

Supplementary

Ligand-Based and Structured-Based in Silico Repurposing Approaches to Predict Inhibitors of SARS-CoV-2 Mpro Protein

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Table S1. Results from molecular docking of known CoV inhibitors on SARS-CoV-2 Mpro.

ID	Vina score	Cluster #
CHEMBL63354	-10.2	C-3
CHEMBL378188	-10	C-3
CHEMBL3808795	-9.7	C-5
BDBM50176856	-9.5	C-5
BDBM50176862	-9.4	C-5
BDBM50176806	-9.4	C-5
BDBM50176807	-9.4	C-5
BDBM50176814	-9.4	C-5
BDBM50176811	-9.4	C-5
BDBM50176812	-9.3	C-5
CHEMBL377324	-9.3	C-3
CHEMBL3099535	-9.3	C-6
BDBM50297257	-9.2	C-3
BDBM50176801	-9.2	C-5
CHEMBL510508	-9.2	C-3
BDBM50176859	-9.1	C-5
BDBM50007792	-9	C-6
BDBM50297254	-9	C-3
BDBM50176809	-9	C-5
BDBM50176863	-9	C-5
BDBM50176802	-9	C-5
BDBM50176813	-9	C-5
CHEMBL1277228	-9	C-5
BDBM50176857	-8.9	C-2
BDBM50176858	-8.9	C-2
BDBM50176810	-8.8	C-5

BDBM50297255	-8.8	C-5
CHEMBL3099546	-8.8	C-6
CHEMBL1277046	-8.8	C-5
BDBM11241	-8.7	C-3
BDBM50176860	-8.7	C-5
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CHEMBL208908	-8.7	C-3
CHEMBL1276871	-8.7	C-5
CHEMBL3099525	-8.7	C-6
BDBM50297252	-8.6	C-3
BDBM23308	-8.6	C-6
CHEMBL1277227	-8.6	C-5
CHEMBL1277047	-8.6	C-5
CHEMBL3099536	-8.6	C-6
BDBM50007789	-8.5	C-6
BDBM11237	-8.5	C-3
BDBM50176803	-8.5	C-5
BDBM50176805	-8.5	C-5
BDBM50343551	-8.5	C-2
CHEMBL2441745	-8.5	C-6
CHEMBL210497	-8.5	C-2
CHEMBL3099539	-8.5	C-6
CHEMBL459393	-8.5	C-3
BDBM11264	-8.4	C-6
BDBM11270	-8.4	C-6
CHEMBL210972	-8.4	C-2
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CHEMBL559870	-8.4	C-3
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CHEMBL3099538	-8.3	C-6
CHEMBL3099534	-8.3	C-6
CHEMBL471187	-8.3	C-3
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BDBM11256	-8.2	C-6
BDBM50343553	-8.2	C-1
50441633	-8.2	C-3
BDBM11259	-8.1	C-6
BDBM50297251	-8.1	C-3
BDBM11283	-8.1	C-2
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CHEMBL210632	-8.1	C-2
CHEMBL210146	-8.1	C-2
CHEMBL1278125	-8.1	C-5
CHEMBL3099540	-8.1	C-6
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BDBM59244	-8	C-2
BDBM11240	-8	C-3

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BDBM78957	-8	C-4
BDBM53105	-8	C-3
BDBM11269	-8	C-6
BDBM50343555	-8	C-1
BDBM11245	-8	C-4
BDBM11243	-8	C-4
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BDBM50167315	-8	C-1
CHEMBL3105075	-8	C-2
CHEMBL187460	-8	C-3
CHEMBL1774324	-8	C-1
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BDBM11235	-7.9	C-3
BDBM11255	-7.9	C-4
BDBM11248	-7.9	C-4
BDBM50423877	-7.9	C-3
BDBM246525	-7.9	C-3
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CHEMBL3099522	-7.9	C-6
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BDBM11257	-7.8	C-4
BDBM50343554	-7.8	C-2
BDBM11284	-7.8	C-2
BDBM11287	-7.8	C-2
BDBM11289	-7.8	C-2
BDBM50188381	-7.8	C-1
BDBM50167309	-7.8	C-1
BDBM50167314	-7.8	C-1
BDBM50167316	-7.8	C-1
CHEMBL4214471	-7.8	C-6
CHEMBL3099547	-7.8	C-6
CHEMBL3099537	-7.8	C-6
CHEMBL207207	-7.8	C-6
BDBM154575	-7.7	C-2
BDBM11234	-7.7	C-3
BDBM11304	-7.7	C-2
BDBM11265	-7.7	C-6
BDBM11271	-7.7	C-6
BDBM11252	-7.7	C-6
BDBM11242	-7.7	C-3
BDBM11249	-7.7	C-4
BDBM11280	-7.7	C-6
BDBM50167306	-7.7	C-1
BDBM50176014	-7.7	C-4

CHEMBL378677	-7.7	C-2
CHEMBL210487	-7.7	C-2
CHEMBL1774323	-7.7	C-6
CHEMBL380470	-7.7	C-2
CHEMBL28	-7.7	C-3
CHEMBL549646	-7.7	C-3
BDBM50007794	-7.6	C-6
BDBM7460	-7.6	C-3
BDBM11251	-7.6	C-4
BDBM11273	-7.6	C-2
BDBM11277	-7.6	C-2
BDBM11278	-7.6	C-6
BDBM51317	-7.6	C-3
BDBM246521	-7.6	C-3
CHEMBL4214066	-7.6	C-6
CHEMBL2316337	-7.6	C-6
CHEMBL3099529	-7.6	C-6
CHEMBL1392147	-7.6	C-2
CHEMBL492772	-7.6	C-3
CHEMBL2391422	-7.6	C-3

Table S2. Compounds obtained from screening the ChEMBL database.

ID	Mol Weight	H acceptor	H donors	Log P	Vina score	Cluster #
CHEMBL2047043	479.28	5	4	3.074	-9.6	C-9
CHEMBL1940937	458.22	7	5	2.856	-9.1	C-35
CHEMBL2042023	447.22	4	3	2.926	-8.9	C-9
CHEMBL3666013	436.19	7	4	2.496	-8.8	C-43
CHEMBL1940941	459.20	8	4	3.154	-8.7	C-35
CHEMBL1963108	444.24	7	5	3.330	-8.7	C-35
CHEMBL1940947	445.22	7	5	3.363	-8.5	C-35
CHEMBL562054	482.25	6	4	1.529	-8.4	C-23
CHEMBL1905705	463.21	6	1	3.950	-8.4	C-35
CHEMBL3742399	471.19	7	4	0.749	-8.4	C-35
CHEMBL4300783	481.24	6	4	4.113	-8.3	C-41
CHEMBL469898	468.24	5	4	1.880	-8.3	C-20
CHEMBL30782	484.30	5	4	3.226	-8.3	C-23
CHEMBL64623	479.28	5	2	4.502	-8.3	C-15
CHEMBL1940942	445.18	7	5	3.065	-8.3	C-35
CHEMBL3233752	458.22	8	3	1.470	-8.3	C-37
CHEMBL3600387	467.24	6	4	4.062	-8.3	C-35
CHEMBL3676493	450.19	7	2	2.903	-8.3	C-43
CHEMBL3900791	465.23	7	3	2.762	-8.3	C-33
CHEMBL318016	447.20	7	3	0.679	-8.2	C-22
CHEMBL549890	499.28	7	4	1.221	-8.2	C-23
CHEMBL1437444	404.17	4	2	3.937	-8.2	C-21
CHEMBL1761701	469.22	6	4	3.500	-8.2	C-43
CHEMBL1941057	493.23	8	5	3.288	-8.2	C-40

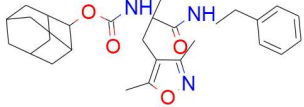
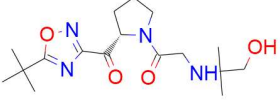
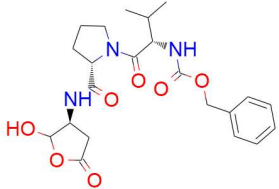
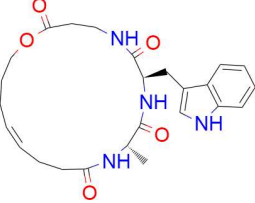
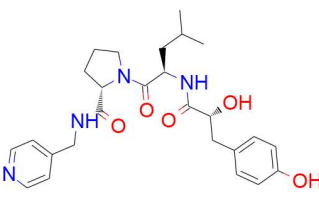
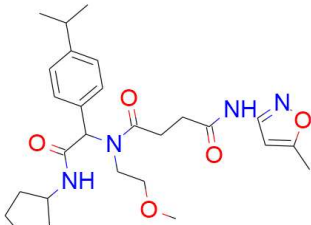
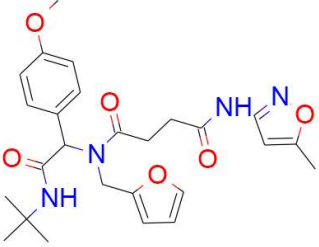
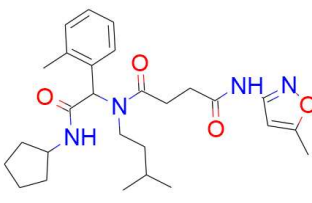
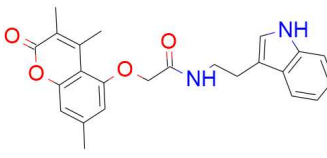
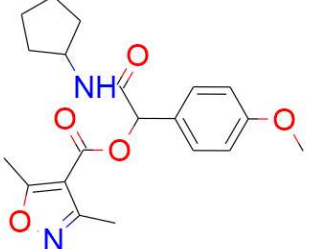
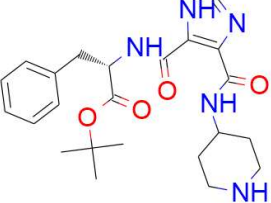
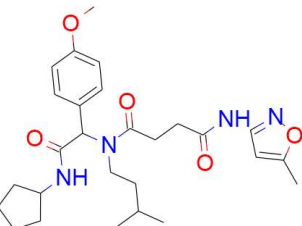
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CHEMBL3233751	457.18	8	1	2.597	-8.2	C-41
CHEMBL3304288	373.20	6	2	2.867	-8.2	C-43
CHEMBL3600789	481.26	6	4	4.453	-8.2	C-35
CHEMBL3752867	498.28	6	3	3.599	-8.2	C-35
CHEMBL3741435	471.19	7	4	0.749	-8.2	C-35
CHEMBL3742031	471.19	7	4	0.749	-8.2	C-35
CHEMBL4088502	369.17	5	2	1.821	-8.2	C-35
CHEMBL231697	352.21	7	2	0.901	-8.1	C-29
CHEMBL237917	475.25	10	3	0.690	-8.1	C-33
CHEMBL294332	410.18	5	2	2.999	-8.1	C-20
CHEMBL31850	454.25	5	2	4.362	-8.1	C-23
CHEMBL1302235	422.20	6	2	2.661	-8.1	C-41
CHEMBL1383217	498.28	6	2	4.100	-8.1	C-26
CHEMBL1504950	410.16	7	1	1.703	-8.1	C-35
CHEMBL1765329	465.16	10	3	2.050	-8.1	C-43
CHEMBL1940938	458.22	7	5	2.856	-8.1	C-35
CHEMBL1941051	459.25	8	4	2.202	-8.1	C-38
CHEMBL1940946	431.21	7	5	3.116	-8.1	C-35
CHEMBL1963050	488.23	9	5	2.625	-8.1	C-35
CHEMBL1940945	431.21	7	5	3.116	-8.1	C-35
CHEMBL2047011	472.23	7	4	2.060	-8.1	C-10
CHEMBL3260634	431.24	5	1	3.079	-8.1	C-22
CHEMBL3676445	400.21	7	2	2.021	-8.1	C-42
CHEMBL3741228	444.18	6	3	1.063	-8.1	C-35
CHEMBL3932144	472.30	5	4	2.066	-8.1	C-13
CHEMBL107883	482.29	4	3	4.202	-8	C-23
CHEMBL461207	461.23	4	2	3.581	-8	C-9
CHEMBL1821856	488.26	6	4	1.432	-8	C-11
CHEMBL1866805	498.28	6	2	4.385	-8	C-27
CHEMBL1209461	370.20	6	3	2.123	-8	C-35
CHEMBL1360513	424.17	7	1	2.093	-8	C-35
CHEMBL1533892	372.17	6	1	3.257	-8	C-17
CHEMBL1761702	469.22	6	4	3.502	-8	C-43
CHEMBL1733669	387.22	6	1	2.711	-8	C-41
CHEMBL3353888	411.14	5	2	3.097	-8	C-14
CHEMBL1941059	478.22	7	4	4.478	-8	C-38
CHEMBL1940927	415.21	6	4	4.145	-8	C-35
CHEMBL1963051	430.22	7	4	2.906	-8	C-39
CHEMBL2047012	470.22	7	3	2.209	-8	C-11
CHEMBL3120427	413.21	4	1	4.026	-8	C-34
CHEMBL3600498	382.19	5	3	4.168	-8	C-35
CHEMBL3799400	407.18	5	2	3.510	-8	C-19
CHEMBL3905703	418.16	7	2	3.724	-8	C-43
CHEMBL3955497	432.18	8	2	3.406	-8	C-43
CHEMBL88718	458.25	6	4	1.761	-7.9	C-29
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CHEMBL399583	479.24	7	3	4.299	-7.9	C-37

