

β -secretase inhibitors for Alzheimer's disease: identification using pharmacoinformatics

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Supplementary data

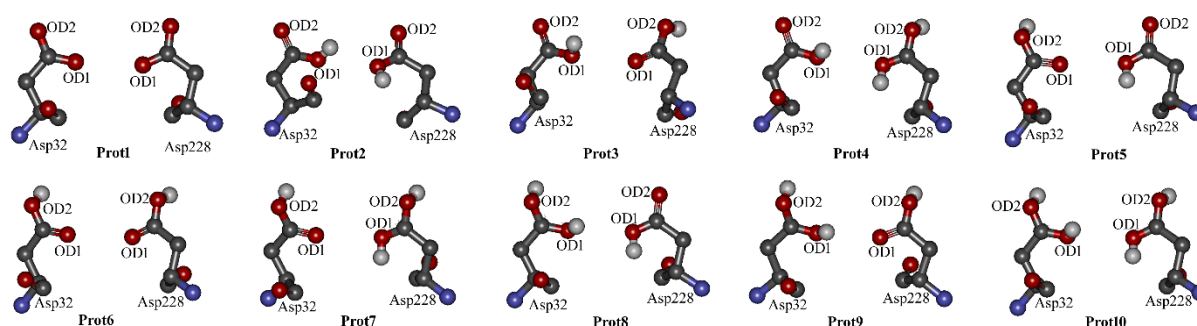


Figure S1: Different protonation states of catalytic dyad Asp32-Asp228 (OD1 – inner oxygen atom; OD2 – outer oxygen atom)

Table S1: Statistical parameters of all eight training and test sets

	n_{tr}	R	$RMSD$	Q^2	se	r_m^2	Δr_m^2	$\Delta cost$	n_{ts}	R^2_{pred}	sp	$r_m^2_{test}$	Δm	Features	No of outliers
Tr1	30	0.922	1.063	0.846	0.514	0.837	0.439	73.943	186	0.603	0.635	0.546	0.128	2xa, p	14
Tr2	30	0.893	1.153	0.795	0.552	0.757	0.189	56.292	189	0.727	0.535	0.680	0.096	2xa, d, p	9
Tr3	30	0.921	2.516	0.802	0.512	0.792	0.176	503.631	193	0.542	0.711	0.481	0.244	3xa, p	7
Tr4	30	0.947	1.919	0.895	0.346	0.889	0.093	461.35	195	0.653	0.584	0.551	0.005	3xa, p	13
Tr5	30	0.865	2.038	0.739	0.622	0.713	0.228	159.967	194	0.751	0.505	0.657	0.052	a, d, p, r	12
Tr6	30	0.938	0.809	0.881	0.385	0.881	0.109	52.008	190	0.601	0.662	0.559	0.147	2xa, d, p	8
Tr7	30	0.950	1.094	0.901	0.332	0.901	0.092	145.882	186	0.756	0.468	0.667	0.079	a, d, p, r	8
Tr8	28	0.877	1.333	0.767	0.617	0.765	0.198	62.825	195	0.564	0.636	0.525	0.183	2xa, d, p	7

Table S2: Observed and predicted activity, and SMILES representation of Tr1, Tr2, Tr3, Tr4, Tr5, Tr6 and Tr8

Set No.	Mol. No.	Activity (<i>pKi</i> nM)		SMILES
		Observed	Predicted	
Training set 1	Tr1-1	4.328	4.702	<chem>O=C1N(C(=N[C@]1/C2=C([H])C([H])=C([H])C([H])=C2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C(C#N)=C4[H])N([H])[H])C([H])([H])[H]</chem>
	Tr1-2	2.083	2.429	<chem>O=C1C([H])=C(OC=2/C1=C(/O[H])C([H])=C(O[H])C=2[H])C3=C(O[H])C([H])=C(O[H])C([H])=C3[H]</chem>
	Tr1-3	5.495	5.881	<chem>O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([H])=C([H])C=1[F])[C@@]2([H])C([H])([H])N/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]</chem>
	Tr1-4	5.770	4.664	<chem>O=C3N(C([H])([H])C([H])([H])C=5C([H])=C(O/C2=C([H])C([H])=C1N=C(N(C([H])([H])C1=C2[H])[C@]([H])(C([H])([H])C3([H])[H])[C@]4([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C4([H])[H])N([H])[H])C([H])([H])C=5[H])[C@@]6([H])C([H])([H])C([H])([H])OC([H])([H])C6([H])[H]</chem>
	Tr1-5	6.398	5.595	<chem>O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C(C([Cl])=C1[H])N([H])C(=O)C([H])([H])N2C([H])([H])C([H])([H])C2([H])[H])N([H])[H])C=3C(=N[S]C=3C([H])([H])[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H]</chem>
	Tr1-6	5.921	6.211	<chem>O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]</chem>
	Tr1-7	2.260	2.421	<chem>O=C3OC=2C(OC([H])([H])[C@]([H])(O[H])C(O[H])C([H])([H])[H])C([H])([H])[H])=C1OC([H])=C([H])C1=C(OC([H])([H])[H])C=2C([H])=C3[H]</chem>
	Tr1-8	2.208	2.469	<chem>O=C3O/C2=C([H])([H])C([H])=C(C([H])([H])C([H])([H])C([H])=C(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C=1OC([H])=C([H])C=1C([H])=C2C([H])=C3[H]</chem>
	Tr1-9	4.879	5.050	<chem>N#C/C1=C([F])C([H])=C([H])C(=C1[H])C=2[S]/C(=C(/[H])C=2[H])[C@@]35N=C(N(C(=O)[C@]3([H])C([H])([H])N/C4=C([H])C([H])=C([F])C([H])=C4[H])C5([H])[H])C([H])([H])[H])N([H])[H]</chem>
	Tr1-10	6.252	6.068	<chem>O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([F])=C([F])C=1[H])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]</chem>
	Tr1-11	6.319	6.430	<chem>O=C2N(C(=N[C@]5(C=1C([H])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)[C@]4([H])C([H])([H])C4([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]</chem>
	Tr1-12	6.347	5.994	<chem>O=C2N(C(=N[C@]4(C=1C([Cl])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]</chem>
	Tr1-13	6.252	6.360	<chem>O=C2N(C(=N[C@]5(C=1C([F])=C([H])C([H])=C([F])C=1[H])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)[C@]4([H])C([H])([H])C4([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]</chem>

Tr1-14	3.418	4.677	O=C3N/C(=N\ [H])N([H])[C@]/C2=C\ [H])C1=C([S]C([H])=C1[H])C([H])=C2[H])(C3([H])[H])C([H])([H])[H]C([H])([H])C4=C([H])C([H])=C([H])C(=C4[H])C(=O)N([H])C([H])([H])C5=C([H])C([H])=C([H])C([H])=C5[H]
Tr1-15	5.796	5.567	O=C1N/C(=N\ [H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@@]([H])N([H])C(=O)N([H])C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H]C([H])([H])[H]
Tr1-16	5.495	5.438	O=C1N/C(=N\ [H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]3([H])C([H])([H])N(C(=O)C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])C3([H])[H]C([H])([H])[H]
Tr1-17	5.409	6.156	O=C1N/C(=N\ [H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@@]([H])N([H])C(=O)C3=C([H])C([H])=NC([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H]C([H])([H])[H]
Tr1-18	3.056	2.892	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([Cl])C([H])=C1[H])N([H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C([H])C([H])=C3[H]
Tr1-19	3.398	3.214	O=C(N([H])C(=NC([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])N([H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]
Tr1-20	5.592	5.611	O=[S]3(=O)N/C(=N\ [H])N([H])[C@](C=1[S]C([H])=C(C=1[H])C2=C([H])C([H])=C([H])C(C#N)=C2[H])(C3([H])[H])C([H])([H])[H]C([H])([H])[H]
Tr1-21	6.000	5.477	O=C(/C1=N/C([H])=C(/N=C1/[H])C([H])([H])[H]N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H]C([H])([H])[H]
Tr1-22	7.023	5.767	O=C(/C1=N/C([H])=C([Cl])C([H])=C1[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]
Tr1-23	5.036	4.242	[H]/C5=C(/C([H])=C1C(O[C@]([H])([C@]3([C@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H])=C5[H])C6=C([H])N=C([H])N=C6[H]
Tr1-24	5.796	6.079	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])C([H])([H])[H])C4([H])[H]N([H])[H]C([H])([H])[H]
Tr1-25	5.056	5.055	[H]/C4=C(/C([H])=C1C(O[C@]([H])([C@]3([C@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])C([H])([H])C([H])([H])C([H])([H])[H])=C4[H])C5=C([H])N=C([H])C(C#CC([H])([H])[H])=C5[H]
Tr1-26	5.418	5.626	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])C([H])([H])[H]C([H])([H])C([H])([H])C=5/N=C(/[H])C([Cl])=C([H])C=5[H]
Tr1-27	5.328	5.728	O=C3N(C(=N[C@](C=1C([H])=C([S]C=1[H])C2=C([H])C(C#CC([H])([H])C([H])=C([H])N=C2[H])(C3([H])[H])C([H])([H])[H]N([H])[H])C([H])([H])[H])
Tr1-28	4.678	4.828	N#CC=1C([H])=C(C([H])=C([H])C=1[H])C=2[S]C([H])=C(C=2[H])[C@]3(N=C(N(C(=O)C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]

	Tr1-29	4.983	5.445	O=C(OC([H])([H])[C@@]([H])(N3C(=N/C2=C([H])C([H])=C(O/C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])=C2C3([H])([H])N([H])[H])[C@]4([H])C([H])([H])OC([H])([H])C([H])([H])C4([H])[H])N([C@@]5([H])C([H])([H])C([H])([H])C([H])([H])C5([H])[H])C([H])([H])[H])
	Tr1-30	5.678	5.694	O=C1N(C(=N[C@@]1(C=2C([H])=C(C([H])=C([H])C=2[H])C3=C([H])C([H])=C([H])N=C3[H])[C@@]4([H])C([H])([H])C4([H])[H])N([H])[H])C([H])([H])[H]
Training set 2	Tr2-1	6.137	6.007	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])([H])N([H])[H])C([H])([H])[H])
	Tr2-2	4.143	3.730	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C([F])=C([H])C([H])=C3[H])N([H])[H])C([H])([H])[H]
	Tr2-3	6.097	5.963	O=C3N(C(=N[C@](C=1C([H])=C([S]C=1[Cl])C=2C([H])=C(C#CC([H])([H])[H])C([H])=NC=2[H])(C3([H])([H])C([H])([H])[H])N([H])[H])C([H])([H])[H])
	Tr2-4	6.620	6.016	O=[S]3(=O)N(C(=N[C@@](C=1[S])/C(=C(/[H])C=1[Cl])C2=C([H])C(C#C([H])([H])[H])=C([H])N=C2[H])(C([H])([H])[H])C3([H])([H])N([H])[H])C([H])([H])[H]
	Tr2-5	6.051	5.930	O=C2N(/C(=N\([H])N([H])[C@]4(C=1C([Cl])=C([H])C([H])=C([F])C=1[H])[C@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])[H])C4([H])([H])C([H])([H])[H])
	Tr2-6	4.668	3.815	[Cl]C=5C([H])=C([H])C([H])=C(/C3=C([H])C([H])=C2OC([C@@]4([C@]1(N=C(OC1([H])([H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])C([H])([H])[H])C([H])([H])[H])C=5[H]
	Tr2-7	4.726	3.795	[Cl]C=5C([H])=C(/C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])([H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])=C([F])C=5[H]
	Tr2-8	4.668	3.811	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@@]4([C@]1(N=C(OC1([H])([H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C5=NC([H])=C(C#N([H])=C5C([H])([H])[H])
	Tr2-9	2.520	3.799	O=C(N([H])C3=C([H])C([H])=C2OC([C@@]4([C@]1(N=C(OC1([H])([H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])C([H])([H])[H])C([H])([H])C=5/N=C(/[H])C([Cl])=C([H])C=5[H]
	Tr2-10	7.023	6.532	O=C(/C1=N/C([H])=C([Cl])C([H])=C1[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])([H])C([H])([H])[H])C([H])([H])[H])
	Tr2-11	4.553	5.159	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C(C([Cl])=C1[H])N([H])[S](=O)(=O)C([H])([H])[H])N([H])[H])C=2C(=N[S]C=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]
	Tr2-12	5.194	5.263	O=C1N(/C(=N\([H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])N(C(=O)C([H])([H])[C@]3([H])C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C4([H])[H])C([H])([H])[H])
	Tr2-13	5.854	6.085	O=C1N(/C(=N\([H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]5([H])C([H])([H])C([H])([H])C([H])([H])C5([H])[H])

			H)C([H])([H])[C@]([H])(N([H])C(=O)N([H])C3=NC=4C(/N=C3/[H])=C([H])C([H])=C([H])C=4[H])C([H])([H])C([H])([H])C5([H])[H])C([H])([H])[H]
Tr2-14	7.000	6.919	O=C1N/C(=N\ [H])N([H])[C@]1(C([H])([H])C([H])([H])[C@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])(N([H])C(=O)N([H])C3=C([H])C([H])=C([Cl])C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])[H]
Tr2-15	5.699	5.818	O=[S]2(=O)N/C(=N/[H])N([H])[C@]4/C1=C([H])C([F])=C([H])C([H])=C1[F])[C@]2([H])C([H])([H])N/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H]C4([H])[H]C([H])([H])[H]
Tr2-16	5.569	6.014	O=[S]2(=O)N/C(=N/[H])N([H])[C@]4/C1=C([H])C([H])=C([H])C([H])=C1[H])[C@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([H])C(=C3[H])C([H])([H])OC([H])([H])[H]C4([H])[H]C([H])([H])[H]
Tr2-17	6.252	6.085	O=C2N(C(=N[C@]4(C=1C([H])=C([F])C([H])=C([H])C=1[F])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H])C4([H])[H]N([H])[H])C([H])([H])[H]
Tr2-18	5.066	5.583	O=[S]2(=O)N/C(=N/[H])N([H])[C@@]4/C1=C([H])C([H])=C([H])C([H])=C1[H])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([H])C([H])=C3[H])C4([H])[H]C([H])([H])[H]
Tr2-19	5.377	5.569	O=[S]2(=O)N/C(=N/[H])N([H])[C@@]5/C1=C([H])C([H])=C([H])C([H])=C1[H])[C@@]2([H])C([H])([H])N/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])[C@@]4([H])C([H])([H])C4([H])[H]C5([H])[H]C([H])([H])[H]
Tr2-20	3.806	3.826	O=[S]2(=O)N/C(=N\ [H])N([H])[C@@]4/C1=C([H])C([H])=C([H])C([H])=C1[H])[C@@]2([H])C([H])([H])N/C3=C([H])C(=C([H])C([H])=C3[H])C([H])([H])[H]C4([H])[H]C([H])([H])[H]
Tr2-21	5.495	5.751	O=C(N2C([H])([H])[C@@]1(N([H])C(=N[H])N([S](=O)(=O)[C@@]1([H])C2([H])[H])C([H])([H])[H])C3=C([H])C(=C([H])C([H])=C3[F])N([H])C(=O)C4=NC([H])=C([F])C([H])=C4[H])C([H])([H])[H]
Tr2-22	6.161	5.885	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([H])=C([F])C=1[H])[C@@]2([H])C([H])([H])N/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])C([H])([H])[H])C4([H])[H]N([H])[H])C([H])([H])[H]
Tr2-23	6.167	5.432	O=C2N(C(=N[C@]5(C=1C([F])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([Cl])C(=N3)[C@]4([H])C([H])([H])C4([H])[H]C5([H])[H]N([H])[H])C([H])([H])[H]
Tr2-24	4.046	4.289	O=C(C=1C([H])=C([H])C([H])=C([H])C=1[H])C4=C([H])C2=C(N=C(N(C2([H])[H])C([H])([H])C([H])([H])C(=O)N(C([H])([H])[H])C3([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C3([H])[H]N([H])[H])C([H])=C4[H]
Tr2-25	3.409	3.826	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C([H])C([H])=C3[H]
Tr2-26	5.699	5.561	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C(C([Cl])=C1[H])N([H])C(=O)C([H])([H])N([H])C([H])([H])C([H])([H])C([H])([H])N([H])[H])C=2C(=N[S]C=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]

