

Supporting information

Chemical Diversity, Medicinal Potentialities, Biosynthesis and Pharmacokinetics of Anthraquinones Derived from Marine Fungi: A Comprehensive Update

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Table S1. Drug-likeness properties of marine-derived fungal anthraquinones. The compounds' numbers are according to the main text.

Molecule	MW	H-bond		Consensus Log P	Fraction Csp3	RB	TPSA	ESOL Log S	ESOL Class	MR	Bioavailability Score	Lipinski	Ghose	Veber	Egan	Muegge
		acceptors	donors													
NIG																
1	596.58	12	8	0.42	0.45	2	222.28	-3.94	S	149.03	0.17	3	3	1	1	3
2	338.35	7	4	0.79	0.59	2	116.45	-2.39	S	85.01	0.55	0	0	0	0	0
3	320.29	7	4	0.17	0.38	1	124.29	-1.93	VS	77.92	0.56	0	0	0	0	0
4	300.26	6	3	1.99	0.12	1	104.06	-4.08	MS	77.28	0.55	0	0	0	0	0
5	284.26	5	2	2.57	0.12	1	83.83	-4.81	MS	75.25	0.55	0	0	0	0	0
6	304.29	6	3	0.91	0.38	1	104.06	-2.54	S	76.76	0.56	0	0	0	0	0
7	324.33	7	5	0.4	0.56	1	127.45	-2.03	S	80.28	0.55	0	0	0	0	0
8	340.33	8	6	-0.53	0.56	1	147.68	-1.51	VS	81.44	0.55	1	1	1	1	1
9	320.29	7	4	0.75	0.38	1	124.29	-2.75	S	78.78	0.56	0	0	0	0	0
10	336.29	8	5	-0.05	0.38	1	144.52	-2.14	S	79.94	0.56	0	1	1	1	0
ASP																
7	324.33	7	5	0.4	0.56	1	127.45	-2.03	S	80.28	0.55	0	0	0	0	0
8	340.33	8	6	-0.53	0.56	1	147.68	-1.51	VS	81.44	0.55	1	1	1	1	1
10	336.29	8	5	-0.05	0.38	1	144.52	-2.14	S	79.94	0.56	0	1	1	1	0
11	460.39	9	5	2.88	0.08	2	165.5	-5.69	MS	121.27	0.55	0	0	1	1	1
12	474.42	9	4	3.14	0.12	3	154.5	-5.9	MS	125.74	0.55	0	0	1	1	1
13	270.24	5	3	1.87	0.07	0	94.83	-3.67	S	70.78	0.55	0	0	0	0	0
14	284.26	5	2	2.27	0.12	1	83.83	-3.87	S	75.25	0.55	0	0	0	0	0
15	288.3	5	3	1.94	0.31	1	86.99	-3.36	S	78.35	0.55	0	0	0	0	0
16	288.3	5	3	1.92	0.31	1	86.99	-3.43	S	78.31	0.55	0	0	0	0	0
17	288.3	5	3	1.92	0.31	1	86.99	-3.43	S	78.31	0.55	0	0	0	0	0
18	286.24	6	4	1.63	0.07	0	115.06	-3.87	S	72.81	0.55	0	0	0	0	0
19	300.26	6	3	1.96	0.12	1	104.06	-4.08	MS	77.28	0.55	0	0	0	0	0
20	402.35	9	4	1.11	0.25	6	150.59	-3.25	S	98.47	0.55	0	0	1	1	1
21	538.54	8	4	4.66	0.19	3	133.52	-7.47	PS	147.55	0.55	1	2	0	1	1

22	524.52	8	5	4.31	0.16	2	144.52	-7.26	PS	143.08	0.55	1	2	1	1	1
23	524.52	8	5	4.27	0.16	2	144.52	-7.26	PS	143.08	0.55	1	2	1	1	1
24	754.78	13	6	5.9	0.33	14	217.35	-9.18	PS	201.5	0.17	3	4	2	2	5
25	726.72	13	8	5.22	0.3	12	239.35	-9.17	PS	192.04	0.17	3	4	2	1	5
26	372.37	7	5	2.52	0.3	5	135.29	-4.69	MS	98	0.55	0	0	0	1	0
27	386.4	7	4	2.8	0.33	6	124.29	-4.69	MS	102.73	0.55	0	0	0	0	0
28	354.35	6	4	3.01	0.2	4	115.06	-4.96	MS	97.16	0.55	0	0	0	0	0
29	400.42	7	3	3.22	0.36	7	113.29	-5.12	MS	106.94	0.55	0	0	0	0	0
30	368.34	7	3	2.32	0.3	0	113.29	-4.33	MS	93.4	0.55	0	0	0	0	0
31	382.36	7	2	2.74	0.33	1	102.29	-4.54	MS	97.87	0.55	0	0	0	0	0
32	396.39	7	1	3.06	0.36	2	91.29	-4.76	MS	102.34	0.55	0	0	0	0	0
33	340.28	7	3	1.7	0.22	0	113.29	-3.75	S	83.75	0.55	0	0	0	0	0
34	356.28	8	4	0.87	0.22	0	133.52	-3.22	S	84.91	0.55	0	0	0	1	0
36	356.33	7	4	1.84	0.26	1	124.29	-3.92	S	91.01	0.55	0	0	0	0	0
37	384.34	8	4	1.52	0.3	0	133.52	-3.8	S	94.56	0.55	0	0	0	1	0
38	412.39	8	2	2.26	0.36	2	111.52	-4.23	MS	103.5	0.55	0	0	0	0	0
39	360.31	8	6	0.79	0.22	4	155.52	-2.81	S	89.55	0.55	1	0	1	1	2
40	388.37	8	4	1.52	0.3	6	133.52	-3.23	S	98.49	0.55	0	0	0	1	0
41	284.26	5	2	2.19	0.12	1	83.83	-3.87	S	75.25	0.55	0	0	0	0	0
42	328.32	6	3	1.97	0.22	3	104.06	-3.74	S	86.03	0.55	0	0	0	0	0
43	368.34	7	1	2.42	0.3	2	91.29	-4.18	MS	92.69	0.55	0	0	0	0	0
44	366.32	7	1	2.42	0.2	2	91.29	-4.36	MS	92.21	0.55	0	0	0	0	0
45	300.26	6	3	1.86	0.12	1	104.06	-3.73	S	77.28	0.55	0	0	0	0	0
46	314.29	6	2	2.23	0.18	2	93.06	-3.95	S	81.75	0.55	0	0	0	0	0
47	238.24	3	1	2.72	0.07	0	54.37	-4.25	MS	66.74	0.55	0	0	0	0	0
48	298.29	5	1	2.26	0.18	3	72.83	-3.6	S	78.52	0.55	0	0	0	0	0
49	222.24	2	0	3.01	0.07	0	34.14	-4.22	MS	64.72	0.55	0	0	0	0	0
50	282.25	5	1	1.84	0.06	2	80.67	-3.46	S	73.65	0.55	0	0	0	0	0
51	240.21	4	2	1.98	0	0	74.6	-3.81	S	63.8	0.55	0	0	0	0	0
52	254.24	4	2	2.23	0.07	0	74.6	-3.82	S	68.76	0.55	0	0	0	0	0
53	270.24	5	3	1.5	0.07	0	94.83	-3.67	S	70.78	0.55	0	0	0	0	0

