1=[C]C2=C([C]=[C]1)O[C]O2)O[C])O[C]	-8.5
746742	C1(=[C]OC2=C([C]=[C]C(=[C]2)O[C]([C])[C])C1=O)C1=[C][C]=C(F)[C]=[C]1	-8.5
630804	O1[C]=C(C(=O)C2=C1C(=C([C]=C2OC(=O)[C])OC(=O)[C])[C][C]=C([C])[C])C1=[C][C]=C([C]=[C]1)OC(=O)[C]	-8.5
342294	O1C2=[C]C(=[C]C(=C2[C][C][C]1C1=[C][C]=[C][C]=[C]1)O[C])O	-8.5
188424	O1C2=C(C(=[C]C(=[C]2)O)O[C])C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O	-8.5
187093	O1C2=[C]C(=[C][C]=C2C(=O)[C][C]1C1=[C]C(=C([C]=[C]1)O[C])O)O	-8.5
185027	O1C2=C([C]=[C]C(=C2/[C]=[C]/C(=[C])[C])O[C])C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1	-8.5
126392	O1C(=[C]C(=O)C2=C1C(=[C][C]=[C]2)[C]C(=O)O[C]N([C])[C])C1=[C][C]=[C][C]=[C]1	-8.5
8395	O1C(=[C]C(=O)C2=[C][C]=C([C]=C12)O[C]C(=O)O[C][C])C1=[C][C]=[C][C]=[C]1	-8.5
1889	O1C2=[C]C(=[C][C]=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O	-8.5
12983023 9	C1(=[C]C(=C([C]=C1c1c(c(=O)c2=C([C]=C([C]=c2o1)O)O)O)O)S(=O)(=O)C1=[C][C]=C([C]=[C]1)[C]	-8.4
12982555 6	o1c2=[C]C(=C(C(=c2c(=O)c(c1C1=[C]C(=C([C]=[C]1)O)/[C]=[C]/C(=[C])[C])O[C])O)O[C])O	-8.4
12981335 4	O1C2=[C]C(=[C][C]=C2C(=O)[C][C]1C1=[C]C(=C(C(=[C]1)O)O)O)O[C]	-8.4
12978128 8	O1[C]=C(C(=C2[C]=[C][C]=[C][C]12)[N]O)C1=[C][C]=[C][C]=[C]1	-8.4
10206428 8	O1C(=[C]C(=O)C2=C1C(=[C][C]=[C]2)/[C]=[C]/[C])C1=[C][C]=[C][C]=[C]1	-8.4
10201716 5	O1C(=[C]C(=O)C2=C([C]=C(C(=C12)[C][C]C(=[C])[C])O)O)C1=[C][C]=[C][C]=[C]1	-8.4

10176363 2	C1(=C(C2=C([C]=C1O)O)[C]=C(C2=O)C1=[C][C]=C([C]=[C]1)O)O)[C]C([C])([C])O	-8.4
10168070 6	C1(=C2C(=[C][C]=C1C(=O)[C]Br)C(=O)[C]=C(O2)C1=[C][C]=[C][C]=[C]1)C(=O)[C]Br	-8.4
10162120 6	O1C2=[C][C]=C([C])[C]=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)N([C])[C]	-8.4
10159128 0	C1(=[C][C]=C2C(=C1O[C])C(=O)[C]=C(O2)C1=[C][C]=C(C(=[C]1)O[C])O)O[C][C][C][C][C]	-8.4
10149923 5	C1(=[C]C(=C(C(=[C]1)O[C])O[C]([C]O)[C](C1=[C][C]=C([C]=[C]1)O)O)O[C])[C]1OC2=C(C(=[C]C(=[C]2)O)O)C(=O)[C]1	-8.4
10102840 4	O1C(=[C]C(=O)C2=C1C(=C([C]=C2O)O)N[C]([C])([C])C1=[C][C]=[C][C]=[C]1	-8.4
10102840 3	O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O)N[C][C]=[C])O)C1=[C][C]=[C][C]=[C]1	-8.4
10094338 5	ClC1=C(C(=[C]C(=[C]1)C1=[C]C(=O)C2=[C][C]=[C][C]=C2O1)S(=O)(=O)Cl)O[C]	-8.4
87771765	[C]1(C(=O)C2=C([C]=[C][C]=[C]2)O[C@]1(C1=[C][C]=[C][C]=[C]1)C(=O)C1=[C]C(=C(C(=[C]1)O)O)O)OS([O])([O])O	-8.4
73829901	O1C2=[C]C3=C(C(=C2C(=O)[C]([C]1C1=[C][C]=[C][C]=[C]1)O)O[C])O[C]O3	-8.4
71621986	C1(=C([C]=C2C(=[C]1)O[C]=C(C2=O)C1=[C][C]=C([C]=[C]1)O)O[C])O[C]1O[C]([C]([C]([C]1O)O)O[C])[C]O	-8.4
70350763	O1C2=[C][C]=[C][C]=C2C(=O)/C(=[C]\O)/[C]1C1=[C][C]=[C][C]=[C]1	-8.4
66783912	C1(=[C]C(=O)C2=C(C3=C([C]=C2O1)O[C]O3)O)C1=[C][C]=C([C]=[C]1)O[C][C]N([C][C])[C][C]	-8.4
57340187	O1C2=[C]C(=[C][C]=C2C(=O)[C]=C1C1=[C][C]=C([C]=[C]1)/[C]=[C]/C(=O)O)O	-8.4
53398699	C1(=[C]C2=C([C]=[C]1)C(=O)C(=[C]O2)C1=[C][C]=C([C]=[C]1)O)O[C]1O[C]([C]([C]([C]1O)O)O)[C]OC(=O)[C]	-8.4
44265523	C1(=[C]C(=O)C2=C(C(=C([C]=C2O)O)C2=[C][C]N([C])[C][C]2)O1)C1=C(I)[C]=[C][C]=[C]1	-8.4
44257645	O1C2=[C]C(=C3C(=O)[C]=C(OC3=C2[C]([C]1)[C](C([C])([C])OC(=O)[C])OC(=O)[C])C1=[C][C]=[C][C]=[C]1)O[C]	-8.4
44257318	O1[C]=C(C(=O)C2=C1C(=C([C]=C2O)O)[C]/[C]=C([C])/[C]O)C1=[C][C]=C([C]=C1O)O	-8.4
25022738	O1C2=[C]C(=C([C]=C2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1)O[C])O	-8.4
23644938	c1(c(c(=O)c2[C]=[C]C(=[C]c2o1)O[C])C1=[C][C]=[C][C]=[C]1)SC1=N[C]=NN1	-8.4
21270125	C1(=[C]OC2=C([C]=C(C(=[C]2)O)O)C1=O)C1=[C][C]=C(Cl)[C]=[C]1	-8.4
18324915	c1(c(c(=O)c2[C]=[C][C]=[C]c2o1)C1=[C]C(=[C][C]=[C]1)F)C1=[C][C]=C([C]=[C]1)S(=O)(=O)[C]	-8.4

16215025	C1(=C2C(=C(C(=[C]1)O[C])O[C])O[C]([C]C2=O)C1=[C][C]=[C][C]=[C]1)O[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-8.4
15491286	o1c(c(c(=O)c2c(c(c(c12)O)O[C])O[C])O[C])O[C]C(=[C]([C])O)O)C1=[C]C(=C([C]=[C]1)O)O[C]	-8.4
15485967	O1C2=C(C(=C(C(=[C]2)O[C])O[C])O[C])O[C]C(=[C]([C])O)C(=O)[C]C1C1=[C][C]=C([C]=[C]1)O	-8.4
15458309	O1C2=C(C(=[C][C]=C2C(=O)[C]C1C1=[C][C]=C([C]=[C]1)O[C])O[C])O[C]	-8.4
15385487	O1C2=[C]C(=[C][C]=C2C(=O)[C]C1C1=[C][C]=C(C(=[C]1)O[C])O)O	-8.4
15301053	O1[C]=C(C(=O)C2=C1[C]=C([C]=C2O)O)C1=[C]C2=C([C]=[C]1)O[C]O2	-8.4
14885875	O1C2=[C]C(=[C]C(=C2[C][C]C1C1=[C][C]=[C][C]=[C]1)O[C])O	-8.4
12813783	O1C2=C([C]=[C][C]=[C]2)C(=O)[C]=C1C1=[C]C(=[C][C]=[C]1)[C]	-8.4
12813780	O1C2=C([C]=[C][C]=[C]2)C(=O)[C]C1C1=[C]C(=[C][C]=[C]1)[C]	-8.4
12407921	O1C2=C([C]=C([C]=[C]2)C(=O)O)C(=O)[C]=C1C1=[C][C]=C([C]=[C]1)O[C][C]O	-8.4
11739635	C1(=[C]C(=C(C(=[C]1)O)O[C])O[C])O[C]C(=[C]([C])O)C1=[C]OC2=[C]C(=[C][C]=C2C1=O)O	-8.4
11704980	o1c2[C]=[C][C]=[C]c2c(=O)c(c1C1=[C]C(=C(C(=[C]1)O[C])O[C])O[C])C(=O)C1=[C][C]=C([C]=[C]1)O[C]	-8.4
11583077	C1(=[C][C]=C2C(=O)[C]=C(OC2=[C]1)C1=[C]C(=C(C(=[C]1)O[C])O[C])O[C])O[C]([C](O)[C]N[C]([C])[C]	-8.4
11494111	C1(=[C]OC2=[C]C(=[C]C(=C2C1=O)O)O)C1=[C][C]=C(C2=C1[C][C]C(O2)([C])[C])O	-8.4
11149874	O1C2=[C][C]=[C][C]=C2C(=O)[C]C1C1=[C][C]=C([C]=[C]1)N(=O)=O	-8.4
10980660	O1C2=C(C(=[C]C(=C2C(=O)[C]C1C1=[C][C]=[C][C]=[C]1)O)O[C])/[C]=[C]/C(=O)[C]	-8.4
10901472	o1c2=[C][C]=[C][C]=c2c(=O)c(c1C1=[C][C]=C([C]=[C]1)[C]=[C])O	-8.4
10659060	O1C2=C([C]=[C][C]=[C]2)C(=O)[C]=C1C1=[C]C(=[C][C]=[C]1)[C]C#N	-8.4
10357090	C1(=[C][C]=[C]C2=C1O[C]=C(C2=O)C1=[C][C]=[C][C]=[C]1)O[C][C]1O[C]1	-8.4
10244935	O1C(=[C]C(=O)C2=C(C(=C([C]=C12)O)N[C][C][C])O)C1=[C][C]=[C][C]=[C]1	-8.4
10108482	C1(=[C][C]=C2C(=O)C(=[C]OC2=[C]1)C1=[C][C]=[C][C]=[C]1)O[C][C]1O[C]1	-8.4
9883305	o1c(c(c(=O)c2=C(C3=C([C]=c12)O[C]O3)O)O)C1=[C][C]=C([C]=[C]1)O	-8.4
5393156	O1C(=[C]C(=O)C2=C([C])[C]=C([C]=C12)O)C1=[C][C]=[C][C]=[C]1	-8.4
5391140	O1C(=[C]C(=O)C2=[C][C]=C([C]=C12)O)C1=[C]C(=[C][C]=[C]1)O	-8.4
5378171	O1C(=[C]C(=O)C2=C([C]=C([C])[C]=C12)O)C1=[C][C]=C([C]=[C]1)O[C]	-8.4
5320693	O1C2=[C]C(=[C][C]=C2C(=O)[C]=C1C1=[C][C]=C([C]=[C]1)O[C])O	-8.4
5317480	O1[C]=C(C(=O)C2=C1C(=C([C]=C2O)O)[C][C]=C([C])[C])C1=[C][C]=C([C]=[C]1)O	-8.4
5281670	o1c2=[C]C(=[C]C(=c2c(=O)c(c1C1=C([C]=C([C]=[C]1)O)O)O)O)O	-8.4
5281601	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O)O[C])C1=[C][C]=C([C]=[C]1)O[C]	-8.4

5272796	O1C2=C([C]=[C][C]=[C]2)C(=O)[C]=C1C1=[C][C]=C([C]=[C]1)C(=O)O	-8.4
2734580	O1C2=C([C]=C([C]=[C]2)O)C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1	-8.4
1232441	O1C2=C([C]=[C][C]=[C]2)[C][C][C]1C1=[C][C]=[C][C]=[C]1	-8.4
688859	O1C2=[C][C]=[C][C]=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O	-8.4
688857	O1C2=C([C]=[C]C(=[C]2)O)C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1	-8.4
688835	o1c2[C]=[C]C(=[C]c2c(=O)c(c1C1=[C]C(=[C][C]=[C]1)O[C])O)O[C]	-8.4
676310	O1C(=[C]C(=O)C2=[C][C]=C(C(=C12)O)O)C1=[C]C(=[C][C]=[C]1)O	-8.4
676309	O1C(=[C]C(=O)C2=C1C(=C([C]=[C]2)O)O)C1=[C][C]=[C][C]=C1O	-8.4
626146	o1c([C])c(c(=O)c2[C]=[C]C(=[C]c12)O[C][C]=[C])C1=[C][C]=[C][C]=[C]1	-8.4
466268	O1C(=[C]C(=O)C2=[C][C]=C([C]=C12)O[C])C1=[C][C]=[C][C]=[C]1	-8.4
373261	O1C2=C(C(=[C]C(=[C]2)O)O)C(=O)[C][C]1C1=[C]C(=C([C]=[C]1)O)O	-8.4
242065	[C]1([C]C(=O)C2=[C][C]=[C][C]=C2O1)C1=[C][C]=C(Cl)[C]=[C]1	-8.4
226342	O1C2=[C][C]=[C][C]=C2C(=O)[C][C]1C1=[C][C]=C(C(=[C]1)O[C])O	-8.4
165506	O1C2=[C][C]=[C][C]=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O	-8.4
145726	O1C2=C([C]=[C][C]=[C]2)C(=O)[C]=C1C1=[C]C(=C([C]=[C]1)O)O	-8.4
97860	O1C2=C([C]=C([C]=[C]2)O[C])C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1	-8.4
55750	C1(=[C][C]=[C]C2=C1OC(=[C]C2=O)C1=[C][C]=[C][C]=[C]1)[C]C(=O)O[C][C]N([C][C])[C][C]	-8.4
27443	o1c(c([C])c(=O)c2=[C]C(=[C][C]=c12)[C]N([C][C])[C][C])C1=[C][C]=[C][C]=[C]1	-8.4
20489	O1C(=[C]C(=O)C2=C([C]=C(C(=C12)O)O[C])O)C1=[C][C]=[C][C]=[C]1	-8.4
1890	O1C2=C([C]=[C]C(=[C]2)O)C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1	-8.4
13253615 8	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2OC(=O)[C]=[C])OC(=O)[C]=[C])C1=[C][C]=C([C]=[C]1)OC(=O)[C]=[C]	-8.3
13247200 6	o1c2[C]=C([C])[C]=C(c2c(=O)c([C])c1C1=[C][C]=C([C])[C]=[C]1)O	-8.3
12986429 4	O1C2=C([C]=[C][C]=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O[C]	-8.3
12985216 0	C1(=c2c(=[C][C]=[C]1)oc(c(c2=O)O)C1=[C][C]=[C][C]=[C]1)[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-8.3

12983569 5	O1C2=[C][C]=[C][C]=C2C(=O)[C@@]([C@]1(C1=[C][C]=[C][C]=[C]1)O)(c1c(=O)c2=[C][C]=[C][C]=c2oc1C1=[C][C]=[C][C] =[C]1)O	-8.3
12982676 9	S=C1C2=C([C]=[C][C]=[C]2)O[C]([C]1)C1=[C][C]=C([C])[C]=[C]1	-8.3
12982445 6	O1C(=[C]C(=C2[C]C(=[C][C]=C12)[C]=O)[N]O)C1=[C][C]=[C][C]=[C]1	-8.3
12973022 2	O1C(=[C]C(=O)C2=C1C(=[C]C(=[C]2)[C])C(=O)[C][C])C1=[C][C]=[C][C]=[C]1	-8.3
12968987 5	O1C(=[C]C(=O)C2=C([C]=[C][C]=C12)OC(O)(O)O)C1=[C][C]=[C][C]=[C]1	-8.3
10236007 9	O1C2=C(C3=C(C(=[C]2)O[C])C(=O)[C][C](O3)C2=[C][C]=[C][C]=[C]2)[C]([C](C1([C])[C])OC(=O)[C])OC(=O)[C]	-8.3
10215422 0	O1C2=[C]C3=C(C(=O)[C]=C(O3)C3=[C][C]=C([C]=[C]3)O)C(=C2[C]([C]C1([C])[C])O)O	-8.3
10209126 7	O1C2=[C][C]=[C][C]=C2[C]([C][C]1C1=[C][C]=[C][C]=[C]1)[N]OC(=O)[C]	-8.3
10184348 4	C1(=[C][C]=[C]C2=C1C(=O)[C]=C(O2)C1=[C][C]=C([C]=[C]1)O)O[C]1O[C]([C]([C]([C]1O)O)O[C])[C]O	-8.3
10168525 1	C1(=[C][C]=C([C]=[C]1)C(=O)N[C][C]O)C1=[C]C(=O)C2=[C][C]=[C][C]=C2O1	-8.3
10168524 9	C1(=[C][C]=C([C]=[C]1)C(=O)N[C][C]O)[C]1OC2=C([C]=[C][C]=[C]2)C(=O)[C]1	-8.3
10159199 8	C1(=[C]C(=C2C(=O)[C]=C(OC2=C1O[C])C1=[C][C]=[C][C]=[C]1)O[C])O[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-8.3
10149923 6	C1(=C([C]=C([C]=C1O[C])C1=[C]C(=O)C2=C([C]=C([C]=C2O)O)O1)O[C])O[C]([C]O)[C](C1=[C][C]=C([C]=[C]1)O)O	-8.3
10102840 8	O1C(=[C]C(=O)C2=C([C]=C(C(=C12)N[C][C][C]([C])[C])O[C])O[C])C1=[C][C]=[C][C]=[C]1	-8.3
10102840 5	O1C(=[C]C(=O)C2=C1C(=C([C]=C2O[C])O[C])N[C]([C])[C])C1=[C][C]=[C][C]=[C]1	-8.3

