

Table S1: Observed, predicted activities and fit values of the test set molecules, obtained using the pharmacophore model *Hypo1*

Comp.	Smiles	Activity $\log(IC_{50})$ nM		Activity scale		Fit value
		Observed	Predicted	Observed	Predicted	
HT1	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])C[C@@](O)([H])CCN3C</chem>	1.322	0.650	+++	+++	13.532
HT2	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])C[C@@]([H])(CCN3C)OC/C4=C/C=C=C4</chem>	1.792	0.580	+++	+++	13.602
HT3	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NCC/C2=C/C=CC=C2)[C@@]3([H])COCCN3C</chem>	1.851	0.672	+++	+++	13.510
HT4	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C/C=C2/[F])[C@@]3([H])COCCN3C</chem>	2.243	2.094	++	++	13.531
HT5	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=CC([F])=C2)[C@@]3([H])COCCN3C</chem>	1.792	1.815	+++	+++	13.515
HT6	<chem>O=C1NC=N/C(=C1/O)C(=O)NC/C2=C/C=C(/[F])C=C2</chem>	1.778	1.877	+++	+++	13.501
HT7	<chem>O=C1NC(=N/C(=C1/O)C(=O)NC/C2=C/C=C(/[F])C=C2)[C@](C)([H])N(C)C</chem>	2.000	0.696	++	+++	13.487
HT8	<chem>OC=1C(=O)NC(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@@]3([H])COCCN3C</chem>	1.000	0.695	+++	+++	13.488
HT9	<chem>OC=2C(=O)N1CC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)C</chem>	0.845	0.647	+++	+++	13.536
HT10	<chem>CN1CCC[C@]1([H])C=2NC(=O)C(O)=C(N=2)C(=O)NC/C3=C/C=C(/[F])C=C3</chem>	2.079	2.050	++	++	13.472
HT11	<chem>O=C1NC(=N/C(=C1/O)C(=O)NC/C2=C/C=C(/[F])C=C2)[C@@]3([H])CCCCN3C</chem>	2.342	2.257	++	++	13.421
HT12	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@@]3([H])CCCN3C</chem>	2.000	2.010	++	++	13.445
HT13	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])CCCCN3C</chem>	2.643	2.654	++	++	13.477
HT14	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])N(C)CC[C@]3(C)[H]</chem>	2.851	2.818	++	++	13.457
HT15	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])C[C@@](C)([H])CN3C</chem>	1.000	0.711	+++	+++	13.472
HT16	<chem>OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)[S](C)(=O)=O</chem>	1.204	0.721	+++	+++	13.462
HT17	<chem>OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)[S](=O)(=O)C4=C(C)N(C)N=C4C</chem>	0.845	0.632	+++	+++	13.551
HT18	<chem>OC=2C(=O)N1CC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)[S](=O)(=O)N(C)C</chem>	1.653	0.631	+++	+++	13.551
HT19	<chem>OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)C(=O)C(=O)N(C)C</chem>	1.544	0.922	+++	+++	13.261
HT20	<chem>OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)[S](=O)(=O)N(C)C</chem>	0.845	0.636	+++	+++	13.546
HT21	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=CC(=C2)OC)[C@]3([H])COCCN3C</chem>	2.146	2.080	++	++	13.478
HT22	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])COCCN3C</chem>	1.322	0.725	+++	+++	13.457
HT23	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])COCCN3C</chem>	1.934	1.902	+++	+++	13.477
HT24	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])C[C@@]([H])(CN3C)OCC</chem>	2.301	2.304	++	++	13.515
HT25	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])C[C@@]([H])(CN3C)OCC=4C=CC=CC=4</chem>	2.114	2.098	++	++	13.582
HT26	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])C[C@@]([H])(CN3C)NC(C)=O</chem>	1.785	1.701	+++	+++	13.529
HT27	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])CC[C@@](C)([H])N3C</chem>	2.839	2.699	++	++	13.543
HT28	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])C[C@@](O)([H])CN3C</chem>	2.000	1.979	++	+++	13.475
HT29	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])C[C@@]([H])(CN3C)OC</chem>	2.255	2.304	++	++	13.535
HT30	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=CC([Cl])=C2)[C@]3([H])COCCN3C</chem>	1.792	1.683	+++	+++	13.521
HT31	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=CC([Br])=C2)[C@]3([H])COCCN3C</chem>	1.279	0.639	+++	+++	13.544
HT32	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@@]3([H])COCCN3C(=O)OC(C)C</chem>	1.301	0.641	+++	+++	13.541
HT33	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=CC=C2)[C@]3([H])COCCN3C</chem>	1.820	1.815	+++	+++	13.436
HT34	<chem>O=C1NC(=N/C(=C1/O)C(=O)NC/C2=C/C=C(/[F])C=C2</chem>	1.699	1.710	+++	+++	13.469

	2)C(C)(C)N(C)C					
HT35	OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])CN(CCN3C)C(=O)C	1.505	0.648	+++	+++	13.535
HT36	OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])CN(C)CCN3C(C)=O	3.602	3.582	+	+	13.531
HT37	OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])CN(CCN3C)C(=O)C=4C=CC=CC=4	1.079	0.674	+++	+++	13.509
HT38	OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])CN(CCN3C)C(=O)CN(C)C	0.602	0.636	+++	+++	13.546
HT39	OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)C	1.839	0.626	+++	+++	13.557
HT40	OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)C	2.740	2.655	++	++	13.524
HT41	OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N4CCCC4	1.799	1.834	+++	+++	13.518
HT42	OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)[S](=O)(=O)N(C)C	0.699	0.636	+++	+++	13.546
HT43	OC=2C(=O)N1CC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)C(=O)C(=O)N(C)C	1.301	0.627	+++	+++	13.556
HT44	OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N4CCOCC4	1.792	1.742	+++	+++	13.441
HT45	OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])CN(CCN3C)[S](=O)(=O)C=4C=CC=CC=4	0.845	0.674	+++	+++	13.508
HT46	OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])CN(CCN3C)[S](=O)(=O)N(C)C	0.903	0.640	+++	+++	13.542
HT47	OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])COCCN3	1.699	1.352	+++	+++	12.831
HT48	OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])COCCN3CC	1.519	1.481	+++	+++	13.514
HT49	OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])COCCN3C(=O)C	1.176	0.691	+++	+++	13.491
HT50	OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)C(=O)C(=O)N(C)C	1.079	0.661	+++	+++	13.522
HT51	OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)C(=O)C(=O)N(C)C	1.114	0.922	+++	+++	13.261
HT52	OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])CC([F])([F])CN3C	1.477	0.743	+++	+++	13.439
HT53	O=C1NC(=N/C(=C1/O)C(=O)NC/C2=C/C=C(/[F])C=C2)CN(C)C	2.301	2.211	++	++	13.513
HT54	OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)C/C4=C/C=CC=C4	0.602	0.650	+++	+++	13.532
HT55	OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)CC=4C=CC=CC=4	1.792	1.742	+++	+++	13.479
HT56	OC=2C(=O)N1CCCC1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3	0.903	0.627	+++	+++	13.556
HT57	OC=2C(=O)N1CCCCC1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3	0.699	0.637	+++	+++	13.546
HT58	OC=2C(=O)N1CC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)C(C)=O	0.954	0.634	+++	+++	13.548
HT59	OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)C(C)=O	0.778	0.815	+++	+++	13.367
HT60	OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)C(C)=O	0.903	1.936	+++	+++	12.246
HT61	OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)C(=O)C([F])([F])[H]	1.255	0.921	+++	+++	13.262
HT62	OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)C(=O)C5=NN4C=CC=NC4=N5	1.000	0.683	+++	+++	13.499
HT63	OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)C(=O)C[S](=O)(=O)N(C)C	0.954	0.655	+++	+++	13.528
HT64	OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)C(=O)C[S](=O)(=O)C	0.778	0.564	+++	+++	13.619
HT65	OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)C(=O)C(=O)N(C)C	0.845	0.661	+++	+++	13.522
HT66	OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)C(=O)C(=O)N(C)C	1.079	0.922	+++	+++	13.261
HT67	O=C1NC(=N/C(=C1/O)C(=O)NC/C2=C/C=CC=C2)C3=CC=C[S]3	1.929	1.834	+++	+++	13.527
HT68	O=C1NC(=N/C(=C1/O)C(=O)NC/C2=C/C=C(/[F])C=C2)C3=CC=C[S]3	1.000	0.651	+++	+++	13.531
HT69	O=C1NC(C)=N/C(=C1/O)C(=O)NC/C2=C/C=C(/[F])C=C2	1.778	1.547	+++	+++	13.547
HT70	O=C1NC(=N/C(=C1/O)C(=O)NC/C2=C/C=CC=C2)C3=CC=CC=3	1.845	1.775	+++	+++	13.467

