

## **Peptide-like and small-molecule inhibitors against Covid-19**

Suyash Pant<sup>1</sup>, Meenakshi Singh<sup>1</sup>, V. Ravichandiran<sup>1</sup>, USN Murty<sup>2</sup>, Hemant Kumar  
Srivastava<sup>2\*</sup>

<sup>1</sup>National Institute of Pharmaceutical Education and Research Kolkata Kolkata-700054, West  
Bengal, India

<sup>2</sup>National Institute of Pharmaceutical Education and Research Guwahati, Guwahati-781039,  
Assam, India, Email: hemantkrsri@gmail.com

**Table S1:** 300 selected compounds based on docking and MM-GBSA calculations

<b>IDs</b>	<b>Score</b>	<b>emodel</b>	<b><math>\Delta G</math> bind</b>	<b>IDs</b>	<b>Score</b>	<b>emodel</b>	<b><math>\Delta G</math> bind</b>
6Y2F#	-12.20	-152.88	-84.48	ZINC14121618	-6.57	-67.21	-69.95
<b>C-1</b>	-11.02	-120.87	-104.89	CHEMBL3287610	-6.57	-84.43	-83.88
<b>C-2</b>	-9.58	-111.13	-89.08	ZINC17666408	-6.55	-90.82	-51.83
ZINC06668537	-9.50	-81.46	-85.95	CHEMBL480373	-6.55	-75.12	-72.46
<b>C-3</b>	-9.28	-98.78	-77.63	ZINC09465822	-6.55	-85.56	-76.82
ZINC05225437	-9.16	-93.83	-83.46	ZINC02801267	-6.54	-68.59	-38.62
ZINC09601385	-9.10	-93.22	-74.55	ZINC25047376	-6.54	-78.53	-70.11
CHEMBL152104	-9.09	-73.20	-78.03	ZINC11841973	-6.53	-77.90	-75.18
ZINC09797971	-8.89	-78.47	-64.31	ZINC33069086	-6.52	-75.04	-71.93
ZINC01031116	-8.84	-70.63	-57.98	ZINC14198502	-6.51	-73.12	-67.89
CHEMBL573507	-8.72	-110.18	-84.79	CHEMBL2028925	-6.51	-70.88	-72.80
CHEMBL2371798	-8.72	-88.83	-85.65	ZINC08710172	-6.51	-71.47	-63.67
<b>C-4</b>	-8.72	-93.67	-93.55	ZINC01060126	-6.51	-71.40	-72.91
ZINC00702508	-8.66	-87.40	-78.12	CHEMBL2376358	-6.50	-77.69	-80.27
CHEMBL207579	-8.56	-111.34	-76.61	ZINC30585960	-6.49	-75.30	-65.17
