

Supplementary Data

Natural products as inhibitors of COVID-19 main protease–A virtual screening by molecular docking

**Marzieh Omrani^{1#}, Mohammad Bayati^{1#}, Parvaneh Mehrbod^{2*}, Kamal Asmari Bardazard¹,
Samad**

Nejad-Ebrahimi^{1*}

¹Department of Phytochemistry, Medicinal Plants and Drugs Research Institute, Shahid Beheshti University, Tehran, Iran.

²Influenza and Respiratory Viruses Department, Pasteur Institute of Iran, Tehran, Iran.

Table S1. The Representing Glide docking and IFD scores with ADME screening results.

No.	Compound	docking score (kcal/mol)	Glide gscore (kcal/mol)	IFD Score (kcal/mol)	ΔG_{bind} (kcal/mol)	PSA	MW	Donor HB	Accept HB	QP Log Po/w	%Oral abs.	CNS
NP-1	ZINC03839114	-11.132	-11.132	-674.28	-51.9	149.6	462.45	3	9.5	1.032	64.756	-2
NP-2	ZINC03841676	-11.068	-11.072	-673.56	-53.07	71.2	394.51	2	6.45	3.854	100	-1
NP-3	ZINC96114284	-10.743	-10.752	-669.73	-37.3	131.4	404.37	1	7	2.537	75.723	-2
NP-4	ZINC98364422	-10.315	-10.317	-669.05	-46.14	104.2	384.39	1	10	1.917	87.351	-1
NP-5	Lonchocarpol A	-10.234	-10.234	-670.01	-39.96	91.7	408.49	2	4	4.845	100	-2
NP-6	ZINC77257242	-10.102	-10.279	-666.89	-36.9	143.2	316.26	2	6.7	0.552	58.759	-2
NP-7	Norkurarinone	-9.91	-9.91	-670.69	-18.92	113.5	424.49	3	4.75	4.199	90.687	-2
NP-8	ZINC72321780	-9.516	-9.516	-669.24	-47.65	96.3	423.38	3	7.4	3.736	100	-1
NP-9	(-)-Catechin	-9.444	-9.444	-668.69	-37.36	116.8	290.27	5	5.45	0.448	59.967	-2
NP-10	Altoxin I	-9.429	-9.429	-664.92	-66.04	133.3	352.34	2	5.95	1.369	66.233	-2
NP-11	ZINC72321775	-9.356	-9.356	-668.71	-47.28	75.9	379.37	3	5.9	3.527	100	-1
NP-12	ZINC35458935	-9.309	-9.349	-667.36	-42.9	148.8	428.39	3	7.65	1.891	72.908	-2
NP-13	ZINC00719192	-9.285	-9.285	-667.72	-38.45	114.5	482.41	1	7.25	4.416	100	-1
NP-14	ZINC72321774	-9.22	-9.22	-667.92	-40.03	89.2	395.37	3	6.65	2.982	89.497	-1
NP-15	ZINC31158868	-9.114	-9.115	-668.84	-41.22	121.9	291.30	3	7.7	1.073	56.981	-2
NP-16	ZINC09033965	-9.069	-9.069	-669.16	-46.67	99.7	433.23	1	8.5	1.621	81.002	-1
NP-17	ZINC02109515	-8.702	-8.86	-669.36	-41.79	75.5	360.33	3	3.5	1.854	65.671	-1
NP-18	ZINC15120609	-8.243	-8.243	-667.9	-37.92	95.5	372.41	2	6.2	3.482	100	-2
NP-19	Isoboldine	-8.049	-8.049	-667.29	-45.22	113.5	424.49	3	4.75	4.199	90.687	-2
NP-20	ZINC08765174	-11.488	-11.488	-673.42	-27.54	74.1	431.57	2	5.5	4.804	100	-1
NP-21	Peramivir	-9.763	-9.763	-670.26	-39.74	113.5	424.49	3	4.75	4.199	90.687	-2
NP-22	Laninamivir	-8.513	-8.513	-671.07	-33.73	113.5	424.49	3	4.75	4.199	90.687	-2
NP-23	Hydroxychloroqui	-7.407	-7.407	-669.57	-39.41	113.5	424.49	3	4.75	4.199	90.687	-2
NP-24	Baloxavir	-7.194	-7.194	-663.34	-40.53	113.5	424.49	3	4.75	4.199	90.687	-2
NP-25	ZINC02130336	-10.58	-10.58	-673.7	-24.1	158.2	464.47	3.25	7.75	2.619	58.193	-2
NP-26	ZINC03869768	-10.324	-10.356	-668.52	-25.91	121.7	286.24	3	4.5	1.035	63.6	-2
NP-27	ZINC03869685	-9.865	-9.897	-668.89	-22.44	143.4	302.24	4	5.25	0.36	51.6	-2

