

Supplementary File

SI 1. Docking score plant-derived natural products against omicron (PDB ID: 7QO7)

Sr. No.	Compounds	Docking score
1	Rutin	-10.224
2	Hesperidin	-9.029
3	Epicatechingallate	-8.202
4	Naringenin	-8.109
5	Luteolin	-7.904
6	Apigenin	-7.857
7	Egcg	-7.7
8	Diosmetin	-7.659
9	Epicatechin	-7.596
10	Daidzein	-7.431
11	Resveratrol	-7.375
12	Beta-glucan	-7.185
13	Epigallocatechin	-6.999
14	Naringin	-6.914
15	Myricetin	-6.877
16	Nigellimine-n-oxide	-6.853
17	Curcumin (enol)	-6.85
18	Glucosamine	-6.819
19	Hesperetin	-6.798
20	Rosamarinic	-6.739
21	Piperolein B	-6.692
22	Thymoquinone	-6.588
23	Taxifolin	-6.472
24	Piperylin A	-6.395
25	Isopelletierine	-6.395
26	Oleocanthal	-6.394
27	Fisetin	-6.376
28	Piperol-B	-6.376
29	Genistein	-6.303
30	Carvacrol	-6.298
31	Chrysin	-6.257
32	Homoorientin	-6.24
33	5-hydroxy-7,8-dimethoxyflavanone	-6.239
34	Withanolide A	-6.153
35	Epigallocatechin	-6.15
36	Tangeretin	-6.124
37	Quercetin	-6.092
38	Thymohydroquinone	-6.075
39	5-hydroxy-7,8-dimethoxyflavone	-6.051

40	Nobiletin	-5.943
41	Gallic acid	-5.928
42	Cuminaldehyde	-5.905
43	Nigellimine	-5.87
44	Withanolide G	-5.817
45	N-acetylcystein	-5.81
46	Isopiperine	-5.806
47	Cadinene	-5.806
48	Elenolic acid	-5.768
49	Cuminic acid	-5.758
50	Kaempferol	-5.748
51	4-terpinol	-5.722
52	Thymol	-5.701
53	A-muurolene	-5.693
54	Carotol	-5.668
55	Anaferine	-5.666
56	P-cymene	-5.649
57	Piperol-A	-5.617
58	Ferulic acid	-5.611
59	Cabenene	-5.6
60	Isochavicine	-5.584
61	Carotol	-5.576
62	Myrcene	-5.547
63	14-deoxy-11,12-didehydroandrographolide	-5.455
64	Piperine	-5.378
65	Sabinene	-5.357
66	Andrograpanin	-5.341
67	Cuscohygrine	-5.336
68	Neoandrographolide	-5.308
69	Nigellicine	-5.261
70	Nigellidine	-5.256
71	Limonene	-5.086
72	14-deoxy-14,15-didehydroandrographolide	-5.035
73	Oleocanthol	-4.97
74	Fenchone	-4.969
75	Apigenin	-4.945
76	Alliin	-4.886
77	Estragole	-4.789
78	B-caryophyllene	-4.787
79	Isoandrographolide	-4.757
80	Galangin	-4.709
81	Sulforaphane	-4.602
82	Dithymoquinone	-4.533
83	Andrographolide	-4.396

84	Withanolide D	-4.166
85	Betapinene	-4.154
86	Pipericine	-4.125
87	Gingerol-6	-4.088
88	Lipoic acid	-4.078
89	Deguelin	-4.069
90	14-deoxyandrographolide	-3.989
91	Kaempferol	-3.799
92	14-deoxy-14,15-didehydroandrographolide	-3.767
93	Fisetin	-3.761
94	Gallic acid	-3.556
95	Withanolide G	-3.533
96	D-citronellol	-3.495
97	Allicin	-2.635
98	Withaferin A	-2.114
99	14-deoxyandrographolide	-2.042
100	Methyl-butyrates	-1.817