	Tr2-27	3.553	3.827	O=C(N([H])C(=NC([H])([H])C=1C([H])=C([H])C([H])=C2C=1C([H])=C([H])C([H])=C2[H])N([H])[H])C=3C(=NOC=3C([H])([H])[H])C4=C([H])C([H])=C([H])C([H])=C4[H]
	Tr2-28	2.083	3.595	O=C1C([H])=C(OC=2/C1=C(/O[H])C([H])=C(O[H])C=2[H])C3=C(O[H])C([H])=C(O[H])C([H])=C3[H]
	Tr2-29	4.367	4.092	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C(=C4[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]
	Tr2-30	4.538	4.486	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C(F)=C4[H])N([H])[H])C([H])([H])[H]
Training set 3	Tr3-1	5.097	4.815	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C(OC([H])([H])[H])=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]
	Tr3-2	2.083	2.557	O=C1C([H])=C(OC=2/C1=C(/O[H])C([H])=C(O[H])C=2[H])C3=C(O[H])C([H])=C(O[H])C([H])=C3[H]
	Tr3-3	2.854	2.513	O=C2C=1C(O[H])=C([H])C(O[H])=C([H])C=1O/C(=C2/O[H])C3=C([H])C([H])=C(O[H])C(O[H])=C3[H]
	Tr3-4	4.060	4.960	O=C(N([H])C(=NC([H])([H])C1=C([H])C=2C(C([H])=C1[H])=C([H])C([H])=C([H])C=2[H])N([H])[H])C=3C(=N[S]C=3C([H])([H])[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H]
	Tr3-5	4.301	5.276	O=C(N([H])C(=NC([H])([H])C=1C([H])=C([H])C([H])=C2C=1C([H])=C([H])C([H])=C2[H])N([H])[H])C=3C(=N[S]C=3C([H])([H])[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H]
	Tr3-6	4.553	5.098	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C(=C1[H])C([H])([H])[H])C([H])([H])[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]
	Tr3-7	4.854	4.962	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C([Cl])=C1[H])C([H])=C([H])C([H])([H])C([H])([H])O[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]
	Tr3-8	3.745	4.640	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C([Cl])=C1[H])C2=C([H])N=C([H])C([H])=C2[H])N([H])[H])C=3C(=NOC=3C([H])([H])[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H]
	Tr3-9	5.796	5.784	[F]C=1C([H])=C([F])C(=C([H])C=1[H])[C@@]24N=C(N(C(=O)[C@]2([H])C([H])([H])N/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])O[H])C4([H])[H])C([H])([H])[H])N([H])[H]
	Tr3-10	5.276	5.444	O=C2N(C(=N[C@]4(C=1C([F])=C([F])C([H])=C([H])C=1[F])[C@@]2([H])C([H])([H])N/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]
	Tr3-11	6.569	6.182	O=C2N(C(=N[C@]5(C=1C([F])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)[C@]4([H])C([H])([H])C4([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]
	Tr3-12	4.521	5.101	O=C1N/C(=N\([H])N([H])[C@]1(C([H])([H])C([H])([H])[C@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])

			<chem>C([H])([H])[C@@]([H])(N([H])C(=O)N([H])C3=C([Cl])C([H])=C([H])C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H]C([H])([H])[H]</chem>
Tr3-13	5.201	5.723	<chem>O=[S](=O)(N3C([H])([H])[C@@]([H])(C([H])([H])[C@@]1(N([H])C(=N([H])N(C1=O)C([H])([H])[H]C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H]C([H])([H])C([H])([H])C3([H])[H]C([H])([H])C([H])([H])C([H])([H])[H]</chem>
Tr3-14	5.638	5.152	<chem>O=C1N(/C(=N\([H])N([H])[C@@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H]C([H])([H])[C@@]4([H])C([H])([H])[C@@]([H])(N([H])[C@@]3([H])C([H])([H])C([H])([H])C([H])([H])C3([H])[H]C([H])([H])C([H])([H])C4([H])[H]C([H])([H])[H])</chem>
Tr3-15	5.357	4.842	<chem>O=C2N(C(=N[C@@]5C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)[C@@]4([H])C([H])([H])C4([H])[H])C([H])([H])[H]C5([H])[H]N([H])[H]C([H])([H])[H]</chem>
Tr3-16	6.899	6.370	<chem>O=C(/C1=N/C([H])=C(C([H])=C1[H])C([F])([F])[F]N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@@]3(N([H])C(=N([H])N([S])(=O)(=O)C3([H])[H])C([H])([H])[H]C([H])([H])[H]</chem>
Tr3-17	7.023	7.339	<chem>O=C(/C1=N/C([H])=C([Cl])C([H])=C1[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@@]3(N([H])C(=N([H])N([S])(=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]</chem>
Tr3-18	5.101	5.035	<chem>O=C(N([H])C3=C([H])C([H])=C2OC([C@@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C(=NC=5[H])OC([H])([H])[H]</chem>
Tr3-19	5.423	4.660	<chem>O=C(N([H])C3=C([H])C([H])=C2OC([C@@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])(C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C([Cl])C([H])=C5[H]</chem>
Tr3-20	5.190	4.669	<chem>O=C(N([H])C3=C([H])C([H])=C2OC([C@@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C([Cl])C([H])=C5C([H])([H])[H]</chem>
Tr3-21	4.504	4.800	<chem>O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C5=NC([H])=C([Cl])C([H])=C5C([H])([H])[H]</chem>
Tr3-22	4.620	4.753	<chem>O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C=5/N=C(/[H])C([Cl])=C([H])C=5[F]</chem>
Tr3-23	5.886	5.628	<chem>O=C2N(/C(=N\([H])N([H])[C@@]4(C=1C([F])=C([H])C([H])=C([Cl])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])[H])C4([H])[H]C([H])([H])[H]</chem>
Tr3-24	2.658	2.751	<chem>O=C4N(C(=N[C@@]([C=1C([H])=C([H])C([H])=C(C=1[H])C2=C([H])C(O)C([H])([H])[H])=C([H])C([H])=C2[H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C4([H])[H])N([H])[H]C([H])([H])[H]</chem>
Tr3-25	3.022	3.645	<chem>O=C4N(C(=N[C@@]([C=1C([H])=C([H])C([H])=C(C=1[H])C2=C([H])C(C#N)=C([H])C([H])=C2[H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C4([H])[H])N([H])[H]C([H])([H])[H]</chem>
Tr3-26	5.244	4.160	<chem>N#CC=1C([H])=C(C([H])=C([H])C=1[H])C=2C([H])=C([S]C=2[H])[C@@]3(N=C(N(C(=O)C3([H])[H])C([H])([H])[H])N([H])[H]C([H])([H])[H]</chem>

	Tr3-27	4.106	4.560	O=C(OC([H])([H])[C@@]([H])(N3C(=N/C2=C([H])C([H])=C(O/C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])=C2C3([H])([H])N([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H])N([C@]5([H])C([H])([H])C([H])([H])C([H])([H])C([H])C([H])([H])C5([H])([H])C([H])([H])[H])
	Tr3-28	5.229	5.463	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])C([H])([H])([H])C([H])([H])([H])C4([H])([H])N([H])([H])C([H])([H])[H])
	Tr3-29	4.569	4.567	O=C1N(C(=N[C@@]1(/C2=C([H])C(=C([H])C([H])=C2[H])C3=C([H])N=C([H])C(C#N)=C3[H])[C@@]4([H])C([H])([H])C4([H])([H])N([H])([H])C([H])([H])([H])[H])
	Tr3-30	4.796	4.562	O=C1N(C(=N[C@]1(/C2=C([H])C(=C([H])C([H])=C2[H])C3=C([H])N=C([H])C([F])=C3[H])[C@@]4([H])C([H])([H])C4([H])([H])N([H])([H])C([H])([H])([H])[H])
Training set 4	Tr4-1	4.812	4.551	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)C([H])([H])([H])C([H])([H])([H])C4([H])([H])N([H])([H])C([H])([H])[H])
	Tr4-2	2.357	3.061	O=C4N(C(=N[C@@]1(/C1=C([H])C([H])=C([H])C(=C1[H])C2=C([H])N=C([H])C([H])=C2[H])C3=C([H])C([H])=C([H])C([H])=C3[H])C4([H])([H])N([H])([H])C([H])([H])[H])
	Tr4-3	5.215	4.697	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)C([H])([H])([H])C([H])([H])([H])C([H])([H])([H])C4([H])([H])N([H])([H])C([H])([H])[H])
	Tr4-4	4.921	4.725	[H]/C5=C(/C([H])=C1C(O[C@@]4([C@]3([C@@]1)2N=C(OC2([H])([H])N([H])([H])C([H])([H])OC3([H])([H])C([H])([H])C([H])([H])C4([H])([H])=C5[H])C6=C([H])N=C([H])C(C#CC([H])([H])([H])=C6[H])
	Tr4-5	4.553	4.649	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@@]4([C@]1(N=C(OC1([H])([H])N([H])([H])C2=C3[H])C([H])([H])C4([H])([H])C=5/N=C(/[H])C(C#N)=C([H])C=5[Cl])
	Tr4-6	6.114	5.707	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([F])=C([F])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])([H])C([H])([H])([H])C4([H])([H])N([H])([H])C([H])([H])[H])
	Tr4-7	5.213	4.680	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1)N=C(OC1([H])([H])N([H])([H])C2=C3[H])C([H])([H])C4([H])([H])C([H])([H])([H])C([H])([H])([H])C5=NC([H])=C(/N=C5/[H])OC([H])([H])([H])
	Tr4-8	7.023	7.338	O=C(/C1=N/C([H])=C([Cl])C([H])=C1[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])([H])C([H])([H])([H])C([H])([H])[H])
	Tr4-9	6.312	6.593	O=C(/C1=N/C([H])=C([F])C([H])=C1[H])N([H])C2=C([F])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])([H])C([H])([H])([H])C([H])([H])[H])
	Tr4-10	5.337	5.521	O=[S]3(=O)N(/C(=N[H])N([H])[C@](C=1[S]C([H])=C(C=1[H])C2=C([H])C([H])=C([F])C(C#N)=C2[H])(C3([H])([H])C([H])([H])([H])C([H])([H])[H])
	Tr4-11	3.092	3.869	O=C(N([H])C1=C([H])C(=C([H])C(=C1[H])C([F])([F])C([F])([F])N([H])C2=C([H])C(=C(C([H])=C2[H])N(C([H])([H])([H])C([H])([H])([H])C(=

			O)N([H])C([H])([H])C([H])([H])C([H])([H])N3C([H])([H])C([H])([H])OC([H])([H])C3([H])[H]
Tr4-12	4.041	4.337	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([Cl])C([H])=C1[H])N([H])([H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]
Tr4-13	4.559	4.549	O=C1N(/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@@]4([H])C([H])([H])[C@@]([H])N([H])C(=O)N([H])C3=C(OC([H])([H])[H])C([H])=C([H])C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])[H]
Tr4-14	5.538	5.114	O=C1N(/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@]2([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]3([H])C([H])([H])N(C(=O)OC(C([H])([H])[H])C([H])([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])[H]
Tr4-15	5.456	5.861	O=[S]2(=O)N(/C(=N/[H])N([H])[C@]4/C1=C([H])C([H])=C([F])C([H])=C1[H])[C@]2([H])C([H])([H])N/C3=N/C(=C/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H]C4([H])[H]C([H])([H])[H]
Tr4-16	5.523	5.464	O=[S]2(=O)N(/C(=N/[H])N([H])[C@]4/C1=C([H])C([H])=C([F])C([H])=C1[F])[C@]2([H])C([H])([H])N/C3=N/C(=C/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H]C4([H])[H]C([H])([H])[H]
Tr4-17	6.000	6.213	O=[S]2(=O)N(/C(=N/[H])N([H])[C@]4/C1=C([H])C([F])=C([H])C([H])=C1[F])[C@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([H])C(=C3[H])C([H])([H])OC([H])([H])[H]C4([H])[H]C([H])([H])[H]
Tr4-18	5.523	5.656	O=[S]2(=O)N(/C(=N/[H])N([H])[C@]4/C1=C([H])C([H])=C([H])C([H])=C1[H])[C@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H]C4([H])[H]C([H])([H])[H]
Tr4-19	5.523	5.324	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([F])=C([F])C=1[F])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])[H])C4([H])([H])N([H])[H])C([H])([H])[H]
Tr4-20	5.409	5.226	O=C2N(C(=N[C@]4/C1=C([H])C([Cl])=C([H])C([H])=C1[H])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])[H])C4([H])[H]N([H])[H]C([H])([H])[H]
Tr4-21	5.285	5.762	O=[S](=O)N(C=2C([H])=C(C([H])=C([H])[C@@]1([H])C([H])([H])[C@]1([H])C([H])([H])[H])C([H])=C(C=2[H])C3=NN=C(O3)[C@@]([H])([H])C([H])([H])C=4C([H])=C([H])C([H])=C([H])C=4[H])[N+]([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])[H]C([H])([H])[H]
Tr4-22	4.801	4.617	O=C(/C1=C([H])C([H])=C([H])C(=C1[H])C([H])([H])N4C(=NC=3C([H])=C([H])C(OC=2C([H])=C([H])C([H])=C([H])C=2[H])=C([H])C=3C4([H])[H])N([H])[H]N(C([H])([H])[H])C5([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C5([H])[H]
Tr4-23	4.458	4.266	O=C2N([H])C1=C([H])C([H])=C([H])C([H])=C1N([H])C3=C2C([H])=C([H])C(=C3[H])C(=O)N([H])C4=N/C(=C/[H])N4[H])C5=C([H])C([H])=NC([H])=C5[H]
Tr4-24	3.770	4.098	O=C(N([H])C(=NC([H])([H])C=1C([H])=C([H])C([H])=C2C=1C([H])=C([H])C([H])=C2[H])N([H])[H])C=3C(=NOC=3C([H])([H])[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H]

