

## Docking Based Identification of Bioactive Diosmin as Potential Multi-Targeted Anti SARS-Cov-2 Agent

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## Supplementary Information

**Table S1.** Stepwise screening of flavonoids on the basis of docking result against 5 targets of SARS-CoV-2.

<b>Step-1 High Throughput Virtual Screening (HTVS) Mode</b>											
S.No	Flavonoids	Main protease (Mpro)		Spike glycoprotein-receptor binding domain (SGp-RBD)		Angiotensin-converting enzyme-2 (ACE2)		RNA - dependent RNA polymerase (RdRp)		Non-structural protein 15(NSP15)	
		Docking Score	Glide Energy	Docking Score	Glide Energy	Docking Score	Glide Energy	Docking Score	Glide Energy	Docking Score	Glide Energy
1	Diosmine	-7.664	-54.561	-6.071	-59.172	-6.101	-56.61	-6.327	-63.908	-6.676	-62.715
2	Astragaline	-7.562	-73.862	-6.904	-56.479	-6.503	-63.64	-6.269	-78.656	-6.501	-59.917
3.	Berberine	-6.849	-65.71	-6.727	-55.21	-6.247	-64.94	-6.099	-59.482	-6.205	-58.722
4.	Hesperidine	-6.622	-67.835	-7.219	-50.497	-6.906	-61.62	-6.693	-65.063	-6.869	-60.212
5.	Baicalin	-6.461	-67.671	-6.906	-59.52	-6.195	-64.784	-6.085	-57.274	-6.737	-58.643
6.	Kuromanin	-6.359	-65.026	-6.833	-53.749	-6.395	-50.441	-6.852	-59.912	-7.684	-50.537
7.	Isoquercitrin	-6.255	-55.35	-6.79	-54.74	-6.715	-53.458	-6.828	-57.594	-6.977	-58.8
8.	Neohesperidine	-6.109	-69.595	-5.69	-52.097	-5.923	-72.435	-6.76	-59.961	-6.605	-53.244
9.	Rutin	-5.964	-59.639	-6.603	-43.857	-5.916	-51.158	-6.697	-51.252	-6.496	-57.671
10.	Jatrorrhizine	-5.818	-53.162	-6.591	-59.531	-6.884	-59.673	-7.566	-65.084	-6.414	-62.027
11.	Daidzein	-5.714	-50.924	-6.569	-63.878	-6.878	-68.77	-7.592	-85.959	-7.24	-74.505
12.	Myricitrin	-5.654	-57.059	-6.553	-72.591	-5.837	-65.418	-6.517	-59.836	-5.80	-51.678
13	Limonin	-5.635	-53.176	-6.473	-63.048	-5.768	-52.284	-6.49	-53.198	-5.961	-56.388
14	Lonicerin	-5.598	-59.971	-6.385	-52.571	-6.47	-58.052	-5.992	-55.166	-6.043	-54.715
15	Icariin	-5.514	-58.348	-6.198	-50.599	-5.941	-52.125	-5.715	-51.059	-6.963	-68.071
16	Laurifolin	-5.167	-61.247	-4.176	-39.413	-5.389	-49.331	-5.289	-55.915	-4.911	-56.853
17	Naringin	-5.113	-56.605	-3.818	-38.83	-5.296	-46.786	-5.024	-47.61	-4.905	-47.157
18	Hyperoside	-5.285	-51.527	-3.807	-36.294	-5.288	-62.637	-4.912	-44.824	-4.7	-36.271
19	Obacunone	-5.034	-52.101	-3.701	-44.741	-5.266	-44.72	-4.827	-45.692	-4.488	-41.09
20	Ononin	-5.106	-45.399	-3.679	-44.604	-5.184	-45.775	-4.622	-39.08	-4.371	-43.73
21	PalmatosideE	-5.253	-47.026	-3.66	-39.327	-5.12	-47.211	-4.423	-47.845	-4.322	-42.405
22	Legalon	-5.676	-51.244	-3.406	-35.217	-4.539	-47.748	-3.827	-40.837	-4.127	-38.911
23	Quercitrin	-5.488	-54.6	-3.303	-37.597	-4.509	-41.581	-3.694	-39.966	-4.025	-41.725
24	Cynaroside	-4.954	-42.45	-3.115	-23.139	-3.783	-34.209	-3.562	-38.514	-3.92	-38.879
25	Eriocitrin	-4.398	-39.097	-2.98	-31.256	-4.101	-46.61	-2.771	-27.199	-4.676	-42.405
26	Fenicularin	-4.664	-40.561	-5.071	-49.172	-5.101	-36.61	-3.327	-35.908	-4.676	-32.715
27	Liquiritin	-4.562	-33.862	-5.004	-36.479	-2.503	-23.64	-2.269	-28.656	-3.501	-39.917
28	Kaempferitin	-4.549	-35.71	-5.227	-41.55	-3.247	-34.94	-5.099	-53.472	-5.205	-50.922
29	Likvirtin	-4.322	-47.835	-5.219	-50.497	-5.206	-51.62	-5.093	-55.063	-5.169	-49.212
30	Prunin	-4.161	-37.671	-5.106	-39.52	-4.195	-39.784	-5.085	-47.274	-5.237	-48.683

