

Supplementary Table 1. Analysis of druglikness properties of 100 physiochemical compounds.

S.No	Compound Names	Physiochemical properties											Pharmacokinetics								
		Formula	Molecular Weight (g/mol)	Num. heavy atoms	Num. arom. heavy atoms	Fracton Csp3	Num. rotatable bonds	Num. H-bond acceptors	Num. H-bond donors	Molar Refractivity	Lipophilicity [Log Po/w (XLOGP3)]	Water Solubility (mol/l)	Solubility Class	GI absorption	BBB permeant	P-gp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor
1	Apigenin	C15H10O5	270.24	20	16	0	1	5	3	73.99	3.02	1.14E-04	Soluble	High	No	No	Yes	No	No	Yes	Yes
2	Berberine	C20H18NO4	336.36	25	16	0.25	2	4	0	94.87	3.62	2.83E-05	Moderately soluble	High	Yes	Yes	Yes	No	No	Yes	Yes
3	Beta-sitosterol	C29H50O	414.71	30	0	0.93	6	1	1	133.23	9.34	1.26E-08	Poorly soluble	Low	No	No	No	No	No	No	No
4	Bisdemethoxycurcumin	C19H16O4	308.33	23	12	0.05	6	4	2	89.82	3.26	1.60E-04	Soluble	High	Yes	No	Yes	No	Yes	No	Yes
5	Brachyamide B	C20H25NO3	327.42	24	6	0.45	8	3	0	99.9	4.78	2.89E-05	Moderately soluble	High	Yes	No	No	Yes	Yes	Yes	Yes
6	Calebin-A	C21H20O7	384.38	28	12	0.14	9	7	2	103.89	3.27	9.85E-05	Moderately soluble	High	No	No	No	No	Yes	No	Yes
7	Campesterol	C28H48O	400.68	29	0	0.93	5	1	1	128.42	8.8	2.90E-08	Poorly soluble	Low	No	No	No	No	No	No	No
8	Chavicine	C17H19NO3	285.34	21	6	0.35	4	3	0	85.47	3.46	1.84E-04	Soluble	High	Yes	No	Yes	Yes	Yes	No	No
9	Cirsilineol	C18H16O7	344.32	25	16	0.17	4	7	2	91.44	3.4	4.72E-05	Moderately soluble	High	No	No	Yes	No	Yes	Yes	Yes
10	Cirsimaritin	C17H14O6	314.29	23	16	0.12	3	6	2	84.95	3.32	6.35E-05	Moderately soluble	High	No	No	Yes	No	Yes	Yes	Yes
11	Cordifolioside A	C22H32O13	504.48	35	6	0.64	10	13	7	116.08	-1.76	4.72E-02	Very soluble	Low	No	No	No	No	No	No	No
12	Cordioside	C26H34O12	538.54	38	5	0.69	6	12	5	126.02	-0.47	2.60E-03	Soluble	Low	No	Yes	No	No	No	No	No
13	Cratogeolic acid	C30H48O4	472.7	34	0	0.9	1	4	3	137.82	6.51	1.56E-07	Poorly	High	No	Yes	No	No	No	No	No

34	Piperine	C17H19NO3	285.34	21	6	0.35	4	3	0	85.47	3.46	1.84E-04	soluble	High	Yes	No	Yes	Yes	Yes	No	No
35	Piperolein (piperolein A)	C19H25NO3	315.41	23	6	0.53	7	3	0	95.56	4.17	7.02E-05	Moderately soluble	High	Yes	No	No	Yes	Yes	Yes	No
36	Piperolein B	C21H29NO3	343.46	25	6	0.57	9	3	0	105.18	5.25	1.38E-05	Moderately soluble	High	Yes	No	No	No	Yes	Yes	Yes