HT71	O=C1NC(=N/C(=C1/O)C(=O)NC/C2=C/C=C(/[F])C=C2/C/C3=C/C=CC=C3	1.699	1.656	+++	+++	13.477
HT72	O=C1NC(=N/C(=C1/O)C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]([H])(C3=CC=CC=C3)N(C)C	2.301	2.323	++	++	13.516
HT73	OC=2C(=O)N1CCC[C@@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)[S](=O)(=O)N4CCN(C)CC4	0.845	0.652	+++	+++	13.531
HT74	OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])C[C@@]([F])([H])CN3C	1.301	0.723	+++	+++	13.459
HT75	OC=2C(=O)N1CCCCC1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3	1.279	0.629	+++	+++	13.553
HT76	OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)C(=O)C[S](C)(=O)=O	1.230	0.548	+++	+++	13.634
HT77	OC=2C(=O)N1CCC[C@]([H])(NC(=O)C[S](=O)(=O)C)C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3	0.845	0.621	+++	+++	13.562
HT78	OC=2C(=O)N1CCC[C@@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)[S](C)(=O)=O	1.079	0.699	+++	+++	13.484
HT79	OC=2C(=O)N1CCC[C@@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N4CCCN(C)[S]4(=O)=O	1.146	0.683	+++	+++	13.500
HT80	OC=2C(=O)N1CCCC[C@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N4CCCN(C)[S]4(=O)=O	0.778	0.794	+++	+++	13.388
HT81	OC=2C(=O)N1CCC[C@@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)[S](=O)(=O)N4CCCC4	0.845	0.756	+++	+++	13.426
HT82	OC=2C(=O)N1CCC[C@@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)[S](=O)(=O)N4CCCC4	0.954	0.691	+++	+++	13.491
HT83	OC=2C(=O)N1CCC[C@@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)[S](=O)(=O)N4CCOCC4	1.041	0.743	+++	+++	13.440
HT84	OC=2C(=O)N1CCC[C@@]([H])(C1=NC=2C(=O)NC/C3=C/C=C(/[F])C=C3)N(C)[S](=O)(=O)N4CCN(C)CC4	0.845	0.652	+++	+++	13.531
HT85	OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])C[S]CCN3C	1.845	1.813	+++	+++	13.478
HT86	OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])C[S](=O)CCN3C	1.568	1.625	+++	+++	13.466
HT87	OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])C[S](=O)(=O)CCN3C	2.146	2.098	++	++	13.555
HT88	OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])CN(C)CCN3C	2.000	1.951	++	+++	13.446
HT89	OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])CN(C)C(=O)CN3C	1.699	1.583	+++	+++	13.522
HT90	OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])CNCCN3C	2.301	2.323	++	++	13.452
HT91	OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])CN(CCN3C)CC	2.398	2.098	++	++	13.505
HT92	OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])CN(CCN3C)C(C)(C)[H]	2.114	2.256	++	++	13.538
HT93	OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C=C(/[F])C=C2)[C@]3([H])CN(CCN3C)C(=O)OC(C)(C)C	1.613	1.710	+++	+++	13.480
HT94	O=C1C(O)=C(N=C(N1C)C(C)(C)NC(=O)C(=O)N(C)C(=O)NC/C2=C/C=C(/[F])C=C2	1.000	1.464	+++	+++	12.718
HT95	O=C1C(O)=C(N=C(N1C)C(C)(C)NC(=O)C(=O)OC)C(=O)NC/C2=C/C=C(/[F])C=C2	1.176	1.498	+++	+++	12.685
HT96	O=C1C(O)=C(N=C(N1C)C(C)(C)NC(C)=O)C(=O)NC/C2=C/C=C(/[F])C=C2	0.845	2.112	+++	++	12.071
HT97	O=C1C(O)=C(N=C(N1C)C(C)(C)NC(=O)C(=O)N(C)C(=O)NC/C2=C/C=CC(OC)=C2OC	1.322	2.522	+++	++	11.661
HT98	O=C1C(O)=C(N=C(N1C)C(C)(C)NC(=O)C(=O)N(C)C(=O)NC/C2=C/C=C(/[F])C=C2[S](C)(=O)=O	0.602	1.065	+++	+++	13.118
HT99	O=C1C(O)=C(N=C(N1C)C(C)(C)NC(=O)C(=O)N(C)C(=O)NC/C2=C/C=C(/[F])C(C[Cl])=C2	0.954	0.878	+++	+++	13.304
HT100	O=C1C(O)=C(N=C(N1C)C(C)(C)NC(=O)C2=CC=CC=N2)C(=O)NC/C3=C/C=C(/[F])C=C3	1.301	1.393	+++	+++	12.790
HT101	O=C1C(O)=C(N=C(N1C)C(C)(C)NC(=O)C2=CC=CN=N2)C(=O)NC/C3=C/C=C(/[F])C=C3	1.176	1.164	+++	+++	13.018
HT102	O=C1C(O)=C(N=C(N1C)C(C)(C)NC(=O)C2=CN=CC=C(N=2)C(=O)NC/C3=C/C=C(/[F])C=C3	0.845	1.089	+++	+++	13.094
HT103	O=C1C(O)=C(N=C(N1C)C(C)(C)NC(=O)C2=CN=CO2)C(=O)NC/C3=C/C=C(/[F])C=C3	0.845	1.065	+++	+++	13.118
HT104	O=C1C(O)=C(N=C(N1C)C(C)(C)NC(=O)C2=C[S]C=N2)C(=O)NC/C3=C/C=C(/[F])C=C3	0.903	1.204	+++	+++	12.978
HT105	O=C1C(O)=C(N=C(N1C)C(C)(C)NC(=O)C2=CN=CN2)C(=O)NC/C3=C/C=C(/[F])C=C3	0.778	1.392	+++	+++	12.790
HT106	[F]/C1=C/C=C(C=C1)CN2CC4=C(C2=O)C(O)=C3N=C=C/C3=C4/OC	1.778	3.171	+++	+	11.012
HT107	[F]/C1=C/C=C(C=C1)C/C2=C/C=C(O2)C(=O)CC(=O)	1.663	1.547	+++	+++	13.581



HT108	[F]/C1=C/C=C(C=C1)CN2C=C/C=C2/C(=O)CC(=O)C(=O)O	1.568	0.851	+++	+++	13.332
HT109	O=C(CC(=O)C(=O)O)C2=CC(CC=1C=CC=CC=1)=CC=C2	1.415	0.544	+++	+++	13.639
HT110	[F]/C1=C([C1])C=C/C=C1/C/C2=C/C=C3C(=C2)C(=O)C(=CN3[C@]([H])(CC)CO)C(=O)O	1.623	1.240	+++	+++	12.943
HT111	[F]/C1=C/C=C(C=C1)CNC(=O)C3=NC(=C2C=CC=N/C2=C3)O)N4CCCC[S]4(=O)=O	1.643	0.927	+++	+++	13.256
HT112	[F]/C1=C/C=C(C=C1)CN4CC3=C(C=C2N=CC=C/C2=C3)OC)C4=O	4.380	4.413	+	+	11.067
HT113	O=C1C(O)=C(N=C(N1C)C(C)(C)NC(=O)N(C)C)C(=O)NC/C2=C/C=C([F])C=C2	1.255	1.854	+++	+++	12.329
HT114	O=C1C(O)=C(N=C(N1C)C(C)(C)N[S](=O)(=O)N(C)C)C(=O)NC/C2=C/C=C([F])C=C2	1.079	0.861	+++	+++	13.322
HT115	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C([F])C=C4)C=5C=CC=CC=5[S](=O)(=O)NC	0.602	0.775	+++	+++	13.408
HT116	OC=2C1=NC=CC=C1C(=NC=2/C4=N/N=C(C/C3=C/C=C([F])C=C3)N4)N5CCCC[S]5(=O)=O	1.041	0.792	+++	+++	13.390
HT117	OC=2C1=NC=CC=C1C(=NC=2/C4=N/N=C(C/C3=C/C=C([F])C=C3)O4)N5CCCC[S]5(=O)=O	0.301	0.772	+++	+++	13.410
HT118	O=C1C(O)=C(N=C(N1C)C(C)(C)NC(=O)C(=O)N2CCN(C)CC2)C(=O)NC/C3=C/C=C([F])C=C3	1.415	1.128	+++	+++	13.054
HT119	O=C1C(O)=C(N=C(N1C)C(C)(C)NC(=O)C2=N/N=C(C)O)C(=O)NC/C3=C/C=C([F])C=C3	1.176	1.295	+++	+++	12.887
HT120	O=C1C(O)=C(N=C(N1C)C(C)(C)NC(=O)C2=N/N=C(C)N2)C(=O)NC/C3=C/C=C([F])C=C3	0.602	1.164	+++	+++	13.018
HT121	O=C1C(O)=C(N=C(N1C)C(C)(C)NC(=O)C(=O)O)C(=O)NC/C2=C/C=C([F])C=C2	0.602	0.922	+++	+++	13.261
HT122	O=C1C(O)=C(N=C(N1C)C(C)(C)N(C)C(=O)C(=O)N(C)C)C(=O)NC/C2=C/C=C([F])C=C2	1.176	2.262	+++	++	11.921
HT123	O=C1C(O)=C(N=C(N1C)C(C)(C)NC(=O)C(=O)N2CCOCC2)C(=O)NC/C3=C/C=C([F])C=C3	1.301	1.767	+++	+++	12.415
HT124	O=C1C(O)=C(N=C(N1C)C(C)(C)N[S](C)(=O)=O)C(=O)NC/C2=C/C=C([F])C=C2	0.903	0.909	+++	+++	13.273
HT125	O=C1C(O)=C(N=C(N1C)C(C)(C)N(C)C)C(=O)NC/C2=C/C=C([F])C=C2	2.362	2.427	++	++	11.755
HT126	O=C1C(O)=C(N=C(N1C)C(C)(C)N2CCOCC2)C(=O)NC/C3=C/C=C([F])C=C3	0.477	0.764	+++	+++	13.419
HT127	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C([F])C=C4)N5CCCC5=O	1.279	1.237	+++	+++	13.403
HT128	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C([F])C=C4)C=5C=COC=5	1.362	0.764	+++	+++	13.418
HT129	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C([F])C=C4)C5=CC=CN5	1.079	0.763	+++	+++	13.419
HT130	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C([F])C=C4)C(=O)NC(C)(C)[H]	2.279	2.251	++	++	13.417
HT131	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C([F])C=C4)C5=CC=C(C=C5)C#N	1.176	0.767	+++	+++	13.416
HT132	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C([F])C=C4)C=5C=CC=CC=5[S](=O)(=O)N(C)C	0.602	0.775	+++	+++	13.407
HT133	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C([F])C=C4)C5=CC=C(C=C5)[S](=O)(=O)N(C)C	1.255	0.774	+++	+++	13.408
HT134	COC=2C=1CN(C)C(=O)C=1C(O)=C3N=CC(=CC=23)C/C4=C/C=C([F])C=C4	2.000	2.760	++	++	11.422
HT135	COC=2C=1CNC(=O)C=1C(O)=C3N=CC(=CC=23)C/C4=C/C=C([F])C=C4	1.146	2.791	+++	++	11.391
HT136	COC=3C=2CN(C/C1=C/C=C([F])C=C1)C(=O)C=2C(O)=C4N=CC(=CC=34)C/C5=C/C=C([F])C=C5	2.778	2.757	++	++	11.426
HT137	CN(C=2C=1CN(C)C(=O)C=1C(O)=C3N=CC(=CC=23)C/C4=C/C=C([F])C=C4)[S](C)(=O)=O	1.903	2.325	+++	++	11.858
HT138	CN(C=2C=1CN(C)C(=O)C=1C(O)=C3N=CC(=CC=23)C/C4=C/C([C1])=C([F])C=C4)[S](C)(=O)=O	2.423	2.267	++	++	11.916
HT139	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C([F])C=C4)C5=CC=C(C=C5)N[S](C)(=O)=O	0.477	0.781	+++	+++	13.401
HT140	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C([F])C=C4)C=5C=CC=CC=5[S](C)(=O)=O	1.041	0.773	+++	+++	13.409
HT141	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C([F])C=C4)C5=CC(=CC=C5)[S](C)(=O)=O	0.778	0.774	+++	+++	13.408
HT142	OC=2C1=NC=CC=C1C=NC=2/C3=N/OC(=N3)C/C4=C/C=C([F])C=C4	2.114	2.162	++	++	13.292
HT143	OC=2C1=NC=CC=C1C=NC=2/C4=N/N=C(C/C3=C/C=CC=C3)N4	2.556	2.505	++	++	13.372
HT144	OC=2C1=NC=CC=C1C=NC=2/C4=N/N=C(C/C3=C/C=C([F])C=C3)N4	2.114	2.218	++	++	13.370

