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Supplementary Materials

Computer-Driven Development of an in Silico Tool for Finding Selective Histone Deacetylase 1 Inhibitors

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Table S1. Experimental (Observed column) and predicted (Predicted column) activity pIC_{50} for compounds used for developing the 3D-QSAR model. (Note: a) compounds included in the training set; b) compounds included in the tests set; (Note: * compounds used for the decoys generation).

Compounds		Observed IC_{50}(μM)	Observed PIC_{50}	Predicted pIC_{50}	Note
1	C1CCN1Cc(cn2)cc(C#N)c2-c3ccc(cc3)C(=O)Nc4c(N)cccc4 (Andrews and Gibson, et al., 2008)	0.01	2.000	1.830	a*
2	c1cccc(N)c1NC(=O)c(cc2)ccc2-c3c(C#N)cc(cn3)CN4CCN(CC4)CC (Andrews and Gibson, et al., 2008)	0.01	2.000	1.880	a*
3	c1cccc(N)c1NC(=O)c(cc2)ccc2-c3c(C#N)cc(cn3)CN4CCN(CC4)C(C)C (Andrews and Gibson, et al., 2008)	0.01	2.000	1.970	a*
4	c1ccsc1-c(ccc2N)cc2NC(=O)c3ccc(cc3)NC(=O)C (Methot and Chakravarty, et al., 2008)	0.007	2.155	1.710	a*
5	c1cscc1-c(ccc2N)cc2NC(=O)c3ccc(cc3)NC(=O)C (Methot and Chakravarty, et al., 2008)	0.007	2.155	1.890	a*
6	c1ccccc1-c(c2)ccc(O)c2NC(=O)c3ccc(cc3)CNc4ccncc4 (Kattar, et al., 2009)	0.01	2.000	1.530	a*
7	c1ccccc1-c(c2)ccc(N)c2NC(=O)c3ccc(cc3)CNc4ccncc4 (Kattar, et al., 2009)	0.01	2.000	1.580	b*
8	c1ccccc1-c(c2)ccc(N)c2NC(=O)c3ccc(cc3)CN(C)c4ccncc4 (Kattar, et al., 2009)	0.01	2.000	2.020	a*
9	c1ccccc1-c(c2)ccc(N)c2NC(=O)c3ccc(cc3)CN(CC4)CCC45NCCC5 (Kattar, et al., 2009)	0.008	2.097	1.790	b*
10	s1cccc1-c(c2)ccc(N)c2NC(=O)c3ccc(cc3)CN(CC4)CCC45NCCC5 (Kattar, et al., 2009)	0.004	2.398	2.130	a*
11	c1sccc1-c(c2)ccc(N)c2NC(=O)c3ccc(cc3)CN(CC4)CCC45NCCC5 (Kattar, et al., 2009)	0.008	2.097	2.250	a*
12	c1ccccc1-c(c2)ccc(N)c2NC(=O)c3ccc(cc3)C(=O)N(CC4)CCC45NCCC5 (Kattar, et al., 2009)	0.008	2.097	2.070	a*
13	C1CNCC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5 (Methot and Hamblett, et al., 2008)	0.008	2.097	1.930	b*
14	C1CNCC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5ccsc5 (Methot and Hamblett, et al., 2008)	0.01	2.000	2.060	a*
15	C1CN(C(=O)C)CC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5 (Methot and Hamblett, et al., 2008)	0.009	2.046	2.090	b*
16	C1CN(S(=O)(=O)C)CC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5 (Methot and Hamblett, et al., 2008)	0.008	2.097	2.190	a*
17	OCCN(CC1)CC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5 (Methot and Hamblett, et al., 2008)	0.006	2.222	2.140	a*
18	CC(=O)N(C1)CCC12CCCN(C2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5	0.008	2.097	2.060	a*

	(Methot and Hamblett, et al., 2008)				
19	C1NC(=O)NC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5 (Methot and Hamblett, et al., 2008)	0.007	2.155	2.280	a*
20	C1OC(=O)NC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5 (Methot and Hamblett, et al., 2008)	0.008	2.097	2.130	a*
21	Nc1ccccc1NC(=O)c2ccc(cc2)CNC(=O)OCc3cccnc3 **Entinostat** (Li et al., 2015)	0.273	0.564	0.410	a
22	Nc1ccccc1NC(=O)c2ccc(cc2)CNc3nccc(n3)-c4cccnc4 **Mocetinostat** (Li et al., 2013)	0.098	1.01	0.800	a
23	Nc1ccccc1NC(=O)c2ccc(cc2)C(C(=O)Nc3ccccc3)C(=O)Nc4ccccc4 (Siliphaivanh et al.,2007)	0.041	1.387	1.320	a
24	Nc1ccccc1NC(=O)c2ccc(cc2)C(C(=O)Nc3cccc(c3)C#N)C(=O)Nc4cc(C#N)ccc4 (Siliphaivanh et al.,2007)	0.034	1.469	1.280	a*
25	Nc1ccccc1NC(=O)c2ccc(cc2)C(C(=O)Nc3ccc(F)cc3)C(=O)Nc4ccc(F)cc4 (Siliphaivanh et al.,2007)	0.063	1.201	1.350	b
26	Nc1ccccc1NC(=O)c2ccc(cc2)C(C(=O)Nc3cc(F)ccc3)C(=O)Nc4cc(F)ccc4 (Siliphaivanh et al.,2007)	0.056	1.252	1.210	a
27	Nc1ccccc1NC(=O)c2ccc(cc2)C(C(=O)Nc3cc(OC)ccc3)C(=O)Nc4cc(OC)cc c4 (Siliphaivanh et al.,2007)	0.035	1.456	1.380	a*
28	Nc1ccccc1NC(=O)c2ccc(cc2)C(C(=O)Nc3c(OC)cccc3)C(=O)Nc4ccccc4OC (Siliphaivanh et al.,2007)	0.047	1.328	1.320	a
29	Nc1ccccc1NC(=O)c2ccc(cc2)C(C(=O)Nc(cc3)cc(c34)OCCO4)C(=O)Nc(c5)ccc(c56)OCCO6 (Siliphaivanh et al.,2007)	0.021	1.678	1.550	a*
30	Nc1ccccc1NC(=O)c2ccc(cc2)C(C(=O)Nc3cc(ccc3)N4CCOCC4)C(=O)Nc5c ccc(c5)N6CCOCC6 (Siliphaivanh et al.,2007)	0.045	1.347	1.280	a
31	Nc1ccccc1NC(=O)c2ccc(cc2)C(C(=O)Nc3cccc(c34)cccn4)C(=O)Nc5cccc(c56)cccn6 (Siliphaivanh et al.,2007)	0.103	0.987	1.060	b
32	Nc1ccccc1NC(=O)c2ccc(cc2)C(C(=O)N(C)c3ccccc3)C(=O)Nc4ccccc4 (Siliphaivanh et al.,2007)	0.196	0.708	0.790	a
33	Nc1ccccc1NC(=O)c2ccc(cc2)C(C(=O)N(C)c3ccccc3)C(=O)N(C)c4ccccc4 (Siliphaivanh et al.,2007)	7.195	-0.857	-0.810	a
34	Nc1ccccc1NC(=O)c2ccc(cc2)C(C(=O)NCc3ccccc3)C(=O)NCc4ccccc4 (Siliphaivanh et al.,2007)	0.199	0.701	0.630	a

35	Nc1ccccc1NC(=O)c2ccc(cc2)C(C(=O)NCCCc3ccccc3)C(=O)NCCCc4ccccc4 (Siliphaivanh et al.,2007)	0.229	0.640	0.690	a
36	Nc1ccccc1NC(=O)c2ccc(cc2)C(F)(C(=O)Nc3ccccc3)C(=O)Nc4ccccc4 (Siliphaivanh et al.,2007)	0.048	1.319	1.100	a
37	Nc1ccccc1NC(=O)c2ccc(cc2)C(O)(C(=O)Nc3ccccc3)C(=O)Nc4ccccc4 (Siliphaivanh et al.,2007)	0.094	1.027	0.740	b
38	Nc1ccccc1NC(=O)c2ccc(cc2)C(C)(C(=O)Nc3ccccc3)C(=O)Nc4ccccc4 (Siliphaivanh et al.,2007)	0.198	0.703	0.660	a
39	Nc1ccccc1NC(=O)c2ccc(cc2)CC(C(=O)Nc3ccccc3)C(=O)Nc4ccccc4 (Siliphaivanh et al.,2007)	0.047	1.328	0.600	b
40	Nc1ccccc1NC(=O)c2ccc(cc2)CC(C)(C(=O)Nc3ccccc3)C(=O)Nc4ccccc4 (Siliphaivanh et al.,2007)	0.200	0.699	0.430	b
41	Nc1ccccc1NC(=O)c2ccc(cc2)CNC(=O)c(c3)c(=O)oc(c34)cc(cc4)OCCC (Abdizadeh et al., 2017)	0.87	0.060	0.270	b
42	Nc1ccccc1NC(=O)c2ccc(cc2)CNC(=O)c(c3)c(=O)oc(c34)cc(cc4)OCc5ccc(Br)cc5 (Abdizadeh et al., 2017)	0.50	0.301	0.330	a
43	Nc1ccccc1NC(=O)c2ccc(cc2)CNC(=O)c(c3)c(=O)oc(c34)cc(cc4)OCc5ccc(cc5)OC (Abdizadeh et al., 2017)	0.71	0.149	0.100	a
44	Nc1ccccc1NC(=O)c2ccc(cc2)CNC(=O)c(c3)c(=O)oc(c34)cc(cc4)OCc5ccc(Cl)c(Cl)c5 (Abdizadeh et al., 2017)	0.47	0.328	0.330	a
45	Nc1ccccc1NC(=O)c2ccc(nc2)N(C)CCN(C)C(=O)OCc3ccccc3 (Hamblett et al., 2007)	0.963	0.016	0.070	a
46	Nc1ccccc1NC(=O)c2ccc(nc2)N3CCN(CC3)C(=O)OCc4ccccc4 (Hamblett et al., 2007)	0.168	0.775	1.010	a
47	Nc1ccccc1NC(=O)c2ccc(nc2)N3CCN[C@H](C3)C (Hamblett et al., 2007)	0.435	0.362	0.520	a
48	Nc1ccccc1NC(=O)c2ccc(nc2)N3CCN([C@H](C3)C)C(=O)OC(C)(C)C (Hamblett et al., 2007)	0.242	0.616	0.930	a
49	Nc1ccccc1NC(=O)c2ccc(nc2)N3CCN([C@H](C3)C)C(=O)OCc4ccccc4 (Hamblett et al., 2007)	0.073	1.137	1.100	b
50	Nc1ccccc1NC(=O)c2ccc(nc2)N3CCN([C@@H](C3)C)C(=O)OCc4ccccc4 (Hamblett et al., 2007)	0.040	1.398	1.140	a
51	Nc1ccccc1NC(=O)c2ccc(nc2)N(C3)CCN(C3(C)C)C(=O)OCc4ccccc4 (Hamblett et al., 2007)	0.169	0.772	0.860	a
52	Nc1ccccc1NC(=O)c2ccc(nc2)N3[C@H](C)CN([C@H](C3)C)C(=O)OCc4ccccc4 (Hamblettet al., 2007)	0.255	0.593	0.510	a