No.	Compound	docking score (kcal/mol)	Glide gscore (kcal/mol)	IFD Score (kcal/mol)	ΔG_{bind} (kcal/mol)	PSA	MW	Donor HB	Accept HB	QP Log Po/w	%Oral abs.	CNS
NP-28	ZINC02138353	-9.545	-9.552	-672.82	-31.88	153.2	448.47	3.25	7.25	3.269	70.889	-2
NP-29	ZINC04098363	-9.504	-9.51	-668.66	-34.78	96.2	340.37	2	4	3.446	91.478	-2
NP-30	ZINC02120464	-9.408	-9.409	-669.98	-26.77	103.8	415.44	1	5.25	4.769	100	-2
NP-31	ZINC09043311	-9.376	-9.429	-670.7	-44.68	78.7	476.61	1	7	4.541	86.791	1
NP-32	ZINC14694365	-9.239	-9.239	-668.78	-31.06	102.2	362.42	4	6.4	2.394	81.199	-2
NP-33	ZINC72321821	-9.17	-9.17	-670.21	-31.56	100	396.36	3	7.65	2.485	85.763	-1
NP-34	ZINC98363648	-9.139	-9.179	-671.53	-32.78	177	376.36	5	9.75	-1.261	27.23	-2
NP-35	ZINC00066182	-8.873	-8.904	-667.14	-27.68	144.4	298.25	2.25	6.25	0.832	61.028	-2
NP-36	ZINC96116208	-8.727	-8.744	-669.31	-53.73	72.6	362.42	1	5.5	3.57	91.49	1
NP-37	ZINC13340416	-8.599	-8.599	-667.18	-27.16	68.43	326.34	2	5.4	2.874	100	0
NP-38	ZINC12603962	-8.047	-8.05	-664.48	-44.71	114.9	266.29	5	8.6	-0.537	52.442	-2
NP-39	ZINC00518554	-7.819	-7.819	-665.74	-27.68	124.8	272.25	5	10	-1.047	53.883	-2
NP-40	ZINC00898438	-7.695	-7.695	-666.67	-29.87	113.5	424.49	3	4.75	4.199	90.687	-2

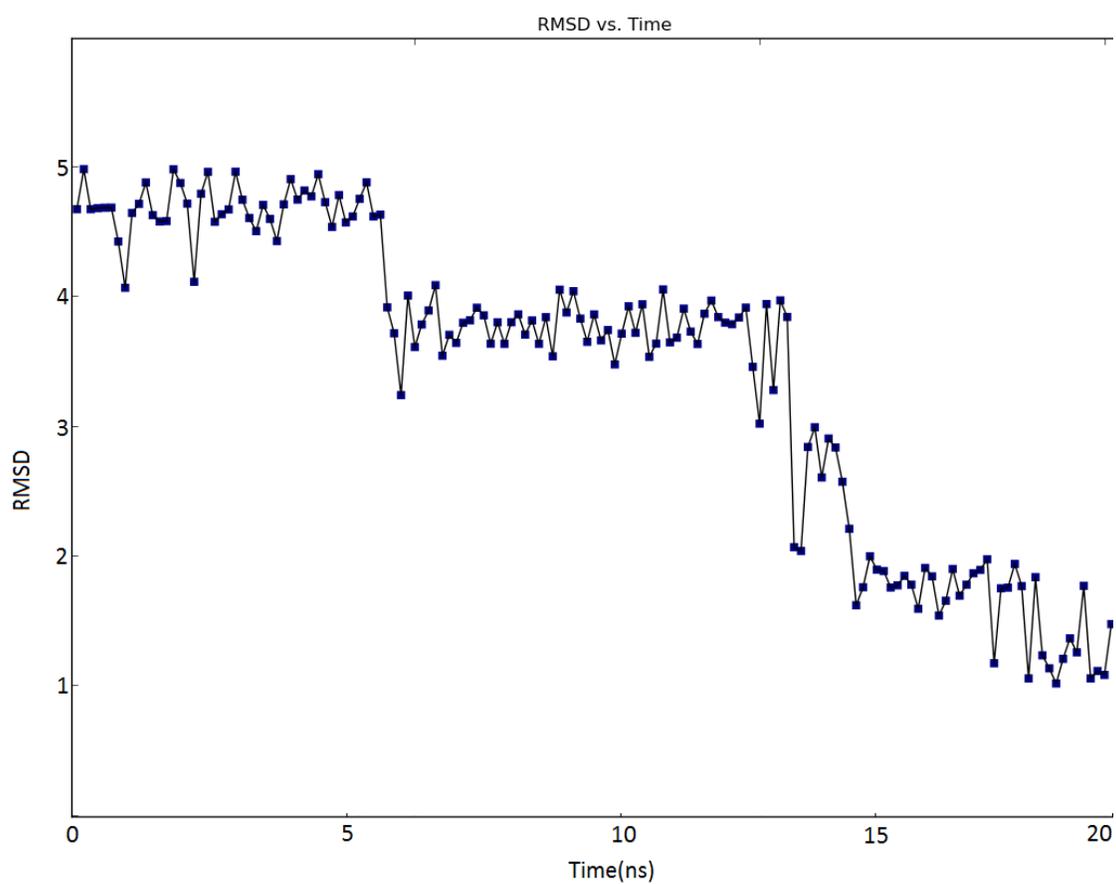


Figure S1. The RMSD versus time plot during the 20 ns molecular dynamics simulation for NP-20