HT145	OC=2C1=NC=CC=C1C=NC=2/C4=N/N=C(/C/C3=C/C=C(/[Cl])C=C3)N4	2.806	2.820	++	++	13.375
HT146	OC=2C1=NC=CC=C1C=NC=2/C4=N/N=C(/C/C3=C/C([Cl])=CC=C3)N4	3.013	3.009	+	+	13.373
HT147	OC=2C1=NC=CC=C1C=NC=2/C4=N/N=C(/C/C3=C/C(=CC=C3)OC)N4	3.447	3.438	+	+	13.371
HT148	OC=2C1=NC=CC=C1C=NC=2/C4=N/N=C(/C/C3=C/C(OC)=C(C=C3)OC)N4	3.799	3.815	+	+	13.372
HT149	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C5=CC=C(C=C5)C(=O)O	0.301	0.771	+++	+++	13.411
HT150	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C5=CC=C(C=C5)C(=O)NC(C)(C)[H]	0.602	0.778	+++	+++	13.404
HT151	OC=2C1=NC=CC=C1C=NC=2/C4=N/N=C(/C/C3=C/C(=CC=C3)O4	2.114	2.098	++	++	13.376
HT152	OC=2C1=NC=CC=C1C=NC=2/C4=N/N=C(/C/C3=C/C=C(/[F])C=C3)O4	1.623	1.701	+++	+++	13.375
HT153	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C(=O)N5CCOCC5	2.114	0.999	++	+++	13.184
HT154	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C5=CC=C(C=C5)C(=O)NC	0.602	0.774	+++	+++	13.409
HT155	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C5=CC=C(C=C5)C(=O)N(C)C	1.255	1.016	+++	+++	13.167
HT156	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C(=O)NC	2.079	2.042	++	++	13.414
HT157	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C5=NC=CC=C5	1.477	1.419	+++	+++	13.407
HT158	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C5=CC(=CC=C5)C(O)=O	0.301	0.771	+++	+++	13.412
HT159	OC=2C1=NC=CC=C1C=NC=2/C3=N/OC(=N3)C/C4=C/C=C=C4	2.978	2.914	++	++	13.298
HT160	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C(=O)NCCO	2.114	0.543	++	+++	13.639
HT161	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C(=O)NCCCCO	1.851	0.562	+++	+++	13.621
HT162	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N5CCN(C)C5=O	1.176	0.769	+++	+++	13.414
HT163	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N5CCCCC5=O	1.944	1.836	+++	+++	13.309
HT164	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N5CCCCC5=O	1.398	1.347	+++	+++	13.406
HT165	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N5CCOC5=O	1.114	0.773	+++	+++	13.409
HT166	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N5CCNC5=O	1.041	0.772	+++	+++	13.410
HT167	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N[S](=O)(=O)C	1.279	1.237	+++	+++	13.410
HT168	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C5=CN=CC=C5	1.041	1.051	+++	+++	13.411
HT169	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C5=CC=NC=C5	0.903	0.779	+++	+++	13.403
HT170	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N5CCNC5=O	1.079	0.776	+++	+++	13.407
HT171	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C5=CC=C(C=C5)[S](C)(=O)=O	0.954	0.771	+++	+++	13.411
HT172	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C(=O)N5CCN(C)CC5	1.643	1.626	+++	+++	13.407
HT173	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C(=O)N5CC[C@@](O)([H])CC5	1.431	0.765	+++	+++	13.417
HT174	OC=2C1=NC=CC=C1C=NC=2/C4=N/N=C(/C/C3=C/N(=CC=C3)N4	3.544	3.406	+	+	13.371
HT175	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C5=CC=C(C=C5)NC(C)=O	0.602	0.776	+++	+++	13.407
HT176	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N5CCN(CCO)C5=O	1.114	0.564	+++	+++	13.618
HT177	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)NC(C)=O	1.857	1.910	+++	+++	13.301
HT178	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N(C)C(C)=O	1.447	1.347	+++	+++	13.400
HT179	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C(=O)N5CC(=O)NCC5	1.869	1.865	+++	+++	13.419
HT180	OC=2C1=NC=CC=C1C=NC=2/C4=N/N=C(C)C(C/C3=C/C=C(/[F])C=C3)=N4	3.898	3.854	+	+	13.363
HT181	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C5=CC(=CC=C5)C(=O)NC(C)(C)[H]	1.000	0.786	+++	+++	13.396

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HT182	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N5C=CC=N5	0.602	0.754	+++	+++	13.428
HT183	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N5C=CC(C)=N5	1.322	1.419	+++	+++	13.430
HT184	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C#N	2.380	2.412	++	++	13.418
HT185	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C(=O)N	2.000	1.979	++	+++	13.414
HT186	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C(=O)O	2.934	2.916	++	++	13.418
HT187	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)NC(=O)C(=O)OCC	1.519	0.768	+++	+++	13.414
HT188	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N(C)C(=O)C(=O)N(C)C	1.929	1.904	+++	+++	13.403
HT189	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N5CCNCC5=O	1.580	0.837	+++	+++	13.346
HT190	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C5=CC(N)=CC=C5	1.176	0.772	+++	+++	13.411
HT191	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C5=CC(=CC=C5)NC(=O)C	1.903	1.893	+++	+++	13.408
HT192	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C5=CC(=CC=C5)N[S](C)(=O)=O	0.903	0.778	+++	+++	13.405
HT193	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C5=CC=C(C=C5)[S](=O)(=O)NC(C)(C)[H]	0.602	0.777	+++	+++	13.405
HT194	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N5CCN(C)[S]5(=O)=O	0.602	0.957	+++	+++	13.225
HT195	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N[S](=O)(=O)C5=C/C=C(/C)C=C5	1.623	1.559	+++	+++	13.412
HT196	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N5CCNC(=O)C5	0.845	0.774	+++	+++	13.409
HT197	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)NC	1.869	0.968	+++	+++	13.215
HT198	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N5CCN(CC5)[S](C)(=O)=O	1.279	0.775	+++	+++	13.407
HT199	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N5CCN(CC5)CC(=O)N(C)C	1.079	0.781	+++	+++	13.401
HT200	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C5=CC=CC=C5	1.462	1.435	+++	+++	13.407
HT201	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N[S](=O)(=O)N(C)C	1.176	0.776	+++	+++	13.406
HT202	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N5CCCN(C)[S]5(=O)=O	0.778	0.823	+++	+++	13.359
HT203	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)N4	3.663	3.653	+	+	13.375
HT204	OC=2C1=NC=CC=C1C(=NC=2/C3=N/N=C(O3)C/C4=C/C=C(/[F])C=C4)C(=O)NCCOC	2.279	2.114	++	++	13.618
HT205	O=C2N1C[S]C[C@@]1([H])C(=O)[S]C=3C=CC([Cl])=CC2=3	5.199	5.329	+	+	8.853
HT206	O=C3N1C[S]C[C@@]1([H])C(=O)[S]C=4C=C2C=CC=CC2=CC3=4	5.000	5.457	+	+	8.726
HT207	O=C2N1CC[S][C@@]1([H])C(=O)[S]C=3C=CC([Cl])=CC2=3	5.179	5.486	+	+	8.697
HT208	O=C2N1C[S]C[C@@]1([H])C(=O)[S]C=3C=CC([Br])=CC2=3	4.940	5.328	+	+	8.854
HT209	O=C2N1[C@@]([H])([S]C[C@@]1([H])C[S]C=3C=C=C=CC2=3)C4=CC=CC=C4	5.571	5.124	+	+	9.058
HT210	O=C2N1C[S](=O)C[C@@]1([H])C(=O)[S]C=3C=CC=CC2=3	5.301	5.254	+	+	8.929
HT211	O=C2N1C[S]C[C@@]1([H])C(=O)[S]C=3C=CC(C)=CC2=3	4.716	5.277	+	+	8.905
HT212	O=C2N1CC[S][C@]1([H])C(=O)[S]C=3C=CC([Br])=CC2=3	4.681	5.481	+	+	8.701
HT213	O=C2N1CC[S][C@@]1([H])C(=O)[S]C=3C=CC(C)=CC2=3	4.740	5.474	+	+	8.708
HT214	O=C(OC)[C@]([H])(NC(=O)C=CC=1/C=C(/OC(=O)C)C(OC(=O)C)=CC=1)COC(=O)C=CC=2/C=C(/OC(=O)C)C(OC(=O)C)=CC=2	3.398	3.268	+	+	13.514
HT215	O=C(OC)[C@]([H])(NC(=O)C=CC=1/C=C(/OC(=O)C)C(OC(=O)C)=CC=1)CNC(=O)C=CC=2/C=C(/OC(=O)C)C(OC(=O)C)=CC=2	4.037	3.980	+	+	13.537
HT216	O=C(O)[C@]([H])(OC(=O)C=CC=1/C=C(/OC(=O)C)C(OC(=O)C)=CC=1)COC(=O)C=CC=2/C=C(/OC(=O)C)C(OC(=O)C)=CC=2	3.322	3.245	+	+	13.594