CHEMBL422440	-8.40	-103.04	-77.02	CHEMBL423112	-6.48	-68.85	-82.37
ZINC08926270	-8.21	-70.64	-85.44	ZINC12630368	-6.48	-71.30	-61.96
ZINC01108942	-8.20	-83.66	-61.22	ZINC06457619	-6.47	-67.62	-63.35
ZINC07238596	-8.16	-90.99	-71.00	ZINC04583765	-6.46	-69.95	-63.28
CHEMBL40589	-8.09	-94.85	-73.47	CHEMBL133803	-6.45	-102.82	-75.55
ZINC12053378	-8.05	-88.25	-81.30	ZINC12615632	-6.44	-59.98	-62.73
ZINC29975718	-8.02	-78.69	-56.88	ZINC21027072	-6.43	-82.36	-57.91
ZINC32929983	-7.97	-82.35	-76.11	ZINC01441524	-6.42	-68.73	-62.75
ZINC03243503	-7.91	-76.36	-66.77	ZINC12041166	-6.42	-64.60	-67.82
ZINC09006550	-7.90	-83.78	-50.77	CHEMBL26285	-6.42	-89.34	-67.88
CHEMBL2396925	-7.89	-95.00	-64.06	ZINC15863650	-6.42	-84.23	-80.64
ZINC11166391	-7.82	-93.09	-69.80	ZINC33539555	-6.41	-72.67	-65.76
ZINC23566409	-7.82	-84.34	-82.08	ZINC03143209	-6.41	-84.46	-77.66
ZINC09934205	-7.82	-93.45	-67.24	ZINC08542354	-6.40	-68.54	-84.74
ZINC09343712	-7.80	-78.32	-70.81	ZINC20745863	-6.39	-80.73	-71.28
ZINC11909002	-7.75	-94.64	-73.56	ZINC04196517	-6.37	-76.61	-50.70
ZINC15532605	-7.74	-79.87	-73.83	ZINC04857894	-6.36	-78.18	-72.51
ZINC13127908	-7.72	-97.78	-62.45	ZINC26687775	-6.36	-68.64	-68.35
ZINC26538087	-7.69	-89.68	-66.28	ZINC02462362	-6.33	-65.30	-70.84
ZINC10912500	-7.69	-91.05	-84.75	CHEMBL285306	-6.33	-81.65	-65.70
ZINC09934141	-7.68	-76.72	-77.00	ZINC08927286	-6.32	-83.23	-64.60
ZINC03192567	-7.67	-89.71	-70.62	ZINC02941457	-6.30	-68.93	-44.73
ZINC09934209	-7.66	-105.46	-111.29	ZINC25056522	-6.30	-79.42	-71.76
ZINC14732819	-7.57	-75.20	-65.42	ZINC09645121	-6.29	-76.59	-67.94
ZINC09934211	-7.57	-97.07	-87.67	ZINC07445512	-6.28	-76.54	-65.43
CHEMBL158806	-7.57	-88.30	-48.88	ZINC03280022	-6.28	-71.03	-65.85