SI 2. Docking score plant-derived natural products against delta (PDB ID: 7W92)

Sr.No.	Compounds	Docking score
1	Rutin	-8.160
2	EgCG	-7.993
3	Hesperidin	-7.873
4	Epicatechin	-7.736
5	Naringin	-7.528
6	Epicatechingallate	-7.454
7	Epicatechin	-7.348
8	Homoorientin	-7.249
9	Naringenin	-7.241
10	Piperol-B	-7.207
11	Epigallocatechin	-7.2
12	EgCG	-6.901
13	Beta-glucan	-6.894
14	Taxifolin	-6.825
15	Nigellimine-n-oxide	-6.815
16	Glucosamine	-6.813
17	Quercetin	-6.795
18	Piperol-A	-6.791
19	Anaferine	-6.706
20	Andrographolide	-6.696
21	14-deoxyandrographolide	-6.685
22	Apigenin	-6.647
23	Rosamarinic	-6.629
24	Hesperetin	-6.611

25	14-deoxy-14,15-didehydroandrographolide	-6.561
26	Myricetin	-6.521
27	Piperylin A	-6.456
28	Nigellidine	-6.377
29	Chrysin	-6.359
30	Kaempferol	-6.273
31	Neoandrographolide	-6.245
32	Withanolide D	-6.242
33	Galangin	-6.238
34	Fisetin	-6.232
35	Withaferin A	-6.205
36	Withanolide G	-6.159
37	Withanolide A	-6.143
38	Isochavicine	-6.119
39	Thymohydroquinone	-6.083
40	14-deoxy-11,12-didehydroandrographolide	-6.054
41	Isoandrographolide	-6.016
42	Homoorientin	-6.012
43	Carotol	-5.947
44	Piperolein B	-5.929
45	Neoandrographolide	-5.912
46	Daidzein	-5.905
47	Genistein	-5.901
48	Deguelin	-5.893
49	Diosmetin	-5.867
50	Andrograpanin	-5.854
51	Nigellimine	-5.82
52	Luteolin	-5.788
53	Carvacrol	-5.774
54	Isopelletierine	-5.772
55	Cabenene	-5.732
56	A-muurolene	-5.725
57	Thymoquinone	-5.686
58	Piperine	-5.684
59	Piperanine	-5.684
60	Withanone	-5.667
61	Masilinic	-5.645
62	Resveratrol	-5.582
63	Cadinene	-5.555
64	Cuscohygrine	-5.549
65	Isopiperine	-5.51
66	5-hydroxy-7,8-dimethoxyflavanone	-5.486
67	Curcumin (enol)	-5.486
68	Nobiletin	-5.447

69	Ursolic acid	-5.436
70	Oleocanthal	-5.428
71	Thymol	-5.359
72	Gallic acid	-5.245
73	Dithymoquinone	-5.209
74	B-caryophyllene	-5.106
75	Terinolene	-5.059
76	5-hydroxy-7,8-dimethoxyflavone	-4.996
77	Nigellicine	-4.984
78	Fenchone	-4.979
79	Tangeretin	-4.95
80	Cuminaldehyde	-4.943
81	Myrcene	-4.886
82	Oleonolic	-4.86
83	P-cymene	-4.843
84	Longifolene	-4.834
85	4-terpinol	-4.777
86	Cuminic acid	-4.709
87	Nigellimine	-4.575
88	Sabinene	-4.528
89	Taxifolin	-4.526
90	Betapinene	-4.521
91	Lipoic acid	-4.444
92	Elenolic	-4.439
93	Alliin	-4.429
94	Dithymoquinone	-4.315
95	T-anethole	-4.147
96	Gingerol-6	-4.141
97	Limonene	-4.069
98	Sulforaphane	-4.068
99	Estragole	-3.888
100	Ferulic acid	-3.867

SI 3. Docking score plant-derived natural products against alpha (PDB ID: 8DLI)