53	Nc1ccccc1NC(=O)c2ccc(nc2)N3CCN([C@H](C3)C(C)C)C(=O)OCc4ccccc4 (Hamblett et al., 2007)	0.326	0.487	0.740	a
54	Nc1ccccc1NC(=O)c2ccc(nc2)N(C3)CCN(C3(C)C)C(=O)OCCc4ccccc4 (Hamblett et al., 2007)	0.077	1.114	0.830	a
55	Nc1ccccc1NC(=O)c2ccc(nc2)N(C3)CCN(C3(C)C)S(=O)(=O)c4ccccc4 (Hamblett et al., 2007)	0.149	0.827	0.950	b
56	Nc1ccccc1NC(=O)c2ccc(nc2)N3CCN([C@H](C3)C)C(=O)Nc4ccccc4 (Hamblett et al., 2007)	0.075	1.125	0.910	b
57	Nc1ccccc1NC(=O)c2ccc(nc2)N3CCN([C@H](C3)C)C(=O)NCc4ccccc4 (Hamblett et al., 2007)	0.039	1.409	1.300	a
58	Nc1ccccc1NC(=O)c2ccc(nc2)N3CCN([C@H](C3)C)C(=O)NCc4ccc(cc4)OC (Hamblett et al., 2007)	0.047	1.328	1.360	a
59	Nc1ccccc1NC(=O)c2ccc(nc2)N3CCN([C@H](C3)C)C(=O)N[C@H](C)c4cc ccc4 (Hamblett et al., 2007)	0.101	0.996	1.280	a
60	Nc1ccccc1NC(=O)c2ccc(nc2)N3CCN([C@H](C3)C)C(=O)N[C@@H](C)c4 ccccc4 (Hamblett et al., 2007)	0.047	1.328	1.270	b
61	Nc1ccccc1NC(=O)c2ccc(nc2)N3CCN([C@H](C3)C)C(=O)NCCc4ccccc4 (Hamblett et al., 2007)	0.047	1.328	1.240	a
62	Nc1ccccc1NC(=O)c2ccc(nc2)N(CC3)CC(N34)CCCC4 (Hamblett et al., 2007)	0.588	0.231	0.250	a
63	Nc1ccccc1NC(=O)c2ccc(nc2)N(CC3)Cc(n34)ncc4-c5ccccc5 (Hamblett et al., 2007)	0.139	0.857	0.580	a
64	Nc1ccccc1NC(=O)c2ccc(nc2)N(CC3)Cc(n34)ncc4Cc5ccccc5 (Hamblett et al., 2007)	0.222	0.654	0.460	b
65	Nc1ccccc1NC(=O)c2ccc(nc2)N(C(C34)CC4)CCN3C(=O)OCc5ccccc5 (Hamblettet al., 2007)	0.140	0.854	1.050	b
66	Nc1ccccc1NC(=O)c2ccc(nc2)N(c(c34)cccc4)CCN3C(=O)OCc5ccccc5 (Hamblett et al., 2007)	0.092	1.036	1.080	b
67	Nc1ccccc1NC(=O)c2ccc(nc2)N3CCN[C@H](C3)CCC (Hamblett et al., 2007) (Ref9)	0.304	0.517	0.600	b
68	Nc1ccccc1NC(=O)c2ccc(nc2)N3CCN[C@H](C3)CCCC (Hamblett et al., 2007) (Ref9)	0.301	0.521	0.440	a
69	Nc1ccccc1NC(=O)c2ccc(nc2)N3[C@H](C)CN[C@H](C3)C (Hamblett et al., 2007)	0.582	0.235	0.300	a
70	Nc1ccccc1NC(=O)c2ccc(nc2)N(C3)CCNC3(C)C (Hamblett et al., 2007)	0.529	0.277	0.600	a
71	Nc1ccccc1NC(=O)c2ccc(nc2)N3CC(C)NC(C3)C (Hamblett et al., 2007)	0.821	0.086	0.400	a
72	Nc1ccccc1NC(=O)c2ccc(nc2)N3CCN(C(=O)OC(C)(C)C)C(C3)Cc4ccccc4	0.352	0.453	0.600	a

	(Hamblett et al., 2007)				
73	Nc1ccccc1NC(=O)c2ccc(nc2)N(CC34)C(C4)CN3 (Hamblett et al., 2007)	0.307	0.513	0.390	b
74	Nc1ccccc1NC(=O)c2ccc(nc2)N(CC34)C(C4)CN3C(=O)OC(C)(C)C (Hamblett et al., 2007)	0.189	0.724	0.940	b
75	Nc1ccccc1NC(=O)c2ccc(nc2)N(CC34)C(C4)CN3C(=O)OCc5ccccc5 (Hamblett et al., 2007)	0.068	1.167	1.250	a
76	Nc1ccccc1NC(=O)c2ccc(nc2)N(CC34)C(C4)CN3Cc5ccccc5 (Hamblett et al., 2007)	0.235	0.629	0.390	b
77	Nc1ccccc1NC(=O)c2ccc(nc2)N(CC34)C(C4)CN3C(=O)CCc5ccccc5 (Hamblett et al., 2007)	0.167	0.777	0.750	a
78	Nc1ccccc1NC(=O)c2ccc(nc2)N(CC34)C(CN3)CC4 (Hamblett et al., 2007)	0.405	0.393	0.590	a
79	Nc1ccccc1NC(=O)c2ccc(nc2)N(CC34)C(CC4)CN3C(=O)OC(C)(C)C (Hamblett et al., 2007)	0.669	0.175	0.480	a
80	Nc1ccccc1NC(=O)c2ccc(nc2)N(CC34)C(CC4)CN3C(=O)OCc5ccccc5 (Hamblett et al., 2007)	0.067	1.174	0.860	b
81	Nc1ccccc1NC(=O)c2ccc(nc2)N(CC34)C(CC4)CN3C(=O)OCc5cccnc5 (Hamblett et al., 2007)	0.091	1.041	0.930	a
82	Nc1ccccc1NC(=O)c2ccc(nc2)N(CC34)CC(CC4)N3C(=O)OC(C)(C)C (Hamblett et al., 2007)	0.167	0.777	0.990	b
83	Nc1ccccc1NC(=O)c2ccc(nc2)N(CC34)CC(CC4)N3C(=O)OCc5ccccc5 (Hamblett et al., 2007)	0.082	1.086	1.110	a
84	Nc1ccccc1NC(=O)c2ncccc2 (Andrews and Stokes, et al., 2008)	2.455	-0.390	-0.310	a
85	Nc1ccccc1NC(=O)c2ccc(cc2)-c3sccn3 (Andrews and Stokes, et al., 2008)	0.123	0.910	0.650	a
86	Nc1ccccc1NC(=O)c2ccc(cc2)C3CCN(CC3)Cc4ccccc4 (Andrews and Stokes, et al., 2008)	0.045	1.347	1.120	a
87	Nc1ccccc1NC(=O)c2ccc(cc2)C3CCN(C)CC3 (Andrews and Stokes, et al., 2008)	0.138	0.860	0.990	b
88	Nc1ccccc1NC(=O)c2ccc(cc2)-c3ncc(s3)CN4CCCCC4 (Andrews and Stokes, et al., 2008)	0.022	1.658	1.570	a*
89	Nc1ccccc1NC(=O)c2ccc(cc2)-c3ncc(s3)CNCC (Andrews and Stokes, et al., 2008)	0.038	1.420	1.450	b
90	Nc1ccccc1NC(=O)c2ccc(cc2)-c3ncc(s3)CNCCC (Andrews and Stokes, et al., 2008)	0.028	1.553	1.420	a*
91	Nc1ccccc1NC(=O)c2ccc(cc2)C3CCN(CC3)CCC(=O)Nc4c(F)cccc4 (Andrews and Stokes, et al., 2008)	0.068	1.167	1.050	a
92	Nc1ccccc1NC(=O)c2ccc(cc2)C3CCN(CC3)Cc4ccc(cc4)C(=O)N(C)C (Andrews and Stokes, et al., 2008)	0.085	1.071	1.140	a

93	Nc1ccccc1NC(=O)c2ccc(cc2)C3CCN(CC3)Cc4ccc(cc4)C(=O)NC5CC5 (Andrews and Stokes, et al., 2008)	0.058	1.237	1.180	a
94	Nc1ccccc1NC(=O)c2ccc(cc2)C3CCN(CC3)Cc4ccc(cc4)C(=O)NCC (Andrews and Stokes, et al., 2008)	0.035	1.456	1.130	b*
95	Nc1ccccc1NC(=O)c2ccc(cc2)C3CCN(CC3)Cc4ccc(cc4)C(=O)NC (Andrews and Stokes, et al., 2008)	0.031	1.509	1.150	b*
96	Nc1ccccc1NC(=O)c2ccc(cc2)-c3c(C#N)cc(cn3)N (Andrews and Gibson, et al., 2008)	0.012	1.921	1.670	a*
97	C1CCN1Cc(cn2)cc(C)c2-c3ccc(cc3)C(=O)Nc4c(N)cccc4 (Andrews and Gibson, et al., 2008)	0.021	1.678	1.660	a*
98	C1CCN1Cc(cn2)cc(Cl)c2-c3ccc(cc3)C(=O)Nc4c(N)cccc4 (Andrews and Gibson, et al., 2008)	0.019	1.721	1.620	a*
99	C1CCN1Cc(cn2)cc(F)c2-c3ccc(cc3)C(=O)Nc4c(N)cccc4 (Andrews and Gibson, et al., 2008)	0.05	1.301	1.410	a
100	c1cccc(N)c1NC(=O)c(cc2)ccc2-c3c(C)cc(cn3)CN4CCN(CC4)CC (Andrews and Gibson, et al., 2008)	0.019	1.721	1.710	a*
101	c1cccc(N)c1NC(=O)c(cc2)ccc2-c3c(Cl)cc(cn3)CN4CCN(CC4)CC (Andrews and Gibson, et al., 2008)	0.016	1.796	1.730	a*
102	c1cccc(N)c1NC(=O)c(cc2)ccc2-c3c(F)cc(cn3)CN4CCN(CC4)CC (Andrews and Gibson, et al., 2008)	0.038	1.420	1.330	a
103	c1cccc(N)c1NC(=O)c(cc2)ccc2-c3c(C)cc(cn3)CN4CCN(CC4)C(C)C (Andrews and Gibson, et al., 2008)	0.019	1.721	1.790	a*
104	c1cccc(N)c1NC(=O)c(cc2)ccc2-c3c(Cl)cc(cn3)CN4CCN(CC4)C(C)C (Andrews and Gibson, et al., 2008)	0.013	1.886	1.700	a*
105	c1cccc(N)c1NC(=O)c(cc2)ccc2-c3c(F)cc(cn3)CN4CCN(CC4)C(C)C (Andrews and Gibson, et al., 2008)	0.033	1.481	1.250	b*
106	s1cccc1-c(ccc2N)cc2NC(=O)c3ccc(cc3)CN(CCO)Cc(c4)ccc(c45)OCO5 (Hirata, et al., 2012)	0.06	1.222	1.410	a
107	Nc1ccccc1NC(=O)c2ccc(cc2)CN(CCO)Cc(c3)ccc(c34)OCO4 (Hirata, et al., 2012)	1.17	-0.068	0.250	a
108	s1cccc1-c(ccc2N)cc2NC(=O)c3ccc(cc3)CNC(=O)CC (Hirata, et al., 2012)	0.04	1.398	1.500	a
109	s1cccc1-c(ccc2N)cc2NC(=O)c3ccc(cc3)CNC(=O)N4CCOCC4 (Hirata, et al., 2012)	0.10	1.000	1.120	a
110	s1cccc1-c(ccc2N)cc2NC(=O)c3ccc(cc3)CNC(=O)N4CCN(C(=O)C4=O)CC (Hirata, et al., 2012)	0.05	1.301	0.960	a
111	s1cccc1-c(ccc2N)cc2NC(=O)c3ccc(cc3)CNC(=O)N4CCN(C)CC4 (Hirata, et al., 2012)	0.08	1.097	1.140	a
112	c1ccccc1-c(ccc2O)cc2NC(=O)c3ccccc3 (Methot and Chakravarty, et al., 2008)	0.058	1.237	1.090	b
113	c1ccccc1-c(ccc2O)cc2NC(=O)c3ccccn3	0.31	0.509	0.760	a