	Tr4-25	3.921	4.015	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C([Cl])=C1[H])C=2C([H])=C([H])[S]C=2[H])N([H])([H])C=3C(=NOC=3C([H])([H])([H])C4=C([H])C([H])=C(OC([H])([H])([H])C([H])=C4[H])
	Tr4-26	4.367	4.304	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C([Cl])=C1[H])C([H])=C([H])([H])N([H])([H])C=2C(=NOC=2C([H])([H])([H])C3=C([H])C([H])=C(OC([H])([H])([H])C([H])=C3[H])
	Tr4-27	4.921	4.297	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C(C([Cl])=C1[H])N([H])([H])N([H])([H])C=2C(=NOC=2C([H])([H])([H])C3=C([H])C([H])=C(OC([H])([H])([H])C([H])=C3[H])
	Tr4-28	4.538	4.497	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])([H])C=2C(=N[S]C=2C([H])([H])([H])C3=C([H])C([H])=C(OC([H])([H])([H])C([H])=C3[H])
	Tr4-29	2.083	2.183	O=C1C([H])=C(OC=2/C1=C(/O[H])C([H])=C(O[H])C=2[H])C3=C(O[H])C([H])=C(O[H])C([H])=C3[H]
	Tr4-30	4.509	4.260	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C=4/N=C(/[H])C([H])=NC=4[H])N([H])([H])C([H])([H])[H])
Training set 5	Tr5-1	4.959	4.253	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C([H])=C4[H])N([H])([H])C([H])([H])[H])
	Tr5-2	2.083	1.933	O=C1C([H])=C(OC=2/C1=C(/O[H])C([H])=C(O[H])C=2[H])C3=C(O[H])C([H])=C(O[H])C([H])=C3[H]
	Tr5-3	2.193	3.693	O=C1C4=C(O/C(=C1/C([H])([H])C([H])=C(C([H])([H])([H])C([H])([H])[H])C=2C([H])=C([H])C(O[H])=C([H])C=2O[H])C3=C(OC(C([H])=C3[H])(C([H])([H])([H])C([H])([H])([H])C([H])=C4O[H])
	Tr5-4	4.071	4.264	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C([Cl])=C1[H])C([H])=C([H])C([H])([H])C([H])([H])C([H])([H])N([H])([H])C=2C(=NOC=2C([H])([H])([H])C3=C([H])C([H])=C(OC([H])([H])([H])C([H])=C3[H])
	Tr5-5	4.824	4.906	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C([Cl])=C1[H])C([H])=C([H])C([H])([H])OC([H])([H])([H])N([H])([H])C=2C(=NOC=2C([H])([H])([H])C3=C([H])C([H])=C(OC([H])([H])([H])C([H])=C3[H])
	Tr5-6	4.530	3.861	O=C2N([H])C1=C([H])C([H])=C([H])C([H])=C1N([H])C=3/C2=C(/[H])C([H])=C(C=3[H])C(=O)N([H])C4=C([H])C([H])=NC([H])=C4[H]
	Tr5-7	5.495	5.414	[F]/C1=C/N=C/N=C1/OC([H])([H])([H])N3C([H])([H])[C@@]2(N=C(N(C(=O)[C@]2([H])C3([H])([H])C([H])([H])([H])N([H])([H])C4=C([H])C([H])=C([F])C([H])=C4[F])C([F])([F])[F])
	Tr5-8	6.276	5.639	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[F])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])([H])=C([F])C(=N3)C([H])([H])C([H])([H])([H])C4([H])([H])N([H])([H])C([H])([H])[H])
	Tr5-9	6.215	6.373	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])([H])=C([F])C(=N3)C([H])([H])C([H])([H])([H])C4([H])([H])N([H])([H])C([H])([H])[H])

Tr5-10	6.745	5.838	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[F])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H])C4([H])([H])N([H])[H])C([H])([H])[H]
Tr5-11	5.215	5.329	O=[S]2(=O)N/C(=N/[H])N([H])[C@]4/C1=C([H])C([H])=C([H])C([H])=C1[H])[C@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([H])C(=C3[H])C([H])([H])OC([H])([H])C([H])([H])[H])C4([H])([H])C([H])([H])[H]
Tr5-12	5.071	5.060	O=C1N/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]3([H])C([H])([H])N(C(=O)N([H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C3([H])[H])C([H])([H])[H]
Tr5-13	4.860	5.110	O=C1N/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@@]1([H])N([H])C(=O)N([H])[C@@]3([H])C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C([H])([H])C4([H])([H])C([H])([H])[H]
Tr5-14	4.907	4.904	O=C1N/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])N(C(=O)C([H])([H])[C@]3([H])C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])[H]
Tr5-15	5.367	4.898	O=C1N/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@@]1([H])N([H])[C@]3([H])C([H])([H])C([H])([H])C([H])([H])C3([H])[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])[H]
Tr5-16	5.886	5.039	O=C1N/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@@]1([H])N([H])C(=O)C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])[H]
Tr5-17	3.009	4.364	O=C(N([H])C1=C([H])C(=C(C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C(=O)N([H])C([H])([H])C([H])([H])C([H])([H])OC([H])([H])C([H])([H])N([H])C2=C([H])C([Cl])=C([H])C([H])=C2[H]
Tr5-18	6.785	6.728	O=C(/C1=N/C([H])=C(/N=C1/[H])OC([H])([H])[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S])(=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]
Tr5-19	7.023	6.646	O=C(/C1=N/C([H])=C([Cl])C([H])=C1[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S])(=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]
Tr5-20	5.039	4.997	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C([F])C([H])=C5[H]
Tr5-21	5.368	5.923	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C(=NC=5[H])OC([H])([H])[H]
Tr5-22	5.991	5.240	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C([Br])=C([H])C=5[H]

	Tr5-23	4.206	4.111	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@@]4([C@]1N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C5=NC([H])=C([Br])C([H])=N5
	Tr5-24	5.044	4.706	[H]/C4=C(/C([H])=C1C(OC([C@@]3([C@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])(C([H])([H])[H])C([H])([H])[H])=C4[H])C5=C([H])N=C([H])C(C#CC([H])([H])[H])=C5[H]
	Tr5-25	4.910	4.188	[H]/C4=C(/C([H])=C1C(OC([H])([H])[C@@]3([C@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])=C4[H])C5=C([H])N=C([H])C(C#CC([H])([H])[H])=C5[H]
	Tr5-26	4.932	5.132	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])(C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C([F])=C([H])C=5[H]
	Tr5-27	4.863	5.872	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])C([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]
	Tr5-28	6.770	6.896	O=C3N(C(=N[C@](C=2[S])C(C=1C([H])=C(C#CC([H])([H])[H])C([H])=N(C=1[H])=C([H])C=2[Cl])(C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]
	Tr5-29	4.523	4.762	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C([Cl])=C([H])C([H])=C3[H])N([H])[H])C([H])([H])[H]
	Tr5-30	3.222	4.427	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C(OC([H])([H])[H])=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]
Training set 6	Tr6-1	5.046	4.937	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C([Cl])=C4[H])N([H])[H])C([H])([H])[H]
	Tr6-2	2.083	2.785	O=C1C([H])=C(OC=2/C1=C(/O[H])C([H])=C(O[H])C=2[H])C3=C(O[H])C([H])=C(O[H])C([H])=C3[H]
	Tr6-3	4.569	3.550	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Br])=C([H])C([Cl])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]
	Tr6-4	3.658	3.481	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C([F])C([H])=C3[H]
	Tr6-5	6.071	6.056	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([H])=C([F])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]
	Tr6-6	4.510	4.590	O=C2N([H])C1=C([H])C([H])=C([H])C([H])=C1N([H])C=3/C2=C(/[H])C([H])=C(C=3[H])C(=O)N([H])C4=NC=5C(N4[H])=C([H])N=C([H])C=5[H]
	Tr6-7	4.533	4.336	O=C2N([H])C=1C([H])=C([H])C([H])=C([H])C=1N([H])C3=C2C([H])=C([H])C(=C3[H])C(=O)N([H])C4=N/C(=C(/[H])N4[H])C5=C([H])C([H])=C([F])C([H])=C5[H]

Tr6-8	4.613	4.529	O=C2N([H])C1=C([H])C([H])=C([H])C([H])=C1N([H])C=3/C2=C(/[H])C([H])=C(C=3[H])C(=O)N([H])C4=NC=5C(N4[H])=C([H])C([F])=C([H])C=5[H]
Tr6-9	2.863	3.571	O=C3OC=2C(OC([H])([H])[H])=C1OC([H])=C([H])C1=C(OC([H])([H])C([H])=C(C([H])([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C=2C([H])=C3[H]
Tr6-10	5.194	4.977	N#C/C1=C([H])C(=C([H])C([H])=C1[H])C2=C([H])[S]/C(=C2/[H])[C@@]35N=C(N(C(=O)[C@]3([H])C([H])([H])N(C=4N=C(C([H])=C([H])C=4[H])C([F])([F])[F])C5([H])[H])C([H])([H])[H])N([H])[H]
Tr6-11	5.854	5.987	O=C2N(C(=N[C@]4(C=1C([H])=C(C#N)C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]
Tr6-12	6.036	6.054	O=C2N(C(=N[C@]4(C=1C([F])=C([Cl])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]
Tr6-13	6.222	6.367	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]
Tr6-14	5.959	6.077	[F]C=1C([H])=C([F])C(=C([H])C=1[H])[C@@]24N=C(N(C(=O)[C@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([F])([F])C([H])([H])[H])C4([H])[H])C([H])([H])[H])N([H])[H]
Tr6-15	5.086	5.161	O=[S]2(=O)N(/C(=N/[H])N([H])[C@]4/C1=C([H])C([H])=C([H])C([H])=C1[H])[C@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])[H]
Tr6-16	4.233	4.775	O=C1N(/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@]2([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]4([H])C([H])([H])[C@]([H])N([H])C(=O)C([H])([H])C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])[H]
Tr6-17	6.357	6.078	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]
Tr6-18	5.310	5.233	O=C1N(/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])[C@]3([H])C([H])([H])N(C(=O)C([H])([H])C([H])([H])C([H])([H])C([H])([H])[H])C([H])([H])C3([H])[H])C([H])([H])[H]
Tr6-19	3.620	3.483	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([Cl])C([H])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C([F])C([H])=C3[H]
Tr6-20	6.523	6.065	O=C(/C1=N/C([H])=C(C([H])=C1[H])C([H])([H])[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]
Tr6-21	7.023	7.183	O=C(/C1=N/C([H])=C([Cl])C([H])=C1[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N[H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]

	Tr6-22	5.278	5.484	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C([H])([H])[H])C([H])([H])C5=NC([H])=C(/N=C5/[H])C([F])([F])[H]
	Tr6-23	4.466	4.641	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@@]4([C@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C=5/N=C(/[H])C(C#N)=C([H])C=5[H]
	Tr6-24	4.971	4.712	[H]/C4=C(/C([H])=C1C(O[C@]([H])([C@]3([C@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])C([H])([H])C([H])([H])=C4[H])C5=C([H])N=C([H])C(C#CC([H])([H])[H])=C5[H]
	Tr6-25	6.328	6.183	O=C2N(/C(=N\([H])N([H])[C@]4(C=1C([F])=C([H])C([F])=C([H])C=1[H])[C@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])[H])C4([H])[H])C([H])([H])[H]
	Tr6-26	4.914	4.999	O=C(N([C@@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])[H])C([H])([H])C([H])([H])[C@]1([H])(N4C(=N/C3=C([H])C([H])=C(OC=2C([H])=C([H])C([H])=C([H])C=2[H])C([H])=C3C4([H])[H])N([H])[H])[C@]5([H])C([H])([H])OC([H])([H])C([H])([H])C5([H])[H]
	Tr6-27	4.432	3.579	O=C1N(C(=N[C@]1(/C2=C([H])C([H])=C([H])C([H])=C2[H])C3=C([H])C(C#N)=C([H])C([H])=C3[H])N([H])[H])C([H])([H])[H]
	Tr6-28	4.337	4.989	O=C1N(C(=N[C@]1(/C2=C([H])C([H])=C([H])C([H])=C2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C(OC([H])([H])C([H])([H])=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]
	Tr6-29	3.420	3.929	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H])N([H])[H])C([H])([H])[H]
	Tr6-30	5.373	5.437	[F]/C1=C([H])C([H])=C(C([H])=C1[H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C3=NN=C(O3)[C@@]([H])([H])([H])C([H])([H])C=4C([H])=C([H])C([H])=C([H])C=4[H])[N+](([H])([H])[H])N(C([H])([H])[H])[S](=O)(=O)C([H])([H])[H])C([H])([H])[H]
Training set 8	Tr8-1	2.721	4.622	O=C3N([H])[C@]([H])(C(=O)N([H])[C@]([H])([C@@]([H])(O[H])C([H])([H])N([H])C([H])([H])C1=C([H])C(=C([H])C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C([H])([H])C2=C([H])C([H])=C([H])C([H])=C2[H])C([H])([H])N3[H]
	Tr8-2	2.083	2.721	O=C1C([H])=C(OC=2/C1=C(/O[H])C([H])=C(O[H])C=2[H])C3=C(O[H])C([H])=C(O[H])C([H])=C3[H]
	Tr8-3	5.658	4.163	O=C3N(C([H])([H])C([H])([H])C=4C([H])=C(OC=2C([H])=C([H])C=1N=C(N(C([H])([H])C=1C=2[H])[C@]([H])(C([H])([H])C3([H])[H])C([H])(C([H])([H])[H])C([H])([H])N([H])[H])C([H])=C([H])C=4[H])[C@@]5([H])C([H])([H])C([H])([H])OC([H])([H])C5([H])[H]
	Tr8-4	5.886	6.572	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C(=O)N3[C@]([H])(C([H])([H])C([H])([H])C3([H])[H])C([H])([H])OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@]4([H])N([H])C([H])([H])C([H])([H])N(C4([H])[H])[S](=O)(=O)C([H])([H])[H]
	Tr8-5	3.097	3.190	[H]C=2C(O[H])=C([H])C=1OC=3C(OC=1C=2O[H])=C([H])C(O[H])=C4OC5=C(OC=34)C(O[H])=C([H])C(O[H])=C5[H]