<b>IDs</b>	<b>Score</b>	<b>emodel</b>	<b><math>\Delta G</math> bind</b>	<b>IDs</b>	<b>Score</b>	<b>emodel</b>	<b><math>\Delta G</math> bind</b>
ZINC09426173	-7.56	-85.01	-65.86	ZINC36049348	-6.26	-87.85	-62.16
ZINC09415205	-7.55	-84.24	-61.84	ZINC09659683	-6.26	-91.26	-70.82
CHEMBL284545	-7.54	-96.49	-88.31	ZINC20734697	-6.26	-86.11	-83.19
CHEMBL130438	-7.54	-83.78	-73.47	ZINC12442116	-6.25	-79.16	-59.23
ZINC03350001	-7.52	-83.40	-73.92	ZINC09957892	-6.25	-93.41	-86.52
ZINC34797125	-7.48	-83.53	-73.49	ZINC00629693	-6.22	-79.73	-62.54
ZINC30731789	-7.47	-78.55	-68.65	ZINC15072856	-6.22	-80.41	-71.10
ZINC04373506	-7.45	-67.70	-54.72	ZINC03374620	-6.22	-66.74	-59.34
CHEMBL93357	-7.44	-105.41	-89.89	ZINC30479921	-6.21	-71.37	-51.86
ZINC12448605	-7.44	-82.47	-49.35	ZINC12714597	-6.20	-68.18	-62.30
CHEMBL303024	-7.43	-72.69	-68.33	ZINC01299293	-6.18	-76.57	-68.92
ZINC02648195	-7.42	-79.70	-79.65	ZINC09112465	-6.18	-68.12	-51.72
ZINC29132087	-7.39	-81.57	-57.11	ZINC32481659	-6.17	-71.20	-56.88
ZINC20744850	-7.39	-87.74	-52.03	ZINC36009996	-6.17	-88.80	-62.18
ZINC30765985	-7.38	-68.81	-85.58	CHEMBL392031	-6.16	-74.59	-51.46
ZINC15108667	-7.38	-94.96	-67.68	ZINC25194263	-6.16	-81.94	-87.37
ZINC14979914	-7.35	-83.86	-73.59	ZINC29895751	-6.15	-78.02	-57.68
ZINC25249923	-7.34	-69.36	-65.72	ZINC33263659	-6.15	-94.45	-75.30
ZINC08867239	-7.34	-94.83	-63.73	ZINC09954459	-6.15	-70.34	-74.88
CHEMBL466151	-7.34	-84.81	-62.58	ZINC33025957	-6.13	-78.70	-60.56
ZINC03584015	-7.33	-71.84	-61.80	ZINC09008513	-6.12	-74.78	-50.50
ZINC18271366	-7.33	-72.46	-68.68	ZINC36061077	-6.12	-81.31	-74.50
CHEMBL134131	-7.33	-99.85	-81.15	ZINC01157055	-6.11	-75.98	-83.95
ZINC08443457	-7.32	-84.86	-77.05	ZINC08876900	-6.11	-81.16	-91.52
ZINC09561809	-7.31	-83.42	-77.00	ZINC33025952	-6.11	-77.30	-89.75
ZINC12478562	-7.29	-84.18	-62.43	ZINC09601385	-6.08	-87.73	-69.31
CHEMBL424947	-7.28	-65.94	-78.16	ZINC13324026	-6.08	-58.80	-47.95
ZINC13785210	-7.23	-91.20	-73.16	ZINC33025943	-6.08	-77.45	-68.55
ZINC33067904	-7.23	-81.35	-79.19	ZINC12146437	-6.08	-72.20	-64.42
ZINC13693037	-7.23	-71.98	-52.92	ZINC04710424	-6.07	-73.41	-85.25
ZINC04520633	-7.22	-74.59	-74.57	ZINC09418846	-6.07	-82.83	-69.54
ZINC12728884	-7.19	-77.22	-77.80	ZINC13000310	-6.06	-94.25	-91.98
ZINC09934282	-7.19	-92.04	-90.81	ZINC20729810	-6.06	-79.47	-62.94
CHEMBL315390	-7.18	-99.97	-79.65	ZINC22313846	-6.06	-69.40	-67.37
ZINC29895854	-7.18	-79.22	-64.59	ZINC08194046	-6.03	-83.00	-67.80
ZINC11663735	-7.17	-65.79	-72.76	ZINC33321018	-6.03	-84.65	-87.29
ZINC16840308	-7.17	-84.25	-84.96	ZINC01061058	-6.03	-81.94	-56.15
ZINC01442374	-7.17	-76.53	-77.74	ZINC12445469	-6.03	-73.23	-80.99
ZINC12433690	-7.15	-65.96	-57.22	ZINC04561360	-6.03	-79.84	-80.84
ZINC24734228	-7.14	-96.14	-75.15	ZINC22868152	-6.03	-78.07	-70.00
CHEMBL346361	-7.14	-80.01	-80.61	ZINC06669611	-6.01	-90.14	-70.81
ZINC08880548	-7.14	-81.14	-47.72	ZINC10912495	-6.01	-79.07	-87.54
ZINC08867240	-7.14	-90.88	-77.28	ZINC09484494	-6.00	-56.80	-62.53