	(Methot and Chakravarty, et al., 2008)				
114	c1ccccc1-c(ccc2O)cc2NC(=O)c3cccnc3 (Methot and Chakravarty, et al., 2008)	0.068	1.167	0.980	b
115	c1ccccc1-c(ccc2O)cc2NC(=O)c3ccncc3 (Methot and Chakravarty, et al., 2008)	0.075	1.125	0.960	a
116	c1ccccc1-c(ccc2O)cc2NC(=O)c3sccc3 (Methot and Chakravarty, et al., 2008)	0.13	0.886	1.070	b
117	c1ccccc1-c(ccc2O)cc2NC(=O)c(c3)sc(c34)cccc4 (Methot and Chakravarty, et al., 2008)	0.13	0.886	1.240	a
118	c1ccccc1-c(ccc2O)cc2NC(=O)c3ccco3 (Methot and Chakravarty, et al., 2008)	0.13	0.886	0.860	b
119	c1ccccc1-c(ccc2O)cc2NC(=O)c3ccno3 (Methot and Chakravarty, et al., 2008)	0.10	1.000	0.800	a
120	c1ccccc1-c(ccc2O)cc2NC(=O)CCCc3ccccc3 (Methot and Chakravarty, et al., 2008)	0.61	0.215	0.110	a
121	c1ccccc1-c(ccc2O)cc2NC(=O)C/C=C/c3ccccc3 (Methot and Chakravarty, et al., 2008)	1.2	-0.079	0.230	a
122	c1cocc1-c(ccc2N)cc2NC(=O)c3cccnc3 (Methot and Chakravarty, et al., 2008)	0.16	0.796	0.430	b
123	c1cncn1-c(ccc2N)cc2NC(=O)c3cccnc3 (Methot and Chakravarty, et al., 2008)	1.00	0.000	0.090	a
124	c1cnccc1-c(ccc2N)cc2NC(=O)c3cccnc3 (Methot and Chakravarty, et al., 2008)	0.65	0.187	0.360	a
125	C1CCCN1c(ccc2N)cc2NC(=O)c3cccnc3 (Methot and Chakravarty, et al., 2008)	0.67	0.174	0.500	a
126	c1cc(F)ccc1-c(ccc2N)cc2NC(=O)c3cccnc3 (Methot and Chakravarty, et al., 2008)	0.14	0.854	0.460	a
127	c1cc(N)ccc1-c(ccc2N)cc2NC(=O)c3cccnc3 (Methot and Chakravarty, et al., 2008)	0.33	0.481	0.150	a
128	c1cc(N(C)C)ccc1-c(ccc2N)cc2NC(=O)c3cccnc3 (Methot and Chakravarty, et al., 2008)	5.3	-0.724	-0.650	a
129	N#CCc(cc1)ccc1-c(ccc2N)cc2NC(=O)c3cccnc3 (Methot and Chakravarty, et al., 2008)	0.25	0.602	0.210	a
130	c1cc(CN)ccc1-c(ccc2N)cc2NC(=O)c3cccnc3 (Methot and Chakravarty, et al., 2008)	2.1	-0.322	-0.020	a
131	c1ncccc1C(=O)Nc2cc(ccc2N)-c3ccc(cc3)CCC(=O)OC (Methot and Chakravarty, et al., 2008)	1.5	-0.176	0.160	b
132	c1ncccc1C(=O)Nc2cc(ccc2N)-c3ccc(cc3)N4CCN(CC4)c5ccccc5 (Methot and Chakravarty, et al., 2008)	50	-1.699	-2.070	a
133	Nc1ccccc1NC(=O)c2ccccc2 (Methot and Chakravarty, et al., 2008)	2.4	-0.380	-0.030	a

134	c1ccccc1-c(ccc2N)cc2NC(=O)c3ccccc3 (Methot and Chakravarty, et al., 2008)	0.060	1.222	0.940	a
135	c1ccsc1-c(ccc2N)cc2NC(=O)c3ccccc3 (Methot and Chakravarty, et al., 2008)	0.048	1.319	0.900	b
136	c1ccccc1- c(ccc2N)cc2NC(=O)c3ccc(nc3)N4CCN([C@H](C4)C)C(=O)OCc5ccccc5 (Methot and Chakravarty, et al., 2008)	0.059	1.229	1.410	a
137	Nc1ccccc1NC(=O)c2ccc(cc2)NC(=O)C **(CI-994)** (Methot and Chakravarty, et al., 2008)	0.57	0.244	0.790	a
138	c1ccccc1-c(ccc2O)cc2NC(=O)c3ccc(cc3)NC(=O)C (Methot and Chakravarty, et al., 2008)	0.018	1.745	1.850	a*
139	c1ccccc1-c(ccc2N)cc2NC(=O)c3ccc(cc3)NC(=O)C (Methot and Chakravarty, et al., 2008)	0.028	1.553	1.800	b*
140	Nc1ccccc1NC(=O)c2ccc(cc2)CNCc3ccc(cc3)-c4cccs4 (Kiyokawa, et al., 2010)	1.00	0.000	0.070	a
141	Nc1ccccc1NC(=O)c2ccc(cc2)CNCc(s3)cc(c34)cccc4 (Kiyokawa, et al., 2010)	1.1	-0.041	0.020	a
142	Nc1ccccc1NC(=O)c2ccc(cc2)CNCc3cc(ccc3)-c4cccs4 (Kiyokawa, et al., 2010)	3.3	-0.519	-0.460	a
143	Nc1ccccc1NC(=O)c2ccc(cc2)CNCc3ccc(cc3)-c4ccccc4 (Kiyokawa, et al., 2010)	0.9	0.046	0.170	b
144	Nc1ccccc1NC(=O)c2ccc(cc2)CN(C)Cc3ccc(cc3)-c4cccs4 (Kiyokawa, et al., 2010)	10	-1.000	-0.810	a
145	Nc1ccccc1NC(=O)c2ccc(cc2)CN(S(=O)(=O)C)Cc3ccc(cc3)-c4cccs4 (Kiyokawa, et al., 2010)	1.2	-0.079	0.070	a
146	Nc1ccccc1NC(=O)c2ccc(cc2)CN(C(=O)N(C)C)Cc3ccc(cc3)-c4cccs4 (Kiyokawa, et al., 2010)	0.8	0.097	0.130	a
147	Nc1ccccc1NC(=O)c2ccc(cc2)CN(CCO)Cc3ccc(cc3)-c4cccs4 (Kiyokawa, et al., 2010)	0.8	0.097	0.010	b
148	Nc1ccccc1NC(=O)c2ccc(cc2)CN(CCO)Cc3ccc(cc3)-c4ccccc4 (Kiyokawa, et al., 2010)	0.7	0.155	0.860	b
149	c1ccccc1-c(c2)ccc(O)c2NC(=O)c3ccc(cc3)CNCC(C)C (Kattar, et al., 2009)	0.112	0.951	1.250	b
150	c1ccccc1-c(c2)ccc(O)c2NC(=O)c3ccc(cc3)CNCc4cnccc4 (Kattar, et al., 2009)	0.032	1.495	1.740	b*
151	c1ccccc1-c(c2)ccc(O)c2NC(=O)c3ccc(cc3)CNC(C)c4ccncc4 (Kattar, et al., 2009)	0.013	1.886	2.080	a*
152	c1c(Cl)ccc(O)c1NC(=O)c2ccc(cc2)CNc3ccncc3 (Kattar, et al., 2009)	5.032	-0.702	-0.740	a
153	c1c(F)ccc(O)c1NC(=O)c2ccc(cc2)CNc3ccncc3	2.013	-0.304	-0.320	a

	(Kattar, et al., 2009)				
154	c1c(Br)ccc(O)c1NC(=O)c2ccc(cc2)CNc3ccncc3 (Kattar, et al., 2009)	5.223	-0.718	-0.700	a
155	c1cccc(O)c1NC(=O)c2ccc(cc2)CNc3ccncc3 (Kattar, et al., 2009)	1.568	-0.195	-0.350	a
156	COc(c1)ccc(O)c1NC(=O)c2ccc(cc2)CNc3ccncc3 (Kattar, et al., 2009)	7.964	-0.901	-0.490	a
157	c1ccccc1-c(c2)ccc(N)c2NC(=O)c3ccc(cc3)CNCc4c(C)n(C)nc4 (Kattar, et al., 2009	0.013	1.886	1.860	a*
158	c1ccccc1-c(c2)ccc(N)c2NC(=O)c3ccc(cc3)CN(CC4)CCC45CNCC5 (Kattar, et al., 2009)	0.033	1.481	1.650	a*
159	c1cccc(F)c1-c(c2)ccc(N)c2NC(=O)c3ccc(cc3)CN(CC4)CCC45NCCC5 (Kattar, et al., 2009)	0.016	1.796	2.110	a*
160	c1ccc(F)cc1-c(c2)ccc(N)c2NC(=O)c3ccc(cc3)CN(CC4)CCC45NCCC5 (Kattar, et al., 2009)	0.047	1.328	2.180	b
161	c1cc(F)ccc1-c(c2)ccc(N)c2NC(=O)c3ccc(cc3)CN(CC4)CCC45NCCC5 (Kattar, et al., 2009)	0.013	1.886	1.730	a*
162	s1cccc1-c(c2)ccc(N)c2NC(=O)c3ccc(cc3)C(=O)N(CC4)CCC45NCCC5 (Kattar, et al., 2009)	0.011	1.959	1.980	b*
163	c1cccc(F)c1-c(c2)ccc(N)c2NC(=O)c3ccc(cc3)C(=O)N(CC4)CCC45NCCC5 (Kattar, et al., 2009)	0.011	1.959	2.040	a*
164	c1cc(F)ccc1-c(c2)ccc(N)c2NC(=O)c3ccc(cc3)C(=O)N(CC4)CCC45NCCC5 (Kattar, et al., 2009)	0.012	1.921	1.640	a*
165	c1ncccc1COC(=O)NCc2ccc(cc2)C(=O)Nc3c(N)cccc3 (Mahboobi, et al., 2009)	0.74	0.131	0.290	a
166	c1ncccc1-c(cn2)cnc2Nc3cc(ccc3C)NC(=O)c4ccc(s4)C(=O)Nc5c(N)cccc5 (Mahboobi, et al., 2009)	0.23	0.638	0.720	a
167	c1ncccc1-c2nc(sc2)Nc3cc(ccc3C)NC(=O)c4cccc(c4)C(=O)Nc5c(N)cccc5 (Mahboobi, et al., 2009)	0.17	0.770	0.890	a
168	c1ncccc1-c2nc(sc2)Nc3cc(ccc3)NC(=O)c4cccc(n4)C(=O)Nc5c(N)cccc5 (Mahboobi, et al., 2009)	0.45	0.347	0.360	a
169	c1ncccc1-c2nc(sc2)Nc3cc(ccc3C)NC(=O)c4cccc(n4)C(=O)Nc5c(N)cccc5 (Mahboobi, et al., 2009)	0.31	0.509	0.290	b
170	c1ncccc1-c2nc(sc2)Nc3cc(ccc3C)NC(=O)c4ccc(s4)C(=O)Nc5c(N)cccc5 (Mahboobi, et al., 2009)	1.13	-0.053	0.200	a
171	c1ccccc1N(CNC2=O)C23CCN(CC3)c(nc4)ccc4C(=O)Nc5ccccc5N (Methot and Hamblett, et al., 2008)	0.039	1.409	1.520	a
172	c1ccccc1S(=O)(=O)N(C2)CCC23CN(CC3)c(nc4)ccc4C(=O)Nc5ccccc5N (Methot and Hamblett, et al., 2008)	0.120	0.921	0.940	a
173	c1cccc(NC2)c1C23CCN(CC3)c(nc4)ccc4C(=O)Nc5ccccc5N (Methot and Hamblett, et al., 2008)	0.130	0.886	0.940	b

