Supplementary Information

Targeting COVID-19 (SARS-CoV-2) RNA dependent RNA polymerase through active phytochemicals of ayurvedic medicinal plants Limonia acidissima Linn. And Ocimum sanctum : A molecular docking study

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Contents:

mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.
1	-9.5	0.000	0.000
2	-9.4	1.496	2.076
3	-9.2	32.560	35.694
4	-8.8	46.223	48.839
5	-8.8	29.674	33.450
6	-8.7	2.559	8.067
7	-8.5	17.497	20.403
8	-8.5	24.069	28.136
9	-8.4	3.207	6.377

Figure 1: Log file of Limonin

mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.
1	-9.0	0.000	0.000
2	-8.6	47.113	50.123
3	-8.5	16.582	19.910
4	-8.4	51.519	53.507
5	-8.2	2.069	7.731
6	-8.2	17.592	21.320
7	-8.2	28.846	32.450
8	-8.1	15.152	17.223
9	-8.1	46.585	51.912

Figure 2: Log file of Obacunone

mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.
1	-8.8	0.000	0.000
2	-8.5	31.019	35.070
3	-8.5	16.614	19.620
4	-8.4	1.865	8.035
5	-8.4	2.215	7.961
6	-8.4	1.473	1.864
7	-8.3	2.256	7.798
8	-8.3	37.319	42.341
9	-8.2	17.174	20.123

Figure 3: Log file of Rutaevin

mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.
1	-8.4	0.000	0.000
2	-8.0	2.526	8.186
3	-7.9	2.538	4.441
4	-7.9	2.823	3.727
5	-7.7	2.715	7.050
6	-7.6	46.294	48.995
7	-7.6	44.650	47.563
8	-7.5	24.697	27.201
9	-7.4	6.771	12.002

Figure 4: Log file of (-)-(2S)-5,3’-Dihydroxy-4’-methoxy-6’’,6’’-dimethylchromeno-(7,8,2’’,3’’)-

Flavanone

mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.
1	-8.3	0.000	0.000
2	-7.9	35.176	37.361
3	-7.7	17.201	20.156
4	-7.6	57.482	60.913
5	-7.6	45.662	49.961
6	-7.4	3.455	5.866
7	-7.4	30.309	34.519
8	-7.3	57.482	61.770
9	-7.1	24.358	27.655

Figure 5: Log file of Lupeol

mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.
1	-8.3	0.000	0.000
2	-7.9	17.925	19.211
3	-7.5	28.541	30.360
4	-7.4	63.714	65.722
5	-7.3	47.609	50.194
6	-7.3	58.616	60.547
7	-7.2	61.641	64.070
8	-7.1	47.727	50.393
9	-7.0	41.255	43.789

Figure 6: Log file of 5-Hydroxy-2-(-hydroxyphenyl)-7-methoxy-6-(3-methylbut-2-enyl)chroman-4-

One

mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.
1	-8.1	0.000	0.000
2	-8.0	24.795	29.046
3	-7.8	3.601	6.846
4	-7.8	26.688	28.606
5	-7.7	2.064	6.051
6	-7.6	45.247	50.143
7	-7.3	18.540	21.629
8	-7.2	18.003	20.991
9	-7.2	49.531	52.399

Figure 7: Log file of Vitexin

mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.
1	-8.1	0.000	0.000
2	-8.0	1.785	5.958
3	-7.7	43.483	47.002
4	-7.5	26.108	28.858
5	-7.5	2.099	5.365
6	-7.4	31.218	33.410
7	-7.3	47.765	50.572
8	-7.1	48.034	51.437
9	-7.0	39.466	43.273

Figure 8: Log file of Orientin

mode	affinity (kcal/mol)	dist from best mode rmsd l.b.	rmsd u.b.
1	-8.1	0.000	0.000
2	-7.9	64.347	67.276
3	-7.7	38.808	40.670
4	-7.7	17.828	19.927
5	-7.5	10.512	14.376
6	-7.3	66.221	69.975
7	-7.2	18.260	20.177
8	-7.2	60.573	62.960
9	-7.2	67.581	69.422

Figure 9: Log file of Urosolic acid