37	Quercetin	C15H10O7	302.24	22	16	0	1	7	5	78.03	1.54	6.98E-04	Soluble	High	No	No	Yes	No	No	Yes	Yes
38	Retrofractamide A	C20H25NO3	327.42	24	6	0.35	9	3	1	97.53	5.55	1.10E-05	Moderately soluble	High	Yes	No	Yes	Yes	Yes	No	Yes
39	Rhamnetin	C16H12O7	316.26	23	16	0.06	2	7	4	82.5	1.87	4.35E-04	Soluble	High	No	No	Yes	No	No	Yes	Yes
40	Rosmarinic acid	C18H16O8	360.31	26	12	0.11	7	8	5	91.4	2.36	3.63E-04	Soluble	Low	No	No	No	No	No	No	No
41	Somniferine A (Somniferine)	C36H36N2O7	608.68	45	12	0.47	3	9	2	171.39	2.61	5.53E-06	Moderately soluble	High	No	Yes	No	No	No	No	No
42	Stigmasterol	C29H48O	412.69	30	0	0.86	5	1	1	132.75	8.56	3.46E-08	Poorly soluble	Low	No	No	No	No	Yes	No	No
43	Tinocordifolioside	C21H32O8	412.47	29	0	0.86	4	8	4	102.01	-0.22	1.01E-02	Very soluble	High	No	Yes	No	No	No	No	No
44	Tinocordioside	C25H34O9	478.53	34	5	0.72	4	9	4	118.47	1.31	3.33E-04	Soluble	High	No	Yes	No	No	No	No	No
45	Tinosporide	C20H22O7	374.38	27	5	0.7	1	7	1	89.54	1.33	8.51E-04	Soluble	High	No	Yes	No	No	No	Yes	No
46	Trichostachine	C16H17NO3	271.31	20	6	0.31	4	3	0	80.67	3.11	3.64E-04	Soluble	High	Yes	No	Yes	Yes	No	No	No
47	Ursolic acid	C30H48O3	456.7	33	0	0.9	1	3	2	136.91	7.34	5.89E-08	Poorly soluble	Low	No	No	No	No	No	No	No
48	Vicenin (Vicenin-2)	C27H30O15	594.52	42	16	0.44	5	15	11	139.23	-2.26	8.83E-03	Soluble	Low	No	No	No	No	No	No	No
49	Withaferin A	C28H38O6	470.6	34	0	0.79	3	6	2	127.49	3.83	1.07E-05	Moderately soluble	High	No	Yes	No	No	No	No	No
50	Withanolide	C28H38O6	470.6	34	0	0.79	2	6	2	127.53	3.12	2.56E-05	Moderately soluble	High	No	Yes	No	No	No	No	No
51	Withanolide B	C28H38O5	454.6	33	0	0.79	2	5	1	126.33	4.66	3.45E-06	Moderately	High	No	Yes	No	No	Yes	No	No

52	Withanone	C28H38O6	470.6	34	0	0.79	2	6	2	127.53	3.05	2.84E-05	Moderately soluble	High	No	Yes	No	No	No	No	No	No
53	Thymoquinone	C10H12O2	164.2	12	0	0.4	1	2	0	47.52	2.2	6.64E-03	Soluble	High	Yes	No	No	No	No	No	No	No
54	Eugenol	C10H12O2	164.2	12	6	0.2	3	2	1	49.06	2.27	3.47E-03	Soluble	High	Yes	No	Yes	No	No	No	No	No
55	Glycyrrhizin	C42H62O16	822.93	58	0	0.86	7	16	8	202.84	2.8	5.70E-07	Poorly soluble	Low	No	Yes	No	No	No	No	No	No
56	Antraquinone	C14H8O2	208.21	16	12	0	0	2	0	59.75	3.39	1.51E-04	Soluble	High	Yes	No	Yes	Yes	No	No	No	No
57	Baicalin	C21H18O11	446.36	32	16	0.24	4	11	6	106.72	1.11	3.87E-04	Soluble	Low	No	Yes	No	No	No	No	No	No