<b>IDs</b>	<b>Score</b>	<b>emodel</b>	<b><math>\Delta G</math> bind</b>	<b>IDs</b>	<b>Score</b>	<b>emodel</b>	<b><math>\Delta G</math> bind</b>
ZINC12420683	-7.12	-73.80	-80.43	CHEMBL2178188	-5.99	-89.66	-78.95
ZINC14732740	-7.12	-65.05	-53.78	ZINC03391962	-5.98	-79.90	-62.23
ZINC29895846	-7.10	-75.99	-75.08	ZINC21038013	-5.97	-85.67	-73.02
ZINC22193334	-7.09	-91.82	-66.66	ZINC08767983	-5.96	-81.45	-78.31
ZINC11791082	-7.09	-89.29	-76.88	ZINC01878170	-5.96	-62.82	-45.65
ZINC09969857	-7.07	-96.67	-81.97	ZINC12150921	-5.95	-86.62	-69.29
CHEMBL2028917	-7.07	-72.24	-71.22	ZINC03144139	-5.95	-88.35	-90.08
CHEMBL26286	-7.06	-87.65	-57.76	ZINC33012857	-5.95	-75.57	-85.95
ZINC29130815	-7.06	-68.77	-69.51	ZINC33291900	-5.94	-90.40	-76.61
ZINC04866918	-7.03	-69.11	-68.64	CHEMBL3288163	-5.94	-67.88	-74.73
ZINC12438679	-7.03	-82.62	-86.31	ZINC05387788	-5.93	-63.22	-62.65
ZINC09586630	-7.02	-79.73	-63.66	ZINC12404176	-5.93	-63.21	-77.33
ZINC20720647	-7.01	-84.15	-69.30	ZINC08612270	-5.93	-90.24	-87.95
ZINC31409555	-7.00	-80.24	-69.76	ZINC12152825	-5.92	-78.02	-81.43
ZINC27538983	-6.98	-81.35	-70.70	ZINC05387787	-5.90	-69.15	-66.46
ZINC12147439	-6.97	-64.74	-62.03	ZINC08816065	-5.90	-74.01	-97.90
ZINC03145822	-6.96	-72.78	-56.57	ZINC05380960	-5.88	-56.16	-51.41
ZINC12784896	-6.96	-71.81	-76.22	ZINC02872512	-5.88	-54.83	-46.33
ZINC15634716	-6.96	-65.69	-65.22	ZINC09318607	-5.87	-65.02	-67.80
ZINC08790010	-6.95	-74.90	-69.58	CHEMBL206482	-5.86	-102.32	-61.59
ZINC33263658	-6.95	-100.48	-85.03	ZINC09057552	-5.86	-83.02	-40.92
ZINC09001590	-6.95	-81.57	-77.74	ZINC20732018	-5.84	-77.54	-63.49
ZINC00720157	-6.95	-82.00	-59.07	ZINC29895846	-5.83	-81.57	-57.85
CHEMBL442612	-6.94	-92.71	-52.53	ZINC14533959	-5.83	-80.41	-80.41
ZINC08704911	-6.93	-80.36	-65.44	ZINC21640961	-5.83	-60.54	-57.49
ZINC27538985	-6.90	-73.79	-76.47	ZINC09152779	-5.81	-70.37	-59.93
ZINC05250880	-6.89	-74.49	-58.81	ZINC25194255	-5.80	-81.61	-80.91
ZINC18092155	-6.88	-69.57	-49.72	ZINC03000060	-5.80	-71.77	-58.07
ZINC00678096	-6.87	-91.41	-60.81	CHEMBL285585	-5.79	-95.51	-60.91
ZINC02721017	-6.87	-64.49	-39.83	ZINC36086055	-5.78	-74.76	-70.08
ZINC09128597	-6.87	-79.46	-76.72	ZINC09409939	-5.78	-79.10	-86.93
CHEMBL196990	-6.87	-96.77	-71.32	ZINC03257715	-5.78	-73.60	-56.68
ZINC01442373	-6.86	-77.72	-82.16	ZINC03558194	-5.77	-86.53	-69.09
ZINC27538980	-6.86	-84.10	-68.24	ZINC02228025	-5.77	-66.14	-65.44
ZINC11820489	-6.85	-80.03	-73.82	ZINC10616133	-5.76	-60.01	-72.25
ZINC23485296	-6.84	-84.15	-91.45	ZINC33025903	-5.76	-74.62	-78.22
ZINC13022096	-6.83	-67.59	-80.25	ZINC09485226	-5.75	-80.72	-81.20
ZINC08583708	-6.82	-91.49	-65.25	ZINC15084955	-5.72	-77.55	-58.66
ZINC09934213	-6.82	-92.53	-72.74	ZINC30903371	-5.71	-67.38	-52.21
ZINC12370971	-6.81	-75.15	-76.88	ZINC01077780	-5.69	-76.01	-62.38
CHEMBL2371797	-6.81	-95.61	-90.41	ZINC03058214	-5.69	-74.15	-64.06
ZINC21649976	-6.80	-85.59	-63.58	CHEMBL1230065	-5.68	-84.95	-70.76
ZINC27663088	-6.80	-76.32	-77.23	ZINC12252277	-5.68	-74.79	-59.19