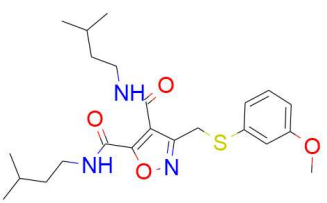
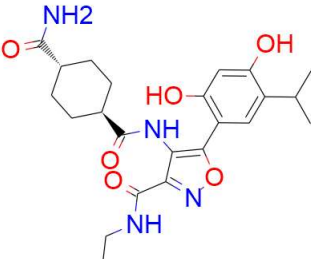
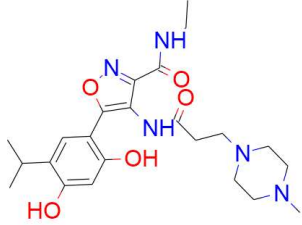
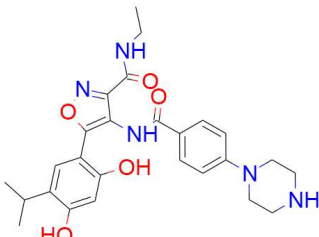
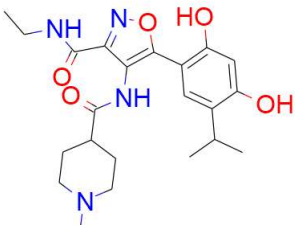
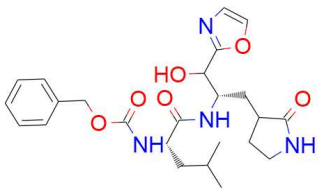
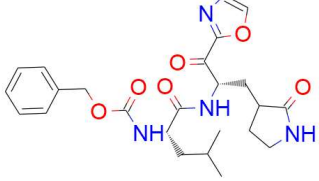

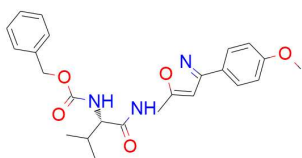
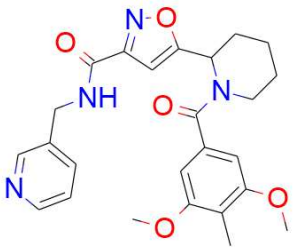
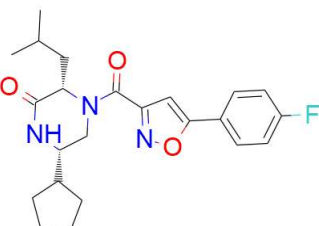
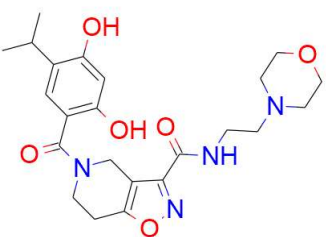
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CHEMBL1761700	469.22	6	4	3.500	-7.9	C-43
CHEMBL1940932	466.20	7	5	3.504	-7.9	C-35
CHEMBL1907379	375.19	8	5	0.167	-7.9	C-20
CHEMBL1963138	458.25	7	5	3.590	-7.9	C-35
CHEMBL2362507	388.21	7	1	2.110	-7.9	C-41
CHEMBL3233753	413.20	6	3	3.080	-7.9	C-37
CHEMBL3427167	486.25	6	4	1.186	-7.9	C-12
CHEMBL3600791	484.23	7	4	2.798	-7.9	C-37
CHEMBL3676490	492.24	7	1	4.753	-7.9	C-43
CHEMBL3676432	388.21	7	3	2.272	-7.9	C-43
CHEMBL3901201	466.12	6	2	3.793	-7.9	C-35
CHEMBL3979436	498.32	5	4	2.783	-7.9	C-13
CHEMBL4227921	438.19	8	1	2.643	-7.9	C-33
CHEMBL252164	465.23	7	3	4.125	-7.8	C-38
CHEMBL254458	479.24	7	3	4.200	-7.8	C-38
CHEMBL1869666	472.23	7	2	1.556	-7.8	C-29
CHEMBL1089046	498.25	7	2	3.257	-7.8	C-35
CHEMBL1303362	404.14	6	2	3.697	-7.8	C-17
CHEMBL1415079	419.18	5	1	3.054	-7.8	C-37
CHEMBL1618953	403.22	8	4	0.770	-7.8	C-35
CHEMBL1940944	431.21	7	5	2.973	-7.8	C-35
CHEMBL1962919	416.21	7	5	2.564	-7.8	C-35
CHEMBL3120428	427.23	4	1	4.416	-7.8	C-35
CHEMBL3120433	429.21	5	1	3.263	-7.8	C-33
CHEMBL3618397	394.16	6	3	2.691	-7.8	C-35
CHEMBL3600514	439.21	6	4	3.282	-7.8	C-35
CHEMBL3593409	490.17	8	3	2.282	-7.8	C-8
CHEMBL3681517	452.21	7	2	3.879	-7.8	C-17
CHEMBL3676430	330.17	6	2	2.131	-7.8	C-43
CHEMBL3753300	435.23	7	1	3.975	-7.8	C-43
CHEMBL3753609	422.21	8	2	3.288	-7.8	C-43
CHEMBL3751894	482.29	5	2	3.933	-7.8	C-13
CHEMBL3885455	426.19	6	3	0.924	-7.8	C-35
CHEMBL214555	444.27	5	5	1.395	-7.7	C-12
CHEMBL1821850	403.21	5	3	1.537	-7.7	C-11
CHEMBL1209617	398.23	6	3	2.759	-7.7	C-35
CHEMBL1209464	384.22	6	3	2.513	-7.7	C-35
CHEMBL1875450	472.20	8	2	1.817	-7.7	C-26
CHEMBL1357672	404.18	7	3	1.779	-7.7	C-35
CHEMBL1331715	486.25	8	2	1.343	-7.7	C-23
CHEMBL1321923	458.22	7	2	2.034	-7.7	C-26
CHEMBL1341095	421.16	6	1	2.446	-7.7	C-37
CHEMBL1392860	496.23	7	2	3.988	-7.7	C-28
CHEMBL1416150	472.20	8	2	1.817	-7.7	C-26
CHEMBL1500139	481.23	8	2	2.298	-7.7	C-23
CHEMBL1581453	442.22	6	2	2.647	-7.7	C-25
CHEMBL1596487	365.12	5	2	1.930	-7.7	C-35