HT217	O/C1=C/C=C(/C=C1/O)C=CC(=O)O[C@@]([H])(C(O)=O)[C@@]([H])(OC(=O)C=C/C2=C/C(/O)C(O)=C2)C(O)=O	2.903	2.680	++	++	13.623
HT218	O=C2N1CCCC[C@@]1([H])C(=O)[S]C=3C=CC=CC2=3	5.609	5.411	+	+	8.772
HT219	O=C(O)[C@@]([H])(OC(=O)C=CC=1/C=C(/OC(=O)C)C(OC(=O)C)=CC=1)[C@@]([H])(OC(=O)C=CC=2/C=C(/OC(=O)C)C(OC(=O)C)=CC=2)C(=O)O	3.663	3.601	+	+	13.628
HT220	O=C(OC)[C@@]([H])(OC(=O)C=CC=1/C=C(/OC(=O)C)C(OC(=O)C)=CC=1)COC(=O)C=CC=2/C=C(/OC(=O)C)C(OC(=O)C)=CC=2	4.004	4.995	+	+	13.622
HT221	O=C(O)[C@@]1([H])CCCC[C@@]1([H])OC(=O)C=CC=2/C=C(/O)C(O)=CC=2)C=CC=3/C=C(/O)C(O)=CC=3	3.881	3.717	+	+	12.881
HT222	O=C(OC)[C@@]([H])(NC(=O)C=CC=1/C=C(/OC(=O)C)C(OC(=O)C)=CC=1)COC(=O)C=CC=2/C=C(/OC(=O)C)C(OC(=O)C)=CC=2	3.447	3.405	+	+	13.514
HT223	O=C(O)[C@@]([H])(OC(=O)C=CC=1/C=C(/OC(=O)C)C(OC(=O)C)=CC=1)[C@@]([H])(OC(=O)C=CC=2/C=C(/OC(=O)C)C(OC(=O)C)=CC=2)C(=O)O	3.792	3.793	+	+	13.628
HT224	O=C(O)[C@@]([H])(NC(=O)C)COC(=O)C=CC=1/C=C(/O)C(O)=CC=1	5.045	6.098	+	+	13.633
HT225	O=C(/C=C/C=1/C=C(/O)C(O)=CC=1)OCCOC(=O)C=CC=2/C=C(/O)C(O)=CC=2	3.875	3.838	+	+	12.921
HT226	O=C(OC)[C@@]([H])(NC(=O)C=CC=1/C=C(/OC(=O)C)C(OC(=O)C)=CC=1)COC(=O)C=CC=2/C=C(/OC(=O)C)C(OC(=O)C)=CC=2	3.447	3.398	+	+	13.514
HT227	O=C(/C=C/C=1/C=C(/OC(=O)C)C(OC(=O)C)=CC=1)NCCOC(=O)C=C/C2=C/C(OC(=O)C)=C(OC(=O)C)C=C2	5.000	5.940	+	+	13.607
HT228	O/C1=C/C=C(/C=C1/O)C=CC(=O)O[C@@]([H])(C(O)=O)[C@@]([H])(OC(=O)C=C/C2=C/C(/O)C(O)=C2)C(=O)O	2.699	2.732	++	++	13.623
HT229	O=C(O)[C@@]([H])(NC(=O)C=CC=1/C=C(/O)C(O)=CC=1)COC(=O)C=CC=2/C=C(/O)C(O)=CC=2	3.230	3.132	+	+	13.620
HT230	O=C(O)[C@@]([H])(OC(=O)C=CC=1/C=C(/O)C(O)=CC=1)COC(=O)C=CC=2/C=C(/O)C(O)=CC=2	3.623	0.541	+	+++	13.642
HT231	O=C2N1C[S]C[C@@]1([H])C(=O)[S]C=3C=CC=CC2=3)OC	5.190	5.125	+	+	9.057
HT232	O=C2N1C[S](=O)C[C@@]1([H])C(=O)[S]C=3C=CC([C])=CC2=3	5.447	5.247	+	+	8.935
HT233	O=C(O)[C@@]([H])(NC(=O)C=CC=1/C=C(/OC(=O)C)C(OC(=O)C)=CC=1)CNC(=O)C=CC=2/C=C(/OC(=O)C)C(OC(=O)C)=CC=2	3.613	0.538	+	+++	13.645
HT234	O=C(/C=C/C=1/C=C(/O)C(O)=CC=1)OCCOC(=O)C=CC=2/C=C(/O)C(O)=CC=2	2.602	2.301	++	++	12.921
HT235	O=C2N1C[S]C[C@@]1([H])C(=O)[S]C=3/C=C(/OC)C(=CC2=3)OC	5.522	5.143	+	+	9.040
HT236	O=C2N1C[S]C[C@@]1([H])C(=O)[S]C=3C=CC=CC2=3	5.318	5.471	+	+	8.712
HT237	O=C2N1C[S](=O)C[C@@]1([H])C(=O)[S]C=3C=CC(=C2=3)OC	5.152	5.150	+	+	9.033
HT238	O=C2[S]C=1C=CC=CC=1CN3C=CC=C23[O-	5.771	7.534	+	+	6.648
HT239][N+](=O)C3=CC=2[S]C(=O)[C@@]1([H])C[S]CN1C(=O)C=2C=C3	5.000	5.123	+	+	9.060
HT240	O=C3N1CC[S][C@@]1([H])C(=O)[S]C=4C=C2C=CC=CC2=CC3=4	4.602	5.489	+	+	8.693
HT241	O=C2N1CC[S](=O)[C@@]1([H])C(=O)[S]C=3C=CC(C)=CC2=3	5.771	5.102	+	+	9.080
HT242	O=C2N1CC[S][C@@]1([H])C(=O)[S]C=3C=CC=CC2=3	5.164	5.577	+	+	8.606
HT243	O/C3=C/C=C(/C=C/C2=N/C1=C(\O)C(=CC=C1C=C2)C(O)=O)C=C3	3.204	5.077	+	+	9.105
HT244][N+](=O)C=3C=CC(/C=C/C2=N/C1=C(\O)C(=CC=C1C=C2)C(=O)O)=CC=3	3.079	5.077	+	+	9.105
HT245	O/C3=C/C=C(/C=C/C2=N/C1=C(\O)C(=CC=C1C=C2)C(O)=O)C(O)=C3	3.447	3.932	+	+	10.251
HT246	OC=1C(=CC=C2C=CC(=NC=12)C=C/C3=C/C=CO3)C(O)=O	3.279	5.076	+	+	9.106
HT247	OC=1C(=CC=C2C=CC(=NC=12)C=C/C3=C/C=CN=C3)C(O)=O	3.613	5.077	+	+	9.105
HT248	O=C(O)C2=CC=C1C=CC(=N/C1=C2\O)C=C/C3=C/[S]C=C3	3.477	5.076	+	+	9.106
HT249	O/C3=C/C/C=C/C2=N/C1=C(\O)C(=CC=C1C=C2)C(O)=O)C=C/C3/OC	2.954	5.053	+	+	9.130

HT250	O/C3=C(/C=C(/C=C/C2=N/C1=C(\O)C(=CC=C1C=C2)C(O)=O)C=C3OC)OC	3.690	3.597	+	+	11.448
HT251	O=C(O)C2=CC=C1C=CC(=N/C1=C2\O)C=CC=3/C=C(/O)C(O)=C(O)C=3	2.602	1.898	+	++	12.285
HT252	O/C3=C(/C=C(/C=C/C2=N/C1=C(\O)C(=CC=C1C=C2)C(O)=O)C=C3O)OC	3.230	2.164	+	++	12.019
HT253	O=C(O)C2=CC=C1C=CC(=N/C1=C2\O)CCC=3/C=C(/O)C(O)=CC=3	3.176	3.185	+	+	13.361
HT254	O=C(O)C2=CC=C1C=CC(=N/C1=C2\O)C=C/C3=C/C=C(/NC(=O)C)C=C3	3.146	5.077	+	+	9.105
HT255	OC=1C(=CC=C2C=CC(=NC=12)C=C/C3=C/C([Br])=C(O)C([Br])=C3)C(O)=O	3.114	5.077	+	+	9.105
HT256	O/C3=C(\[I])C=C(/C=C/C2=N/C1=C(\O)C(=CC=C1C=C2)C(O)=O)C=C3O	3.602	3.462	+	+	11.283
HT257	O=C(O)C2=CC=C1C=CC(=N/C1=C2\O)C=CC=3/C=C(/OC)C(O)=CC=3	3.568	3.538	+	+	10.644
HT258	O/C3=C/C=C(/C=C/C2=N/C1=C(\O)C(=CC=C1C=C2)C(O)=O)C=C3O	3.380	2.514	+	++	11.669
HT259	O=C(O)C2=CC=C1C=CC(=N/C1=C2\O)C=C/C3=C/C(O)=CC(O)=C3	3.505	1.891	+	+++	12.291
HT260	O=C(O)C2=CC=C1C=CC(=N/C1=C2\O)C=C/C3=C/C=CC=C3	3.724	5.077	+	+	9.105
HT261	OC=1C(=CC=C2C=CC(=NC=12)C=C/C3=C/C=C(N)C=C3)C(O)=O	3.342	5.077	+	+	9.105
HT262	O=C(O)C(=O)CC(=O)C2=CC(C/C1=C/C=C(/[Cl])C=C1)=CC=C2	2.699	2.554	++	++	13.584
HT263	O=C(O)C(=O)CC(=O)C=1[S]C(=CC=1)C/C2=C/C=CC=C2	2.699	2.544	++	++	13.533
HT264	O=C(CC(=O)C(=O)O)C=1C=CC=CC=1C/C2=C/C=CC=C2	3.754	3.686	+	+	13.357
HT265	O=C(CC(=O)C(=O)O)C1=CC=CN1C/C2=C/C=CC=C2	2.342	2.299	++	++	13.344
HT266	O=C(O)C(=O)CC(=O)C1=CN(C=C1)C/C2=C/C=CC=C2	2.699	2.485	++	++	13.599
HT267	O=C(CC(=O)C(=O)O)C=1C=C[S]C=1C/C2=C/C=CC=C2	2.255	2.244	++	++	13.398
HT268	O=C(O)C(=O)CC(=O)C=2/C=C(/C/C1=C/C=CC=C1)C(=CC=2)OC	2.176	1.997	++	+++	13.615
HT269	O=C(O)C(=O)CC(=O)C=1C=C([S]C=1)C/C2=C/C=CC=C2	2.204	2.176	++	++	13.564
HT270	O=C(C=2OC1=CC=CN=C1C=2O)C4=CC(C/C3=C/C=CC=C3)=CC=C4	3.000	0.928	+	+++	13.254
HT271	O=C(C=2/C=C(/CC=1C=CC=CC=1)C=C(C=2)CN3CC C[S]3(=O)=O)C5=NC=C4C=CC=N/C4=C5\O	1.000	0.557	+++	+++	13.626
HT272	O=C(/C1=C/C(=CC=C1)CC=2C=CC=CC=2)C4=NC=C3C=CC=N/C3=C4\O	1.602	1.646	+++	+++	13.411
HT273	O=C(/C1=C/C(=CC=N1)CC=2C=CC=CC=2)C4=CC=C3C=CC=N/C3=C4\O	1.699	0.672	+++	+++	13.511
HT274	O=C4NNC(=O)C=1C=CC=CC=1[S][S]C=2C=CC=CC=2C(=O)NNC(=O)C=3C=CC=CC=3[S][S]C=5C=CC=CC4=5	3.845	5.144	+	+	9.038
HT275	O=C(NNC(=O)C=1C=CC=CC=1[S])C=2C=CC=CC=2[S]	4.301	5.015	+	+	9.168
HT276	O=C(NNC(=O)C=1C=CC=CC=1[S])C=2C=CC=CC=2[S][S]C=3C=CC=CC=3C(=O)NNC(=O)C=4C=CC=CC=4[S]	4.041	4.928	+	+	13.572
HT277	O=C(/C2=C/C=C1C=CC=N/C1=C2\O)C4=CC(C/C3=C/C=CC=C3)=CC=C4	2.568	2.591	++	++	13.331
HT278	O=C1C=4C(OC2=CC=C(C=C12)C/C3=C/C=CC=C3)=C/C=C(/O)C=4O	2.778	2.512	++	++	12.940
HT279	O=C(O)C(=O)CC(=O)C3=CC(OCC=1C=CC=CC=1CO C=2C=C(C=CC=2)C(=O)CC(=O)C(=O)O)=CC=C3	3.255	3.182	+	+	13.636
HT280	O=C(O)C(=O)CC(=O)C2=CC(CC=1C=CC=CC=1[F])=CC=C2	3.398	3.268	+	+	13.560
HT281	O=C(NCCNC(=O)C(=O)CC(=O)C2=CC(CC=1C=CC=CC=1[F])=CC=C2)C(=O)CC(=O)C4=CC(CC=3C=CC=CC=3[F])=CC=C4	3.763	3.628	+	+	13.600
HT282	O=C(O)C(=O)CC(=O)C=1C=C(C=C=1)C([H])(C2=C(C=CC=C2)C(=O)CC(=O)C(=O)O)C=3C=CC=CC=3[F]	3.255	3.147	+	+	13.632
HT283	O=C(NCCCCNC(=O)C(=O)CC(=O)C2=CC(CC=1C=CC=CC=1[F])=CC=C2)C(=O)CC(=O)C4=CC(CC=3C=CC=CC=3[F])=CC=C4	3.681	3.716	+	+	13.652
HT284	O=C(NCCCCNC(=O)C(=O)CC(=O)C2=CC(CC=1C=CC=CC=1[F])=CC=C2)C(=O)CC(=O)C4=CC(CC=3C=CC=CC=3[F])=CC=C4	2.301	2.256	++	++	13.651