Sr.No	Compounds	docking score
1	Hesperidin	-8.993
2	Withanolide G	-8.766
3	Rosamarinic	-8.761
4	Naringin	-8.614
5	Rutin	-8.589
6	Homoorientin	-8.545
7	Alliin	-7.914
8	Egcg	-7.851
9	Epicatechin	-7.799

10	Epigallocatechin	-7.765
11	Epicatechingallate	-7.738
12	Andrographolide	-7.702
13	Anaferine	-7.509
14	Withanolide D	-7.386
15	Taxifolin	-7.258
16	Nigellicine	-7.252
17	14-deoxy-14,15-didehydroandrographolide	-7.232
18	Naringenin	-7.181
19	Beta-glucan	-7.165
20	Withanolide A	-7.161
21	Glucosamine	-7.022
22	Elenolic	-7.015
23	Homovanillic	-6.984
24	Gallic acid	-6.964
25	Piperol-B	-6.955
26	Myricetin	-6.916
27	Withanolide G	-6.899
28	Quercetin	-6.825
29	Piperol-A	-6.772
30	Fisetin	-6.722
31	Neoandrographolide	-6.683
32	Withaferin A	-6.672
33	Resveratrol	-6.524
34	Isopelletierine	-6.49
35	Daidzein	-6.471
36	Hesperetin	-6.458
37	Andrograpanin	-6.435
38	Isopiperine	-6.424
39	Andrographolide	-6.408
40	Cuscohygrine	-6.399
41	Galangin	-6.353
42	Oleocanthol	-6.352
43	Nigellidine	-6.319
44	Kaempferol	-6.208
45	Isoandrographolide	-6.199
46	N-acetylcystein	-6.178
47	Diosmetin	-6.173
48	Genistein	-6.119
49	Lipoic acid	-6.109
50	Luteolin	-6.093
51	Carotol	-6.078
52	Dithymoquinone	-6.065
53	Apigenin	-6.043

54	5-hydroxy-7,8-dimethoxyflavone	-5.99
55	Andrograpanin	-5.971
56	14-deoxy-11,12-didehydroandrographolide	-5.97
57	Isoandrographolide	-5.967
58	14-deoxyandrographolide	-5.939
59	5-hydroxy-7,8-dimethoxyflavanone	-5.926
60	N-acetylcystein	-5.919
61	Ferulic acid	-5.866
62	Nigellimine-n-oxide	-5.831
63	Oleocanthol	-5.807
64	Withanone	-5.782
65	Piperine	-5.761
66	Piperanine	-5.761
67	Curcumin (enol)	-5.725
68	Nobiletin	-5.669
69	Isochavicine	-5.662
70	Ursolic acid	-5.638
71	4-terpinol	-5.622
72	Carvacrol	-5.455
73	Chrysin	-5.43
74	Tangeretin	-5.423
75	Cabenene	-5.414
76	Piperylin A	-5.309
77	Cadinene	-5.306
78	Piperolein B	-5.243
79	Cuminic acid	-5.23
80	Nigellimine	-5.176
81	A-muurolene	-5.167
82	Fenchone	-5.163
83	Longifolene	-5.112
84	Cuminaldehyde	-5.081
85	Cabenene	-5.05
86	Dithymoquinone	-4.98
87	T-anethole	-4.953
88	B-caryophyllene	-4.768
89	Thymol	-4.761
90	Terpinolene	-4.747
91	Sabinene	-4.67
92	Oleonolic	-4.547
93	Sulforaphane	-4.183
94	Myrcene	-4.16
95	Masilinic	-3.832
96	Limonene	-3.679
97	Allicin	-3.394

98	Gingerol-6	-2.85
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SI 4. Docking score plant-derived natural products against beta (PDB ID: 7LYQ)