Tr8-6	3.745	3.584	O=C(N([H])C(=NC([H])([H])C=1C([H])=C([H])C([H])=C2C=1C([H])=C([H])C([H])=C2[H])N([H])([H])C=3C(=NOC=3C([H])([H])([H])C4=C([H])C([H])=C([F])C([H])=C4[H])
Tr8-7	4.678	4.496	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])([H])C=2C(=NN([H])C=2C([H])([H])([H])C3=C([H])C([H])=C(OC([H])([H])([H])C([H])=C3[H])
Tr8-8	4.319	4.822	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C(O[H])C([Cl])=C1[H])N([H])([H])C=2C(=NOC=2C([H])([H])([H])C3=C([H])C([H])=C(OC([H])([H])([H])C([H])=C3[H])
Tr8-9	3.398	4.104	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])([H])C2=C(N(/N=C2/C([H])([H])([H])C([H])([H])([H])C3=C([H])C([H])=C(OC([H])([H])([H])C([H])=C3[H])
Tr8-10	6.046	6.051	N#C/C1=C([H])C=C([H])C([H])=C1[H]C2=C([H])[S]/C(=C2/[H])[C@@]35N=C(N(C(=O)[C@]3([H])C([H])([H])N/C4=N/C([H])=C(C([H])=N4)C([H])([H])([H])C5([H])([H])C([H])([H])([H])N([H])([H])
Tr8-11	5.585	4.767	O=C2N(C(=N[C@]5(C=1C([H])=C([F])C([H])=C([H])C=1[F])[C@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)[C@]4([H])C([H])([H])C4([H])([H])C([H])([H])([H])C5([H])([H])N([H])([H])C([H])([H])([H])
Tr8-12	6.187	6.215	O=C2N(C(=N[C@]5(C=1C([F])=C([H])C([H])=C([F])C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])([H])=C([Cl])C(=N3)[C@]4([H])C([H])([H])C4([H])([H])([H])C5([H])([H])N([H])([H])C([H])([H])([H])
Tr8-13	6.155	6.419	O=[S]2(=O)N/C(=N/[H])N([H])[C@]4/C1=C([H])C([H])=C([H])C([H])=C1[F])[C@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])([H])=C([H])C(=C3[H])C([H])([H])OC([H])([H])([H])C4([H])([H])C([H])([H])([H])
Tr8-14	6.155	5.634	O=[S]2(=O)N/C(=N/[H])N([H])[C@]4/C1=C([H])C([F])=C([F])C([H])=C1[F])[C@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])([H])=C([H])C(=C3[H])C([H])([H])OC([H])([H])([H])C4([H])([H])C([H])([H])([H])
Tr8-15	5.495	5.751	O=[S]2(=O)N/C(=N/[H])N([H])[C@]4/C1=C([H])C([F])=C([F])C([H])=C1[F])[C@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])([H])C([H])([H])([H])C4([H])([H])C([H])([H])([H])
Tr8-16	5.721	5.834	O=[S]2(=O)N/C(=N/[H])N([H])[C@]4/C1=C([H])C([H])=C([H])C([H])=C1[F])[C@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])([H])C([H])([H])([H])C4([H])([H])C([H])([H])([H])
Tr8-17	5.292	5.710	O=[S]2(=O)N/C(=N/[H])N([H])[C@]4/C1=C([H])C([H])=C([H])C([H])=C1[H])[C@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])([H])C([H])([H])([H])C4([H])([H])C([H])([H])([H])
Tr8-18	5.071	4.497	O=C1N(/C(=N\([H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C2([H])([H])C([H])([H])[C@]3([H])C([H])([H])N([H])C([H])([H])C([H])([H])C3([H])([H])C([H])([H])([H])
Tr8-19	7.000	6.926	O=C1N(/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])[C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C2([H])([H])C([H])([H])[C@]4([H])C([H])([H])[C@@]([H])([H])N([H])C(=O)N([H])C3=C([H])C([H])=C(OC([H])([H])([H])C([H])=C3[H])C([H])([H])C([H])([H])C4([H])([H])C([H])([H])([H])

Tr8-20	6.979	6.609	<chem>O=C/C1=N/C([H])=C(/N=C1/[H])OC([H])([H])[H]N([H])C2=C([H])C(=C([F])C([F])=C2[H])[C@]3(N([H])C(=N([H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]</chem>
Tr8-21	7.023	6.723	<chem>O=C/C1=N/C([H])=C([Cl])C([H])=C1[H]N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N([H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]</chem>
Tr8-22	5.148	5.062	<chem>[H]/C5=C(/C([H])=C1C(O[C@]([H])([C@]3([C@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H])=C5[H])C6=C([H])N=C([H])C/C#CC([H])([H])[H])=C6[H]</chem>
Tr8-23	4.061	4.521	<chem>[F]C([F])([F])C([H])([H])C([H])([H])[C@]3([H])O/C1=C([H])C([H])=C(C([H])=C1[C@]2(N=C(OC2([H])[H])N([H])[H])[C@]34C([H])([H])OC4([H])[H])C5=C([H])N=C([H])C/C#CC([H])([H])[H])=C5[H]</chem>
Tr8-24	3.987	4.479	<chem>O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C=5/N=C(/[H])C([F])=C([H])C=5[H]</chem>
Tr8-25	5.569	5.091	<chem>O=[S]3(=O)N(C(=N[C@]4/C1=C([H])C(=C([H])C([H])=C1[F])N([H])C(=O)C2=NC([H])=C(/N=C2/[H])C([F])([F])[H])[C@@]3([H])C([H])([H])OC4([H])[H])N([H])[H])C([H])([H])[H]</chem>
Tr8-26	6.108	5.121	<chem>O=C3N(C(=N[C@](C=2[S]C([H])=C(/C1=C([H])C(C#CC([H])([H])[H])=C([H])N=C1[H])C=2[H])(C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]</chem>
Tr8-27	3.721	3.891	<chem>O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=NC([H])=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]</chem>
Tr8-28	3.481	2.881	<chem>O=C1N(C(=N[C@]1/C2=C([H])C([H])=C([H])C([H])=C2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C([H])=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]</chem>

Table S3: Statistical parameters of decoy set screening

Parameters	Model	Tr2	Tr3	Tr3	Tr4	Tr5	Tr6	Tr7	Tr8
Total compounds in database (D)		1478	1478	1478	1478	1478	1478	1478	1478
Total number of actives in database (A)		30	30	30	30	30	30	30	30
Total hits (Ht)		125	42	437	332	194	106	69	148
Active hits (TP)		15	12	21	16	18	18	21	19
True negative (TN)		1338	1418	1032	1132	1265	1360	1400	1219
Enrichment factor or enhancement (E)		0.00	26.28	0.00	0.00	29.56	0.00	9.85	19.71
False negatives (FN = A - TP)		15	18	9	14	12	12	9	11
False positives (FP = Ht - TP)		110	30	416	316	183	88	48	229
Accuracy = (TP + TN)/(TP + TN + FP + FN)		0.92	0.97	0.71	0.78	0.87	0.93	0.96	0.84
Precision = TP/(TP + FP)		0.120	0.286	0.048	0.048	0.090	0.170	0.304	0.077
Sensitivity = TP/(TP + FN)		0.500	0.400	0.700	0.533	0.600	0.600	0.700	0.633
Specificity = TN/(TN + FP)		0.924	0.979	0.713	0.782	0.874	0.939	0.967	0.842
AUC curve		0.480	0.400	0.560	0.430	0.570	0.570	0.680	0.580

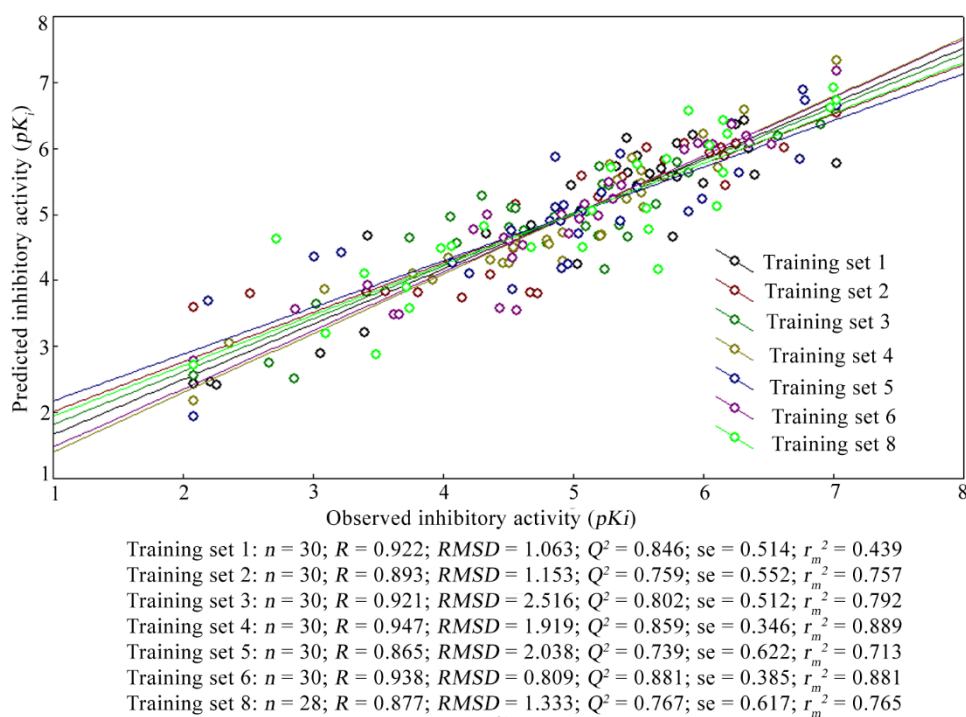


Figure S2: Observed and predicted activity of all training sets except Tr7

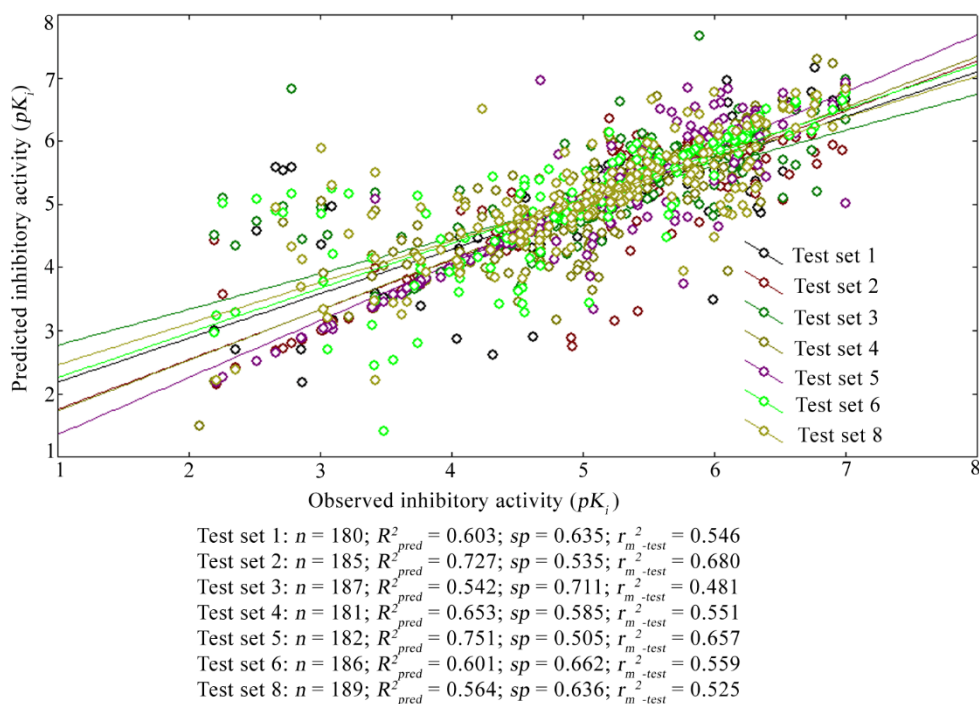


Figure S3: Observed and predicted activity of all test sets except Ts7

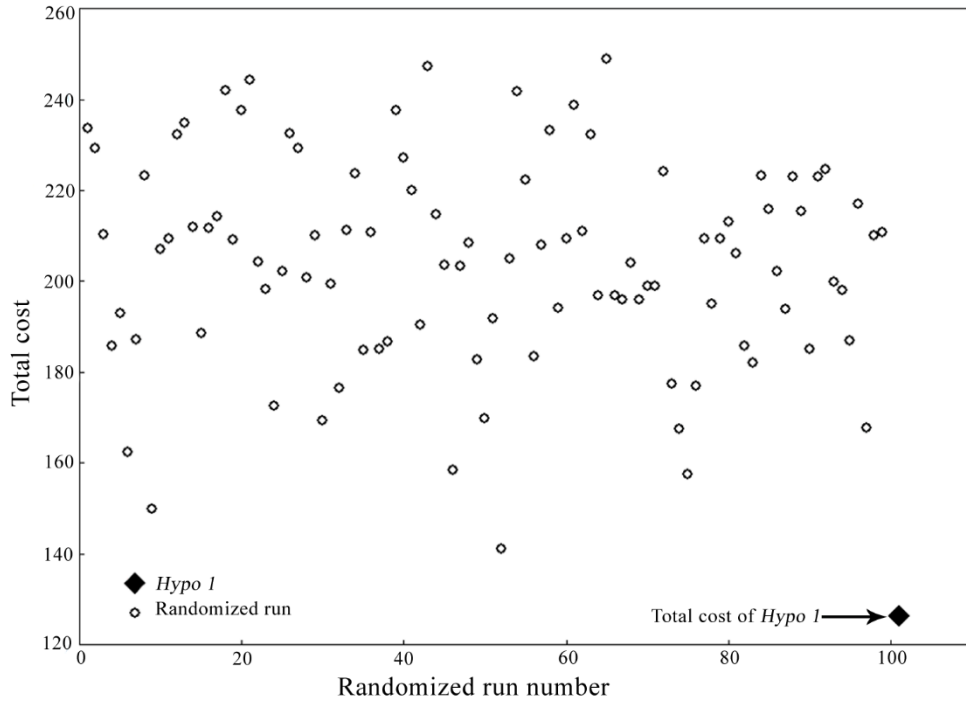


Figure S4: Lowest total cost of 99 randomized runs and *Hypo 1*.