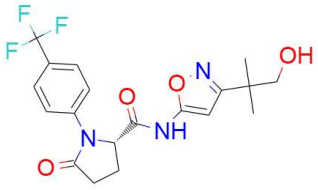
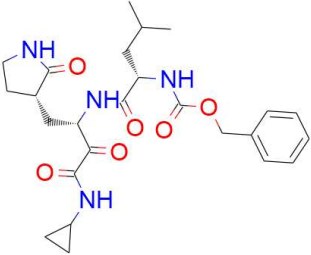
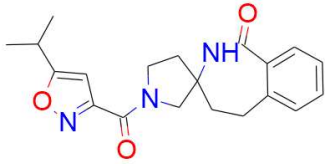
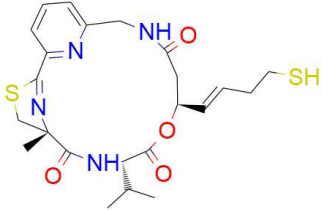
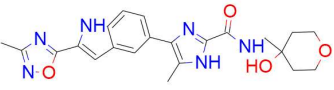
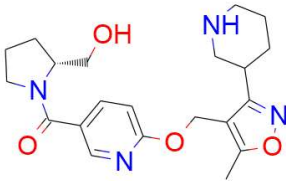
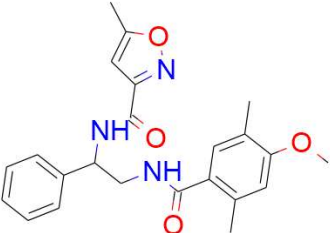
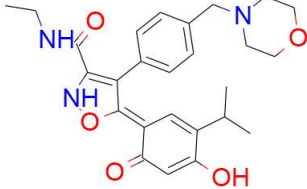
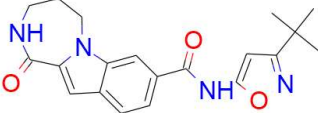
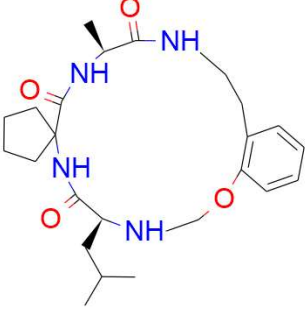
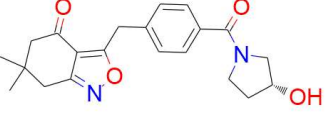
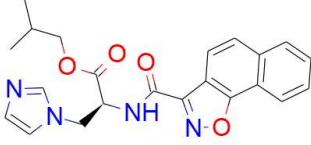
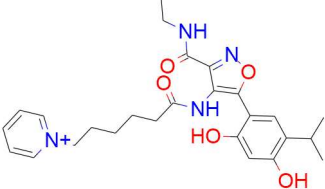
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CHEMBL1733581	357.17	5	1	2.221	-7.7	C-37
CHEMBL1736030	456.24	6	2	3.381	-7.7	C-29
CHEMBL1740647	441.24	6	4	1.574	-7.7	C-24
CHEMBL2047013	488.21	7	4	2.529	-7.7	C-11
CHEMBL2356571	464.21	7	1	3.693	-7.7	C-36
CHEMBL3108881	410.16	7	2	1.459	-7.7	C-35
CHEMBL3126614	494.25	8	3	3.484	-7.7	C-43
CHEMBL3233488	373.16	6	3	2.157	-7.7	C-37
CHEMBL3600497	396.20	5	3	4.558	-7.7	C-35
CHEMBL3676497	493.23	8	3	1.927	-7.7	C-43
CHEMBL3676438	406.20	7	3	2.220	-7.7	C-43
CHEMBL3752799	498.28	6	3	3.599	-7.7	C-35
CHEMBL3967098	461.21	8	3	2.748	-7.7	C-43
CHEMBL4092885	457.26	5	3	2.669	-7.7	C-11
CHEMBL4207348	368.17	5	1	2.627	-7.7	C-32
CHEMBL469274	446.22	7	4	3.874	-7.6	C-9
CHEMBL477398	473.25	6	3	2.253	-7.6	C-11
CHEMBL1807681	414.23	4	5	1.563	-7.6	C-9
CHEMBL1209463	356.18	6	3	1.733	-7.6	C-35
CHEMBL1209686	426.26	6	3	3.540	-7.6	C-35
CHEMBL1209685	412.25	6	3	3.150	-7.6	C-35
CHEMBL1870133	486.21	8	2	2.207	-7.6	C-26
CHEMBL1221416	455.24	6	2	2.740	-7.6	C-20
CHEMBL1377499	492.24	6	2	2.825	-7.6	C-29
CHEMBL1471649	419.18	5	2	4.333	-7.6	C-19
CHEMBL1436544	399.22	5	1	2.904	-7.6	C-41
CHEMBL1483149	476.24	6	2	2.796	-7.6	C-23
CHEMBL1525744	460.23	7	3	2.187	-7.6	C-26
CHEMBL1619336	441.24	6	4	1.779	-7.6	C-23
CHEMBL1899611	447.22	6	2	4.527	-7.6	C-18
CHEMBL1735999	477.12	10	1	1.847	-7.6	C-33
CHEMBL1730265	401.21	7	1	1.126	-7.6	C-41
CHEMBL1941050	446.22	8	4	2.287	-7.6	C-41
CHEMBL1935666	396.20	4	2	3.460	-7.6	C-10
CHEMBL1940948	445.22	7	5	3.363	-7.6	C-35
CHEMBL1894431	426.24	7	3	0.847	-7.6	C-11
CHEMBL2172593	437.20	6	2	3.917	-7.6	C-16
CHEMBL2315031	417.23	5	3	1.580	-7.6	C-11
CHEMBL3126619	494.25	8	3	3.484	-7.6	C-43
CHEMBL3126613	494.25	8	3	3.484	-7.6	C-43
CHEMBL3126433	480.24	8	3	3.175	-7.6	C-43
CHEMBL3121964	499.21	8	3	3.753	-7.6	C-43
CHEMBL3447382	353.17	4	1	2.759	-7.6	C-31
CHEMBL3618393	395.15	6	4	2.693	-7.6	C-35
CHEMBL3754533	482.29	5	3	3.899	-7.6	C-35
CHEMBL3912437	366.17	5	2	3.313	-7.6	C-30
CHEMBL3910409	383.22	5	3	3.657	-7.6	C-33
CHEMBL3901559	488.24	6	2	4.753	-7.6	C-43

CHEMBL3933573	498.32	5	4	2.927	-7.6	C-13
CHEMBL4227331	406.16	7	1	3.175	-7.6	C-7
CHEMBL4217568	468.26	7	3	0.958	-7.6	C-22

Table S3. Leaders from ChEMBL clusters.

		
CHEMBL64623 -8.3 kcal/mol	CHEMBL231697 -8.1 kcal/mol	CHEMBL318016 -8.2 kcal/mol
		
CHEMBL469898 -8.3 kcal/mol	CHEMBL562054 -8.4 kcal/mol	CHEMBL1383217 -8.1 kcal/mol
		
CHEMBL1392860 -7.7 kcal/mol	CHEMBL1431465 -7.9 kcal/mol	CHEMBL1437444 -8.2 kcal/mol
		
CHEMBL1533892	CHEMBL1740647	CHEMBL1866805

-8.0 kcal/mol	-7.7 kcal/mol	-8.0 kcal/mol
		
CHEMBL1899611 -7.6 kcal/mol	CHEMBL1940937 -9.1 kcal/mol	CHEMBL1941051 -8.1 kcal/mol
		
CHEMBL1941057 -8.2 kcal/mol	CHEMBL1963051 -8.0 kcal/mol	CHEMBL2047011 -8.1 kcal/mol
		
CHEMBL2047012 -8.0 kcal/mol	CHEMBL2047043 -9.6 kcal/mol	CHEMBL2172593 -7.6 kcal/mol
		
CHEMBL2356571 -7.7 kcal/mol	CHEMBL3120427 -8.0 kcal/mol	CHEMBL3233752 -8.3 kcal/mol

		
CHEMBL3353888 -8.0 kcal/mol	CHEMBL3427167 -7.9 kcal/mol	CHEMBL3447382 -7.6 kcal/mol
		
CHEMBL3593409 -7.8 kcal/mol	CHEMBL3666013 -8.8 kcal/mol	CHEMBL3676445 -8.1 kcal/mol
		
CHEMBL3799400 -8.0 kcal/mol	CHEMBL3900791 -8.3 kcal/mol	CHEMBL3912437 -7.6 kcal/mol
		
CHEMBL3932144 -8.1 kcal/mol	CHEMBL4207348 -7.7 kcal/mol	CHEMBL4227331 -7.6 kcal/mol
		

	CHEMBL4300783 -8.3 kcal/mol	
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Table S4. Compounds obtained from screening the DrugBank database.

ID	Mol Weight	H acceptor	H donors	Log P	Vina score	Cluster #
DB07458	438.52	6	2	4.441	-8.6	C-63
DB11799	449.38	7	2	1.963	-8.5	C-63
DB09371	298.42	5	1	3.637	-8.5	C-45
DB01003	468.37	9	3	2.114	-8.4	C-45
DB07456	438.52	6	2	4.441	-8.4	C-63
DB12200	369.42	3	2	3.921	-8.4	C-63
DB11703	465.51	8	2	3.905	-8.4	C-63
DB11942	443.31	7	2	3.851	-8.4	C-63
DB12207	442.32	6	2	4.456	-8.4	C-63
DB01897	466.49	5	2	2.854	-8.4	C-63
DB08124	393.42	6	2	4.467	-8.4	C-63
DB02194	439.46	6	3	2.474	-8.4	C-63
DB12760	489.89	9	3	3.108	-8.4	C-63
DB15133	492.57	7	0	3.946	-8.4	C-63
DB12571	394.44	6	2	4.422	-8.4	C-63
DB00894	300.39	6	0	3.59	-8.3	C-45
DB11827	436.88	7	4	1.357	-8.3	C-45
DB12812	406.43	5	1	4.596	-8.3	C-45
DB09280	452.41	7	2	4.82	-8.3	C-63
DB08362	384.39	8	3	3.661	-8.3	C-63
DB06858	413.56	8	4	3.8	-8.3	C-63
DB15247	439.48	7	3	3.216	-8.3	C-63
DB15399	461.49	8	3	3.816	-8.3	C-63
DB07265	400.38	5	3	3.281	-8.3	C-63
DB12385	364.35	6	2	1.785	-8.3	C-63
DB02152	467.47	7	2	3.984	-8.3	C-63
DB08930	419.38	8	2	1.682	-8.3	C-63
DB12387	406.44	7	3	3.803	-8.3	C-63
DB01609	373.36	6	3	3.711	-8.3	C-63
DB13029	422.44	4	1	3.497	-8.3	C-63
DB15295	415.42	5	2	4.902	-8.3	C-63
DB06964	388.8	6	3	4.222	-8.3	C-63
DB15157	469.84	5	3	4.261	-8.3	C-63
DB14917	412.51	7	2	3.941	-8.3	C-63
DB00591	452.49	9	2	2.367	-8.2	C-45
DB04392	336.29	8	0	2.213	-8.2	C-45
DB02241	455.46	7	3	2.971	-8.2	C-63
DB11952	416.86	5	2	4.557	-8.2	C-63
DB12108	460.53	7	1	3.875	-8.2	C-63
DB12121	411.46	6	2	3.991	-8.2	C-63
DB15418	399.37	8	2	2.294	-8.2	C-63
DB11832	443.54	6	1	4.682	-8.2	C-63
DB06435	448.52	5	1	4.049	-8.2	C-63
DB13874	473.37	8	3	4.439	-8.2	C-63

DB08232	404.38	6	4	4.824	-8.2	C-63
DB07337	375.81	6	3	4.449	-8.2	C-63
DB07020	370.36	5	3	3.933	-8.2	C-63
DB08899	464.44	7	1	4.513	-8.2	C-63
DB02084	472.45	8	4	3.442	-8.2	C-63
DB14846	411.38	9	1	1.919	-8.2	C-63
DB15456	426.38	9	3	3.793	-8.2	C-63
DB15085	487.38	5	1	2.697	-8.2	C-63
DB09195	405.46	6	0	3.562	-8.2	C-63
DB01405	417.38	5	2	3.298	-8.2	C-63
DB14823	409.91	5	0	4.304	-8.2	C-63
DB01267	426.48	5	1	3.019	-8.2	C-63
DB12523	432.49	5	1	3.477	-8.2	C-63
DB12221	340.46	6	0	4.37	-8.1	C-45
DB15048	416.46	7	4	1.126	-8.1	C-45
DB08907	444.52	6	4	2.968	-8.1	C-45
DB07152	362.36	6	2	3.561	-8.1	C-63
DB08553	373.45	5	2	3.99	-8.1	C-63
DB15197	388.39	6	3	3.801	-8.1	C-63
DB08448	385.42	9	3	3.806	-8.1	C-63
DB08036	311.34	2	3	4.528	-8.1	C-63
DB14878	366.46	4	1	4.975	-8.1	C-63
DB11877	445.46	7	0	3.652	-8.1	C-63
DB08454	301.35	4	2	4.145	-8.1	C-63
DB12168	406.41	6	1	3.674	-8.1	C-63
DB07275	411.47	6	2	3.969	-8.1	C-63
DB11701	482.55	8	1	4.304	-8.1	C-63
DB13993	397.38	6	0	3.045	-8.1	C-63
DB11925	462.54	9	1	3.023	-8.1	C-63
DB07006	416.43	5	3	3.198	-8.1	C-63
DB08174	441.93	7	2	4.415	-8.1	C-63
DB15219	340.38	7	3	2.616	-8.1	C-63
DB15268	485.43	9	2	3.219	-8.1	C-63
DB11491	385.36	5	2	2.771	-8.1	C-63
DB04030	398.45	4	2	4.237	-8.1	C-63
DB03383	443.9	6	3	3.614	-8.1	C-63
DB14970	437.49	5	2	4.786	-8.1	C-63
DB14034	420.48	6	1	4.688	-8.1	C-63
DB08138	360.29	5	3	3.478	-8.1	C-63
DB08239	397.46	5	1	4.476	-8.1	C-63
DB06169	389.83	4	1	4.632	-8.1	C-63
DB08358	340.38	4	2	3.907	-8.1	C-63
DB12269	479.92	9	3	3.251	-8.1	C-63
DB12899	395.46	7	0	3.452	-8.1	C-63
DB13113	377.35	5	0	3.213	-8.1	C-63
DB11901	477.43	8	1	4.052	-8.1	C-63
DB01138	404.48	5	0	4.791	-8.1	C-63
DB11984	479.98	8	2	3.319	-8.1	C-63
DB07220	453.56	7	2	4.558	-8.1	C-63
DB05552	346.34	8	4	3.492	-8.1	C-63
DB01741	460.41	4	3	0.318	-8.1	C-63
DB07396	455.81	7	3	4.549	-8.1	C-63
DB09034	450.92	7	0	4.114	-8.1	C-63
DB13643	464.9	9	0	2.268	-8.1	C-63
DB13040	469.94	6	2	4.039	-8.1	C-63
DB06831	450.9	7	1	4.006	-8.1	C-63
DB03960	449.5	9	4	3.32	-8.1	C-63