174	c1cccc(CNC2)c1C23CCN(CC3)c(nc4)ccc4C(=O)Nc5ccccc5N (Methot and Hamblett, et al., 2008)	0.089	1.051	1.080	a
175	s1cccc1-c(ccc2N)cc2NC(=O)c3cccnc3 (Methot and Hamblett, et al., 2008)	0.065	1.187	0.580	a
176	C1CNCC12CCN(CC2)c(nc3)ccc3C(=O)Nc4ccccc4N (Methot and Hamblett, et al., 2008)	0.160	0.796	0.630	b
177	C1CNCC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5ccccc5 (Methot and Hamblett, et al., 2008)	0.011	1.959	1.890	b*
178	C1CNCC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cn(C)nc5 (Methot and Hamblett, et al., 2008)	0.036	1.444	1.480	a
179	C1CNCC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cc[nH]n5 (Methot and Hamblett, et al., 2008)	0.018	1.745	1.590	a*
180	C1CNCC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cn(cn5)C (Methot and Hamblett, et al., 2008)	0.022	1.658	1.690	a*
181	CCNC(=O)N(CC1)CC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5 (Methot and Hamblett, et al., 2008)	0.014	1.854	1.830	a*
182	n1cccnc1N(CC2)CC23CCN(CC3)c(nc4)ccc4C(=O)Nc5cc(ccc5N)-c6cccs6 (Methot and Hamblett, et al., 2008)	0.028	1.553	1.590	a*
183	FC(F)(F)CN(CC1)CC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5 (Methot and Hamblett, et al., 2008)	0.017	1.770	1.980	b*
184	OC(=O)CN(CC1)CC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5 (Methot and Hamblett, et al., 2008)	0.017	1.770	1.770	a*
185	NC(=O)CN(CC1)CC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5 (Methot and Hamblett, et al., 2008)	0.013	1.886	1.790	b*
186	CC(=O)N(C1)CCC12CN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5 (Methot and Hamblett, et al., 2008)	0.012	1.921	1.950	a*
187	CC(=O)N(C1)CC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5 (Methot and Hamblett, et al., 2008)	0.023	1.638	1.910	b*
188	C1CCN(C(=O)C)C12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5 (Methot and Hamblett, et al., 2008)	0.023	1.638	1.940	a*
189	C1CCC(=O)C12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5 (Methot and Hamblett, et al., 2008)	0.013	1.886	1.740	a*
190	C1CCC(O)C12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5 (Methot and Hamblett, et al., 2008)	0.029	1.538	2.020	b*
191	C1CNC(=O)C12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5 (Methot and Hamblett, et al., 2008)	0.021	1.678	1.950	a*
192	C1NC(=O)C12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5 (Methot and Hamblett, et al., 2008)	0.011	1.959	2.110	b*
193	C1C(=O)NCC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5 (Methot and Hamblett, et al., 2008)	0.013	1.886	2.000	a*
194	N1CNC(=O)C12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5	0.011	1.959	2.280	b*

	(Methot and Hamblett, et al., 2008				
195	c1ccccc1NC(=O)CNCCCC(=O)Nc2ccccc2N (Rajak, et al., 2012)	9.2	-0.964	-0.890	a
196	Brc1ccc(cc1)NC(=O)CNCCCC(=O)Nc2ccccc2N (Rajak, et al., 2012)	1.7	-0.230	-0.160	a
197	Clc1ccccc1NC(=O)CNCCCC(=O)Nc2ccccc2N (Rajak, et al., 2012)	2.9	-0.462	-0.470	a
198	Clc1cccc(c1)NC(=O)CNCCCC(=O)Nc2ccccc2N (Rajak, et al., 2012)	1.8	-0.255	-0.060	a
199	Clc1ccc(cc1)NC(=O)CNCCCC(=O)Nc2ccccc2N (Rajak, et al., 2012)	1.4	-0.146	-0.140	b
200	O=[N+]([O-])c1ccccc1NC(=O)CNCCCC(=O)Nc2ccccc2N (Rajak, et al., 2012)	3.1	-0.491	-0.360	a
201	O=[N+]([O-])c1cccc(c1)NC(=O)CNCCCC(=O)Nc2ccccc2N (Rajak, et al., 2012)	2.3	-0.362	-0.120	b
202	O=[N+]([O-])c1ccc(cc1)NC(=O)CNCCCC(=O)Nc2ccccc2N (Rajak, et al., 2012)	0.9	0.046	-0.230	a
203	COc1ccc(cc1)NC(=O)CNCCCC(=O)Nc2ccccc2N (Rajak, et al., 2012)	3.6	-0.556	-0.710	b
204	c1ccccc1NC(=O)CNc2ccc(cc2)C(=O)Nc3c(N)cccc3 (Rajak, et al., 2012)	7.4	-0.869	-0.670	a
205	Brc1ccc(cc1)NC(=O)CNc2ccc(cc2)C(=O)Nc3c(N)cccc3 (Rajak, et al., 2012)	1.6	-0.204	-0.500	b
206	Clc1ccccc1NC(=O)CNc2ccc(cc2)C(=O)Nc3c(N)cccc3 (Rajak, et al., 2012)	2.9	-0.462	-0.400	a
207	Clc1cccc(c1)NC(=O)CNc2ccc(cc2)C(=O)Nc3c(N)cccc3 (Rajak, et al., 2012)	2.5	-0.398	-0.590	a
208	O=[N+]([O-])c1ccccc1NC(=O)CNc2ccc(cc2)C(=O)Nc3c(N)cccc3 (Rajak, et al., 2012)	2.00	-0.301	-0.550	a
209	COc1ccc(cc1)NC(=O)CNc2ccc(cc2)C(=O)Nc3c(N)cccc3 (Rajak, et al., 2012)	3.1	-0.491	-0.490	b
210	Cc1ccc(cc1)NC(=O)CNc2ccc(cc2)C(=O)Nc3c(N)cccc3 (Rajak, et al., 2012)	4.5	-0.653	-0.480	b
211	Clc1ccc(Cl)c(c1)NC(=O)CNc2ccc(cc2)C(=O)Nc3c(N)cccc3 (Rajak, et al., 2012)	8.6	-0.934	-0.710	a
212	c1cccc(N)c1NC(=O)\C=C\c(cc2)ccc2-c3nnc(o3)Cc4cccc(c45)cccc5 (Valente, et al., 2014)	1.00	0.000	-0.220	a
213	c1cccc(N)c1NC(=O)\C=C\c(cc2)ccc2-c3nnc(o3)Cc(c4)ccc(c45)cccc5 (Valente, et al., 2014)	2.4	-0.380	-0.570	a
214	c1cccc(N)c1NC(=O)\C=C\c(cc2)ccc2-c3nnc(o3)Cc4c[nH]c(c45)cccc5 (Valente, et al., 2014)	1.5	-0.176	-0.200	a

215	c1cccc(N)c1NC(=O)\C=C\c(cc2)ccc2Cc3nnc(o3)Cc4cccc(c45)cccc5 (Valente, et al., 2014)	4.1	-0.613	-0.620	a
216	c1cccc(N)c1NC(=O)c(cc2)ccc2-c3nnc(o3)Cc4cccc(c45)cccc5 (Valente, et al., 2014)	0.3	0.523	0.250	a
217	c1cccc(N)c1NC(=O)c(cc2)ccc2Cc3nnc(o3)Cc4cccc(c45)cccc5 (Valente, et al., 2014)	0.2	0.699	0.240	b
218	s1ccnc1C(=O)NCCCCCC(=O)Nc2ccc(F)cc2N (Rusche, et al., 2016)	18	-1.255	-1.480	a
219	Nc1ccccc1NC(=O)CCCCCNC(=O)C(=N2)C(C)c(c23)cccc3 (Rusche, et al., 2016)	0.371	0.431	0.720	a
220	Nc1ccccc1NC(=O)CCCCCNC(=O)C(=N2)Cc(c23)c(OC)ccc3 (Rusche, et al., 2016)	0.299	0.524	0.570	a
221	Nc1ccccc1NC(=O)CCCCCNC(=O)C(=N2)Cc(c23)c(ccc3)OCC (Rusche, et al., 2016)	0.262	0.582	0.590	a
222	Nc1ccccc1NC(=O)CCCCCNC(=O)C(=N2)Cc(c23)c(F)ccc3 (Rusche, et al., 2016)	0.436	0.361	0.540	a
223	Nc1ccccc1NC(=O)CCCCCNC(=O)C(=N2)Cc(c23)c(Cl)ccc3 (Rusche, et al., 2016)	0.254	0.595	0.530	a
224	Nc1ccccc1NC(=O)CCCCCNC(=O)C(=N2)Cc(c23)cc(cc3)OC(F)(F)F (Rusche, et al., 2016)	0.550	0.260	0.380	a
225	Nc1ccccc1NC(=O)CCCCCNC(=O)C(=N2)Cc(c23)cc(C)cc3 (Rusche, et al., 2016)	0.426	0.371	0.470	a
226	Nc1ccccc1NC(=O)CCCCCNC(=O)C(=N2)Cc(c23)cc(F)cc3 (Rusche, et al., 2016)	0.384	0.416	0.350	b
227	Nc1ccccc1NC(=O)CCCCCNC(=O)C(=N2)Cc(c23)cc(Cl)cc3 (Rusche, et al., 2016)	0.203	0.693	0.610	a
228	Nc1ccccc1NC(=O)CCCCCNC(=O)C(=N2)Cc(c23)cccc3OC (Rusche, et al., 2016)	0.392	0.407	0.490	b
229	Nc1ccccc1NC(=O)CCCCCNC(=O)C(=N2)Cc(c23)cccc3C (Rusche, et al., 2016)	0.059	1.229	0.640	b
230	Nc1ccccc1NC(=O)CCCCCNC(=O)C(=N2)Cc(c23)cccc3F (Rusche, et al., 2016)	0.079	1.102	1.180	a
231	Nc1ccccc1NC(=O)CCCCCNC(=O)C(=N2)Cc(c23)ccc(c3)N(C)C (Rusche, et al., 2016)	0.081	1.092	1.260	a
232	Nc1ccccc1NC(=O)CCCCCNC(=O)C(=N2)Cc(c23)c(OC(F)F)ccc3 (Rusche, et al., 2016)	0.041	1.387	1.500	a
233	Nc1ccccc1NC(=O)CCCCCNC(=O)c(n2C)cc(c23)cccc3 (Rusche, et al., 2016)	0.135	0.870	0.580	a
234	Nc1ccccc1NC(=O)CCCCCNC(=O)c(n2C)cc(c23)cc(F)cc3 (Rusche, et al., 2016)	0.081	1.092	0.810	a
235	Nc1ccccc1NC(=O)CCCCCNC(=O)c(n2C)cc(c23)cc(Cl)cc3	0.061	1.215	0.770	b

	(Rusche, et al., 2016)				
236	Nc1ccccc1NC(=O)CCCCCNC(=O)c(n2CCOC)cc(c23)cccc3 (Rusche, et al., 2016)	0.195	0.710	0.850	a
237	Nc1ccccc1NC(=O)CCCCCNC(=O)c2ccccc2CC (Rusche, et al., 2016)	3.756	-0.575	-0.570	a
238	Nc1ccccc1NC(=O)CCCCCNC(=O)c2cccc(c2)N(C)C (Rusche, et al., 2016)	0.585	0.233	0.270	b
239	Nc1ccccc1NC(=O)CCCCCNC(=O)C=2CN=c(c23)c(OC)ccc3 (Rusche, et al., 2016)	0.196	0.708	0.520	b
240	Nc1ccccc1NC(=O)CCCCCNC(=O)c(cc2)cc(c23)n(C)cc3 (Rusche, et al., 2016)	0.378	0.423	0.540	a
241	Nc1ccccc1NC(=O)CCCCCNC(=O)c(ccc2)c(c23)[nH]c(C)c3C (Rusche, et al., 2016)	0.207	0.684	0.600	a
242	c1ccc(OC(F)(F)F)cc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	0.468	0.330	0.250	a
243	FC(F)(F)Oc(cc1)ccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	0.501	0.300	0.180	a
244	c1cccc(c12)n(C)cc2C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.174	0.759	0.600	a
245	CCOc(cc1)cc(c12)CC(=N2)C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.359	0.445	0.590	a
246	CCNc(cc1)ccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	0.403	0.395	0.660	a
247	Cc1c(C)[nH]c(c12)ccc(c2)C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.270	0.569	0.070	b
248	c1ccc(Cl)c(c12)=NCC=2C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.172	0.764	0.700	a
249	c1cc(C)ccc1C(=O)NCCCCCC(=O)Nc2c(O)cccc2 (Rusche, et al., 2016)	0.224	0.650	0.760	a
250	c1c(C)cccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	0.527	0.278	0.250	b
251	Cc1cc(C)ccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	2.143	-0.331	-0.210	a
252	c1cc(C(F)F)ccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	0.362	0.441	0.180	a
253	c1cc(C(C)(C)O)ccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	0.402	0.396	0.430	b
254	C1CCN1c(cc2)ccc2C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.272	0.565	0.530	a
255	C1CN(C)CCN1c(c2)cccc2C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.365	0.438	0.400	a