	$C(=O)O)CC=4C=C(C(NC(=O)C=3C=C(C=CC=3)[N+]($ $[O-])=O)=CC=4)C(=O)O$					
HT323	$O=C(N/N=C(\backslash)CC(=O)N/C1=C(\backslash)C=C(C)C=C1)C$ $=2C=CC(O)=CC=2O$	5.176	5.148	+	+	13.336
HT324	$O/C1=C(/C(=C)N/C1=C/C=2OC(=CC=2)CNC(=O)C(=$ $O)N/C3=C/C=C(/C)C=C3)C(=O)OC$	4.908	4.815	+	+	13.018
HT325	$O=C(CC(=O)C(=O)OCC)C2=CN(C/C1=C/C=C(/[F])C=$ $C1)C3=CC=CC=C23$	3.079	3.097	+	+	13.548
HT326	$[Cl]C=1C=C2C(=CC=1)N/C=C2/C(=O)CC(=O)C(=O)$ O	2.716	2.350	++	++	12.202
HT327	$O=C(CC(=O)C=1NC=NN=1)C2=CNC3=C/C=C(/[Cl])$ $C=C23$	3.301	3.050	+	+	12.077
HT328	$O=C2OC1=CC(O)=C(O)C=C1/C=C2/OC=3C=CC(/C=$ $C/C(=O)O)=CC=3O$	3.301	3.093	+	+	11.090
HT329	$O=C2OC1=CC(O)=C(O)C=C1/C=C2/OC=3/C=C(/C=C$ $/C(=O)O)C=CC=3O$	3.000	3.093	+	+	11.090
HT330	$O=C2OC1=CC(O)=C(O)C=C1/C=C2/O$	3.301	5.691	+	+	8.492
HT331	$O=C(CC(=O)C(=O)OCC)C2=CN(C/C1=C/C=C(/[F])C=$ $C1)C3=CC=C(C=C23)OC$	5.116	5.084	+	+	13.558
HT332	$O=C(OC(C)(C)[H])C(=O)CC(=O)C1=CC=CN1C/C2=C$ $/C=C(/[F])C=C2$	5.000	4.984	+	+	13.325
HT333	$O=C(CC(=O)C(=O)OCC)C2=CN(C/C1=C/C=CC=C1)C$ $3=CC=C(C=C23)OC$	2.176	0.570	++	+++	13.613
HT334	$O=C(O)C(=O)CC(=O)C1=CC=C(C=C1)C(=O)CC(=O)$ $C(=O)O$	3.107	3.271	+	+	10.911
HT335	$O=C(NC=1C=C(C=CC=1)C(=O)CC(=O)C(=O)O)C2=C$ $C=CC=C2$	4.544	4.455	+	+	13.629
HT336	$O=C(CC(=O)C(=O)O)C2=CN(C/C1=C/C=CC=C1)C3=$ $C/C=C(/[Cl])C=C23$	2.987	3.036	++	+	13.634
HT337	$O=C(CC(=O)C(=O)O)C2=CN(C/C1=C/C=C(/[F])C=C1$ $)C3=C/C=C(/[Cl])C=C23$	2.301	2.182	++	++	13.509
HT338	$O=C(CC(=O)C(=O)O)C2=CN(C/C1=C/C=CC=C1)C3=$ $CC=C(C=C23)OC$	3.334	3.268	+	+	13.628
HT339	$O=C(CC(=O)C(=O)O)C1=CNC2=CC=CC=C12$	3.155	1.910	+	++	12.273
HT340	$O=C(CC(=O)C(=O)O)C2=CN(C/C1=C/C=C(/[F])C=C1$ $)C3=CC=C(C=C23)OC$	0.602	0.647	+++	+++	13.536
HT341	$O=C(CC(=O)C(=O)OCC)C2=CN(C/C1=C/C=C(/[F])C=$ $C1)C3=C/C=C(/[Cl])C=C23$	2.591	2.549	++	++	13.524
HT342	$O=C(CC(=O)C(=O)O)C=1C=CN=C2C=CC=CC=12$	5.000	4.777	+	+	12.037
HT343	$O=C(O)C(=O)CC(=O)C2=C/C=C(/O/C1=C/C=CC=C1)$ $C=C2$	4.057	4.011	+	+	13.465
HT344	$O=C(CC(=O)C(=O)OCC)C2=CN(C/C1=C/C=CC=C1)C$ $3=C/C=C(/[Cl])C=C23$	4.008	3.952	+	+	13.507
HT345	$O=C1NC(=O)C[C@@]([H])(N1)C=2N=C(C(O)=C3N=$ $CC=CC=23)C(=O)NCC=4C=CC([F])=CC=4$	1.000	0.625	+++	+++	13.558
HT346	$O=C1N(C)C(=O)C[C@]([H])(N1C)C=2N=C(C(O)=C3$ $N=CC=CC=23)C(=O)NCC=4C=CC([F])=CC=4$	1.544	0.700	+++	+++	13.483
HT347	$O/C4=N/C(=O)C[C@]([H])(C=1N=C(C(O)=C2N=C$ $C=CC=12)C(=O)NCC=3C=CC([F])=CC=3)N4C$	1.097	0.700	+++	+++	13.483
HT348	$O=C(CC(=O)C(=O)CC)C1=CNC2=C/C=C(/[Cl])C=C1$ 2	3.839	3.719	+	+	12.271
HT349	$O=C(CC(=O)C(=O)OCC)C2=CN(C/C1=C/C=CC=C1)C$ $3=CC=CC=C23$	2.881	2.892	++	++	13.374
HT350	$O=C(CC(=O)C(=O)O)C=2/C=C(/C/C1=C/C=CC=C1)C$ $=CC=2OC$	2.000	1.834	++	+++	13.540
HT351	$O=C(O)C(=O)CC(=O)C2=CC(OC/C1=C/C=CC=C1)=C$ $C=C2$	2.544	2.477	++	++	13.615
HT352	$O=C(NC=2N=C(C(O)=C1N=CC=CC1=2)C(=O)NCC=$ $3C=CC([F])=CC=3)C(=O)N$	1.602	0.869	+++	+++	13.314
HT353	$O=C(CC(=O)C(=O)O)C2=CN(C/C1=C/C=C(/[F])C=C1$ $)C3=CC=CC=C23$	1.176	0.664	+++	+++	13.518
HT354	$O=C(CC(=O)C(=O)OCCCC)C1=CC=CN1C/C2=C/C=C$ $(/[F])C=C2$	5.000	5.134	+	+	12.900
HT355	$O=C(O)C(=O)CC(=O)C1=CC=CC=C1$	4.384	3.587	+	+	10.595
HT356	$O=C(O)C(=O)CC(=O)C=1C=C(C=CC=1)C(=O)CC(=O)$ $C(=O)O$	3.255	3.252	+	+	10.931
HT357	$O=C(CC(=O)C=1NN=NN=1)C2=CNC3=CC=CC=C23$	3.290	3.094	+	+	12.150
HT358	$O=C(O)C(=O)CC(=O)C1=CC([Br])=CC=C1$	3.398	3.602	+	+	10.580
HT359	$CC=1C=CC(=CC=1)[S](=O)(=O)N/C2=C/C=C/C2/$ $N=C/C=4[S]C3=CC=CC=C3C=4O$	4.944	4.932	+	+	13.239
HT360	$O=C(CC(=O)C=2N=CN=C1N(C=NC1=2)C/C3=C/C=C$ $C=C3)C(=O)O$	5.898	5.903	+	+	13.506
HT361	$O=C(N/C(=C\C=C\C=C\C=C=CC=C1)C(=O)N=N/C2=C($ $\backslash)NC3=C/C=C(/[F])C=C23)C4=CC=CC=C4$	4.778	4.742	+	+	13.397
HT362	$O=C(NC=1C=CC(O)=C(C=1)C3=NC2=CC([Cl])=CC=$	4.000	4.952	+	+	11.918

