

### ***Supplementary Material***

**Table S1** Docking based virtual screening results of the 50 phytochemical compound dataset against wild-type Spike protein, predicted by PyRx.

<b>Sl No.</b>	<b>Compound</b>	<b>Binding energy (kcal/mol)</b>
1	Lupeol	−9.4
2	Betulin	−9
3	Hypericin	−8.8
4	Corilagin	−8.7
5	Rutaecarpine	−7.8
6	Geraniin	−7.8
7	Rutin	−8.5
8	Hyperoside	−8.5
9	Mulberroside C	−8.5
10	Pentagalloylglucose	−8.3
11	Chebolic acid	−8.2
12	Mimusopic acid	−8.1
13	Berberine	−8.0
14	Neoandrographolide	−7.9
15	Chebulaigic acid	−7.9
16	Chebulinic acid	−7.9
17	Quercetin	−7.9

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18	Kaemferol	-7.9
19	Germacrone	-7.8
20	Baicelein	-7.8
21	Ellagic acid	-7.7
22	Epigallocatechin gallate	-7.7
23	Glycyrrhizic acid	-7.7
24	Fisetin	-7.7
25	Palmitine	-7.7
26	Torvoside H	-7.7
27	Myricetin	-7.6
28	Rosmarinic acid	-7.5
29	Cordycepin	-7.4
30	Andrographolide	-7.4
31	Carvacrol	-7.3
32	Apigenin	-7.4
33	Piperine	-7.4
34	Curcumin	-7.2
35	Quinic acid	-7.1
36	Thymol	-7.1
37	Eugenol	-7.0

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38	P-Coumaric acid	−6.9
39	Gingerol	−6.3
40	Gallic acid	−5.3
41	Ferulic acid	−5.1
42	E-cinnamaldehyde	−5.0
43	Menthol	−4.5
44	Ajoene	−3.7
45	Allicin	−3.4
46	Methyl allyl thiosulfinate	−3.3
47	Diallyl trisulfide	−3.2
48	Gingerone A	−3.0
49	Ursolic acid	−2.9
50	Emblicanin A	−2.9

**Table S2** Docking based virtual screening results of the 50 phytochemical compound dataset against Delta Spike protein, predicted by PyRx.

Sl No.	Compound	Binding energy (kcal/mol)
1	Lupeol	-7.5
2	Betulin	-7.5
3	Corilagin	-7.4
4	Hypericin	-7.4
5	Rutaecarpine	-7.4
6	Geraniin	-7.3
7	Rutin	-7.2
8	Hyperoside	-7.0
9	Pentagalloylglucose	-6.9
10	Mulberroside C	-6.8
11	Mimusopic acid	-6.8
12	Chebolic acid	-6.8
13	Kaemferol	-6.7
14	Quercetine	-6.7
15	Neoandrographolide	-6.3
16	Berberine	-6.2
17	Germacrone	-5.8
18	Ellagic acid	-5.6

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19	Glycyrrhizic acid	−5.5
20	Fisetin	−4.9
21	Palmitine	−4.8
22	Torvoside H	−4.8
23	Myricetin	−4.4
24	Chebularic acid	−4.1
25	Chebulinic acid	−3.6
26	Rosmarinic acid	−3.6
27	Baicalein	−3.6
28	Cordycepin	−3.4
29	Epigallocatechin gallate	−3.2
30	Carvacrol	−3.2
31	Piperine	−3.1
32	Curcumin	−3.0
33	Apigenin	−2.9
34	Andrographolide	−2.9
35	Thymol	−2.7
36	Eugenol	−2.6
37	Quinic acid	−2.4
38	P-coumaric acid	−2.4
39	Ferulic acid	−2.3

