

# Molecular docking, validation, dynamics simulations, and pharmacokinetic prediction of natural compounds against SARS-CoV-2 Main-Protease

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Table S1: Binding scores and Ki values of natural ligands

S. No	Ligand	Binding score (kcal/mol)	Ki value
1.	Theaflavin-3-3'-digallate	-12.41	794.96 pM
2.	Rutin	-11.33	4.98 nM
3.	Hypericin	-11.17	6.54 nM
4.	Robustaflavone	-10.92	9.85 nM
5.	Solenolide A	-10.81	11.88 nM
6.	Rhusflavone	-10.77	12.75 nM
7.	Ginkgetin	-10.47	20.98 nM
8.	Rhinacanthin E	-10.43	22.73 nM
9.	Sorbarin	-10.02	45.41 nM
10.	Betulinic acid	-9.99	47.91 nM
11.	Vaticinone	-9.91	54.24 nM
12.	Clemastanin B	-9.89	55.90 nM
13.	Vitexin	-9.86	59.46 nM
14.	Theaflavin	-9.81	64.76 nM
15.	Prunin	-9.74	72.15 nM
16.	Lucialdehyde D	-9.63	87.64 nM
17.	Taiwanschirin D	-9.58	94.48 nM
18.	Scytovirin	-9.33	146.00 nM
19.	Scutellarin	-9.29	154.15 nM
20.	Alpha-amyrin	-9.29	154.58 nM
21.	Hypocrellin A	-9.28	157.01 nM
22.	Sitosterol	-9.26	163.72 nM
23.	Agathisflavone	-9.25	167.13 nM
24.	Genkanolb	-9.24	168.81 nM
25.	Violathin	-9.23	171.23 nM
26.	Biflavone	-9.20	179.35 nM
27.	Glycyrrhetic acid	-9.19	182.97 nM
28.	Garciosaterpene A	-9.19	183.31 nM
29.	CVL	-9.17	188.51 nM
30.	Silibinin	-9.11	210.49 nM
31.	Epitarascerol	-9.11	210.67 nM

32.	Uvaol	-9.10	214.62 nM
33.	Proanthocyanidins	-9.03	238.80 nM
34.	Swertisin	-8.96	272.74 nM
35.	Cercosporin	-8.89	302.47 nM
36.	Rhoifolin	-8.89	302.78 nM
37.	Mangiferin	-8.89	306.46 nM
38.	Schizarin B	-8.88	309.77 nM
39.	Moronic acid	-8.85	324.55 nM
40.	Rhinacanthin F	-8.84	331.91 nM
41.	Garciosaterpene C	-8.80	355.43 nM
42.	Honokiol	-8.75	385.20 nM
43.	Oroxindin	-8.75	388.01 nM
44.	Yatein	-8.71	414.52 nM
45.	Maslinic acid	-8.68	435.99 nM
46.	Ursolic acid	-8.65	459.59 nM
47.	Genkwanolc	-8.61	489.62 nM
48.	Kaempferol	-8.59	508.35 nM
49.	Xanthohumol	-8.58	514.85 nM
50.	Dihydroquercetin	-8.57	525.45 nM
51.	Polydatin	-8.56	531.85 nM
52.	Sophoricoside	-8.45	644.68 nM
53.	Hinokinin	-8.41	680.02 nM
54.	TMP	-8.37	735.56 nM
55.	Sesamin	-8.36	742.01 nM
56.	Morin	-8.33	778.53 nM
57.	Spongiadiol	-8.28	850.58 nM
58.	Myricitrin	-8.25	898.88 nM
59.	Glabranine	-8.24	909.83 nM
60.	Agastaquinone	-8.23	928.61 nM
61.	Phleichrome	-8.17	1.03 $\mu$ M
62.	Guineesin	-8.14	1.09 $\mu$ M
63.	Tetrahydroxyflavone	-8.03	1.30 $\mu$ M
64.	Diphyllin	-8.02	1.33 $\mu$ M
65.	Rubrifloralignan A	-8.01	1.35 $\mu$ M
66.	Oxyayanin A	-7.93	1.54 $\mu$ M
67.	Epicatechin gallate	-7.93	1.55 $\mu$ M
68.	Cosmosiin	-7.92	1.57 $\mu$ M
69.	Chrysosplenol E	-7.90	1.61 $\mu$ M
70.	Acacetin	-7.90	1.63 $\mu$ M
71.	Chrysin	-7.87	1.70 $\mu$ M
72.	Phillygenin	-7.86	1.72 $\mu$ M
73.	Tectochrysin	-7.84	1.79 $\mu$ M
74.	Uncinosideb	-7.83	1.81 $\mu$ M
75.	Scutellarein	-7.83	1.82 $\mu$ M
76.	Dolabelladienetriol	-7.82	1.85 $\mu$ M
77.	Epigallocatechin gallate	-7.80	1.92 $\mu$ M
78.	UDA 680	-7.77	2.02 $\mu$ M
79.	Chrysoeriol	-7.73	2.17 $\mu$ M