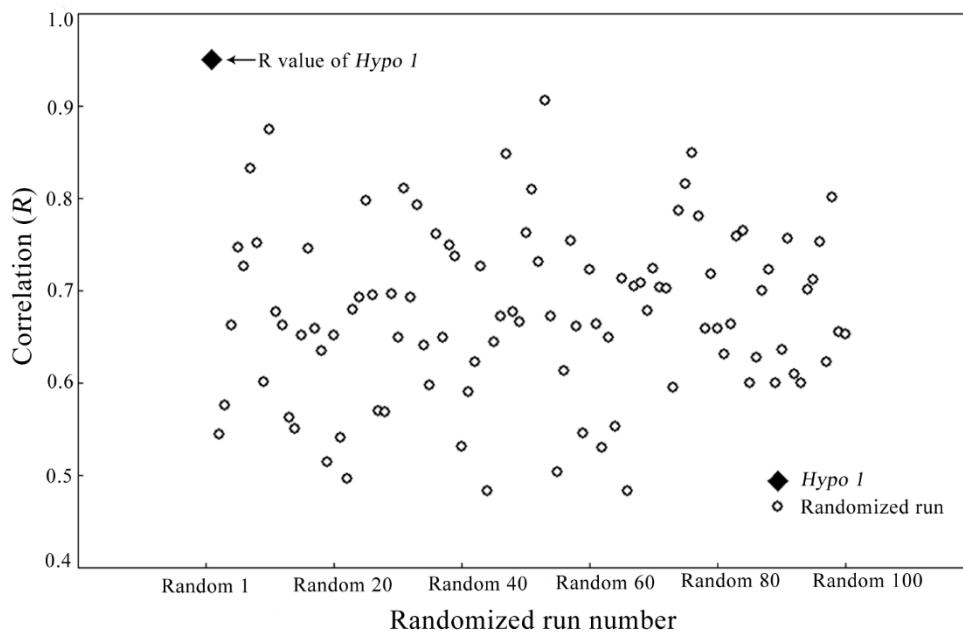


Figure S5: Best correlation coefficient of 99 randomized runs and *Hypo 1*.

Table S4: Observed and predicted activity, fit value and smiles representation of the Ts7 molecules.

Mol	Activity (pK _i nM)		Error	Activity scale		Fit value	SMILES
	Obs.	Pred.		Obs.	Pred.		
T1	5.373	5.293	+1.015	+++	+++	8.941	[F]/C1=C([H])C([H])=C(C([H])=C1[H])[C@]([H])(N([H])C(=O)C2=C([H])C(=C([H])C(=C2[H])C3=NN=C(O3)[C@@]([H])([H])([H])C([H])([H])C=4C([H])=C([H])C([H])=C([H])C=4[H])[N+](H)([H])([H])N(C([H])([H])([H])[S](=O)(=O)C([H])([H])([H])C([H])([H])[H])
T2	6.137	6.043	+1.016	+++	+++	9.303	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[H])[C@@]2([H])C([H])([H])N/C3=N/C(=C/[F])C(=N3)OC([H])([H])([H])C([H])([H])([H])C4([H])[H])N([H])([H])C([H])([H])[H])
T3	3.222	3.224	-0.999	++	++	8.005	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C(OC([H])([H])[H])=C([H])C([H])=C4[H])N([H])([H])C([H])([H])[H])
T4	4.523	4.210	+1.074	++	++	7.865	O=C1N(C(=N[C@@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C([Cl])=C([H])C([H])=C3[H])N([H])([H])C([H])([H])[H])
T5	4.796	4.824	-0.994	++	++	8.145	O=C1N(C(=N[C@]1/C2=C([H])C(=C([H])C([H])=C2[H])C3=C([H])N=C([H])C([F])=C3[H])[C@]4([H])C([H])([H])C4([H])[H])N([H])([H])C([H])([H])[H])
T6	4.569	4.582	-0.997	++	++	8.656	O=C1N(C(=N[C@@]1/C2=C([H])C(=C([H])C([H])=C2[H])C3=C([H])N=C([H])C(C#N)=C3[H])[C@@]4([H])C([H])([H])C4([H])[H])N([H])([H])C([H])([H])[H])
T7	3.481	3.510	-0.992	++	++	7.754	O=C1N(C(=N[C@]1/C2=C([H])C([H])=C([H])C([H])=C2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C([H])=C([H])C([H])=C4[H])N([H])([H])C([H])([H])[H])
T8	5.678	5.387	+1.054	+++	+++	8.420	O=C1N(C(=N[C@@]1(C=2C([H])=C(C([H])=C([H])C=2[H])C3=C([H])C([Cl])=C([H])N=C3[H])[C@]4([H])C([H])([H])C4([H])[H])N([H])([H])C([H])([H])[H])
T9	3.420	3.450	-0.991	++	++	9.375	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C([H])=C(OC([H])([H])[H])C([H])=C4[H])N([H])([H])C([H])([H])[H])
T10	4.143	4.109	+1.008	++	++	4.824	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C([F])=C([H])C([H])=C3[H])N([H])([H])C([H])([H])[H])
T11	4.337	4.962	-0.874	++	++	9.036	O=C1N(C(=N[C@]1/C2=C([H])C([H])=C([H])C([H])=C2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C(OC([H])([H])C([H])([H])[H])=C([H])C([H])=C4[H])N([H])([H])C([H])([H])[H])
T12	5.229	5.302	-0.986	+++	+++	9.376	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N/C3=N/C(=C/[F])C(=N3)OC([H])([H])C([H])([H])([H])C([H])([H])[H])C4([H])[H])N([H])([H])C([H])([H])[H])
T13	4.432	1.167	+3.797	++	+	5.241	O=C1N(C(=N[C@]1/C2=C([H])C([H])=C([H])C([H])=C2[H])C3=C([H])C(C#N)=C([H])C([H])=C3[H])N([H])([H])C([H])([H])[H])
T14	3.721	3.671	+1.014	++	++	8.019	O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=N(C([H])=C([H])C([H])=C4[H])N([H])([H])C([H])([H])[H])
T15	4.914	5.580	-0.881	++	+++	8.719	O=C(N([C@]1([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C1([H])[H])C([H])([H])([H])C([H])([H])C([H])([H])[C@@]([H])([H])N4C(=N/C3=C([H])C([H])=C(OC=2C([H])=C([H])C([H])=C([H])C=2[H])C([H])=C3C4([H])[H])N([H])([H])[C@@]5([H])C([H])([H])OC([H])([H])C([H])([H])C5([H])[H])

T16	4.983	5.400	-0.923	++	+++	9.474	O=C(OC([H])([H])[C@]([H])(N3C(=N/C2=C([H])C([H])=C(O/C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])=C2C3([H])[H]N([H])[H])[C@]4([H])C([H])([H])OC([H])([H])C([H])([H])C4([H])[H]N([C@]5([H])C([H])([H])C([H])([H])C([H])([H])C5([H])[H])C([H])([H])[H])
T17	4.106	4.110	-0.999	++	++	9.189	O=C(OC([H])([H])[C@]([H])(N3C(=N/C2=C([H])C([H])=C(O/C1=C([H])C([H])=C([H])C([H])=C1[H])C([H])=C2C3([H])[H]N([H])[H])C4=C([H])C([H])=C([H])C([H])=C4[H]N([C@]5([H])C([H])([H])C([H])([H])C([H])([H])C5([H])[H])C([H])([H])[H]N#CC=1C([H])=C(C([H])=C([H])C=1[H])C=2[S]C([H])=C(C=2[H])[C@]3(N=C(N(C(=O)C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H])
T18	4.678	4.573	+1.023	++	++	9.248	O=C3N(C(=N[C@](C=2[S]C([H])=C(/C1=C([H])C(C#CC([H])([H])[H])=C([H])N=C1[H])C=2[H])(C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H])
T19	6.108	5.324	+1.147	+++	+++	9.398	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@]2([H])C([H])([H])N(/C3=N/C(=C(/F)C(=N3)C([H])([H])[H])C([H])([H])C4([H])[H])N([H])[H])C([H])([H])[H])
T20	4.812	4.813	-1.000	++	++	9.344	O=C3N(C(=N[C@](C=1C([H])=C([S]C=1[Cl])C=2C([H])=C(C#CC([H])([H])[H])C([H])=NC=2[H])(C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]N#CC=1C([H])=C(C([H])=C([H])C=1[H])C=2C([H])=C([S]C=2[H])[C@]3(N=C(N(C(=O)C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H])
T21	6.097	6.180	-0.987	+++	+++	9.510	O=C3N(C(=N[C@](C=1C([H])=C([S]C=1[H])C2=C([H])C(C#CC([H])([H])[H])=C([H])N=C2[H])(C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]N#CC=1C([H])=C(C([H])=C([H])C=1[H])C=2C([H])=C([S]C=2[H])[C@]3(N=C(N(C(=O)C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H])
T22	5.244	5.234	+1.002	+++	+++	9.308	O=C4N(C(=N[C@](/C1=C([H])C([H])=C([H])C(=C1[H])C2=C([H])N=C([H])C([H])=C2[H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C4([H])[H])N([H])[H])C([H])([H])[H])
T23	5.328	5.424	-0.982	+++	+++	9.498	O=C3N(C(=N[C@](C=1C([H])=C([S]C=1[H])C2=C([H])C(C#CC([H])([H])[H])=C([H])N=C2[H])(C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H])
T24	2.357	2.374	-0.993	+	+	9.983	O=C4N(C(=N[C@](/C1=C([H])C([H])=C([H])C(=C1[H])C2=C([H])N=C([H])C([H])=C2[H])(C3=C([H])C([H])=C([H])C([H])=C3[H])C4([H])[H])N([H])[H])C([H])([H])[H])
T25	6.770	6.403	+1.057	+++	+++	9.543	O=C3N(C(=N[C@](C=2[S]C(C=1C([H])=C(C#CC([H])([H])[H])C([H])=NC=1[H])=C([H])C=2[Cl])(C3([H])[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]N#CC=1C([H])=C(C([H])=C([H])C=1[H])C=2C([H])=C([S]3(=O)N(C(=N[C@]4(C=1C([H])C(=C([H])C([H])=C1[F])N([H])C(=O)C2=NC([H])=C(/N=C2/[H])C([F])([F])[H])[C@]3([H])C([H])([H])OC4([H])[H])N([H])[H])C([H])([H])[H])
T26	5.569	5.572	-0.999	+++	+++	9.646	O=[S]3(=O)N(C(=N[C@](C=1[S]C(=C([H])C=1[Cl])C2=C([H])C(C#CC([H])([H])[H])=C([H])N=C2[H])(C([H])([H])[H])C3([H])[H])N([H])[H])C([H])([H])[H])
T27	6.620	7.719	-0.858	+++	+++	11.793	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])C([H])([H])C4([H])[H]N([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H])C([F])=C([H])C=1[H])[C@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])[H])C4([H])[H])C([H])([H])[H])
T28	4.863	4.850	+1.003	++	++	9.460	O=C2N(/C(=N[H])N([H])[C@]4(C=1C([F])=C([H])C([F])=C([H])C=1[H])[C@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])[H])C4([H])[H])C([H])([H])[H])
T29	6.328	5.410	+1.170	+++	+++	9.484	O=C2N(/C(=N[H])N([H])[C@]4(C=1C([F])=C([H])C([F])=C([H])C=1[H])[C@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])[H])C4([H])[H])C([H])([H])[H])
T30	5.886	5.879	+1.001	+++	+++	9.481	O=C2N(/C(=N[H])N([H])[C@]4(C=1C([F])=C([H])C([F])=C([H])C=1[H])[C@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])[H])C4([H])[H])C([H])([H])[H])
T31	6.051	5.463	+1.108	+++	+++	9.537	O=C2N(/C(=N[H])N([H])[C@]4(C=1C([Cl])=C([H])C([H])=C([F])C=1[H])[C@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])[H])C4([H])[H])C([H])([H])[H])
T32	5.418	5.410	+1.001	+++	+++	8.495	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])C([H])([H])[H])C([H])([H])[H])C=5/N=C(/[H])C([Cl])=C([H])C=5[H])
T33	4.932	4.942	-0.998	++	++	9.016	O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])