10091405 2	C1(=[C][C]=C([C]=[C]1)c1c(c(=O)c2[C]=[C][C]=[C]c2o1)O)N1[C][C]O[C][C]O[C][C]O[C][C]O[C][C]1	-8.3
89858365	o1c(c(c(=O)c2C(=[C][C]=[C]c12)C(=O)[C])O)C1=[C][C]=[C][C]=[C]1	-8.3
86236611	C1(=[C][C]=C2C(=O)[C]=C(OC2=[C]1)C1=[C]C(=C([C]=[C]1)O[C])O[C])O[C][C]1O[C]1	-8.3
85751070	[N](C1=C2C(=[C][C]=[C][C]2)OC(=[C]1)C1=[C][C]=[C][C]=[C]1)NC(=S)N	-8.3
71762131	O1C(=[C]C(=O)C2=C1C(=C([C]=[C]2)O)O[C])C1=[C][C]=[C][C]=[C]1	-8.3
71621984	C1(=[C]C(=C2C(=O)C(=[C]OC2=[C]1)C1=[C][C]=C([C]=[C]1)O)O)O[C]1O[C]([C]([C]([C]1O)O)O[C])[C]O	-8.3
69234627	O([C@@]1([C][C]C2=[C][C]=[C][C]=C2O1)C1=[C][C]=[C][C]=[C]1)[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-8.3
67114276	o1c(c(c(=O)c2=C([C]=[C][C]=c12)C(=O)[C])C(=O)[C])C1=[C][C]=[C][C]=[C]1	-8.3
66650373	C1(=[C][C]=[C]C2=C1C(=O)[C]=C(O2)C1=[C][C]=[C][C]=[C]1)[C]Br	-8.3
66561376	o1c(c(c(=O)c2c(c3c(c(c12)O[C])O[C]O3)O)O[C])C1=[C]C2=C([C]=[C]1)O[C]O2	-8.3
57409964	C1(=[C]C(=C(C(=[C]1)[C][C](C(=[C])O)O)[C]/[C]=C(/[C])\)[C]O)c1oc2=[C]C(=C(C(=c2c(=O)c1O[C])O)O[C])O	-8.3
57340184	C1(=[C]C(=O)C2=C([C]=C([C]=[C]2)O)O1)C1=[C][C]=C(F)[C]=[C]1	-8.3
54553686	O1C2=C([C]=[C][C]=[C]2)C(=O)[C][C]1C1=[C]C(=[C][C]=[C]1)C#N	-8.3
53247999	C1(=[C][C]=C([C]=[C]1)[C]1[C]C(=O)C2=[C][C]=[C][C]=C2O1)O[C]1O[C]([C]([C]([C]1O)O)O)[C]	-8.3
53247946	C1(=[C]C2=C([C]=[C]1)O[C]([C]C2=O)C1=[C][C]=C([C]=[C]1)O)O[C]1O[C]([C]([C]([C]1O)O)O[C])[C]O	-8.3
45933941	O1C2=[C][C]=[C][C]=C2C(=O)[C]=C1C1=[C]C(=[C]C(=[C]1)O)O	-8.3
44380894	O1C(=[C]C(=O)C2=C([C]=C(C(=C12)N[C][C][C])O)O)C1=[C][C]=[C][C]=[C]1	-8.3
44259965	o1c(c(c(=O)c2=C([C]=C(C(=c12)O)O[C])O)O)C1=[C][C]=C([C]=[C]1)O	-8.3
44259864	o1c(c(c(=O)c2c(c(c3c([C]=[C]O3)c12)O[C])O[C])O[C])C1=[C]C2=C([C]=[C]1)O[C]O2	-8.3
44258614	O1c2c3C(=O)[C]=C(Oc3c(c(c2[C]=[C]C1([C])[C])O[C])O[C])C1=[C][C]=C(C(=[C]1)O[C])O[C]	-8.3
44258526	O1C(=[C]C(=O)C2=C1[C]=C(C1=C2O[C]O1)O[C])C1=[C][C]=C2C(=[C]1)O[C]O2	-8.3
42608071	O1C2=C(C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O)O[C])[C][C]=C([C])[C]	-8.3
42608069	O1C2=C(C(=[C]C3=C2[C]=[C]C(O3)([C])[C])O[C])C(=O)[C][C]1C1=[C]C(=[C][C]=[C]1)O[C])O[C]	-8.3
23644937	c1(c(c(=O)c2[C]=[C]C(=[C]c2o1)O[C])C1=[C][C]=[C][C]=[C]1)SC1=N[C]=[C]N1[C]	-8.3
20452436	O1C2=C([C]=[C][C]=[C]2)[C][C][C]1C1=[C][C]=C([C]=[C]1)O	-8.3
20394007	C1(=[C][C]=C2C(=O)C(=[C]OC2=[C]1)C1=[C][C]=[C][C]=[C]1)O[C]([C])[C][C]	-8.3
20301086	O1C2=[C][C]=[C][C]=C2C(=O)C(=[C])[C]1C1=[C]C(=[C][C]=[C]1)N(=O)=O	-8.3
15896301	O1C(=[C]C(=O)c2c(c(c(c12)O[C])O[C])O[C])O)C1=[C][C]=[C]C(=C1O)O[C]	-8.3

14034288	O1C2=C(C(=[C]C(=C2O)O[C])O)C(=O)[C][C]1C1=[C][C]=[C][C]=C1O	-8.3
12674946	o1c2=[C][C]=[C][C]=c2c(=O)c(c1C1=[C][C]=[C][C]=[C]1)C(=O)O	-8.3
12114693	O1[C]([C]C(=O)C2=C1C(=C([C]=C2O)O)C([C])([C])[C]=[C])C1=[C][C]=C([C]=[C]1)O	-8.3
12098358	O1C2=C(C(=[C]C(=C2O[C])O[C])O)C(=O)[C][C]1C1=[C][C]=[C][C]=C1O	-8.3
11661570	C1(=[C]C2=C([C]=[C]1)C(=O)[C]=C(O2)C1=[C]C(=[C]C(=[C]1)O[C])O[C])O[C][C](O)[C]N[C]([C])[C]	-8.3
11382711	C1(=C(C2=C([C]=C1O)O[C]=C(C2=O)C1=[C][C]=C([C]=[C]1)O)O)[C][C]C([C])([C])O	-8.3
11246736	c1(c(c(=O)c2[C]=[C]C(=[C]c2o1)O[C])C1=[C][C]=C([C]=[C]1)O[C])S[C]C1=[C][C]=N[C]=[C]1	-8.3
11176755	c1(c(c(=O)c2[C]=[C]C(=[C]c2o1)O[C])C1=[C][C]=C([C]=[C]1)[C])S[C]C1=[C][C]=N[C]=[C]1	-8.3
10904774	C1(=C([C]=C(C2=C1O[C]=C(C2=O)C1=C([C]=C([C]=[C]1)O)O)O)[C][C]C([C])([C])O	-8.3
10902653	C1(=[C]C(=O)C2=[C][C]=[C][C]=C2O1)C1=[C][C]=C([C]=[C]1)S(=O)(=O)[C]	-8.3
10777811	O1C2=[C][C]=[C][C]=C2C(=O)[C]=C1C1=[C][C]=C([C]=[C]1)[C]C#N	-8.3
10742453	O1[C]([C]C(=O)C2=C1C(=C([C]=C2O)O)[C][C](C(=[C])[C])[C][C]C([C])([C])O)C1=C([C]=C([C]=[C]1)O)O[C]	-8.3
10736576	O1C2=[C]C3=C(C(=O)C(=[C]O3)C3=[C][C]=C([C]=[C]3)O)C(=C2[C]=[C]C1([C])[C])O[C]	-8.3
10498462	O1C2=C(C(=C(C(=[C]2)O)C([C])([C])[C]=[C])O)C(=O)[C][C]1C1=[C]C(=[C]=[C]1)O)O	-8.3
10335613	O1C(=[C]C(=O)C2=C(C(=C([C]=C12)O)N[C]([C])[C])O)C1=[C][C]=[C][C]=[C]1	-8.3
10022760	C1(=[C]c2c(C(=[C]1)O)c(=O)c(c(o2)C1=[C]C(=C([C]=[C]1)O)O)OS([O])([O])O	-8.3
9813808	O1C2=[C][C]=[C][C]=C2[C][C]([C]1C1=[C]C(=[C]=[C]1)O)O)O	-8.3
9562299	[N]([C]1C2=[C][C]=[C][C]=C2O[C]([C]1)C1=[C][C]=[C][C]=[C]1)NC(=S)N	-8.3
5321859	O1C(=[C]C(=O)c2c(c(c(c12)O[C])O)O[C])O)C1=[C]C(=[C]=[C]1)O)O	-8.3
5317435	O1C2=[C]C(=[C][C]=C2C(=O)[C]([C]1C1=[C][C]=C(C(=[C]1)O)O)O)O	-8.3
5316733	O1C2=[C]C(=C(C(=C2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1)O)O[C])O	-8.3
5282073	O1C(=[C]C(=O)C2=[C][C]=C([C]=C12)O)C1=[C][C]=C([C]=[C]1)O	-8.3
5281894	O1C(=[C]C(=O)C2=[C][C]=C([C]=C12)O)C1=[C][C]=[C][C]=[C]1	-8.3
5281674	O1C(=[C]C(=O)C2=C([C]=C(C(=C12)O)O)O)C1=[C][C]=[C][C]=[C]1	-8.3
5280445	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O)O)C1=[C][C]=C(C(=[C]1)O)O	-8.3
3826106	O1C2=C([C]=[C][C]=[C]2)[C]([C][C]1)C1=[C][C]=[C][C]=[C]1	-8.3
740761	C1(=[C]OC2=C([C]=[C]C(=[C]2)O[C]([C])[C])C1=O)C1=C(F)[C]=[C][C]=[C]1	-8.3
688853	O1C(=[C]C(=O)C2=[C][C]=C(C(=C12)O)O)C1=[C][C]=C([C]=[C]1)O	-8.3
688672	O1C(=[C]C(=O)C2=[C][C]=C([C]=C12)O[C])C1=[C]C(=[C][C]=[C]1)O[C]	-8.3

676034	O1C2=C([C]=C([C]=[C]2)O)C(=O)[C]=C1C1=C([C]=[C][C]=[C]1)O[C]	-8.3
676033	O1C2=C([C]=[C][C]=[C]2)C(=O)[C]=C1C1=C(C(=[C][C]=[C]1)O[C])O[C]	-8.3
619834	O1C2=C([C]=[C][C]=[C]2)C(=O)[C]=C1C1=[C][C]=[C]C(=[C]1)O[C]	-8.3
441251	O1[C]=C(C(=O)C2=C(C(=C([C]=C12)O[C]))[C][C]=C([C])[C])O)C1=C([C]=C([C]=[C]1)O)O	-8.3
439652	O1C2=C([C]=[C][C]=[C]2)C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1	-8.3
369609	O1C2=C([C]=C([C]=C2[C]([C][C]1C1=[C][C]=C(C(=[C]1)O[C])O[C])O)[C][C]=[C])O[C]	-8.3
238782	O1C2=C(C(=[C]C(=[C]2)O)O)C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1	-8.3
177032	O1C2=C(C(=C(C(=[C]2)O)O[C])O)C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1	-8.3
102928	O1C2=C([C]=[C][C]=[C]2)C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O[C]	-8.3
76573	O1C(=[C]C(=O)c2c(c([C])c(c([C])c12)O[C])O)C1=[C][C]=C([C]=[C]1)O[C]	-8.3
41449	C1(=[C][C]=C([C]=[C]1)C1=[C]C(=O)C2=[C][C]=[C][C]=C2O1)O[C][C](O)[C]N[C]([C])[C]	-8.3
18721	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2OC(=O)[C])OC(=O)[C])C1=[C][C]=C([C]=[C]1)OC(=O)[C]	-8.3
11095	O1C2=C(C(=[C]C(=[C]2)O)O)C(=O)[C][C]1C1=[C]C(=C([C]=[C]1)O)O	-8.3
10251	O1C2=C([C]=[C][C]=[C]2)C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1	-8.3
3747	C1(=[C][C]=C2C(=O)C(=[C]OC2=[C]1)C1=[C][C]=[C][C]=[C]1)O[C]([C])[C]	-8.3
13840297 3	O1[C]=C(C(=O)C2=C1[C]=C(C(=[C]2)O)[C][C][C]O)C1=[C][C]=C([C]=[C]1)O	-8.2
13482072 6	O1C(=[C]C(=O)C2=[C]C(=[C]C(=C12)O[C])O[C])C1=[C][C]=C([C]=[C]1)O[C]	-8.2
12988240 4	O1[C]=C(C(=O)C2=C1[C]=[C][C]=[C]2)C1=[C][C]=C([C]=[C]1)[C]N	-8.2
12986605 2	o1c2[C]=[C][C]=[C]c2c(=O)c(c1C1=[C][C]=[C][C]=[C]1)[C]1[C]N[C][C]N1[C]C1=[C][C]=[C][C]=[C]1	-8.2
12982447 9	O1[C]2[C]=[C][C]=[C]C2=C([C]=C1C1=[C][C]=C([C]=[C]1)[C]=O)[N]O	-8.2
12982075 5	C1(=[C][C]=c2c(=[C]1)c(=O)c(c(o2)C1=[C][C]=[C][C]=[C]1)O)[C](O)[C][C][C][C]	-8.2
12976293 0	O1C2=C(C(=[C]C(=[C]2)O[C])O)C(=O)[C][C@]1(C1=[C][C]=C([C]=[C]1)O)O[C]	-8.2

12966237 4	o1c2=[C][C]=[C][C]=c2c(=O)c(c1[C])C1=[C][C]=C([C]=[C]1)N(=O)=O	-8.2
12148792 9	O1C2=[C][C]=[C][C]=C2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1	-8.2
10232004 0	O1[C]=C(C(=O)c2c(c(c(c12)O)O)O[C])O)C1=[C][C]=C([C]=[C]1)O	-8.2
10113705 4	C1(=C([C]=C(C2=C1O[C]=C(C2=O)C1=[C][C]=C([C]=C1O)O)O)[C]C([C])([C])O	-8.2
10102840 7	O1C(=[C]C(=O)C2=C([C]=C(C(=C12)N[C][C]([C])([C])O[C])O[C])C1=[C][C]=[C][C]=[C]1	-8.2
71777365	O1C2=[C][C]=[C][C]=C2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1	-8.2
71621987	C1(=[C][C]=C2C(=O)C(=[C]OC2=[C]1)C1=[C][C]=C([C]=[C]1)O)O[C]1O[C]([C]([C]([C]1O)O)O[C])([C])O	-8.2
69029207	C1(=[C][C]=C2C(=O)[C]=C(OC2=[C]1)C1=[C]C=C([C]=[C]1)O[C])O[C])O[C][C][C]Br	-8.2
57340186	O1C2=[C]C(=[C][C]=C2C(=O)[C]=C1C1=[C][C]=C([C]=[C]1)/[C]=[C]/C(=O)O[C][C])O	-8.2
49788612	o1c2=[C]C(=[C]C(=c2c(=O)c(c1C1=[C]C2=C([C]=[C]1)O[C]O2)O)O)O[C]	-8.2
44380950	O1C(=[C]C(=O)C2=C1C(=C([C]=C2O)O)N[C][C]=[C])C1=[C][C]=[C][C]=[C]1	-8.2
29920547	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2[C])OC(=O)O[C][C])C1=[C][C]=[C][C]=[C]1	-8.2
25201487	O1[C](C(=O)C(=O)C2=[C][C]=[C][C]=C12)C1=[C][C]=[C][C]=[C]1	-8.2
24866263	C1(=[C][C]=C([C]=[C]1)C1=[C]C(=O)C2=C([C]=C([C]=C2O1)O)O)O[C]1O[C]([C]([C]([C]1O)O)O)[C]	-8.2
24866262	C1(=C([C]=C([C]=[C]1)C1=[C]C(=O)C2=C([C]=C([C]=C2O1)O)O)O[C])O[C]1O[C]([C]([C]([C]1O)O)O)[C]	-8.2
23644936	c1(c(c(=O)c2[C]=[C]C(=[C]c2o1)O[C])C1=[C][C]=[C][C]=[C]1)SC1=N[C]=[C]N1	-8.2
21576250	O1[C]=C(C(=O)C2=C([C]=C(C(=C12)C([C])([C])[C]=[C])O)O)C1=[C][C]=C([C]=C1O)O	-8.2
20522556	c1(c(c(=O)c2C(=[C]C(=[C]c2o1)O[C])O)O[C])C1=[C][C]=C(C(=[C]1)O[C])OC(=O)C([C])([C])[C]	-8.2
19835350	C1(=C2C(=[C][C]=[C]1)C(=O)[C]=C(O2)C1=[C][C]=[C][C]=[C]1)O[C][C]1O[C]1	-8.2
18324995	c1(c(c(=O)c2[C]=[C][C]=[C]c2o1)C1=C([C]=[C][C]=[C]1)F)C1=[C][C]=C([C]=[C]1)S(=O)(=O)N	-8.2
15817847	o1c2=[C]C(=C([C]=c2c(=O)c(c1C1=[C][C]=C(C(=[C]1)O[C])O)O)O)O	-8.2
15160703	O1C2=C([C]=C(C3=C2[C]=[C]C(O3)([C])([C])O[C])C(=O)[C][C]1C1=[C]C(=C([C]=[C]1)O[C])O[C]	-8.2
13942547	o1c(c(c(=O)c2=C([C]=C(C(=c12)O[C])O[C][C]=C([C])([C])O[C])O[C])C1=[C]C2=C([C]=[C]1)O[C]O2	-8.2
13908971	O1C2=C(C3=C(C(=[C]2)O)C(=O)C(=[C]O3)C2=C([C]=C([C]=[C]2)O)O)[C][C]1C(=[C])[C]	-8.2

