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STEROIDS OF SOFT CORAL *Scleronephthya* sp. FROM THE SOUTH CHINA SEA

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The soft coral *Scleronephthya* sp. belongs to the family Alcyoniidae. A literature survey revealed that chemical studies on the genus *Scleronephthya* were relatively rare, and only a few metabolites, mainly pregnane steroids, have been reported to date. Most of these steroids exhibited potent bioactivities, including cytotoxic, antiviral, and antibacterial activities [1–5].

In our investigation on bioactive compounds from *Scleronephthya* sp. collected from the South China Sea, nine steroids, including three ergosterol derivatives and six cholesterol derivatives, were isolated from the EtOH extract. Their structures were identified as ergosta-6α-hydroxy-4,22-dien-3-one (**1**) [6], ergosta-4,22-dien-3-one (**2**) [7], cholesta-4,22-dien-3-one (**3**) [8], cholesta-4-en-3-one (**4**) [8], cholesterol (**5**) [9], dendronesterol A (**6**) [10], cholesta-7,22-diene-3β,5α,6β-triol (**7**) [11], ergosta-7,22-diene-3β,5α,6β-triol (**8**) [12], and cholesta-7-en-3β,5α,6β-triol (**9**) [11] on the basis of their spectral data and by comparison with those reported in the literature. All of these steroids, including four sterones and five sterols, were isolated from the genus *Scleronephthya* for the first time.

To our knowledge, it is also the first time that compounds **1** and **2** were isolated from corals [6, 13–15]. Thus, the occurrence of **1** and **2** in *Scleronephthya* sp. is chemotaxonomically important. Based on a search of the literature [10, 16–18], besides many other class organisms, the concurrence of compounds **3**, **4**, and **6** in corals of both genus *Scleronephthya* and *Dendronephthya* suggested that there might be a biogenic association between the two different genus.

All of these steroids exhibited potent lethal activity against brine shrimp *Artemia salina* with a lethality of more than 50.0% at a concentration of 50.0 μg/mL. Compounds **2**, **4**, **6**, and **9** were selected to evaluate antifouling activity, and all of these four steroids showed no activity against the larval settlement of barnacle *Balanus amphitrite* at a concentration of 50.0 μg/mL.

Animal Material. The soft coral *Scleronephthya* sp. was collected from the Meishan coral reef in the South China Sea at 10 m depth in September 2006 and was identified by Prof. Huang Hui, South China Sea Institute of Oceanology, Chinese Academy of Science. A voucher specimen (HN-SYM-20060029) was deposited in the Key Laboratory of Marine Drugs, Ministry of Education, Ocean University of China, Qingdao, China.

Extraction and Isolation. The fresh specimens *Scleronephthya* sp. (900.0 g) were immediately chilled to –20°C and kept frozen until they were exhaustively extracted with ethanol (v/v 95%) at room temperature. After removal of the solvent under reduced pressure, the EtOH extract was evaporated to give a residue (24.4 g) and was then subjected to silica gel (100–200 mesh) vacuum column chromatography (VLC) eluted with petroleum ether–EtOAc mixtures of increasing polarity, yielding seven fractions (Fr. 1–Fr. 7). Fraction 3, 5, and 7 were further purified by column chromatography on silica gel and Sephadex LH-20 and by prep-HPLC to yield compounds **1** (2.0 mg), **2** (3.0 mg), **3** (3.0 mg), **4** (5.0 mg), **5** (3.0 mg), **6** (4.5 mg), **7** (2.0 mg), **8** (7.7 mg), and **9** (2.5 mg).

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Assessment of Bioactivities. Lethal activity to brine shrimp *A. salina* was tested according to the modified Solis method [19, 20]. Antifouling activity on larval settlement of *B. amphitrite* was evaluated according to standard protocols [21, 22].

