SUPPLEMENTARY MATERIAL

Isolation of a new cytotoxic polyhydroxysterol from the South China Sea soft coral *Sinularia* sp.

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A new polyhydroxysterol, (22*E*)-24-methylencholestane-22-ene-3 β ,5 α ,6 β -triol (**1**), together with four known analogues (**2-5**), were isolated from the South China Sea soft coral *Sinularia* sp.. Their structures were elucidated by spectroscopic analyses and comparison with previously reported data. All these compounds exhibited cytotoxic effect against both HepG2 and HeLa cell lines with IC₅₀ values ranging from 8.36 to 37.30 μ M. Preliminary structure-activity relationship study identified that the presence of double bonds in the side chains of these polyhydroxysterols significantly reduced the biological effect obtained.

Keywords: Soft coral; *Sinularia* sp.; Sterols; Cytotoxicity

Figure legends

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

Figure S2. ^1H NMR (300 MHz, CDCl_3) of **1**

Figure S3. ^{13}C NMR (75 MHz, CDCl_3) of **1**

Figure S4. COSY (300 MHz, CDCl_3) of **1**

Figure S5. HSQC (300 MHz, CDCl_3) of **1**

Figure S6. HMBC (300 MHz, CDCl_3) of **1**

Figure S7. HRMS of **1**

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Figure S5. HSQC (300 MHz, CDCl₃) of compound **1**.

Figure S6. HMBC (300 MHz, CDCl_3) of compound **1**

● Spectrum from DataSample-N-1.wiff (sample 1) - Sample001, Experiment 1, -TOF MS (100 - 1000) from 0.086 to 0.108 min
 ● C₂₈H₄₆O₃ +Cl

Compound Name (Library Hit)	Formula	Intensity	Threshold	Expected m/z	Found at m/z	Error (ppm)
430.34469576 (No Match)	C ₂₈ H ₄₆ O ₃	6280	50	465.3135	465.3131	0.3

Figure S7. HRMS of compound **1**.