13250353	<chem>O1C2=C(C(=[C][C]=[C]2)O)[C][C][C]1C1=[C][C]=[C][C]=[C]1</chem>	-8.2
12735893	<chem>o1c(c(c(=O)c2[C]=[C]C3=C([C]=[C]O3)c12)O[C])C1=[C][C]=C([C]=[C]1)O[C]</chem>	-8.2
12407866	<chem>O1C(=[C]C(=O)C2=C1[C]=[C]C(=[C]2)C(=O)O[C])C1=C([C]=[C][C]=[C]1)O</chem>	-8.2
12261178	<chem>O1C2=C([C]=[C][C]=[C]2)C(=O)[C]=C1C1=[C][C]=C([C]=[C]1)[C]=O</chem>	-8.2
12136839	<chem>O1C2=C([C]=[C][C]=[C]2)C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1</chem>	-8.2
11847318	<chem>c1(c(c(=O)c2[C]=[C][C]=[C]c2o1)[C]N1[C]=N[C]=[C]1)C1=[C][C]=C(Br)[C]=[C]1</chem>	-8.2
11847316	<chem>o1c2=[C][C]=[C][C]=c2c(=O)c(c1C1=[C][C]=[C][C]=[C]1)[C]N1[C]=N[C]=[C]1</chem>	-8.2
11417114	<chem>c1(c(c(=O)c2[C]=[C]C(=[C]c2o1)O)C1=[C][C]=[C][C]=[C]1)S[C]C1=[C]N=[C][C]=[C]1</chem>	-8.2
11142360	<chem>O1[C]=C(C(=O)C2=C1[C]=C1C(=[C]2)O[C]O1)C1=[C]C(=C2C(=[C]1)O[C]O2)O[C]</chem>	-8.2
11032058	<chem>[C]1([C]C(=O)C2=C([C]=[C][C]=[C]2)O1)C1=[C][C]=C(F)[C]=[C]1</chem>	-8.2
10685123	<chem>C1(=[C][C]=C2C(=[C]1)C(=O)[C]=C(O2)C1=[C][C]=[C][C]=[C]1)[C]N=C=S</chem>	-8.2
10613051	<chem>C1(=[C]C(=O)C2=C([C]=[C][C]=[C]2)O1)C1=[C][C]=C([C]=[C]1)[S@](=O)[C]</chem>	-8.2
6450959	<chem>O1[C]=C(C(=O)C2=C([C]=C(C(=C12)[C]/[C]=C([C])/[C]O)O)O)C1=[C][C]=C([C]=[C]1)O</chem>	-8.2
5487268	<chem>C1(=C([C]=C(C(=[C]1)O)C1=[C]OC2=[C]C(=[C]C(=C2C1=O)O)O)C([C])([C])[C]=[C])O</chem>	-8.2
5466137	<chem>o1c2=[C]C(=[C]C(=c2c(=O)c(c1C1=[C]C2=C([C]=[C]1)O[C]O2)O[C])O)O[C]</chem>	-8.2
5417907	<chem>o1c2[C]=C([C]=[C]c2c(=O)c(c1[C])C1=[C][C]=C([C]=[C]1)N(=O)=O)O</chem>	-8.2
5356690	<chem>O1C2=[C][C]=[C][C]=C2[C]([C][C]1C1=[C][C]=[C][C]=[C]1)[N]O</chem>	-8.2
5317481	<chem>O1[C]=C(C(=O)C2=C([C]=C(C(=C12)[C]/[C]=C([C])/[C]O)O)O)C1=[C][C]=C(C(=[C]1)O)O[C]</chem>	-8.2
5317284	<chem>O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O)O[C])O)C1=[C][C]=C(C(=[C]1)O)O</chem>	-8.2
5310669	<chem>C1(=[C]OC2=C([C]=[C]C(=[C]2)O)C1=O)C1=[C][C]=C(F)[C]=[C]1</chem>	-8.2
5281954	<chem>O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O)O[C])C1=[C][C]=[C][C]=[C]1</chem>	-8.2
5281805	<chem>C1(=[C]OC2=[C]C(=[C][C]=C2C1=O)O)C1=[C]C2=C(O[C]O2)[C]=[C]1</chem>	-8.2
5281703	<chem>O1C(=[C]C(=O)C2=C([C]=C(C(=C12)O[C])O)O)C1=[C][C]=[C][C]=[C]1</chem>	-8.2
5281692	<chem>o1c2[C]=C([C]=[C]c2c(=O)c(c1C1=[C]C(=C(C(=[C]1)O)O)O)O)O</chem>	-8.2
5281616	<chem>o1c(c(c(=O)c2=C([C]=C([C]=c12)O)O)O)C1=[C][C]=[C][C]=[C]1</chem>	-8.2
5281614	<chem>o1c2[C]=C([C]=[C]c2c(=O)c(c1C1=[C]C(=C([C]=[C]1)O)O)O)O</chem>	-8.2
5281612	<chem>O1C2=[C]C(=[C]C(=C2C(=O)[C]=C1C1=[C][C]=C(C(=[C]1)O)O[C])O)O</chem>	-8.2
5280863	<chem>o1c(c(c(=O)c2C(=[C]C(=[C]c12)O)O)O)C1=[C][C]=C([C]=[C]1)O</chem>	-8.2
5280442	<chem>O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O)O)C1=[C][C]=C([C]=[C]1)O[C]</chem>	-8.2

5272801	<chem>O1C2=C([C]=[C][C]=[C]2)C(=O)[C]=C1C1=[C][C]=C([C]=[C]1)C1=N[C][C]O1</chem>	-8.2
3890073	<chem>[N]([C]1C2=[C][C]=[C][C]=C2O[C]([C]1)C1=[C][C]=[C][C]=[C]1)NC(=S)N</chem>	-8.2
3070240	<chem>c1(c([C])c(=O)c2[C]=[C]C(=C(c2o1)[C]N([C])[C])O[C])C1=[C][C]=C(F)[C]=[C]1</chem>	-8.2
689010	<chem>O1C2=C([C]=[C][C]=[C]2)C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1</chem>	-8.2
676299	<chem>O1C(=[C]C(=O)C2=C1C(=C([C]=[C]2)O[C])O)C1=[C][C]=[C][C]=[C]1</chem>	-8.2
462697	<chem>O1C2=[C]C(=[C]C(=C2C(=O)[C]([C]1C1=[C]C(=C([C]=[C]1)O[C])O[C]C1=[C][C]=[C][C]=[C]1)O[C])O)O</chem>	-8.2
439712	<chem>O1C2=[C][C]=[C][C]=C2[C]([C][C]1C1=[C][C]=[C][C]=[C]1)O</chem>	-8.2
439246	<chem>O1C2=[C]C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O)O</chem>	-8.2
378567	<chem>O1C2=[C]C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1)O[C])O[C]</chem>	-8.2
373260	<chem>O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O)O)O[C])C1=[C][C]=C(C(=[C]1)O)O[C]</chem>	-8.2
344546	<chem>o1c(c(c(=O)c2[C]=[C][C]=C([C]=c12)O[C])O)C1=[C][C]=[C][C]=[C]1</chem>	-8.2
229016	<chem>O1C2=C([C]=[C][C]=[C]2)C(=O)[C]=C1C1=[C][C]=C([C]=[C]1)O</chem>	-8.2
188308	<chem>O1C2=[C]C(=C(C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O)O)O</chem>	-8.2
176925	<chem>O1C2=C([C]=[C][C]=[C]2)C(=O)[C][C]1C1=[C][C]=[C][C]=C1O</chem>	-8.2
160921	<chem>O1C(=[C]C(=O)c2c(c(c(c12)O[C])O)O[C])O)C1=[C][C]=C([C]=[C]1)O[C]</chem>	-8.2
137327	<chem>O1C(=[C]C(=O)C2=[C]C(=[C]C(=C12)[C]C(=O)O)[C])C1=[C][C]=[C][C]=[C]1</chem>	-8.2
136418	<chem>O1C(=[C]C(=O)C2=C(C(=C([C]=C12)OC(=O)[C])OC(=O)[C])OC(=O)[C])C1=[C][C]=C([C]=[C]1)OC(=O)[C]</chem>	-8.2
100633	<chem>o1c(c(c(=O)c2[C]=[C]C3=C([C]=[C]O3)c12)O[C])C1=[C][C]=[C][C]=[C]1</chem>	-8.2
77793	<chem>O1C2=C([C]=[C][C]=[C]2)C(=O)[C]=C1C1=[C][C]=C([C]=[C]1)O[C]</chem>	-8.2
72281	<chem>O1C2=[C]C(=[C]C(=C2C(=O)[C][C]1C1=[C]C(=C([C]=[C]1)O[C])O)O)O</chem>	-8.2
72279	<chem>O1C(=[C]C(=O)C2=C1[C]=[C]C(=[C]2)O)C1=[C][C]=[C][C]=[C]1</chem>	-8.2
51459	<chem>o1c2=[C][C]=[C][C]=c2c(=O)c([C])c1C1=[C][C]=[C][C]=[C]1</chem>	-8.2
11055	<chem>O1C(=[C]C(=O)C2=C([C]=[C]C(=C12)O)O)C1=[C][C]=[C][C]=[C]1</chem>	-8.2
3593	<chem>O1C2=[C]C(=[C]C(=C2C(=O)[C][C]1C1=[C]C(=C([C]=[C]1)O[C])O)O)O</chem>	-8.2
1880	<chem>O1C(=[C]C(=O)C2=[C][C]=C(C(=C12)O)O)C1=[C][C]=[C][C]=[C]1</chem>	-8.2
932	<chem>O1C2=[C]C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O)O</chem>	-8.2
14668157	<chem>o1c(c(c(=O)c2C(=C3C(=[C]c12)O[C]O3)O)O[C](O)O)C1=[C][C]=[C][C]=[C]1</chem>	-8.1

12985837 0	O1C2=C([C]=[C]C=[C]2)O[C]C(=O)O)C(=O)[C]=C1C1=[C]C(=C(C=[C]1)O[C])O[C])O[C]	-8.1
12985288 2	[S]([C]1C(=O)c2c(c(c(c2O[C]1C1=[C]C(=C([C]=[C]1)O[C])O[C])O[C])O[C])O[C])O[C])([O])[O]	-8.1
12983454 0	C1(=C([C]=C2C(=C1O)C(=O)[C]=C(O2)C1=[C][C]=C([C]=[C]1)[C])O)S([O])([O])O	-8.1
12982959 8	o1c(c(c(=O)c2c(c(c(c12)O)O)O)O[C])O)C1=[C][C]=[C][C]=[C]1	-8.1
12982449 0	O1C2=[C][C]=[C][C]C2=C([C]=C1C1=[C][C]=C([C]=[C]1)[C]=O)[N]O[C][C]	-8.1
12981955 7	O1C2=C([C]=[C][C]=[C]2)C(=O)[C]([C]1C1=[C][C]=[C][C]=[C]1)O	-8.1
12973227 0	o1c2=[C][C]=[C][C]=c2c(=O)c(c1C1=[C][C]=[C][C]=[C]1)OO	-8.1
12971127 8	C1(=[C][C]=[C]C2=C1C(=O)[C]=C(O2)C1=[C][C]=[C][C]=[C]1)C(O)(O)[C]([C]([C])O)	-8.1
12968466 8	o1c(c(c(=O)c2c(c(c(c12)O)O)/[C]=[C]/C(=[C])[C])O)O)C1=[C][C]=[C][C]=[C]1	-8.1
10257792 6	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O)O)C1=[C][C]=C([C]=[C]1)O[C]O[C]	-8.1
10200537 4	C1(=[C]C(=O)C2=C(C(=C([C]=C2O[C])O[C]))[C]2[C][C][C][C][C]2O)O1)C1=C(Cl)[C]=[C][C]=[C]1	-8.1
10193061 3	O1[C]2[C]=[C][C]=[C]C2=[C][C]=C1C1=[C][C]=C([C]=[C]1)NC([C])([C])[C]	-8.1
73829902	O1C2=C(C(=[C][C]=C2C(=O)[C]([C]1C1=[C][C]=C(C(=[C]1)O)O)O)O)O	-8.1
70018578	O1C2=[C]C(=[C][C]=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O[C])O	-8.1
57368437	o1c(c(c(=O)c2[C]=C([C]=C(c12)O)O)O)C1=[C][C]=C([C]=[C]1)O	-8.1
57363368	o1c(c(c(=O)c2[C]=C([C]=C(c12)O)O)O)C1=[C][C]=C([C]=[C]1)O[C]	-8.1
54070148	C1(=[C][C]=C([C]=[C]1)O[C][C]O)[C]1OC2=[C][C]=[C][C]=C2[C][C]1	-8.1
53233892	C1(=[C]C2=C([C]=[C]1)OC(=[C]C2=O)C1=[C][C]=[C][C]=[C]1)OP(=O)(O[C][C])O[C][C]	-8.1

44260056	$O1C(=[C]C(=O)c2c(c(c(c12)O[C])O[C])OC(=O)[C]([C])([C])O)C1=[C][C]=C([C]=[C]1)O$	-8.1
44260022	$o1c(c(c(=O)c2C(=[C]C(=C(c12)O[C])O[C][C]=C([C])([C])O)O[C])C1=[C][C]=C(C(=[C]1)O[C])O$	-8.1
44258732	$o1c(c(c(=O)c2c(c([C])c(c([C])c12)O[C])O)O)C1=[C][C]=[C][C]=[C]1$	-8.1
44258533	$O1C(=[C]C(=O)C2=C(C(=C([C]=C12)O[C])O[C])O[C])C1=[C]C(=C(C(=[C]1)O[C])O[C][C]=C([C])([C])O[C])$	-8.1
44257359	$O1[C]=C(C(=O)C2=C1[C]=C1C(=C2O[C])O[C]O1)C1=[C]C(=C([C]=[C]1)O[C])O$	-8.1
42608063	$O1C2=C(C(=[C]C3=C2[C]=[C]C(O3)([C])([C])O[C])C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O[C])$	-8.1
25022469	$O1C(=[C]C(=O)C2=C(C(=[C]C(=C12)O[C])O[C])O[C])C1=C([C]=[C]C(=[C]1)O[C])O[C]$	-8.1
21636237	$O1C2=C(C(=[C]C(=C2O[C])O[C])O)C(=O)[C][C]1C1=[C][C]=[C][C]=C1O[C]$	-8.1
21626042	$O1[C]=C(C(=O)C2=C1[C]=C1C(=C2O[C])O[C]O1)C1=C([C]=C2C(=[C]1)O[C]O2)O[C]$	-8.1
21325037	$C1(=[C]C2=C([C]=[C]1)OC(=[C]C2=O)C1=C([C]=[C][C]=[C]1)O[C]([C])([C])C(=O)Cl$	-8.1
21270134	$C1(=[C]OC2=C([C]=C(C(=[C]2)O)O)C1=O)C1=[C]C(=[C][C]=[C]1)Cl$	-8.1
20452422	$O1C2=C([C]=[C][C]=[C]2)[C][C][C]1C1=[C][C]=C([C]=[C]1)N([C])[C]$	-8.1
18325002	$c1(c(c(=O)c2[C]=[C][C]=[C]c2o1)C1=C([C]=[C][C]=[C]1)F)C1=[C][C]=C([C]=[C]1)S(=O)(=O)[C]$	-8.1
14804713	$o1c(c(c(=O)c2=C([C])[C]=C([C]=c12)O[C])O[C])C1=[C][C]=C([C]=[C]1)O$	-8.1
12310641	$O1C2=[C]C(=[C][C]=C2C(=O)[C]([C]1C1=[C][C]=C(C(=[C]1)O)O)O)O$	-8.1
11847319	$o1c2=[C][C]=[C][C]=c2c(=O)c(c1C1=[C][C]=C([C]=[C]1)C\#N)[C]N1[C]=N[C]=[C]1$	-8.1
11810763	$O1[C]=C(C(=O)C2=C(C3=C([C]=C12)O[C]O3)O[C])C1=[C]C(=C2C(=[C]1)O[C]O2)O[C]$	-8.1
11485667	$c1(c(c(=O)c2[C]=[C]C(=[C]c2o1)O[C])C1=[C][C]=[C][C]=[C]1)S[C]C1=[C][C]=[C][C]=N1$	-8.1
11316719	$O1C(=[C]C(=O)C2=C1[C]=C(C(=C2OC(=O)[C])OC(=O)[C])O[C]C1=[C][C]=[C][C]=[C]1)C1=[C][C]=[C][C]=[C]1$	-8.1
11164739	$c1(c(c(=O)c2=[C][C]=C([C]=c2o1)O[C])C1=[C][C]=[C][C]=[C]1)S[C]C1=[C][C]=[C]N=[C]1$	-8.1
11153057	$c1(c(c(=O)c2[C]=[C]C(=[C]c2o1)O[C])C1=[C][C]=[C][C]=[C]1)S[C]C1=[C][C]=N[C]=[C]1$	-8.1
10814211	$o1c(c(c(=O)c2c(c(c(c12)O[C])O[C][C]=C([C])([C])O[C])O[C])O[C])C1=[C][C]=C2C(=[C]1)O[C]O2$	-8.1
10665235	$o1c(c(c(=O)c2=C([C]=C(C(=c12)O[C])O[C])O)O)C1=[C]C(=C([C]=[C]1)O)O$	-8.1
10612616	$O1C(=[C]C(=O)C2=C1[C]=[C][C]=C2O[C][C]=[C])C1=[C][C]=[C][C]=[C]1$	-8.1
10069029	$c1(c(c(=O)c2[C]=[C]C(=[C]c2o1)O)C1=[C][C]=C([C]=[C]1)O[C])S[C]C1=[C][C]=N[C]=[C]1$	-8.1
9821032	$c1(c(c(=O)c2=[C][C]=[C][C]=c2o1)C1=[C][C]=[C][C]=[C]1)C1=[C][C]=C([C]=[C]1)S(=O)(=O)[C]$	-8.1
6077518	$O1C2=C([C]=[C][C]=[C]2)[C]([C][C]1C1=[C][C]=[C][C]=[C]1)[N]O[C][C]N([C][C])[C][C]$	-8.1
5491929	$O1[C]=C(C(=O)C2=C1[C]=C1C(=C2O)O[C]O1)C1=C([C]=[C][C]=[C]1)O[C]$	-8.1
5490139	$O1C2=[C]C3=C(C(=O)C(=[C]O3)C3=[C][C]=C([C]=[C]3)O)C(=C2[C]=[C]C1([C])([C])O$	-8.1

