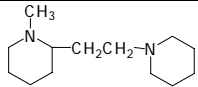
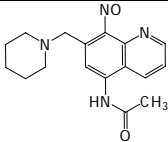
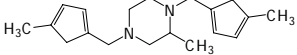
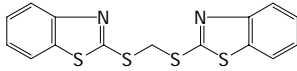
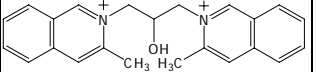
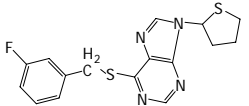
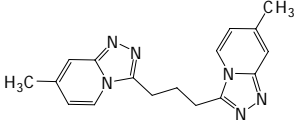
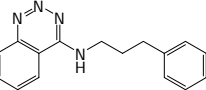
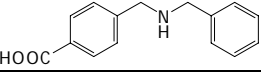
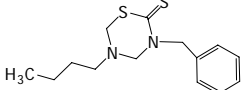
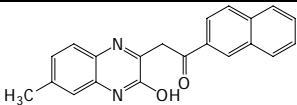
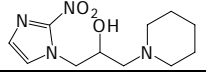
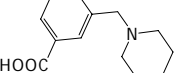


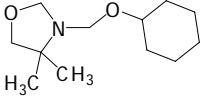
Table S1 Selected hit compounds

	Diversity/ NSC no.	Structure	Pharmacokinetic properties				Pharmacodynamic properties								
			MW	Log P (XLOGP)	HBD <5	HBA <10	RB	Ls- AChBP		Ac- AChBP		Bt- AChBP		Ligand Efficiency	
								Cluster# (%member)	Docking ΔG	Cluster# (%member)	Docking ΔG	Cluster# (%member)	Docking ΔG	Binding/ non H	Docking/ non H
1	1917 NSC 600067		324	1.16	0	2	5	1 (91)	-13.84	1 (27) 2 (70)	-14.47 -13.0	1 (93)	-13.03	-0.51 -0.47 -0.47	-0.58 -0.54 -0.54
2	0713 NSC 5 9486		326	2.34	1	1	5	1 (92)	-13.05	1 (73)	-12.75	1 (20) 2(33)	-10.78 -10.6	-0.53 -0.51 -0.42	-0.57 -0.55 -0.46
3	1002 NSC 95926		447	1.5	2	2	5	1 (75)	-12.81	1 (80)	-11.72	1 (56)	-10.83	-0.40 -0.34 -0.31	-0.43 -0.39 -0.36
4	1759 NSC326381		311	3.04	2	4	5	1 (100)	-12.81	1 (38)	-11.66	1 (23) 5 (56)	-10.97 -9.05	-0.51 -0.49 -0.35	-0.58 -0.53 -0.41
5	1066 NSC102852		240	0.55	0	4	4	1 (100)	-12.53	1 (100)	-12.63	1 (98)	-11.51	-0.65 -0.65 -0.59	-0.74 -0.74 -0.68
6	1922 NSC606535		314	-0.92	2	8	5	1 (99)	-12.47	1 (35) 2 (63)	-11.63 -11.1	1 (84)	-11.21	-0.52 -0.45 -0.44	-0.57 -0.51 -0.51
7	0763 NSC66183		220	-0.15	2	4	5	1 (98)	-12.31	1 (94)	-12.55	1 (74)	-10.73	-0.65 -0.68 -0.56	-0.77 -0.78 -0.67
8	1080 NSC105900		284	3.34	1	3	5	1 (77)	-12.27	1 (60)	-11.42	1 (71)	-11.14	-0.54 -0.51 -0.48	-0.61 -0.57 -0.56
9	0498 NSC42258		417	4.15	2	3	4	1 (68)	-12.12	1 (86)	-11.46	1 (94)	-11.82	-0.43 -0.42 -0.39	-0.47 -0.44 -0.45
10	0726 NSC61810		384	0.56	1	4	5	1 (84)	-11.80	1 (52)	-10.62	1 (57)	-10.70	-0.52 -0.50 -0.46	-0.54 -0.48 -0.49
11	0797 NSC72861*		305	1.50	1	4	5	1 (78)	-11.80	1 (55)	-10.38	1 (52)	-10.50	-0.51 -0.49 -0.44	-0.54 -0.47 -0.48

