

Phytochemical communication

A new steroid from *Selaginella pulvinata*

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Abstract

A new steroid, 3 β , 16 α -dihydroxy-(5 α)-cholestan-21-oic acid, was isolated from the aerial parts of *Selaginella pulvinata*. Its structure was elucidated on the basis of spectral analysis.

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Keywords: *Selaginella pulvinata*; Steroids; Spectral analysis

1. Plant

Selaginella pulvinata, collected in Kunming, Yunnan Province of China, was identified by Prof. S. K. Wu, a Botanist of Kunming Institute of Botany. A voucher specimen was deposited in the Herbarium of Kunming Institute of Botany, Chinese Academy of Sciences.

2. Uses in traditional medicine

S. pulvinata has been used to treat tumor, diabetes, stomachache and asthma [1].

3. Previously isolated constituents

Sterols and flavonoids [2,3].

4. New isolated constituent

3 β , 16 α -Dihydroxy-(5 α)-cholestan-21-oic acid (**1**, Fig. 1, yield: 0.0003%).

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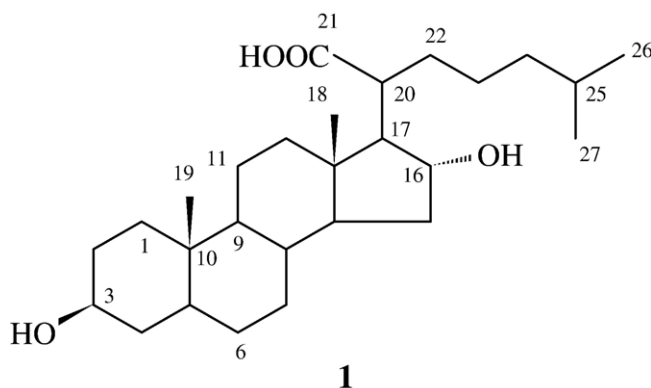


Fig. 1.

White powder, mp 213–215 °C; EI-MS m/z : 434 $[M]^+$, 416 $[M-H_2O]^+$, 388 $[M-COOH-H]^+$, 291 $[M-C_8H_{15}O_2 \text{ (side chain)}]^+$; HRMS m/z : 434.3403. Calculated for $C_{27}H_{46}O_4$: 434.3396. 1H NMR (300 M Hz, C_5D_5N): δ 4.41 (16 β -H, m), 3.80 (3 α -H, m), 1.01 (3H, s , 19 Me), 0.79 (3H, d , J 6.6 Hz, 27 Me), 0.77 (3H, s , 18 Me), 0.76 (3H, d , J 6.6 Hz, 26 Me); ^{13}C NMR (75 M Hz, C_5D_5N): δ 37.5 (C-1), 32.5 (C-2), 70.7 (C-3), 38.9 (C-4), 45.3 (C-5), 29.2 (C-6), 32.9 (C-7), 35.4 (C-8), 54.8 (C-9), 35.9 (C-10), 21.3 (11), 39.5 (C-12), 44.3 (C-13), 53.7 (C-14), 37.8 (C-15), 76.1 (C-16), 63.2 (C-17), 12.6 (C-18), 14.2 (C-19), 47.9 (C-20), 178.8 (C-21), 32.5 (C-22), 26.3 (C-23), 39.3 (C-24), 28.5 (C-25), 22.6 (C-26), 22.9 (C-27).

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