5469524	$O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O)O[C])O)C1=[C][C]=C(C(=[C]1)O)O[C]$	-8.1
5465888	$O1C2=[C][C]=[C][C]=C2/C(=N/N(C(=O)[C])C(=O)[C])/[C][C]1C1=[C][C]=[C][C]=[C]1$	-8.1
5393152	$o1c(c(c(=O)c2=[C][C]=C([C]=c12)O)O)C1=[C][C]=[C][C]=[C]1$	-8.1
5385026	$o1c(c(c(=O)c2C(=C(C(=[C]c12)O)O[C])O[C])O)C1=[C][C]=[C][C]=[C]1$	-8.1
5378518	$O1C2=C([C]=[C]C(=[C]2)O)C(=O)[C]=C1C1=[C]C(=C([C]=[C]1)O[C])O[C]$	-8.1
5378202	$C1(=C([C]=C(C2=C1O[C]=C(C2=O)C1=[C][C]=C([C]=[C]1)O)O)O)[C][C]C([C])([C])O$	-8.1
5353357	$O1C(=[C]C(=O)C2=[C]C(=C([C]=C12)O)O)C1=[C][C]=[C][C]=[C]1$	-8.1
5321861	$o1c(c(c(=O)c2=C([C]=C(C(=c12)O)O)O[C])C1=[C]C(=C([C]=[C]1)O[C])O$	-8.1
5320438	$O1C(=[C]C(=O)C2=C(C(=C([C]=C12)O)O[C])O)C1=[C][C]=C([C]=[C]1)O[C]$	-8.1
5319422	$O1[C]=C(C(=O)C2=C1[C]=C([C]=[C]2)O)C1=[C]C(=C([C]=[C]1)O)O[C]$	-8.1
5318869	$o1c(c(c(=O)c2C(=[C]C(=[C]c12)O[C])O)O[C])C1=[C][C]=C([C]=[C]1)O$	-8.1
5284648	$O1[C]=C(C(=O)C2=C1[C]=C([C]=[C]2)O)C1=[C]C(=C([C]=[C]1)O)O$	-8.1
5282074	$O1[C]=C(C(=O)C2=C1[C]=C([C]=C2O)O)C1=[C][C]=C([C]=C1O)O$	-8.1
5281950	$o1c(c(c(=O)c2=C([C]=C(C(=c12)C([C])([C])[C]=[C])O)O)O)C1=[C][C]=[C][C]=[C]1$	-8.1
5281949	$o1c(c(c(=O)c2C(=[C]C(=C(c12)C([C])([C])[C]=[C])O)O)O)C1=[C][C]=C([C]=[C]1)O[C]$	-8.1
5281811	$O1[C]=C(C(=O)C2=C(C(=C([C]=C12)O)O[C])O)C1=[C][C]=C([C]=[C]1)O$	-8.1
5281691	$o1c(c(c(=O)c2C(=[C]C(=[C]c12)O[C])O)O)C1=[C][C]=C(C(=[C]1)O)O$	-8.1
5281628	$O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O)O[C])O)C1=[C][C]=C([C]=[C]1)O$	-8.1
5281617	$O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O)O[C])C1=[C][C]=C([C]=[C]1)O$	-8.1
5281611	$o1c2=[C]C(=[C][C]=c2c(=O)c(c1C1=[C][C]=C([C]=[C]1)O)O)O$	-8.1
5280961	$O1[C]=C(C(=O)C2=C1[C]=C([C]=C2O)O)C1=[C][C]=C([C]=[C]1)O$	-8.1
5280448	$O1[C]=C(C(=O)C2=C1[C]=C([C]=[C]2)O)C1=[C][C]=C(C(=[C]1)O)O[C]$	-8.1
5280443	$O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O)O)C1=[C][C]=C([C]=[C]1)O$	-8.1
5280417	$o1c(c(c(=O)c2=C([C]=C([C]=c12)O[C])O)O[C])C1=[C]C(=C([C]=[C]1)O)O$	-8.1
4231835	$O1C2=[C][C]=[C][C]=C2C(=O)[C]=C1C1=C([C]=[C]C(=[C]1)O[C])O[C]$	-8.1
3083783	$O1C(=[C]C(=O)c2c(c(c(c12)O)O[C])O[C])O)C1=[C][C]=C([C]=[C]1)O[C]$	-8.1
1232440	$O1C2=[C][C]=[C][C]=C2[C][C][C]1C1=[C][C]=[C][C]=[C]1$	-8.1
847733	$O1C2=[C][C]=[C][C]=C2[C][C]([C]1C1=[C][C]=[C][C]=[C]1)O$	-8.1
689014	$O1C(=[C]C(=O)C2=C1C(=C([C]=[C]2)O[C])O[C])C1=[C][C]=[C][C]=[C]1$	-8.1

688715	$o1c2=[C][C]=[C][C]=c2c(=O)c(c1C1=[C][C]=C([C]=[C]1)O)O$	-8.1
688671	$O1C(=[C]C(=O)C2=[C][C]=C([C]=C12)O[C])C1=C([C]=[C][C]=[C]1)O[C]$	-8.1
688659	$o1c(c(c(=O)c2[C]=C([C]=[C]c12)O)O)C1=[C][C]=[C][C]=[C]1$	-8.1
676295	$o1c2=[C][C]=[C][C]=c2c(=O)c(c1C1=[C][C]=[C]C(=[C]1)O)O$	-8.1
676290	$O1C2=[C][C]=[C][C]=C2C(=O)[C]=C1C1=C([C]=C([C]=[C]1)O)O$	-8.1
676289	$O1C2=C([C]=[C][C]=[C]2)C(=O)[C]=C1C1=C(C(=[C][C]=[C]1)O)O$	-8.1
636496	$O1C2=[C]C3=C(C(=O)C(=[C]O3)C3=C([C]=C([C]=[C]3)O[C])O)C(=C2[C]=[C]C1([C])([C])O[C]$	-8.1
633124	$O1C(=[C]C(=O)c2c(c(c(c12)O[C])O)O[C])O)C1=[C]C(=C(C(=[C]1)O[C])O[C])O$	-8.1
578729	$o1c2=[C][C]=[C][C]=c2c(=O)c(c1C1=[C][C]=[C][C]=C1O[C])O$	-8.1
468911	$O1C2=C(C(=[C]C(=C2O)O)O)C(=O)[C]([C]1C1=[C][C]=C([C]=[C]1)O)O$	-8.1
443638	$O1C2=C(C(=[C]C(=[C]2)O)O)[C]([C][C]1C1=[C][C]=C([C]=[C]1)O)O$	-8.1
369616	$O1C2=C([C]=C([C]=C2O[C])[C][C]=[C])[C]([C][C]1C1=[C][C]=C(C(=[C]1)O[C])O[C])OC(=O)[C]$	-8.1
369615	$O1C2=C([C]=[C][C]=C2O[C])C(=[C])[C][C]1C1=[C]C(=C([C]=[C]1)O)O[C]$	-8.1
321346	$O1C2=[C]C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O[C])O)O[C]$	-8.1
161271	$O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O)O[C])O[C])C1=[C][C]=C([C]=[C]1)O[C]$	-8.1
154227	$O1C2=C([C]=[C]C(=[C]2)O[C])C(=O)[C]=C1C1=[C][C]=C(C(=[C]1)O[C])O[C]$	-8.1
94156	$O1C2=[C][C]=[C][C]=C2[C][C][C]1C1=[C][C]=[C][C]=[C]1$	-8.1
73202	$O1C2=C(C(=[C]C(=[C]2)O)O)C(=O)[C]([C]1C1=[C][C]=[C][C]=[C]1)O$	-8.1
72304	$O1[C]=C(C(=O)C2=C1[C]=[C][C]=[C]2)C1=[C][C]=[C][C]=[C]1$	-8.1
55748	$O1C(=[C]C(=O)C2=[C][C]=[C]C(=C12)[C]C(=O)O)C1=[C][C]=[C][C]=[C]1$	-8.1
53645	$O1C(=[C]C(=O)C2=[C][C]=[C]C(=C12)O)C1=[C][C]=[C][C]=[C]1$	-8.1
25585	$o1c([C])c(c(=O)c2=[C][C]=[C]C(=c12)O[C]N([C])[C])C1=[C][C]=C([C]=[C]1)O[C]$	-8.1
20399	$O1C2=[C]C(=[C][C]=C2C(=O)[C]([C]1C1=[C]C(=C(C(=[C]1)O)O)O)O)O$	-8.1
10680	$O1C2=C([C]=[C][C]=[C]2)C(=O)[C]=C1C1=[C][C]=[C][C]=[C]1$	-8.1
13903075	$O1[C]=C(C(=O)C2=C1C(=C([C]=[C]2)[C][C][C]O)O[C])C1=[C][C]=C([C]=[C]1)O[C]$	-8
7		
13482227	$O1[C]=C(C(=O)C2=C(C3=C([C]=C12)O[C]O3)O)C1=[C][C]=C([C]=[C]1)O[C]$	-8
8		

12986463 5	O1C(=[C]C(=O)C2=C1[C]=[C][C]=C2O[C]O)C1=[C][C]=[C][C]=[C]1	-8
12984791 0	O1C2=C(C(=[C]C(=[C]2)O)O)[C](C(=O)[C]1C1=[C][C]=[C]C(=[C]1)O[C])O	-8
12984790 9	o1c(c(c(=O)c2=[C][C]=C([C]=c12)O[C](O)O)O[C]O)C1=[C][C]=[C][C]=[C]1	-8
12982170 5	o1c(c([C])c(=O)c2[C]=C(C(=C(c12)N([C])[C])O)O)C1=[C][C]=C([C]=[C]1)O	-8
10166596 2	o1c2=[C]C(=[C][C]=c2c(=O)c(c1C1=[C][C]=C(C(=[C]1)O[C][C]O)O[C][C]O)O[C][C]O)O[C][C]O	-8
10102840 9	O1C(=[C]C(=O)C2=C1C(=C([C]=C2O[C])O[C])N[C][C]=[C])C1=[C][C]=[C][C]=[C]1	-8
10102840 6	O1C(=[C]C(=O)C2=C1C(=C([C]=C2O[C])O[C])N[C][C][C])C1=[C][C]=[C][C]=[C]1	-8
10094337 9	C1(=[C][C]=C([C]=[C]1)C1=[C]C(=O)C2=[C][C]=[C][C]=C2O1)S(=O)(=O)N([C][C])[C][C]	-8
86606987	C1(=[C][C]=C2C(=O)[C]=C(OC2=[C]1)C1=[C]C(=C(C(=[C]1)O[C])O[C])O[C])O[C][C]1O[C]1	-8
86083806	O1[C]2[C]=[C][C]=[C]C2=[C][C]=C1C1=[C][C]=C([C]=[C]1)NC(=O)[C]	-8
73265447	C1(=[C]OC2=C([C]=[C]C(=C2[C])O)C1=O)C1=[C][C]=C([C]=[C]1)C(F)(F)F	-8
70696494	O1C2=[C]C(=[C]C(=C2C(=O)[C][C]1C1=[C]C(=[C]C(=[C]1)O)O)O)O[C]	-8
66968868	C1(=[C][C]=c2c(=[C]1)c(=O)c(c(o2)C1=[C][C]=C([C]=[C]1)N([C][C])[C][C])O)[C]Br	-8
54073202	C1(=[C]C2=C(C(=[C]1)O)C(=O)[C][C](O2)C1=[C]C(=C([C]=[C]1)O[C])O)O[C][C]Br	-8
49788611	o1c(c(c(=O)c2=C([C]=C(C(=c12)O[C])O[C])O)O)C1=[C]C2=C([C]=[C]1)O[C]O2	-8
44260080	o1c(c(c(=O)c2c(c3c(c(c12)O[C])O[C]O3)O[C])O[C])C1=[C]C2=C(C(=[C]1)O[C])O[C]O2	-8
25232840	O1C2=C(C(=[C]C(=[C]2)O)O)[C][C][C]1C1=[C][C]=C([C]=[C]1)O[C]	-8
24721178	o1c(c(c(=O)c2[C]=[C]C(=C(c12)O)O)O)C1=[C][C]=[C][C]=C1O	-8
23724666	C1(=[C]OC2=[C]C(=[C][C]=C2C1=O)O)C1=[C]C2=C(O[C]O2)[C]=C1O	-8
21291576	O1[C]=C(C(=O)C2=C([C]=C([C])C(=C12)O)C1=[C][C]=C([C]=[C]1)O	-8
20394006	o1c([C])c(c(=O)c2=C([C]=C([C]=c12)OC(=O)[C])OC(=O)[C])C1=[C][C]=[C][C]=[C]1	-8
18702583	O1C(=[C]C(=O)C2=C(C(=[C][C]=C12)O[C])O)C1=[C]C(=C([C]=[C]1)O)O	-8

18324974	c1(c(=O)c2=[C][C]=[C][C]=c2oc1C1=[C][C]=C([C]=[C]1)S(=O)(=O)[C])C1=[C][C]=C(Cl)[C]=[C]1	-8
18324902	c1(c(c(=O)c2=[C][C]=[C][C]=c2o1)C1=[C][C]=C([C]=[C]1)F)C1=[C][C]=C([C]=[C]1)S(=O)(=O)[C]	-8
16213663	O1C(=[C]C(=C2[C]=[C]C(=[C][C]12)N([C][C])[C][C])C1=C([C]=[C][C]=[C]1)C(=O)O)C1=[C][C]=C([C]=[C]1)N([C])[C]	-8
14886014	o1c2=C(C(=[C]C(=c2c(=O)c(c1C1=[C]C2=C([C]=[C]1)O[C]O2)O[C])O[C])O[C])O[C]	-8
14791392	O1C2=C([C]=[C]C(=[C]2)O)C(=O)[C]=C1C1=[C][C]=C([C]=[C]1)N	-8
14730798	O1C2=[C]C(=[C][C]=C2C(=O)[C]([C]1C1=[C][C]=[C][C]=[C]1)O)O	-8
14704648	o1c(c(c(=O)c2C(=C3C(=[C]c12)O[C]O3)O[C])O[C])C1=[C]C(=C2C(=[C]1)O[C]O2)O[C]	-8
14440496	o1c2[C]=C([C]=[C]c2c(=O)c(c1C1=C([C]=[C][C]=[C]1)O[C])O)O[C]	-8
13889022	O1C(=[C]C(=O)C2=C1C(=C([C]=C2O)O[C])O[C])C1=C([C]=[C][C]=C1O[C])O	-8
13873818	O1C(=[C]C(=O)C2=C(C(=C([C]=C12)O[C]C1=[C][C]=[C][C]=[C]1)O[C])O[C])C1=[C]C(=C([C]=[C]1)O[C])O[C]	-8
12444947	C1(=[C]C2=C(C(=O)C(=[C]O2)C2=[C][C]=C([C]=[C]2)O[C])[C]=C1O[C])O[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-8
12318033	O1C2=[C][C]=[C][C]=C2[C]C(=O)[C]1C1=[C][C]=[C][C]=[C]1	-8
12310757	C1(=C([C]=C(c2c(=O)c(c(oc12)C1=[C][C]=C([C]=[C]1)O[C])O)O)O)[C][C]C([C])([C])O	-8
11777425	O1C(=[C]C(=O)C2=[C]C(=[C][C]=C12)[C]C#N)C1=[C][C]=[C][C]=[C]1	-8
11609345	O1C(=[C]C(=O)c2c(c(c(c12)O[C])O)O[C])O)C1=[C][C]=[C][C]=[C]1	-8
11289628	O1C2=[C]C(=[C]C(=C2C(=O)[C][C]1C1=[C]C(=[C]C(=[C]1)O)O)O)O[C]	-8
10759582	O1C2=[C]C(=C(C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O)C([C])([C])[C]=[C])O	-8
10643413	Br c1c(=O)c2=[C][C]=[C][C]=c2oc1C1=[C][C]=C([C]=[C]1)S(=O)(=O)[C]	-8
10542374	O1[C]=C(C(=O)C2=C1C(=C([C]=C2O)O)O)C1=[C][C]=C(C(=[C]1)O)O	-8
10491973	O1C(=[C]C(=O)C2=C1[C]=[C][C]=C2O[C][C])C1=[C][C]=[C][C]=[C]1	-8
9864504	c1(c(c(=O)c2=[C][C]=[C][C]=c2o1)C1=[C][C]=[C][C]=[C]1)C1=[C][C]=C([C]=[C]1)S(=O)(=O)N	-8
6028923	C1(=[C]C(=O)C2=[C][C]=C([C]=C2O1)O)C1=[C][C]=C(Br)[C]=[C]1	-8
5748553	o1c(c(c(=O)c2=C([C]=C(C(=c12)O[C])O)O)O[C])C1=[C]C(=C([C]=[C]1)O)O	-8
5492944	O1[C]=C(C(=O)C2=C1C(=C([C]=C2O)O)O)C1=[C][C]=C([C]=[C]1)O	-8
5481647	O1C(=[C]C(=O)C2=C(C(=C([C]=C12)O)O[C])O[C])C1=[C][C]=[C][C]=[C]1	-8
5468257	O1C2=[C][C]=[C][C]=C2[C]([C][C]1C1=[C][C]=[C][C]=[C]1)N]N	-8
5395695	o1c([C])c(c(=O)c2=C([C]=C([C]=c12)O)O)C1=[C][C]=[C][C]=[C]1	-8
5321538	O1C2=C([C]=C(C(=[C]2)O)O[C])C(=O)[C][C]1C1=[C]C(=C([C]=[C]1)O)O	-8
5317747	O1C2=[C]C(=[C]C(=C2C(=O)[C]([C]1C1=[C][C]=[C][C]=[C]1)O)O)O[C]	-8

