SUPPLEMENTARY MATERIAL

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

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A new polyhydroxysterol, (22E)-24-methylenecholestan-22-ene-3β,5α,6β-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 µM. 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 $^1$H-$^1$H COSY and HMBC correlations of 1

Figure S2. $^1$H 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
Figure S1. Key $^1$H-$^1$H COSY and HMBC correlations of 1.
Figure S2. $^1$H NMR (300 MHz, CDCl$_3$) of compound 1.
Figure S3. $^{13}$C NMR (75 MHz, CDCl$_3$) of compound 1.
Figure S4. $^1$H-$^1$H COSY (300 MHz, CDCl$_3$) of compound 1.
Figure S5. HSQC (300 MHz, CDCl₃) of compound 1.
Figure S6. HMBC (300 MHz, CDCl$_3$) of compound 1
| Compound Name (Library Hit) | Formula  | Intensity | Threshold | Expected m/z | Found at m/z | Error (ppm) |
|-----------------------------|----------|-----------|-----------|--------------|--------------|-------------|
| 430.34469576 (No Match)    | C28H46O3 | 6280      | 50        | 465.3135     | 465.3131     | 0.3         |

Figure S7. HRMS of compound 1.