IDs	Score	emodel	$\Delta G$ bind	IDs	Score	emodel	$\Delta G$ bind
ZINC26889990	-6.80	-74.30	-66.45	ZINC06142224	-5.68	-84.62	-59.93
ZINC09664063	-6.80	-72.50	-65.43	ZINC00960048	-5.67	-72.76	-65.37
ZINC13027874	-6.79	-90.37	-67.51	ZINC15679848	-5.67	-65.57	-66.92
ZINC03626921	-6.77	-72.88	-53.45	ZINC09262267	-5.67	-83.13	-53.86
ZINC33057728	-6.77	-82.62	-64.47	ZINC32724155	-5.66	-73.95	-54.52
ZINC20574379	-6.76	-82.75	-62.68	ZINC09877598	-5.66	-79.33	-58.22
ZINC08583708	-6.75	-86.93	-69.00	ZINC12686569	-5.66	-73.17	-90.02
ZINC34831394	-6.74	-81.27	-89.44	ZINC09031542	-5.65	-65.51	-44.88
ZINC09224066	-6.73	-83.41	-63.19	ZINC12712423	-5.63	-71.48	-64.13
ZINC05526887	-6.70	-65.89	-57.94	ZINC12035928	-5.61	-75.10	-46.34
CHEMBL204540	-6.69	-71.37	-66.06	ZINC15767769	-5.59	-69.36	-64.52
ZINC08662068	-6.68	-84.18	-61.86	ZINC16993657	-5.57	-72.66	-52.37
ZINC09883605	-6.67	-85.16	-59.90	CHEMBL561734	-5.55	-74.24	-64.54
ZINC17598974	-6.67	-80.57	-56.35	ZINC35354266	-5.54	-70.93	-51.18
ZINC09598771	-6.66	-75.75	-60.56	ZINC11162302	-5.54	-90.72	-52.59
ZINC11614597	-6.66	-70.83	-64.22	ZINC08856275	-5.53	-72.12	-77.56
ZINC21037410	-6.66	-83.47	-69.40	ZINC01432842	-5.53	-66.54	-49.37
ZINC21639175	-6.65	-87.92	-67.90	ZINC19696231	-5.52	-68.58	-51.22
ZINC06809320	-6.64	-54.96	-57.25	ZINC20095139	-5.51	-81.94	-70.27
ZINC34789480	-6.61	-81.15	-89.53	ZINC01059896	-5.50	-69.31	-76.79
ZINC09442002	-6.60	-101.65	-62.15	ZINC32641706	-5.49	-72.33	-80.39
ZINC32643347	-6.58	-69.78	-66.60	ZINC32645018	-5.48	-70.74	-74.30
ZINC32929984	-6.58	-79.46	-67.86	ZINC12314057	-5.46	-68.79	-60.91