256	C1CN(C)CCN1c2ccccc2C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	3.581	-0.554	-0.650	a
257	C1COCCN1c(cc2)ccc2C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.334	0.476	0.560	a
258	c1cccc(Cl)c1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	2.035	-0.309	-0.150	a
259	c1c(F)c(F)ccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	0.772	0.112	-0.200	b
260	c1cccc(c12)=NCC=2C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.246	0.609	0.470	a
261	COc(c1)ccc(c12)=NCC=2C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.218	0.662	0.640	b
262	C1CCCCC1c2ccccc2C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	2.768	-0.442	-0.260	a
263	c1cccc(COC)c1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	3.278	-0.516	-0.370	a
264	c1cc(OC)cc(c12)=NCC=2C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.248	0.606	0.450	b
265	N1=CCc(c12)c(ccc2)C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.524	0.281	0.150	b
266	Cn1ccc(c12)c(ccc2)C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.448	0.349	0.340	a
267	Nc1ccccc1NC(=O)CCCCCNC(=O)c(c2)ccc(c23)[nH]cc3 (Rusche, et al., 2016)	0.210	0.678	0.370	a
268	c1cn(C)c(c12)ccc(c2)C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.218	0.662	0.280	b
269	c1cccc(c12)n(C)nc2C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.299	0.524	0.530	a
270	c1n[nH]c(c12)c(ccc2)C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.371	0.431	0.480	a
271	C=CCc1ccccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	2.698	-0.431	-0.440	a
272	CCOc1ccccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	0.549	0.260	0.360	b
273	CCCOc1ccccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	0.399	0.399	0.290	a
274	c1cccc(SCC)c1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	1.333	-0.125	-0.140	a
275	O=S(=O)(C)c1ccccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	4.447	-0.648	-0.190	b
276	N#Cc1ccccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2	0.426	0.371	0.090	b

	(Rusche, et al., 2016)				
277	O=C(C)c1ccccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	2.644	-0.422	-0.370	a
278	c1ccccc1C(=O)c(cccc2)c2C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	2.720	-0.435	-0.430	a
279	c1ccccc1-c2ccccc2C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	5.732	-0.758	-0.830	a
280	FC(F)Oc1ccccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	1.479	-0.170	0.030	b
281	COCCOc1ccccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	2.396	-0.379	-0.310	a
282	FC(F)(F)c1ccccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	3.564	-0.552	-0.490	a
283	Fc1ccccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	1.135	-0.055	-0.230	b
284	COc1ccccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	0.674	0.171	-0.080	b
285	Brc1ccccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	2.719	-0.434	-0.160	a
286	COc1cccc(c12)=NCC=2C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.197	0.706	0.500	a
287	c1c[nH]c(c12)c(ccc2)C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.278	0.556	0.360	b
288	c1n[nH]c(c12)cc(cc2)C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.582	0.235	0.100	a
289	COc(c1)ccc(c12)CC(=N2)C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.193	0.714	0.860	a
290	c1cc(NC)ccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	0.449	0.348	0.090	b
291	C1CC1Nc(cc2)ccc2C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.315	0.502	-0.010	b
292	C1CN(C)CCN1c(cc2)ccc2C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.445	0.352	0.190	b
293	c1c(C)ccc(c12)CC(=N2)C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.177	0.752	0.650	a
294	CCOc(cc1)cc(c12)cc(n2C)C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.327	0.485	0.500	a
295	Cc1c(C)[nH]c(c12)cc(cc2)C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.201	0.697	0.750	a
296	c1c(C)ccc(c12)n[nH]c2C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.220	0.658	0.720	a

297	c1c(Cl)ccc(c12)=NCC=2C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.263	0.580	0.490	a
298	c1c[nH]c(c12)cc(cc2)C(=O)NCCCCCC(=O)Nc3c(N)cccc3 (Rusche, et al., 2016)	0.234	0.631	0.120	b
299	c1ccccc1S(=O)(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	7.00	-0.845	-0.850	a
300	c1cc(C)ccc1C(=O)NCCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	0.19	0.721	0.220	b
301	c1cccc(c12)cc(o2)C(=O)NCCCCCC(=O)Nc3c(N)cc(F)cc3 (Rusche, et al., 2016)	0.76	0.119	0.30	a
302	c1cc(C)ccc1C(=O)NCCCCCC(=O)Nc2c(O)cc(F)cc2 (Rusche, et al., 2016)	1.00	0.00	-0.11	b
303	n1ccccc1C(=O)NCCCCCC(=O)Nc2c(N)cc(F)cc2 (Rusche, et al., 2016)	3.890	-0.59	-0.55	a
304	c1ncccc1C(=O)NCCCCCCC(=O)Nc2cc(ccc2N)-c3cccs3 (Rusche, et al., 2016)	0.021	1.678	1.72	a*
305	c1cc(F)ccc1C(=O)NCCCCCC(=O)Nc2ccccc2N (Rusche, et al., 2016)	1.8	-0.255	-0.03	a
306	c1cc(Cl)ccc1C(=O)NCCCCCC(=O)Nc2ccccc2N (Rusche, et al., 2016)	0.7	0.155	0.25	b
307	c1cc(OC)ccc1C(=O)NCCCCCC(=O)Nc2ccccc2N (Rusche, et al., 2016)	1.7	-0.230	-0.18	a
308	c1c(Cl)cccc1C(=O)NCCCCCC(=O)Nc2ccccc2N (Rusche, et al., 2016)	2	-0.301	-0.11	a
309	c1cc(N(C)C)ccc1C(=O)NCCCCCC(=O)Nc2ccccc2N (Rusche, et al., 2016)	1.00	0.00	0.160	b
310	c1cc(C(C)(C)C)ccc1C(=O)NCCCCCC(=O)Nc2ccccc2N (Rusche, et al., 2016)	0.6	0.222	0.45	b
311	c1cc(C(F)(F)F)ccc1C(=O)NCCCCCC(=O)Nc2ccccc2N (Rusche, et al., 2016)	1.1	-0.041	-0.08	a
312	c1cc([N+]([O-])=O)ccc1C(=O)NCCCCCC(=O)Nc2ccccc2N (Rusche, et al., 2016)	1.2	-0.079	0.05	b
313	[O-][N+](=O)c(c1)cccc1C(=O)NCCCCCC(=O)Nc2ccccc2N (Rusche, et al., 2016)	0.8	0.097	0.01	b
314	FC(F)(F)c(c1)cccc1C(=O)NCCCCCC(=O)Nc2ccccc2N (Rusche, et al., 2016)	0.7	0.155	0.00	a
315	c1cc(C#N)ccc1C(=O)NCCCCCC(=O)Nc2ccccc2N (Rusche, et al., 2016)	0.7	0.155	-0.14	b
316	c1c(Cl)cc(Cl)cc1C(=O)NCCCCCC(=O)Nc2ccccc2N (Rusche, et al., 2016)	0.4	0.398	0.270	b
317	c1ccsc1C(=O)NCCCCCC(=O)Nc2ccccc2N	0.649	0.188	0.13	a

	(Rusche, et al., 2016)				
318	c1cc(C)ccc1C(=O)NCCCCCC(=O)Nc2cc(c(F)cc2N)-n3cccn3 (Rusche, et al., 2016)	0.442	0.355	0.210	a
319	O1COc(c12)c(N)c(cc2)NC(=O)CCCCCNC(=O)c3ccc(C)cc3 (Rusche, et al., 2016)	2.89	-0.461	-0.5	a
320	n1ccsc1C(=O)NCCCCCC(=O)Nc2ccccc2N (Rusche, et al., 2016)	0.973	0.012	-0.030	a
321	n1c(C)csc1C(=O)NCCCCCC(=O)Nc2ccccc2N (Rusche, et al., 2016)	0.721	0.142	0.470	a
322	n1cc(C)sc1C(=O)NCCCCCC(=O)Nc2ccccc2N (Rusche, et al., 2016)	0.816	0.088	-0.100	a
323	c1cc(Cl)cc(Cl)c1C(=O)NCCCCCC(=O)Nc2ccccc2N (Rusche, et al., 2016)	2.270	-0.356	-0.230	a
324	c1cc(S(=O)(=O)C)ccc1S(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	0.57	0.244	0.140	b
325	c1cc(S(=O)(=O)N)ccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	1.104	-0.043	-0.03	a
326	c1cnccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	1.260	-0.100	-0.150	b
327	n1ccncc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	2.045	-0.311	-0.410	a
328	c1nnccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	2.565	-0.409	-0.460	a
329	c1ccoc1C(=O)NCCCCCC(=O)Nc2ccccc2N (Rusche, et al., 2016)	0.99	0.004	0.130	a
330	c1cocc1C(=O)NCCCCCC(=O)Nc2ccccc2N (Rusche, et al., 2016)	1.24	-0.093	-0.040	a
331	c1cscc1C(=O)NCCCCCC(=O)Nc2ccccc2N (Rusche, et al., 2016)	0.76	0.119	0.000	b
332	[nH]1cccc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	0.463	0.334	0.240	a
333	[nH]1cnnc1C(=O)NCCCCCC(=O)Nc2c(N)cccc2 (Rusche, et al., 2016)	2.689	-0.43	-0.20	a
334	Nc1ccccc1NC(=O)CCCCCNC(=O)c2oncc2 (Rusche, et al., 2016)	1.372	-0.137	-0.230	a
335	Nc1ccccc1NC(=O)CCCCCNC(=O)c2ncsc2 (Rusche, et al., 2016)	1.039	-0.017	-0.090	a
336	Nc1ccccc1NC(=O)CCCCCNC(=O)c2cc(ncc2)N3CCCCC3 (Rusche, et al., 2016)	0.238	0.623	0.620	b
337	Nc1ccccc1NC(=O)CCCCCNC(=O)c2n[nH]c(c2)-c3ccccc3 (Rusche, et al., 2016)	0.388	0.411	0.490	b

338	Nc1ccccc1NC(=O)CCCCCNC(=O)c(cc2)cc(c23)OCCO3 (Rusche, et al., 2016)	0.754	0.123	0.420	b
339	Nc1ccccc1NC(=O)CCCCCNC(=O)c(c2)oc(c23)cccc3 (Rusche, et al., 2016)	0.418	0.379	0.440	a
340	Nc1ccccc1NC(=O)CCCCCNC(=O)c(cc2)cc(c23)scn3 (Rusche, et al., 2016)	0.433	0.364	0.570	b
341	Nc1ccccc1NC(=O)CCCCCNC(=O)CCC(=O)c2cccs2 (Rusche, et al., 2016)	0.78	0.108	0.060	a
342	Nc1ccccc1NC(=O)CCCCCNC(=O)c(cc2)cc(c23)non3 (Rusche, et al., 2016)	1.238	-0.093	-0.150	a
343	Nc1ccccc1NC(=O)CCCCCNC(=O)c(cc2)cc(c23)nccn3 (Rusche, et al., 2016)	1.027	-0.012	-0.220	a
344	Nc1ccccc1NC(=O)CCCCCNC(=O)c(cc2)cc(c23)nccc3 (Rusche, et al., 2016)	0.617	0.210	-0.190	b
345	Nc1ccccc1NC(=O)CCCCCNC(=O)c(c2)ccc(c23)cccc3 (Rusche, et al., 2016)	0.187	0.728	0.550	a
346	Nc1ccccc1NC(=O)CCCCCNC(=O)c(cc2)cc(c23)NC(=O)C3 (Rusche, et al., 2016)	0.725	0.140	0.120	a
347	Nc1ccccc1NC(=O)CCCCCNC(=O)c2cc(ccc2)-c3nnn[nH]3 (Rusche, et al., 2016)	0.466	0.332	0.290	a
348	Nc1ccccc1NC(=O)CCCCCNC(=O)c2ccc(cc2)-c3nnn[nH]3 (Rusche, et al., 2016)	0.371	0.431	0.440	a
349	Nc1ccccc1NC(=O)CCCCCNC(=O)CCc2oc(cn2)-c3ccccc3 (Rusche, et al., 2016)	0.312	0.506	0.460	a
350	Nc1ccccc1NC(=O)CCCCCNC(=O)c(no2)cc2-c3cscc3 (Rusche, et al., 2016)	0.484	0.315	0.370	a
351	Nc1ccccc1NC(=O)CCCCCNC(=O)C(=N2)Cc(c23)cc(cc3)OC (Rusche, et al., 2016)	0.258	0.588	0.720	b
352	Nc1ccccc1NC(=O)CCCCCNC(=O)c2noc(c2)C3CC3 (Rusche, et al., 2016)	0.673	0.172	0.040	b
353	Nc1ccccc1NC(=O)CCCCCNC(=O)c2n[nH]c(c23)cccc3 (Rusche, et al., 2016)	0.107	0.971	0.310	b
354	Nc1ccccc1NC(=O)CCCCCNC(=O)c(nc2)cc(c23)cccc3 (Rusche, et al., 2016)	0.264	0.578	0.550	a
355	Nc1ccccc1NC(=O)CCCCCNC(=O)c(cn2)cc(c23)cccc3 (Rusche, et al., 2016)	0.479	0.320	0.160	b
356	Nc1ccccc1NC(=O)CCCCCNC(=O)c(cnn2)c(c23)cccc3 (Rusche, et al., 2016)	4.312	-0.635	-0.490	a
357	Nc1ccccc1NC(=O)CCCCCNC(=O)c(cn2)nc(c23)cccc3 (Rusche, et al., 2016)	0.388	0.411	0.410	a
358	Nc1ccccc1NC(=O)CCCCCNC(=O)c2csc(n2)-c3ccncc3	0.3	0.523	0.580	b