ID	Chemical Structure	4.973	5.076	+	+	9.106
HT363	O=C(OCC)C1=CC(CCC(=O)OCC)=C(/C=C1/CCC(=O)OCC)C(=O)OCC	4.973	5.076	+	+	9.106
HT364	O=C(N/C1=C/C=C(O)C(=C1)C3=NC2=CC=CC=C2O3)C=4C=CC=C5C=CC=CC=45	4.146	3.952	+	+	11.893
HT365	O/C1=C/C=C(/C=C1/OC)C/N=N/C2=N/C(O)=C([S]2)C C(=O)N/C3=C/C=C(/[Cl])C([Cl])=C3	4.949	4.902	+	+	13.480
HT366	C/C1=N/N(C(O)=C1[C@]([H])(C2=C/C=C(/O)C(O)=C2)C=3C(=O)N(N(C)C=3C)C4=CC=CC=C4)C5=CC=C C=C5	4.949	5.042	+	+	12.289
HT367	O=C2N(CC(C)(C)[H])C1=CC=CC=C1C(O)=C2C(=O) NC=3C=CC=CC=3[S](=O)(=O)N	4.602	4.512	+	+	12.372
HT368	C[S](=O)(=O)N(CC(=O)N/N=C/C=1C(O)=CC=C2C=C C=CC=12)C=3/C=C(/[Cl])C(=CC=3)OC	4.771	4.786	+	+	13.369
HT369	[Cl]C=1C=CC(=CC=1)[C@]3([H])N(CCC/C2=C/N=CN2)C(=O)C(=O)[C@]3([H])C(=O)C4=C/C=C(/C)C=C4	4.968	4.654	+	+	13.613
HT370	[Cl]C=1C=CC(=CC=1)C=CC(=O)N/C2=C/C=C(C=C2) NC(=O)C=3OC=CC=3	4.954	5.187	+	+	8.995
HT371	O=C(CC(=O)C(O)=O)C2=NC1=CN=CN=C1N2C/C3=C/C=CC=C3	5.000	6.043	+	+	13.422
HT372	O=C3C=2N=CN(C/C1=C/C=CC=C1)C=2N=C(N3CC=4C=CC=CC=4)C(=O)CC(=O)C(O)=O	4.477	4.333	+	+	13.600
HT373	O/C(=C/C(=O)C(O)=O)C3=NC2=C(N=CN(C/C1=C/C=CC=C1)C2=O)N3C/C4=C/C=CC=C4	4.498	4.453	+	+	13.587
HT374	O=C2N(C/C1=C/C=C/C1/[F])C(=O)N(/C=C2/C(O)=CC(=O)C(O)=O)CC=3C=CC=CC=3[F]	3.613	3.513	+	+	13.635
HT375	O=C2N(C/C1=C/C=C(/[F])C=C1)C(=O)N(/C=C2/C(O)=CC(=O)C(O)=O)C/C3=C/C=C(/[F])C=C3	3.591	0.540	+	+++	13.643
HT376	O=C2N(C/C1=C/C=CC=C1)C(=O)N(/C=C2/C(O)=CC(=O)C(O)=O)C/C3=C/C=CC=C3	2.301	0.538	++	+++	13.644
HT377	O=C1NC(=O)N(/C=C1/C(=O)CC(=O)C(O)=O)C/C2=C /C=CC=C2	2.699	2.602	++	++	13.636
HT378	O=C(N/C1=C/C=C(/[Cl])C=C1[Cl])C[S]/C3=N/C(C[S]/C2=C/C=C(/[Cl])C=C2)=CC(=O)N3	4.380	4.312	+	+	13.323
HT379	O=C(NC=1C=CC=C(C=1)[N+](=O)[O-])CC(=O)C=3[S]C(N/C2=C/C=CC=C2)=C(C=3)C(=O)C	4.987	5.955	+	+	13.619
HT380	O=C(N/C(=C\C=C\C=C\C=C=CC=C1)C(=O)N/N=C/C2=C/C([Br])=C/C=C2/O)C3=CC=CC=C3	4.954	4.819	+	+	12.899
HT381	O=C(NC=1C=CC=C(C=1)N(C(=O)CC(=O)C=3[S]C(N/C2=C/C=CC=C2)=C(C=3)C(=O)C	4.903	4.978	+	+	13.609
HT382	O/C1=C/C=C/C=C1/NC(=[S])NC(=O)C=CC=2OC=CC=2	4.447	4.333	+	+	12.117
HT383	O=C(OCC)C1=C([S]/C=C1/C2=C/C=C=CC=C2)N[C@]([H])(NC(=O)C=3OC=CC=3)C(=O)C4=C/C=C(/C)C=C4	4.898	4.877	+	+	13.392
HT384	O=C(C=1C=CC=CC=1)C2=CC([Br])=C/C=C2/NC(=O)C=3NC=NC=3C(O)=O	4.230	4.271	+	+	13.589
HT385	O=C(NC=1C=CC=C(C=1)N(C(=O)CC(=O)C=3[S]C(N/C2=C/C=CC=C2)=C(C=3)C(=O)C	4.944	5.833	+	+	13.628
HT386	O=C(NC=1C=CC(O)=C(C=1)C3=NC2=CC=CC=C2O3)C4=C/C=C(/OC)C(=C4)[N+](=O)[O-]	3.845	2.565	+	++	11.618
HT387	O/C1=C/C=C/C=C1/C=N/CC(O)([H])C/N=C/C2=C/C=C/C=C2/O	4.785	5.780	+	+	13.558
HT388	O=C(NC=1C=CC=CC=1)C5=C/C=C(/C=C/C(=O)N/C2=C/C=C(/O)C(=C2)C4=NC3=CC=CC=C3O4)O5	4.362	4.268	+	+	12.909
HT389	O=C2NC1=CC=CC=C1[S][C@]2([H])CC(=O)N/C3=C/C=CC(=C3)C(O)=O	4.851	4.846	+	+	13.444
HT390	[Cl]/C3=C/C(N[C@]([H])(OC)C2=N/C1=C(\O)C=CC=C1C=C2)=C([Cl])C=C3[N+](=O)[O-]	5.362	6.453	+	+	11.186
HT391	[Cl]C=3C=C/C=C(/C=C/C2=N/C1=C(\O)C=CC=C1C=C2)C=3	5.362	5.266	+	+	8.917
HT392	[Cl]C=3C=C/C=C(/C=C/C2=N/C1=CC(=CC=C1C=C2)C(=O)O)C=3	5.362	5.838	+	+	8.345
HT393	O=C(CC=1C=CC=CC=1)N/C2=C/C=C(/C=C2/C(O)=O)NC(=O)C/C3=C/C=CC=C3)C(O)=O	3.954	3.819	+	+	13.615
HT394	O=C(CC(=O)C(=O)N=N/C1=C(\O)NC2=C/C=C(/[Br])C=C12)C3=C/C=C(/[Cl])C=C3	4.447	4.404	+	+	13.380
HT395	OC(=O)C1=CC=C(C=C1)C(=O)C=2C=CC3=C(C=2)C(=O)N(C3=O)C=4[S]C(=NN=4)[S]CC	4.813	4.796	+	+	13.028
HT396	O/C1=C/C=C(=CC(O)=C1)C(=O)N/N=C/C=2C=CC(=CC=2)C=NNC(=O)C3=CC(O)=CC(O)=C3	4.881	3.376	+	+	10.806

HT397	O=C2OC1=CC=C(C=C1/C=C2/C=3N=C([S]C=3)N=N C/C4=C/C=C/C=C4/O)OC	4.477	4.400	+	+	13.018
HT398	O=C(C[S])C2=N/C1=CC=CC=C1N2C/C3=C/C=CC=C 3)N/N=C/C4=C/C([Br])=C/C=C4/O	4.708	4.700	+	+	13.501
HT399	COC=1C=CC(=CC=1OC)CCNC(=O)CC(=O)N/N=C/C =2OC=CC=2	4.954	4.979	+	+	13.341
HT400	O=C3C(=O)N(CCN1CCNCC1)[C@]([H])(C=2C=CC= CC=2[F])[C@@]3([H])C(=O)C4=CC=C(C=C4)OC	5.799	3.203	+	+	10.979
HT401	O=C(NCC=1OC(=CC=1)C=C2NC(=C)C(=C2O)C(=O) OCC)C(=O)NC=3C=CC=CC=3	4.602	4.629	+	+	13.256
HT402	O=C2C1=CC=CC=C1C(=O)C4=C2C(O)=CC(O/C3=C/ C=C(C=C3)[S](=O)(=O)NCCOC)=C4O	5.000	4.988	+	+	13.279
HT403	O=C1OC=4C(/C=C1/C=3[S][C@]2([H])C=CC=C[C @]2([H])N=3=C/C=C(/O)C=4CN(CCO)CCO	5.929	3.041	+	+	11.142
HT404	O=C2OC1=CC=CC=C1/C=C2/C(=O)NC=3[S]/C=C(/C C=3C(=O)OCC)C(N)=O	4.954	4.818	+	+	12.722
HT405	OC(=O)C2=CN(C1=CC=C(C=C1C2=O)C/C3=C/C=CC ([Cl])=C3[F])[C@]([H])(CO)C(C)[H]	0.914	1.294	+++	+++	12.888
HT406	O=C2C1=CC(=CC=C1N/C=C2/C(O)=O)CCO)CC=3C =C/C=C(/[Cl])C=3[F]	1.384	1.234	+++	+++	12.948
HT407	OC(=O)C2=CN=C1C=CC(=C/C1=C2/O)C/C3=C/C=C C=C3	3.204	3.042	+	+	13.055
HT408	OC=2C1=CC(=CC=C1N=CC=2C(O)=O)CC=3C=C/C= C(/[Cl])C=3[F]	1.638	1.171	+++	+++	13.012
HT409	O=C(NC/C1=C/C=C(/[F])C=C1)C3=NC(=C2C=CC=N/ C2=C3\O)N4CCN(C)CC4	1.602	0.957	+++	+++	13.225
HT410	O=C(NC/C1=C/C=C(/[F])C=C1)C3=NC(=C2C=CC=N/ C2=C3\O)N(C)CC(=O)N(C)C	1.763	1.723	+++	+++	13.298
HT411	O=C(NC/C1=C/C=C(/[F])C=C1)C3=NC(=C2C=CC=N/ C2=C3\O)N(C)C(=O)C(=O)N(C)C	1.602	0.951	+++	+++	13.231
HT412	O=C(NC/C1=C/C=C(/[F])C=C1)C3=NC(=C2C=CC=N/ C2=C3\O)N(C)C(=O)C(N)=O	1.301	0.852	+++	+++	13.331
HT413	O=C(NC/C1=C/C=C(/[F])C=C1)C3=NC(=C2C=CC=N/ C2=C3\O)N4CCN(CC4)C(C)=O	1.398	0.984	+++	+++	13.198
HT414	O=C(NC/C1=C/C=C(/[F])C=C1)C3=NC(=C2C=CC=N/ C2=C3\O)N(C)C(=O)C(=O)NC	1.176	0.847	+++	+++	13.336
HT415	O=C(NC/C1=C/C=C(/[F])C=C1)C3=NC(=C2C=CC=N/ C2=C3\O)N(C)CCN(C)C(C)=O	2.193	2.085	++	++	13.564
HT416	O=C(NC/C1=C/C=C(/[F])C=C1)C3=NC(=C2C=CC=N/ C2=C3\O)N(C)C(=O)C(=O)N4CCCC4	1.602	0.908	+++	+++	13.275
HT417	O=C(NC/C1=C/C=C(/[F])C=C1)C3=NC(=C2C=CC=N/ C2=C3\O)N(C)C(=O)C(=O)N4CCCC4	0.845	0.949	+++	+++	13.234
HT418	O=C(NC/C1=C/C=C(/[F])C=C1)C3=NC(=C2C=CC=N/ C2=C3\O)N4CCN(CC)C(=O)C4=O	1.000	0.992	+++	+++	13.191
HT419	O=C3C2=CC(CC=1C=C/C=C(/[Cl])C=1[F])=C(C=C2N (/C=C3/C(O)=O)[C@]([H])(CO)C(C)[H])OC	0.857	1.691	+++	+++	12.492
HT420	OC(=O)C2=CN(CCO)C1=CC(OC)=C(C=C1C2=O)C/C 3=C/C=CC([Cl])=C3[F]	0.959	1.363	+++	+++	12.820
HT421	N[C@](C)([H])C(=O)N[C@](C)([H])C(=O)N[C@@]([H])(C/C1=C/C=C(/O)C=C1)C(=O)N[C@]([H])(C/C2 =C/C=CC=C2)C(=O)N[C@]([H])(CC(C)C)[H])C(=O) N[C@@]([H])(CC(C)C)[H])C(=O)N[C@]([H])(C CCCN)C(=O)N[C@]([H])(CC(C)C)[H])C(=O)N[C@]](C)([H])C(=O)NCC(=O)N[C@]([H])(CCC/N=C(N) N)C(=O)N[C@]([H])(C/C3=C/NC4=CC=CC=C34)C(O)=O	5.000	4.844	+	+	13.212
HT422	O=C2C1=CC(=CC=C1N/C=C2/C(=O)CC(=O)C(=O)O CC)C/C3=C/C=C(/[F])C=C3)C(=O)CC(=O)C(=O)OCC	2.462	2.093	++	++	13.628
HT423	OC=2C1=CC(=CC=C1N=CC=2C(=O)CC(=O)C(=O)O C(=O)CC(=O)C(O)=O	4.342	4.547	+	+	13.187
HT424	OC=2C1=CC(=CC=C1N=CC=2C(=O)CC(=O)C(=O)O CC)C(=O)CC(=O)C(=O)OCC	4.591	4.522	+	+	13.175
HT425	O=C2C1=CC(=CC=C1N/C=C2/C(=O)CC(=O)C(=O)O)C/C3=C/C=C(/[F])C=C3)C(=O)CC(=O)C(O)=O	2.643	2.624	++	++	13.617
HT426	O=C2C=1C(O)=C/C=C(/O)C=1C3=NN(CCNCCO)C4= C/C=C(/NCCCN)C2=C34	4.255	3.038	+	+	11.145
HT427	[F]C=5C=CC(CN3CC2=C(C1=CC=CN=C1C(O)=C2C3 =O)C(=O)NC/C4=C/C=CC=N4)=CC=5	2.279	1.963	++	+++	12.220
HT428	[F]/C4=C/C=C(/CN3CC2=CC1=CC=CN=C1C(O)=C2C 3=O)C=C4	1.845	3.792	+++	+	10.391
HT429	[F]C=5C=CC(CN3CC2=C(C1=CC=CN=C1C(O)=C2C3 =O)C(=O)N4CCOCC4)=CC=5	1.556	1.066	+++	+++	13.117
HT430	N[C@](C)([H])C(=O)N[C@]([H])([S])C(=O)N[C@ @]([H])(C/C1=C/NC2=CC=CC=C12)C(=O)N[C@]([H])(C/C3=C/NC4=CC=CC=C34)C(=O)N[C@](C)([H])	4.954	6.043	+	+	13.615