DB15099	368.81	5	2	4.002	-8.1	C-63
DB11466	385.84	5	1	3.981	-8.1	C-63
DB12570	397.47	8	2	2.685	-8.1	C-63
DB06160	426.41	5	2	4.796	-8.1	C-63
DB12690	445.42	5	1	4.36	-8.1	C-63
DB12540	483.56	8	0	3.585	-8.1	C-63
DB04888	385.46	3	1	4.113	-8.1	C-63
DB07146	398.5	4	2	4.819	-8.1	C-63
DB07297	399.49	5	2	4.214	-8.1	C-63
DB14882	418.49	5	1	2.012	-8.1	C-63
DB15186	382.42	9	1	1.614	-8.1	C-63
DB15442	446.55	8	2	3.129	-8.1	C-63
DB08005	398.89	6	3	4.286	-8.1	C-63
DB04204	470.29	6	4	4.706	-8.1	C-45
DB11487	497.56	9	2	3.155	-8.1	C-45
DB11698	404.45	5	4	2.146	-8.1	C-45
DB12802	414.41	8	1	2.409	-8.1	C-45
DB00693	332.31	5	2	3.666	-8.1	C-45
DB01977	289.33	4	3	4.249	-8	C-54
DB02840	368.34	7	4	3.144	-8	C-63
DB07826	365.81	4	1	4.662	-8	C-63
DB07514	397.47	5	2	4.761	-8	C-63
DB07430	374.46	6	2	4.831	-8	C-63
DB13919	440.45	7	2	4.029	-8	C-63
DB08353	347.42	6	2	3.878	-8	C-63
DB08354	375.81	6	2	4.151	-8	C-63
DB08248	402.47	8	3	4.557	-8	C-63
DB08495	462.97	7	2	4.629	-8	C-63
DB15145	439.53	8	2	3.791	-8	C-63
DB04405	471.5	8	1	4.65	-8	C-63
DB03925	454.52	8	3	3.02	-8	C-63
DB08395	423.39	6	1	4.196	-8	C-63
DB08015	404.39	6	1	4.149	-8	C-63
DB15407	401.4	6	2	3.437	-8	C-63
DB12963	451.91	7	1	2.835	-8	C-63
DB04591	439.46	7	2	3.985	-8	C-63
DB01261	407.31	5	1	2.655	-8	C-63
DB15233	498.56	8	1	3.438	-8	C-63
DB11697	472.58	6	1	3.76	-8	C-63
DB11734	462.58	7	1	4.134	-8	C-63
DB15029	457.47	6	1	3.921	-8	C-63
DB08815	492.68	8	0	4.197	-8	C-63
DB08091	444.5	5	2	4.714	-8	C-63
DB11751	405.35	7	2	1.292	-8	C-63
DB00685	416.35	8	2	2.66	-8	C-63
DB14935	363.37	6	1	2.716	-8	C-63
DB02008	463.5	5	2	3.496	-8	C-63
DB12183	473.93	8	2	4.166	-8	C-63
DB15170	429.51	7	2	4.947	-8	C-63
DB12412	489.36	7	1	2.95	-8	C-63
DB06852	419.91	6	3	4.242	-8	C-63
DB04908	390.4	3	1	3.174	-8	C-63
DB08058	380.42	5	2	2.355	-8	C-64
DB15408	349.77	5	2	4.951	-8	C-63
DB07666	448.46	8	1	4.742	-8	C-63
DB12914	435.22	7	2	2.098	-8	C-63
DB12242	362.42	6	4	4.02	-8	C-63

DB04049	411.45	6	3	4.4	-8	C-63
DB15183	468.4	7	2	3.862	-8	C-63
DB08338	363.42	7	3	3.456	-8	C-63
DB08345	345.36	7	3	2.263	-8	C-63
DB07131	384.52	7	3	4.067	-8	C-63
DB07253	418.85	8	2	4.976	-8	C-63
DB07605	476.96	5	1	4.568	-8	C-63
DB14845	425.5	7	1	3.067	-8	C-63
DB14966	389.49	5	1	4.334	-8	C-63
DB15121	421.35	7	1	2.49	-8	C-63
DB12854	462.89	7	3	4.695	-8	C-63
DB14569	370.34	8	1	1.461	-8	C-63
DB06817	444.42	9	3	1.693	-8	C-63
DB09054	415.42	7	2	3.827	-8	C-63
DB04739	479.58	8	2	4.304	-8	C-63
DB11795	433.42	5	1	4.32	-8	C-63
DB12158	420.48	6	0	4.244	-8	C-63
DB12910	404.46	7	1	3.575	-8	C-63
DB12725	455.59	7	2	3.873	-8	C-63
DB01933	482.53	7	3	4.565	-8	C-63
DB11511	399.39	5	1	2.722	-8	C-63
DB06916	420.46	9	1	2.483	-8	C-63
DB06888	403.43	7	2	2.026	-8	C-63
DB08738	444.53	7	0	2.943	-8	C-63
DB12096	405.49	5	1	3.638	-8	C-63
DB01349	411.46	7	1	3.485	-8	C-63
DB15227	454.48	7	1	3.273	-8	C-63
DB15327	487.53	8	3	4.658	-8	C-63
DB15579	296.36	3	0	3.443	-8	C-45
DB01108	329.43	7	2	3.467	-8	C-45
DB11824	386.44	6	4	0.997	-8	C-45
DB11994	368.29	8	1	2.011	-8	C-45
DB04064	378.33	7	2	2.406	-8	C-45
DB13062	348.39	4	3	4.42	-8	C-45
DB09074	434.46	7	1	2.636	-7.9	C-64
DB04982	337.37	6	1	2.498	-7.9	C-63
DB07415	386.38	6	2	4.535	-7.9	C-63
DB04797	322.34	3	0	4.314	-7.9	C-63
DB14974	399.39	6	3	3.672	-7.9	C-63
DB12924	363.41	5	2	3.828	-7.9	C-63
DB12535	349.36	5	3	3.699	-7.9	C-63
DB11632	413.17	5	2	4.598	-7.9	C-63
DB08141	349.34	7	4	2.215	-7.9	C-63
DB07594	352.38	5	3	3.797	-7.9	C-63
DB07422	474.26	5	2	4.674	-7.9	C-63
DB01793	377.18	6	3	3.573	-7.9	C-63
DB07528	396.37	4	1	4.938	-7.9	C-63
DB11769	429.35	5	0	4.317	-7.9	C-63
DB06976	366.42	9	4	3.182	-7.9	C-63
DB08267	305.33	4	3	2.748	-7.9	C-63
DB04154	343.38	5	0	3.441	-7.9	C-63
DB12903	356.38	4	3	3.933	-7.9	C-63
DB02071	427.47	8	2	4.385	-7.9	C-63
DB08591	318.35	6	1	3.018	-7.9	C-63
DB07540	363.41	7	3	4.332	-7.9	C-63
DB07568	425.48	9	2	4.289	-7.9	C-63
DB12382	413.45	9	2	2.734	-7.9	C-63

DB06957	462.95	7	3	3.951	-7.9	C-63
DB00203	474.58	8	1	2.568	-7.9	C-63
DB08426	427.5	8	2	3.662	-7.9	C-63
DB08745	475	7	0	4.118	-7.9	C-63
DB06140	478.4	5	0	4.353	-7.9	C-63
DB07827	424.45	4	1	3.041	-7.9	C-63
DB07229	357.41	2	3	3.819	-7.9	C-63
DB01725	328.37	4	4	4.687	-7.9	C-63
DB05611	418.49	8	1	3.222	-7.9	C-63
DB11666	410.39	7	2	1.873	-7.9	C-63
DB12238	395.43	6	0	3.418	-7.9	C-63
DB12140	456.42	6	3	3.012	-7.9	C-63
DB00275	446.5	7	3	3.657	-7.9	C-63
DB11526	498.64	6	2	4.628	-7.9	C-63
DB15190	458.52	8	2	3.674	-7.9	C-63
DB13059	474.48	8	3	4.533	-7.9	C-63
DB14980	408.45	7	2	2.849	-7.9	C-63
DB12021	396.49	5	2	3.212	-7.9	C-63
DB01166	369.46	6	1	3.603	-7.9	C-63
DB12966	387.84	7	2	3.546	-7.9	C-63
DB00218	401.43	8	2	2.764	-7.9	C-63
DB12134	448.52	7	1	1.416	-7.9	C-63
DB12742	447.51	8	1	3.695	-7.9	C-63
DB07227	405.88	5	0	3.308	-7.9	C-63
DB15305	401.46	6	1	2.357	-7.9	C-63
DB06144	440.94	4	1	4.832	-7.9	C-63
DB08882	472.54	8	1	1.913	-7.9	C-63
DB01852	286.24	5	4	2.282	-7.9	C-47
DB14029	293.34	3	1	3.696	-7.9	C-58
DB09268	437.44	9	2	4.787	-7.9	C-59
DB07756	426.43	5	3	4.979	-7.9	C-63
DB14814	412.53	5	1	3.808	-7.9	C-63
DB12507	496.89	9	3	3.188	-7.9	C-63
DB08607	441.54	8	2	4.703	-7.9	C-63
DB08111	302.33	4	1	3.088	-7.9	C-63
DB06446	442.59	4	0	4.949	-7.9	C-63
DB04760	410.42	6	2	4.013	-7.9	C-63
DB07343	373.2	7	2	4.822	-7.9	C-63
DB12446	308.38	4	3	3.413	-7.9	C-63
DB07204	395.46	6	2	4.822	-7.9	C-63
DB04716	309.34	2	2	3.994	-7.9	C-63
DB03903	483.52	8	1	3.873	-7.9	C-63
DB08731	403.38	8	2	3.158	-7.9	C-63
DB00973	409.43	4	2	4.953	-7.9	C-63
DB04014	293.28	3	2	3.899	-7.9	C-63
DB13939	393.83	8	2	4.049	-7.9	C-63
DB08137	324.31	5	3	3.199	-7.9	C-63
DB12055	422.35	7	2	3.541	-7.9	C-63
DB07495	387.82	6	4	3.958	-7.9	C-63
DB15391	437.44	8	2	3.306	-7.9	C-63
DB06741	375.21	4	3	4.898	-7.9	C-63
DB12517	470.59	4	1	4.657	-7.9	C-63
DB12659	468.4	6	1	4.585	-7.9	C-63
DB02195	305.31	3	1	4.142	-7.9	C-63
DB07549	448.44	6	4	1.612	-7.9	C-63
DB07686	387.46	8	3	4.187	-7.9	C-63
DB07247	358.39	5	4	4.862	-7.9	C-63