	(Rusche, et al., 2016)				
359	Nc1ccccc1NC(=O)CCCCCNC(=O)c2sc(nc2C)-c3cnccc3 (Rusche, et al., 2016)	0.352	0.453	0.430	b
360	Nc1ccccc1NC(=O)CCCCCNC(=O)c2ccc(cc2)-n3cccc3 (Rusche, et al., 2016)	0.258	0.588	0.020	a
361	Nc1ccccc1NC(=O)CCCCCNC(=O)C2CCN(CC2)c3ccncc3 (Rusche, et al., 2016)	1.725	-0.237	-0.290	a
362	Nc1ccccc1NC(=O)CCCCCNC(=O)c2c(C)nc(s2)-c3ccccn3 (Rusche, et al., 2016)	0.483	0.316	0.450	b
363	Nc1ccccc1NC(=O)CCCCNC(=O)C(=N2)Cc(c23)cc(cc3)OC (Rusche, et al., 2016)	3.709	-0.569	-0.630	a
364	Nc1ccccc1NC(=O)CCCCNC(=O)c(c2)ccc(c23)ncs3 (Rusche, et al., 2016)	11.39	-1.057	-1.150	a
365	Nc1ccccc1NC(=O)CCCCNC(=O)c2nc(sc2)-c3ccncc3 (Rusche, et al., 2016)	2.766	-0.442	-0.510	a
366	Nc1ccccc1NC(=O)CCCCNC(=O)c2ccnc(c2)N3CCCCC3 (Rusche, et al., 2016)	18.24	-1.261	-1.220	a
367	Nc1ccccc1NC(=O)CCCCNC(=O)c(c2)ccc(c23)OCCO3 (Rusche, et al., 2016)	4.615	-0.664	-0.050	b
368	Nc1ccccc1NC(=O)CCCCNC(=O)C2=NN=C(C2)c3ccccc3 (Rusche, et al., 2016)	2.026	-0.307	0.060	b
369	Nc1ccccc1NC(=O)CCCCNC(=O)c2cc(no2)-c(cn3)cn3C (Rusche, et al., 2016)	7.274	-0.862	-0.800	a
370	c1cc(C)ccc1NC(=O)CCCCCC(=O)Nc2ccccc2N (Rusche, et al., 2016)	3.050	-0.484	-0.510	a

Table S2. Experimental (Observed column) and predicted (Predicted column) activity pIC_{50} for compounds included in the external test set. (Note: * compounds used for the decoys generation).

Compounds		Observed IC_{50}(μM)	Observed pIC_{50}	Predicted pIC_{50}	Note
371	Nc1ccccc1NC(=O)c2ccc(cc2)CCNC(=O)/C=C/c(cn3)n(c34)cccc4 (Li et al., 2015)	0.217	0.66	0.34	
372	Nc1ccccc1NC(=O)c2ccc(cc2)CCNC(=O)/C=C/c(c(n3)C)n(c34)cccc4 (Li et al., 2015)	0.169	0.77	0.35	
373	Nc1cc(F)ccc1NC(=O)c2ccc(cc2)CNC(=O)/C=C/c(cn3)n(c34)nccc4 (Li et al., 2015)	0.131	0.81	0.28	
374	Nc1ccccc1NC(=O)c2ccc(cc2)CNc3nc(ccn3)-c(cn4)n(c45)ccnc5 (Li et al., 2013)	0.110	0.96	0.81	
375	Nc1ccccc1NC(=O)c2ccc(cc2)CNc3nc(ccn3)-c(c(n4)C)n(c45)cccc5 (Li et al., 2013)	0.108	0.97	0.69	
376	Nc1ccccc1NC(=O)c2ccc(cc2)CNc3nc(ccn3)-c(c(n4)C)n(c45)cccn5 (Li et al., 2013)	0.127	0.90	0.67	
377	Nc1ccccc1NC(=O)c2ccc(cc2)CNc3nc(ccn3)-c(c(n4)C)n(c45)ccnc5 (Li et al., 2013)	0.097	1.01	0.69	
378	Nc1ccccc1NC(=O)c2ccc(cc2)CCNc3nc(ccn3)-c(c(n4)C)n(c45)cccn5 (Li et al., 2013)	0.154	0.81	0.96	
379	Nc1ccc(F)cc1NC(=O)c2ccc(cc2)CNc3nc(ccn3)-c(c(n4)C)n(c45)cccc5 (Li et al., 2013)	0.097	1.01	0.75	
380	Nc1cc(F)ccc1NC(=O)c2ccc(cc2)CNc3nc(ccn3)-c(c(n4)C)n(c45)cccc5 (Li et al., 2013)	0.135	0.87	0.71	
381	Nc1ccccc1NC(=O)c2ccc(cc2)CNc3nc(ccn3)-c(c(n4)C)n(c45)cc(Br)cc5 (Li et al., 2013)	0.125	0.90	0.73	
382	Nc1ccccc1NC(=O)c2ccc(cc2)CSc3[nH]ccn3 (Frechette et al., 2008)	0.5	0.30	0.10	
383	Nc1ccccc1NC(=O)c2ccc(cc2)CSc3n(C)ccn3 (Frechette et al., 2008)	1	0.00	0.11	
384	Nc1ccccc1NC(=O)c2ccc(cc2)CNc3sc(Br)cn3 (Frechette et al., 2008)	0.4	0.40	0.31	
385	Nc1ccccc1NC(=O)c2ccc(cc2)CNc3n[nH]c(n3)SC (Frechette et al., 2008)	0.2	0.70	0.62	
386	Nc1ccccc1NC(=O)c2ccc(cc2)CNc3cc([nH]n3)-c4ccccc4 (Frechette et al., 2008)	0.07	1.15	0.82	
387	Nc1ccccc1NC(=O)c2ccc(cc2)CNc3sc(cn3)-c4ccc(Cl)cc4 (Frechette et al., 2008)	0.3	0.52	0.52	
388	Nc1ccccc1NC(=O)c2ccc(cc2)CSc(s3)nc(c34)ccc(c4)NCc5cccnc5 (Frechette et al., 2008)	0.8	0.1	0.31	

389	Nc1ccccc1NC(=O)c2ccc(cc2)CSC3=N[C@H](CN3)c4ccccc4 (Marson et al., 2015)	0.24	0.62	0.31	
390	Nc1ccccc1NC(=O)c2ccc(cc2)CSC3=N[C@H](CN3)c4ccccc4 (Marson et al., 2015)	0.38	0.420	0.067	
391	Nc1ccccc1NC(=O)c2ccc(cc2)CSC3=N[C@H](CO3)Cc4ccccc4 (Marson et al., 2015)	0.70	0.15	0.23	
392	Nc1ccccc1NC(=O)c2ccc(cc2)CNC3=N[C@H](CO3)c4ccccc4 (Marson et al., 2015)	0.53	0.27	0.42	
393	Nc1ccccc1NC(=O)c2ccc(cc2)CNC3=NC(CO3)c4ccc(F)cc4 (Marson et al., 2015)	0.19	0.72	0.33	
394	Nc1ccccc1NC(=O)c2ccc(cc2)CNC3=NC(CO3)c4cc(F)ccc4 (Marson et al., 2015)	0.24	0.62	0.35	
395	Nc1ccccc1NC(=O)c2ccc(cc2)CNC3=NC(CO3)c4ccc(O)cc4 (Marson et al., 2015)	0.29	0.54	0.34	
396	Nc1ccccc1NC(=O)c2ccc(cc2)CNC3=NC(CO3)c4cccnc4 (Marson et al., 2015)	0.26	0.58	0.25	
397	Nc1ccccc1NC(=O)c2ccc(cc2)CNC3=N[C@H](CO3)Cc4ccccc4 (Marson et al., 2015)	0.20	0.50	0.57	
398	Nc1ccccc1NC(=O)c2ccc(cc2)CNC3=NC[C@@H](O3)c4ccccc4 (Marson et al., 2015)	0.39	0.41	0.36	
399	Nc1ccccc1NC(=O)c2ccc(cc2)CNC3=N[C@@H](CO3)Cc4c[nH]cn4 (Marson et al., 2015)	0.13	0.89	0.48	
400	Fc1ccc(c(c1)N)NC(=O)c2ccc(cc2)NC(=O)NCc3ccccc3 (Zhu et al., 2017)	0.772	0.11	0.41	
401	Nc1ccccc1NC(=O)c2ccc(cc2)CNC(=O)Nc3cc(C(F)(F)F)ccc3 (Zhu et al., 2017)	0.182	0.74	0.37	
402	Nc1ccccc1NC(=O)c2ccc(cc2)CNC(=O)Nc3ccc(C(F)(F)F)cc3 (Zhuet et al., 2017)	0.190	0.72	0.29	
403	Nc1ccccc1NC(=O)c2ccc(cc2)CNC(=O)Nc3ccc(Cl)cc3 (Zhu et al., 2017)	0.234	0.63	0.35	
404	Nc1ccccc1NC(=O)c2ccc(cc2)CNC(=O)Nc3cc(Cl)c(F)cc3 (Zhu et al., 2017)	0.624	0.20	0.31	
405	Nc1ccccc1NC(=O)c2ccc(cc2)CNC(=O)Nc3cc(C(F)(F)F)c(Cl)cc3 (Zhu et al., 2017)	0.211	0.67	0.30	
406	Nc1ccccc1NC(=O)c2ccc(cc2)CNC(=O)NCc3ccccc3 (Zhu et al., 2017)	0.123	0.91	0.59	
407	Fc1ccc(c(c1)N)NC(=O)c2ccc(cc2)CNC(=O)NCc3ccccc3 (Zhu et al., 2017)	1.14	-0.06	0.034	
408	c1cccc(N)c1NC(=O)c2ccc(cc2)CNc3cc(c(C)cc3)Nc4nc(ccn4)- c5cccnc5 (Mahboobi et al., 2009)	0.208	0.68	0.83	