54	284.26	5	2	1.98	0.12	1	83.83	-3.53	S	75.25	0.55	0	0	0	0	0
55	316.26	7	3	1.52	0.12	2	117.2	-3.27	S	82.93	0.55	0	0	0	0	0
56	270.24	5	3	2	0.07	0	94.83	-4.02	MS	70.78	0.55	0	0	0	0	0
57	298.29	5	1	2.6	0.18	2	72.83	-4.08	MS	79.72	0.55	0	0	0	0	0
58	284.26	5	2	2.43	0.12	1	83.83	-4.23	MS	75.25	0.55	0	0	0	0	0
59	288.25	6	4	1.95	0.13	0	107.22	-3.83	S	73.91	0.55	0	0	0	0	0
60	302.28	6	3	2.34	0.19	1	96.22	-4.04	MS	78.38	0.55	0	0	0	0	0
61	388.32	9	5	0.87	0.21	5	161.59	-3.38	S	94	0.55	0	0	1	1	1
62	300.26	6	3	1.42	0.12	2	104.06	-3.1	S	76.41	0.55	0	0	0	0	0
63	300.26	6	3	1.5	0.12	2	104.06	-3.1	S	76.41	0.55	0	0	0	0	0
64	300.26	6	3	1.97	0.12	1	104.06	-4.08	MS	77.28	0.55	0	0	0	0	0
65	340.28	7	3	1.7	0.22	0	113.29	-3.75	S	83.75	0.55	0	0	0	0	0
66	340.28	7	3	1.6	0.22	0	113.29	-3.75	S	83.75	0.55	0	0	0	0	0
67	370.35	7	4	2.46	0.25	5	132.13	-4.74	MS	97.26	0.55	0	0	0	1	0
68	386.4	7	4	2.94	0.33	6	124.29	-4.9	MS	102.47	0.55	0	0	0	0	0
69	400.42	7	3	3.3	0.36	7	113.29	-4.9	MS	107.2	0.55	0	0	0	0	0
70	428.47	7	4	3.9	0.42	9	124.29	-5.51	MS	117.15	0.55	0	0	0	0	1
71	406.81	7	5	3.02	0.3	5	135.29	-5.29	MS	103.01	0.55	0	0	0	1	0
72	420.84	7	4	3.42	0.33	6	124.29	-5.5	MS	107.48	0.55	0	0	0	0	0
73	420.84	7	4	3.42	0.33	6	124.29	-5.29	MS	107.74	0.55	0	0	0	0	0
74	434.87	7	3	3.81	0.36	7	113.29	-5.5	MS	112.21	0.55	0	0	0	0	0
75	462.92	7	4	4.41	0.42	9	124.29	-6.11	PS	122.16	0.55	0	0	0	0	1
76	388.8	6	4	3.55	0.2	4	115.06	-5.56	MS	102.17	0.55	0	0	0	0	1
77	402.82	6	3	3.94	0.24	5	104.06	-5.78	MS	106.64	0.55	0	0	0	0	1
78	465.29	7	4	3.44	0.33	6	124.29	-5.82	MS	110.17	0.55	0	0	0	0	1
79	479.32	7	3	3.9	0.36	7	113.29	-5.82	MS	114.9	0.55	0	0	0	0	1
80	414.45	7	2	3.54	0.39	8	102.29	-5.12	MS	111.67	0.55	0	0	0	0	0

