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Phytochemical communication

A new ellagic acid glycoside from Paeonia delavayi

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Abstract

A new ellagic acid glycoside, 4'-O-methylellagic acid 4-O- β -D-glucopyranoside (1), was isolated from the root cortex of *Paeonia delavayi*. The structure was elucidated on the basis of spectroscopic methods. © 2008 Elsevier B.V. All rights reserved.

Keywords: Paeonia delavayi; 4'-O-Methylellagic acid 4-O-β-D-glucopyranoside; Spectroscopic methods

1. Plant

Paeonia delavayi Franch (Paeoniaceae), roots collected from Lijiang County of Yunnan Province, PR China in August 1998, and identified by Mr. Zheng-Wei Lu, Kunming Institute of Botany, The Chinese Academy of Sciences, Kunming, Yunnan, where a voucher specimen is deposited.

2. Uses in traditional medicine

The root cortex, as one of the most important crude drugs in Chinese traditional medicine, is an analgesic, sedative and antiinflammatory agent. It is also frequently used as a remedy for cardiovascular, extravasated blood, stagnated blood and female diseases in traditional oriental medicine [1-3].

3. Previously isolated classes of constituents

Monoterpenoids [4–6] and triterpenoids [7].

4. New-isolated constituent

4'-O-methylellagic acid 4-O-β-D-glucopyranoside (1, Fig. 1) (12 mg from 5 kg of dried material): white amorphous powder; mp 293–295 °C; UV max (MeOH): 254, 276, 359 nm; IR bands (KBr): 3444, 1723, 1622, 1573, 1496, 1450,

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Fig. 1. Structure of compound 1.

Fig. 2. Some HMBC correlations of compound 1.

1348, 1087, 1046, 918, 757 cm⁻¹; ¹H-NMR (500 MHz, pyridine- d_5): δ 8.45 (1H, s, H-5), 7.82 (1H, s, H-5'), 5.90 (1H, d, J7.7 Hz, H-1"), 4.36 (1H, m, H-2"), 4.28 (1H, m, H-3"), 4.13 (1H, m, H-4"), 4.40 (1H, m, H-5"), 4.53 (1H, m, H-6"a), 4.42 (1H, m, H-6"b), 3.84 (3H, s, 4'-OMe); ¹³C-NMR (125 MHz, pyridine- d_5): δ 108.4 (C-1), 137.6 (C-2), 138.0 (C-3), 149.2 (C-4), 113.6 (C-5), 115.2 (C-6), 160.2 (C-7), 108.4 (C-1'), 142.7 (C-2'), 143.9 (C-3'), 151.4 (C-4'), 107.5 (C-5'), 114.5 (C-6'), 160.0 (C-7'), 103.7 (C-1"), 74.9 (C-2"), 78.4 (C-3"), 71.1 (C-4"), 79.2 (C-5"), 62.2 (C-6"), 56.5 (4'-OMe); long-range C-H connectivities: C-4 with H-1" (δ 5.90); C-3, C-4, C-6 and C-7 with H-5 (δ 8.45); C-3', C-4', C-6' and C-7' with H-5' (δ 7.82); C-4' with 4'-OMe (δ 3.84) (Fig. 2); Negative FAB-MS: m/z 477 [M-1]⁻ (100%), 447 (6), 315 (12), 297 (5), 229 (8); Negative HRFAB-MS: m/z [M-1]⁻ 477.0843 (calcd. for C₂₁H₁₈O₁₃, 478.0859).

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