

Supplementary file

Article

Cyclodepsipeptides: Isolation from Endophytic Fungi of *Sarcophyton ehrenbergi* and Verification of Their Larvicidal Activity via In-Vitro and In-Silico Studies

Table S1. ¹H-NMR, and ATP spectral data of compound 1.

Position	δ _c (ppm)	δ _H (ppm), multiplicity and J (Hz)	*Ref. δ _c (ppm)	*Ref. δ _H (ppm)	Position	δ _c (ppm)	δ _H (ppm), multiplicity and J (Hz)	*Ref. δ _c (ppm)	*Ref. δ _H (ppm)
Phenylalanine					Valine				
1	172.66	--	173.6		1	171.79	--	173.4	
2	53.25	4.83 (m)	55.3	4.79, m	2	57.93	4.21, m	59.9	4.20, m
3	38.55	3.12 (d, J = 8.1 Hz) 3.09 (d, J = 8.1 Hz)	39.4	3.18, d 3.03, d	3	31.11	2.18(m)	31.0	2.19, m
4	135.76	--	137.8		4	18.21	0.93 (d, J = 3.5 Hz)	19.0	0.98, d
5/9	129.10	7.16 (m)	130.3	7.24, m	5	19.60	0.93 (d, J = 3.5 Hz)	19.7	0.97, d
6/8	128.52	7.28 (m)	129.6	7.28, m	Glycine				
7	127.07	7.21 (m)	128.0	7.21, m	1	171.9		171.9	
Alanine					2	43.14	3.44 (dd, J = 17.2, 4.1 Hz) 4.43 (d, J = 8.0 Hz)	44.0	4.24,d 3.53, d
1	172.70	--	174.1		Hydroxy methyl decanoic acid (HMDA)				
2	49.53	4.24 (m)	50.3	4.29, q	1	172.81	--	174.5	
3	17.50	1.29 (d, J = 7.3 Hz)	17.6	1.27, d	2	40.98	2.40 (m)	40.9	2.42, m
Leucine					3	78.14	4.64 (m)	78.6	4.77, m
1	173.28	--	175.1		4	37.92	1.58 (m)	39.0	1.54, m
2	54.00	4.16 (m)	54.7	4.19, m	5	32.12	0.91(m) 1.21 (m)	33.6	1.22.m 0.95, m
3	39.15	1.58 (m)	40.3	1.58, m	6	29.24	1.21 (m)	30.6	1.30, m
4	24.66	1.68 (m)	26.0	1.68, m	7	29.06	1.21 (m)	28.2	1.29, m

5	22.43	0.95 (d, $J = 2.5$ Hz)	23.1	1.00, d	8	33.20	1.28 (m)	33.0	1.26, m
6	22.01	0.91 (d, $J = 2.2$ Hz)	22.3	0.95, d	9	22.69	1.22 (m)	23.7	1.31, m
					10	13.92	0.85 (t)	14.42	0.91, t
					11	13.52	0.78 (d, $J = 6.7$ Hz)	14.41	0.83, d

* These reference data are according to reported data by Yu et al. [29].

Table S2. ^1H -NMR and ATP spectral data of compound 2.

Position	δ_{C} (ppm)	δ_{H} (ppm), multiplicity and J (Hz)	*Ref. δ_{C} (ppm)	*Ref. δ_{H} (ppm)	Position	δ_{C} (ppm)	δ_{H} (ppm), multiplicity and J (Hz)	*Ref. δ_{C} (ppm)	*Ref. δ_{H} (ppm)
Phenylalanine					Valine				
1	172.29	--	173.6	--	1	171.81	--	173.4	
2	53.49	4.72 – 4.64 (m)	55.3	4.79, m	2	58.05	4.21 (t)	59.9	4.20, m
3	40.93	2.98 (dd, $J = 13.5, 7.5$ Hz) 3.12 (dd, $J = 13.5, 8.5$ Hz)	39.4	3.18, dd 3.03, dd	3	28.25	2.27 (m)	31.0	2.18, m
4	135.74	--	137.8	--	4	18.39	0.97 (d, $J = 2.3$ Hz)	19.0	0.98, d
5/9	129.13	7.17 (m)	130.3	7.24, m	5	19.65	0.97 (d, $J = 2.3$ Hz)	19.7	0.97, d
6/8	128.55	7.26 (m)	129.6	7.28, m	Glycine				
7	127.09	7.22 (m)	128.0	7.21, m		171.1	--	171.9	
Alanine					2	43.21	4.46 (d, $J = 8.0$ Hz) 3.47 (dd, $J = 17.2, 4.0$ Hz)	44.0	4.24, d 3.53, d
					Hydroxy methyl lactonic acid (HMOA)				
1	172.64	--	174.1		1	172.91	--	174.5	
2	49.43	4.14 (q)	50.3	4.29, q	2	41.2	2.41(m)	40.9	2.41, m
3	17.89	1.29 (d, $J = 7.3$ Hz)	17.6	1.28, d	3	77.98	4.80 (m)	78.6	4.77, m
Leucine					4	37.74	1.50 (m) 1.2 (m)	39.0	1.54m 1.22 m
1	172.94	--	175.1		5	32.48	1.19 (m) 0.91 (m)	33.3	0.96 m 1.32 m
2	53.23	4.27 (t)	54.7	4.19, m	6	29.34	1.10 (m)	30.5	1.32 m
3	39.06	1.60 – 1.57 (m)	40.4	1.58, m	7	22.59	1.24 (m)	23.8	1.16 m
4	24.52	1.64 (m)	26.0	1.69, m	8	13.67	0.87 (t)	14.38	0.90 t
5	22.02	0.97 (d, $J = 2.2$ Hz)	23.1	0.99, d	9	14.05	0.75 (d, $J = 6.7$ Hz)	14.41	0.83 d
6	22.55	0.95 (d, $J = 2.2$ Hz)	22.3	0.95, d					

* This reference data are according to reported data by Yu et al. [29].

Reference

Yu, Z.; Lang, G.; Kajahn, I.; Schmaljohann, R.; Imhoff, J.F. Scopularides A and B, Cyclodepsipeptides from a Marine Sponge-Derived Fungus, *Scopulariopsis brevicaulis*. *J. Nat. Prod.* **2008**, *71*, 1052–1054.