PEN

13	270.24	5	3	1.87	0.07	0	94.83	-3.67	S	70.78	0.55	0	0	0	0	0
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17	288.3	5	3	1.92	0.31	1	86.99	-3.43	S	78.31	0.55	0	0	0	0	0
26	372.37	7	5	2.52	0.3	5	135.29	-4.69	MS	98	0.55	0	0	0	1	0
27	386.4	7	4	2.8	0.33	6	124.29	-4.69	MS	102.73	0.55	0	0	0	0	0
37	384.34	8	4	1.52	0.3	0	133.52	-3.8	S	94.56	0.55	0	0	0	1	0
81	520.48	10	6	2.96	0.25	2	181.82	-6.52	PS	134.57	0.11	2	2	1	1	3
82	536.48	11	7	2.25	0.25	3	202.05	-5.76	MS	135.73	0.11	3	2	1	1	3
83	254.24	4	2	2.38	0.07	0	74.6	-4.11	MS	68.76	0.55	0	0	0	0	0
84	286.24	6	4	1.08	0.07	1	115.06	-2.9	S	71.95	0.55	0	0	0	0	0
85	376.74	7	2	2.46	0.17	4	110.13	-4.14	MS	91.16	0.55	0	0	0	0	0
86	366.3	9	4	0.44	0.07	3	166.81	-2.82	S	82.14	0.11	0	0	1	1	1
87	350.3	8	3	1.29	0.07	2	146.58	-3.59	S	80.98	0.56	0	0	1	1	0
88	270.24	5	3	1.5	0.07	1	94.83	-3.04	S	69.92	0.55	0	0	0	0	0
89	413.38	8	4	1.79	0.24	6	150.23	-4.14	MS	104.13	0.55	0	0	1	1	1
90	399.35	8	5	1.52	0.2	5	161.23	-3.92	S	99.81	0.11	0	0	1	1	1
91	433.8	8	5	1.95	0.2	5	161.23	-4.52	MS	104.82	0.11	0	0	1	1	1
92	427.4	8	4	2.11	0.27	7	150.23	-4.37	MS	108.94	0.55	0	0	1	1	1
93	413.38	8	5	1.73	0.24	6	161.23	-4.16	MS	104.62	0.11	0	0	1	1	1
94	447.82	8	5	2.27	0.24	6	161.23	-4.76	MS	109.63	0.11	0	0	1	1	1
95	447.82	8	5	2.23	0.24	6	161.23	-4.76	MS	109.63	0.11	0	0	1	1	1
96	371.3	8	5	0.84	0.11	4	161.23	-3.23	S	90.2	0.11	0	0	1	1	1
97	300.22	7	4	1.07	0	1	132.13	-3.22	S	72.78	0.56	0	0	0	1	0
98	320.68	6	4	1.62	0.07	1	115.06	-3.49	S	76.96	0.55	0	0	0	0	0

STE

99	336.29	8	5	-0.67	0.38	1	144.52	-1.2	VS	79.36	0.55	0	1	1	1	0
100	322.31	7	5	-0.11	0.44	1	127.45	-1.49	VS	78.94	0.55	0	1	0	0	0
101	304.29	6	3	1.11	0.38	1	104.06	-2.42	S	77.04	0.55	0	0	0	0	0
102	308.33	6	4	0.72	0.56	1	107.22	-2.17	S	78.25	0.55	0	0	0	0	0
103	346.33	7	2	1.55	0.39	3	110.13	-2.88	S	86.78	0.55	0	0	0	0	0

104	320.29	7	4	0.24	0.38	1	124.29	-1.81	VS	78.2	0.55	0	0	0	0	0
105	324.33	7	5	-0.22	0.56	1	127.45	-1.64	VS	79.42	0.55	0	1	0	0	0
106	366.36	8	4	0.31	0.56	3	133.52	-2.12	S	89.15	0.55	0	0	0	1	0
107	340.33	8	6	-0.91	0.56	1	147.68	-1.12	VS	80.58	0.55	1	1	1	1	1
108	284.26	5	2	2.22	0.12	1	83.83	-3.87	S	75.25	0.55	0	0	0	0	0
109	364.33	8	2	1.65	0.12	3	135.58	-3.8	S	85.45	0.56	0	0	0	1	0
110	488.44	11	4	0.93	0.38	6	169.05	-3.52	S	117.11	0.55	1	1	1	1	2
111	352.29	9	5	-0.9	0.5	1	157.05	-1.06	VS	78.89	0.55	0	1	1	1	1
112	618.54	13	7	1.08	0.25	3	228.35	-4.65	MS	153.61	0.17	3	3	1	1	4
113	618.54	13	7	1.08	0.25	3	228.35	-4.65	MS	153.61	0.17	3	3	1	1	4
114	566.51	10	4	3.95	0.12	3	167.66	-7.22	PS	149.5	0.55	1	2	1	1	2
115	670.57	16	10	-1.82	0.38	3	289.04	-2.11	S	157.72	0.17	3	4	1	1	5
116	670.57	16	10	-1.82	0.38	3	289.04	-2.11	S	157.72	0.17	3	4	1	1	5
117	618.54	13	7	1.02	0.25	3	228.35	-4.65	MS	153.61	0.17	3	3	1	1	4
118	566.51	10	4	3.94	0.12	3	167.66	-7.22	PS	149.5	0.55	1	2	1	1	2
119	566.51	10	4	3.95	0.12	3	167.66	-7.22	PS	149.5	0.55	1	2	1	1	2
120	622.57	13	7	0.74	0.38	3	228.35	-3.92	S	154.24	0.17	3	3	1	1	4
121	606.57	12	6	1.64	0.38	3	208.12	-4.52	MS	153.08	0.17	3	3	1	1	4
122	566.51	10	4	3.86	0.12	3	167.66	-7.22	PS	149.5	0.55	1	2	1	1	2
123	602.54	12	6	2	0.25	3	208.12	-5.27	MS	152.45	0.17	3	2	1	1	4
124	602.54	12	6	1.98	0.25	3	208.12	-5.27	MS	152.45	0.17	3	2	1	1	4
125	618.54	13	7	1.19	0.25	3	228.35	-4.65	MS	153.61	0.17	3	3	1	1	4
126	618.54	13	7	1	0.25	3	228.35	-4.65	MS	153.61	0.17	3	3	1	1	4
127	618.54	13	7	1	0.25	3	228.35	-4.65	MS	153.61	0.17	3	3	1	1	4
128	632.57	13	6	1.43	0.27	4	217.35	-5.01	MS	158.34	0.17	3	3	1	1	4
129	446.4	10	5	0.64	0.36	4	162.98	-3.4	S	107.38	0.55	0	0	1	1	1
130	606.57	12	6	1.74	0.38	3	208.12	-4.52	MS	153.08	0.17	3	3	1	1	4

