

## Supplementary Tables

## Supplementary 1. Binding affinity of spike glycoprotein-ligands

PubChem ID	Ligand	Binding Affinity (kcal/mol)
91472	Friedelin	-8.5
73170	alpha-Amyrin	-8.4
3034659	Pseudotaraxasterol	-8.3
6436598	Lantadene A	-8.3
633072	Chitranone	-8.2
3003153	Lantanolic acid	-8.2
5280794	Stigmasterol	-8.2
9890209	Ursonic acid	-8.2
183757	3,3'-Biplumbagin	-8.1
15560077	Lantadene B	-8.1
101316804	Lantanilic acid	-8.1
73145	beta-Amyrin	-8.1
<b>10621</b>	<b>Hesperidin</b>	<b>-7.9</b>
441686	Taraxasterol	-7.9
5280459	Quercitrin	-7.9
5280637	Cynaroside	-7.9
259846	Lupeol	-7.8
382831	Pomolic acid	-7.8
10423777	Artemisitene	-7.7
5315628	Camaroside	-7.6
222284	beta-Sitosterol	-7.5
11106485	beta-Cedrene	-7.5
12314703	psi-Santonin	-7.5
92231	Spathulenol	-7.4
185689	(-)-Occidentalol	-7.4
439531	Stachyose	-7.4
5280441	Vitexin	-7.4
5281672	Myricetin	-7.4
6508206	αhumulene	-7.4
14989	Aloin	-7.3
65575	Cedrol	-7.3
442355	(-)-alpha-Copaene	-7.3
5280343	Quercetin	-7.3
42608192	(-)-1-Silphinene	-7.3
101596917	beta-Maaliene	-7.3
10208	Chrysophanol	-7.2
5281608	Chrysosplenetin	-7.2
5281677	Pachypodol	-7.2
5281678	Patuletin	-7.2
5281697	Scutellarein	-7.2
6543478	Arteannuin B	-7.2
10744475	CHEMBL496041	-7.2
102090429	Prerotundifuran	-7.2
68229	Seselin	-7.1

PubChem ID	Ligand	Binding Affinity (kcal/mol)
68827	Artemisinin	-7.1
188323	Cirsimaritin	-7.1
237619	beta-Santonin	-7.1
5280863	Kaempferol	-7.1
5317570	(-)-Germacrene D	-7.1
10207	Aloe-emodin	-7.0
5280417	3,7-Di-O-methylquercetin	-7.0
5280445	Luteolin	-7.0
5280699	Chrysosplenol	-7.0
5280805	Rutin	-7.0
5281654	isorhamnetin	-7.0
5281699	Tamarixetin	-7.0
5317287	Eupatin	-7.0
5320946	Rhamnocitrin	-7.0
10856614	alpha-Selinene	-7.0
482576	Dihydrotamarixetin	-6.9
1268142	Nootkatone	-6.9
1549992	Bisabolol	-6.9
5280443	Apigenin	-6.9
5280804	Isoquercetin	-6.9
5281603	Axillarin	-6.9
5281691	Rhamnetin	-6.9
5320462	Penduletin	-6.9
6432005	gamma-Eudesmol	-6.9
101321311	Cinnamoylechinaldiol	-6.9
102247458	[[2S,3R,4S,5S,6R]-4,5-Dihydroxy-6-(hydroxymethyl)-2-[5-methyl-4-oxo-2-(2-oxopropyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-8-yl]oxan-3-yl] (E)-3-phenylprop-2-enoate	-6.9
11256019	Blumeatin B	-6.8
101321314	Cinnamoylechinoxanthol	-6.8
72	Protocatechuic	-6.7
6949	Guaiene	-6.7
439514	Scopolin	-6.7
5281515	beta-Caryophyllene	-6.7
6430754	10-Epi-gamma-Eudesmol	-6.7
6918391	beta-Elemene	-6.7
92138	Elemol	-6.6
158311	Arcapillin	-6.6
290897	5-Methoxyseselin	-6.6
442739	Droserone	-6.6
11020369	Occidol	-6.6
68486	Suberosin	-6.5
121052	2-Phenylbenzaldehyde	-6.5
5280682	Ayanin	-6.5
5352005	Retusin	-6.5
15560536	Mikanin	-6.5