DB14765	397.47	6	2	4.822	-7.9	C-63
DB08512	356.38	5	4	3.801	-7.9	C-63
DB07786	424.88	7	2	4.699	-7.9	C-63
DB08708	361.36	4	1	4.628	-7.9	C-63
DB08006	325.37	4	1	4.556	-7.9	C-63
DB12048	345.36	6	0	1.879	-7.9	C-63
DB07546	376.41	6	2	3.127	-7.9	C-63
DB12015	441.47	7	2	4.546	-7.9	C-63
DB07062	493.56	9	3	3.593	-7.9	C-63
DB04698	343.32	9	2	2.414	-7.9	C-63
DB07252	419.84	9	3	4.92	-7.9	C-63
DB00862	488.6	8	1	3.027	-7.9	C-63
DB00705	456.56	8	3	3.947	-7.9	C-63
DB07848	454.93	8	2	2.295	-7.9	C-63
DB07024	403.41	7	3	3.571	-7.9	C-63
DB08676	453.54	9	1	3.989	-7.9	C-63
DB08011	346.28	6	1	2.621	-7.9	C-63
DB07606	465.72	5	3	4.633	-7.9	C-63
DB08349	449.45	5	2	4.411	-7.9	C-63
DB00678	422.91	5	2	4.267	-7.9	C-63
DB07213	427.5	5	4	3.912	-7.9	C-63
DB14770	443.5	9	2	2.69	-7.9	C-63
DB08057	406.91	6	2	4.853	-7.9	C-63
DB14885	414.39	6	0	3.189	-7.9	C-63
DB13094	376.43	4	1	3.055	-7.9	C-63
DB04289	393.48	3	1	4.572	-7.9	C-63
DB07570	446.54	5	1	4.851	-7.9	C-63
DB08365	476.71	5	3	3.014	-7.9	C-63
DB12185	435.45	6	2	3.173	-7.9	C-63
DB06961	457.91	7	3	3.984	-7.9	C-63
DB11943	440.76	7	3	2.564	-7.9	C-63
DB11665	368.43	7	3	2.087	-7.9	C-63
DB05424	485.94	8	2	4.475	-7.9	C-63
DB06518	388.37	6	1	3.063	-7.9	C-63
DB00734	410.48	4	0	3.528	-7.9	C-63
DB15431	449.86	6	2	4.971	-7.9	C-63
DB14844	386.49	3	0	1.853	-7.9	C-63
DB05928	392.43	5	3	3.129	-7.9	C-63
DB13080	366.43	4	0	3.252	-7.9	C-64
DB13292	293.43	2	0	4.617	-7.9	C-45
DB01406	337.46	5	1	4.221	-7.9	C-45
DB14664	478.57	7	1	4.326	-7.9	C-45
DB11939	454.87	7	4	1.496	-7.9	C-45
DB13016	434.48	6	3	4.906	-7.9	C-45
DB07435	304.34	6	3	2.895	-7.9	C-45
DB00266	336.29	4	2	2.901	-7.9	C-45
DB06588	348.39	4	2	4.415	-7.9	C-45
DB11521	348.4	7	4	1.705	-7.8	C-62
DB02473	384.47	5	3	4.686	-7.8	C-61
DB07586	417.46	7	3	4.199	-7.8	C-49
DB15465	403.47	8	0	3.653	-7.8	C-64
DB12721	437.96	4	0	4.456	-7.8	C-64
DB14769	298.31	3	2	2.306	-7.8	C-64
DB14775	299.71	4	2	3.959	-7.8	C-63
DB04861	405.44	5	3	2.755	-7.8	C-63
DB07063	376.35	3	1	4.344	-7.8	C-63
DB03878	382.42	7	2	4.384	-7.8	C-63

DB08079	383.4	6	0	3.927	-7.8	C-63
DB12941	398.85	6	3	3.061	-7.8	C-63
DB08710	398.41	7	2	2.67	-7.8	C-63
DB12009	393.46	5	0	4.946	-7.8	C-63
DB11946	388.87	5	2	4.87	-7.8	C-63
DB07074	377.39	7	4	4.05	-7.8	C-63
DB04971	392.4	6	1	3.347	-7.8	C-63
DB03744	425.86	7	3	3.034	-7.8	C-63
DB15498	446.55	8	2	4.875	-7.8	C-63
DB04764	399.53	4	1	4.984	-7.8	C-63
DB14627	401.41	6	1	3.962	-7.8	C-63
DB06995	398.36	7	3	4.67	-7.8	C-63
DB12364	451.91	8	3	4.381	-7.8	C-63
DB06578	391.82	5	2	4.076	-7.8	C-63
DB05944	466.94	8	2	4.831	-7.8	C-63
DB08400	380.36	5	1	4.763	-7.8	C-63
DB15254	471.46	9	2	4.229	-7.8	C-63
DB07137	337.38	7	1	2.27	-7.8	C-63
DB05575	373.45	6	3	4.639	-7.8	C-63
DB07704	335.36	5	3	2.757	-7.8	C-63
DB11990	455.56	5	1	4.376	-7.8	C-63
DB04480	293.34	2	0	4.006	-7.8	C-63
DB12784	389.43	6	2	4.474	-7.8	C-63
DB07853	381.43	6	2	4.775	-7.8	C-63
DB08539	341.41	4	1	4.354	-7.8	C-63
DB07324	321.33	5	2	1.92	-7.8	C-63
DB11836	309.33	6	2	3.542	-7.8	C-63
DB07664	425.44	9	4	4.283	-7.8	C-63
DB06589	437.52	8	2	4.993	-7.8	C-63
DB07934	466.62	9	4	2.926	-7.8	C-63
DB07261	453.54	9	2	4.497	-7.8	C-63
DB07029	388.38	7	0	4.284	-7.8	C-63
DB15009	432.43	9	1	3.449	-7.8	C-63
DB08042	420.46	8	2	4.272	-7.8	C-63
DB03865	362.83	2	4	4.026	-7.8	C-63
DB13093	445.47	8	2	3.619	-7.8	C-63
DB02656	307.34	3	0	3.362	-7.8	C-63
DB04957	457.95	7	0	2.977	-7.8	C-63
DB15393	409.83	7	2	4.417	-7.8	C-63
DB11867	416.38	8	1	2.957	-7.8	C-63
DB08087	307.3	8	1	1.616	-7.8	C-63
DB02132	441.64	4	1	2.851	-7.8	C-63
DB11953	395.46	7	1	1.434	-7.8	C-63
DB07917	377.48	5	1	3.341	-7.8	C-63
DB12494	405.42	5	1	4.06	-7.8	C-63
DB07340	393.49	7	3	3.889	-7.8	C-63
DB13950	426.51	4	0	4.538	-7.8	C-63
DB14895	444.53	6	3	3.168	-7.8	C-63
DB12050	464.44	8	3	2.939	-7.8	C-63
DB08730	444.5	5	1	4.645	-7.8	C-63
DB06469	439.46	5	3	3.803	-7.8	C-63
DB07145	433.5	8	2	3.835	-7.8	C-63
DB00978	351.35	5	2	2.19	-7.8	C-63
DB14795	459.9	8	1	4.258	-7.8	C-63
DB08916	485.94	8	2	4.536	-7.8	C-63
DB15345	451.49	7	1	2.382	-7.8	C-63
DB06605	459.5	8	1	3.53	-7.8	C-63

DB08588	359.42	6	1	3.009	-7.8	C-63
DB13471	476.56	6	2	3.028	-7.8	C-64
DB07816	384.43	6	3	4.254	-7.8	C-51
DB08883	349.38	3	0	4.438	-7.8	C-50
DB08184	249.31	2	3	4.227	-7.8	C-52
DB00875	434.52	5	1	4.478	-7.8	C-56
DB13841	400.96	5	1	4.112	-7.8	C-57
DB03285	256.25	4	3	2.7	-7.8	C-47
DB07352	270.24	4	3	2.577	-7.8	C-46
DB08121	318.37	4	1	4.428	-7.8	C-48
DB07809	344.41	5	3	4.39	-7.8	C-53
DB04059	263.3	5	3	3.531	-7.8	C-55
DB07949	335.31	7	1	0.777	-7.8	C-60
DB12211	367.83	4	2	4.762	-7.8	C-63
DB06635	446.5	6	3	4.407	-7.8	C-63
DB11900	348.37	3	1	4.312	-7.8	C-63
DB08022	372.45	7	1	3.864	-7.8	C-63
DB08976	406.36	6	3	3.58	-7.8	C-63
DB03623	272.3	3	1	4.156	-7.8	C-63
DB00197	441.54	7	2	4.703	-7.8	C-63
DB08513	377.4	8	4	3.845	-7.8	C-63
DB07589	485.52	9	4	4.739	-7.8	C-63
DB01871	460.52	9	3	3.595	-7.8	C-63
DB11645	393.5	5	1	4.472	-7.8	C-63
DB06972	408.28	4	0	4.698	-7.8	C-63
DB06977	383.45	7	2	3.733	-7.8	C-63
DB07507	329.35	4	1	4.233	-7.8	C-63
DB06922	389.36	8	2	2.768	-7.8	C-63
DB11450	334.37	5	2	2.863	-7.8	C-63
DB02712	236.2	5	2	1.301	-7.8	C-63
DB15406	484.99	6	1	4.991	-7.8	C-63
DB14774	428.42	5	0	3.419	-7.8	C-63
DB12848	372.38	7	1	1.674	-7.8	C-63
DB08927	401.49	5	1	4.491	-7.8	C-63
DB14969	341.31	4	2	4.355	-7.8	C-63
DB07963	447.17	5	3	3.537	-7.8	C-63
DB06874	450.29	7	2	4.7	-7.8	C-63
DB11764	423.44	8	3	4.472	-7.8	C-63
DB07256	383.79	8	3	4.291	-7.8	C-63
DB06997	422.38	6	3	4.988	-7.8	C-63
DB07226	389.79	4	3	4.558	-7.8	C-63
DB08997	362.46	4	1	3.487	-7.8	C-63
DB04260	337.22	7	4	1.224	-7.8	C-63
DB04196	312.28	9	4	1.672	-7.8	C-63
DB07203	357.84	5	2	4.782	-7.8	C-63
DB08241	366.42	7	3	3.928	-7.8	C-63
DB14716	353.76	5	0	3.447	-7.8	C-63
DB08218	373.37	7	0	2.58	-7.8	C-63
DB07382	332.36	6	4	3.587	-7.8	C-63
DB06314	359.41	6	0	3.224	-7.8	C-63
DB08584	359.41	6	0	3.224	-7.8	C-63
DB04669	382.24	4	2	3.053	-7.8	C-63
DB08538	381.38	6	2	3.875	-7.8	C-63
DB01906	272.22	8	3	0.778	-7.8	C-63
DB03496	401.84	5	3	3.242	-7.8	C-63
DB06974	468.53	8	2	3.886	-7.8	C-63
DB08614	488.48	9	3	3.599	-7.8	C-63