ALT

100	322.31	7	5	-0.11	0.44	1	127.45	-1.49	VS	78.94	0.55	0	1	0	0	0
101	304.29	6	3	1.11	0.38	1	104.06	-2.42	S	77.04	0.55	0	0	0	0	0
102	308.33	6	4	0.72	0.56	1	107.22	-2.17	S	78.25	0.55	0	0	0	0	0
104	320.29	7	4	0.24	0.38	1	124.29	-1.81	VS	78.2	0.55	0	0	0	0	0
105	324.33	7	5	-0.22	0.56	1	127.45	-1.64	VS	79.42	0.55	0	1	0	0	0
107	340.33	8	6	-0.91	0.56	1	147.68	-1.12	VS	80.58	0.55	1	1	1	1	1
108	284.26	5	2	2.22	0.12	1	83.83	-3.87	S	75.25	0.55	0	0	0	0	0
114	566.51	10	4	3.95	0.12	3	167.66	-7.22	PS	149.5	0.55	1	2	1	1	2
131	586.54	11	5	2.66	0.25	3	187.89	-5.71	MS	151.29	0.17	2	2	1	1	2
132	602.54	12	6	1.7	0.25	3	208.12	-5.27	MS	152.45	0.17	3	2	1	1	4
133	602.54	12	6	1.96	0.25	3	208.12	-5.27	MS	152.45	0.17	3	2	1	1	4
134	638.57	14	8	-0.29	0.38	3	248.58	-3.09	S	154.29	0.17	3	4	1	1	4
135	602.54	12	6	1.62	0.25	3	208.12	-5.27	MS	152.45	0.17	3	2	1	1	4
136	308.33	6	4	0.78	0.56	1	107.22	-2.17	S	78.25	0.55	0	0	0	0	0
137	308.33	6	4	0.72	0.56	1	107.22	-2.17	S	78.25	0.55	0	0	0	0	0
138	308.33	6	4	0.73	0.56	1	107.22	-2.17	S	78.25	0.55	0	0	0	0	0
139	350.36	7	3	1.18	0.56	3	113.29	-2.63	S	87.99	0.55	0	0	0	0	0
140	488.48	10	5	0.39	0.6	1	162.98	-2.51	S	118.47	0.11	0	1	1	1	1
141	300.26	6	3	1.92	0.12	1	104.06	-3.73	S	77.28	0.55	0	0	0	0	0
142	288.3	5	2	1.88	0.38	1	83.83	-2.94	S	75.88	0.55	0	0	0	0	0

TRI																
13	270.24	5	3	1.87	0.07	0	94.83	-3.67	S	70.78	0.55	0	0	0	0	0
83	254.24	4	2	2.38	0.07	0	74.6	-4.11	MS	68.76	0.55	0	0	0	0	0
84	286.24	6	4	1.08	0.07	1	115.06	-2.9	S	71.95	0.55	0	0	0	0	0
143	276.28	5	4	0.55	0.4	0	97.99	-2.01	S	71.41	0.55	0	0	0	0	0
144	276.28	5	4	0.54	0.4	0	97.99	-2.01	S	71.41	0.55	0	0	0	0	0
145	254.24	4	2	2.22	0.07	0	74.6	-3.82	S	68.76	0.55	0	0	0	0	0

146	270.24	5	3	1.43	0.07	1	94.83	-3.04	S	69.92	0.55	0	0	0	0	0
147	238.24	3	1	2.73	0.07	0	54.37	-4.25	MS	66.74	0.55	0	0	0	0	0
148	314.29	6	4	1.68	0.18	2	115.06	-3.53	S	81.56	0.55	0	0	0	0	0
149	254.24	4	2	1.94	0.07	1	74.6	-3.47	S	67.9	0.55	0	0	0	0	0
150	290.27	6	4	0.28	0.33	0	115.06	-1.84	VS	71.83	0.55	0	0	0	0	0
151	290.27	6	4	0.29	0.33	1	115.06	-1.68	VS	71.83	0.55	0	0	0	0	0
152	254.24	4	2	2.4	0.07	0	74.6	-4.16	MS	68.76	0.55	0	0	0	0	0
153	254.24	4	1	2.39	0.07	1	63.6	-4.02	MS	68.26	0.55	0	0	0	0	0
154	276.28	5	4	0.52	0.4	0	97.99	-2.01	S	71.41	0.55	0	0	0	0	0
155	290.27	6	4	0.28	0.33	0	115.06	-1.84	VS	71.83	0.55	0	0	0	0	0