31	Miquelianin	-4.159	-35.026	-4.833	-43.749	-5.095	-42.441	-5.252	-59.917	-5.384	-50.637
32	Norswertianolin	-4.125	-35.35	-4.79	-54.74	-4.015	-54.458	-5.328	-57.594	-5.277	-48.8
33	Nicotiflorin	-4.09	-40.595	-4.69	-46.097	-5.123	-49.435	-5.26	-50.961	-5.105	-52.244
34	Oenin	-3.964	-36.639	-4.603	-43.857	-4.916	-48.158	-4.697	-46.252	-5.496	-43.671
35	Orientin	3.718	-33.162	-4.591	-49.531	-5.284	-52.673	-5.136	-50.084	-5.414	-47.027
36	OroxinA	-3.614	-32.924	-4.569	-48.878	-4.878	-48.77	-5.052	-51.959	-5.24	-44.505
37	Persiconin	-3.496	-37.059	-4.553	-42.591	-5.837	-65.418	-5.517	-49.836	-5.2	-51.678
38	Genistoside	-3.42	-41.176	-4.473	-46.048	-5.268	-50.284	-5.22	-51.198	-5.161	-46.388
39	Gossypin	-3.393	-40.971	-4.385	-49.571	-4.47	-48.052	-5.392	-55.166	-5.043	-44.715
40	Guaiaverin	3.235	-38.348	-4.198	-40.599	-5.441	-52.125	-5.315	-51.059	-4.963	-48.071
41	Helichryoside	-3.167	-41.247	-4.176	-39.413	-5.389	-49.331	-5.289	-55.915	-4.911	-56.853
42	Hirsutrin	-3.113	-36.605	-3.818	-38.83	-4.296	-46.786	-4.024	-47.61	-4.905	-47.157
43	Isoorientin	-2.985	-31.527	-3.807	-36.294	-5.288	-62.637	-4.912	-44.824	-4.7	-36.271
44	Tectoridin	-2.834	-32.101	-3.701	-44.741	-5.266	-44.72	-4.827	-45.692	-4.488	-41.09
45	Tilianin	-2.706	-40.399	-4.679	-44.604	-5.184	-45.775	-4.622	-39.08	-4.371	-43.73
46	Juglanin	-2.553	-37.026	-3.66	-39.327	-5.12	-47.211	-4.423	-47.845	-4.322	-42.405
47	Linarin	-2.476	-31.244	-4.406	-35.217	-4.539	-47.748	-3.827	-40.837	-4.127	-38.911
48	Tiliroside	-2.388	-34.6	-3.303	-37.597	-4.509	-41.581	-4.694	-39.966	-4.025	-41.725
49	Tribuloside	-2.154	-40.45	-3.115	-23.139	-3.783	-54.209	-3.562	-38.514	-3.92	-38.879
50	Trifolin	-2.025	-32.097	-2.98	-31.256	-5.101	-56.61	-5.771	-27.199	-3.676	-32.405
<b>Step-2 Standard Precision (SP) Docking Mode</b>											
S.No	Flavonoids	Main protease (Mpro)		Spike glycoprotein-receptor binding domain (SGp-RBD)		Angiotensin-converting enzyme-2 (ACE2)		RNA - dependent RNA polymerase (RdRp)		Non-structural protein 15(NSP15)	
		Docking Score	Glide Energy	Docking Score	Glide Energy	Docking Score	Glide Energy	Docking Score	Glide Energy	Docking Score	Glide Energy
1	Diosmine	-10.674	-68.111	-9.612	-73.774	-8.784	-59.326	-9.664	-66.263	-7.929	-61.168
2	Astragalin	-10.562	-61.746	-8.612	-71.176	-8.651	-60.577	-7.562	-60.131	-7.84	-65.973
3.	Berberine	-9.501	-69.702	-7.549	-68.758	-6.543	-62.627	-8.510	-62.332	-8.752	-63.525
4.	Hesperidine	-9.322	-62.067	-6.521	-69.02	-6.851	-67.353	-7.367	-67.525	-7.433	-62.282
5.	Baicalin	-8.964	-62.611	-6.841	-68.686	-7.161	-59.333	-6.661	-61.335	-7.313	-65.974
6.	Kuromanin	-7.718	-65.509	-6.695	-65.414	-7.854	-60.131	-6.965	-63.231	-6.798	-60.376
7.	Isoquercitrin	-7.614	-65.509	-8.155	-64.981	-7.576	-58.141	-7.195	-65.817	-6.779	-67.402
8.	Neohesperidine	-7.09	-61.15	-6.745	-62.805	-6.965	-69.817	-6.924	-61.587	-6.702	-66.282
9.	Rutin	-6.964	-60.491	-6.661	-63.846	-6.881	-57.669	-6.764	-65.051	-6.669	-65.633
10.	Jatrorrhizine	-6.858	-56.157	-6.718	-58.663	-6.734	-66.486	-6.718	-62.202	-6.631	-59.395