PubChem ID	Ligand	Binding Affinity (kcal/mol)
10205	Plumbagin	-6.4
28237	(-)-beta-Selinene	-6.4
65188	Xanthyletin	-6.4
5315263	Casticin	-6.4
5318355	Penduletin 4'-methyl ether	-6.4
5320351	Artemetin	-6.4
11020893	Dihydroartemisinic acid	-6.4
15560330	Selin-11-en-4alpha-ol	-6.4
21600809	alpha-Epoxydihydroartemisinic acid	-6.4
21636178	Vitexilactone	-6.4
76332505	Isoaloeserin D	-6.4
323	Coumarin	-6.3
76689	4-Phenylbenzaldehyde	-6.3
179396	Theviridoside	-6.3
226343	Vanillil	-6.3
1742210	Caryophyllene oxide	-6.3
5280460	Scopoletin	-6.3
5281517	beta-Farnesene	-6.3
5284507	Nerolidol	-6.3
5316832	Quercetagenin-6,7-3',4'-tetramethyl Ether	-6.3
10704181	Humulene epoxide II	-6.3
97548366	Cinnamoyl epoxyechinadiol	-6.3
4133	Methyl salicylate	-6.2
89316	Cyclohexene	-6.2
5280598	Farnesal	-6.2
6989	Thymol	-6.1
66548	Xanthoxyletin	-6.1
338	Salicylic acid	-6.0
445713	Farnesyl diphosphate	-6.0
2758	Eucalyptol	-5.9
11463	Terpinolene	-5.9
14896	beta Pinen	-5.9
79035	Tricyclene	-5.9
523035	1,3,3-Trimethyl-2-oxa bicyclo[2.2.2]oct-5-ene	-5.9
637542	P-Coumaric Acid	-5.9
5318565	Isofraxidin	-5.9
10922465	Artemisinic acid	-5.9
6654	Alpha pinen	-5.8
442461	(-)-3-Carene	-5.8
2537	Camphor	-5.7
7462	alpha-Terpinene	-5.7
88302	trans-Pinocarveol	-5.7
443777	Isoshinanolone	-5.7
1201518	(-)-Borneol	-5.7
326	4-Isopropylbenzaldehyde	-5.6

PubChem ID	Ligand	Binding Affinity (kcal/mol)
8294	Linalyl acetate	-5.6
8417	Scoparone	-5.6
10364	Carvacrol	-5.6
17100	Alpha terpineol	-5.6
94147	(+)-cis-Sabinol	-5.6
442463	Chrysanthenone	-5.6
6321405	Isoborneol	-5.6
<b>121304016</b>	<b>Remdesivir</b>	<b>-5.6</b>
5988	Sucrose	-5.5
7460	1-Phellandren	-5.5
7463	p-cimene,	-5.5
11230	Terpinen-4-ol	-5.5
111274	(1r,4r)-1-Methyl-4-(prop-1-en-2-yl)cyclohex-2-en-1-ol	-5.5
440917	D-Limonene	-5.5
638500	Farnesyl acetate	-5.5
5280934	Linolenic acid	-5.5
5320128	cis-Nerolidol	-5.5
7461	gamma-Terpinene	-5.4
637563	Anethole	-5.4
6251	D-mannitol	-5.3
66654	Xanthoxylin	-5.3
445639	Oleic acid	-5.3
3314	Eugenol	-5.2

### Supplementary 2. Binding affinity of RdRp-ligands

PubChem ID	Ligand	Binding Affinity (kcal/mol)
5280805	Rutin	-9.6
441686	Taraxasterol	-9.3
183757	3,3'-Biplumbagin	-9.2
73145	beta-Amyrin	-9.0
3003153	Lantanolic acid	-9.0
91472	Friedelin	-8.9
73170	alpha-Amyrin	-8.9
<b>10621</b>	<b>Hesperidin</b>	<b>-8.8</b>
633072	Chitranone	-8.8
382831	Pomolic acid	-8.6
101316804	Lantanilic acid	-8.5
9890209	Ursonic acid	-8.5
10744475	CHEMBL496041	-8.5
3034659	Pseudotaraxasterol	-8.5
121304016	Remdesivir	-8.4
5280637	Cynaroside	-8.4
15560077	Lantadene B	-8.3
5280441	Vitexin	-8.3
5280459	Quercitrin	-8.3
5280804	Isoquercetin	-8.3