EUR

13	270.24	5	3	1.87	0.07	0	94.83	-3.67	S	70.78	0.55	0	0	0	0	0
15	288.3	5	3	1.94	0.31	1	86.99	-3.36	S	78.35	0.55	0	0	0	0	0
18	286.24	6	4	1.63	0.07	0	115.06	-3.87	S	72.81	0.55	0	0	0	0	0
19	300.26	6	3	1.96	0.12	1	104.06	-4.08	MS	77.28	0.55	0	0	0	0	0
20	402.35	9	4	1.11	0.25	6	150.59	-3.25	S	98.47	0.55	0	0	1	1	1
60	302.28	6	3	2.34	0.19	1	96.22	-4.04	MS	78.38	0.55	0	0	0	0	0
63	300.26	6	3	1.5	0.12	2	104.06	-3.1	S	76.41	0.55	0	0	0	0	0
97	300.22	7	4	1.07	0	1	132.13	-3.22	S	72.78	0.56	0	0	0	1	0
154	276.28	5	4	0.52	0.4	0	97.99	-2.01	S	71.41	0.55	0	0	0	0	0
156	272.25	5	3	2.34	0.13	0	86.99	-3.98	S	71.89	0.55	0	0	0	0	0
157	286.28	5	2	2.7	0.19	1	75.99	-4.18	MS	76.36	0.55	0	0	0	0	0
158	418.39	9	4	1.49	0.38	4	134.91	-3.93	S	102.51	0.55	0	0	0	1	0
159	416.38	9	4	1.02	0.33	4	142.75	-3.63	S	101.41	0.55	0	0	1	1	0
160	588.6	10	6	3.59	0.33	4	173.98	-6.46	PS	159.7	0.17	2	3	1	1	2
161	432.38	10	5	0.25	0.33	5	162.98	-2.86	S	102.57	0.55	0	1	1	1	1
162	420.41	9	5	0.81	0.48	4	145.91	-3.13	S	104.5	0.55	0	0	1	1	0

163	276.28	5	4	0.51	0.4	0	97.99	-2.01	S	71.41	0.55	0	0	0	0	0
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FUS

5	284.26	5	2	2.57	0.12	1	83.83	-4.81	MS	75.25	0.55	0	0	0	0	0
6	304.29	6	3	0.91	0.38	1	104.06	-2.54	S	76.76	0.56	0	0	0	0	0
7	324.33	7	5	0.4	0.56	1	127.45	-2.03	S	80.28	0.55	0	0	0	0	0
8	340.33	8	6	-0.53	0.56	1	147.68	-1.51	VS	81.44	0.55	1	1	1	1	1
10	336.29	8	5	-0.05	0.38	1	144.52	-2.14	S	79.94	0.56	0	1	1	1	0
164	304.29	6	3	0.97	0.38	1	104.06	-2.54	S	76.76	0.56	0	0	0	0	0
165	324.33	7	5	0.37	0.56	1	127.45	-2.03	S	80.28	0.55	0	0	0	0	0
166	306.31	6	3	1.24	0.56	1	96.22	-2.56	S	76.93	0.55	0	0	0	0	0
167	340.33	8	6	-0.43	0.56	1	147.68	-1.51	VS	81.44	0.55	1	1	1	1	1
168	324.33	7	5	0.36	0.56	1	127.45	-2.03	S	80.28	0.55	0	0	0	0	0
169	352.38	5	0	3.21	0.29	5	69.67	-3.98	S	97.29	0.55	0	0	0	0	0
170	328.27	7	3	1.68	0.12	2	121.13	-4.07	MS	82.5	0.55	0	0	0	0	0

ENG

171	616.57	12	5	2.53	0.33	4	197.12	-5.66	MS	153.75	0.11	2	3	1	1	3
172	616.57	12	5	2.57	0.33	4	197.12	-5.66	MS	153.75	0.11	2	3	1	1	3
173	616.57	12	5	2.61	0.33	4	197.12	-5.66	MS	153.75	0.11	2	3	1	1	3
174	616.57	12	3	2.85	0.36	5	182.96	-5.44	MS	152.77	0.11	2	3	1	1	3
175	634.58	13	5	2.15	0.36	8	214.19	-4.86	MS	156.54	0.11	2	3	1	1	3
176	634.58	13	5	2.34	0.36	8	214.19	-4.86	MS	156.54	0.11	2	3	1	1	3
177	616.57	12	3	2.88	0.36	5	182.96	-5.44	MS	152.77	0.11	2	3	1	1	3

SPO

101	304.29	6	3	1.11	0.38	1	104.06	-2.42	S	77.04	0.55	0	0	0	0	0
178	320.29	7	4	0.26	0.38	1	124.29	-1.81	VS	78.2	0.55	0	0	0	0	0
179	338.31	8	5	-0.39	0.5	1	144.52	-1.46	VS	79.88	0.55	0	1	1	1	0
180	356.32	9	7	-1.43	0.56	1	167.91	-0.68	VS	81.82	0.55	1	1	1	1	3
181	340.33	8	6	-0.79	0.56	1	147.68	-1.07	VS	80.62	0.55	1	1	1	1	1
182	372.75	8	5	-0.12	0.5	1	144.52	-1.99	VS	84.71	0.55	0	1	1	1	0
183	338.31	8	5	-0.49	0.56	1	139.98	-1.21	VS	78.46	0.55	0	1	0	1	0