12	0872 NSC83391		310	1.91	0	5	5	1 (95)	-11.80	1 (91)	-10.88	1 (97)	-11.30	-0.50 -0.47 -0.47	-0.59 -0.54 -0.56
13	0155 NSC13378		358	3.0	2	4	4	1 (53)	-11.74	1 (76)	-12.13	1 (35)	-10.78	-0.50 -0.52 -0.45	-0.56 -0.58 -0.51
14	0490 NSC41805		300	1.55	2	5	4	1 (85)	-11.68	1 (20) 2 (36)	-10.42 -10.2	1 (91)	-10.66	-0.50 -0.43 -0.44	-0.56 -0.49 -0.51
15	0584 NSC47938		345	4.83	0	4	5	1 (43)	-11.68	1 (53)	-10.47	1 (82)	-10.68	-0.42 -0.37 -0.39	-0.45 -0.40 -0.41
16	1539 NSC190382		361	4.27	0	2	5	1 (82)	-11.68	1 (52)	-12.81	1 (69)	-11.64	-0.45 -0.48 -0.44	-0.53 -0.58 -0.53
17	1040 NSC99676		346	2.36	1	1	5	1 (65)	-11.66	1 (32) 2 (41)	-12.02 -10.5	1 (19) 2 (64)	-10.59 -9.8	-0.43 -0.39 -0.35	-0.51 -0.46 -0.43
18	0307 NSC24048		442	4.7	1	3	4	1 (80)	-11.65	1 (30) 2 (67)	-11.56 -10.4	1 (53)	-10.12	-0.47 -0.39 -0.38	-0.48 -0.44 -0.42
19	1131 NSC112796		268	3.01	1	3	5	1 (85)	-11.58	1 (71)	-11.78	1 (99)	-10.68	-0.48 -0.53 -0.45	-0.58 -0.59 -0.53
20	0250 NSC18877		406	4.86	0	5	4	1 (99)	-11.56	1 (68)	-10.64	1 (71)	-11.86	-0.37 -0.37 -0.38	-0.41 -0.38 -0.42
21	0384 NSC33052*		314	6.4	0	0	4	1 (100)	-11.51	1 (100)	-11.21	1 (79)	-10.51	-0.44 -0.42 -0.42	-0.50 -0.49 -0.46
22	0038 NSC3535		253	2.82	0	3	5	1 (94)	-11.47	1 (99)	-11.03	1 (89)	-10.59	-0.56 -0.54 -0.52	-0.67 -0.65 -0.62
23	0863 NSC81747		279	4.89	1	1	5	1 (100)	-11.45	1 (76)	-11.36	1 (100)	-11.30	-0.50 -0.49 -0.49	-0.57 -0.57 -0.56
24	1975 NSC668394		452	3.74	2	5	5	1 (75)	-11.42	1 (55)	-10.64	1 (36)	-10.43	-0.42 -0.40 -0.37	-0.48 -0.44 -0.43

25	0342 NSC27476		283	2.04	0	3	3	1 (100)	-11.39	1 (100)	-11.45	1 (100)	-10.65	-0.68 -0.69 -0.63	-0.76 -0.76 -0.71
26	1304 NSC130876		299	1.17	2	4	4	1 (89)	-11.27	1 (47)	-11.09	1 (63)	-11.59	-0.43 -0.42 -0.44	-0.49 -0.48 -0.50
27	1823 NSC360218		361	1.45	1	4	4	1 (40) 2 (60)	-11.25 -10.4	1 (1) 2 (78)	-11.36 -9.53	1 (98)	-10.77	-0.46 -0.48 -0.44	-0.50 -0.51 -0.51
28	0410 NSC35582		347	3.91	0	2	4	1 (99)	-11.20	1 (80)	-11.98	1 (67)	-10.58	-0.47 -0.51 -0.43	-0.53 -0.57 -0.50
29	0395 NSC34352		504	4.3	1	2	5	1 (100)	-11.19	1 (38)	-11.12	1 (40) 2 (50)	-11.03 -10.2	-0.41 -0.39 -0.35	-0.43 -0.43 -0.39
30	0689 NSC56939		346	3.65	0	1	4	1 (98)	-11.15	1 (62)	-11.42	1 (76)	-10.93	-0.45 -0.44 -0.45	-0.48 -0.50 -0.48
31	1678 NSC303530		292	4.28	0	4	3	1 (96)	-11.14	1 (51)	-10.39	1 (71)	-11.07	-0.45 -0.41 -0.43	-0.48 -0.45 -0.48
32	1507 NSC174201		364	3.06	1	3	4	1 (22) 3 (63)	-11.05 -10.7	1 (9) 2 (79)	-10.98 -10.3	1 (99)	-10.77	-0.47 -0.45 -0.48	-0.54 -0.52 -0.54
33	1255 NSC122451		241	2.86	2	3	5	1 (38) 4 (50)	-11.04 -9.64	1 (23) 2 (54)	-10.66 -9.38	1 (71)	-10.23	-0.45 -0.48 -0.48	-0.54 -0.57 -0.57
34	1607 NSC246981		280	2.99	0	1	5	1 (13) 2 (34)	-11.02 -10.6	1 (100)	-10.48	1 (81)	-10.48	-0.52 -0.50 -0.50	-0.59 -0.58 -0.58
35	1871 NSC373058		328	4.93	1	3	4	1 (92)	-11.01	1 (20) 2 (41)	-10.71 -10.5	1 (37)	-10.86	-0.42 -0.41 -0.40	-0.44 -0.42 -0.43
36	1887 NSC380540		254	1.00	1	4	4	1 (48)	-11.01	1 (79)	-11.14	1 (50)	-10.68	-0.51 -0.55 -0.47	-0.61 -0.62 -0.59
37	0260 NSC19496		256	0.64	1	4	3	1 (65)	-11.00	1 (67)	-10.54	1 (92)	-10.31	-0.61 -0.59 -0.57	-0.69 -0.66 -0.64