Ergosta-6α-hydroxy-4,22-dien-3-one (**1**): white amorphous powder, $C_{28}H_{44}O_2$; $[\alpha]_D^{25}$ +156.0° (*c* 0.43, MeOH); mp 129–138°C. UV spectrum (MeOH, λ_{max}, nm): 245. IR spectrum (KBr, ν_{max}, cm^{-1}): 3422, 2930, 1666. ^1H NMR (600 MHz, $CDCl_3$, δ, ppm, J/Hz): 1.95 (1H, m, H-1a), 1.70 (1H, m, H-1b), 1.26 (1H, m, H-2a), 2.41(1H, m, H-2b), 6.19 (1H, s, H-4), 4.36 (1H, dd, J = 13.0, 4.5, H-6), 1.35 (1H, m, H-7a), 2.02 (1H, m, H-7b), 1.95 (1H, m, H-8), 0.95 (1H, m, H-9), 1.74 (2H, m, H-11), 2.01 (1H, m, H-12a), 1.28 (1H, m, H-12b), 1.03 (1H, m, H-14), 1.75 (2H, m, H-15), 1.04 (2H, m, H-16), 1.24 (1H, m, H-17), 0.75 (3H, s, H-18), 1.21 (3H, s, H-19), 2.04 (1H, m, H-20), 0.94 (3H, d, J = 7.0, H-21), 5.21 (1H, dd, J = 15.0, 9.5, H-22), 5.17 (1H, dd, J = 15.0, 7.5, H-23), 2.39 (1H, m, H-24), 2.04 (1H, m, H-25), 0.87 (3H, d, J = 6.5, H-26), 0.85 (3H, d, J = 6.5, H-27), 1.03 (3H, d, J = 6.5, H-28). ^{13}C NMR (150 MHz, $CDCl_3$, δ, ppm): 199.8 (C-3), 171.9 (C-5), 136.1 (C-23), 132.6 (C-22), 120.1 (C-4), 69.1 (C-6), 56.2 (C-17), 56.1 (C-14), 54.2 (C-9), 43.5 (C-24), 42.7 (C-13), 41.9 (C-7), 40.7 (C-12), 39.7 (C-20), 39.7 (C-10), 36.7 (C-1), 34.6 (C-2), 34.2 (C-8), 33.6 (C-25), 29.3 (C-15), 24.1 (C-16), 21.4 (C-21), 21.3 (C-11), 20.6 (C-27), 20.0 (C-26), 18.7 (C-19), 18.5 (C-28), 12.5 (C-18); ESI-MS *m/z* 413 $[M + H]^+$.

Ergosta-4,22-dien-3-one (**2**): white amorphous powder, $C_{28}H_{44}O$. ^1H NMR (600 MHz, $CDCl_3$, δ, ppm): 5.72 (1H, s, H-4), 0.72 (3H, s, H-18), 1.18 (3H, s, H-19), 0.99 (3H, d, J = 6.6, H-21), 5.20 (1H, dd, J = 15.0, 8.6, H-22), 5.29 (1H, dd, J = 15.0, 8.6, H-23), 0.87 (3H, d, J = 6.6, H-26), 0.85 (3H, d, J = 6.6, H-27), 0.92 (3H, d, J = 6.6, H-28). ^{13}C NMR (150 MHz, $CDCl_3$, δ, ppm): 199.5 (C-3), 171.5 (C-5), 135.6 (C-22), 131.9 (C-23), 123.8 (C-4), 56.0 (C-17), 56.0 (C-14), 53.9 (C-9), 42.8 (C-24), 42.3 (C-13), 40.1 (C-20), 39.5 (C-12), 38.6 (C-1), 35.7 (C-10), 35.6 (C-8), 34.0 (C-2), 33.1 (C-25), 32.9 (C-6), 32.1 (C-7), 28.5 (C-16), 24.2 (C-15), 21.0 (C-11), 20.9 (C-21), 20.0 (C-26), 19.6 (C-27), 17.6 (C-28), 17.4 (C-19), 12.2 (C-18); ESI-MS *m/z* 397 $[M + H]^+$.

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