OTH

184	282.29	4	0	2.8	0.18	2	52.6	-3.88	S	77.7	0.55	0	0	0	0	0
185	254.24	4	2	2.41	0.07	0	74.6	-4.16	MS	68.76	0.55	0	0	0	0	0
186	240.21	4	2	2.04	0	0	74.6	-3.81	S	63.8	0.55	0	0	0	0	0
187	284.26	5	2	2.2	0.12	1	83.83	-3.87	S	75.25	0.55	0	0	0	0	0
188	298.29	5	1	2.56	0.18	2	72.83	-4.08	MS	79.72	0.55	0	0	0	0	0
189	268.26	4	1	2.6	0.12	1	63.6	-4.02	MS	73.23	0.55	0	0	0	0	0
190	314.29	6	2	2.15	0.18	2	93.06	-3.95	S	81.75	0.55	0	0	0	0	0
191	256.21	5	3	1.62	0	0	94.83	-3.67	S	65.82	0.55	0	0	0	0	0
192	300.26	6	3	1.96	0.12	1	104.06	-4.08	MS	77.28	0.55	0	0	0	0	0
193	336.29	8	5	0.05	0.38	1	144.52	-2.02	S	80.23	0.55	0	0	1	1	0
194	332.35	6	3	1.73	0.44	2	104.06	-3.01	S	86.81	0.55	0	0	0	0	0
195	268.26	4	1	2.63	0.12	1	63.6	-4.02	MS	73.23	0.55	0	0	0	0	0
196	316.26	7	5	1.08	0.12	1	135.29	-3.42	S	78.78	0.55	0	0	0	1	0
197	330.29	7	4	1.42	0.18	2	124.29	-3.42	S	83.51	0.55	0	0	0	0	0
198	346.29	8	5	1.13	0.18	2	144.52	-3.27	S	85.53	0.55	0	0	1	1	0
199	286.24	6	3	1.53	0.07	1	104.06	-3.43	S	72.31	0.55	0	0	0	0	0
200	574.49	12	6	0.69	0.33	2	208.12	-3.73	S	138.35	0.11	3	2	1	1	4
201	272.21	6	4	1.11	0	0	115.06	-3.23	S	67.84	0.55	0	0	0	0	0
202	538.46	10	6	3.64	0.07	1	189.66	-7.49	PS	140.56	0.17	2	2	1	1	3

203	298.29	5	1	2.63	0.18	2	72.83	-4.08	MS	79.72	0.55	0	0	0	0	0
204	352.38	5	1	3.78	0.24	4	72.83	-5.17	MS	98.48	0.55	0	0	0	0	0
205	284.26	5	2	2.25	0.12	1	83.83	-3.87	S	75.25	0.55	0	0	0	0	0
206	300.26	6	4	1.4	0.12	1	115.06	-3.56	S	76.75	0.55	0	0	0	0	0
207	328.27	7	3	1.48	0.12	3	121.13	-3.33	S	81.68	0.55	0	0	0	0	0
208	398.41	7	2	2.95	0.36	3	102.29	-4.69	MS	104.75	0.55	0	0	0	0	0

S: Soluble

PS: Poorly Soluble

MS: Moderately soluble

VS: Very Soluble

Table S2. Pharmacokinetics behavior of anthraquinones. Compounds number according to the main text.

Molecule	GI absorption	BBB permeant	Pgp substrate	CYP1A2 inhibition					
				CYP1A2	CYP2C19	CYP2C9	CYP2D6	CYP3A4	
NIG									
1	Low	No	Yes	No	No	No	No	No	No
2	High	No	Yes	No	No	No	No	No	No
3	High	No	No	No	No	No	No	No	No
4	High	No	No	Yes	No	Yes	No	Yes	Yes
5	High	No	No	Yes	No	Yes	No	Yes	Yes
6	High	No	No	No	No	No	No	No	No
7	High	No	Yes	No	No	No	No	No	No
8	Low	No	No	No	No	No	No	No	No
9	High	No	Yes	No	No	No	No	No	No
10	Low	No	No	No	No	No	No	No	No
ASP									
7	High	No	Yes	No	No	No	No	No	No
8	Low	No	No	No	No	No	No	No	No
10	Low	No	No	No	No	No	No	No	No
11	Low	No	No	No	No	Yes	No	No	No
12	Low	No	No	No	No	Yes	No	No	No
13	High	No	No	Yes	No	No	No	No	Yes
14	High	No	No	Yes	No	Yes	No	Yes	Yes
15	High	No	Yes	Yes	No	No	No	No	No
16	High	No	Yes	No	No	No	No	No	No
17	High	No	Yes	No	No	No	No	No	No
18	High	No	No	No	No	No	No	No	Yes
19	High	No	No	Yes	No	Yes	No	Yes	Yes
20	Low	No	Yes	No	No	No	No	No	No
21	Low	No	No	No	No	Yes	No	No	No

22	Low	No	No	No	No	Yes	No	No
23	Low	No	No	No	No	Yes	No	No
24	Low	No	Yes	No	No	No	No	No
25	Low	No	No	No	No	No	No	No
26	High	No	No	No	No	Yes	Yes	Yes
27	High	No	No	No	No	Yes	Yes	Yes
28	High	No	No	Yes	No	Yes	Yes	Yes
29	High	No	No	No	No	Yes	No	Yes
30	High	No	Yes	No	No	Yes	Yes	Yes
31	High	No	Yes	No	No	Yes	Yes	Yes
32	High	No	No	No	Yes	Yes	Yes	Yes
33	High	No	No	Yes	No	Yes	No	Yes
34	High	No	No	No	No	No	No	No
36	High	No	Yes	No	No	Yes	No	Yes
37	High	No	Yes	No	No	No	No	No
38	High	No	No	No	No	Yes	Yes	Yes
39	Low	No	Yes	No	No	No	No	No
40	High	No	Yes	No	No	No	No	No
41	High	No	No	Yes	No	No	No	Yes
42	High	No	No	No	No	No	No	Yes
43	High	No	No	No	Yes	Yes	Yes	Yes
44	High	No	No	Yes	No	Yes	Yes	Yes
45	High	No	No	Yes	No	Yes	No	Yes
46	High	No	No	Yes	No	Yes	No	Yes
47	High	Yes	No	Yes	Yes	No	No	Yes
48	High	Yes	No	Yes	Yes	Yes	No	Yes
49	High	Yes	No	Yes	Yes	No	No	No
50	High	No	No	Yes	No	No	No	Yes
51	High	Yes	No	Yes	No	No	No	Yes
52	High	Yes	No	Yes	No	No	No	Yes
53	High	No	Yes	No	No	No	No	Yes