)]OC4([H])([H])(C([H])([H])([H])C([H])([H])([H])C=5/ N=C/[H])C([F])=C([H])C=5[H]
T34	4.620	4.720	-0.979	++	++	8.794	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@] 4([C@@]1(N=C(OC1([H])([H])N([H])([H])C2=C3[H]) C([H])([H])C4([H])([H])C=5/N=C/[H])C([Cl])=C([H] C=5[F]
T35	3.987	3.984	+1.001	++	++	8.938	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@] 4([C@@]1(N=C(OC1([H])([H])N([H])([H])C2=C3[H]) C([H])([H])C4([H])([H])C=5/N=C/[H])C([F])=C([H]) C=5[H]
T36	5.215	5.206	+1.002	+++	+++	9.280	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H] C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(=C/[F])C(=N3)C([H])([H])C([H])([H])C([H])([H])([H]) C4([H])([H])N([H])([H])C([H])([H])([H]) [H]/C4=C/C([H])=C1C(OC([H])([H])[C@]3([C@]12 N=C(OC2([H])([H])N([H])([H])C([H])([H])OC3([H]) [H])=C4[H])C5=C([H])N=C([H])C(C#CC([H])([H])(H)=C5[H]
T37	4.910	4.805	+1.022			7.896	[H]/C4=C/C([H])=C1C(O[C@@])([H])([C@@]3([C @]12N=C(OC2([H])([H])N([H])([H])C([H])([H])OC3([H])([H])C([H])([H])C([H])([H])C([H])([H])=C4[H])C5=C([H])N=C([H])C(C#CC([H])([H])([H])=C5[H]
T38	4.971	5.000	-0.994	++	++	8.773	[H]/C4=C/C([H])=C1C(O[C@@])([H])([C@@]3([C @]12N=C(OC2([H])([H])N([H])([H])C([H])([H])OC3([H])([H])C([H])([H])C([H])([H])C([H])([H])=C4[H])C5=C([H])N=C([H])C(C#CC([H])([H])([H])=C5[H]
T39	5.056	5.147	-0.982	+++	+++	8.840	[H]/C4=C/C([H])=C1C(O[C@@])([H])([C@@]3([C @]12N=C(OC2([H])([H])N([H])([H])C([H])([H])OC3([H])([H])C([H])([H])C([H])([H])C([H])([H])=C4[H])C5=C([H])N=C([H])C(C#CC([H])([H])([H])=C5[H] [F]C([F])([F])C([H])([H])C([H])([H])C([H])([H])O/ C1=C([H])C([H])=C(C([H])=C1[C@@]2(N=C(OC2([H])([H])N([H])([H])C([H])([H])OC4([H])([H]))C5=C([H])N=C([H])C(C#CC([H])([H])([H])=C5[H] [H]/C5=C/C([H])=C1C(O[C@]4([C@@]3([C@@]12 N=C(OC2([H])([H])N([H])([H])C([H])([H])OC3([H]) [H])C([H])([H])C([H])([H])C4([H])([H])=C5[H])C6=C([H])N=C([H])C(C#CC([H])([H])([H])=C6[H]
T40	4.061	4.620	-0.879	++	++	8.694	[H]/C4=C/C([H])=C1C(OC([C@@]3([C@]12N=C(O C2([H])([H])N([H])([H])C([H])([H])OC3([H])([H])C([H])([H])([H])C([H])([H])C([H])([H])=C4[H])C5=C([H])N=C([H])C(C#CC([H])([H])([H])=C5[H]
T41	4.921	4.892	+1.006	++	++	8.558	[Cl]C=5C([H])=C([H])C([H])=C(/C3=C([H])C([H])= C2OC([C@]4([C@]1(N=C(OC1([H])([H])N([H])([H]) C2=C3[H])C([H])([H])OC4([H])([H])C([H])([H])([H]) C([H])([H])([H])C=5[H]
T42	5.044	4.981	+1.013	+++	++	7.928	[Cl]C=5C([H])=C(/C3=C([H])C([H])=C2OC([C@@] 4([C@@]1(N=C(OC1([H])([H])N([H])([H])C2=C3[H]) C([H])([H])OC4([H])([H])C([H])([H])([H])C([H])([H]) [H])C([H])=C([F])C=5[H]
T43	4.668	4.611	+1.012	++	++	8.015	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@] 4([C@]1(N=C(OC1([H])([H])N([H])([H])C2=C3[H])C([H])([H])C4([H])([H])C5=NC([H])=C([Br])C([H])=N5 O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H] C=1[H])[C@@]2([H])C([H])([H])N(/C3=N/C(OC([H])([H])([H])=C([F])C(=N3)C([H])([H])C([H])([H])(H))C4([H])([H])N([H])([H])C([H])([H])([H])
T44	4.726	4.728	-0.999	++	++	7.242	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@] 4([C@]1(N=C(OC1([H])([H])N([H])([H])C2=C3[H])C([H])([H])C4([H])([H])C=5/N=C/[H])C(C#N)=C([H]) C=5[Cl]
T45	4.206	4.331	-0.971	++	++	7.414	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@] 4([C@]1(N=C(OC1([H])([H])N([H])([H])C2=C3[H])C([H])([H])C4([H])([H])C=5/N=C/[H])C(C#N)=C([H]) C=5[Cl]
T46	5.796	5.350	+1.083	+++	+++	9.424	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@] 4([C@]1(N=C(OC1([H])([H])N([H])([H])C2=C3[H]) C([H])([H])([H])C4([H])([H])C5=NC([H])=C([Cl])C([H])= C5C([H])([H])([H])
T47	4.668	3.802	+1.228	++	++	7.876	O=C(N([H])C3=C([H])C([H])=C2OC([C@@]4([C@ @]1(N=C(OC1([H])([H])N([H])([H])C2=C3[H]) C([H])([H])([H])C4([H])([H])C5=NC([H])=C(C#N)C([H]) =C5C([H])([H])([H])
T48	4.553	4.560	-0.998	++	++	8.830	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@] 4([C@]1(N=C(OC1([H])([H])N([H])([H])C2=C3[H])C([H])([H])([H])C4([H])([H])C=5/N=C/[H])C(C#N)=C([H]) C=5[Cl]
T49	4.504	4.086	+1.102	++	++	8.160	O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@] 4([C@]1(N=C(OC1([H])([H])N([H])([H])C2=C3[H]) C([H])([H])([H])C4([H])([H])C5=NC([H])=C([Cl])C([H])= C5C([H])([H])([H])
T50	5.190	5.229	-0.993	++++	+++	10.116	O=C(N([H])C3=C([H])C([H])=C2OC([C@@]4([C@ @]1(N=C(OC1([H])([H])N([H])([H])C2=C3[H])C([H])

T51	4.466	3.490	+1.280	++	++	7.564	<chem>([H])OC4([H])[H](C([H])([H])[H])C([H])([H])[H]C5=NC([H])=C([Cl])C([H])=C5C([H])([H])[H]O=C(N([H])C3=C([H])C([H])=C2OC([H])([H])[C@]4([C@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C=5N=C([H])C(C#N)=C([H])C=5[H]</chem>
T52	5.036	4.875	+1.033	+++	++	8.949	<chem>[H]/C5=C/C([H])=C1C(O[C@]([H])([C@@]3([C@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H])=C5[H])C6=C([H])N=C([H])N=C6[H]</chem>
T53	5.148	5.033	+1.023	+++	+++	8.301	<chem>[H]/C5=C/C([H])=C1C(O[C@]([H])([C@]3([C@]12N=C(OC2([H])[H])N([H])[H])C([H])([H])OC3([H])[H])C([H])([H])C4=C([H])C([H])=C([H])C([H])=C4[H])=C5[H])C6=C([H])N=C([H])C(C#CC([H])([H])[H])=C6[H]</chem>
T54	6.114	6.085	+1.005	+++	+++	9.391	<chem>O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([F])=C([F])C=1[H])[C@@]2([H])C([H])([H])N/(C3=N/C(=C/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]</chem>
T55	5.991	5.942	+1.008	+++	+++	8.570	<chem>O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])C([H])([H])[H])C([H])([H])[H])C=5/N=C([H])C([Br])=C([H])C=5[H]</chem>
T56	5.368	5.211	+1.030	+++	+++	9.047	<chem>O=C(N([H])C3=C([H])C([H])=C2OC([C@@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])C([H])([H])[H])C([H])([H])[H])C=5N=C([H])C(=NC=5[H])OC([H])([H])[H]</chem>
T57	5.423	5.618	-0.965	+++	+++	7.690	<chem>O=C(N([H])C3=C([H])C([H])=C2OC([C@@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C([Cl])C([H])=C5[H]</chem>
T58	5.039	4.970	+1.014	+++	++	8.045	<chem>O=C(N([H])C3=C([H])C([H])=C2OC([C@@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C([F])C([H])=C5[H]</chem>
T59	5.213	5.388	-0.968	+++	+++	8.149	<chem>O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C(/N=C5/[H])OC([H])([H])[H]</chem>
T60	5.278	5.313	-0.993	+++	+++	8.041	<chem>O=C(N([H])C3=C([H])C([H])=C2OC([C@@]4([C@@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])C4([H])[H])C([H])([H])[H])C([H])([H])[H])C5=NC([H])=C(/N=C5/[H])C([F])([F])[H]</chem>
T61	5.101	5.225	-0.976	+++	+++	8.518	<chem>O=C(N([H])C3=C([H])C([H])=C2OC([C@@]4([C@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])C([H])([H])[H])C([H])([H])[H])C=5/N=C([H])C(=NC=5[H])OC([H])([H])[H]</chem>
T62	2.520	2.520	+1.000	+	+	8.793	<chem>O=C(N([H])C3=C([H])C([H])=C2OC([C@]4([C@]1(N=C(OC1([H])[H])N([H])[H])C2=C3[H])C([H])([H])OC4([H])[H])C([H])([H])[H])C([H])([H])[H])C=5/N=C([H])C([Cl])=C([H])C=5[H]</chem>
T63	6.899	7.954	-0.867	+++	+++	12.028	<chem>O=C(/C1=N/C([H])=C(C([H])=C1[H])C([F])([F])[F])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N([H])N([S])(=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]</chem>
T64	5.357	5.266	+1.017	+++	+++	9.340	<chem>O=C2N(C(=N[C@]5(C=1C([H])=C([H])C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N/(C3=N/C(=C/[F])C(=N3)[C@]4([H])C([H])([H])C4([H])[H])C([H])([H])[H])C5([H])[H])N([H])[H])C([H])([H])[H]</chem>
T65	6.000	6.122	-0.980	+++	+++	11.335	<chem>O=C(/C1=N/C([H])=C(/N=C1/[H])C([H])([H])[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])[C@]3(N([H])C(=N([H])N([S])(=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]</chem>
T66	6.979	7.151	-0.976	+++	+++	11.225	<chem>O=C(/C1=N/C([H])=C(/N=C1/[H])OC([H])([H])[H])N([H])C2=C([H])C(=C([F])C([F])=C2[H])[C@]3(N([H])C(=N([H])N([S])(=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H]</chem>

T67	6.523	6.178	+1.056	+++	+++	10.252	O=C(/C1=N/C([H])=C(C([H])=C1[H])C([H])([H])[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])C@]3(N([H])C(=N([H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H])
T68	6.312	6.895	-0.915	+++	+++	10.969	O=C(/C1=N/C([H])=C([F])C([H])=C1[H])N([H])C2=C([F])C(=C([F])C([H])=C2[H])C@]3(N([H])C(=N([H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H])
T69	5.592	5.377	+1.040	+++	+++	9.451	O=[S]3(=O)N(/C(=N\([H])N([H])[C@](C=1[S]C([H])=C(C=1[H])C2=C([H])C([H])=C([H])C(C#N)=C2[H])(C3([H])[H])C([H])([H])[H])C([H])([H])[H])
T70	5.337	5.400	-0.988	+++	+++	9.474	O=[S]3(=O)N(/C(=N\([H])N([H])[C@](C=1[S]C([H])=C(C=1[H])C2=C([H])C([H])=C([F])C(C#N)=C2[H])(C3([H])[H])C([H])([H])[H])C([H])([H])[H])
T71	6.785	7.635	+0.889	+++	+++	11.709	O=C(/C1=N/C([H])=C(/N=C1/[H])OC([H])([H])[H])N([H])C2=C([H])C(=C([F])C([H])=C2[H])C@]3(N([H])C(=N([H])N([S](=O)(=O)C3([H])[H])C([H])([H])[H])C([H])([H])[H])
T72	3.092	3.083	+1.003	++	++	9.349	O=C(N([H])C1=C([H])C(=C([H])C(=C1[H])C([F])([F])C([F])([F])N([H])C2=C([H])C(=C(C([H])=C2[H])N(C([H])([H])[H])C([H])([H])[H])C(=O)N([H])C([H])([H])C([H])([H])C([H])([H])N3C([H])([H])C([H])([H])OC([H])([H])C3([H])[H])
T73	3.009	3.052	+0.986	++	++	9.273	O=C(N([H])C1=C([H])C(=C(C([H])=C1[H])N(C([H])([H])[H])C([H])([H])[H])C(=O)N([H])C([H])([H])C([H])([H])C([H])([H])OC([H])([H])C([H])([H])[H])N([H])C2=C([H])C([Cl])=C([H])C([H])=C2[H])
T74	4.553	4.480	+1.016	++	++	8.349	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C(C([Cl])=C1[H])N([H])[S](=O)(=O)C([H])([H])[H])N([H])C(=2C(=N[S]C=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H])
T75	3.398	3.113	+1.092	++	++	8.222	O=C(N([H])C(=NC([H])([H])C1=C([H])C([H])=C([H])C([H])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H])
T76	3.620	3.621	-1.000	++	++	8.478	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([Cl])C([H])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C([F])C([H])=C3[H])
T77	4.041	3.920	+1.031	++	++	7.994	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([Cl])C([H])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H])
T78	3.056	4.118	-0.742	++	++	8.192	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([Cl])C([H])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C([H])C([H])=C3[H])
T79	5.409	5.440	-0.994	+++	+++	11.622	O=C1N(/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])C@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])C@]4([H])C([H])([H])[C@]([H])N([H])C(=O)C3=C([H])C([H])=NC([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])[H])
T80	5.638	5.212	+1.082	+++	+++	9.286	O=C1N(/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])C@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])C@]4([H])C([H])([H])[C@]([H])N([H])C(=O)C3=C([H])C([H])=NC([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])[H])
T81	5.886	6.031	-0.976	+++	+++	11.568	O=C1N(/C(=N/[H])N([H])[C@]1(C([H])([H])C([H])([H])C@]2([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])C@]4([H])C([H])([H])[C@]([H])N([H])C(=O)C3=C([H])C([H])=C([H])C([H])=C3[H])C([H])([H])C([H])([H])C4([H])[H])C([H])([H])[H])
T82	5.367	5.186	+1.035	+++	+++	9.260	O=C1N(/C(=N\([H])N([H])[C@]1(C([H])([H])C([H])([H])C@@]2([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C2([H])[H])C([H])([H])C@@]4([H])C([H])([H])[C@]([H])N([H])[C@@]3([H])C([H])([H])C([H])([H])[H])