80.	Galangin	-7.72	2.19 $\mu$ M
81.	Cirsimaritin	-7.69	2.31 $\mu$ M
82.	NDGA	-7.69	2.31 $\mu$ M
83.	Liquiritin	-7.68	2.34 $\mu$ M
84.	Naringin	-7.67	2.39 $\mu$ M
85.	Coumarin	-7.63	2.54 $\mu$ M
86.	Avarone	-7.61	2.66 $\mu$ M
87.	Apigenin	-7.60	2.67 $\mu$ M
88.	Pectolarigenin	-7.60	2.68 $\mu$ M
89.	Axillarin	-7.60	2.69 $\mu$ M
90.	Neotripterifordin	-7.59	2.75 $\mu$ M
91.	Hesperidin	-7.58	2.79 $\mu$ M
92.	Resveratrol	-7.57	2.81 $\mu$ M
93.	Chrysosplenol C	-7.56	2.90 $\mu$ M
94.	Wogonin	-7.54	2.99 $\mu$ M
95.	Pectolarin	-7.53	3.01 $\mu$ M
96.	Lycolene	-7.51	3.12 $\mu$ M
97.	Luteolin	-7.49	3.25 $\mu$ M
98.	Curcumin	-7.48	3.27 $\mu$ M
99.	Dehydroandrographolide	-7.47	3.32 $\mu$ M
100.	Chrysosplenol B	-7.42	3.66 $\mu$ M
101.	Myricetin	-7.39	3.82 $\mu$ M
102.	Piperlonguminine	-7.37	3.97 $\mu$ M
103.	Embinin	-7.35	4.07 $\mu$ M
104.	Equol	-7.35	4.10 $\mu$ M
105.	Chrysosplenoside B	-7.33	4.21 $\mu$ M
106.	Limaquinone	-7.33	4.27 $\mu$ M
107.	2,5-Bis(2-thienylethynyl) thiophene	-7.30	4.49 $\mu$ M
108.	Vasicoline	-7.28	4.60 $\mu$ M
109.	Epigallocatechin	-7.28	4.63 $\mu$ M
110.	Avarol	-7.27	4.66 $\mu$ M
111.	Cirsimaritin	-7.27	4.70 $\mu$ M
112.	Quercetagenin	-7.26	4.74 $\mu$ M
113.	Artemisin	-7.26	4.78 $\mu$ M
114.	Baicalin	-7.21	5.17 $\mu$ M
115.	6-Shogaol	-7.21	5.18 $\mu$ M
116.	Genistein	-7.21	5.20 $\mu$ M
117.	5,6,7- trimethoxyflavone	-7.20	5.23 $\mu$ M
118.	Diosmetin	-7.19	5.35 $\mu$ M
119.	Orientin	-7.17	5.55 $\mu$ M
120.	Aesculin	-7.15	5.73 $\mu$ M
121.	Chrysosplenoside A	-7.13	5.96 $\mu$ M
122.	Iridins	-7.12	6.08 $\mu$ M
123.	Baicalein	-7.11	6.15 $\mu$ M
124.	Chrysosplenol D	-7.06	6.66 $\mu$ M
125.	Bicyclol	-6.99	7.57 $\mu$ M
126.	ACBP-thiophene	-6.97	7.74 $\mu$ M
127.	Amentoflavone	-6.89	8.88 $\mu$ M