Sr. No.	Compounds	Docking score
1.	Egcg	-8.369
2.	Diosmetin	-8.2
3.	Myricetin	-8.102
4.	Homoorientin	-8.39
5.	Naringin	-8.139
6.	Rutin	-8.095
7.	Beta-glucan	-7.889
8.	Hesperidin	-7.559
9.	Epicatechingallate	-7.429
10.	Taxifolin	-7.425
11.	Apigenin	-7.393
12.	Epicatechin	-7.367
13.	Withanolide D	-7.273
14.	Epigallocatechin	-7.272
15.	Rosamarinic	-7.187
16.	Kaempferol	-7.179
17.	Fisetin	-7.15
18.	Neoandrographolide	-7.126
19.	Withaferin A	-6.98
20.	Luteolin	-6.92
21.	Isoandrographolide	-6.906
22.	Nigellidine	-6.866
23.	Quercetin	-6.844
24.	Gallic acid	-6.807
25.	Glucosamine	-6.667
26.	Withanolide G	-6.59
27.	Thymohydroquinone	-6.564
28.	Neoandrographolide	-6.548
29.	Homovanillic	-6.421
30.	Anaferine	-6.421
31.	14-deoxy-11,12-didehydroandrographolide	-6.394
32.	Andrographolide	-6.376
33.	Daidzein	-6.329
34.	Dithymoquinone	-6.326
35.	Genistein	-6.318
36.	Deguelin	-6.313
37.	Chrysin	-6.302
38.	Tangeretin	-6.283
39.	Curcumin (enol)	-6.266
40.	Piperol-B	-6.257

41.	Naringenin	-6.243
42.	Piperol-A	-6.241
43.	Resveratrol	-6.18
44.	Galangin	-6.166
45.	5-hydroxy-7,8-dimethoxyflavanone	-6.153
46.	Isochavicine	-6.008
47.	A-muurolene	-5.992
48.	14-deoxyandrographolide	-5.991
49.	Elenolic	-5.986
50.	Carvacrol	-5.934
51.	14-deoxy-14,15-didehydroandrographolide	-5.925
52.	Nobiletin	-5.866
53.	Nigellicine	-5.855
54.	Anaferine	-5.84
55.	Andrograpanin	-5.763
56.	Withanolide A	-5.763
57.	Carotol	-5.704
58.	Nigellimine-n-oxide	-5.69
59.	Withanolide G	-5.688
60.	4-terpinol	-5.65
61.	Isopelletierine	-5.614
62.	Cabenene	-5.556
63.	Thymol	-5.545
64.	Piperylin A	-5.545
65.	Cadinene	-5.4
66.	Fenchone	-5.354
67.	Ferulic acid	-5.327
68.	Isopiperine	-5.309
69.	Oleocanthol	-5.298
70.	Piperine	-5.273
71.	Piperanine	-5.273
72.	Cuminaldehyde	-5.254
73.	Longifolene	-5.25
74.	Thymoquinone	-5.18
75.	N-acetylcystein	-5.175
76.	Myrcene	-5.106
77.	B-caryophyllene	-5.089
78.	Epigallocatechin	-5.046
79.	4-terpinol	-5.04
80.	Nigellimine	-5.037
81.	Myrcene	-5.029
82.	Cadinene	-5.028
83.	Cabenene	-4.981
84.	Piperolein B	-4.941

85.	Lipoic acid	-4.892
86.	Terinolene	-4.832
87.	Sabinene	-4.802
88.	Cuminic acid	-4.612
89.	T-anethole	-4.542
90.	Withanolide D	-4.54
91.	Betapinene	-4.504
92.	Cuscohygrine	-4.102
93.	Estragole	-4.088
94.	Sulforaphane	-3.934
95.	Alliin	-3.919
96.	Hesperetin	-3.623
97.	Gingerol-6	-3.395
98.	D-citronellol	-3.279
99.	Methyl-butyrates	-1.972
100.	Oleonolic	-1.904