58	Honokiol	C18H18O2	266.33	20	12	0.11	5	2	2	84.14	4.98	1.81E-05	Moderately soluble	High	Yes	No	Yes	Yes	Yes	Yes	Yes	Yes
59	Myricetin	C15H10O8	318.24	23	16	0	1	8	6	80.06	1.18	9.88E-04	Soluble	Low	No	No	Yes	No	No	No	No	Yes
60	Andrographolide	C20H30O5	350.45	25	0	0.75	3	5	3	95.21	2.16	6.67E-04	Soluble	High	No	Yes	No	No	No	No	No	No
61	Naringenin	C15H12O5	272.25	20	12	0.13	1	5	3	71.57	2.52	3.21E-04	Soluble	High	No	Yes	Yes	No	No	No	No	Yes
62	6-Gingerol	C17H26O4	294.39	21	6	0.59	10	4	2	84.55	2.76	1.11E-03	Soluble	High	Yes	No	Yes	No	No	Yes	No	No
63	Bavachinin	C21H22O4	338.4	25	12	0.29	4	4	1	97.74	4.45	1.47E-05	Moderately soluble	High	Yes	No	No	Yes	Yes	Yes	Yes	Yes
64	Neobavaisoflavone	C20H18O4	322.35	24	16	0.15	3	4	2	95.69	4.4	1.24E-05	Moderately soluble	High	Yes	No	Yes	No	Yes	No	Yes	Yes
65	Isobavachalcone	C20H20O4	324.37	24	12	0.15	5	4	3	96.04	5.1	7.87E-06	Moderately soluble	High	No	No	Yes	No	Yes	No	Yes	Yes
66	4'-O-methylbavachalcone	C22H24O4	352.42	26	12	0.23	7	4	1	104.98	5.76	2.93E-06	Moderately soluble	High	Yes	No	Yes	Yes	Yes	Yes	No	Yes
67	Psoralidin	C20H16O5	336.34	25	17	0.15	2	5	2	97.53	4.69	5.61E-06	Moderately soluble	High	No	No	Yes	Yes	Yes	Yes	No	No
68	corylifol A	C25H26O4	390.47	29	16	0.24	6	4	2	119.25	6.25	6.16E-07	Poorly soluble	High	No	No	No	Yes	No	No	No	Yes

69	lycorine	C16H17NO4	287.31	21	6	0.5	0	5	2	78.4	-0.02	1.51E-02	Very soluble	High	No	Yes	No	No	No	Yes	No
70	kappa-Carrageenan	C24H36O25S2	788.66	51	0	1	12	25	8	143.4	-8.35	2.10E+01	Highly soluble	Low	No	Yes	No	No	No	No	No
71	lamda-Carrageenan	C14H26O19S3	594.54	36	0	1	11	19	6	107.87	-3.94	4.81E-01	Very soluble	Low	No	Yes	No	No	No	No	No
72	beta-Carrageenan	C14H24O9	336.33	23	0	1	4	9	4	73.14	-1.79	2.93E-01	Very soluble	Low	No	Yes	No	No	No	No	No
73	Nelfinavir	C32H45N3O4S	567.78	40	12	0.56	12	5	4	166.17	5.67	4.34E-07	Poorly soluble	Low	No	Yes	No	Yes	No	No	Yes
74	Hinokinin	C20H18O6	354.35	26	12	0.35	4	6	0	91.23	3.65	3.85E-05	Moderately soluble	High	Yes	No	Yes	Yes	Yes	Yes	Yes
75	Luteolin	C15H10O6	286.24	21	16	0	1	6	4	76.01	2.53	1.97E-04	Soluble	High	No	No	Yes	No	No	Yes	Yes
76	Aloe-emodin	C15H10O5	270.24	20	12	0.07	1	5	3	69.92	1.82	9.12E-04	Soluble	High	No	No	Yes	No	No	No	Yes
77	Hypericin	C30H16O8	504.44	38	22	0.07	0	8	6	144.83	5.71	1.02E-07	Poorly soluble	Low	No	No	No	Yes	Yes	No	No
78	Glabridin	C20H20O4	324.37	24	12	0.3	1	4	2	93.25	3.89	2.48E-05	Moderately soluble	High	Yes	Yes	Yes	Yes	Yes	Yes	Yes