5317652	O1C2=[C][C]=C(C=C2[C]=[C]C1([C])[C])O)C1=[C]OC2=C([C]=[C]C(=[C]2)O)C1=O	-8
5284649	O1[C]=C(C(=O)C2=[C]C(=[C]([C]=C12)O)O)C1=[C][C]=C([C]=[C]1)O	-8
5281607	O1C(=[C]C(=O)C2=C([C]=C([C]=C12)O)O)C1=[C][C]=[C][C]=[C]1	-8
5281603	o1c(c(c(=O)c2=C(C(=C([C]=c12)O)O[C])O)O[C])C1=[C][C]=C(C(=[C]1)O)O	-8
5280681	o1c2=[C]C(=[C]C(=c2c(=O)c(c1C1=[C]C(=[C]([C]=[C]1)O)O)O[C])O)O	-8
5280362	c1(c(=O)c2C(=[C]C(=[C]c2oc1C1=[C]C(=[C]([C]=[C]1)O)O)O)O)OS([O])([O])O	-8
5280343	o1c(c(c(=O)c2C(=[C]C(=[C]c12)O)O)O)C1=[C][C]=C(C(=[C]1)O)O	-8
5106787	O1C2=C([C]=C([C]=[C]2)O)C(=O)[C][C]1C1=[C][C]=[C][C]=C1O	-8
4872981	O1C2=C(C(=[C]C(=[C]2)O[C])O)C(=O)[C][C]1C1=[C]C(=[C]([C]=[C]1)O)O	-8
4183640	C1(=[C]C2=C([C]=[C]1)C(=O)C(=[C]O2)C1=[C][C]=C([C]=[C]1)O)O[C]1O[C]([C]([C]([C]1O)O)O)[C]O	-8
4169706	FC1=[C]C2=C([C]=[C]1)O[C]([C]C2=O)C1=[C][C]=[C][C]=[C]1	-8
3070245	c1(c([C])c(=O)c2[C]=[C]C(=C(c2o1)[C]N([C])[C])O[C])C1=[C][C]=C(Cl)[C]=[C]1	-8
911486	o1c2=[C]C(=[C][C]=c2c(=O)c(c1[C])C1=[C][C]=C([C]=[C]1)N(=O)=O)O[C]	-8
688836	o1c(c(c(=O)c2=[C][C]=C([C]=c12)O[C])O)C1=[C]C(=[C][C]=[C]1)O[C]	-8
555407	o1c(nc(=O)c2=[C][C]=[C][C]=c12)C1=[C][C]=[C][C]=[C]1	-8
471706	O1[C]=C(C(=O)C2=[C]C(=[C]([C]=C12)OC(=O)[C])OC(=O)[C])C1=[C][C]=C([C]=[C]1)OC(=O)[C]	-8
466277	BrC1=[C][C]=C2C(=O)[C]=C(OC2=[C]1)C1=[C][C]=[C][C]=[C]1	-8
462691	O1C2=C([C]=[C][C]=C2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1)[C]C(=O)O	-8
455313	o1c2[C]=[C][C]=[C]c2c(=O)c(c1C1=C([C]=[C][C]=[C]1)O)O	-8
369599	O1C(=[C]C(=O)C2=C(C(=C([C]=C12)O[C])[C])O)C1=[C][C]=[C][C]=[C]1	-8
348130	O1C2=[C]C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O)O[C]	-8
250312	O1C(=[C]C(=C2[C][C]=[C][C]=C12)[N]O)C1=[C][C]=[C][C]=[C]1	-8
213728	O1C(=[C]C(=O)C2=C1C(=[C][C]=[C]2)O[C])C1=[C][C]=[C][C]=[C]1	-8
194690	O1C(=[C]C(=O)C2=[C]C(=[C]C(=C12)O[C])O[C])C1=[C][C]=[C][C]=[C]1	-8
182026	O1C2=C(C(=C(C(=[C]2)O)[C])O)C(=O)[C]([C]1C1=[C]C(=[C]([C]=[C]1)O)O)O	-8
161860	O1C2=C([C]=[C][C]=[C]2)C(=O)[C]=C1C1=[C][C]=[C][C]=C1O	-8
147157	O1C(=[C]C(=O)C2=[C]C(=[C][C]=C12)O[C])C1=[C][C]=[C][C]=[C]1	-8
97214	O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O)O[C])O[C])C1=[C][C]=C(C(=[C]1)O)O[C]	-8
88881	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O[C])O[C])C1=[C][C]=[C][C]=[C]1	-8

73571	<chem>O1C2=[C]C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O)O)O[C]</chem>	-8
11349	<chem>o1c2=[C][C]=[C][C]=c2c(=O)c(c1C1=[C][C]=[C][C]=[C]1)O</chem>	-8
10185	<chem>O1C2=[C]C(=[C]C(=C2C(=O)[C]([C]1C1=[C][C]=C(C(=[C]1)O)O)O)O)O</chem>	-8
1686	<chem>C1(=[C]C(=O)C2=[C][C]=[C][C]=C2O1)C1=[C][C]=C(Br)[C]=[C]1</chem>	-8
13512149 8	<chem>c1(c(c(=O)c2C(=[C][C]=[C]c2o1)O)O)C1=[C]C(=C2C(=[C]1)[C]2)O[C]</chem>	-7.9
12984453 1	<chem>O1C2=[C]C(=[C]C(=C2C(=O)[C@@]([C])([C]1C1=[C][C]=C(C(=[C]1)[C])O)O)O)O</chem>	-7.9
12982239 0	<chem>O1C(=[C]C(=O)c2c(c(c(c12)N(=O)=O)OC(=O)[C])OC(=O)[C])OC(=O)[C])C1=[C][C]=[C][C]=[C]1</chem>	-7.9
12978776 5	<chem>O1C(=[C]C(=C2[C][C]=[C][C]=C12)[N]N)C1=[C][C]=[C][C]=[C]1</chem>	-7.9
12973416 4	<chem>o1c(c(c(=O)c2c(c(c(c12)O)O[C])O[C])O[C])O)C1=[C][C]=[C][C]=C1O</chem>	-7.9
12972874 3	<chem>c1(c(c(=O)c2=[C][C]=[C][C]=c2o1)C1=[C][C]=[C][C]=[C]1)[C]1O[C]([C]([C]([C]1O)O)O)[C]O</chem>	-7.9
12971614 9	<chem>C1(=C([C]=C2C(=C1O)C(=O)C(=[C]O2)C1=[C][C]=C([C]=[C]1)O)O)[C]([C]1O[C]1)[C][C]=C([C])[C]</chem>	-7.9
12970411 8	<chem>O1C(=[C]C(=O)C2=C([C]=C([C]=C12)O[C]O)O[C]O)C1=[C][C]=[C][C]=[C]1</chem>	-7.9
12967047 6	<chem>O1C2=C([C])[C]=[C]C(=C2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1)[C]O</chem>	-7.9
10174053 8	<chem>C1(=[C]C2=C(C(=O)[C]=C(O2)C2=[C][C]=[C][C]=[C]2)C(=C1O[C])O)OS([O])([O])O</chem>	-7.9
10121493 7	<chem>o1c(c(c(=O)c2[C]=C([C]=[C]c12)[C]N([C][C])[C][C])O)C1=[C][C]=C([C]=[C]1)N([C][C])[C][C]</chem>	-7.9
86641845	<chem>O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O)O[C]C#[C])C1=[C][C]=C(C(=[C]1)O[C])O[C]</chem>	-7.9
86236608	<chem>C1(=[C]C2=C([C]=[C]1)C(=O)[C]=C(O2)C1=[C]C(=[C]C(=[C]1)O[C])O[C])O[C][C]1O[C]1</chem>	-7.9
69033169	<chem>C1(=[C]C2=C([C]=[C]1)C(=O)[C]=C(O2)C1=[C]C(=C(C(=[C]1)O[C])O[C])O[C])O[C][C]Br</chem>	-7.9
69030799	<chem>C1(=[C]C2=C([C]=[C]1)C(=O)[C]=C(O2)C1=[C]C(=C(C(=[C]1)O[C])O[C])O[C])O[C][C][C]Br</chem>	-7.9

69030155	C1(=[C][C]=C2C(=O)[C]=C(OC2=[C]1)C1=[C]C(=[C]C(=[C]1)O[C])O[C])O[C][C][C]Br	-7.9
56649088	O1C(=[C]C(=O)C2=C(C(=C([C]=C12)O[C][C]=[C])O)O)C1=[C][C]=[C][C]=[C]1	-7.9
25073757	O1C2=[C]C(=[C]C(=C2C(=O)[C][C]1C1=C([C]=[C]C(=[C]1)O)O)O)O	-7.9
22134047	o1c(c(c(=O)c2C=C([C]=[C]c12)O[C])O[C])O)C1=[C][C]=[C][C]=[C]1	-7.9
21673114	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O)O[C]O[C])C1=[C][C]=[C][C]=[C]1	-7.9
17585058	C1(=[C][C]=C2C(=O)C(=[C]OC2=[C]1)C1=[C][C]=[C][C]=[C]1)O[C][C]Br	-7.9
14504257	C1(=C(C(=[C]C(=C1C1=[C]OC2=C([C]=[C]C(=[C]2)O)C1=O)O)O)O[C])[C][C]C([C])([C])O	-7.9
13942548	o1c(c(c(=O)c2c(c3c(c(c12)O[C])O[C]O3)O[C])O[C])C1=[C]C2=C([C]=[C]1)O[C]O2	-7.9
13886894	O1C2=[C]C(=[C][C]=C2[C]([C]([C]1C1=[C][C]=C([C]=[C]1)O)O)O)O	-7.9
13568446	o1c2[C]=[C][C]=[C]c2c(=O)c(c1C1=[C][C]=[C][C]=[C]1)C(=O)[C]	-7.9
12000157	O1C2=[C]C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=C1O)O)O)O[C]	-7.9
11499970	O1C2=C([C]=[C][C]=[C]2)C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)N([C])[C]	-7.9
11033582	O1C2=C(C(=[C][C]=C2[C][C]([C]1C1=[C][C]=C(C(=[C]1)O)O)O)O)O	-7.9
10761665	O1C2=[C]C(=C(C(=C2C(=O)[C][C]1C1=[C][C]=C(C(=[C]1)O[C])O)O)C([C])([C])[C]=[C])O	-7.9
10468234	O1C2=[C][C]=[C][C]=C2C(=O)[C@@]([C])([C]1C1=[C][C]=C([C])[C]=[C]1)O	-7.9
10315196	O1C2=C(C(=C(C(=[C]2)O)C([C])([C])[C]=[C])O)C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O	-7.9
5487855	o1c2[C]=C([C]=C(c2c(=O)c(c1C1=[C][C]=C(C(=[C]1)O[C])O[C])O)O)O	-7.9
5385091	C1(=[C]OC2=C([C]=[C]C(=[C]2)O)C1=O)C1=[C]C2=C(O[C]O2)[C]=C1O[C]	-7.9
5380976	o1c2=[C]C(=[C][C]=c2c(=O)c(c1[C])C1=[C][C]=[C][C]=[C]1)O	-7.9
5378260	O1[C]=C(C(=O)C2=C1C(=C([C]=[C]2)O)O)C1=[C][C]=C([C]=C1O)O	-7.9
5362017	o1c(c(c(=O)c2C(=[C]C(=C(c12)O)O)O)O)C1=[C][C]=[C][C]=[C]1	-7.9
5360930	o1c(c(c(=O)c2=C([C]=C(C(=c12)O)O)O)O[C])C1=[C][C]=[C][C]=[C]1	-7.9
5351234	O1C2=C(C(=[C]C(=[C]2)O)O)C(=O)[C]=C1C1=[C]C(=[C]=[C]1)O[C])O[C]	-7.9
5322009	O1C(=[C]C(=O)C2=C1[C]=C(C(=C2OC(=O)[C])O[C])OC(=O)[C])C1=[C][C]=C([C]=[C]1)OC(=O)[C]	-7.9
5320287	o1c(c(c(=O)c2=C([C]=C([C]=c12)O[C])O)O)C1=[C]C(=[C]=[C]1)O[C]O	-7.9
5316653	O1[C]=C(C(=O)C2=C1[C]=C1C(=C2O)O[C]O1)C1=[C]C(=C(C(=[C]1)O)O[C])O[C]	-7.9
5315202	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O[C])O)C1=[C][C]=C([C]=[C]1)O	-7.9
5282154	o1c2=[C]C(=[C]C(=c2c(=O)c(c1C1=[C]C(=C(C(=[C]1)O)O)O[C])O)O)O	-7.9
5281804	O1[C]=C(C(=O)C2=C1[C]=C([C]=C2O)O[C])C1=[C][C]=C([C]=[C]1)O	-7.9

5281801	O1[C]=C(C(=O)C2=C([C]=C([C]=C12)O)O)C1=[C][C]=C(C(=[C]1)O)O	-7.9
5281779	O1[C]=C(C(=O)C2=C(C3=C([C]=C12)O[C]O3)O)C1=[C][C]=C([C]=[C]1)O	-7.9
5281708	O1[C]=C(C(=O)C2=C1[C]=C([C]=[C]2)O)C1=[C][C]=C([C]=[C]1)O	-7.9
5281702	O1C2=C(C(=[C]C(=[C]2)O)O)C(=O)[C]=C1C1=[C]C(=C(C(=[C]1)O[C])O)O[C]	-7.9
5281697	O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O)O)O)C1=[C][C]=C([C]=[C]1)O	-7.9
5280378	O1[C]=C(C(=O)C2=C1[C]=C([C]=[C]2)O)C1=[C][C]=C([C]=[C]1)O[C]	-7.9
5271991	O1C(=[C]C(=O)C2=C1C(=C([C]=C2O)O)O[C])C1=C(C(=[C][C]=C1O)O)O[C]	-7.9
3080750	O1C(=[C]C(=O)c2c(c(c(c12)O[C])O[C])O[C])O)C1=[C][C]=C(C(=[C]1)O)O[C]	-7.9
3070241	c1(c([C])c(=O)c2=[C][C]=C(C(=c2o1)[C]N([C][C])[C][C])O[C])C1=[C][C]=C(F)[C]=[C]1	-7.9
688827	o1c2=[C][C]=[C][C]=c2c(=O)c(c1c1=[C]C(=C(C(=[C]1)O[C])O[C])O[C])O	-7.9
586090	O1C2=C(C(=[C][C]=[C]2)O)C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1	-7.9
513103	O1C2=[C][C]=[C][C]=C2C(=O)[C]([C]1)[C]C1=[C][C]=[C][C]=[C]1	-7.9
439533	O1C2=C(C(=[C]C(=[C]2)O)O)C(=O)[C]([C]1C1=[C]C(=C([C]=[C]1)O)O)O	-7.9
369608	O1C2=C([C]=C([C]=C2[C]([C][C]1C1=[C][C]=[C][C]=[C]1)O)[C][C]=[C])O[C]	-7.9
265699	o1c(c(c(=O)c2[C]=[C]C(=[C]c12)O[C])O)C1=[C][C]=C([C]=[C]1)O[C]	-7.9
125540	ClC1=C2C(=C([C]=C1O)O)C(=O)[C]([C])[C](O2)C1=[C][C]=C([C]=[C]1)O	-7.9
125526	O1C2=C(C(=[C]C(=[C]2)O)O)C(=O)[C]([C])[C]1C1=[C][C]=C([C]=[C]1)O	-7.9
68112	O1C(=[C]C(=O)C2=C1[C]=[C][C]=C2O)C1=[C][C]=[C][C]=[C]1	-7.9
31161	O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O)O)O[C])C1=[C][C]=C(C(=[C]1)O)O	-7.9
3078	o1c(c([C])c(=O)c2[C]=[C]C(=C(c12)[C]N([C])[C])O[C])C1=[C][C]=[C][C]=[C]1	-7.9
13251736 8	O1C(=[C]C(=O)c2c(c([C])c(c(c12)C([C])([C])O)O[C])O)C1=[C][C]=C([C]=[C]1)O[C]	-7.8
13227966 3	O1[C]=C(C(=O)C2=C1[C]=C(C(=C2O[C])O[C])O)C1=C2C(=[C][C]=[C]1)O[C]O2	-7.8
12988748 1	o1c(c(c(=O)c2C(=C([C]=[C]c12)O)O[C])C1=[C][C]=[C][C]=[C]1)O[C]	-7.8
12984795 9	O1C2=C([C]=[C]C(=C2O)O)[C]([C]([C]1C1=[C][C]=C([C]=[C]1)O)O)O	-7.8

12983719 5	o1c(c(c(=O)c2c(c(c(c12)O)O)O)O[C])O[C])C1=[C][C]=[C][C]=C1O	-7.8
12982451 0	O1C(=[C]C(=O)C2=C1C(=C([C]=C2O[C])O[C])C1=[C]C(=C(C(=[C]1)O[C])O[C])O[C])C1=[C][C]=[C][C]=[C]1	-7.8
12971122 2	O1C2=C([C]C(=O)[C]=[C]2)[C][C][C]1C1=[C][C]=[C][C]=[C]1	-7.8
10232003 9	O1[C]=C(C(=O)c2c(c(c(c12)O)O)O[C])O[C])C1=[C]C(=C([C]=[C]1)O)O[C]	-7.8
10214569 8	O1C2=C([C]=C(C(=[C]2)O[C])O)C(=O)[C][C]1C1=[C][C]=C(C(=[C]1)O)O	-7.8
10189069 3	O1c2c([C])c(c([C])c(c2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1)O[C])O	-7.8
10162437 3	O1C2=[C]C(=[C][C]=C2[C]([C][C]1C1=[C][C]=[C][C]=[C]1)O)O[C]	-7.8
10159128 1	C1(=C(c2c(C(=[C]1)O[C])c(=O)c(c(o2)C1=[C][C]=C(C(=[C]1)O[C])O)O[C])O[C])O[C][C][C][C][C]	-7.8
10158423 2	O1C2=C(C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1)O[C])O[C])/[C]=[C]/C(=[C])[C]	-7.8
71586772	O1C(=[C]C(=O)C2=C(C(=C([C]=C12)OC(=O)[C])O[C])OC(=O)[C])C1=[C][C]=[C][C]=[C]1	-7.8
56648912	O1C(=[C]C(=O)C2=C1[C]=C(C(=C2OC(=O)[C])OC(=O)[C])O[C][C]=[C])C1=[C][C]=[C][C]=[C]1	-7.8
54728923	o1c(=O)c(c(c2C(=[C]C(=[C]c12)O)O)O)C1=[C][C]=C([C]=[C]1)O	-7.8
53796934	O1[C]=C(C(=O)C2=C([C]=C([C]=C12)O[C])O)C1=[C][C]=C([C]=C1O)O[C]	-7.8
21315732	O1C2=C([C]=C([C]=[C]2)C(=O)O[C][C])C(=O)[C]=C1C1=[C]C(=[C][C]=C1O[C]([C])[C])[C]	-7.8
19972541	o1c(c([C])c(=O)c2[C]=[C][C]=C(c12)C(=O)O[C][C])C1=[C][C]=[C][C]=[C]1	-7.8
15761525	O1C2=[C][C]=[C][C]=C2C(=O)C([C]1C1=[C][C]=[C][C]=[C]1)([C]O)[C]O	-7.8
15126657	O1[C]=C(C(=O)C2=C1C(=C([C]=[C]2)O)[C])C1=[C][C]=C([C]=[C]1)O	-7.8
14057034	O1C2=C(C3=C(C(=[C]2)O)C(=O)C(=[C]O3)C2=[C]C(=C([C]=C2O[C])O)O[C])[C]=[C]C1([C])[C]	-7.8
13916267	o1c(c(c(=O)c2=C([C]=C(C(=c12)O[C])O)O[C])O[C])C1=[C]C(=C([C]=[C]1)O[C])O[C]	-7.8
11772232	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O)O[C]O[C][C]O[C])C1=[C][C]=[C][C]=[C]1	-7.8
10755200	O1C2=C([C]=C([C]=[C]2)N)C(=O)[C]=C1C1=[C][C]=C([C]=[C]1)N([C])[C]	-7.8