409	c1ncccc1-c(cn2)cnc2Nc3cc(ccc3)NC(=O)c4cccc(c4)C(=O)Nc5c(N)cccc5 (Mahboobi et al., 2009)	0.76	0.12	0.170	
410	c1ncccc1-c(cn2)cnc2Nc3cc(ccc3C)NC(=O)c4cccc(c4)C(=O)Nc5c(N)cccc5 (Mahboobi et al., 2009)	0.27	0.57	0.161	
411	c1ncccc1-c2nc(sc2)Nc3cc(ccc3)NC(=O)c4cccc(c4)C(=O)Nc5c(N)cccc5 (Mahboobi et al., 2009)	0.23	0.64	0.77	
412	c1ncccc1-c2nc(sc2)Nc3cc(ccc3)NC(=O)c4ccc(s4)C(=O)Nc5c(N)cccc5 (Mahboobi et al., 2009)	0.47	0.33	0.16	
413	c1cncc(n12)ncc2-c(n3)ccnc3NCc4ccc(cc4)C(=O)Nc5ccccc5N (Li et al., 2013)	0.110	0.96	0.81	
414	c1cccc(n12)nc(C)c2-c(n3)ccnc3NCc4ccc(cc4)C(=O)Nc5ccccc5N (Li et al., 2013)	0.108	0.97	0.75	
415	c1ccnc(n12)nc(C)c2-c(n3)ccnc3NCc4ccc(cc4)C(=O)Nc5ccccc5N (Li et al., 2013)	0.127	0.90	0.64	
416	c1cncc(n12)nc(C)c2-c(n3)ccnc3NCc4ccc(cc4)C(=O)Nc5ccccc5N (Li et al., 2013)	0.097	1.01	0.69	
417	Nc1ccccc1NC(=O)c(cc2)ccc2CCNc3nccc(n3)-c4c(C)nc(n45)cccc5 (Li et al., 2013)	0.131	0.88	1.04	
418	Nc1ccccc1NC(=O)c(cc2)ccc2CCNc3nccc(n3)-c4cnc(n45)nccc5 (Li et al., 2013)	0.154	0.81	0.85	
419	c1cccc(n12)nc(C)c2-c(n3)ccnc3NCc4ccc(cc4)C(=O)Nc5cc(F)ccc5N (Li et al., 2013)	0.097	1.01	0.77	
420	c1cccc(n12)nc(C)c2-c(n3)ccnc3NCc4ccc(cc4)C(=O)Nc5ccc(F)cc5N (Li et al., 2013)	0.135	0.90	0.74	
421	c1c(Br)ccc(n12)nc(C)c2-c(n3)ccnc3NCc4ccc(cc4)C(=O)Nc5ccccc5N (Li et al., 2013)	0.125	0.90	0.68	
422	c1ccncc1COC(=O)NCc2ccc(cc2)C(=O)Nc3c(N)ccc(c3)-c4ccsc4 (Harrington et al., 2013)	0.0058	2.22	1.75	*
423	c1ccncc1COC(=O)NCc2ccc(cc2)C(=O)Nc3c(O)ccc(c3)-c4ccccc4 (Harrington et al., 2013)	0.02	1.70	1.49	*
424	CC(C)(C)OC(=O)NCc1ccc(cc1)C(=O)Nc2c(O)ccc(c2)-c3ccccc3 (Harrington et al., 2013)	0.07	1.15	1.50	
425	NCc1ccc(cc1)C(=O)Nc2c(O)ccc(c2)-c3ccccc3 (Harrington et al., 2013)	0.028	1.55	1.23	*
426	COC(=O)NCc1ccc(cc1)C(=O)Nc2cc(ccc2N)-c3ccccc3 (Harrington et al., 2013)	0.017	1.77	1.34	*
427	CCCOC(=O)NCc1ccc(cc1)C(=O)Nc2c(N)ccc(c2)-c3ccccc3 (Harrington et al., 2013)	0.029	1.54	1.36	*

428	CC(C)COC(=O)NCc1ccc(cc1)C(=O)Nc2c(N)ccc(c2)-c3ccccc3 (Harrington et al., 2013)	0.045	1.35	1.35	
429	c1ccncc1CCC(=O)NCc2ccc(cc2)C(=O)Nc3cc(ccc3N)-c4ccccc4 (Harrington et al., 2013)	0.011	1.96	1.49	*
430	c1ccccc1COC(=O)NCc2ccc(cc2)C(=O)Nc3cc(ccc3N)-c4ccccc4 (Harrington et al., 2013)	0.058	1.24	1.51	
431	CC(C)OC(=O)NCc1ccc(cc1)C(=O)Nc2c(N)ccc(c2)-c3cccs3 (Harrington et al., 2013)	0.019	1.72	1.30	*
432	CCCOC(=O)NCc1ccc(cc1)C(=O)Nc2c(N)ccc(c2)-c3cccs3 (Harrington et al., 2013)	0.019	1.72	1.47	*
433	CC(C)COC(=O)NCc1ccc(cc1)C(=O)Nc2c(N)ccc(c2)-c3cccs3 (Harrington et al., 2013)	0.031	1.51	1.23	*
434	c1ccccc1OC(=O)NCc2ccc(cc2)C(=O)Nc3c(N)ccc(c3)-c4cccs4 (Harrington et al., 2013)	0.077	1.11	1.15	
435	c1ccccc1COC(=O)NCc2ccc(cc2)C(=O)Nc3c(N)ccc(c3)-c4cccs4 (Harrington et al., 2013)	0.053	1.27	1.33	
436	CC(=O)NCc1ccc(cc1)C(=O)Nc2c(N)ccc(c2)-c3ccccc3 (Harrington et al., 2013)	0.018	1.74	1.33	*
437	CCC(=O)NCc1ccc(cc1)C(=O)Nc2cc(ccc2N)-c3ccccc3 (Harrington et al., 2013)	0.017	1.77	1.33	*
438	CC(C)(C)C(=O)NCc1ccc(cc1)C(=O)Nc2c(N)ccc(c2)-c3ccccc3 (Harrington et al., 2013)	0.025	1.60	1.11	*
439	C1CCCCC1C(=O)NCc2ccc(cc2)C(=O)Nc3cc(ccc3N)-c4ccccc4 (Harrington et al., 2013)	0.042	1.38	1.24	
440	C1CCCC1C(=O)NCc2ccc(cc2)C(=O)Nc3c(N)ccc(c3)-c4ccccc4 (Harrington et al., 2013)	0.021	1.68	1.27	*
441	c1ccccc1CC(=O)NCc2ccc(cc2)C(=O)Nc3c(N)ccc(c3)-c4ccccc4 (Harrington et al., 2013)	0.072	1.14	1.21	
442	C1CCCCC1C(=O)NCc2ccc(cc2)C(=O)Nc3cc(ccc3N)-c4cccs4 (Harrington et al., 2013)	0.034	1.47	1.12	*
443	C1CCCC1C(=O)NCc2ccc(cc2)C(=O)Nc3c(N)ccc(c3)-c4cccs4 (Harrington et al., 2013)	0.020	1.70	1.23	*
444	c1cccnc1CC(=O)NCc2ccc(cc2)C(=O)Nc3c(N)ccc(c3)-c4ccccc4 (Harrington et al., 2013)	0.019	1.72	1.65	*
445	c1ccncc1CCC(=O)NCc2ccc(cc2)C(=O)Nc3cc(ccc3N)-c4ccccc4 (Harrington et al., 2013)	0.016	1.79	1.50	*
446	c1cnccc1CC(=O)NCc2ccc(cc2)C(=O)Nc3c(N)ccc(c3)-c4cccs4 (Harrington et al., 2013)	0.018	1.74	1.24	*
447	c1ccncc1CCC(=O)NCc2ccc(cc2)C(=O)Nc3c(N)ccc(c3)-c4cccs4 (Harrington et al., 2013)	0.013	1.89	1.51	*
448	C1CCN[C@@H]1C(=O)NCc2ccc(cc2)C(=O)Nc3c(N)ccc(c3)-c4cccs4	0.018	1.74	1.44	*

	(Harrington et al., 2013)				
449	C1CCN[C@@H]1C(=O)NCc2ccc(cc2)C(=O)Nc3c(N)ccc(c3)-c4ccccc4 (Harrington et al., 2013)	0.024	1.62	1.26	*
450	c1cccnc1COC(=O)NCc2ccc(cc2)C(=O)Nc3cc(ccc3N)-c4ccccc4 (Harrington et al., 2013)	0.020	1.70	1.27	*
451	c1cnccc1NCc2ccc(cc2)C(=O)Nc3cc(ccc3N)-c4ccccc4 (Harrington et al., 2013)	0.010	2	1.61	*
452	c1cnccc1N(C)Cc2ccc(cc2)C(=O)Nc3cc(ccc3N)-c4ccccc4 (Harrington et al., 2013)	0.010	2	2.02	*
453	Cc1n(C)ncc1CNCc2ccc(cc2)C(=O)Nc3cc(ccc3N)-c4ccccc4 (Harrington et al., 2013)	0.013	1.89	1.97	*
454	c1ccccc1-c2ccc(N)c(c2)NC(=O)c3ccc(cc3)CN(C)CCCNC (Harrington et al., 2013)	0.018	1.74	1.81	*
455	c1ccccc1-c2ccc(N)c(c2)NC(=O)c3ccc(cc3)CNCC(C)C (Harrington et al., 2013)	0.035	1.45	1.30	*
456	c1ccccc1-c2ccc(N)c(c2)NC(=O)c3ccc(cc3)CNC(C)COC (Harrington et al., 2013)	0.023	1.64	1.40	*
457	c1cnccc1NCc2ccc(cc2)C(=O)Nc3cc(ccc3N)-c4ccccc4F (Harrington et al., 2013)	0.023	1.64	1.63	*
458	c1cnccc1NCc2ccc(cc2)C(=O)Nc3cc(ccc3N)-c4cccc(F)c4 (Harrington et al., 2013)	0.027	1.57	1.67	*
459	c1cnccc1NCc2ccc(cc2)C(=O)Nc3cc(ccc3N)-c4cc(cs4)C (Harrington et al., 2013)	0.015	1.82	1.46	*
460	c1ccccc1-c2ccc(O)c(c2)NC(=O)c3ccc(cc3)CNC4CC4 (Harrington et al., 2013)	0.076	1.12	1.22	
461	c1ccccc1NCc2ccc(cc2)C(=O)Nc3cc(ccc3O)-c4ccccc4 (Harrington et al., 2013)	0.089	1.05	1.2	
462	c1ccccc1-c2ccc(O)c(c2)NC(=O)c3ccc(cc3)CNCC4CC4 (Harrington et al., 2013)	0.072	1.14	1.33	
463	c1ccncc1CNCc2ccc(cc2)C(=O)Nc3cc(ccc3O)-c4ccccc4 (Harrington et al., 2013)	0.032	1.49	1.34	*
464	c1cnccc1NCc2ccc(cc2)C(=O)Nc3cc(ccc3O)-c4ccccc4 (Harrington et al., 2013)	0.0099	2.0	1.53	*
465	c1ccccc1-c2ccc(O)c(c2)NC(=O)c3ccc(cc3)CNCCNC(C)C (Harrington et al., 2013)	0.044	1.36	1.72	
466	c1ccccc1-c(ccc2O)cc2NC(=O)c3ccc(cc3)CNCCC(C)C (Harrington et al., 2013)	0.100	1.00	1.33	
467	c1ccccc1-c2cc(c(O)cc2)NC(=O)c3ccc(cc3)CN(C)CC (Harrington et al., 2013)	0.031	1.51	1.84	*
468	c1ccccc1-c2cc(c(O)cc2)NC(=O)c3ccc(cc3)CN(C)CCCNC (Harrington et al., 2013)	0.018	1.74	1.65	*