79	Sageone	C19H24O3	300.39	22	6	0.53	1	3	2	89.49	3.67	7.07E-05	Moderately soluble	High	Yes	Yes	No	No	No	No	No
80	Psoralidin	C20H16O5	336.34	25	17	0.15	2	5	2	97.53	4.69	5.61E-06	Moderately soluble	High	No	No	Yes	Yes	Yes	No	No
81	Emodin	C15H10O5	270.24	20	12	0.07	0	5	3	70.78	2.72	2.12E-04	Soluble	High	No	No	Yes	No	No	No	Yes
82	Cinanserin	C20H24N2OS	340.48	24	12	0.25	9	2	1	104.21	4.09	4.97E-05	Moderately soluble	High	Yes	No	Yes	Yes	Yes	Yes	Yes
83	Liquiritigenin	C15H12O4	256.25	19	12	0.13	1	4	2	69.55	2.3	5.26E-04	Soluble	High	Yes	Yes	Yes	No	No	No	No
84	Lapachol	C15H14O3	242.27	18	6	0.2	2	3	1	69.95	2.79	6.10E-04	Soluble	High	Yes	No	Yes	Yes	No	No	No
85	Hibiscus Acid	C6H6O7	190.11	13	0	0.5	2	7	3	34.87	-1.23	7.73E-01	Very soluble	Low	No	No	No	No	No	No	No

86	Hydroxytyrosol	C8H10O3	154.16	11	6	0.25	2	3	3	41.42	-0.72	2.43E-01	Very soluble	High	No	No	No	No	No	No	No
87	Carvacrol	C10H14O	150.22	11	6	0.4	1	1	1	48.01	3.49	4.92E-04	Soluble	High	Yes	No	Yes	No	No	No	No
88	Cinnamic	C9H8O2	148.16	11	6	0	2	2	1	43.11	2.13	4.25E-03	Soluble	High	Yes	No	No	No	No	No	No
89	Methyl Cinnamate	C10H10O2	162.19	12	6	0.1	3	2	0	47.43	2.62	2.15E-03	Soluble	High	Yes	No	No	No	No	No	No
90	Thymohydroquinone	C10H14O2	166.22	12	6	0.4	1	2	2	50.03	2.94	9.40E-04	Soluble	High	Yes	No	Yes	No	No	No	No
91	Thymol	C10H14O	150.22	11	6	0.4	1	1	1	48.01	3.3	6.49E-04	Soluble	High	Yes	No	Yes	No	No	No	No
92	Cinnamaldehyde	C9H8O	132.16	10	6	0	2	1	0	41.54	1.9	6.79E-03	Soluble	High	Yes	No	No	No	No	No	No
93	Ajoene	C9H14OS3	234.4	13	0	0.33	8	1	0	67.41	1.71	1.44E-02	Very soluble	High	No	No	No	No	Yes	No	No
94	Allicin	C6H10OS2	162.27	9	0	0.33	5	1	0	45.88	1.31	4.56E-02	Very soluble	High	Yes	No	No	No	No	No	No
95	Diallyl Trisulfide	C6H10S3	178.34	9	0	0.33	6	0	0	52.78	2.64	6.12E-03	Soluble	High	Yes	No	No	No	No	No	No
96	Saikosaponin	C42H68O13	780.98	55	0	0.95	6	13	8	199.82	2.52E+00	1.34E-06	Moderately soluble	low	No	Yes	No	No	No	No	No
97	Myricitrin	C21H20O12	464.38	33	16	0.29	3	12	8	111.02	0.51	6.29E-04	Soluble	Low	No	No	No	No	No	No	No
98	Corydine	C20H23NO4	341.4	25	12	0.4	3	5	1	100.47	2.57	1.85E-04	Soluble	High	Yes	Yes	Yes	No	No	Yes	Yes
99	Aloin	C21H22O9	418.39	30	12	0.38	3	9	7	101.96	-0.12	3.50E-03	Soluble	Low	No	No	No	No	No	No	No
100	Catechin	C15H14O6	290.27	21	12	0.2	1	6	5	74.33	0.36	5.98E-03	Soluble	High	No	Yes	No	No	No	No	No