11.	Daidzein	-6.765	-58.33	-6.614	-65.079	-6.581	-58.781	-6.614	-61.81	-6.622	-60.573
12.	Myricitrin	-6.696	-60.874	-6.762	-64.022	-6.796	-67.503	-6.596	-58.846	-6.621	-57.623
13	Limonin	-6.62	-63.632	-6.784	-60.113	-8.42	-69.326	-7.137	-68.891	-6.929	-63.544
14	Lonicerin	-6.574	-57.863	-6.941	-63.774	-6.893	-60.577	-6.753	-59.728	-6.827	-59.134
15	Icariin	-6.521	-56.913	-7.664	-61.176	-7.664	-62.627	-7.664	-66.381	-6.75	-55.668
<b>Step-3 Extra Precision Docking (XP) Mode</b>											
S.No	Flavonoids	Main protease (Mpro)		Spike glycoprotein-receptor binding domain (SGp-RBD)		Angiotensin-converting enzyme-2 (ACE2)		RNA - dependent RNA polymerase (RdRp)		Non-structural protein 15(NSP15)	
		Docking Score	Glide Energy	Docking Score	Glide Energy	Docking Score	Glide Energy	Docking Score	Glide Energy	Docking Score	Glide Energy
1	Diosmine	-12.16	-77.24	-11.52	-74.49	-9.75	-65.18	-11.25	-69.90	-10.25	-67.15
2	Astragalin	-11.04	-72.83	-9.51	-67.52	-10.51	-70.38	-10.82	-71.25	-9.74	-68.74
3.	Berberine	-9.54	-68.52	-10.74	-69.82	-8.95	-67.18	-9.12	-68.14	-8.82	-65.15
4.	Hesperidine	-8.56	-66.24	-8.52	-70.48	-8.73	-66.05	-8.62	-66.47	-8.93	-66.98