10422310	O1C(=[C]C(=O)C2=C1[C]=[C][C]=C2N)C1=[C][C]=C([C]=[C]1)N	-7.8
7454026	O1[C]=C(C(=O)C2=[C][C]=C([C]=C12)O)C1=[C][C]=C([C]=[C]1)N(=O)=O	-7.8
6253276	C1(=C(C(=[C]C(=C1C(=O)/[C]=[C]/C1=[C][C]=C([C]=[C]1)O[C])O)O[C])O[C])O[C]	-7.8
5748605	O1[C]=C(C(=O)C2=C1[C]=C([C]=[C]2)O)C1=[C]C(=C([C]=[C]1)O[C])O[C]	-7.8
5491412	o1c2[C]=C([C]=C(c2c(=O)c(c1c1=[C]C(=C(C(=[C]1)O)O[C])O)O[C])O)O[C]	-7.8
5466136	o1c2[C]=C(C(=C(c2c(=O)c(c1c1=[C][C]=C2C(=[C]1)O[C]O2)O[C])O)O[C])O[C]	-7.8
5465885	O1C2=[C][C]=[C][C]=C2[C]([C][C]1C1=[C][C]=[C][C]=[C]1)[N]N	-7.8
5386297	o1c(c(c(=O)c2C(=C(C(=[C]c12)O)O[C])O)C1=[C]C(=C([C]=C1O[C])O[C])O[C])C(=O)O	-7.8
5383438	o1c2=[C]C(=[C]C(=c2c(=O)c(c1c1=[C]C(=C([C]=[C]1)O[C])O[C])O[C])O)O	-7.8
5381920	O1C2=C([C]=[C]C(=[C]2)O)C(=O)[C]=C1C1=[C]C(=C(C(=[C]1)O[C])O[C])O[C]	-7.8
5380905	o1c2=[C]C(=[C]C(=c2c(=O)c(c1c1=[C]C(=C([C]=[C]1)O[C])O)O[C])O)O	-7.8
5379265	O1C2=C(C(=[C]C(=[C]2)O)O)C(=O)[C]=C1C1=[C]C(=C(C(=[C]1)O[C])O[C])O[C]	-7.8
5378210	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O)O)C1=[C][C]=[C][C]=C1O[C]	-7.8
5377945	o1c(c(c(=O)c2=C(C(=C([C]=c12)O)O[C])O)O)C1=[C][C]=C([C]=[C]1)O	-7.8
5376891	O1[C]=C(C(=O)C2=C1[C]=C([C]=[C]2)O)C1=[C][C]=[C][C]=[C]1	-7.8
5353911	O1[C]=C(C(=O)C2=C([C]=C(C(=C12)O[C])O)O)C1=[C][C]=C([C]=[C]1)O	-7.8
5352032	o1c(c(c(=O)c2=C(C(=C([C]=c12)O)O[C])O)O[C])C1=[C][C]=C([C]=[C]1)O	-7.8
5352005	o1c2=[C]C(=[C]C(=c2c(=O)c(c1c1=[C]C(=C([C]=[C]1)O[C])O[C])O[C])O)O[C]	-7.8
5320945	o1c(c(c(=O)c2C(=[C]C(=[C]c12)O[C])O)O)C1=[C][C]=C(C(=[C]1)O[C])O	-7.8
5320181	O1C(=[C]C(=O)C2=C(C(=C([C]=C12)O)O)O)C1=[C]C(=C([C]=[C]1)O)O[C]	-7.8
5281695	o1c(c(c(=O)c2=C(C(=C([C]=c12)O)O[C])O)O[C])C1=[C][C]=C([C]=[C]1)O[C]	-7.8
5281654	o1c2[C]=C([C]=C(c2c(=O)c(c1c1=[C][C]=C(C(=[C]1)O[C])O)O)O)O	-7.8
5280666	O1C2=[C]C(=[C]C(=C2C(=O)[C]=C1C1=[C][C]=C(C(=[C]1)O[C])O)O)O	-7.8
5271551	O1C2=C(C(=[C]C(=[C]2)O[C])O[C])C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O	-7.8
3245800	C1(=[C]C(=O)C2=[C][C]=[C][C]=C2O1)C1=[C][C]=C([C]=[C]1)S[C]	-7.8
3084508	O1C(=[C]C(=O)c2c(c(c(c12)O[C])O[C])O[C])O)C1=[C]C(=C(C(=[C]1)O)O[C])O	-7.8
3070246	c1(c([C])c(=O)c2=[C][C]=C(C(=c2o1)[C]N([C][C])[C][C])O[C])C1=[C][C]=C(CI)[C]=[C]1	-7.8
2734290	O1[C]=C(C(=O)C2=C1[C]=C([C]=C2[C])O[C])C1=[C][C]=[C][C]=[C]1	-7.8
2017481	C1(=[C][C]=C2C(=O)C(=[C]OC2=[C]1)C1=[C][C]=[C][C]=[C]1)OS([C])([O])[O]	-7.8

1241435	O1C2=C([C]=[C][C]=[C]2)C(=O)[C]=C1C1=[C][C]=C([C]=[C]1)N([C])[C]	-7.8
736738	O1C2=[C][C]=[C][C]=C2C(=O)[C]([C]1C1=[C][C]=[C][C]=[C]1)O	-7.8
632255	O1C(=[C]C(=O)c2c(c(c(c12)O[C])O[C])O)O)C1=[C][C]=C(C(=[C]1)O[C])O[C]	-7.8
631782	o1c2[C]=C([C]=[C]c2c(=O)c(c1[C])C1=C([C]=C([C]=[C]1)O[C])O[C])O[C][C]=[C]	-7.8
369612	O1C2=C([C]=C([C]=C2[C]([C][C]1C1=[C][C]=C(C(=[C]1)O[C])O[C])O[C])[C][C]=[C])O[C]	-7.8
343083	C1(=[C]OC2=C([C]=[C]C(=[C]2)O[C])C1=O)C1=[C]C2=C(O[C]O2)[C]=C1O[C]	-7.8
321347	O1C2=[C]C(=[C]C(=C2C(=O)[C][C]1C1=[C]C(=[C]=[C]1)O)O[C])O)O[C]	-7.8
246330	O1C2=[C]C(=[C][C]=C2C(=O)[C]([C]1C1=[C][C]=C(C(=[C]1)O)O)O)O	-7.8
195603	O1C2=C(C(=[C]C(=[C]2)O[C])O)C(=O)[C][C]1C1=C([C]=[C][C]=C1O)O	-7.8
188323	O1C(=[C]C(=O)C2=C(C(=C([C]=C12)O[C])O[C])O)C1=[C][C]=C([C]=[C]1)O	-7.8
177000	o1c2=[C]C(=[C][C]=c2c(=O)c([C])c1C1=[C]C(=C(C(=[C]1)O[C])O[C])O[C])O[C]	-7.8
160237	O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O)O[C])O[C])C1=[C][C]=C(C(=[C]1)O)O	-7.8
158311	O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O)O[C])O[C])C1=C([C]=C(C(=[C]1)O[C])O)O	-7.8
153441	O1C(=[C]C(=O)c2c(c(c(c12)O)O[C])O[C])O)C1=[C][C]=[C][C]=[C]1	-7.8
102674	O1C2=[C][C]=[C][C]=C2[C]([C][C]1C1=[C][C]=[C][C]=[C]1)[N]N	-7.8
96539	O1C(=[C]C(=O)c2c(c(c(c12)O[C])O[C])O[C])O)C1=[C][C]=C([C]=[C]1)O[C]	-7.8
26034	o1c(c(c(=O)c2=C([C]=C([C]=C12)O[C])O[C])O)C1=[C]C(=[C]=[C]1)O)O	-7.8
9064	O1C2=[C]C(=[C]C(=C2[C][C]([C]1C1=[C][C]=C(C(=[C]1)O)O)O)O)O	-7.8
471	O1C2=[C]C(=[C]C(=C2C(=O)[C]([C]1C1=[C]C(=[C]=[C]1)O)O)O)O)O	-7.8
13959263 0	O1C2=C([C]=[C]C(=[C]2)O)[C]2[C][C]1[C]1[C][C]=[C][C](O[C]O2)[C]1	-7.7
13845452 9	O1C2=[C][C]=[C][C]=C2C(=O)[C]([C@]1(C1=[C][C]=[C][C]=[C]1)OC(O)(O)O)O	-7.7
12986426 5	O1C2=C([C]=[C][C]=C2C(=O)[C][C@]1(C1=[C][C]=[C][C]=[C]1)O)O[C]	-7.7
12982238 6	Brc1c(c(c(c2C(=O)[C]=C(Oc12)C1=[C][C]=[C][C]=[C]1)OC(=O)[C])OC(=O)[C])OC(=O)[C]	-7.7
10233021 7	O1C2=C([C]=[C]C(=[C]2)O[C])C(=O)[C]([C]1C1=[C][C]=C([C]=[C]1)O[C])O	-7.7

10232161 0	C1(=[C]OC2=[C]C(=[C]C(=C2C1=O)O)O)C1=C(C2=C(O[C]O2)[C]=[C]1)O[C]	-7.7
10201716 3	o1c(c(c(=O)c2=C([C]=C(C(=c12)[C][C]C(=[C])[C])O)O)O)C1=[C][C]=[C][C]=[C]1	-7.7
10159128 2	C1(=C(c2c(C(=[C]1)O[C])c(=O)c(c(o2)C1=[C][C]=C(C(=[C]1)O[C])O[C])O[C])O[C])O[C][C][C][C][C]	-7.7
10117916 5	o1c(c(c(=O)c2=C([C]=C([C]=c12)O[C])O[C][C][C]O)O[C])C1=[C]C=C([C]=[C]1)O[C])O[C]	-7.7
90000191	o1c(c(c(=O)c2c(c(c(c12)O[C])O[C])O[C])O)O)C1=C(C(=[C][C]=[C]1)O[C])O[C]	-7.7
74977227	O1C2=[C]C(=[C]C(=C2[C][C][C]1C1=[C][C]=C(C(=[C]1)O[C])O[C])O)O	-7.7
70253991	o1c(c(c(=O)c2c(c(c(c12)O)O[C])O[C])O)O)C1=[C][C]=[C][C]=[C]1	-7.7
69030367	O1C2=[C]C(=[C][C]=C2C(=O)[C]=C1C1=[C]C(=[C]C(=[C]1)O[C])O[C])O	-7.7
54140898	o1c(c(c(=O)c2=C(C(=[C][C]=c12)O[C][C])O[C][C])O[C][C])C1=[C][C]=[C][C]=[C]1	-7.7
44412009	O1C2=C([C])C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1)O[C])O[C]	-7.7
44266353	O1C2=[C][C]=[C][C]=C2C(=O)/C(=[C]/C2=[C][C]=N[C]=[C]2)/[C]1C1=[C][C]=[C][C]=[C]1	-7.7
44259869	o1c(c(c(=O)c2=C(C(=C([C]=c12)O)O[C])O)O)C1=[C][C]=C(C(=[C]1)O[C])O[C]	-7.7
44258621	O1c2c3C(=O)[C]=C(Oc3c(c2[C]=[C]C1([C])[C])O[C])O[C])C1=[C]C(=C(C(=[C]1)O[C])O[C])O[C]	-7.7
35028119	O1C(=[C]C(=O)c2c(c(c(c12)O[C])O[C])O[C])O[C])C1=[C][C]=[C]C(=[C]1)O[C]	-7.7
25068463	O1C2=[C]C(=[C]C(=C2[C]C(=O)[C]1C1=[C][C]=C(C(=[C]1)O[C])O[C])O[C])O[C]	-7.7
18324985	lc1c(=O)c2=[C][C]=[C][C]=c2oc1C1=[C][C]=C([C]=[C]1)S(=O)(=O)[C]	-7.7
15389441	O1C2=C([C]=C3C(=[C]2)O[C]=C(C3=O)C2=[C]C(=C([C]=C2O[C])O[C])O[C])[C]=[C]C1([C])[C]	-7.7
14372618	O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O[C])O)O[C])C1=[C][C]=[C][C]=[C]1	-7.7
14254494	O1[C]=C(C(=O)C2=C1[C]=C([C]=C2[C])O)C1=[C][C]=[C][C]=[C]1	-7.7
13964544	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O[C])O)C1=[C][C]=C(C(=[C]1)O[C])O[C]	-7.7
13916278	o1c(c(c(=O)c2C(=[C]C(=C(c12)O[C])O)O)O[C])C1=[C][C]=C([C]=[C]1)O[C]	-7.7
12360936	O1C2=[C]C(=[C][C]=C2[C]([C][C]1C1=[C][C]=[C][C]=[C]1)O)O[C]	-7.7
12241083	O1[C]=C(C(=O)C2=C1[C]=C([C]=C2O)O)C1=[C][C]=C([C]=[C]1)N(=O)=O	-7.7
12132943	O1c2c(c(c([C])c(c2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1)O)O[C])[C]=O	-7.7
12132870	O1[C]=C(C(=O)C2=C1[C]=C(C(=[C]2)O)O[C])C1=[C][C]=C([C]=[C]1)O[C]	-7.7

11726019	O1C(=[C]C(=O)c2c(c(c(c12)O)O[C])O[C])O)C1=[C][C]=C(C(=[C]1)O[C])O	-7.7
10594862	Br1c(=O)c2=[C][C]=[C][C]=c2oc1C1=[C][C]=C([C]=[C]1)[S@@](=O)[C]	-7.7
5491643	O1C(=[C]C(=O)C2=C(C(=C([C]=C12)O)O[C])O[C])C1=[C][C]=C(C(=[C]1)O[C])O[C]	-7.7
5488781	O1[C]=C(C(=O)C2=C1[C]=C(C(=C2O)O[C])O)C1=[C][C]=C(C(=[C]1)O)O[C]	-7.7
5386961	o1c(c(c(=O)c2=C([C]=C(C(=c12)O[C])O)O)O[C])C1=[C]C=C([C]=[C]1)O)O[C]	-7.7
5317287	o1c(c(c(=O)c2=C(C(=C([C]=c12)O[C])O[C])O)O)C1=[C]C=C([C]=[C]1)O[C])O	-7.7
5316900	o1c2=[C]C(=[C]C(=c2c(=O)c(c1C1=[C]C=C([C]=[C]1)O)O[C])O[C])O)O	-7.7
5281706	O1[C]=C(C(=O)C2=C([C]=C([C]=C12)O[C])O)C1=C([C]=C([C]=[C]1)O)O	-7.7
5281666	o1c(c(c(=O)c2=C([C]=C([C]=c12)O)O)O)C1=[C][C]=C([C]=[C]1)O[C]	-7.7
5280373	O1[C]=C(C(=O)C2=C1[C]=C([C]=C2O)O)C1=[C][C]=C([C]=[C]1)O[C]	-7.7
4303567	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2OC(=O)[C])OC(=O)[C])C1=[C][C]=C([C]=[C]1)O[C]	-7.7
3825918	o1c2[C]=[C][C]=[C]c2c(=O)c(c1C1=[C][C]=[C][C]=[C]1)N1[C]=NN=N1	-7.7
1666397	o1c2=[C][C]=[C][C]=c2c(=O)c(c1C1=[C][C]=[C][C]=[C]1)OC(=O)[C]	-7.7
634113	o1c2=[C]C(=[C]C(=c2c(=O)c(c1C1=[C]C=C(C(=[C]1)O[C])O[C])O[C])O[C])O[C])O[C]	-7.7
631791	o1c(c(c(=O)c2c(c(c3c([C]=[C]O3)c12)O[C])O[C])O[C])C1=[C][C]=[C][C]=[C]1	-7.7
624789	O1[C]=C(C(=O)C2=C1[C]=C(C(=[C]2)O[C])O[C])C1=[C][C]=[C][C]=[C]1	-7.7
602425	O1C2=C(C(=[C][C]=C2C(=O)[C])([C]1C1=[C][C]=C(C(=[C]1)O[C])O[C])O[C])O[C]	-7.7
586387	O1C2=[C]C(=[C]C(=C2C(=O)[C])([C]1C1=[C][C]=C([C]=[C]1)O[C])O)O)O	-7.7
462696	O1C2=[C]C(=[C]C(=C2C(=O)[C][C]1C1=[C]C=C(C(=[C]1)O[C])O[C])O[C])O)O	-7.7
442621	o1c(c(c(=O)c2C=C(C(=[C]c12)O[C])O)O)O[C])C1=[C][C]=C(C(=[C]1)O)O[C]	-7.7
343081	O1[C]=C(C(=O)C2=C1C1=C([C]=[C]2)O[C]O1)C1=[C]C=C([C]=[C]1)O[C])O[C]	-7.7
331149	O1C(=[C]C(=O)c2c(c(c(c12)O[C])O[C])O[C])O[C])C1=[C]C2=C(C(=[C]1)O[C])O[C]O2	-7.7
147806	O1C2=[C][C]=[C][C]=C2C(=O)[C]([C]1C1=[C][C]=[C][C]=[C]1)O	-7.7
129394	O1c2c(c(c([C])c(c2[C]([C][C]1C1=[C][C]=[C][C]=[C]1)O)O[C])O)[C]=O	-7.7
49676	o1c(c([C])c(=O)c2=[C][C]=C(C(=c12)[C]N([C][C])[C][C])O[C])C1=[C][C]=[C][C]=[C]1	-7.7
41451	C1(=[C][C]=C([C]=[C]1)c1c([C])c(=O)c2=[C][C]=[C][C]=c2o1)O[C][C](O)[C]N[C]([C])[C]	-7.7
13415942	o1c2[C]=[C][C]=[C]c2c(=O)c(c1C1=C([C]=C(C(=[C]1)O)O)C(=O)O)C1=[C][C]=[C][C]=[C]1	-7.6