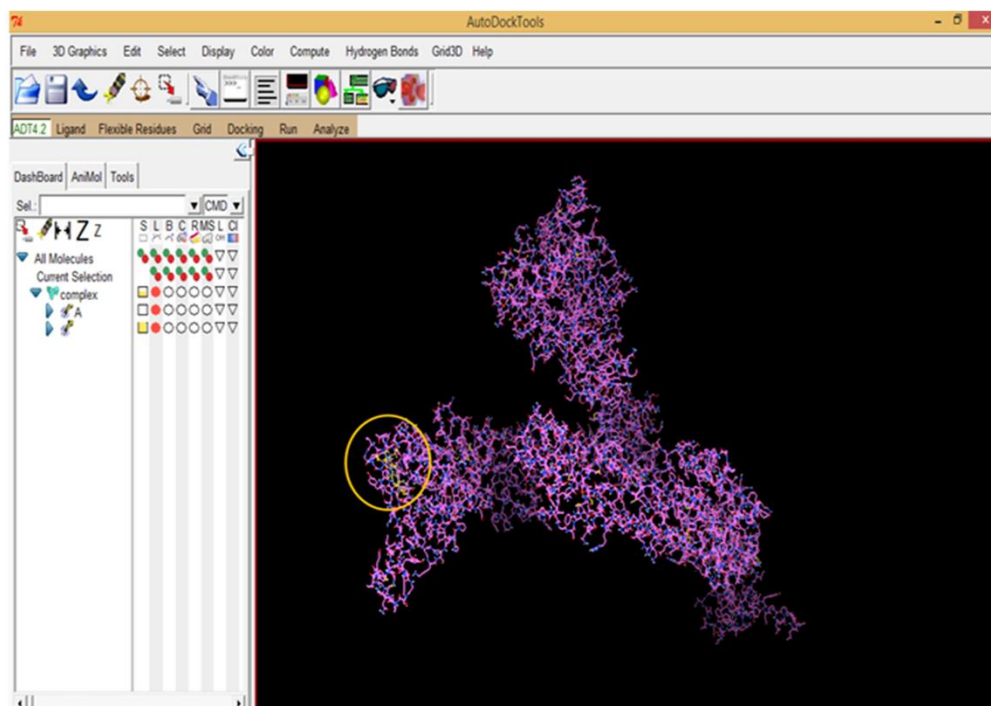
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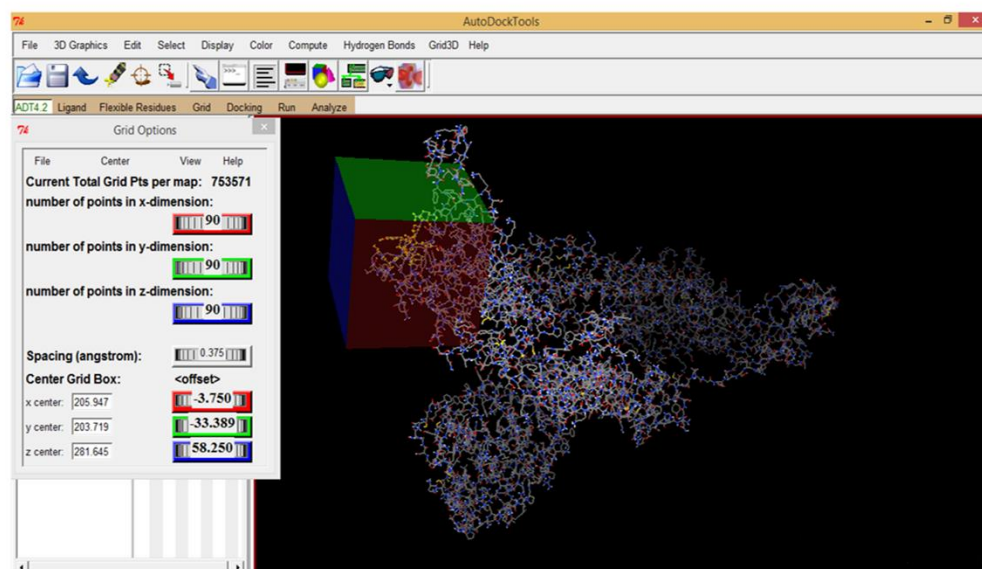
40	Gingerol	−2.1
41	Gallic acid	−2.0
42	E-cinnamaldehyde	−1.9
43	Menthol	−1.8
44	Ajoene	−1.7
45	Allicin	−1.7
46	Methyl allyl thiosulfinate	−1.7
47	Diallyl trisulfide	−1.6
48	Ursolic acid	−1.6
49	Gingerone A	−1.5
50	Emblicanin A	−1.3

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**A)**



**B)**



**Figure S1.** (A) A snapshot of the grid box enclosing the binding pocket of the representative macromolecule (B) Dimensions of the grid box set up around the ligand binding cavity of the protein.