DB07531	350.37	7	2	4.028	-7.8	C-63
DB08481	362.42	7	1	3.753	-7.8	C-63
DB07534	349.38	7	3	3.942	-7.8	C-63
DB12068	411.3	7	3	4.609	-7.8	C-63
DB02519	342.33	9	3	3.262	-7.8	C-63
DB07126	402.47	8	3	4.557	-7.8	C-63
DB08487	462.97	7	2	4.629	-7.8	C-63
DB08488	436.94	6	1	3.879	-7.8	C-63
DB08303	428.57	9	2	3.655	-7.8	C-63
DB08613	423.41	5	2	2.905	-7.8	C-63
DB08703	424.49	4	1	4.348	-7.8	C-63
DB07140	358.44	6	2	4.943	-7.8	C-63
DB03159	327.38	1	3	3.81	-7.8	C-63
DB08356	296.32	4	3	3.472	-7.8	C-63
DB08445	401.39	8	1	3.661	-7.8	C-63
DB12174	434.49	8	3	4.662	-7.8	C-63
DB11865	441.46	7	2	4.117	-7.8	C-63
DB12443	421.83	9	4	0.876	-7.8	C-63
DB12130	406.41	7	1	3.32	-7.8	C-63
DB12417	383.45	8	2	1.37	-7.8	C-63
DB11763	414.46	8	2	3.506	-7.8	C-63
DB13308	372.8	5	2	3.739	-7.8	C-63
DB07059	398.46	9	3	3.129	-7.8	C-63
DB12432	388.47	5	2	3.818	-7.8	C-63
DB07186	448.54	6	2	3.389	-7.8	C-63
DB04685	472.51	7	1	4.171	-7.8	C-63
DB14896	380.42	6	1	3.063	-7.8	C-63
DB08068	445.91	8	1	4.023	-7.8	C-63
DB00377	296.41	4	0	2.532	-7.8	C-63
DB05327	420.19	6	1	1.581	-7.8	C-63
DB07875	490.94	9	3	2.507	-7.8	C-63
DB12658	375.42	5	1	3.831	-7.8	C-63
DB12949	433.52	7	2	2.807	-7.8	C-63
DB06600	371.43	6	2	2.982	-7.8	C-63
DB09047	398.39	9	2	1.616	-7.8	C-63
DB12447	360.38	5	2	2.372	-7.8	C-63
DB00365	359.39	5	2	2.674	-7.8	C-63
DB03034	361.37	6	1	1.547	-7.8	C-63
DB07973	405.53	4	1	4.63	-7.8	C-63
DB07967	428.49	7	1	4.295	-7.8	C-63
DB00317	446.9	7	1	4.287	-7.8	C-63
DB01184	425.91	3	2	3.291	-7.8	C-63
DB00450	379.43	3	1	3.616	-7.8	C-63
DB12867	381.44	4	1	4.119	-7.8	C-63
DB08530	355.41	4	1	0.5	-7.8	C-63
DB15323	357.38	5	1	1.299	-7.8	C-64
DB07629	472	8	3	4.456	-7.8	C-64
DB07707	316.43	8	2	3.482	-7.8	C-45
DB09123	311.42	5	1	3.837	-7.8	C-45
DB05830	288.42	6	1	3.735	-7.8	C-45
DB07638	318.31	6	2	4.36	-7.8	C-45
DB12214	434.55	7	4	2.225	-7.8	C-45
DB07036	362.37	7	2	4.507	-7.8	C-45
DB15359	354.4	5	3	4.217	-7.8	C-45
DB14008	300.26	5	3	2.585	-7.8	C-45
DB08978	484.61	8	1	4.954	-7.8	C-64
DB02398	318.37	5	4	4.408	-7.8	C-55

DB08639	329.4	5	2	4.907	-7.8	C-56
DB07743	363.31	4	1	3.749	-7.8	C-60
DB06454	348.41	3	1	4.762	-7.7	C-63
DB00800	305.76	4	4	3.063	-7.7	C-63
DB13217	329.8	3	1	4.758	-7.7	C-63
DB08449	377.34	4	1	3.739	-7.7	C-63
DB07064	324.42	5	1	3.576	-7.7	C-63
DB02455	434.46	9	4	4.739	-7.7	C-63
DB11962	333.36	6	1	3.95	-7.7	C-63
DB02014	413.35	7	2	3.763	-7.7	C-63
DB03921	272.3	3	1	3.687	-7.7	C-63
DB12011	426.41	5	1	4.523	-7.7	C-63
DB08752	405.53	9	2	2.129	-7.7	C-63
DB07124	384.43	8	1	1.015	-7.7	C-63
DB07245	304.39	3	1	4.706	-7.7	C-63
DB05686	394.34	6	3	4.898	-7.7	C-63
DB06930	318.37	4	3	4.023	-7.7	C-63
DB00485	470.33	9	2	3.531	-7.7	C-63
DB08707	322.75	4	1	4.769	-7.7	C-63
DB07244	355.38	5	3	4.996	-7.7	C-63
DB09199	381.42	5	1	4.781	-7.7	C-63
DB06834	362.42	4	3	3.613	-7.7	C-63
DB12573	374.44	5	1	3.949	-7.7	C-63
DB07075	384.48	4	3	4.392	-7.7	C-63
DB07470	278.31	4	1	2.055	-7.7	C-63
DB14654	417.41	7	1	3.95	-7.7	C-63
DB07078	332.35	4	3	4.027	-7.7	C-63
DB07236	277.27	3	2	4.059	-7.7	C-63
DB07070	427.39	6	2	4.827	-7.7	C-63
DB07419	416.75	5	2	4.211	-7.7	C-63
DB12078	389.33	6	2	3.29	-7.7	C-63
DB07941	477.3	4	1	4.825	-7.7	C-63
DB04434	289.33	5	2	2.967	-7.7	C-63
DB07692	460.47	8	0	3.469	-7.7	C-63
DB12306	390.24	3	3	4.811	-7.7	C-63
DB07535	254.29	3	3	2.2	-7.7	C-63
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DB08463	431.53	8	3	4.41	-7.7	C-63
DB01938	280.32	5	3	2.845	-7.7	C-63
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DB14717	319.32	4	0	2.794	-7.7	C-63
DB08300	275.31	4	1	3.347	-7.7	C-63
DB08536	380.24	4	1	4.239	-7.7	C-63
DB01765	292.29	3	2	2.561	-7.7	C-63
DB06983	331.37	5	2	2.969	-7.7	C-63
DB08242	358.4	6	2	3.691	-7.7	C-63
DB07133	365.47	7	2	3.201	-7.7	C-63
DB07369	455.96	5	1	3.488	-7.7	C-63
DB12285	409.41	8	2	2.645	-7.7	C-63
DB06629	424.43	9	1	3.86	-7.7	C-63
DB08123	401.46	8	3	3.797	-7.7	C-63
DB07325	389.43	9	3	3.214	-7.7	C-63
DB01289	449.52	9	3	3.926	-7.7	C-63
DB07817	444.53	9	2	3.923	-7.7	C-63
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DB12512	406.48	6	1	4.658	-7.7	C-63

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DB13042	459.56	7	0	4.303	-7.7	C-63
DB08931	422.42	9	2	3.605	-7.7	C-63
DB11950	426.58	9	1	1.836	-7.7	C-63
DB07406	440.52	9	4	2.808	-7.7	C-63
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DB06090	361.44	6	1	3.592	-7.7	C-63
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DB06306	409.52	6	2	2.938	-7.7	C-63
DB05532	422.43	8	1	1.623	-7.7	C-63
DB15102	487.5	8	1	3.725	-7.7	C-63
DB15173	410.8	7	1	3.355	-7.7	C-63
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DB08739	405.4	8	0	1.345	-7.7	C-64
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DB07795	286.24	5	4	2.282	-7.7	C-47
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DB07856	389.88	4	2	4.672	-7.7	C-63
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DB11711	410.46	6	2	3.466	-7.7	C-63
DB07604	336.38	7	2	2.766	-7.7	C-63
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DB02611	370.4	9	4	2.525	-7.7	C-63
DB01147	435.88	9	2	2.878	-7.7	C-63
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DB11870	469.4	6	3	4.723	-7.7	C-63

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DB15091	380.37	5	2	3.237	-7.7	C-63
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DB01411	481.5	7	2	4.7	-7.7	C-63
DB12776	472.49	9	2	4.541	-7.7	C-63
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DB07031	399.46	5	3	4.618	-7.7	C-63
DB02848	422.5	7	2	4.86	-7.7	C-63
DB13327	376.41	7	2	3.127	-7.7	C-63
DB07751	415.44	9	3	3.689	-7.7	C-63
DB13872	335.18	4	1	2.626	-7.7	C-63
DB07180	329.78	7	3	3.666	-7.7	C-63
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DB14672	328.75	5	1	2.592	-7.7	C-63
DB07578	372.44	3	0	4.154	-7.7	C-63
DB00699	484.39	6	0	3.849	-7.7	C-63
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DB01215	294.74	3	0	2.707	-7.7	C-63
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DB14998	357.41	5	2	1.883	-7.7	C-63

