

Supporting Information

Cortistatins and Plakinamines Steroidal Alkaloids from the Marine Sponges of the Genus *Corticium*: Insights into their Chemistry, Pharmacology, Pharmacokinetics and Structure Activity Relationships (SARs)

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Table S1. Physicochemical properties of Coristatins and Plakinamines.

No	Compound	MW	LogP	nHD	nHA	TPSA	RB	NC	QED	SA	LogS
1	<i>Corticium</i> sp	420.685	6.876	1.0	2.0	38.38	4.0	5.0	0.494	5.408	-5.988
2	<i>Corticium</i> sp	422.701	6.955	1.0	2.0	38.38	4.0	5.0	0.488	5.334	-5.882
3	<i>C.simplex</i>	472.629	4.348	2.0	5.0	65.82	2.0	7.0	0.680	6.447	-3.487
4	<i>C.simplex</i>	488.628	3.319	3.0	6.0	86.05	2.0	7.0	0.601	6.643	-2.935
5	<i>C.simplex</i>	486.612	3.527	2.0	6.0	82.89	2.0	7.0	0.675	6.554	-3.252
6	<i>C.simplex</i>	502.611	2.631	3.0	7.0	103.12	2.0	7.0	0.580	6.668	-2.724
7	<i>C.simplex</i>	480.781	6.695	0.0	3.0	15.71	5.0	6.0	0.435	6.614	-4.394
8	<i>C.simplex</i>	478.765	6.471	0.0	3.0	15.71	5.0	6.0	0.450	6.742	-4.383
9	<i>C.simplex</i>	458.690	6.744	0.0	3.0	25.36	4.0	6.0	0.499	6.493	-5.523
10	<i>C.simplex</i>	460.706	6.663	0.0	3.0	25.36	5.0	6.0	0.490	6.340	-5.435
11	<i>C.simplex</i>	438.615	6.182	0.0	3.0	25.36	2.0	7.0	0.559	6.301	-4.837
12	<i>C.simplex</i>	440.631	6.406	0.0	3.0	25.36	2.0	7.0	0.539	6.157	-5.005
13	<i>C.simplex</i>	456.630	5.377	1.0	4.0	45.59	2.0	7.0	0.659	6.327	-4.317
14	<i>Corticium</i> sp	466.754	6.673	1.0	3.0	35.83	4.0	5.0	0.469	5.173	-5.693
15	<i>Corticium</i> sp	480.737	6.248	2.0	3.0	61.69	4.0	5.0	0.467	5.144	-6.133
16	<i>Corticium</i> sp	510.807	6.103	1.0	4.0	43.78	6.0	5.0	0.438	5.186	-5.119
17	<i>Corticium</i> sp	510.807	6.247	1.0	4.0	43.78	6.0	5.0	0.429	5.185	-4.840
18	<i>Corticium</i> sp	478.765	6.518	0.0	3.0	23.55	4.0	5.0	0.429	5.062	-5.157
19	<i>Corticium</i> sp	424.717	7.035	1.0	2.0	38.38	4.0	5.0	0.483	5.066	-6.456
20	<i>Corticium</i> sp	440.760	6.895	1.0	2.0	29.26	4.0	5.0	0.481	4.977	-4.488
21	<i>Corticium</i> sp	482.753	6.184	1.0	3.0	49.54	4.0	5.0	0.295	5.351	-5.608
22	<i>Corticium</i> sp	464.738	6.881	0.0	3.0	32.67	4.0	5.0	0.424	5.146	-6.514
23	<i>Corticium</i> sp	436.684	6.124	2.0	2.0	55.12	3.0	5.0	0.523	5.060	-4.992
24	<i>Corticium</i> sp	464.738	6.176	1.0	3.0	32.34	4.0	5.0	0.504	5.127	-5.035
25	<i>Corticium</i> sp	452.727	5.707	2.0	3.0	49.49	3.0	5.0	0.539	5.078	-4.292
26	<i>Corticium</i> sp	426.733	6.553	2.0	2.0	38.05	4.0	5.0	0.499	5.015	-4.413
27	<i>C.niger</i>	450.755	6.924	0.0	2.0	6.48	1.0	6.0	0.399	5.297	-4.652
28	<i>C.niger</i>	438.744	6.671	1.0	2.0	29.26	4.0	5.0	0.496	5.194	-4.298
29	<i>C.niger</i>	496.780	6.419	2.0	4.0	50.36	5.0	5.0	0.3405	5.185	-4.873

30	<i>C.niger</i>	498.796	6.355	2.0	4.0	50.36	6.0	5.0	0.330	5.176	-4.550
31	<i>Corticium</i> sp	500.812	6.518	1.0	4.0	55.56	6.0	5.0	0.421	5.051	-4.436
32	<i>Corticium</i> sp	508.791	6.539	1.0	4.0	41.57	5.0	5.0	0.338	5.106	-5.065
33	<i>Corticium</i> sp	482.841	8.055	0.0	2.0	6.48	8.0	4.0	0.322	4.863	-5.284
34	<i>Corticium</i> sp	498.840	7.026	1.0	3.0	26.71	8.0	4.0	0.364	5.103	-4.352
35	<i>C.niger</i>	424.717	6.617	2.0	2.0	38.05	3.0	5.0	0.499	5.028	-4.809
36	<i>C.niger</i>	482.753	6.158	2.0	4.0	64.35	4.0	5.0	0.372	5.169	-4.790

Table S2. Molecular drugs like filters for Coristatins and Plakinamines.