12988767 6	O1C2=C([C]=C(C(=[C]2)O)O[C])C(=O)[C]([C]1C1=[C][C]=[C][C]=[C]1)O	-7.6
12985870 7	O1C2=C(C(=[C]C(=[C]2)O)O)C(=O)[C@]([C]1C1=[C]C=C([C]=[C]1)O)O)(O)O[C]	-7.6
12985834 1	O1C2=C([C]=[C]C(=C2O[C])O[C])C(=O)C([C@@]1(C1=[C][C]=[C][C]=[C]1)O)(O)O	-7.6
12984454 3	O1[C]=C(C(=O)c2c(c(c(c12)O)O)O[C])O)C1=[C]C=C(C(=[C]1)O)O[C])O[C]	-7.6
12971122 0	O1C2=C([C]=[C][C]C2=O)[C][C][C]1C1=[C][C]=[C][C]=[C]1	-7.6
12971080 8	O1C2=[C][C]=[C][C]=C2C(=O)[C][C@@]1(C1=[C][C]=[C][C]=[C]1)/[C]=[C]/C(=[C])[C]	-7.6
12968025 6	O1C2=[C][C]=[C][C]=C2[C]C([C]1C1=[C][C]=[C][C]=[C]1)(O)O	-7.6
12966151 7	O1C2=[C]C(=[C]C(=C2[C](C(=O)[C]1C1=[C][C]=[C][C]=[C]1)O)O)O	-7.6
12963357 8	o1c(c(c(=O)c2[C]=[C]C=C(c12)O[C])O[C])O)C1=[C][C]=C(C(=[C]1)O[C])O[C]	-7.6
10158423 6	O1C2=C(C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1)O[C])O[C])/[C]=[C]\C([C])([C])O	-7.6
67743168	O1C2=[C]C(=[C]C(=C2[C]([C]([C]1C1=[C]C(=[C][C]=[C]1)O)O)O)O)O	-7.6
67425485	C1(=[C]C2=C(C(=[C]1)O[C])C(=O)[C]=C(O2)C1=[C][C]=C(C(=[C]1)O[C])O[C])O[C]P(=O)([C]([C])[C])([C])([C])[C]	-7.6
57340185	C1(=[C]C(=O)C2=C([C]=C([C]=[C]2)O)O1)C1=[C][C]=C(I)[C]=[C]1	-7.6
54423602	c1(c(c(=O)c2=[C][C]=[C][C]=c2o1)C1=[C][C]=[C][C]=[C]1)O[C]([C])[C]	-7.6
51041990	o1c2=[C]C(=[C]C(=c2c(=O)c(c1C1=[C]C(=[C]C(=C1[C][C]=C([C])([C])O)O[C])O[C])O)O	-7.6
44258304	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O[C])O[C])C1=[C]C=C([C]=[C]1)O)O	-7.6
44257206	o1c([C])c(c(=O)c2=[C][C]=C(C(=c12)C(=O)[C])O)C1=[C][C]=[C][C]=[C]1	-7.6
44257187	O1C2=C(C(=[C]C(=C2[C][C]C([C])([C])O)O[C])O[C])[C][C][C]1C1=[C][C]=[C][C]=[C]1	-7.6
23786424	O1C2=C(C(=[C]C(=C2O[C])O)O[C])C(=O)[C][C]1C1=[C][C]=[C][C]=[C]1	-7.6
21270152	O1[C]=C(C(=O)C2=[C][C]=C(C(=C12)[C])O)C1=[C][C]=C([C]=[C]1)N(=O)=O	-7.6

16681753	O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O)O[C])O[C])C1=[C]C(=C(C(=[C]1)O[C])O)O[C]	-7.6
14732294	O1C2=[C]C(=[C]C(=C2[C][C]([C]1C1=[C][C]=C(C(=[C]1)O)O)O)O[C])O[C]	-7.6
14057036	O1C2=C(C3=C(C(=[C]2)O)C(=O)C(=[C]O3)C2=[C]C(=C([C]=C2O[C])O[C])O[C])[C]=[C]C1([C])[C]	-7.6
13291608	o1c(c(c(=O)c2C(=C(C(=[C]c12)O[C])O[C])O)O)C1=[C][C]=[C][C]=[C]1	-7.6
13045799	O1C2=[C][C]=[C][C]=C2[C][C]([C]1C1=[C][C]=[C][C]=[C]1)OC(=O)[C]	-7.6
10665307	BrC1c(=O)c2[C]=[C][C]=[C]c2oc1C1=[C][C]=C([C]=[C]1)S[C]	-7.6
10475482	o1c(c(c(=O)c2c(c(c(c12)O[C])O[C])O[C])O)O)C1=[C]C(=C([C]=[C]1)O)O[C]	-7.6
9798295	O1C2=C(C(=C(C(=[C]2)O[C])O[C])O[C])C(=O)[C][C]1C1=[C]C(=C([C]=[C]1)O)O	-7.6
5491798	o1c(c(c(=O)c2=C([C]=C(C(=c12)O[C])O[C])O)O)C1=[C][C]=[C][C]=[C]1	-7.6
5490001	o1c2=[C]C(=[C][C]=c2c(=O)c(c1C1=[C]C(=C(C(=[C]1)O[C])O[C])O[C])O	-7.6
5381919	O1C(=[C]C(=O)C2=C([C]=C([C])[C]=C12)O)C1=[C]C(=C(C(=[C]1)O[C])O[C])O[C]	-7.6
5378391	o1c([C])c(c(=O)c2=[C][C]=C(C(=c12)[C][C]=[C])O)C1=[C][C]=[C][C]=[C]1	-7.6
5281606	c1(c(c(=O)c2C(=[C]C(=C(c2o1)O[C])O[C])O)O)C1=C(C(=[C][C]=[C]1)Cl)O	-7.6
5273755	O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O)O[C])O)C1=[C][C]=C(C(=[C]1)O[C])O[C]	-7.6
5272653	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O)O[C])C1=[C][C]=C(C(=[C]1)O[C])O[C]	-7.6
3082330	O1C2=C(C(=[C]C(=[C]2)O)O)C(=O)[C]([C]1C1=[C][C]=[C][C]=C1O)O	-7.6
2064449	O1C2=C(C(=[C]C(=[C]2)O[C])O[C])C(=O)[C]([C]1C1=[C]C(=C([C]=[C]1)O[C])O[C])O	-7.6
636642	ClC1=C([C]=C2C(=C1O)[C][C]([C](O2)C1=[C][C]=C(C(=[C]1)O)O)O)O	-7.6
628555	o1c2=[C]C(=[C][C]=c2c(=O)c(c1C1=[C][C]=C([C]=[C]1)O[C])O[C])O[C]	-7.6
493376	O1C2=[C]C(=[C]C(=C2C(=O)[C]=C1C1=[C]C(=C(C(=[C]1)O[C])O[C])O[C])O[C]	-7.6
315709	O1C(=[C]C(=O)C2=C1[C]=C(C(=[C]2)O[C])O[C])C1=[C][C]=C(C(=[C]1)O[C])O[C]	-7.6
282014	O1C2=[C]C(=[C]C(=C2[C][C]([C]1C1=[C][C]=C([C]=[C]1)O)O)O)O	-7.6
189551	O1C(=C(C(=O)[C@]2([C][C]=[C]C(=C12)O[C])O)O[C])C1=[C][C]=[C][C]=[C]1	-7.6
182659	O1C2=[C]C(=[C]C(=C2[C][C]([C]1C1=[C][C]=C(C(=[C]1)O[C])O[C])O)O[C])O[C]	-7.6
124211	O1C(=[C]C(=O)c2c(c(c(c12)O[C])O[C])O[C])O)C1=C([C]=[C][C]=C1O)O[C]	-7.6
97332	o1c(c(c(=O)c2C(=[C]C(=[C]c12)O[C])O[C])O[C])C1=[C]C(=C([C]=[C]1)O[C])O[C]	-7.6
97142	o1c(c(c(=O)c2=C([C]=C([C]=c12)O[C])O[C])O)C1=[C]C(=C([C]=[C]1)O[C])O[C]	-7.6
12988102	O1[C]=C(C(=O)C2=[C][C]=C(C(=C12)[C]O)O)C1=[C]C(=C(C(=[C]1)[C]O)O)[C]O	-7.5

12981827 7	O1C2=[C]C(=[C][C]=C2[C](C(=O)[C]1C1=[C][C]=[C][C]=[C]1)O[C])O	-7.5
12966152 7	O1C2=[C]C(=[C]C(=C2[C](C(=O)[C@@]1(C1=[C][C]=[C][C]=[C]1)O)O)O)O	-7.5
10219490 9	o1c(c(c(=O)c2c(c(c(c12)O[C])O[C][C]=C([C])[C])O[C])O[C])O[C])C1=[C][C]=C(C(=[C]1)O[C])O[C]	-7.5
91727421	O1C2=C(C(=[C]C(=[C]2)O[C])O[C])C(=O)[C]([C]1C1=[C][C]=C(C(=[C]1)O[C])O[C])OC(=O)[C]	-7.5
69047096	C1(=C([C]=C([C]=[C]1)O[C]O[C])O[C]O[C])[C]1OC2=[C][C]=[C][C]=C2C(=O)[C]1	-7.5
56658060	O1C2=[C]C(=[C]C(=C2C(=O)[C]([C]1C1=[C][C]=C(C(=[C]1)O[C])O)O)O)O	-7.5
54368735	c1(c(=O)c2[C]=[C][C]=[C]c2oc1C1=[C]C=C(C(=[C]1)O[C])O[C])O[C])C(=O)N[C][C]Br	-7.5
44566483	O1C2=[C]C(=C(C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O[C])O[C])O)O[C]	-7.5
44260053	o1c(c(c(=O)c2c(c(c(c12)OC(=O)[C][C]([C])[C])O)O[C])O)O[C])C1=[C][C]=C([C]=[C]1)O[C]	-7.5
44257043	O1C(=[C][C]=C2[C](C(=C([C]=C12)O)O)O[C])C1=[C][C]=C(C(=[C]1)O)O[C]	-7.5
44133602	O1[C]=C(C(=O)C2=C(C(=C([C]=C12)O)O[C])O)C1=[C]C=C(C(=[C]1)O[C])O)O[C]	-7.5
42608126	O1c2c(c(c(c2C(=O)[C][C]1C1=[C]C(=C2C(=[C]1)O[C]O2)O[C])O[C])O[C])O[C]	-7.5
25058047	o1c(c(c(=O)c2C(=[C]C(=C(c12)[C][C]=C([C])[C])O[C][C]O)O)O[C][C]O)C1=[C][C]=C([C]=[C]1)O[C]	-7.5
19358638	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O[C])O[C][C]O)C1=[C][C]=C(C(=[C]1)O[C])O[C]	-7.5
15761521	o1c2=[C][C]=[C][C]=c2c(=O)c(c1C1=[C][C]=[C][C]=[C]1)[C]([C])C#N	-7.5
14055876	O1C(=[C]C(=O)C2=C1[C]=[C]C(=C2O[C])O[C])C1=[C][C]=C(C(=[C]1)O[C])O[C]	-7.5
11795367	o1c(c(c(=O)c2c(c(c(c12)O[C])O)O[C])O[C])O[C])C1=[C]C2=C([C]=[C]1)O[C]O2	-7.5
11709692	o1c(c(c(=O)c2C(=[C]C(=[C]c12)O)O[C])O)C1=[C][C]=C([C]=C1O[C])O	-7.5
11610052	O1[C]=C(C(=O)C2=C1[C]=C([C]=C2O)O)C1=C(C(=C([C]=[C]1)O)O)[C][C]=C([C])[C]	-7.5
11500888	O1C2=C(C(=[C]C(=[C]2)O)O[C])C(=O)[C]([C]1C1=[C][C]=C([C]=C1O[C])O)O	-7.5
11471620	O1[C]=C(C(=O)C2=C1[C]=C([C]=[C]2)O[C])C1=[C][C]=C([C]=C1O)O	-7.5
9972910	o1c(c(c(=O)c2=C([C]=C(C(=c12)O[C])O)O)O[C])C1=[C][C]=[C][C]=[C]1	-7.5
7309334	O1C2=[C][C]=[C][C]=C2[C][C]([C]1C1=[C][C]=[C][C]=[C]1)O	-7.5
6453535	o1c(c(c(=O)c2C(=C(C(=[C]c12)O[C])O[C])O)O)C1=[C][C]=C(C(=[C]1)O[C])O	-7.5
5459184	o1c(c(c(=O)c2=C([C]=C(C(=c12)O[C])O[C])O)O[C])C1=[C]C=C([C]=[C]1)O)O[C]	-7.5
5407860	O1[C]=C(C(=O)C2=C1C(=C([C]=[C]2)O)O)C1=[C][C]=[C][C]=[C]1	-7.5

5380187	o1c(c(c(=O)c2C(=[C]C(=[C]c12)O)O)C1=[C][C]=C([C]=[C]1)O[C])C(=O)O[C][C]	-7.5
5379262	o1c(c(c(=O)c2c(c(c(c12)O[C])O[C])O[C])O)O)C1=[C][C]=[C][C]=[C]1	-7.5
5377381	O1[C]=C(C(=O)C2=C1[C]=C([C]=C2O)O)C1=[C][C]=[C][C]=[C]1	-7.5
5321435	o1c(c(c(=O)c2C(=C(C(=[C]c12)O)O[C])O)O)C1=[C][C]=C(C(=[C]1)O[C])O	-7.5
5318041	O1C(=[C]C(=O)c2c(c(c(c12)O[C])O[C])O[C])O[C])C1=[C][C]=C(C(=[C]1)O)O	-7.5
5281781	O1[C]=C(C(=O)C2=C1[C]=C(C(=C2O)O[C])O)C1=[C][C]=C([C]=[C]1)O[C]	-7.5
5281676	o1c2=[C]C(=[C]C(=c2c(=O)c(c1C1=[C]C(=C([C]=C1O)O[C])O)O[C])O)O[C]	-7.5
5280699	o1c(c(c(=O)c2C(=C(C(=[C]c12)O[C])O[C])O)O[C])C1=[C]C(=C([C]=[C]1)O)O	-7.5
3083840	O1[C]=C(C(=O)C2=[C]C(=C([C]=C12)OC(=O)[C])O[C])C1=[C][C]=C([C]=[C]1)O[C]	-7.5
638006	O1[C]=C(C(=O)C2=C1[C]=C([C]=[C]2)O[C])C1=[C][C]=[C][C]=[C]1	-7.5
634724	o1c(c(c(=O)c2C(=C(C(=[C]c12)O[C][C])O[C])O[C][C])O[C])C1=[C]C(=C([C]=[C]1)O[C][C])O[C]	-7.5
631176	O1[C]=C(C(=O)C2=[C]C(=C([C]=C12)O[C])O[C])C1=[C][C]=C(C(=[C]1)O[C])O[C]	-7.5
631171	o1c2=[C]C(=[C][C]=c2c(=O)c(c1C1=[C]C(=C([C]=[C]1)O[C])O[C])O[C])O[C]	-7.5
442583	O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O[C])O[C])O[C])C1=[C][C]=[C][C]=[C]1	-7.5
386331	o1c(c(c(=O)c2=C(C(=C([C]=c12)O[C])O[C])O[C])O[C])C1=[C]C(=C([C]=[C]1)O[C])O[C]	-7.5
358832	O1C(=[C]C(=O)c2c(c(c(c12)O[C])O[C])O[C])O)C1=[C][C]=C(C(=[C]1)O[C])O[C]	-7.5
253959	O1C2=[C][C]=[C][C]=C2[C]([C][C]1C1=[C][C]=[C][C]=[C]1)O	-7.5
245874	O1C2=[C]C(=C(C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O[C])O[C])O)O[C]	-7.5
181092	O1C(=[C]C(=O)c2c(c(c(c12)O[C])O[C])O[C])O)C1=[C]C(=C([C]=[C]1)O)O[C]	-7.5
167616	O1C2=C(C(=[C]C(=[C]2)O[C])O[C])C(=O)[C][C]1C1=[C]C(=C([C]=[C]1)O[C])O[C]	-7.5
162464	O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O)O[C])O[C])C1=[C][C]=C(C(=[C]1)O[C])O	-7.5
136420	O1[C]=C(C(=O)C2=C([C]=C([C]=C12)O[C])O[C])C1=[C][C]=C([C]=[C]1)O[C]	-7.5
97151	O1C(=[C]C(=O)c2c(c(c(c12)O[C])O[C])O[C])O[C])C1=[C][C]=C2C(=[C]1)O[C]O2	-7.5
54799	o1c(c(c(=O)c2c(c(c(c12)O[C])O[C])O[C])O)O[C])C1=[C][C]=C(C(=[C]1)O)O	-7.5
12988780	o1c2=[C][C]=C(C(=c2c(=O)c(c1C1=[C]C(=C([C]=[C]1)O[C])O[C])O[C])O)O	-7.4
1		
12982055	o1c(c(c(=O)c2=C([C]=C(C(=c12)O[C])O[C])O[C])O)C1=[C]C(=C([C]=[C]1)O[C])O[C]	-7.4
4		