54	High	No	No	Yes	No	No	No	Yes
55	High	No	No	Yes	No	No	No	Yes
56	High	No	No	Yes	No	No	No	Yes
57	High	Yes	No	Yes	Yes	Yes	No	Yes
58	High	No	No	Yes	No	Yes	No	Yes
59	High	No	No	Yes	No	No	No	Yes
60	High	No	No	Yes	No	No	No	Yes
61	Low	No	Yes	No	No	No	No	No
62	High	No	No	No	No	No	No	Yes
63	High	No	No	Yes	No	No	No	Yes
64	High	No	No	Yes	No	Yes	No	Yes
65	High	No	No	Yes	No	Yes	No	Yes
66	High	No	No	Yes	No	No	No	Yes
67	High	No	No	Yes	No	Yes	No	Yes
68	High	No	No	No	No	Yes	Yes	Yes
69	High	No	No	No	No	Yes	No	Yes
70	Low	No	No	No	Yes	Yes	No	Yes
71	Low	No	No	Yes	No	Yes	Yes	Yes
72	High	No	No	Yes	Yes	Yes	No	Yes
73	High	No	No	Yes	Yes	Yes	No	Yes
74	High	No	No	Yes	Yes	Yes	No	Yes
75	Low	No	No	No	Yes	Yes	No	Yes
76	High	No	No	Yes	No	Yes	No	Yes
77	High	No	No	Yes	No	Yes	No	Yes
78	High	No	No	Yes	Yes	Yes	No	Yes
79	High	No	No	Yes	Yes	Yes	No	Yes
80	High	No	No	No	Yes	Yes	No	Yes

PEN								
13	High	No	No	Yes	No	No	No	Yes

17	High	No	Yes	No	No	No	No	No
26	High	No	No	No	No	Yes	Yes	Yes
27	High	No	No	No	No	Yes	Yes	Yes
37	High	No	Yes	No	No	No	No	No
81	Low	No	No	No	No	Yes	No	No
82	Low	No	No	No	No	Yes	No	No
83	High	Yes	No	Yes	No	No	No	Yes
84	High	No	No	No	No	No	No	Yes
85	High	No	No	Yes	No	Yes	No	Yes
86	Low	No	No	No	No	No	No	No
87	Low	No	No	No	No	No	No	No
88	High	No	No	Yes	No	No	No	Yes
89	Low	No	Yes	No	No	Yes	No	No
90	Low	No	Yes	No	No	No	No	No
91	Low	No	Yes	No	No	Yes	No	Yes
92	Low	No	Yes	No	No	Yes	No	Yes
93	Low	No	Yes	No	No	No	No	No
94	Low	No	Yes	No	No	Yes	No	Yes
95	Low	No	Yes	No	No	Yes	No	Yes
96	Low	No	Yes	No	No	No	No	No
97	High	No	No	No	No	No	No	No
98	High	No	No	No	No	No	No	Yes

STE

99	Low	No	No	No	No	No	No	No
100	High	No	No	No	No	No	No	No
101	High	No	Yes	No	No	No	No	No
102	High	No	Yes	No	No	No	No	No
103	High	No	No	No	No	No	No	No

104	High	No	No	No	No	No	No	No
105	High	No	No	No	No	No	No	No
106	High	No	Yes	No	No	No	No	No
107	Low	No	No	No	No	No	No	No
108	High	No	No	Yes	No	Yes	No	Yes
109	High	No	No	No	No	No	No	No
110	Low	No	Yes	No	No	No	No	No
111	Low	No	No	No	No	No	No	No
112	Low	No	No	No	No	Yes	No	No
113	Low	No	No	No	No	Yes	No	No
114	Low	No	No	No	Yes	Yes	No	No
115	Low	No	Yes	No	No	No	No	No
116	Low	No	Yes	No	No	No	No	No
117	Low	No	No	No	No	Yes	No	No
118	Low	No	No	No	Yes	Yes	No	No
119	Low	No	No	No	Yes	Yes	No	No
120	Low	No	No	No	Yes	No	No	No
121	Low	No	No	No	Yes	Yes	No	No
122	Low	No	No	No	Yes	Yes	No	No
123	Low	No	No	No	No	Yes	No	No
124	Low	No	No	No	No	Yes	No	No
125	Low	No	No	No	No	Yes	No	No
126	Low	No	No	No	No	Yes	No	No
127	Low	No	No	No	No	Yes	No	No
128	Low	No	No	No	No	Yes	No	No
129	Low	No	Yes	No	No	No	No	No
130	Low	No	No	No	Yes	Yes	No	No