#Co-crystalized ligand of PDB-ID 6Y2F

CHEMBL shows compounds selected from CHEMBL database

ZINC shows compounds selected from ZINC15 database

IDs are compound IDs from databases

The score is the glide docking score

emodel is the glide emodel score

$\Delta G$ -bind is MM-GBSA based binding free energy

**C-1:** CHEMBL206650; **C-2:** CHEMBL303543; **C-3:** CHEMBL127888; **C-4:** CHEMBL573507 (these four compounds were selected for MD simulations)

**Table S2:** Name of FDA selected approved drugs for repurposing against Covid-19

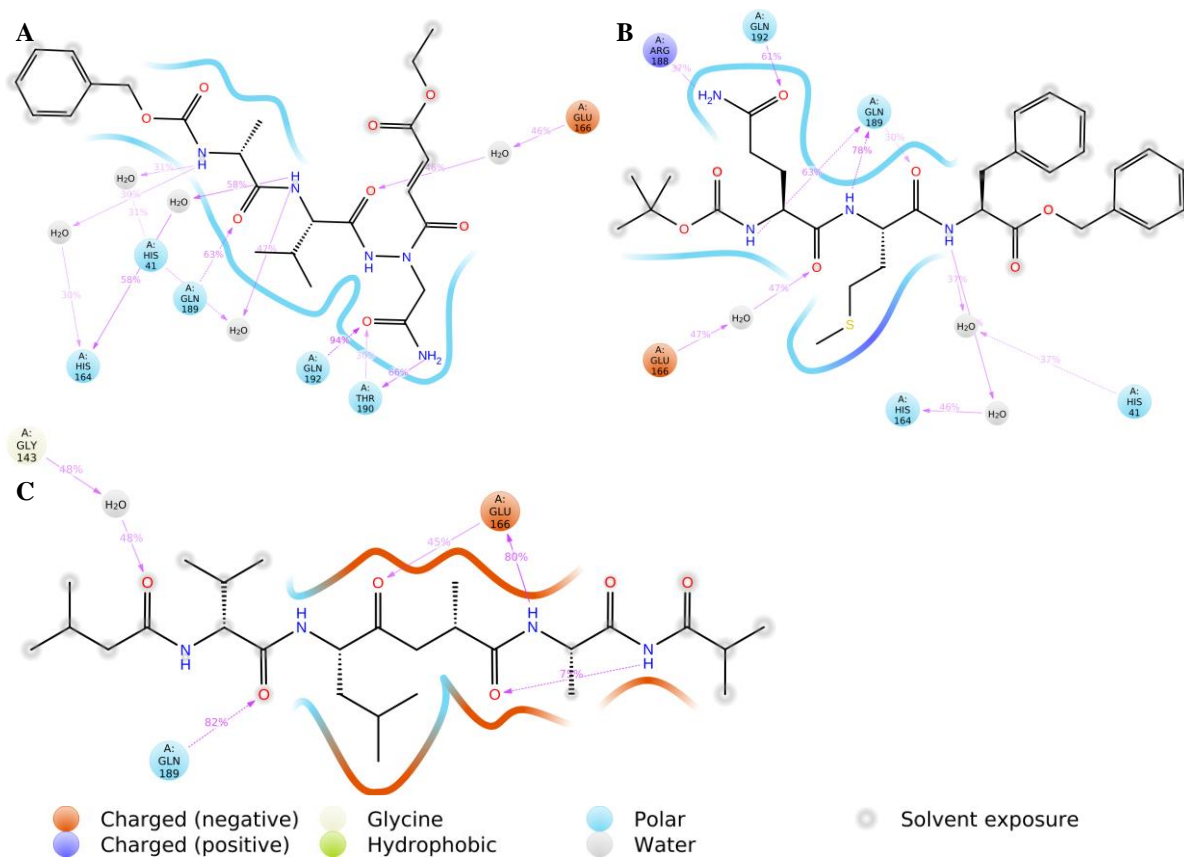
IDs	Score	emodel	$\Delta G$ bind	IDs	Score	emodel	$\Delta G$ bind
6W63 <sup>#</sup>	-5.99	-58.64	-52.57	Abacavir	-6.56	-51.49	-44.95
Cobicistat	-9.35	-107.34	-80.01	Betaxolol	-6.56	-57.50	-63.01
Oxytocin	-9.29	-74.72	-68.29	Pitavastatin	-6.56	-55.61	-40.79
Ritonavir	-8.88	-106.65	-67.65	Chlorthalidone	-6.56	-63.55	-38.58
Teniposide	-8.43	-46.10	-54.79	Ruxolitinib	-6.53	-51.11	-42.56
Lopinavir	-8.36	-86.41	-73.33	Apixaban	-6.52	-66.20	-60.40
Dobutamine	-8.15	-60.50	-62.66	Avanafil	-6.47	-71.64	-54.42
Nelfinavir mesylate	-8.13	-80.50	-77.12	Apicidine	-6.39	-68.28	-55.56
Formoterol	-8.05	-66.82	-64.27	Zileuton	-6.35	-46.86	-38.20
Pentagastrin	-8.04	-90.84	-73.95	Lorazepam	-6.34	-51.40	-44.25
Latanoprost	-7.82	-63.81	-57.43	Lacosamide	-6.32	-52.30	-40.12
Octreotide acetate	-7.79	-77.15	-60.41	Cefuroxime	-6.29	-53.34	-34.59
Pravastatin sodium	-7.74	-54.54	-39.18	Levorphanol	-6.29	-39.12	-53.29
Cangrelor	-7.72	-81.40	-51.27	Mebendazole	-6.18	-62.52	-58.10
Protirelin	-7.70	-77.40	-57.95	Amlodipine	-6.18	-53.53	-51.72
