

Appendix 3. Physicochemical Properties of Selected Phytochemicals

Mol ID	MOL012940	MOL003410	MOL005360	MOL008034	MOL008647
Molecule Name	<u>Spiradine A</u>	<u>Jujubogenin</u>	<u>Malkangunin</u>	<u>Ceanothic Acid</u>	<u>Moupinamide</u>
MW	311.5	472.8	432.6	486.8	313.4
AlogP	1.24	4.39	1.84	5.36	2.86
Hdon	1	2	2	3	3
Hacc	3	4	7	5	5
OB (%)	113.52	66.95	57.71	73.52	86.71
Caco-2	0.29	0.49	0.22	-0.05	0.55
BBB	0.14	-0.1	-0.2	-0.5	-0.5
DL	0.6	0.6	0.6	0.8	0.3
FASA-	0.27	0.24	0.3	0.31	0.33
HL	15.7	10	4.09	14.2	3.71
Hepatotoxicity	No	No	No	No	No
Carcinogenicity	No	No	No	No	No
Cytotoxicity	No	No	No	No	No
Mutagenicity	No	No	No	No	No

Appendix 4. Molecular docking results for Jujubogenin against EGFR, HSP90AA1, and STAT3 using CB-Dock2.

Complex	CurPocket ID	Vina score	Cavity volume (Å³)	Center (x, y, z)	Docking size (x, y, z)
Jujubogenin-EGFR	C4	-8.7	355	-61, 8, -33	23, 23, 23
Jujubogenin-HSP90AA1	C1	-7.5	1723	-8, -9, -24	23, 23, 23
Jujubogenin-STAT3	C1	-8.2	830	0, 25, 31	23, 23, 23