SUPPLEMENTARY MATERIAL

Two New Eunicellin Diterpenoids from the South China Sea Gorgonian *Muricella sibogae* and Their Bioactivities

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Abstract

A systematic re-study on gorgonian *Muricella sibogae* from South China Sea yielded ten eunicellin-based diterpenoids including two new ones, sibogins C and D (**1–2**). Their structures were elucidated by extensive spectroscopic analyses (1D and 2D NMR, IR and HRMS) and by comparison with data reported in literatures. All the isolates were tested for cytotoxic and antifouling activities. Compounds **3** and **5** showed significant antifouling activity against the green mussel *Perna viridis*, especially **3** was suggested as a potent low-toxic antifouling agent with a large LC₅₀/EC₅₀ value of 18.6. This was the first report on the antifouling activity of the eunicellin-type diterpenoids against the green mussel.

Keywords: Gorgonian; *Muricella sibogae*; eunicellin-based diterpenoids; cytotoxicity; antifouling activity.

List of Supplementary Material

Figure S1. ^1H - ^1H COSY, key HMBC and NOE correlations for compound **1**.

Figure S2. HR-ESI-MS of compound **1**.

Figure S3. ^1H NMR spectrum (600 MHz, CDCl_3) of compound **1**.

Figure S4. ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **1**.

Figure S5. DEPT spectrum (150 MHz, CDCl_3) of compound **1**.

Figure S6. HMQC spectrum (600 MHz, CDCl_3) of compound **1**.

Figure S7. ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound **1**.

Figure S8. HMBC spectrum (600 MHz, CDCl_3) of compound **1**.

Figure S9. NOESY spectrum (600 MHz, CDCl_3) of compound **1**.

Figure S10. HR-ESI-MS of compound **2**.

Figure S11. ^1H NMR spectrum (600 MHz, CDCl_3) of compound **2**.

Figure S12. ^{13}C NMR spectrum (150 MHz, CDCl_3) of compound **2**.

Figure S13. ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound **2**.

Figure S14. HMBC spectrum (600 MHz, CDCl_3) of compound **2**.

Figure S15. NOESY spectrum (600 MHz, CDCl_3) of compound **2**.

Figure S1. ^1H - ^1H COSY, key HMBC and NOE correlations for compound **1**.

20120507-zxw-2-2-3_120507144508 #45-46 RT: 1.16-1.19 AV: 2 NL: 3.54E7
T: FTMS + p ESI Full ms [100.00-1000.00]

Figure S2. HRESI-MS of compound 1.

Figure S3. ^1H NMR spectrum (600 MHz, CDCl_3) of compound 1.

Figure S4. ¹³C NMR spectrum (150 MHz, CDCl₃) of compound **1**.

Figure S5. DEPT spectrum (150 MHz, CDCl₃) of compound **1**.

Figure S6. HMQC spectrum (600 MHz, CDCl_3) of compound **1**.

Figure S7. ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound **1**.

Figure S8. HMBC spectrum (600 MHz, CDCl_3) of compound **1**.

Figure S9. NOESY spectrum (600 MHz, CDCl₃) of compound 1.

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20130125 ZXW2-2-5_130124092337 #22-24 RT: 0.58-0.64 AV: 3 NL: 9.06E5

T: FTMS + p ESI Full ms [130.00-1500.00]

433.2567

$C_{23}H_{38}O_6Na = 433.2561$

1.5678 ppm

Figure S10. HRESI-MS of compound 2.

Figure S11. ^1H NMR spectrum (600 MHz, CDCl_3) of compound **2**.

Figure S12. ¹³C NMR spectrum (150 MHz, CDCl₃) of compound 2.

Figure S13. ^1H - ^1H COSY spectrum (600 MHz, CDCl_3) of compound **2**.

Figure S14. HMBC spectrum (600 MHz, CDCl₃) of compound **2**.

Figure S15. NOESY spectrum (600 MHz, CDCl₃) of compound **2**.