

Supplement E. SwissADME-derived molecular properties of alkaloids.

S.No	Compound	Molecular weight	Mlog P	Number of rotatable bonds	HBAs	HBDs	Total surface area (Å2)	# of Lipinski fails	Lipinski evalaution	# of Veber fails	Veber evalaution
1	Vindoline	336.43	3.12	2	3	1	41.75	0	yes	0	yes
2	Cryptolepine	232.28	3.29	0	1	0	17.82	0	yes	0	yes
3	Harmane	182.22	1.90	0	1	1	28.68	0	Yes	0	Yes
4	Palmatine	352.40	2.01	4	4	0	40.80	0	Yes	0	Yes
5	Pinoline	202.25	1.22	1	2	2	37.05	0	Yes	0	Yes
6	Jatrorrhizine	338.38	1.78	3	4	1	51.80	0	Yes	0	Yes
7	Magnoflorine	342.41	-1.71	2	4	2	58.92	0	Yes	0	Yes
8	Groenlandicine	322.33	1.96	1	4	1	51.80	0	Yes	0	Yes
9	Galegine	127.19	0.69	2	1	2	64.40	0	Yes	0	Yes
10	Radicamine B	225.24	-0.83	2	5	5	92.95	0	Yes	0	Yes
11	Vindoline	456.53	1.74	6	7	1	88.54	0	Yes	0	Yes
12	Norharman	168.19	1.62	0	1	1	28.68	0	Yes	0	Yes
13	Berberine	336.36	2.19	2	4	0	40.80	0	Yes	0	Yes
14	Catharanthine	336.43	2.96	3	3	1	45.33	0	Yes	0	Yes
15	Casurine 6-O- α -glucoside	365.38	-3.22	4	10	8	174.31	1	Yes	1	No
16	Tembetarine	344.42	-1.71	4	4	2	58.92	0	Yes	0	Yes
17	Lupinine	169.26	0.86	1	2	1	23.47	0	Yes	0	Yes
18	Mahanimbine	331.45	4.66	3	1	1	25.02	1	Yes	0	Yes
19	Piperumbellaatm A	265.26	2.34	1	3	2	62.32	0	Yes	0	Yes
20	Echinulin	461.64	3.55	8	2	3	73.99	0	Yes	0	Yes
21	Radicamine A	255.27	-1.09	3	6	5	102.18	1	Yes	0	Yes
22	Tecostanine	183.29	1.81	1	2	1	23.47	0	Yes	0	Yes
23	Vasicine	188.23	1.57	0	2	1	35.83	0	Yes	0	Yes
24	Vasicinol	204.23	0.99	0	3	2	56.06	0	Yes	0	Yes
25	Epiberberine	336.36	2.19	2	4	0	40.80	0	Yes	0	Yes
26	Coptisine	320.32	2.37	0	4	0	40.80	0	Yes	0	Yes
27	Conophylline	794.89	1.42	8	12	4	163.82	2	No	1	No
28	Physostigmine	275.35	2.04	3	3	1	44.81	0	Yes	0	Yes
29	Capsaicin	305.41	2.69	10	3	2	58.56	0	Yes	0	Yes
30	Sanguinarine	332.33	2.72	0	4	0	40.80	0	Yes	0	Yes
31	Matrine	248.36	2.27	0	2	0	23.55	0	Yes	0	Yes