T109	5.215	5.539	-0.941	+++	+++	9.613	N/C3=N/C(OC([H])([H])[H])=C([H])C(=C3[H])C([H])([H])OC([H])([H])[H]C4([H])[H]C([H])([H])[H]O=[S]2(=O)N/C(=N\ [H])N([H])[C@@]4/C1=C([H])C([H])=C([H])C([H])=C1[H][C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([H])C(=C3[H])C([H])([H])OC([H])([H])[H]C4([H])[H]C([H])([H])[H])
T110	5.569	5.546	+1.004	+++	+++	9.620	O=[S]2(=O)N/C(=N\ [H])N([H])[C@@]4/C1=C([H])C([H])=C([H])C([H])=C1[H][C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([H])C(=C3[H])C([H])([H])OC([H])([H])[H]C4([H])[H]C([H])([H])[H]O=C2N(C(=N[C@]4(C=1C([H])=C([F])C([H])=C([H])C=1[F])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H]C4([H])([H])N([H])[H]C([H])([H])[H])
T111	6.252	5.442	+1.149	+++	+++	9.516	O=[S]2(=O)N/C(=N\ [H])N([H])[C@@]4/C1=C([H])C([H])=C([H])C([H])=C1[H][C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H]C4([H])([H])[H]O=[S]2(=O)N/C(=N\ [H])N([H])[C@@]4/C1=C([H])C([H])=C([H])C([H])=C1[H][C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H]C4([H])([H])[H])
T112	5.523	5.539	-0.997	+++	+++	9.613	O=[S]2(=O)N/C(=N\ [H])N([H])[C@@]4/C1=C([H])C([H])=C([H])C([H])=C1[H][C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H]C4([H])([H])[H]O=[S]2(=O)N/C(=N\ [H])N([H])[C@@]4/C1=C([H])C([H])=C([H])C([H])=C1[H][C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([H])C(=C3[H])C4([H])[H]C([H])([H])[H])
T113	5.066	5.114	-0.990	+++	+++	9.645	O=[S]2(=O)N/C(=N\ [H])N([H])[C@@]4/C1=C([H])C([H])=C([H])C([H])=C1[H][C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([H])C(=C3[H])C4([H])[H]C([H])([H])[H]O=[S]2(=O)N/C(=N\ [H])N([H])[C@@]4/C1=C([H])C([H])=C([H])C([H])=C1[H][C@@]2([H])C([H])([H])N/C3=N/C(=C/[F])C(=N3)OC([H])([H])[H]C4([H])([H])[H]O=[S]2(=O)N/C(=N\ [H])N([H])[C@@]5/C1=C([H])C([H])=C([H])C([H])=C1[H][C@@]2([H])C([H])([H])N/C3=N/C(=C/[F])C(=N3)OC([H])([H])[H][C@@]4([H])C([H])([H])C4([H])[H]C5([H])[H]C([H])([H])[H])
T114	5.086	5.136	-0.990	+++	+++	9.710	O=[S]2(=O)N/C(=N\ [H])N([H])[C@@]4/C1=C([H])C([H])=C([H])C([H])=C1[H][C@@]2([H])C([H])([H])N/C3=N/C(=C/[F])C(=N3)OC([H])([H])[H]C4([H])([H])[H]O=[S]2(=O)N/C(=N\ [H])N([H])[C@@]4/C1=C([H])C([H])=C([H])C([H])=C1[H][C@@]2([H])C([H])([H])N/C3=N/C(=C/[F])C(=N3)OC([H])([H])[H][C@@]4([H])C([H])([H])C4([H])[H]C5([H])[H]C([H])([H])[H])
T115	5.377	5.500	-0.978	+++	+++	9.574	O=[S]2(=O)N/C(=N\ [H])N([H])[C@@]4/C1=C([H])C([H])=C([H])C([H])=C1[H][C@@]2([H])C([H])([H])N/C3=N/C(=C/[F])C(=N3)OC([H])([H])[H][C@@]4([H])C([H])([H])C4([H])[H]C5([H])[H]C([H])([H])[H])
T116	3.806	3.843	-0.990	++	++	9.544	O=[S]2(=O)N/C(=N\ [H])N([H])[C@@]4/C1=C([H])C([H])=C([H])C([H])=C1[H][C@@]2([H])C([H])([H])N/C3=N/C(=C/[F])C(=N3)OC([H])([H])[H]C4([H])([H])[H]O=[S]2(=O)N/C(=N\ [H])N([H])[C@@]4/C1=C([H])C([H])=C([H])C([H])=C1[H][C@@]2([H])C([H])([H])N/C3=N/C(=C/[F])C(=N3)OC([H])([H])[H][C@@]4([H])C([H])([H])C4([H])[H]C5([H])[H]C([H])([H])[H])
T117	5.495	5.572	-0.986	+++	+++	9.646	O=C(N2C([H])([H])[C@@]1(N([H])C(=N[H])N([S](=O)(=O)[C@]1([H])C2([H])[H])C([H])([H])[H])C3=C([H])C(=C([H])C([H])=C3[F])N([H])C(=O)C4=NC([H])=C([F])C([H])=C4[H]C([H])([H])[H]O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[F])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)OC([H])([H])[H]C4([H])([H])N([H])[H]C([H])([H])[H])
T118	6.745	6.913	-0.976	+++	+++	9.459	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([F])=C([F])C=1[F])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])[H]C4([H])[H])N([H])[H]C([H])([H])[H]O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[F])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])C([H])([H])[H])C4([H])[H]N([H])[H]C([H])([H])[H])
T119	5.523	5.394	+1.024	+++	+++	9.468	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([F])=C([F])C=1[F])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])[H]C4([H])[H])N([H])[H]C([H])([H])[H]O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[F])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])C([H])([H])[H])C4([H])[H]N([H])[H]C([H])([H])[H])
T120	6.215	5.200	+1.195	+++	+++	9.274	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[F])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])C([H])([H])[H])C4([H])[H]N([H])[H]C([H])([H])[H]O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([F])=C([F])C=1[F])[C@@]2([H])C([H])([H])N/C3=N/C(=C/[F])C(=N3)OC([H])([H])[H]C4([H])([H])[H])C4([H])[H]N([H])[H]C([H])([H])[H])
T121	6.161	5.357	+1.150	+++	+++	9.431	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([F])=C([F])C=1[F])[C@@]2([H])C([H])([H])N/C3=N/C(=C/[F])C(=N3)OC([H])([H])[H]C4([H])([H])[H])C4([H])[H]N([H])[H]C([H])([H])[H])
T122	6.276	6.246	+1.005	+++	+++	9.414	O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([F])=C([H])C=1[F])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])C([H])([H])[H])C4([H])[H]N([H])[H]C([H])([H])[H]O=C2N(C(=N[C@]4/C1=C([H])C([C1])=C([H])C([H])=C1[H][C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])C([H])([H])[H])C4([H])[H]N([H])[H]C([H])([H])[H])
T123	5.409	5.386	+1.004	+++	+++	9.460	O=C2N(C(=N[C@]4/C1=C([H])C([C1])=C([H])C([H])=C1[H][C@@]2([H])C([H])([H])N/C3=N/C(OC([H])([H])[H])=C([F])C(=N3)C([H])([H])C([H])[H]C4([H])([H])N([H])[H]C([H])([H])[H])
T124	5.285	5.237	+1.009	+++	+++	8.777	O=[S](=O)N(C=2C([H])=C(C([H])=C([H])[C@]1([H])C([H])([H])[C@]1([H])C([H])([H])[H])C([H])=C(C(=2[H])C3=NN=C(O3)[C@@]([C([H])([H])[H])C([H])

							([H])C=4C([H])=C([H])C([H])=C([H])C=4[H][N+](H)([H])([H])C([H])([H])C([H])([H])C([H])([H])([H])C ([H])([H])[H]
T125	6.252	5.371	+1.164	+++	+++	9.445	O=C2N(C(=N[C@]5(C=1C(F))=C([H])C([H])=C([F]))C=1[H])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H]))([H])[H]=C([F])C(=N3)[C@]4([H])C([H])([H])C4(H)[H])C5([H])[H]N([H])[H]C([H])([H])[H]
T126	6.187	5.351	+1.156	+++	+++	9.425	O=C2N(C(=N[C@]5(C=1C(F))=C([H])C([H])=C([F]))C=1[H])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H]))([H])[H]=C([Cl])C(=N3)[C@]4([H])C([H])([H])C4(([H])[H])C5([H])[H]N([H])[H]C([H])([H])[H]
T127	5.585	5.350	+1.044	+++	+++	9.424	O=C2N(C(=N[C@]5(C=1C([H])=C([F])C([H])=C([H]))C=1[F])[C@@]2([H])C([H])([H])N/C3=N/C(=C/[F]))C(=N3)[C@@]4([H])C([H])([H])C4([H])[H]C([H]) ([H])[H]C5([H])[H]N([H])[H]C([H])([H])[H]
T128	6.569	6.338	+1.036	+++	+++	9.379	O=C2N(C(=N[C@]5(C=1C(F))=C([H])C([F])=C([H]))C=1[H])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H]))([H])[H]=C([F])C(=N3)[C@@]4([H])C([H])([H])C 4([H])[H]C5([H])[H]N([H])[H]C([H])([H])[H]
T129	6.167	5.293	+1.165	+++	+++	9.367	O=C2N(C(=N[C@]5(C=1C(F))=C([H])C([F])=C([H]))C=1[H])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H]))([H])[H]=C([Cl])C(=N3)[C@]4([H])C([H])([H])C4(([H])[H])C5([H])[H]N([H])[H]C([H])([H])[H]
T130	5.959	5.939	+1.003	+++	+++	9.362	[F]C=1C([H])=C([F])C(=C([H])C=1[H])[C@@]24N= C(N(C(=O)[C@]2([H])C([H])([H])N/C3=N/C(=C/[F]))C(=N3)OC([H])([H])[H]C([F])([F])C([H])([H])[H] C4([H])[H]C([H])([H])[H]N([H])[H]
T131	5.495	5.397	+1.018	+++	+++	9.471	[F]/C1=C/N=C/N=C1/OC([H])([H])[H]N3C([H])([H])[C@@]2(N=C(N(C(=O)[C@]2([H])C3([H])[H])C([H])([H])[H]N([H])[H])C4=C([H])C([H])=C([F])C(H)=C4[F])C([F])([F])[F]
T132	6.222	5.314	+1.171	+++	+++	9.388	O=C2N(C(=N[C@]4(C=1C(F))=C([H])C([H])=C([H]))C=1[H])[C@@]2([H])C([H])([H])N/C3=N/C(=C/[F]))C(=N3)OC([H])([H])[H]C([H])([H])[H]C4([H])[H] N([H])[H]C([H])([H])[H]
T133	6.036	5.388	+1.120	+++	+++	9.462	O=C2N(C(=N[C@]4(C=1C(F))=C([Cl])C([F])=C([H]))C=1[H])[C@@]2([H])C([H])([H])N/C3=N/C(=C/[F]))C(=N3)OC([H])([H])[H]C([H])([H])[H]C4([H])(H)N([H])[H]C([H])([H])[H]
T134	4.046	4.285	-0.944	++	++	8.359	O=C(C=1C([H])=C([H])C([H])=C([H])C=1[H])C4=C ([H])C2=C(N=C(N(C2([H])[H])C([H])([H])C([H])([H]))C(=O)N(C([H])([H])[H])C3([H])C([H])([H])C([H])([H])C([H])([H])C([H])([H])C3([H])[H]N([H])[H]C(H)=C4[H]
T135	5.854	5.438	+1.077	+++	+++	9.512	O=C2N(C(=N[C@]4(C=1C([H])=C(C#N)C([H])=C([H])C=1[H])[C@@]2([H])C([H])([H])N/C3=N/C(=C/ [F])C(=N3)OC([H])([H])[H]C([H])([H])[H]C4([H]) [H])N([H])[H]C([H])([H])[H]
T136	5.276	5.406	+0.976	+++	+++	9.480	O=C2N(C(=N[C@]4(C=1C(F))=C([F])C([H])=C([H]))C=1[F])[C@@]2([H])C([H])([H])N/C3=N/C(=C/[F]))C(=N3)OC([H])([H])[H]C([H])([H])[H]C4([H])[H] N([H])[H]C([H])([H])[H]
T137	5.796	5.376	+1.078	+++	+++	9.450	[F]C=1C([H])=C([F])C(=C([H])C=1[H])[C@@]24N= C(N(C(=O)[C@]2([H])C([H])([H])N/C3=N/C(=C/[F]))C(=N3)OC([H])([H])[H]C([H])([H])O[H]C4([H])(H)C([H])([H])[H]N([H])[H]
T138	6.347	5.436	+1.168	+++	+++	9.510	O=C2N(C(=N[C@]4(C=1C([Cl])=C([H])C([F])=C([H]))C=1[H])[C@@]2([H])C([H])([H])N/C3=N/C(=C/[F]))C(=N3)OC([H])([H])[H]C([H])([H])[H]C4([H])(H)N([H])[H]C([H])([H])[H]
T139	6.319	5.236	+1.207	+++	+++	9.310	O=C2N(C(=N[C@]5(C=1C([H])=C([H])C([F])=C([H]))C=1[H])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H]))([H])[H]=C([F])C(=N3)[C@]4([H])C([H])([H])C4(H)[H])C5([H])[H]N([H])[H]C([H])([H])[H]
T140	6.252	5.235	+1.194	+++	+++	9.309	O=C2N(C(=N[C@]4(C=1C(F))=C([H])C([F])=C([F]))C=1[H])[C@@]2([H])C([H])([H])N/C3=N/C(OC([H]))([H])[H]=C([F])C(=N3)[C@]4([H])C([H])([H])C4(H)[H])C5([H])[H]N([H])[H]C([H])([H])[H]