Fluvastatin	-7.35	-56.40	-41.43	Trandolapril	-6.15	-59.10	-32.16
Ipratropium bromide	-7.34	-53.77	-55.03	Estradiol	-6.12	-47.15	-45.18
Darunavir	-7.21	-69.20	-64.49	Cephalexin	-6.11	-52.26	-40.52
Carfilzomib	-7.20	-85.26	-79.74	Rotigotine	-6.09	-49.33	-57.93
Hydroxyzine pamoate	-7.08	-57.43	-33.62	Testosterone	-6.00	-49.41	-47.07
Dipyridamole	-7.07	-60.39	-72.81	Fenofibrate	-5.99	-52.18	-35.63
Pergolide mesylate	-7.06	-67.70	-68.79	Mesoridazine	-5.99	-59.15	-63.10
Podofilox	-6.99	-59.11	-69.97	Temazepam	-5.94	-47.74	-38.06
Saquinavir	-6.98	-89.99	-72.08	Levallorphan	-5.93	-40.84	-45.79
Labetalol	-6.96	-58.30	-39.02	Nimodipine	-5.67	-73.60	-68.42
Fluvoxamine maleate	-6.94	-49.20	-53.58	Lisinopril	-5.64	-59.20	-36.54
Enalapril maleate	-6.83	-57.19	-41.72	Cephadrine	-5.64	-53.22	-38.04
Pyruvium pamoate	-6.83	-58.25	-33.91	Olopatadine	-5.61	-50.72	-38.26
Cabergoline	-6.71	-76.53	-71.46	Boceprevir	-5.59	-52.48	-65.46
Epirubicin	-6.67	-68.46	-70.85	Zaleplon	-5.59	-50.55	-47.66
Etidocaine	-6.66	-52.09	-50.14	Metolazone	-5.56	-60.21	-56.25
Fluorometholone	-6.64	-57.71	-50.77	Lansoprazole	-5.42	-54.46	-48.22
Ascorbic acid	-6.63	-33.92	-30.52	Moexipril	-5.41	-55.33	-45.59

<sup>#</sup>Co-crystallized ligand of PDB-ID 6W63

The score is the glide docking score

emodel is the glide emodel score

$\Delta G$ -bind is MM-GBSA based binding free energy



**Figure S1:** Hydrogen bond interaction network during 20ns of molecular dynamics simulations for C-2 (A), C-3 (B), and C-4 (C).

C-2: CHEMBL303543; C-3: CHEMBL127888; C-4: CHEMBL573507