SUPPLEMENTARY MATERIAL

A new sesquiterpene from the South China Sea gorgonian coral *Subergorgia suberosa*

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A new sesquiterpene, namely suberosoid (**1**), was isolated from the South China Sea gorgonian coral *Subergorgia suberosa*.. The chemical structure of **1** was established as an unusual sesquiterpene containing 4-methylenecyclohex-2-enone system, by extensive analyses of NMR spectroscopy and high-resolution mass spectrometry. Suberosoid (**1**) exhibited cytotoxic effect against HeLa cell lines with IC₅₀ value being 10.6 µM.

Keywords: Gorgonian coral; *Subergorgia suberosa*; Sesquiterpene; Cytotoxicity

Table S1: ^1H (500 MHz), ^{13}C (125 MHz) data of compound **1** in CD_3OD

No.	1	
	δ_{C} (mult.)	δ_{H} (mult., J in Hz)
1	207.1 (C)	
2	125.8 (CH)	5.86 (d, $J = 10.0$ Hz)
3	149.3 (CH)	7.21 (d, $J = 10.0$ Hz)
4	144.1 (C)	
5	24.7 (CH_2)	2.19 (ddd, $J = 14.0, 2.0, 1.5$) 1.70 (ddd, $J = 14.0, 12.0, 1.5$)
6	43.7 (CH)	1.63 (m)
7	22.2 (CH_2)	1.61 (m), 1.40 (m)
8	33.9 (CH_2)	1.52 (m), 1.34 (m)
9	47.0 (C)	
10	44.0 (CH)	2.74 (dd, $J = 2.0, 1.5$)
11	122.9 (CH_2)	5.65 (s), 5.54 (s)
12	73.2 (C)	
13	27.2 (CH_3)	1.19 (s)
14	26.8 (CH_3)	1.20 (s)
15	20.0 (CH_3)	1.26 (s)

Figure legends

Figure S1. Key ^1H - ^1H COSY and HMBC correlations of **1**

Figure S2. Key NOESY correlations of **1**

Figure S3. ^1H NMR (500 MHz, CD_3OD) of **1**

Figure S4. ^{13}C NMR (125 MHz, CD_3OD) of **1**

Figure S5. COSY (500 MHz, CD_3OD) of **1**

Figure S6. HSQC (500 MHz, CD_3OD) of **1**

Figure S7. HMBC (500 MHz, CD_3OD) of **1**

Figure S8. HMBC (500 MHz, CD_3OD) of **1** (part 1)

Figure S9. HMBC (500 MHz, CD_3OD) of **1** (part 2)

Figure S10. HMBC (500 MHz, CD_3OD) of **1** (part 3)

Figure S11. NOESY (500 MHz, CD_3OD) of **1**

Figure S12. NOESY (500 MHz, CD_3OD) of **1** (part 1)

Figure S13. NOESY (500 MHz, CD_3OD) of **1** (part 2)

Figure S14. HRMS of **1**

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Figure S13. NOESY (500 MHz, CD₃OD) of compound **1** (part 2)

Figure S14. HRMS of compound **1**.