)([H])[H]=C([F])C(=N3)C([H])([H])C([H])([H])[H] C4([H])([H])N([H])[H]C([H])([H])[H] N#C/C1=C([H])C=C([H])C([H])=C1[H]C2=C([H]) [S]/C(=C2/[H])[C@@]35N=C(N(C(=O)[C@]3([H])C T141 6.046 5.207 +1.161 +++ +++ 9.281 ([H])([H])N(C4=N/C([H])=C(C([H])=N4)C([H])([H]) [H])C5([H])[H]C([H])([H])[H]N([H])[H] N#C/C1=C([H])C=C([H])C([H])=C1[H]C2=C([H]) T142 5.194 5.297 -0.980 +++ +++ 9.371 [S]/C(=C2/[H])[C@@]35N=C(N(C(=O)[C@]3([H])C ([H])([H])N(C=4N=C(C([H])=C([H])C=4[H])C([F])([F])[F])C5([H])[H]C([H])([H])[H]N([H])[H] O=C/C1=C([H])C([H])=C([H])C=C1[H]C([H])([H] T143 4.801 4.722 +1.017 ++ ++ 8.037 [H])N4C(=NC=3C([H])=C([H])C(OC=2C([H])=C([H])C ([H])=C([H])C=2[H])=C([H])C=3C4([H])[H]N([H])C [H])N(C([H])([H])[H])C5([H])C([H])([H])C([H])([H]) C([H])([H])C([H])([H])C5([H])[H] N#C/C1=C([F])C([H])=C([H])C=C1[H]C=2[S]/C(= T144 4.879 4.860 +1.004 ++ ++ 9.240 C/[H])C=2[H])[C@@]35N=C(N(C(=O)[C@]3([H])C ([H])([H])N(C4=C([H])C([H])=C([F])C([H])=C4[H])C5([H])[H]C([H])([H])[H]N([H])[H] O=C2N([H])C1=C([H])C([H])=C([H])C([H])=C1N([T145 4.613 4.686 -0.984 ++ ++ 8.760 H])C=3/C2=C/[H])C([H])=C(C=3[H])C(=O)N([H])C 4=NC=5C(N4[H])=C([H])C([F])=C([H])C=5[H] O=C2N([H])C1=C([H])C([H])=C([H])C([H])=C1N([T146 4.530 4.568 -0.992 ++ ++ 8.642 H])C=3/C2=C/[H])C([H])=C(C=3[H])C(=O)N([H])C 4=C([H])C([H])=NC([H])=C4[H] O=C2N([H])C1=C([H])C([H])=C([H])C([H])=C1N([T147 4.458 4.872 -0.915 ++ ++ 8.946 H])C3=C2C([H])=C([H])C=C3[H])C(=O)N([H])C4= N/C(=C/[H])N4[H])C5=C([H])C([H])=NC([H])=C5[H] O=C2N([H])C=1C([H])=C([H])C([H])=C([H])C=1N([T148 4.533 5.293 -0.856 ++ +++ 9.367 H])C3=C2C([H])=C([H])C=C3[H])C(=O)N([H])C4= N/C(=C/[H])N4[H])C5=C([H])C([H])=C([F])C([H])= C5[H] O=C2N(C(=N[C@]4(C=1C([H])=C([H])C([H])=C([H] T149 5.921 5.261 +1.125 +++ +++ 9.335 [H])C=1[H])[C@@]2([H])C([H])([H])N(C3=N/C(=C/[F])C(=N3)OC([H])([H])[H]C([H])([H])[H]C4([H])(H])N([H])[H]C([H])([H])[H] O=C2N([H])C1=C([H])C([H])=C([H])C([H])=C1N([T150 4.510 4.506 +1.001 [H])C=3/C2=C/[H])C([H])=C(C=3[H])C(=O)N([H])C 4=NC=5C(N4[H])=C([H])N=C([H])C=5[H] O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C(C(T151 6.398 5.476 +1.168 +++ +++ 9.550 [Cl])=C1[H])N([H])C(=O)C([H])([H])N2C([H])([H]) C([H])([H])C2([H])[H]N([H])[H]C=3C(=N[S]C=3C ([H])([H])[H])C4=C([H])C([H])=C(OC([H])([H])[H]) C([H])=C4[H] O=C(N([H])C(=NC([H])([H])C=1C([H])=C([H])C([H] T152 3.770 3.811 -0.989 ++ ++ 8.337 [H])=C2C=1C([H])=C([H])C([H])=C2[H]N([H])[H]C= 3C(=NOC=3C([H])([H])[H])C4=C([H])C([H])=C(OC ([H])([H])[H]C([H])=C4[H] O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C(T153 3.745 3.819 -0.980 ++ ++ 9.868 [Cl])=C1[H])C2=C([H])N=C([H])C([H])=C2[H]N([H])[H]C=3C(=NOC=3C([H])([H])[H])C4=C([H])C([H])=C(OC([H])([H])[H]C([H])=C4[H] O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C(T154 3.921 4.000 -0.980 ++ ++ 11.081 [Cl])=C1[H])C=2C([H])=C([H])[S]C=2[H]N([H])[H])C=3C(=NOC=3C([H])([H])[H])C4=C([H])C([H])=C(OC([H])([H])[H]C([H])=C4[H] O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C(T155 4.854 4.868 -0.997 ++ ++ 9.184 [Cl])=C1[H])C([H])=C([H])C([H])([H])C([H])([H])O(H])N([H])[H]C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H]C([H])=C3[H] O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C(T156 4.367 4.742 -0.921 ++ ++ 8.816 [Cl])=C1[H])C([H])=C([H])[H]N([H])[H]C=2C(=N OC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H]C([H])=C3[H] O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C(T157 4.553 4.518 +1.008 ++ ++ 8.479 =C1[H])C([H])([H])[H]C([H])([H])[H]N([H])[H]C
--	--	--	--	--	--	--	--	--

							=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(O C([H])([H])[H])C([H])=C3[H]
T158	4.921	4.869	+1.011	++	++	7.945	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C(C([Cl])=C1[H])N([H])[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]
T159	4.824	4.884	-0.988	++	++	9.586	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C([Cl])=C1[H])C([H])=C([H])C([H])([H])OC([H])([H])[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]
T160	6.071	6.303	-0.963	+++	+++	9.431	O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([H])=C([F])C=1[H])C@]2([H])C([H])([H])N(/C3=N/C(=C(/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H])
T161	4.071	4.031	+1.010	++	++	8.105	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C([H])C([Cl])=C1[H])C([H])=C([H])C([H])([H])C([H])([H])C([H])([H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]
T162	4.319	5.437	-0.794	++	+++	9.511	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C(O[H])C([Cl])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]
T163	4.678	4.774	-0.980	++	++	9.240	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C=2C(=NN([H])C=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]
T164	4.301	4.301	+1.000	++	++	9.374	O=C(N([H])C(=NC([H])([H])C=1C([H])=C([H])C([H])=C2C=1C([H])=C([H])C([H])=C2[H])N([H])[H])C=3C(=N[S]C=3C([H])([H])[H])C4=C([H])C([H])=C(O C([H])([H])[H])C([H])=C4[H]
T165	4.538	4.270	+1.063	++	++	8.344	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C=2C(=N[S]C=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]
T166	3.658	3.809	-0.960	++	++	8.260	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C([F])C([H])=C3[H]
T167	3.409	3.411	-0.999	++	++	8.391	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Cl])=C([H])C([Cl])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C([H])C([H])=C3[H]
T168	4.569	4.664	-0.980	++	++	8.162	O=C(N([H])C(=NC([H])([H])C1=C([H])C([Br])=C([H])C([Cl])=C1[H])N([H])[H])C=2C(=NOC=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]
T169	4.060	4.208	-0.965	++	++	7.865	O=C(N([H])C(=NC([H])([H])C1=C([H])C=2C(C([H])=C1[H])=C([H])C([H])=C([H])C=2[H])N([H])[H])C=3C(=N[S]C=3C([H])([H])[H])C4=C([H])C([H])=C(O C([H])([H])[H])C([H])=C4[H]
T170	3.745	1.935	+1.935	++	+	8.056	O=C(N([H])C(=NC([H])([H])C=1C([H])=C([H])C([H])=C2C=1C([H])=C([H])C([H])=C2[H])N([H])[H])C=3C(=NOC=3C([H])([H])[H])C4=C([H])C([H])=C([F])C([H])=C4[H]
T171	5.699	5.375	+1.060	+++	+++	9.449	O=C(N([H])C(=NC([H])([H])C1=C([H])C(=C(C([Cl])=C1[H])N([H])C(=O)C([H])([H])N([H])C([H])([H])C([H])([H])[H])C([H])([H])N([H])[H])C=2C(=N[S]C=2C([H])([H])[H])C3=C([H])C([H])=C(OC([H])([H])[H])C([H])=C3[H]
T172	3.553	3.598	-0.987	++	++	8.981	O=C(N([H])C(=NC([H])([H])C=1C([H])=C([H])C([H])=C2C=1C([H])=C([H])C([H])=C2[H])N([H])[H])C=3C(=NOC=3C([H])([H])[H])C4=C([H])C([H])=C([H])C([H])=C4[H]
T173	3.097	3.107	-0.997	++	++	8.253	[H]C=2C(O[H])=C([H])C=1OC=3C(OC=1C=2O[H])=C([H])C(O[H])=C4OC5=C(OC=34)C(O[H])=C([H])C(O[H])=C5[H]
T174	2.854	2.826	+1.010	+	+	5.999	O=C2C=1C(O[H])=C([H])C(O[H])=C([H])C=1O/C(=C2/O[H])C3=C([H])C([H])=C(O[H])C(O[H])=C3[H]

T175	5.886	6.176	-0.953	+++	+++	10.250	[F]C=1C([H])=C(C([H])=C([F])C=1[H])C([H])([H])[C@@]([H])(N([H])C(=O)C2=C([H])C=C([H])C(=C2[H])C(=O)N3[C@]([H])(C([H])([H])C([H])([H])C3([H])[H])C([H])([H])OC([H])([H])[H])C([H])([H])[C@]([H])(O[H])[C@]4([H])N([H])C([H])([H])C([H])([H])N(C4([H])[H])[S](=O)(=O)C([H])([H])[H]O=C3N(C([H])([H])C([H])([H])C=4C([H])=C(OC=2C([H])=C([H])C=1N=C(N(C([H])([H])C=1C=2[H])C@@]([H])(C([H])([H])C3([H])[H])C([H])(C([H])([H])C([H])([H])N([H])C([H])=C([H])C=4[H])[C@@]5([H])C([H])([H])C([H])([H])OC([H])([H])C5([H])[H]O=C3N(C([H])([H])C([H])([H])C=5C([H])=C(O/C2=C([H])C([H])=C1N=C(N(C([H])([H])C1=C2[H])C@[H])(C([H])([H])C3([H])[H])[C@@]4([H])C([H])([H])C([H])([H])C([H])([H])C4([H])[H]N([H])[H])C([H])=C([H])C=5[H])[C@]6([H])C([H])([H])C([H])([H])OC([H])([H])C6([H])[H]O=C1C4=C(O/C(=C1/C([H])([H])C([H])=C(C([H])([H])[H])C([H])([H])[H])C=2C([H])=C([H])C(O[H])=C([H])C=2O[H])C3=C(OC(C([H])=C3[H])C([H])([H])C([H])([H])[H])C([H])=C4O[H]O=C2N(C(=N[C@]4(C=1C([F])=C([H])C([H])=C([H])C=1[F])C@@]2([H])C([H])([H])N/C3=N/C(=C/[F])C(=N3)OC([H])([H])[H])C([H])([H])[H])C4([H])[H])N([H])[H])C([H])([H])[H]O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C(=C4[H])C([H])([H])[H])N([H])[H])C([H])([H])[H]O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C([F])=C4[H])N([H])[H])C([H])([H])[H]O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C(#N)=C4[H])N([H])[H])C([H])([H])[H]O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])C(OC([H])([H])[H])=C([H])C([H])=C4[H])N([H])C([H])([H])[H]O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C([Cl])=C4[H])N([H])[H])C([H])([H])[H]O=C1N(C(=N[C@]1(C=2C([H])=C([H])C([H])=C([H])C=2[H])C3=C([H])C(=C([H])C([H])=C3[H])C4=C([H])N=C([H])C([H])=C4[H])N([H])[H])C([H])([H])[H]
T176	5.658	5.543	+1.021	+++	+++	8.290	
T177	5.770	5.621	+1.026	+++	+++	7.350	
T178	2.193	2.201	-0.997	+	+	9.509	
T179	5.495	5.340	+1.029	+++	+++	9.414	
T180	4.367	4.236	+1.031	++	++	8.310	
T181	4.509	3.973	+1.135	++	++	8.047	
T182	4.538	4.561	-0.995	++	++	8.832	
T183	4.328	3.920	+1.104	++	++	7.994	
T184	5.097	4.967	+1.026	+++	++	9.041	
T185	5.046	5.048	-1.000	+++	+++	8.783	
T186	4.959	5.015	-0.989	++	+++	8.602	

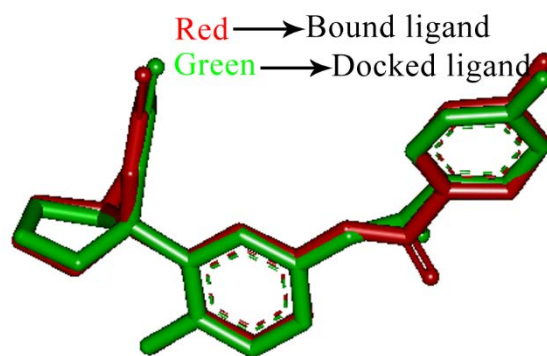


Figure S6: Superimposed bound ligand in crystal structure and docked pose of same

Table S5: Dock score, binding energy and number of binding interactions of proposed and most active molecules with different protonated state of Asp32 and Asp228 dyad.

		Prot1	Prot2	Prot3	Prot4	Prot5	Prot6	Prot7	Prot8	Prot9	Prot10
B26	DS	7.164	6.199	5.898	6.156	5.446	6.321	6.093	6.344	6.387	5.536
	BE	-74.552	-14.611	-18.563	-1.203	-18.419	-16.843	-17.163	-20.815	-23.228	-38.719
	NBI	0	0	0	0	0	0	0	0	0	0
NSC11408	DS	61.663	60.490	60.148	60.250	60.642	60.107	60.323	60.726	27.726	60.207
	BE	-45.069	-28.989	-34.551	-12.606	-45.068	-16.565	-13.985	-24.515	-21.161	-8.366
	NBI	2	0	0	1	0	0	0	0	0	0
NSC367261	DS	33.372	26.048	27.394	27.537	27.494	27.796	27.939	26.715	56.950	27.938
	BE	-28.964	-26.994	-0.376	-15.345	-23.677	-10.632	-15.012	-20.569	-17.072	-3.333
	NBI	5	0	0	0	1	1	1	2	1	1
NSC694875	DS	56.494	50.936	51.201	51.459	56.133	56.869	56.719	54.487	56.950	56.687
	BE	-78.853	-67.725	-69.471	-20.768	-41.861	-39.072	-50.952	-16.407	-56.727	-59.383
	NBI	0	0	0	0	0	0	0	0	0	0
STOCKIN033-31	DS	77.878	67.532	67.05	67.596	68.079	67.988	68.074	67.936	67.709	67.953
	BE	903.925	-32.512	-34.086	130.374	-17.194	-0.202	140.159	182.699	180.072	373.984
	NBI	3	0	0	0	0	0	0	0	0	0
STOCK3334396	DS	67.614	61.231	61.029	61.093	60.900	60.661	60.665	61.037	60.521	60.921
	BE	-32.760	-27.756	-26.759	-31.602	-9.342	-8.348	-15.138	-19.303	-17.516	-31.390
	NBI	3	1	1	1	2	2	2	2	2	2
STOCK6874113	DS	77.509	73.719	73.730	73.985	73.545	73.081	73.509	74.170	73.436	73.607
	BE	-22.694	-17.324	-7.928	-14.829	-12.621	-4.553	-15.915	-22.246	-12.079	-20.362
	NBI	1	0	0	0	1	1	1	1	1	1

DS – Dock score; BE – Binding energy; NBI – Number of binding interactions with Asp32 and Asp228