	N[C@](C)([H])C(=O)NCC(=O)N[C@]([H])(C(=O)N[C@@]([H])(CCCCN)C(=O)N[C@]([H])(CCC(=O)N)C(=O)N[C@]([H])(CCC(=O)O)C(=O)N[C@]([H])(C/C3=C/C=CC=C3)C(=O)N[C@]([H])CC							
HT442	N[C@]([H])(C(=O)N[C@](C)([H])C(=O)N[C@@]([H])(C/C1=C/C=C(O)C=C1)C(=O)N[C@@]([H])(C/C2=C/C=CC=C2)C(=O)N[C@@]([H])(CC(C)(C)[H])C(=O)N[C@@]([H])(CC(C)(C)[H])C(=O)N[C@@]([H])(C(=O)N[C@@]([H])(CC(C)(C)[H])C(=O)N[C@@]([H])(C(=O)NCC(=O)N[C@@]([H])(CCC/N=C(N)N)C(=O)N[C@@]([H])(C/C3=C/NC4=CC=CC=C34)C(=O)O)[C@](O)(C)[H])	5.053	6.009	+	+			13.546
HT443	N[C@@]([H])(C(=O)N[C@@](C)([H])C(=O)N[C@]([H])(C/C1=C/C=C(O)C=C1)C(=O)N[C@@]([H])(C/C2=C/C=CC=C2)C(=O)N[C@@]([H])(CC(C)(C)[H])C(=O)N[C@@]([H])(CC(C)(C)[H])C(=O)N[C@@]([H])(CCCCN)C(=O)N[C@@]([H])(CC(C)(C)[H])C(=O)N[C@@]([H])(C(=O)NCC(=O)N[C@@]([H])(CCC/N=C(N)N)C(=O)N[C@@]([H])(C/C3=C/NC4=CC=CC=C34)C(=O)N)[C@@](O)(C)[H])	4.114	3.895	+	+			13.202
HT444	N[C@](C)([H])C(=O)N[C@@]([H])(C[S])C(=O)N[C@@]([H])(C/C1=C/NC2=CC=CC=C12)C(=O)N[C@@]([H])(C/C3=C/NC4=CC=CC=C34)C(=O)N[C@@]([H])(C(=O)NCC(=O)N[C@@]([H])(C(=O)N[C@@]([H])(C(=O)N[C@@]([H])(C(=O)N[C@@]([H])(C(=O)N[C@@]([H])(C/C5=C/C=CC=C5)C(=O)O)[C@](C)([H])CC	4.740	4.765	+	+			13.584
HT445	N[C@](C)([H])C(=O)N[C@@](C)([H])C(=O)N[C@@]([H])(C/C1=C/NC2=CC=CC=C12)C(=O)N[C@@]([H])(C/C3=C/NC4=CC=CC=C34)C(=O)N[C@@]([H])(C(=O)NCC(=O)N[C@@]([H])(C(=O)N[C@@]([H])(CCCCN)C(=O)N[C@@]([H])(CCC(=O)N)C(=O)N[C@@]([H])(CCC(=O)O)C(=O)N[C@@]([H])(C/C5=C/C=CC=C5)C(=O)O)[C@](C)([H])CC	5.442	5.450	+	+			13.541
HT446	[F]/C4=C/C=C(/CN3C/C2=C(\OC(=O)N(C)C)C1=CC=CN=C1C(O)=C2C3=O)C=C4	2.881	2.909	++	++			11.273
HT447	[F]C=5C=CC(CN3CC2=C(C1=CC=CN=C1C(O)=C2C3=O)C4=CC(=CC=C4)C(=O)OCC)=CC=5	3.322	2.634	+	++			11.549
HT448	[F]C=5C=CC(CN3CC2=C(C1=CC=CN=C1C(O)=C2C3=O)C4=C([F])C=C/C=C4/[F])=CC=5	2.525	3.202	++	+			10.980
HT449	[F]/C4=C/C=C(/CN3C(=O)C2=C(OC)C1=CC=CN=C1C(O)=C2C3=O)C=C4	1.903	3.051	+++	+			11.131
HT450	OC=2C1=NC=CC=C1C=CC=2C(=O)NC/C3=C/C=C(/F)C=C3	3.301	3.165	+	+			11.018
HT451	[F]C=5C=CC(CN3CC2=C(C1=CC=CN=C1C(O)=C2C3=O)C4=CC=C/C=C4/C(=O)OCC)=CC=5	2.544	1.711	++	+++			12.471
HT452	[F]C=4C=CC(CN3C(=O)C2=C(OC(=O)N(C)C)C1=CC=CN=C1C(O)=C2C3=O)=CC=4	3.380	3.162	+	+			12.402
HT453	[F]C=5C=CC(CN3CC2=C(C1=CC=CN=C1C(O)=C2C3=O)C4=CC=C(C=C4)OCC)=CC=5	3.079	3.070	+	+			11.113
HT454	[F]/C4=C/C=C(/CN3C/C2=C(\OC)C1=NC=CN=C1C(O)=C2C3=O)C=C4	2.322	2.961	++	++			11.222
HT455	[F]/C4=C/C=C(/CN3C/C2=C(\OC)C1=CC([F])=CN=C1C(O)=C2C3=O)C=C4	0.857	3.273	+++	+			10.909
HT456	[F]/C4=C/C=C(/CN3C/C2=C(\OC)C1=CC(=CN=C1C(O)=C2C3=O)C=C4	2.929	3.592	++	+			10.591
HT457	[F]C=4C=CC(CN3C/C2=C(\O[S](=O)(=O)N(C)C)C1=NC=CN=C1C(O)=C2C3=O)=CC=4	1.519	1.857	+++	+++			12.326
HT458	[F]C=4C=CC(CN3C/C2=C(\O[S](=O)(=O)N(C)C)C1=CC=CN=C1C(O)=C2C3=O)=CC=4	2.407	1.939	++	+++			12.243
HT459	[F]/C4=C/C=C(/CN3C/C2=C(\OC)C1=CC(=CN=C1C(O)=C2C3=O)OC)C=C4	1.968	3.117	+++	+			11.066
HT460	[F]C=5C=CC(CN4CC=3C(OC)=C1C(N=CN1C/C2=C/C=CC=C2)=C(O)C=3C4=O)=CC=5	4.380	4.099	+	+			12.881
HT461	O=C(CC(=O)C(=O)OC)C1=CC=CN1C/C2=C/C=C(/F)C=C2	4.681	4.586	+	+			13.224
HT462	N[C@]([H])(C(=O)N[C@](C)([H])C(=O)N[C@@]([H])(C/C1=C/C=C(O)C=C1)C(=O)N[C@@]([H])(C/C2=C/C=CC=C2)C(=O)N[C@@]([H])(CC(C)(C)[H])C(=O)N[C@@]([H])(CCCCN)C(=O)N[C@@]([H])(CC(C)(C)[H])C(=O)N[C@@]([H])(C(=O)NCC(=O)N[C@@]([H])(C(=O)N[C@@]([H])(C/C3=C/NC4=CC=CC=C34)C(=O)O)[C@](O)(C)[H])	4.903	4.916	+	+			13.245
HT463	N[C@]([H])(C(=O)N[C@](C)([H])C(=O)N[C@@]([H])(C/C1=C/C=C(O)C=C1)C(=O)N[C@@]([H])(C/C2=C/C=CC=C2)C(=O)N[C@@]([H])(CC(C)(C)[H])C(=O)N[C@@]([H])(CCCCN)C(=O)N[C@@]([H])(CC(C)(C)[H])C(=O)N[C@@]([H])(C(=O)NCC(=O)N[C@@]([H])(CCC/N=C(N)N)C(=O)N[C@@]([H])(C/C3=C/NC4=CC=CC=C34)C(=O)O)[C@](O)(C)[H])	5.498	5.492	+	+			13.441

HT485	<chem>C/C([Cl])=C([F])C=C2)C3=O)C(C)(C)[H]</chem> OC=1C(=O)N(C(CCC(=O)OC)=C3C=1C(=O)N(C/C2=C/C([Cl])=C([F])C=C2)C3=O)C(C)(C)[H]	3.851	3.836	+	+	13.370
HT486	<chem>OC=1C(=O)NC(COC(=O)C)=C3C=1C(=O)N(C/C2=C/C([Cl])=C([F])C=C2)C3=O</chem>	4.090	4.054	+	+	13.423
HT487	<chem>OC=1C(=O)NC(CO)=C3C=1C(=O)N(C/C2=C/C([Cl])=C([F])C=C2)C3=O</chem>	3.813	3.512	+	+	12.483
HT488	<chem>OC=1C(=O)N(C)C(=NC=1C(=O)NC/C2=C/C(/[F])C=C2)C(C)(C)C(=O)C3=N/N=C(/C)O3</chem>	1.826	1.378	+++	+++	12.804
HT489	<chem>[F]C=3C=CC(CN1CCC2=CC(=CC=C12)C(=O)NO)=C([F])C=3</chem>	4.924	3.103	+	+	11.080
HT490	<chem>O=C2N(O)C(=O)C1=CC=CC=C1[C@]2([H])[C@]3([H])CCCCC3</chem>	3.130	5.160	+	+	9.023
HT491	<chem>O=C(NNCC=1C=CC=CC=1O)C=2C=CC=CC=2O</chem>	2.845	1.425	+++	++	12.758
HT492	<chem>CC=2C(CC(=O)C1=CC(C=O)=C(O)C=C1C)=CC=C(C=2O)C(=O)OC</chem>	5.090	6.164	+	+	13.020
HT493	<chem>O=C(O)C=2C(=O)N(C)C1=CC=C(C=C1C=2O)C=3C=CC([F])=CC=3</chem>	4.362	3.587	+	+	10.596
HT494	<chem>[F]C=1C=C2C(=CC=1)N(C=C(C2=O)C(=O)CC(=O)C(=O)O)C/C3=C/C(/[F])C=C3</chem>	3.362	3.333	+	+	13.566
HT495	<chem>O=C4C=1C=CC=CC=1C(=O)C(=CC=3C(O)=C2C=CC=C/C2=C(O)C=3O)C4=O</chem>	4.301	3.122	+	+	11.061
HT496	<chem>OC=1C=CC=CC=1C(=O)N3N=C/C(=C/C2=C/C=CC(O)=C2)C3=O</chem>	3.869	3.966	+	+	12.252
HT497	<chem>O=C(NC/C2=C/C1=CC=CC=C1[S]2)C=3N=C(NC(=O)C=3O)C=4[S]C=CC=4</chem>	1.000	0.562	+++	+++	13.621
HT498	<chem>O=C4OC1=CC=CC=C1C=3OC=2C=CC=CC=2[C@]([H])(C=34)C6=C(O)C5=CC=CC=C5OC6=O</chem>	5.086	4.516	+	+	9.666
HT499	<chem>OC=1C=CC=CC=1CNNC[C@@]([O])([H])CO/C2=C/C=CC=C2</chem>	5.301	6.220	+	+	13.561
HT500	<chem>O=C1N(NC(=C)C1=C/C2=C/C(/O)C=C2)C(=O)C3=C/C=C(/[Cl])C=C3</chem>	5.467	5.278	+	+	12.327
HT501	<chem>OC=1C=CC=CC=1C(=O)NNC(=O)C2=CC=CC(O)=C2O</chem>	2.699	1.892	++	+++	12.290
HT502	<chem>O=C(OC)C2=CC=C1C=C(OC1=C2)CC/C3=C/C(/O)C(O)=C3</chem>	4.641	4.624	+	+	12.449
HT503	<chem>O=C(NC=1N=CN=C2C=1N=CN2C/C3=C/C(/[F])C=C3)C=5C=CC4=CC=CN=C4C=5O</chem>	4.049	3.931	+	+	13.568
HT504	<chem>O=C(NC/C1=C/C=C(/[Cl])C([Cl])=C1)C=2N=C(NC(=O)C=2O)C=3[S]C=CC=3</chem>	1.000	0.650	+++	+++	13.533

