

Table 1S: Docking summary results in form of Binding energy (Kcal/mol), Ki Value, Cluster and Confirmation. Herein we mentioned the results in terms of energy order from lower energy to higher energy.

No .	Compound Name	Binding Energy Kcal/mol	Ki Value	Cluster	Confirmation
1.	Carnosic acid	-7.21	5.23 μ M	1	100
2.	Girinimbine	-7.13	5.96 μ M	1	100
3.	Gingerol	-7.1	6.29 μ M	12	22
4.	Shogaol	-7.07	6.61 μ M	8	25
5.	Tannin	-7.04	6.96 μ M	1	100
6.	Cubebin	-6.97	7.73 μ M	18	30
7.	Piperine	-6.85	9.52 μ M	5	46
8.	6_paradol	-6.77	10.99 μ M	6	57
9.	Dehydrozingerone	-6.75	12.67 μ M	7	80
10.	Galangin	-6.65	13.45 μ M	4	60
11.	Capsaicin	-6.62	13.96 μ M	26	18
12.	Alkanet_root	-6.54	16.04 μ M	9	45
13.	Copaene.	-6.45	18.76 μ M	1	100
14.	Beta-cadinene	-6.37	21.45 μ M	1	100
15.	Caryophyllene_oxide	-6.18	29.44 μ M	1	100
16.	Crocetin	-6.01	39.1 μ M	1	100
17.	Thymoquinone	-5.96	42.83 μ M	2	100
18.	Beta-caryophyllene	-5.95	43.85 μ M	1	100
19.	Luteic_acid	-5.93	44.69 μ M	7	75
20.	Cubebene	-5.92	46.06 μ M	4	92
21.	Umbelliferone	-5.64	73.72 μ M	2	95
22.	Safranal	-5.11	179.56 μ M	2	82
23.	Terpinolene_oxide	-5.08	190.42 μ M	2	55
24.	Pinene	-5.04	202.8 μ M	1	100
25.	Beta-pinene	-5	217.05 μ M	1	100
26.	Crocin	-4.98	224.32 μ M	1	100
27.	Alpha-phellandrene	-4.95	236.66 μ M	1	100
28.	Eugenol	-4.95	237.15 μ M	3	80
29.	Cuminaldehyde	-4.94	241.01 μ M	1	100
30.	Alpha-TERPINEOL	-4.92	248.03 μ M	4	46
31.	Ferulic_acid	-4.91	253.55 μ M	3	72
32.	Sabinene.	-4.86	272.65 μ M	2	92
33.	Carene	-4.83	289.93 μ M	1	100
34.	Cinnamaldehyde	-4.76	322.51 μ M	1	100
35.	Limonene	-4.62	410.37 μ M	1	100
36.	Thujene	-4.55	465.45 μ M	2	90
37.	P-cymene	-4.36	636.99 μ M	1	100
38.	Myrcene	-4.25	762.16 μ M	3	95

39.	Terpinene	-4.24	785.21 μ M	1	100
40.	Diallyl trisulfide	-3.52	2.65 mM	4	46
41.	Diallyl disulfide	-3.41	3.17 mM	4	75
42.	Diallyl sulfide	-2.8	8.87 mM	4	47