No	Compound	Lipinski	Veber	Rule of 3	Rule of 4
1	<i>Corticium</i> sp	No	Yes	Yes	Yes
2	<i>Corticium</i> sp	No	Yes	Yes	Yes
3	<i>C.simplex</i>	No	Yes	Yes	Yes
4	<i>C.simplex</i>	No	Yes	Yes	Yes
5	<i>C.simplex</i>	No	Yes	Yes	Yes
6	<i>C.simplex</i>	No	Yes	Yes	Yes
7	<i>C.simplex</i>	No	Yes	Yes	Yes
8	<i>C.simplex</i>	No	Yes	Yes	Yes
9	<i>C.simplex</i>	No	Yes	Yes	Yes
10	<i>C.simplex</i>	No	Yes	Yes	Yes
11	<i>C.simplex</i>	No	Yes	Yes	Yes
12	<i>C.simplex</i>	No	Yes	Yes	Yes
13	<i>C.simplex</i>	No	Yes	Yes	Yes
14	<i>Corticium</i> sp	No	Yes	Yes	Yes
15	<i>Corticium</i> sp	No	Yes	Yes	Yes
16	<i>Corticium</i> sp	No	Yes	No	Yes
17	<i>Corticium</i> sp	No	Yes	No	Yes
18	<i>Corticium</i> sp	No	Yes	Yes	Yes
19	<i>Corticium</i> sp	No	Yes	Yes	Yes
20	<i>Corticium</i> sp	No	Yes	Yes	Yes
21	<i>Corticium</i> sp	No	Yes	Yes	Yes
22	<i>Corticium</i> sp	No	Yes	Yes	Yes
23	<i>Corticium</i> sp	No	Yes	Yes	Yes
24	<i>Corticium</i> sp	No	Yes	Yes	Yes
25	<i>Corticium</i> sp	No	Yes	Yes	Yes
26	<i>Corticium</i> sp	No	Yes	Yes	Yes
27	<i>C.niger</i>	No	Yes	Yes	Yes
28	<i>C.niger</i>	No	Yes	Yes	Yes
29	<i>C.niger</i>	No	Yes	Yes	Yes
30	<i>C.niger</i>	No	Yes	Yes	Yes
31	<i>Corticium</i> sp	No	Yes	No	Yes

32	<i>Corticium</i> sp	No	Yes	No	Yes
33	<i>Corticium</i> sp	No	No	Yes	Yes
34	<i>Corticium</i> sp	No	No	Yes	Yes
35	<i>C.niger</i>	No	Yes	Yes	Yes
36	<i>C.niger</i>	No	Yes	Yes	Yes

Table S3. *In-silico* ADMET prediction of Coristatins and Plakinamines.

No	Absorption and distribution			Metabolism				Excretion and toxicity		
	Blood-Brain Barrier (LogBB)	Human Intestinal absorption (HIA)	Volume of Distribution (VDss)	CYP1A2 Inhibitor	CYP2D6 Substrate	CYP3A4 Inhibitor	CYP3A4 Substrate	Clearance	AMES	hERG inhibition
1	0.104	91.863	0.95	No	No	No	Yes	0.1	No	No
2	0.017	92.49	0.716	No	No	No	Yes	-0.004	No	No
3	-0.307	97.651	0.384	No	No	No	Yes	0.491	No	No
4	-0.762	96.628	0.46	No	No	No	No	0.464	No	No
5	-0.853	98.802	0.118	No	No	Yes	Yes	0.48	No	No
6	-0.918	88.63	0.809	No	No	No	No	0.588	No	No
7	0.888	91.261	0.804	No	Yes	No	Yes	0.361	No	No
8	0.848	92.413	0.873	No	No	No	Yes	0.276	No	No
9	0.367	95.375	1.149	No	No	No	Yes	0.533	No	No
10	0.467	95.564	1.168	No	No	No	Yes	0.744	No	No
11	0.175	95.912	1.791	No	No	No	Yes	0.689	No	No
12	0.232	95.954	1.782	No	Yes	No	Yes	0.82	No	No
13	-0.026	96.415	1.155	No	Yes	No	Yes	0.768	No	No
14	0.004	95.967	0.323	No	Yes	No	Yes	0.013	No	No
15	-0.414	96.61	-0.118	No	No	No	Yes	0.387	No	No
16	-0.197	94.04	0.503	No	No	No	Yes	0.078	No	No
17	-0.079	91.022	0.574	No	No	No	Yes	0.209	No	No
18	0.809	94.368	0.598	No	No	No	Yes	-0.046	No	No
19	-0.092	95.156	0.712	No	No	No	Yes	-0.004	No	No
20	0.751	92.356	0.821	No	No	No	Yes	0.021	No	No
21	-0.153	96.55	0.207	No	No	No	Yes	0.059	No	No
22	0.033	96.846	0.739	No	No	No	Yes	0.064	No	No
23	-0.312	92.867	0.034	No	No	No	Yes	-0.033	No	No
24	-0.076	94.578	0.585	No	No	No	Yes	0.079	No	No
25	-0.242	93.719	0.119	No	Yes	No	Yes	-0.011	No	No
26	-0.091	92.566	0.806	No	No	No	Yes	0.131	No	No
27	0.883	94.319	1.322	No	Yes	No	Yes	-0.018	No	No
28	0.753	92.832	0.774	No	Yes	No	Yes	-0.105	No	No
29	-0.009	94.273	0.434	No	No	No	Yes	0.135	No	No
30	-0.101	93.67	0.244	No	No	No	Yes	0.025	No	No
31	-0.281	93.133	0.008	No	No	No	Yes	-0.054	No	No
32	-0.021	94.384	0.064	No	No	No	Yes	-0.089	No	No
33	1.026	92.112	0.548	No	No	No	Yes	0.024	No	No
34	0.863	92.549	0.03	No	No	No	Yes	-0.051	No	No
35	0.001	93.169	1.013	No	No	No	Yes	0.24	No	No
36	-0.145	94.292	0.393	No	No	No	Yes	0.081	No	No