38	0679 NSC55462		286	1.62	1	1	5	1 (4) 4 (79)	-11.00 -10.1	1 (34)	-10.97	1 (20) 2 (77)	-10.48 -10.3	-0.44 -0.46 -0.44	-0.51 -0.55 -0.52
39	1281 NSC126347		328	2.26	0	3	3	1 (51)	-10.99	1 (32) 2 (42)	-10.34 -10.0	1 (86)	-10.30	-0.50 -0.45 -0.47	-0.55 -0.50 -0.51
40	1468 NSC166302		196	1.80	1	2	3	1 (100)	-10.98	1 (100)	-11.06	1 (100)	-10.18	-0.70 -0.71 -0.64	-0.78 -0.79 -0.73
41	0581 NSC47924		279	4.15	2	3	4	1 (85)	-10.97	1 (100)	-10.43	1 (63)	-10.36	-0.47 -0.39 -0.45	-0.52 -0.45 -0.49
42	0817 NSC74429		308	2.99	4	2	4	1 (6) 2 (73)	-10.97 -10.3	1 (21) 2 (79)	-11.58 -9.76	1 (72)	-10.61	-0.45 -0.41 -0.43	-0.47 -0.44 -0.48
43	0421 NSC36369		474	4.8	0	1	5	1 (91)	-10.96	1 (31) 2 (69)	-11.81 -11.5	1 (79)	-11.33	-0.41 -0.42 -0.42	-0.46 -0.48 -0.47
44	0291 NSC23082		270	2.46	1	1	4	1 (6) 3 (80)	-10.91 -10.5	1 (17) 2 (71)	-10.57 -10.2	1 (87)	-10.18	-0.47 -0.47 -0.47	-0.55 -0.54 -0.54
45	1434 NSC158011		309	4.75	1	0	5	1 (87)	-10.84	1 (25) 2 (66)	-10.77 -10.1	1 (84)	-10.30	-0.44 -0.41 -0.41	-0.52 -0.48 -0.49
46	1303 NSC130843		317	-0.1	2	3	4	1 (35)	-10.82	1 (38) 2 (40)	-11.29 -10.7	1 (82)	-10.12	-0.48 -0.47 -0.44	-0.54 -0.54 -0.51
47	1041 NSC99785		244	1.84	2	3	4	1 (46)	-10.81	1 (60)	-10.81	1 (66)	-10.55	-0.56 -0.55 -0.53	-0.60 -0.60 -0.59
48	0007 NSC1199		225	3.35	1	2	4	1 (99)	-10.79	1 (98)	-10.34	1 (100)	-10.31	-0.63 -0.60 -0.59	-0.67 -0.65 -0.64
49	0437 NSC37372		294	2.6	0	2	3	1 (21) 2 (60)	-10.76 -10.4	1 (10) 3 (76)	-10.97 -10.1	1 (88)	-10.89	-0.51 -0.48 -0.52	-0.55 -0.54 -0.57
50	0617 NSC49455		301	3	0	1	5	1 (87)	-10.70	1 (62)	-10.75	1 (97)	-10.89	-0.46 -0.46 -0.47	-0.53 -0.54 -0.54

51	1679 NSC303534		213	2.45	0	3	3	1 (100)	-10.49	1 (100)	-10.78	1 (100)	-10.00	-0.62 -0.65 -0.60	-0.70 -0.72 -0.67
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