Supplementary material

Cytotoxic 19-oxygenated steroids from the South China Sea gorgonian *Pacifigorgia senta*

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Abstract: Bioassay guided chemical investigation of a gorgonian *Pacifigorgia senta* led to the discovery of a new 19-oxygenated steroid, cholesta-5,24-diene-3 β ,7 β ,19-triol (**1**), as well as three known steroids (**2–4**). The structure of **1** was determined by extensive spectroscopic analysis including NMR and MS spectra. All of the compounds exhibited cytotoxicities against HepG2, Hep3B, MCF-7/ADR, PC-3, and HCT-116 cell lines with the IC₅₀ values ranging from 7.0 to 29.7 μ M. It is the first report on the chemical constituents of the coral species *P. senta*.

Keywords: gorgonian; *Pacifigorgia senta*; 19-oxygenated steroid; cytotoxicity

List of Supplementary Material

Figure S1. Selected ^1H , ^1H -COSY (bold line) and HMBC (arrow) correlations of **1**

Figure S2. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **1**

Figure S3. ^{13}C NMR (150 MHz, CDCl_3) spectrum of compound **1**

Figure S4. ^1H - ^1H COSY (CDCl_3) spectrum of compound **1**

Figure S5. HMQC (CDCl_3) spectrum of compound **1**

Figure S6. HMBC (CDCl_3) spectrum of compound **1**

Figure S7. HRESI-MS spectrum of compound **1**

Figure S1. Selected ¹H, ¹H-COSY (bold line) and HMBC (arrow) correlations of **1**

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Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

145 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

YG-13-13A

20101105-YG-13-13A 64 (2.282) AM (Cen.8, 80.00, Ht.5000.0.0.0.1.00); Sm (Md, 3.00); Cm (64.69)

Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
439.3185	439.3188	-0.3	-0.7	5.5	1	C27 H44 O3 Na

Figure S7. HRESI-MS spectrum of compound **1**