

Supplement F. ADME properties of the selected alkaloids using SwissADME tool.

S.No	Compound Name	Absorption					Distribution		Metabolism				
		C Log P	Ali Class	GI absorption	log Kp (cm/s)	Pgp substrate	BBB permeant	Bioavailability Score	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor
1	Vindoline	2.59	Soluble	High	-6.29	No	Yes	0.55	No	No	No	yes	No
2	Cryptolepine	3.29	Soluble	High	-5.35	Yes	Yes	0.55	Yes	yes	No	yes	Yes
3	Harmane	2.70	Moderately soluble	High	-5.08	Yes	Yes	0.55	No	No	No	No	Yes
4	Palmatine	2.64	Moderately soluble	High	-5.79	Yes	Yes	0.55	No	No	No	Yes	Yes
5	Pinoline	1.78	Moderately Soluble	High	-6.50	Yes	Yes	0.55	No	No	No	No	No
6	Jatrorrhizine	2.31	Moderately soluble	High	-5.94	Yes	Yes	0.55	Yes	No	No	Yes	Yes
7	Magnoflorine	0.65	Moderately soluble	High	-6.44	Yes	Yes	0.55	Yes	No	No	No	Yes
8	Groenlandicine	2.18	Moderately soluble	High	-5.93	Yes	Yes	0.55	Yes	No	No	Yes	Yes
9	Galegine	0.50	Soluble	High	-6.83	Yes	Yes	0.55	Yes	No	No	Yes	Yes
10	Radicamine B	-0.53	Soluble	High	-8.07	No	No	0.55	Yes	No	No	No	No
11	Vindoline	1.78	Soluble	High	-8.02	No	No	0.55	No	No	No	Yes	Yes
12	Norman	2.41	Soluble	High	-5.08	Yes	Yes	0.55	Yes	No	No	No	Yes
13	Berberine	2.53	Moderately soluble	High	-5.78	Yes	Yes	0.55	Yes	No	No	Yes	Yes
14	Catharanthine	3.10	Soluble	High	-6.36	Yes	Yes	0.55	No	No	No	Yes	Yes
15	Casurine 6-O- α -glucoside	-3.19	Soluble	Low	-11.10	Yes	No	0.55	No	No	No	No	No
16	Tembetarine	0.78	Moderately soluble	High	-6.25	Yes	Yes	0.55	No	No	No	Yes	Yes
17	Lupinine	1.46	Very soluble	High	-6.45	No	Yes	0.55	No	No	No	No	No
18	Mahanimbine	5.62	Poorly soluble	High	-3.61	Yes	No	0.55	No	No	No	No	No
19	Piperumbellatm A	2.58	Moderately soluble	High	-5.82	No	Yes	0.55	Yes	No	No	Yes	No
20	Echinulin	5.33	Poorly soluble	High	-4.12	Yes	No	0.55	No	Yes	Yes	No	Yes
21	Radicamine A	-0.40	Very soluble	High	-8.28	No	No	0.55	Yes	No	No	No	No
22	Tecostanine	1.59	Very soluble	High	-6.15	No	Yes	0.55	No	No	No	No	No
23	Vasicine	1.23	Very soluble	High	-7.14	No	No	0.55	No	No	No	No	No
24	Vasicinol	0.77	Very soluble	High	-7.48	Yes	No	0.55	No	No	No	No	No
25	Epiberberine	2.50	Moderately soluble	High	-5.78	Yes	Yes	0.55	Yes	No	No	No	Yes
26	Coptisine	2.40	Moderately soluble	High	-5.78	Yes	Yes	0.55	Yes	No	No	No	Yes
27	Conophylline	3.21	Poorly soluble	Low	-8.53	Yes	No	0.17	No	No	No	No	No
28	Physostigmine	2.04	Soluble	High	-6.86	Yes	Yes	0.55	No	No	No	Yes	No
29	Capsaicin	2.69	Moderately soluble	High	-5.62	No	Yes	0.55	Yes	No	No	Yes	Yes
30	Sanguinarine	2.72	Moderately soluble	High	-5.17	Yes	Yes	0.55	Yes	Yes	No	No	No
31	Matrine	2.27	Very soluble	High	-6.69	No	Yes	0.55	No	No	No	No	No