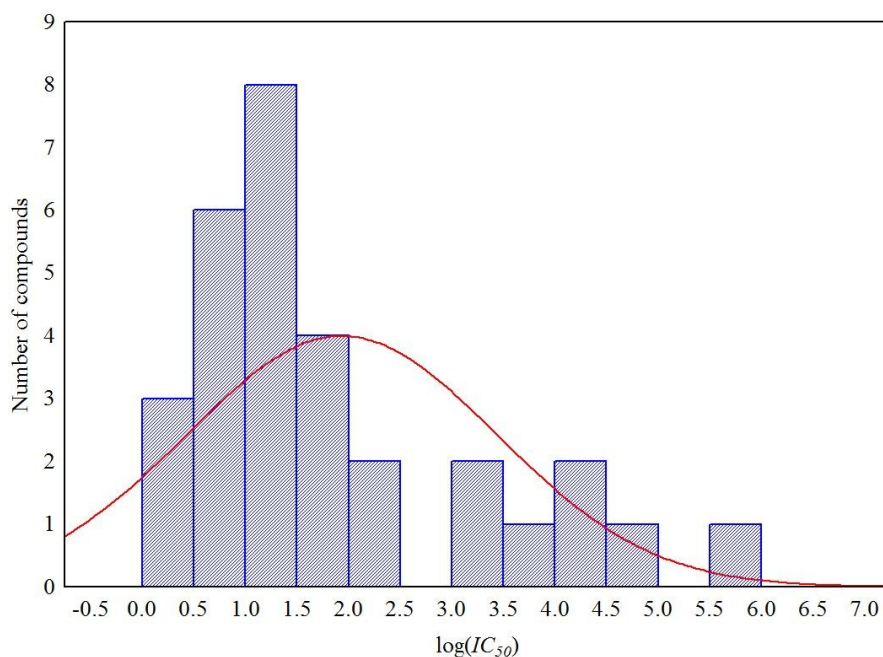


Figure S1: Activity value distribution of training set molecules.

Table S2: Statistical parameters of Sets 1, 2, 3 and 4

Parameters	Set 1	Set 2	Set 3	Set 4
<i>R</i>	0.940	0.791	0.931	0.729
<i>s</i>	2.847	5.897	3.576	6.164
<i>Q</i> ²	0.912	0.624	0.899	0.542
<i>R</i> ² _{pred}	0.847	0.429	0.511	0.394
<i>s</i> _p	0.697	1.170	1.112	1.231

Table S3: SMILES, fit value observed and estimated activity of set 2

SN	SMILES	Activity Log(IC ₅₀)		Fit Value
		¹ Obs.	² Est.	
1	<chem>O=C(C=1N=C(N(C(=O)C=1O[H])C([H])([H])[H])C@@]2([H])N(C([H])([H])C([H])([H])OC2([H])([H])C([H])([H])C([H])([H])N([H])C([H])([H])C3=C([H])C([H])=C([F])C([H])=C3[H])</chem>	1.519	0.763	10.360
2	<chem>O=C1C(O[H])=C(N=C(N1C([H])([H])[H])C2(N(C([H])([H])[H])C([H])([H])[H])C([H])([H])OC([H])([H])C2([H])[H])C(=O)N([H])C([H])([H])C=3C([H])=C([H])C([F])=C([H])C=3[H]</chem>	0.301	0.930	10.193
3	<chem>O=C(C=1N=C2N(C(=O)C=1O[H])C([H])([H])C([H])([H])C([H])([H])C@@]2([H])N(C([H])([H])[H])[S](=O)(=O)N(C([H])([H])[H])C([H])([H])[H])N([H])C([H])([H])C3=C([H])C([H])=C([F])C([H])=C3[H]</chem>	0.699	0.937	10.186
4	<chem>[F]/C1=C([H])C([H])=C(C([H])=C1[H])C([H])([H])C2=NN=C(O2)C4=NC(=C3C([H])=C([H])C([H])=N/C3=C4/O[H])C=5C([H])=C(C([H])C=C([H])C=5[H])[S](=O)(=O)N([H])C([H])(C([H])([H])[H])C([H])([H])[H]</chem>	0.602	0.953	10.171
5	<chem>O=C1C(O[H])=C(N=C(N1C([H])([H])[H])C(N([H])[S](=O)(=O)N(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C(=O)N([H])C([H])([H])C=2C([H])=C([H])C([F])=C([H])C=2[H]</chem>	1.079	0.963	10.160
6	<chem>O=C1C(O[H])=C(N=C(N1C([H])([H])[H])C(N2C([H])([H])C([H])([H])OC([H])([H])C2([H])[H])C([H])([H])[H])C([H])([H])[H])C(=O)N([H])C([H])([H])C=3C([H])=C([H])C([F])=C([H])C=3[H]</chem>	0.477	1.034	10.089
7	<chem>O=C/C2=N/C(=C1C/N=C(/[H])C([H])=C1[H])=C2O[H])N3C([H])([H])C([H])([H])N(C(=O)C([H])([H])[H])C([H])([H])C3([H])[H])N([H])C([H])([H])C4=C([H])C([H])=C([F])C([H])=C4[H]</chem>	1.398	1.260	9.863
8	<chem>O=C1C(O[H])=C(N=C(N1[H])C=2[S]C([H])=C([H])C=2[H])C(=O)N([H])C([H])([H])C=3C([H])=C([H])C([H])=C([H])C=3[H]</chem>	1.929	1.397	9.726
9	<chem>[F]/C1=C([H])C([H])=C(C([H])=C1[H])C([H])([H])N4C(=O)C=3C(O[H])=C2/N=C(/[H])C(OC([H])([H])[H])=C([H])C2=C(OC([H])([H])[H])C=3C4([H])[H]</chem>	1.968	1.555	9.568
10	<chem>O=C/C2=N/C(=C1C/N=C(/[H])C([H])=C1[H])=C2O[H])N(C(=O)C(=O)N3C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])[H])N([H])C([H])([H])C4=C([H])C([H])=C([F])C([H])=C4[H]</chem>	0.845	1.605	9.519
11	<chem>[F]/C1=C([H])C([H])=C(C([H])=C1[H])C([H])([H])C2=NN=C(O2)C4=NC(=C3C([H])=C([H])C([H])=N/C3=C4/O[H])C=5C([H])=C(C([H])=C([H])C=5[H])C(=O)O[H]</chem>	0.301	1.781	9.342
12	<chem>O=[S](=O)(=O)C([H])=C([H])C=1C([H])=C(O[H])C(O[H])=C(O[H])C=1[H])C([H])([H])[S](=O)(=O)C([H])=C([H])C=2C([H])=C(O[H])C(O[H])=C(O[H])C=2[H]</chem>	3.255	2.004	9.119
13	<chem>O=C(OC([H])([H])C([H])([H])OC(=O)C([H])=C([H])C=1C([H])=C(O[H])C(O[H])=C([H])C=1[H])C([H])=C([H])C=2C([H])=C(O[H])C(O[H])=C([H])C=2[H]</chem>	2.602	2.037	9.087
14	<chem>O=C(O[C@]([H])(C(=O)O[H])[C@]([H])(OC(=O)C([H])=C([H])C1=C([H])C([H])=C(O[H])C(O[H])=C1[H])C(=O)O[H])C([H])=C([H])C2=C([H])C([H])=C(O[H])C(O[H])=C2[H]</chem>	2.699	2.813	8.310
15	<chem>O=C/C3=C([S][S]/C2=C([C(=O)N([H])N([H])C(=O)C1=C([S][H])C([H])=C([H])C([H])=C1[H])C([H])=C([H])C([H])=C2[H])C([H])=C([H])C([H])=C3[H])N([H])N([H])C(=O)C4=C([S][H])C([H])=C([H])C([H])=C4[H]</chem>	4.041	2.821	8.302
16	<chem>O=C(O[C@@]([H])(C(=O)O[H])[C@@]([H])(OC(=O)C([H])=C([H])C1=C([H])C([H])=C(O[H])C(O[H])=C1[H])C(=O)O[H])C([H])=C([H])C2=C([H])C(O[H])=C(O[H])C([H])=C2[H]</chem>	2.903	2.965	8.158

26	([H])C([H])([H])N([H])C([H])([H])C4([H])[H] O=C(C=1N(C=3C(C=1[H])=C([H])C=2OC([H])([H])OC=2C=3[H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H])C([H])([H])C(=O)C(=O)O[H]	3.301	3.995	6.357
27	O=[S](=O)(C([H])=C([H])C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])([H])[S](=O)(=O)C([H])=C([H])C=2C([H])=C(/C(=C(/OC([H])([H])[H])C=2[H])C(=O)C([H])([H])[H])C(=O)C([H])([H])[H]	4.903	4.006	6.345
28	[Cl]C=1C([H])=C([H])C(=C([H])C=1[H])C([H])([H])C4=N/N=C(/C3=N/C([H])=C2C([H])=C([H])C([H])=N/C2=C3\O[H])N4[H]	2.806	4.100	6.251
29	O=C(/C2=C(\O[H])C=1/N=C(/[H])C([H])=C([H])C=1C([H])=C2[H])C3=C([H])C(=C([H])C([H])=C3[H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H]	2.568	4.109	6.242
30	O=C(O[H])C3=C([H])C([H])=C1C(N=C(C([H])=C1[H])C([H])=C([H])C2=C([H])C([Br])=C(O[H])C([Br])=C2[H])=C3O[H]	3.114	4.243	6.109

¹Observed; ²Estimated