ALT

100	High	No	No	No	No	No	No	No
101	High	No	Yes	No	No	No	No	No
102	High	No	Yes	No	No	No	No	No
104	High	No	No	No	No	No	No	No
105	High	No	No	No	No	No	No	No
107	Low	No	No	No	No	No	No	No
108	High	No	No	Yes	No	Yes	No	Yes
114	Low	No	No	No	Yes	Yes	No	No
131	Low	No	No	No	No	Yes	No	No
132	Low	No	No	No	No	Yes	No	No
133	Low	No	No	No	No	Yes	No	No
134	Low	No	Yes	No	No	No	No	No
135	Low	No	No	No	No	Yes	No	No
136	High	No	Yes	No	No	No	No	No
137	High	No	Yes	No	No	No	No	No
138	High	No	Yes	No	No	No	No	No
139	High	No	Yes	No	No	No	No	No
140	Low	No	Yes	No	Yes	No	No	No
141	High	No	No	Yes	No	Yes	No	Yes
142	High	No	No	Yes	No	No	No	No

TRI								
13	High	No	No	Yes	No	No	No	Yes
83	High	Yes	No	Yes	No	No	No	Yes
84	High	No	No	No	No	No	No	Yes
143	High	No	No	No	No	No	No	No
144	High	No	No	No	No	No	No	No
145	High	Yes	No	Yes	No	No	No	Yes

146	High	No	No	Yes	No	No	No	Yes
147	High	Yes	No	Yes	Yes	No	No	Yes
148	High	No	No	No	No	No	No	No
149	High	No	No	Yes	No	No	No	Yes
150	High	No	No	No	No	No	No	No
151	High	No	No	No	No	No	No	No
152	High	Yes	No	Yes	No	No	No	Yes
153	High	Yes	No	Yes	No	Yes	No	Yes
154	High	No	No	No	No	No	No	No
155	High	No	No	No	No	No	No	No

EUR

13	High	No	No	Yes	No	No	No	Yes
15	High	No	Yes	Yes	No	No	No	No
18	High	No	No	No	No	No	No	Yes
19	High	No	No	Yes	No	Yes	No	Yes
20	Low	No	Yes	No	No	No	No	No
60	High	No	No	Yes	No	No	No	Yes
63	High	No	No	Yes	No	No	No	Yes
97	High	No	No	No	No	No	No	No
154	High	No	No	No	No	No	No	No
156	High	No	No	Yes	No	No	No	Yes
157	High	Yes	No	Yes	No	Yes	Yes	Yes
158	High	No	Yes	No	No	No	No	No
159	Low	No	Yes	No	No	No	No	No
160	Low	No	No	No	No	Yes	No	No
161	Low	No	Yes	No	No	No	No	No
162	Low	No	Yes	No	No	No	No	No

163	High	No	No	No	No	No	No	No	No
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FUS

5	High	No	No	Yes	No	Yes	No	Yes
6	High	No	No	No	No	No	No	No
7	High	No	Yes	No	No	No	No	No
8	Low	No	No	No	No	No	No	No
10	Low	No	No	No	No	No	No	No
164	High	No	No	No	No	No	No	No
165	High	No	Yes	No	No	No	No	No
166	High	No	Yes	No	No	No	No	No
167	Low	No	No	No	No	No	No	No
168	High	No	Yes	No	No	No	No	No
169	High	Yes	No	Yes	Yes	Yes	No	Yes
170	High	No	No	No	No	Yes	No	Yes

ENG

171	Low	No	Yes	No	No	Yes	No	No
172	Low	No	Yes	No	No	Yes	No	No
173	Low	No	Yes	No	No	Yes	No	No
174	Low	No	Yes	No	No	No	No	No
175	Low	No	No	No	No	No	No	No
176	Low	No	No	No	No	No	No	No
177	Low	No	Yes	No	No	No	No	No

SPO

101	High	No	Yes	No	No	No	No	No
178	High	No	No	No	No	No	No	No
179	Low	No	No	No	No	No	No	No
180	Low	No	No	No	No	No	No	No
181	Low	No	No	No	No	No	No	No
182	Low	No	No	No	No	No	No	No
183	Low	No	No	No	No	No	No	No

OTH

184	High	Yes	No	Yes	Yes	Yes	No	Yes
185	High	Yes	No	Yes	No	No	No	Yes
186	High	Yes	No	Yes	No	No	No	Yes
187	High	No	No	Yes	No	No	No	Yes
188	High	Yes	No	Yes	Yes	Yes	No	Yes
189	High	Yes	No	Yes	Yes	Yes	No	Yes
190	High	No	No	Yes	No	Yes	No	Yes
191	High	No	No	No	No	No	No	Yes
192	High	No	No	Yes	No	Yes	No	Yes
193	Low	No	No	No	No	No	No	No
194	High	No	Yes	No	No	No	No	No
195	High	Yes	No	Yes	Yes	Yes	No	Yes
196	High	No	No	No	No	No	No	No
197	High	No	Yes	No	No	No	No	Yes
198	Low	No	Yes	No	No	No	No	Yes
199	High	No	No	No	No	No	No	Yes
200	Low	No	Yes	No	Yes	No	No	No
201	High	No	No	No	No	No	No	Yes
202	Low	No	No	No	Yes	Yes	No	No

203	High	Yes	No	Yes	Yes	Yes	No	Yes
204	High	Yes	No	Yes	Yes	Yes	No	Yes
205	High	No	No	Yes	No	Yes	No	Yes
206	High	No	No	No	No	No	No	No
207	High	No	No	No	No	No	No	No
208	High	No	Yes	No	No	Yes	No	Yes

Figure S1: List of 20 anthraquinones-containing compounds with promising drug likeness properties

