

Supplementary Table on

Pharmacophore-based virtual screening, quantum mechanics calculations, and molecular dynamics simulation approaches identified potential natural antiviral drug candidates against MERS-CoV S1-NTD.

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Table S1: A list of 32 compounds generated as hits during pharmacophore based virtual screening process with there geometric fit score, conformation number and binding affinity (kcal/mol) with desire protein.

Compound Name	Pharmacophore Fit Score	Number of conformations	Binding Affinity
Amb6600135	66.6	25	-9.2
Amb23604132	65.48	25	-9.1
Amb23604659	65.55	25	-8.6
Amb1153724	66.64	25	-8.1
Amb24326239	67.57	25	-8.0
Amb22172700	67.12	12	-7.7
Amb22407028	67.12	8	-7.7
Amb19746939	67.51	25	-7.6
Amb24326238	66.88	25	-7.6
Amb28533232	65.46	25	-7.6
Amb21855756	66.6	25	-7.5
Amb22407027	67.12	14	-7.5
Amb22735040	66.88	25	-7.5
Amb22800823	66.21	25	-7.5
Amb29085648	66	16	-7.5
Amb22888458	66.84	25	-7.4
Amb29085659	67.1	25	-7.4
Amb29085660	66.85	25	-7.4
Amb22584586	66.83	25	-7.3
Amb18003253	66.77	25	-7.2
Amb29085723	66.83	25	-7.2
Amb19886350	67.46	25	-7.1
Amb19893465	66.38	25	-7.1
Amb24323825	66.81	25	-7.1
Amb28532929	66.59	25	-7.1
Amb29085710	67.75	25	-7.1
Amb19928430	65.71	9	-6.9
Amb22584350	66.54	25	-6.9
Amb22888476	66.95	25	-6.9
Amb22896309	66.27	25	-6.7
Amb8514723	66.58	25	-6.6
Amb22584735	66.63	25	-6.4

Table S2: List of HOMO, LUMO, HOMO-LUMO gap, softness and hardness of the selected three compound.

Compound Name	HOMO (a.u)	LUMO (a.u)	Area (HOMO)	Area (LUMO)	HLG (a.u)	Softness	Hardness	Iso-value
Amb1153724	-0.207	-0.0425	70.947	62.03	0.1645	0.0822	12.157	-0.05
Amb23604132	-0.211	-0.079	107.067	85.507	0.1326	0.0663	15.084	-0.05
Amb23604659	-0.217	-0.057	120.442	58.779	0.1601	0.0801	12.488	-0.05

Table S3: List of MM/GBSA component and their energy with standard error value of the selected three compound.

Compound Name	ΔG Bind	ΔG Bind Coulomb	ΔG Bind Covalent	ΔG Bind Hbond	ΔG Bind Lipo	ΔG Bind Packing	ΔG Bind Solv GB	ΔG Bind vdW
Amb1153724	-32.47 \pm 6	-22.45 \pm 4	2.5 \pm 1	-2.08 \pm 1	-7.51 \pm 3	-6.91 \pm 2	16.2 \pm 4	-14.22 \pm 4
Amb23604132	-24.75 \pm 4	-12.25 \pm 5	1.41 \pm .5	-1.01 \pm .6	-7.28 \pm 2	-9.79 \pm 3	16.28 \pm 5	-10.3 \pm 3
Amb23604659	-26.18 \pm 5	-6.43 \pm 4	1.7 \pm .6	-1.04 \pm .5	-5.4 \pm 3	-5.86 \pm 1	10.03 \pm 3	-17.78 \pm 7