

Supplementary Information

Biologically active isoquinoline alkaloids with drug-like properties from the genus *Corydalis*

Iranshahy M¹, Quinn RJ², Iranshahi M^{1*}

¹*Biotechnology Research Center and School of Pharmacy, Mashhad University of Medical Sciences, Mashhad, Iran*

²*Eskitis institute, Griffith University, Brisbane QLD 4111, Australia*

***To whom correspondence should be addressed:**

Mehrdad Iranshahi, Pharm.D., Ph.D.

Professor of Pharmacognosy

Biotechnology Research Center

School of Pharmacy, Mashhad University of Medical Sciences, Mashhad, Iran

E-mail: Iranshahim@mums.ac.ir

Tel: +98-511-8823255

Fax: +98-511-8823251

Full table 2. *In silico* physico-chemical properties of CA. For oral bioavailability, NROT, HBA, HBD, cLogP, PSA and MW should less than 10, 10, 5, 5, 140 and 500, respectively. Log D_{5.5} is defined as Log P at pH 5.5 (pH of the small intestine) and is a more appropriate measure than Log P where oral drug absorption occurs. All physiochemical parameters used for the prediction of drug-likeness were calculated using Marvin Sketch (version 5.11, academic package, Chem Axon).

No	MW	NROT	HBA	HBD	PSA	cLog P	Log D _{5.5}	Bioavailability prediction
1	327	2	5	2	62.18	2.86	1.98	√
2	369	3	7	1	77.46	2.93	0.20	√
3	355	3	7	2	86.25	2.55	0.08	√
4	371	5	7	2	86.25	2.61	0.14	√
5	371	5	7	2	86.25	2.61	0.14	√
6	283	4	3	1	30.49	3.33	0.17	√
7	283	4	3	1	30.49	3.33	0.17	√
8	336	2	4	0	40.80	-1.28	-1.28	√
9	369	5	6	0	57.23	3.05	1.39	√
10	367	0	6	1	60.39	2.55	2.20	√
11	365	0	6	0	49.39	3.34	3.34	√
12	381	0	7	1	77.49	1.90	1.90	√
13	352	4	4	0	40.80	-1.22	-1.22	√
14	366	4	4	0	40.80	-0.71	-0.71	√
15	320	0	4	0	40.80	-1.34	-1.34	√
16	350	2	4	0	40.80	-0.77	-0.77	√

17	336	2	4	0	40.80	-1.28	-1.28	√
18	324	2	4	2	62.80	-1.51	-1.59	√
19	322	1	4	1	51.80	-1.43	-1.45	√
20	274	0	0	0	3.88	0.95	0.95	√
21	304	0	2	0	22.34	0.06	0.06	√
22	366	4	4	0	40.80	-0.71	-0.71	√
23	336	2	4	0	40.80	-1.28	-1.28	√
24	320	0	4	0	40.80	-1.34	-1.34	√
25	336	1	4	1	51.80	-0.92	-0.93	√
26	336	1	4	1	51.80	-0.92	-0.94	√
27	339	0	6	1	66.02	2.21	0.11	√
28	367	0	6	0	57.23	3.14	3.01	√
29	353	0	7	1	83.09	2.09	1.56	√
30	353	0	6	0	57.23	2.59	2.49	√
31	660	8	10	0	97.81	5.62	5.33	×
32	650	8	8	1	79.88	5.68	2.23	√
33	355	3	5	1	51.16	3.42	3.12	√
34	353	4	5	0	40.16	3.47	3.41	√
35	323	3	4	0	30.93	3.63	3.57	√
36	369	4	6	1	60.39	3.17	3.13	√
37	367	4	5	0	40.16	3.98	3.90	√
38	341	4	5	1	48.95	2.69	-0.48	√
39	311	3	4	1	39.72	2.85	-0.33	√

40	355	4	5	0	40.16	3.07	1.47	√
41	325	3	4	0	30.93	3.23	1.31	√
42	341	3	5	1	51.16	2.92	1.28	√
43	353	4	6	0	66.35	2.56	2.56	√
44	311	1	4	1	49.77	2.44	0.43	√
45	414	7	7	2	89.49	1.99	-1.26	√
46	366	3	5	0	50.03	-1.44	-1.44	√
47	364	1	5	0	67.10	-1.85	-1.85	√
48	364	1	5	0	67.10	-1.85	-1.85	√
49	327	2	5	2	62.16	2.78	1.35	√
50	341	3	5	1	51.16	2.92	1.28	√
51	355	3	5	1	51.16	3.37	3.03	√
52	385	5	6	0	49.39	2.72	2.87	√
53	339	2	5	0	40.16	3.09	3.08	√
54	355	4	5	0	40.16	3.15	2.84	√
55	400	4	7	1	96.98	3.31	3.17	√
56	384	2	7	1	96.98	3.25	2.02	√
57	353	2	5	0	40.16	3.45	2.99	√
58	353	2	5	0	40.16	3.45	2.99	√
59	323	0	5	0	40.16	3.03	2.76	√
60	405	4	6	0	57.23	3.66	3.88	√
61	332	0	4	0	40.80	-0.94	-0.94	√
62	382	4	6	1	78.10	-2.08	-3.46	√

63	420	5	4	0	55.84	3.25	3.25	√
64	367	4	5	0	57.23	2.26	2.26	√
65	299	4	4	1	41.93	3.06	0.85	√
66	363	1	6	0	49.39	3.99	3.99	√
67	285	3	4	3	61.72	2.86	-0.36	√
68	327	2	5	2	62.16	2.86	2.03	√
69	418	4	8	3	155	-0.77	2.45	√
70	432	4	8	2	150.56	-1.43	0.12	√
71	356	4	4	1	41.36	-0.35	2.84	√
72	371	4	5	0	63.80	2.02	2.02	√
73	326	3	3	1	32.13	-0.2	2.73	√
74	324	0	4	1	41.36	-0.48	2.76	√
75	342	3	4	2	52.36	-0.50	2.61	√
76	340	2	4	1	41.36	-0.41	2.80	√
77	357	3	5	1	74.80	1.88	1.88	√
78	357	3	5	1	74.80	1.88	1.88	√
79	338	0	4	0	36.92	-1.14	-1.14	√
80	328	2	5	2	63.36	-0.65	2.73	√
81	328	2	5	2	63.36	-0.65	2.03	√
82	340	1	5	1	52.36	-0.20	2.83	√
83	342	3	5	1	52.36	-0.5	2.80	√
84	369	0	7	2	80.62	1.40	-0.27	√
85	367	1	6	0	66.46	2.66	0.75	√

86	367	1	6	0	66.46	2.66	0.75	√
87	365	0	6	0	49.39	3.34	3.34	√