12973375 0	Cl[C]1C2=C([C]=[C][C]=[C]2)O[C]([C]1O)C1=[C][C]=[C][C]=[C]1	-7.4
12973362 2	O1C2=C(C(=C([C]=[C]2)O[C])O)C(=O)C([C@@]1(C1=[C][C]=[C][C]=[C]1)O)(O)O	-7.4
12967478 1	O1C2=C([C]=[C][C]=[C]2)[C][C]([C]1C1=[C][C]=[C][C]=[C]1)O[C]	-7.4
12903597 6	O1C2=C([C]=[C][C]=[C]2)[C][C]([C]1C1=[C][C]=[C][C]=[C]1)O	-7.4
10218073 9	o1c2[C]=[C][C]=[C]c2c(=O)c(c1C1=C(C(=C([C]=[C]1)O[C])O[C])O[C])C1=[C][C]=C([C]=[C]1)O[C]	-7.4
10156189 8	o1c2[C]=[C][C]=[C]c2c(=O)c(c1C1=[C][C]=[C][C]=[C]1)O[C]C#[C]	-7.4
86641846	O1C(=[C]C(=O)C2=C([C]=C([C]=C12)O[C]C#[C])O[C])C1=[C]C(=C([C]=[C]1)O[C])O[C]	-7.4
71428798	O1[C]=C(C(=O)C2=C1C(=C([C]=[C]2)O)O[C])C1=[C][C]=C([C]=[C]1)O	-7.4
71346541	o1c2[C]=[C][C]=[C]c2c(=O)c(c1C1=[C][C]=C([C]=[C]1)N([C])[C])O[C]	-7.4
67200543	O1C2=C([C]=[C][C]=[C]2)C(=O)[C]([C]1C1=[C][C]=[C][C]=[C]1)C(=O)OC([C])([C])[C]	-7.4
66916672	o1c2=[C][C]=[C][C]=c2c(=O)c(c1C(=O)[C])C1=[C][C]=[C][C]=[C]1	-7.4
66692593	O1C2=C([C]=[C][C]=[C]2)[C][C]([C]1C1=[C][C]=[C][C]=[C]1)O	-7.4
59331779	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O[C])O[C]C#N)C1=[C][C]=C(C(=[C]1)O[C])O[C]	-7.4
54140747	c1(c(=O)c2=[C][C]=[C][C]=c2oc1C1=[C][C]=[C][C]=[C]1)OS([O])([O])O	-7.4
23644935	o1c2=[C]C(=[C][C]=c2c(=O)c(c1N1[C]=N[C]=N1)C1=[C][C]=[C][C]=[C]1)O[C]	-7.4
23644932	o1c2=[C]C(=[C][C]=c2c(=O)c(c1N1[C]=N[C]=[C]1)C1=[C][C]=C([C]=[C]1)O[C])O[C]	-7.4
23644623	o1c2=[C]C(=[C][C]=c2c(=O)c(c1N1[C]=N[C]=[C]1)C1=[C][C]=[C][C]=[C]1)O[C]	-7.4
21270160	O1[C]=C(C(=O)C2=[C][C]=C(C(=C12)[C])O)C1=[C][C]=C([C]=[C]1)[C]	-7.4
15625549	O1c2c(c(c(c2C(=O)[C][C]1C1=[C]C(=C([C]=[C]1)O[C])O[C])O[C])O[C])O[C]	-7.4
14756305	O1C2=[C]C(=[C]C(=C2C(=O)[C]([C])[C]1C1=[C][C]=C([C]=[C]1)O)O)O	-7.4
14630603	O1[C]=C(C(=O)C2=C(C3=C([C]=C12)O[C]O3)O[C])C1=[C][C]=[C]C(=C1O[C])O[C]	-7.4
13045744	O1C2=C(C(=[C]C(=[C]2)O[C])O[C])[C][C][C]1C1=[C]C(=C([C]=[C]1)O[C])O[C]	-7.4
13045742	O1C2=C(C(=[C]C(=[C]2)O[C])O[C])[C][C][C]1C1=[C]C(=C([C]=[C]1)O[C])O[C]	-7.4
11797078	o1c(c(c(=O)c2c(c(c(c12)O[C])O[C])O[C]O[C])O[C])O)C1=[C]C(=C([C]=[C]1)O)O[C]	-7.4

10937632	O1C2=C(C(=C(C(=[C]2)O[C])O[C])O[C])C(=O)[C][C]1C1=[C]C(=C([C]=[C]1)O[C])O[C]	-7.4
5386963	o1c(c(c(=O)c2c(c(c(c12)O[C])O)O[C])O)O[C]C1=[C]C(=C(C(=[C]1)O[C])O[C])O[C]	-7.4
5384810	o1c(c(c(=O)c2=C([C]=C(C(=c12)OC(=O)[C][C][C])O[C])O)O)C1=[C][C]=C([C]=[C]1)O[C]	-7.4
5281704	O1[C]=C(C(=O)C2=C1[C]=C(C(=[C]2)O[C])O)C1=[C][C]=C([C]=[C]1)O[C]	-7.4
5003667	O1C2=[C]C(=[C]C(=C2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O[C])O[C])O[C]	-7.4
3084507	O1C(=[C]C(=O)c2c(c(c(c12)O[C])O[C])O[C])O)C1=[C]C(=C(C(=[C]1)O[C])O[C])O	-7.4
1560918	C1(=[C]C2=C([C]=[C]1)C(=O)C(=[C]O2)C1=C([C]=[C][C]=[C]1)O[C])OS([C])([O])[O]	-7.4
633456	o1c2=[C]C(=[C][C]=c2c(=O)c(c1[C])C1=C([C]=C(C(=[C]1)O[C])O[C])O[C])OC(=O)[C]	-7.4
631170	O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O[C])O[C])C1=[C][C]=C(C(=[C]1)O[C])O[C]	-7.4
631095	o1c(c(c(=O)c2C(=[C]C(=[C]c12)O[C])O[C])O[C])C1=[C][C]=C([C]=[C]1)O[C]	-7.4
628412	o1c(c(c(=O)c2C(=[C]C(=[C]c12)O[C])O[C])O[C])C1=[C][C]=[C][C]=C1O[C]	-7.4
614295	[C]1(C(=O)C2=C([C]=[C][C]=[C]2)O[C]1C1=[C][C]=[C][C]=[C]1)S[C][C][C]	-7.4
462698	O1c2c(c(c(c2C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O[C])O[C])O[C])O[C]O[C]	-7.4
462695	O1C2=C(C(=[C]C(=[C]2)O[C])O[C])C(=O)[C]([C]1C1=[C]C(=C([C]=[C]1)O[C])O[C])O	-7.4
242486	O1C2=C(C(=C(C(=[C]2)O[C])O[C])O[C])C(=O)[C][C]1C1=[C][C]=C([C]=[C]1)O[C]	-7.4
12986412 1	o1c2[C]=C([C]=C(c2c(=O)c(c1C1=[C][C]=C([C]=[C]1)O[C](C(=[C])[C])[C]O)O[C])O)O[C]	-7.3
12983478 8	o1c(c(c(=O)c2C(=C(C(=[C]c12)O[C])O[C])O[C])O[C][C])C1=[C][C]=C(C(=[C]1)O[C][C])O[C]	-7.3
12982594 3	O1C2=[C]C(=[C]C(=C2C(=O)[C]=C1C1=[C][C]=[C][C]=C1C(=O)[C][C][C][C])O)O[C]	-7.3
44257042	O1C(=[C][C]=C2[C](C(=C([C]=C12)O)O)O[C])C1=[C][C]=C(C(=[C]1)O)O	-7.3
14606539	o1c(c(c(=O)c2=C(C(=C([C]=c12)O[C])O[C])O[C])O)C1=[C][C]=[C][C]=[C]1	-7.3
14304977	o1c2=[C][C]=[C][C]=c2c(=O)c(c1C1=[C]C(=C(C(=[C]1)O[C])O[C])O[C])C(=O)O	-7.3
12578908	O1C2=[C]C(=[C]C(=C2C(=O)[C]([C]1)C1=[C][C]=[C][C]=[C]1)O)O	-7.3
12088189	o1c2[C]=[C][C]=[C]c2c(=O)c(c1C1=[C][C]=C([C]=[C]1)N([C][C])[C][C])O	-7.3
11244229	c1(c(c(=O)c2[C]=[C]C(=[C]c2o1)O[C])C1=[C][C]=[C][C]=[C]1)S[C][C]=[C]	-7.3
10386481	O1C(=[C]C(=O)c2c(c(c(c12)O[C])O[C])O[C])O)C1=[C]C(=C(C(=[C]1)O[C])O)O[C]	-7.3
6710704	O1[C]=C(C(=O)C2=C([C]=C([C]=C12)O[C])O[C])C1=[C][C]=[C][C]=[C]1	-7.3

5318979	$O1C2=[C][C]=[C][C]=C2[C]([C]([C]1C1=[C][C]=[C][C]=[C]1)O)O$	-7.3
631105	$o1c2[C]=C([C]=C(c2c(=O)c(c1C1=C([C]=C([C]=[C]1)O[C])O[C])O[C])O[C]O[C]$	-7.3
150893	$o1c(c(c(=O)c2c(c(c(c12)O[C])O[C])O[C])O[C])O[C])C1=[C]C=C([C]=[C]1)O[C]O[C]$	-7.3
96118	$O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O[C])O[C])O[C])C1=[C][C]=C([C]=[C]1)O[C]$	-7.3
79730	$O1C(=[C]C(=O)C2=C1[C]=C([C]=C2O[C])O[C])C1=[C][C]=C([C]=[C]1)O[C]$	-7.3
12989197 2	$O1[C]=C(C(=O)C2=[C][C]=C(C(=C12)O[C])O)C1=[C][C]=C([C]=C1O)O[C]$	-7.2
12976274 2	$O1C2=C(C(=[C]C(=[C]2)O[C])O)C(=O)C([C]1C1=[C][C]=C([C]=[C]1)O[C])(O)O$	-7.2
12967461 9	$[C]1(C2=C([C]=[C][C]=[C]2)O[C]([C]1)C1=[C][C]=[C][C]=[C]1)S$	-7.2
12403736 3	$O1C2=C([C]=[C][C]=[C]2)[C]([C]([C]1C1=[C][C]=[C][C]=[C]1)O)O$	-7.2
91584129	$O1C2=[C]C(=C(C(=C2C(=O)[C]=C1C1=[C][C]=C(C(=C1O[C])O[C])O)O)O[C])O$	-7.2
44257041	$O1C(=[C][C]=C2[C](C(=C([C]=C12)O)O)O[C])C1=[C][C]=C([C]=[C]1)O$	-7.2
21573556	$O1C2=C(C(=[C]C(=[C]2)O[C])O[C])C(=O)[C][C]1C1=[C][C]=C(C(=C1O[C])O[C])O[C]$	-7.2
12405140	$O1C2=[C]C(=C(C(=C2C(=O)[C][C]1C1=[C][C]=C(C(=[C]1)O[C])O[C])O[C])O[C])O[C]$	-7.2
6399103	$O1C2=[C][C]=[C][C]=C2C(=O)[C]([N]O)[C]1C1=[C][C]=[C][C]=[C]1$	-7.2
5487785	$O1[C]=C(C(=O)C2=C(C(=C([C]=C12)O[C])O[C])O)C1=[C][C]=C([C]=[C]1)O$	-7.2
1546800	$O1C2=C([C]=[C][C]=[C]2)C(=O)[C]([C]1C1=[C][C]=[C][C]=[C]1)O$	-7.2
632958	$O1[C]=C(C(=O)C2=[C]C(=C([C]=C12)O[C])O[C])C1=[C]C(=C([C]=C1O[C])O[C])O[C]$	-7.2
632135	$O1C(=[C]C(=O)C2=C([C]=C(C(=C12)O[C])O[C])O[C])C1=[C]C(=C([C]=[C]1)O[C])O[C]$	-7.2
624831	$o1c(c(c(=O)c2=C([C]=C([C]=C12)O[C])O[C])O)C1=[C][C]=C([C]=[C]1)O[C]$	-7.2
462694	$O1C2=[C]C(=[C][C]=C2C(=O)[C]([C]1C1=[C][C]=C([C]=[C]1)O[C])O[C])O$	-7.2
261859	$O1C(=[C]C(=O)c2c(c(c(c12)O[C])O[C])O[C])O)C1=[C]C(=C(C(=[C]1)O[C])O[C])O[C]$	-7.2
155365	$O1C2=C(C3=C(C(=[C]2)O[C])C(=O)[C]=C(O3)C2=[C][C]=[C][C]=[C]2)[C]([C]1)[C](C([C])([C])OC(=O)[C])OC(=O)[C]$	-7.2
145659	$O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O[C])O[C])O[C])C1=[C][C]=C(C(=[C]1)O[C])O[C]$	-7.2
117900	$o1c(c(c(=O)c2C(=[C]C(=[C]c12)O[C])O[C])O[C])C1=[C][C]=[C][C]=[C]1$	-7.2
68077	$O1C(=[C]C(=O)c2c(c(c(c12)O[C])O[C])O[C])O[C])C1=[C][C]=C([C]=[C]1)O[C]$	-7.2

13250796 0	O1[C]=C(C(=O)C2=[C]C(=C([C]=C12)[C]O)O[C])C1=[C][C]=C([C]=[C]1)O	-7.1
12988909 7	O1C2=C(C(=[C][C]=[C]2)[C])[C@]([C])([C@]([C])([C@]1([C])C1=[C][C]=[C][C]=[C]1)O)O	-7.1
12988275 2	O1[C]=C(C(=O)C2=C([C]=C(C(=C12)O[C])O[C])O[C])C1=[C][C]=C([C]=[C]1)O	-7.1
12988261 5	O1[C]([C]2C(=O)[C]3[C]=[C][C][C]1[C]3C2=O)C1=[C][C]=[C][C]=[C]1	-7.1
12984868 0	o1c(c(c(=O)c2C=C([C]=C(c12)O[C])O[C])O[C])O[C])C1=[C][C]=C(C(=[C]1)O[C])O[C]	-7.1
23270524	O1C2=[C]C(=[C]C(=C2C(=O)[C])([C]1C1=C([C]=C([C]=[C]1)O[C])O[C])OC(=O)[C])O[C])O[C]	-7.1
15761527	C1(C(=O)C2=[C][C]=[C][C]=C2O[C]1C1=[C][C]=[C][C]=[C]1)([C]Cl)[C]Cl	-7.1
14034216	o1c(c(c(=O)c2=C([C]=C(C(=c12)O[C])O[C])O)O)C1=[C]C=C([C]=[C]1)O[C])O[C]	-7.1
10526049	o1c(c(c(=O)c2c(c(c(c12)O[C])O[C])O[C]O[C])O[C])O)C1=[C][C]=C([C]=[C]1)O[C]	-7.1
5320351	o1c(c(c(=O)c2=C(C(=C([C]=c12)O[C])O[C])O)O)C1=[C][C]=C(C(=[C]1)O[C])O[C]	-7.1
72344	O1C(=[C]C(=O)c2c(c(c(c12)O[C])O[C])O[C])O[C])C1=[C][C]=C(C(=[C]1)O[C])O[C]	-7.1
13903076 7	O1[C]=C(C(=O)C2=[C][C]=C(C(=C12)O[C])C(=O)[C][C]O)C1=[C][C]=C([C]=[C]1)O[C]	-7
12982441 8	O1C2=[C][C]=[C][C]=C2[C][C]([C@]1(C1=[C][C]=[C][C]=[C]1)[C]C(=O)O)O	-7
12981808 8	Br[C@]1(C(=O)C2=[C][C]=[C][C]=C2O[C]1C1=[C][C]=[C][C]=[C]1)N(=O)=O	-7
66780856	O1C2=C(C(=[C][C]=[C]2)O)C(=O)C([C@]1(C1=[C][C]=[C][C]=[C]1)O[C])(O)O	-7
44257040	O1C(=[C][C]=C2[C](C(=C([C]=C12)O)O)O[C])C1=[C][C]=C([C]=[C]1)O[C]	-7
24850296	O1C2=[C]C(=[C]C(=C2C(=O)[C@]([C@]1(C1=[C][C]=C(C(=[C]1)O)O)O[C])(O)[C]C(=O)O[C])O)O	-7
631156	O1[C]=C(C(=O)C2=C1C(=C([C]=[C]2)O[C])O[C])C1=C([C]=C([C]=[C]1)O[C])O[C]	-7
185670	O1C(=[C]C(=O)C2=C1[C]=C(C(=C2O[C])O[C])O[C])C1=[C]C=C(C(=[C]1)O[C])O[C])O[C]	-7
165203	O1[C]=C(C(=O)C2=C1[C]=C([C]=[C]2)O[C])C1=[C]C=C(C([C]=C1O[C])O[C])O[C]	-7
10195886 2	O1C2=[C][C]=[C][C]=C2C(=O)[C][C@]1(C1=[C][C]=[C][C]=[C]1)C(=O)O	-6.9

44257169	O1c2c3[C]=[C]Oc3c(c(c2[C])([C]([C]1C1=[C][C]=[C][C]=[C]1)O[C])O[C])O[C]	-6.9
389000	o1c(c(c(=O)c2c(c(c(c12)O[C])O[C])O[C])O[C])O[C])C1=[C]C(=C(C(=[C]1)O[C])O[C])O[C]	-6.9
13228149 8	O1C2=C(C(=C(C(=[C]2)O[C])O[C])O[C])C(=O)C([C@]1(C1=[C][C]=[C][C]=[C]1)O[C])(O[C])O[C]	-6.8
12987610 5	O1C2=[C][C]=[C][C]=C2C(=O)[C][C@]1(C1=[C]NN=[C]1)C1=[C][C]=[C][C]=[C]1	-6.8
11741814	o1c(c(c(=O)c2c(c(c(c12)O[C])O[C])O[C])O[C])O[C])C1=[C][C]=C([C]=[C]1)O[C]	-6.8
634440	o1c(c(c(=O)c2C(=C(C(=[C]c12)O[C])O[C][C])O[C][C])O[C])C1=[C]C(=C([C]=[C]1)O[C])O[C][C]	-6.8
12971327 4	Cl[C@@]1([C]C(=S)C2=[C][C]=[C][C]=C2O1)C1=[C][C]=[C][C]=[C]1	-6.7
12967896 8	[C]1(C2=[C][C]=[C][C]=C2O[C@]([C]1)(C1=[C][C]=[C][C]=[C]1)O[C])SOC(=O)[C]	-6.7
629965	O1C(=[C]C(=O)C2=C1[C]=[C]C(=C2O[C])O[C])C1=C([C]=[C][C]=C1O[C])O[C]	-6.7
12977612 2	O1C2=[C]C(=C(C(=C2C(=O)C([C]1C1=[C][C]=[C][C]=[C]1)(O[C])O[C])O)O)O[C]	-6.6
12967470 6	O1C2=C([C]=[C][C]=[C]2)[C][C]([C@]1(C1=[C][C]=[C][C]=[C]1)[C]=O)O	-6.6
90690372	O1C2=[C][C]=[C][C]=C2C(=O)C([C@@]1(C1=[C][C]=[C][C]=[C]1)O[C])(O[C])O[C]	-6.3
238791	C1(=C([C]=C([C]=C1C1=C(C(=[C]C(=[C]1)C(=O)[C])O[C])O[C])C(=O)[C])O[C])O[C]	-6.3
16092266	ClC1=[C]C(=N[C]=N1)N1[C][C]N[C][C]1	-6