DB12501	493.56	7	2	3.891	-7.7	C-63
DB12301	425.75	5	1	2.655	-7.7	C-63
DB07474	397.43	5	3	3.492	-7.7	C-63
DB07444	321.37	3	2	3.1	-7.7	C-63
DB15419	394.4	8	3	2.354	-7.7	C-63
DB07156	426.31	5	2	4.108	-7.7	C-63
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DB06457	324.4	2	2	3.138	-7.7	C-63
DB15003	389.4	7	1	1.864	-7.7	C-63
DB14857	286.29	6	2	1.175	-7.7	C-63
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DB07257	354.79	3	2	2.673	-7.7	C-63
DB05482	392.4	6	2	2.348	-7.7	C-63
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DB08351	431.53	7	2	3.643	-7.7	C-63
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DB00547	376.46	6	2	2.781	-7.7	C-45
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DB12479	401.39	8	2	1.374	-7.7	C-64
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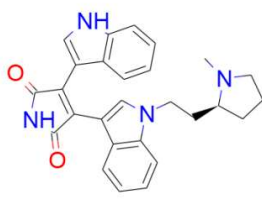
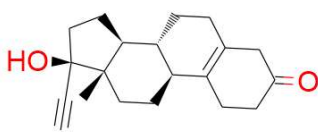
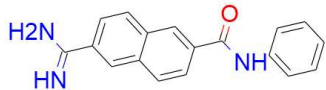
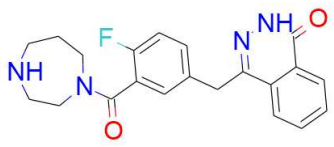
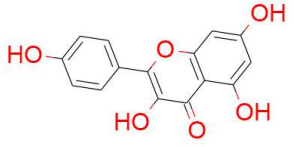
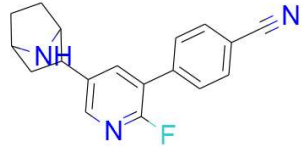
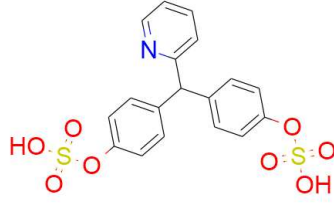
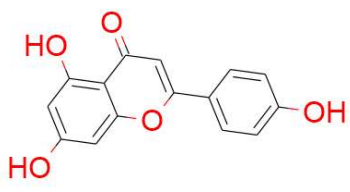
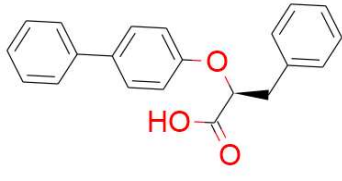
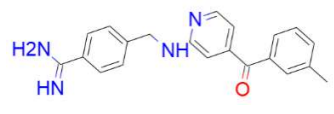
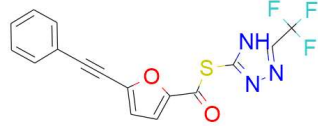
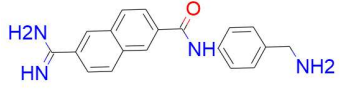
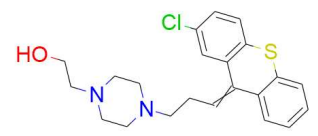
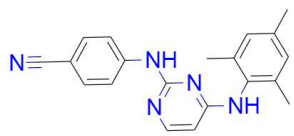
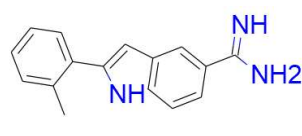
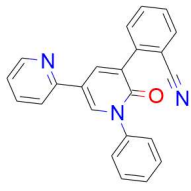
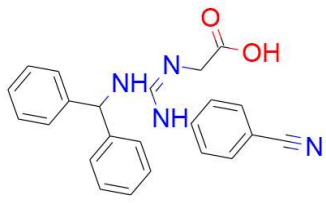
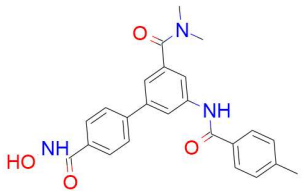
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DB08088	359.73	8	1	2.842	-7.6	C-63
DB04709	350.37	8	0	4.262	-7.6	C-63
DB13022	444.31	5	2	4.764	-7.6	C-63
DB00713	401.44	9	2	2.224	-7.6	C-63
DB04862	452.46	9	3	4.546	-7.6	C-63
DB08063	384.43	5	1	4.098	-7.6	C-63
DB08130	475.21	5	3	4.719	-7.6	C-63
DB13520	403.52	6	1	4.394	-7.6	C-63
DB07085	364.76	6	3	3.577	-7.6	C-63
DB06992	326.41	3	0	4.396	-7.6	C-63
DB03205	330.21	9	4	0.55	-7.6	C-63
DB04823	317.34	4	3	3.522	-7.6	C-63
DB07769	402.3	5	2	4.117	-7.6	C-63
DB07761	415.44	9	3	3.689	-7.6	C-63
DB03996	314.77	5	1	3.117	-7.6	C-63
DB07040	273.22	5	2	2.443	-7.6	C-63
DB03444	356.17	5	3	3.692	-7.6	C-63
DB08498	400.77	9	2	2.437	-7.6	C-63
DB07493	341.16	6	2	3.697	-7.6	C-63
DB14715	465.68	7	2	3.2	-7.6	C-63
DB00455	382.88	4	0	4.826	-7.6	C-63
DB12115	465.62	3	0	4.818	-7.6	C-63
DB02583	340.38	8	2	3.005	-7.6	C-63
DB08361	340.42	9	4	3.856	-7.6	C-63
DB07647	344.41	5	3	4.158	-7.6	C-63
DB07648	360.41	6	4	3.13	-7.6	C-63
DB07042	354.41	8	4	2.736	-7.6	C-63
DB04239	312.39	5	3	3.538	-7.6	C-63
DB12357	289.72	4	2	3.076	-7.6	C-63
DB12332	323.36	3	3	3.699	-7.6	C-63
DB07728	307.32	3	2	3.498	-7.6	C-63
DB08285	354.45	7	3	3.189	-7.6	C-63
DB08634	364.44	3	1	3.425	-7.6	C-63
DB09017	393.69	3	0	3.84	-7.6	C-63
DB00897	343.21	3	0	3.669	-7.6	C-63
DB12588	348.77	7	3	3.153	-7.6	C-63
DB07210	380.24	4	1	4.239	-7.6	C-63
DB07595	381.25	3	2	3.658	-7.6	C-63
DB06845	371.48	8	4	2.63	-7.6	C-63
DB08051	419.44	6	1	4.01	-7.6	C-63
DB07414	396.46	7	1	3.511	-7.6	C-63
DB08000	335.29	8	2	1.786	-7.6	C-63
DB12229	409.5	5	1	4.96	-7.6	C-63
DB01128	430.37	6	2	4.033	-7.6	C-63
DB00436	421.41	7	3	4.954	-7.6	C-63

DB00795	398.39	9	3	4.855	-7.6	C-63
DB08122	329.37	7	3	3.683	-7.6	C-63
DB08125	398.46	7	3	4.714	-7.6	C-63
DB12505	336.37	5	2	4.174	-7.6	C-63
DB11982	456.21	6	3	2.939	-7.6	C-63
DB07688	388.44	8	2	4.081	-7.6	C-63
DB12623	478.52	8	1	4.203	-7.6	C-63
DB06887	385.44	9	3	2.792	-7.6	C-63
DB12135	463.31	8	4	4.569	-7.6	C-63
DB08561	392.43	4	0	2.928	-7.6	C-63
DB07840	364.34	3	1	4.748	-7.6	C-63
DB08350	372.42	5	1	4.002	-7.6	C-63
DB08694	293.28	7	3	2.372	-7.6	C-63
DB06932	334.37	6	2	4.589	-7.6	C-63
DB08741	354.4	8	2	3.596	-7.6	C-63
DB03173	335.4	2	3	3.465	-7.6	C-63
DB01905	283.31	4	4	1.109	-7.6	C-63
DB03016	253.26	5	4	2.415	-7.6	C-63
DB02875	270.26	2	3	1.678	-7.6	C-63
DB06940	382.42	8	3	2.985	-7.6	C-63
DB07188	355.26	5	1	4.124	-7.6	C-63
DB07280	400.48	7	1	3.069	-7.6	C-63
DB11958	370.38	5	2	3.518	-7.6	C-63
DB15281	440.86	6	2	3.23	-7.6	C-63
DB08339	427.28	5	2	4.611	-7.6	C-63
DB14768	431.88	8	2	2.137	-7.6	C-63
DB00177	435.52	7	2	4.162	-7.6	C-63
DB00209	392.51	5	1	3.729	-7.6	C-63
DB06899	414.52	9	3	3.842	-7.6	C-63
DB12321	440.53	6	2	4.506	-7.6	C-63
DB12436	432.44	6	2	3.992	-7.6	C-63
DB12247	463.57	7	3	4.118	-7.6	C-63
DB07081	421.34	7	1	3.216	-7.6	C-63
DB07011	377.44	6	0	3.582	-7.6	C-63
DB07879	368.41	6	2	2.715	-7.6	C-63
DB12666	401.46	5	0	2.846	-7.6	C-63
DB13783	415.82	6	1	3.471	-7.6	C-63
DB11881	479.57	7	3	4.628	-7.6	C-63
DB07601	389.83	6	3	3.314	-7.6	C-63
DB00537	331.34	5	2	1.977	-7.6	C-63
DB01165	361.37	6	1	1.547	-7.6	C-63
DB07982	435.52	8	2	2.69	-7.6	C-63
DB13276	423.5	7	1	3.19	-7.6	C-63
DB08391	403.43	9	0	3.313	-7.6	C-63
DB12877	426.55	3	1	4.003	-7.6	C-63
DB06203	339.39	5	1	1.16	-7.6	C-64
DB01452	369.41	7	0	1.926	-7.6	C-64
DB00704	341.4	7	2	1.463	-7.6	C-64
DB15241	385.48	5	3	2.057	-7.6	C-64
DB07242	377.27	5	1	3.567	-7.6	C-64
DB08166	328.8	5	2	2.962	-7.6	C-64
DB08666	268.2	6	3	2.037	-7.6	C-60
DB05015	318.35	6	3	3.551	-7.6	C-45
DB08975	302.32	3	1	4.535	-7.6	C-45
DB06499	266.29	2	1	4.288	-7.6	C-45
DB00635	358.43	8	2	1.766	-7.6	C-45
DB12081	344.44	4	2	2.731	-7.6	C-45

DB06693	390.51	6	1	3.949	-7.6	C-45
DB07706	288.38	6	3	3.315	-7.6	C-45
DB12025	360.4	6	1	1.103	-7.6	C-45
DB08905	302.41	6	1	3.973	-7.6	C-45
DB07119	270.71	2	2	4.571	-7.6	C-45
DB04824	318.32	4	2	3.56	-7.6	C-45
DB07830	392.37	7	1	3.357	-7.6	C-64
DB01538	343.42	8	0	2.234	-7.6	C-64
DB14210	470.51	9	3	2.435	-7.6	C-64
DB12013	457.61	7	3	2.896	-7.6	C-64
DB00967	310.82	2	1	4.348	-7.6	C-58
DB11770	363.49	6	4	4.123	-7.6	C-63
DB00821	273.71	2	2	4.163	-7.6	C-63
DB06472	367.4	7	4	3.125	-7.6	C-63
DB09227	491.54	7	1	4.61	-7.6	C-63
DB01659	267.28	5	2	2.438	-7.6	C-63
DB11814	419.9	5	1	4.756	-7.6	C-63
DB12739	324.37	4	1	3.464	-7.6	C-63
DB06945	445.41	7	2	4.798	-7.6	C-63
DB09292	411.49	8	2	4.226	-7.6	C-63
DB08251	342.3	9	3	1.61	-7.6	C-63
DB13317	285.27	3	1	3.822	-7.6	C-63
DB08974	313.28	5	2	3.125	-7.6	C-63
DB08034	336.34	6	3	3.414	-7.6	C-63
DB01250	302.24	8	4	2.91	-7.6	C-63
DB08252	292.29	5	2	4.659	-7.6	C-63
DB07663	355.3	9	3	1.32	-7.6	C-63
DB14918	393.48	6	3	4.256	-7.6	C-63
DB08705	367.2	3	2	4.049	-7.6	C-63
DB07729	283.26	5	2	2.331	-7.6	C-63
DB02833	328.35	6	2	4.32	-7.6	C-63
DB12206	414.46	5	2	4.455	-7.6	C-63
DB01496	368.33	5	2	3.313	-7.6	C-63
DB07503	285.22	6	1	2.661	-7.6	C-63
DB00408	327.81	4	0	3.083	-7.6	C-63
DB07061	340.5	3	2	4.503	-7.6	C-63
DB00353	339.43	5	3	2.253	-7.6	C-63
DB15256	384.38	6	2	3.155	-7.6	C-63
DB06620	310.35	5	2	2.64	-7.6	C-63
DB12492	430.59	5	1	4.268	-7.6	C-63
DB11679	393.39	7	1	4.244	-7.6	C-63
DB07054	465.44	8	3	4.569	-7.6	C-63
DB07451	422.25	8	3	4.423	-7.6	C-63
DB15028	461.9	8	1	4.592	-7.6	C-63
DB02052	277.28	5	3	2.93	-7.6	C-63
DB00186	321.16	4	2	2.675	-7.6	C-63
DB01545	360.77	5	1	2.774	-7.6	C-63
DB12680	353.44	5	1	3.952	-7.6	C-63
DB13463	319.4	2	0	4.709	-7.6	C-63
DB07653	345.35	5	2	4.126	-7.6	C-63
DB03987	340.38	8	2	3.005	-7.6	C-63
DB02919	370.41	9	2	3.014	-7.6	C-63
DB07537	366.46	6	3	4.58	-7.6	C-63
DB04751	388.89	7	3	4.379	-7.6	C-63
DB06873	382.41	5	2	1.673	-7.6	C-63
DB00683	325.77	2	0	3.76	-7.6	C-63
DB07168	360.42	7	4	3.891	-7.6	C-63