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6436598	Lantadene A	-8.3
259846	Lupeol	-8.2
439531	Stachyose	-8.2
102247458	[(2S,3R,4S,5S,6R)-4,5-Dihydroxy-6-(hydroxymethyl)-2-[5-methyl-4-oxo-2-(2-oxopropyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-8-yl]oxan-3-yl] (E)-3-phenylprop-2-enoate	-8.1
5280794	Stigmasterol	-8.0
5315628	Camaroside	-8.0
482576	Dihydrotamarixetin	-7.9
10208	Chrysophanol	-7.8
68827	Artemisinin	-7.8
10423777	Artemisitene	-7.8
14989	Aloin	-7.8
5281677	Pachypodol	-7.8
5280445	Luteolin	-7.6
5281678	Patuletin	-7.5
5281697	Scutellarein	-7.5
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5281672	Myricetin	-7.3
5281699	Tamarixetin	-7.3
5315263	Casticin	-7.3
10207	Aloe-emodin	-7.2
102090429	Prerotundifuran	-7.2
10856614	alpha-Selinene	-7.2
21636178	Vitexilactone	-7.2
237619	beta-Santonin	-7.2
5280343	Quercetin	-7.2
5280863	Kaempferol	-7.2
5281603	Axillarin	-7.2
101321311	Cinnamoylchinaldiol	-7.1
188323	Cirsimaritin	-7.1
439514	Scopolin	-7.1
5280699	Chrysosplenol	-7.1
5281654	Isorhamnetin	-7.1
5320946	Rhamnocitrin	-7.1
68486	Suberosin	-7.0
5281608	Chrysosplenetin	-7.0
5316832	Quercetagenin-6,7-3',4'-tetramethyl Ether	-7.0
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1549992	Bisabolol	-6.2
442739	Droserone	-6.2

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6918391	beta-Elemene	-6.1
5280460	Scopoletin	-6.1
5988	Sucrose	-6.1
8417	Scoparone	-6.0
5281516	alpha-Farnesene	-5.9
5318565	Isofraxidin	-5.9
10364	Carvacrol	-5.8
638500	Farnesyl acetate	-5.8
7460	alpha-Phellandrene	-5.6
5280435	Phytol	-5.6
5280598	Farnesal	-5.6
5280934	Linolenic acid	-5.6
79035	Tricyclene	-5.5
94147	(+)-cis-Sabinol	-5.5
72	3,4-Dihydroxybenzoic acid	-5.5
7461	gamma-Terpinene	-5.5
7462	alpha-Terpinene	-5.5
7463	P-Cymene	-5.5
10453	Isophytol	-5.5
11463	Terpinolene	-5.5
323	Coumarin	-5.5
5284507	Nerolidol	-5.5
6989	Thymol	-5.4
14896	beta-Pinene	-5.4
17100	alpha-Terpineol	-5.4
440917	D-Limonene	-5.4
445639	Oleic acid	-5.4
5281517	beta-Farnesene	-5.4
6321405	Isoborneol	-5.4
637542	4-Hydroxycinnamic acid	-5.4
6654	alpha-Pinene	-5.4
88302	trans-Pinocarveol	-5.3
111274	(1r,4r)-1-Methyl-4-(prop-1-en-2-yl)cyclohex-2-en-1-ol	-5.3
11230	Terpinen-4-ol	-5.3
1549018	Jasmone	-5.3
326	4-Isopropyl benzaldehyde	-5.3
338	Salicylic acid	-5.3
1201518	(-)-Borneol	-5.2
4133	Methyl salicylate	-5.2
442461	(-)-3-Carene	-5.2
3314	Eugenol	-5.1
442463	Chrysanthenone	-5.1

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5317319	cis-beta-Farnesene	-5.1
5320128	cis-Nerolidol	-5.1
637563	Anethole	-5.1
523035	1,3,3-Trimethyl-2-oxabicyclo[2.2.2]oct-5-ene	-5.0
637566	Geraniol	-5.0
12315281	(+)-Santolina alcohol	-4.9
2537	Camphor	-4.9
2758	Eucalyptol	-4.9
445638	Palmitoleic acid	-4.9
6251	D-mannitol	-4.9
5320250	(Z)-beta-Ocimene	-4.8
8181	Methyl palmitate	-4.7
8294	Linalyl acetate	-4.7
1110	Succinic acid	-4.7
5281553	(E)-beta-Ocimene	-4.7
5367681	cis-3-Hexenyl isovalerate	-4.7
6654	alpha-Pinene	-4.6
637523	Hexyl tiglate	-4.6
6549	Linalool	-4.6
11635	Octadecane	-4.5
8103	1-Hexanol	-4.4
31253	Myrcene	-4.4
996	Phenol	-4.3
11005	Myristic acid	-4.3
12398	Heptadecane	-4.3
3893	Lauric acid	-4.3
61455	Hexyl isovalerate	-4.3
750	Glycine	-4.2
5281167	cis-3-Hexen-1-ol	-4.2
612	Lactic acid	-4.2
25612	9-Decen-1-OL	-4.1
24020	Ethyl-2-methylbutyrate	-4.0
454	Octanal	-3.9
18827	1-Octen-3-OL	-3.8