469	c1cnccc1N(C)Cc2ccc(cc2)C(=O)Nc3c(O)ccc(c3)-c4ccccc4 (Harrington et al., 2013)	0.013	1.89	2.26	*
470	c1cnccc1CCN(C)Cc2ccc(cc2)C(=O)Nc3c(O)ccc(c3)-c4ccccc4 (Harrington et al., 2013)	0.033	1.48	1.76	*
471	c1ccccc1-c2ccc(O)c(c2)NC(=O)c3ccc(cc3)CNCCN (Harrington et al., 2013)	0.072	1.14	1.43	
472	c1ccccc1-c2ccc(O)c(c2)NC(=O)c3ccc(cc3)CNCCCc4ccncc4 (Harrington et al., 2013)	0.100	1.00	1.40	
473	c1ccccc1-c2ccc(O)c(c2)NC(=O)c3ccc(cc3)CNCC4CCN(C4)C (Harrington et al., 2013)	0.180	0.74	0.73	
474	c1ccccc1-c2ccc(O)c(c2)NC(=O)c3ccc(cc3)CNCCn4nccc4 (Harrington et al., 2013)	0.033	1.48	1.95	*
475	c1ccccc1-c2cc(c(O)cc2)NC(=O)c3ccc(cc3)CN(C)Cc4cn(C)nc4 (Harrington et al., 2013)	0.024	1.62	1.88	*
476	c1ccccc1[C@@H](COC2=O)N2Cc3ccc(cc3)C(=O)Nc4c(N)ccc(c4)-c5ccccc5 (Harrington et al., 2013)	0.064	1.19	1.27	
477	c1ccccc1C[C@H](COC2=O)N2Cc3ccc(cc3)C(=O)Nc4c(N)ccc(c4)-c5ccccc5 (Harrington et al., 2013)	0.089	1.05	1.27	
478	c1ccccc1C[C@@H](COC2=O)N2Cc3ccc(cc3)C(=O)Nc4c(N)ccc(c4)-c5ccccc5 (Harrington et al., 2013)	0.096	1.02	1.31	
479	c1ccccc1[C@H](COC2=O)N2Cc3ccc(cc3)C(=O)Nc4c(N)ccc(c4)-c5ccccc5 (Harrington et al., 2013)	0.058	1.24	1.36	
480	Cn1nnc(c1)CN(C(=O)C)Cc(cc2)ccc2C(=O)Nc3c(N)ccc(c3)-c4sccc4 (Harrington et al., 2013)	0.0095	2.04	1.80	*
481	OC(=O)CNCc1ccc(cc1)C(=O)Nc2c(N)ccc(c2)-c3cccs3 (Harrington et al., 2013)	0.034	1.47	1.46	*
482	OC(=O)CNCc1ccc(cc1)C(=O)Nc2c(N)ccc(c2)-c3ccsc3 (Harrington et al., 2013)	0.042	1.38	1.63	
483	c1ccncc1CN(C(=O)[O-])Cc2ccc(cc2)C(=O)Nc(c3N)cc(cc3)-c4ccccc4 (Harrington et al., 2013)	0.016	1.80	1.51	*

Table S3. Active compounds used for generating a decoys set.

Compound	
1	C1CCN1Cc(cn2)cc(C#N)c2-c3ccc(cc3)C(=O)Nc4c(N)cccc4
2	c1cccc(N)c1NC(=O)c(cc2)ccc2-c3c(C#N)cc(cn3)CN4CCN(CC4)CC
3	c1cccc(N)c1NC(=O)c(cc2)ccc2-c3c(C#N)cc(cn3)CN4CCN(CC4)C(C)C
4	c1ccsc1-c(ccc2N)cc2NC(=O)c3ccc(cc3)NC(=O)C
5	c1cscc1-c(ccc2N)cc2NC(=O)c3ccc(cc3)NC(=O)C
6	c1ccccc1-c(c2)ccc(O)c2NC(=O)c3ccc(cc3)CNc4ccncc4
7	c1ccccc1-c(c2)ccc(N)c2NC(=O)c3ccc(cc3)CNc4ccncc4
8	c1ccccc1-c(c2)ccc(N)c2NC(=O)c3ccc(cc3)CN(C)c4ccncc4
9	c1ccccc1-c(c2)ccc(N)c2NC(=O)c3ccc(cc3)CN(CC4)CCC45NCCC5
10	s1cccc1-c(c2)ccc(N)c2NC(=O)c3ccc(cc3)CN(CC4)CCC45NCCC5
11	c1sccc1-c(c2)ccc(N)c2NC(=O)c3ccc(cc3)CN(CC4)CCC45NCCC5
12	c1ccccc1-c(c2)ccc(N)c2NC(=O)c3ccc(cc3)C(=O)N(CC4)CCC45NCCC5
13	C1CNCC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5
14	C1CNCC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5ccsc5
15	C1CN(C(=O)C)CC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5
16	C1CN(S(=O)(=O)C)CC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5
17	OCCN(CC1)CC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5
18	CC(=O)N(C1)CCC12CCCN(C2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5
19	C1NC(=O)NC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5
20	C1OC(=O)NC12CCN(CC2)c(nc3)ccc3C(=O)Nc4cc(ccc4N)-c5cccs5
24	Nc1ccccc1NC(=O)c2ccc(cc2)C(C(=O)Nc3cccc(c3)C#N)C(=O)Nc4cc(C#N)ccc4
27	Nc1ccccc1NC(=O)c2ccc(cc2)C(C(=O)Nc3cc(OC)ccc3)C(=O)Nc4cc(OC)ccc4
29	Nc1ccccc1NC(=O)c2ccc(cc2)C(C(=O)Nc(cc3)cc(c34)OCCO4)C(=O)Nc(c5)ccc(c56)OCCO6
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90	Nc1ccccc1NC(=O)c2ccc(cc2)-c3ncc(s3)CNCCC
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95	Nc1ccccc1NC(=O)c2ccc(cc2)C3CCN(CC3)Cc4ccc(cc4)C(=O)NC
96	Nc1ccccc1NC(=O)c2ccc(cc2)-c3c(C#N)cc(cn3)N
97	C1CCN1Cc(cn2)cc(C)c2-c3ccc(cc3)C(=O)Nc4c(N)cccc4
98	C1CCN1Cc(cn2)cc(Cl)c2-c3ccc(cc3)C(=O)Nc4c(N)cccc4
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425	NCc1ccc(cc1)C(=O)Nc2c(O)ccc(c2)-c3ccccc3
426	COC(=O)NCc1ccc(cc1)C(=O)Nc2cc(ccc2N)-c3ccccc3
427	CCCOC(=O)NCc1ccc(cc1)C(=O)Nc2c(N)ccc(c2)-c3ccccc3
429	c1ccncc1CCC(=O)NCc2ccc(cc2)C(=O)Nc3cc(ccc3N)-c4ccccc4
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437	CCC(=O)NCc1ccc(cc1)C(=O)Nc2cc(ccc2N)-c3ccccc3
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452	c1cnccc1N(C)Cc2ccc(cc2)C(=O)Nc3cc(ccc3N)-c4ccccc4
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459	c1cnccc1NCc2ccc(cc2)C(=O)Nc3cc(ccc3N)-c4cc(cs4)C
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464	c1cnccc1NCc2ccc(cc2)C(=O)Nc3cc(ccc3O)-c4ccccc4
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468	c1ccccc1-c2cc(c(O)cc2)NC(=O)c3ccc(cc3)CN(C)CCCNC
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480	Cn1nnc(c1)CN(C(=O)C)Cc(cc2)ccc2C(=O)Nc3c(N)ccc(c3)-c4sccc4
481	OC(=O)CNCc1ccc(cc1)C(=O)Nc2c(N)ccc(c2)-c3cccs3
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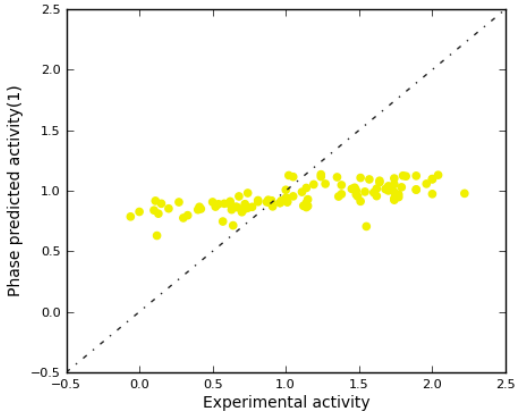

Figure S1. Scatter plot for the predicted (phase predicted activity) and observed (experimental activity) pIC_{50} values (μM) as calculated by the 3D-QSAR model with 1 factor applied to the external test set ($r^2_{ext\_ts}$ = 0.421).

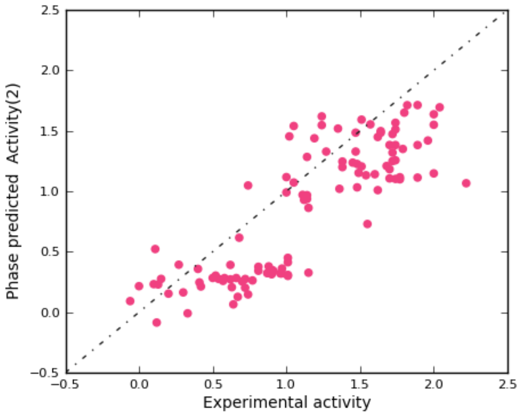

Figure S2. Scatter plot for the predicted (phase predicted activity) and observed (experimental activity) pIC_{50} values (μM) as calculated by the 3D-QSAR model with 2 factors applied to the external test set ($r^2_{ext\_ts}$ = 0.698).

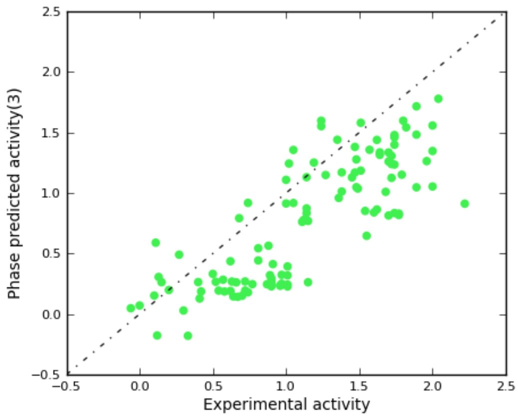

Figure S3. Scatter plot for the predicted (phase predicted activity) and observed (experimental activity) pIC_{50} values (μM) as calculated by the 3D-QSAR model with 3 factors applied to the external test set ($r^2_{ext\_ts}$ = 0.657).

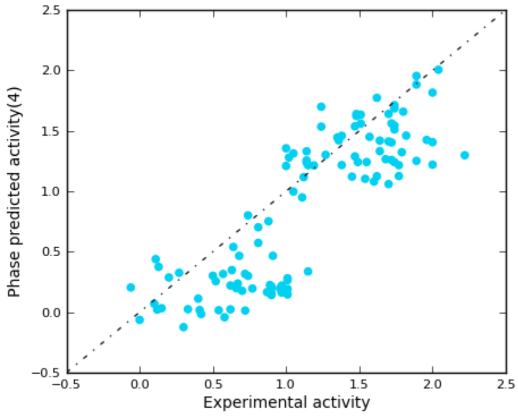

Figure S4. Scatter plot for the predicted (phase predicted activity) and observed (experimental activity) pIC_{50} values (μM) as calculated by the 3D-QSAR model with 4 factors applied to the external test set ($r^2_{ext\_ts}$ = 0.712).

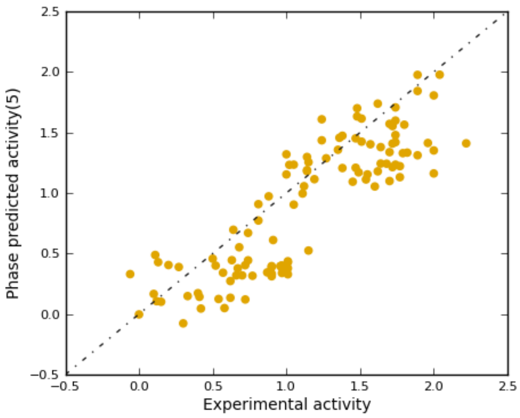

Figure S5. Scatter plot for the predicted (phase predicted activity) and observed (experimental activity) pIC_{50} values (μM) as calculated by the 3D-QSAR model with 5 factors applied to the external test set ($r^2_{ext\_ts}$ = 0.735).

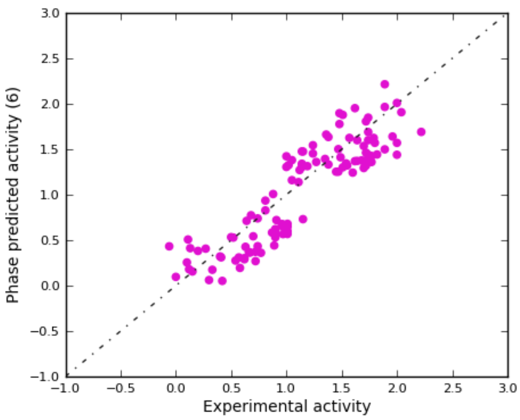

Figure S6. Scatter plot for the predicted (phase predicted activity) and observed (experimental activity) pIC_{50} values (μM) as calculated by the 3D-QSAR model with 6 factors applied to the external test set ($r^2_{ext\_ts}$ = 0.787).

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