128.	Apiin	-6.89	8.92 $\mu\text{M}$
129.	A-terthienyl	-6.81	10.13 $\mu\text{M}$
130.	Paradol	-6.80	10.34 $\mu\text{M}$
131.	Hyperin	-6.77	10.90 $\mu\text{M}$
132.	Emodin	-6.66	13.17 $\mu\text{M}$
133.	Cona	-6.63	13.82 $\mu\text{M}$
134.	SCL	-6.60	14.61 $\mu\text{M}$
135.	Glucuronide	-6.58	15.05 $\mu\text{M}$
136.	Aloe emodin	-6.57	15.21 $\mu\text{M}$
137.	Visnagin	-6.50	17.31 $\mu\text{M}$
138.	Harmalol	-6.49	17.56 $\mu\text{M}$
139.	Anthraquinone chrysophanic acid	-6.47	18.11 $\mu\text{M}$
140.	Isorhamnetin	-6.46	18.34 $\mu\text{M}$
141.	Harmaline	-6.45	18.85 $\mu\text{M}$
142.	Harmine	-6.44	19.17 $\mu\text{M}$
143.	Chrysosplenoside D	-6.43	19.32 $\mu\text{M}$
144.	Vasicinone	-6.43	19.38 $\mu\text{M}$
145.	Chitosan oligosaccharide lactate	-6.38	21.04 $\mu\text{M}$
146.	Geniposide	-6.36	21.81 $\mu\text{M}$
147.	B-Caryophyllene	-6.34	22.44 $\mu\text{M}$
148.	Harmol	-6.34	22.42 $\mu\text{M}$
149.	B-Caryophyllene oxide	-6.29	24.70 $\mu\text{M}$
150.	Khellin	-6.19	28.85 $\mu\text{M}$
151.	3-hydroxy caruilignan	-6.12	32.74 $\mu\text{M}$
152.	Farnesol	-6.06	36.36 $\mu\text{M}$
153.	Niranthin	-5.95	43.38 $\mu\text{M}$
154.	Harmane	-5.94	44.48 $\mu\text{M}$
155.	1,8-cineole	-5.93	44.95 $\mu\text{M}$
156.	Sandalwood oil	-5.91	46.88 $\mu\text{M}$
157.	8-gingerol	-5.90	47.10 $\mu\text{M}$
158.	8-methoxypsoralen	-5.89	47.83 $\mu\text{M}$
159.	Aesculetin	-5.85	81.87 $\mu\text{M}$
160.	Terpinen-4-ol	-5.82	54.62 $\mu\text{M}$
161.	10-gingerol	-5.76	60.34 $\mu\text{M}$
162.	$\alpha$ -Pinene	-5.75	60.93 $\mu\text{M}$
163.	Vasicol	-5.75	60.99 $\mu\text{M}$
164.	Angelicin	-5.73	63.33 $\mu\text{M}$
165.	Dictamnine	-5.72	64.23 $\mu\text{M}$
166.	Phenylheptatriyne	-5.63	74.43 $\mu\text{M}$
167.	NPL	-5.63	75.15 $\mu\text{M}$
168.	Deoxyvasicinone	-5.62	77.06 $\mu\text{M}$
169.	Borneol	-5.57	82.69 $\mu\text{M}$
170.	Chlorogenic acid	-5.53	87.75 $\mu\text{M}$
171.	Zingerone	-5.50	93.55 $\mu\text{M}$
172.	Vasicine	-5.48	96.83 $\mu\text{M}$
173.	A-Terpineol	-5.45	100.43 $\mu\text{M}$
174.	Carvone	-5.44	102.58 $\mu\text{M}$
175.	Deoxyvasicine	-5.42	106.38 $\mu\text{M}$

176.	Perillic acid	-5.25	141.19 $\mu\text{M}$
177.	Thymoquinone	-5.25	142.07 $\mu\text{M}$
178.	A-Terpinene	-5.23	147.63 $\mu\text{M}$
179.	Limonene	-5.22	149.29 $\mu\text{M}$
180.	Myristicin	-5.20	155.30 $\mu\text{M}$
181.	Salvianic acid A	-5.19	157.53 $\mu\text{M}$
182.	Eugenol	-4.99	220.17 $\mu\text{M}$
183.	Hydroxyanthanilic acid	-4.95	236.52 $\mu\text{M}$
184.	Thymol	-4.93	244.27 $\mu\text{M}$
185.	Arecoline hydrochloride	-4.90	256.46 $\mu\text{M}$
186.	Thiarubrine-A	-4.90	257.03 $\mu\text{M}$
187.	Anise oil	-4.89	262.29 $\mu\text{M}$
188.	Citral	-4.88	263.24 $\mu\text{M}$
189.	P-Cymene	-4.86	274.44 $\mu\text{M}$
190.	Trans-Anethole	-4.85	278.08 $\mu\text{M}$
191.	Caffeic acid	-4.83	286.94 $\mu\text{M}$
192.	Beta-myrcene	-4.68	371.35 $\mu\text{M}$
193.	Thiophene-A	-4.63	406.86 $\mu\text{M}$
194.	Ligustrazine hydrochloride	-4.60	423.11 $\mu\text{M}$
195.	GNA	-4.36	634.30 $\mu\text{M}$
196.	Gallic acid	-4.36	640.06 $\mu\text{M}$
197.	MVL	-4.36	641.49 $\mu\text{M}$
198.	Thyme oil	-4.28	725.43 $\mu\text{M}$
199.	OAA	-3.94	1.28 mM
200.	Tea tree oil	-1.98	35.31 mM

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