SUPPLEMENTARY MATERIAL

A New Steroid from the Red Sea Soft Coral *Lobophytum lobophytum*

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Abstract: Chemical investigations of the soft coral *Lobophytum lobophytum* collected from the Red Sea led to isolation of a new compound gorgostan-5,25-dien-3 β -ol (**1**), and two known gorgosterol (**2**), and alismol (**3**). Structures were elucidated by employing extensive NMR and HR-EI-MS experiments.

Keywords: *Nephtheasp.*, Terpenes, Cytotoxicity, Breast cancer cells MCF-7

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Table S1. ¹H (600 MHz) and ¹³C (150 MHz) NMR Data for **1**.

	¹³ C	¹ H
1α	37.3	2.27 m
1β		1.45 m
2	31.7	1.84 m, 1.49 m
3	71.9	3.51 m
4	42.3	2.21 m, 1.27 m
5	140.8	---
6	121.7	5.33 m
7	31.9	1.82 m, 1.42 m
8	32.0	1.92 m
9	50.2	1.07 m
10	35.8	---
11	24.3	1.12 m
12	39.8	1.62 m, 1.30 m
13	42.8	---
14	56.7	1.22 m
15	24.6	1.49 m, 1.04 m
16	28.2	1.64 m, 1.22 m
17	58.0	1.27 m
18	11.9	0.66 s
19	19.4	0.99 s
20	36.6	1.10 m
21	21.1	0.99 s
22	31.7	0.15 ddd (4.0, 6.0, 9.0)
23	25.8	---
24	50.2	0.22 dq (7.0, 8.0)
25	156.9	---
26a	106.0	4.64 s
26b		4.69 s
27	22.0	0.97 d (6.0)
28	15.4	1.82 s
29	14.3	0.88 s
30a	22.2	- 0.14 dd (4.0, 4.0)
30b		0.43 dd (4.0, 9.0)

Full assignment S1. Assignment of known compounds (**2-3**) (^1H (600 MHz) and ^{13}C (150 MHz) NMR]

3.3.1. *Gorgosterol* (**2**):

Amorphous powder, ^1H -NMR [CDCl_3] δ_{H} 5.32 (1H, s, H-6), 3.49 (1H, m, H-3), 2.25, 1.43 (2H, m, H-1), 2.20, 1.26 (2H, m, H-4), 1.89 (1H, m, H-8), 1.88, 1.48 (2H, m, H-2), 1.81, 1.44 (2H, m, H-7), 1.68, 1.19 (2H, m, H-16), 1.58, 1.44 (2H, m, H-12), 1.56, 1.08 (2H, m, H-15), 1.26 (1H, m, H-17), 1.16 (1H, m, H-14), 1.13 (2H, m, H-11), 1.10 (3H, s, Me-19), 1.08 (1H, m, H-20), 1.06 (1H, m, H-9), 0.97 (3H, s, Me-21), 0.92 (3H, s, Me-26), 0.87 (3H, s, Me-29), 0.87 (3H, s, Me-28), 0.83 (3H, s, Me-27), 0.65 (3H, s, Me-18), 0.42 (1H, dd, $J = 4.0, 9.0$ Hz, H-30a), 0.22 (1H, dq, $J = 7.0, 8.0$, H-24), -0.14 (1H, dd, $J = 4.0, 4.0$ Hz, H-30b). ^{13}C -NMR [CDCl_3] δ_{C} 140.8 (C-5), 121.7 (CH, C-6), 71.8 (CH, C-3), 58.0 (CH, C-17), 56.7 (CH, C-14), 50.2 (CH, C-9), 50.2 (CH, C-24), 42.4 (CH_2 , C-4), 42.3 (C-13), 39.2 (CH_2 , C-12), 37.4 (CH_2 , C-1), 36.5 (CH, C-20), 35.3 (C-10), 32.1 (CH, C-8), 32.0 (CH_2 , C-7), 32.0 (CH, C-25), 31.7 (CH, C-22), 31.6 (CH_2 , C-2), 28.3 (CH_2 , C-16), 25.8 (C-23), 24.6 (CH_2 , C-15), 24.4 (CH_2 , C-11), 22.2 (CH_2 , C-30), 21.5 (CH_3 , C-27), 21.3 (CH_3 , C-26), 21.2 (CH_3 , C-21), 19.4 (CH_3 , C-19), 15.5 (CH_3 , C-28), 14.3 (CH_3 , C-29), 11.9 (CH_3 , C-18) (Tanaka et al. 1982; Mohamed et al., 2012).

3.3.2. *Alismol* (**3**):

Colorless crystals, ^1H NMR (CDCl_3) δ_{H} 5.52 (1H, br s, H-6), 4.73, 4.68 (2H, s, H₂-14), 1.22 (3H each, s, Me-15), 0.96, 0.95 (3H each, d, $J = 5.0$ Hz, Me-13, Me-12). ^{13}C NMR (CDCl_3): δ_{C} 153.9 (C-10), 149.8 (C-7), 121.8 (CH, C-6), 106.5 (CH_2 , C-14), 80.8 (C-4), 55.1 (CH, C-5), 47.3 (CH, C-1), 40.3 (CH_2 , C-3), 37.4 (CH, C-11), 37.1 (CH_2 , C-9), 30.0 (CH_2 , C-8), 24.8 (CH_2 , C-2), 24.1 (CH_3 , C-15) 21.5 (CH_3 , C-13), 21.4 (CH_3 , C-12) (Jing et al., 2011).

Figure S1. Selected ^1H - ^1H COSY (---) and HMBC ($\text{--}\rightarrow$) correlations of **1**.

Figure S2. ^1H -NMR Spectrum of Compound **1**.

Figure S3. ^{13}C NMR Spectrum of Compound 1.

Figure S4. ^1H -NMR Spectrum of Compound 2.

Figure S5. ^{13}C NMR Spectrum of Compound 2.

Figure S6. ^1H -NMR Spectrum of Compound **3**.

Figure S7. ^{13}C NMR Spectrum of Compound **3**.