DB08008	293.25	4	1	3.268	-7.6	C-63
DB13767	324.77	4	0	2.851	-7.6	C-63
DB06625	321.34	6	2	3.165	-7.6	C-63
DB06853	399.53	8	4	3.41	-7.6	C-63
DB06942	378.47	7	3	3.34	-7.6	C-63
DB07143	351.44	7	2	2.893	-7.6	C-63
DB07779	383.46	7	2	3.536	-7.6	C-63
DB14941	454	7	4	3.601	-7.6	C-63
DB07403	478.87	7	2	4.28	-7.6	C-63
DB08961	370.84	7	3	3.695	-7.6	C-63
DB07175	354.43	6	2	4.794	-7.6	C-63
DB11464	300.34	6	2	3.748	-7.6	C-63
DB11967	441.23	6	3	3.475	-7.6	C-63
DB03598	471.57	9	1	4.151	-7.6	C-63
DB02118	372.44	7	0	3.15	-7.6	C-63
DB08213	400.45	8	0	3.162	-7.6	C-63
DB08305	427.58	8	1	3.691	-7.6	C-63
DB11829	468.55	5	1	3.843	-7.6	C-63
DB12191	317.38	2	2	3.923	-7.6	C-63
DB08519	406.44	8	3	4.32	-7.6	C-63
DB02287	253.28	3	4	1.1	-7.6	C-63
DB02288	345.19	2	3	2.609	-7.6	C-63
DB12167	406.48	5	1	3.213	-7.6	C-63
DB04667	354.34	7	3	0.083	-7.6	C-63
DB11732	377.36	5	1	3.287	-7.6	C-63
DB11816	401.43	8	2	3.079	-7.6	C-63
DB12612	404.46	6	2	4.023	-7.6	C-63
DB02001	353.44	7	2	4.009	-7.6	C-63
DB00889	312.41	4	1	2.647	-7.6	C-63
DB12591	432.52	6	1	3.568	-7.6	C-63
DB12579	372.34	4	1	3.861	-7.6	C-63
DB06228	435.88	9	1	3.041	-7.6	C-63
DB12774	465.54	9	1	2.773	-7.6	C-63
DB12092	392.49	5	1	3.413	-7.6	C-63
DB08143	492.93	8	2	3.484	-7.6	C-63
DB07981	428.91	5	2	4.121	-7.6	C-63
DB12459	433.5	6	2	3.011	-7.6	C-63
DB06525	381.47	6	1	4.237	-7.6	C-63
DB01044	375.39	6	2	2.374	-7.6	C-63
DB04576	369.34	5	1	1.702	-7.6	C-63
DB08590	440.45	7	2	4.127	-7.6	C-63
DB01254	488.01	9	3	3.462	-7.6	C-63
DB11818	494.58	8	1	2.244	-7.6	C-63
DB08436	325.37	6	1	3.109	-7.6	C-63
DB07937	446.49	7	1	3.087	-7.6	C-63
DB01029	428.53	6	1	4.151	-7.6	C-63
DB08743	393.44	7	1	1.046	-7.6	C-63

Table S5. Leaders from DrugBank clusters.

		
DB07458 -8.6 kcal/mol	DB09371 -8.5 kcal/mol	DB01977 -8.0 kcal/mol
		
DB08058 -8.0 kcal/mol	DB01852 -7.9 kcal/mol	DB14029 -7.9 kcal/mol
		
DB09268 -7.9 kcal/mol	DB07352 -7.8 kcal/mol	DB08121 -7.8 kcal/mol
		
DB07809 -7.8 kcal/mol	DB07743 -7.8 kcal/mol	DB02398 -7.8 kcal/mol
		
DB13841 -7.8 kcal/mol	DB08639 -7.8 kcal/mol	DB08184 -7.8 kcal/mol
		
DB08883	DB07816	DB07586

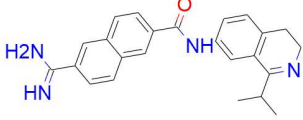
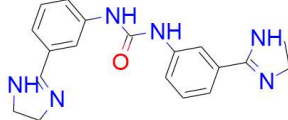
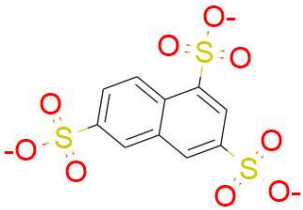
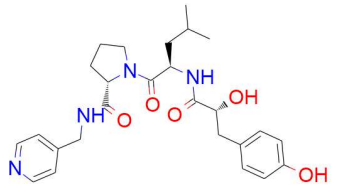
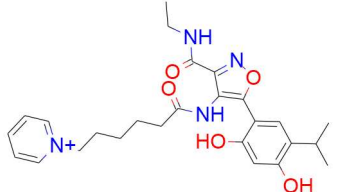
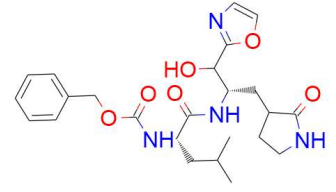
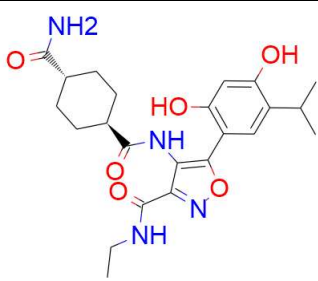
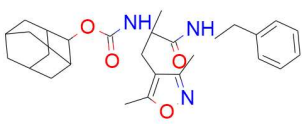
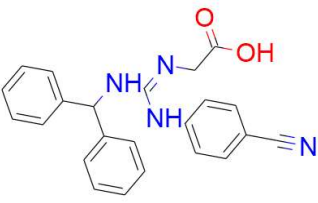
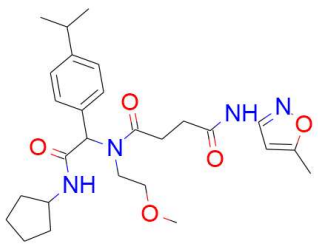
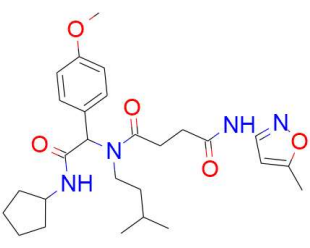
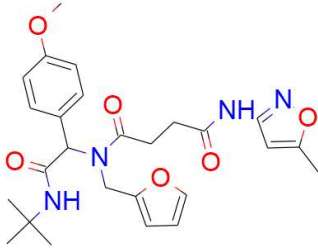
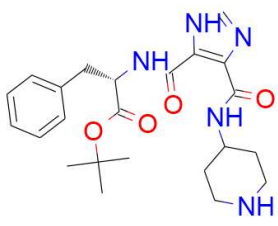
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DB02473 -7.8 kcal/mol	DB11521 -7.8 kcal/mol	DB04409 -7.7 kcal/mol

Table S6. List of non-covalent bindings of SARS-CoV2.

CrystalName	CompoundCode	CompoundSMILES	Deposition_PDB_ID
Mpro-x0072	Z45617795	CS(=O)(=O)NCCC=1C=CC=CC1	5R7Y
Mpro-x0104	Z1220452176	CC(=O)NCCC1=CNC=2C=CC(F)=CC12	5R7Z
Mpro-x0107	Z1129283193	CC(=O)NC=1C=NC=CC1C	5RE4
Mpro-x0161	Z18197050	COC(=O)C=1C=CC(=CC1)S(=O)(=O)N	5R80
Mpro-x0195	Z1367324110	CN1CCCC=2C=CC(=CC12)S(=O)(=O)N	5R81
Mpro-x0305	Z219104216	CCNC=1C=CC(C#N)=CN1	5R82
Mpro-x0354	Z2856434836	CN1CCN(CC1)C(=O)COC=2C=CC(C)=CC2	5RE9
Mpro-x0387	Z2856434899	OC1CCN(CC=2C=CSC2)CC1	5REB
Mpro-x0395	Z1619978933	CC1=NN=C(CN2CCC=C(F)C2)S1	5RGH
Mpro-x0397	Z369936976	CN(CC=1C=C(C)ON1)C(=O)NC2CC2	5RGI
Mpro-x0426	Z1310876699	FC=1C=CC=CC1C(=O)NCCC=2C=CN=CC2	5RGK
Mpro-x0434	Z44592329	O=C(NC=1C=CC=CC1)NC=2C=CC=NC2	5R83
Mpro-x0540	Z111507846	O=C(NCCC=1C=CN=CC1)NC2CCCCC2	5REH
Mpro-x0678	Z31792168	O=C(CC1CCCCC1)NC=2C=CC=NC2	5R84
Mpro-x0874	POB0129	O=C([C@H]1[C@H](C2=CSC=C2)CCC1)N	5REZ
Mpro-x0946	NCL-00023830	BrC1=CC=C(S(N)(=O)=O)C=C1	5RF1
Mpro-x0967	NCL-00024905	CC(=O)NC(Cc1ccc(cc1)O)C(=O)NCC#CBr	5RG1
Mpro-x0991	Z1741969146	Cl.CCC(=N)N	5RF2
Mpro-x0995	Z1741970824	NC=1C=NC=NC1	5RF3
Mpro-x1077	Z1348371854	N#CC=1C=CC(=CN1)N2CCCOCC2	5RF6
Mpro-x1093	Z316425948_minor	CN1CCN(CC1)C(=O)CC1=CNC2=NC=CC=C12	5RF7
Mpro-x1249	Z509756472	O=C(NCC=1C=CC(C#N)=CC1)N2CCOCC2	5RFE

Table S7: 2D structure of the predict inhibitors of SARS-CoV-2 Mpro protein.

		
CHEMBL562054	CHEMBL4300783	CHEMBL2047011

-8.4 kcal/mol 9 I. I.	-8.3 kcal/mol 9 I. I.	-8.1 kcal/mol 9 I. I.
		
CHEMBL1940937 -9.1 kcal/mol 8 I. I.	CHEMBL64623 -8.3 kcal/mol 8 I. I.	DB07816 -7.8 kcal/mol 8 I. I.
		
CHEMBL1383217 -8.1 kcal/mol 8 I. I.	CHEMBL1866805 -8.0 kcal/mol 8 I. I.	CHEMBL1392860 -7.7 kcal/mol 8 I. I.
		
	CHEMBL1740647 -7.7 kcal/mol 7 I. I.	