SI 5. Docking score plant-derived natural products against gamma (PDB ID: 7SBT)

Sr. No.	Compounds	Docking score
1	Rosmarinic	-9.235
2	Epicatechin	-8.896
3	Quercetin	-8.021
4	Taxifolin	-7.948
5	Kaempferol	-7.923
6	Naringenin	-7.878
7	Apigenin	-7.674
8	Homoorientin	-7.663
9	Fisetin	-7.603
10	Genistein	-7.537
11	egcg	-7.532
12	Naringin	-7.354
13	Resveratrol	-7.157
14	14-deoxy-14,15-didehydroandrographolide	-6.917
15	Beta-glucan	-6.835
16	Glucosamine	-6.827
17	Piperol-A	-6.756
18	Isoandrographolide	-6.676
19	Epicatechingallate	-6.615
20	Hesperetin	-6.589
21	4-terpinol	-6.487
22	Daidzein	-6.469
23	Chrysin	-6.463
24	Galangin	-6.446
25	Diosmetin	-6.439

26	Nigellicine	-6.431
27	Carvacrol	-6.392
28	Neoandrographolide	-6.387
29	Nigellimine-n-oxide	-6.331
30	Thymohydroquinone	-6.254
31	Gallic acid	-6.239
32	Elenolic	-6.224
33	Carotol	-6.214
34	Andrographolide	-6.2
35	Andrograpanin	-6.147
36	Myricetin	-5.968
37	14-deoxy-11,12-didehydroandrographolide	-5.934
38	Piperol-B	-5.921
39	curcumin (enol)	-5.911
40	Rutin	-5.891
41	Isochavicine	-5.89
42	Thymol	-5.888
43	Cuminaldehyde	-5.877
44	Epicatechingallate	-5.857
45	Isopelletierine	-5.776
46	Anaferine	-5.75
47	5-hydroxy-7,8-dimethoxyflavone	-5.741
48	A-murolene	-5.713
49	Nigellimine	-5.683
50	Cadinene	-5.67
51	5-hydroxy-7,8-dimethoxyflavanone	-5.657
52	Nigellidine	-5.64
53	thymoquinone	-5.593
54	P-cymene	-5.49
55	Homovanillic	-5.409
56	Fenchone	-5.363
57	Cuscohygrine	-5.353
58	Cabenene	-5.352
59	Piperolein B	-5.342
60	Piperine	-5.334
61	Piperanine	-5.334
62	Luteolin	-5.296
63	14-deoxyandrographolide	-5.262
64	Cuminic acid	-5.229
65	Isopiperine	-5.213
66	deguelin	-5.226
67	Ferulic acid	-5.153
68	Oleocanthol	-5.148
69	nobiletin	-5.022

70	N-acetylcystein	-4.967
71	Apigenin	-4.942
72	Myrcene	-4.915
73	Piperylin A	-4.904
74	Dithymoquinone	-4.862
75	B-caryophyllene	-4.856
76	Longifolene	-4.849
77	Sabinene	-4.841
78	Kaempferol	-4.798
79	Alliin	-4.705
80	Naringenin	-4.637
81	Lipoic acid	-4.457
82	Tangeretin	-4.456
83	Withanolide G	-4.443
84	Limonene	-4.442
85	T-anethole	-4.437
86	deguelin	-4.277
87	Galangin	-4.276
88	Cabenene	-4.275
89	Sulforaphane	-4.231
90	Withanolide D	-4.23
91	Pipericine	-4.227
92	Betapinene	-4.206
93	Hesperidin	-4.055
94	Estragole	-3.601
95	D-citronellol	-3.574
96	Gingerol-6	-3.43
97	Withaferin A	-3.205
98	Allicin	-2.937
99	Methyl-butyrates	-1.924

SI 6. The reactive sites of (A) Alpha, (B) Beta (C) Gamma (D) Delta (E) Omicron variants of SARS-CoV-2.

