Phytochemical Communication

Novel prenylated flavonoid from stem of
Pithecellobium dulce

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Plant. Pithecellobium dulce Benth. (Mimosaceae), stems collected locally from University Campus in July, 1996 and authenticated by Dr Pradeep Tiwari, Department of Botany, Dr H.S. Gour University Sagar, voucher specimen No. XXXII B (Department of Chemistry, Dr H.S. Gour University, Sagar).

Uses in traditional medicines. Astringent and abortifacient agent [1].

Previously isolated constituents. Flavonoids from the seeds [2], triterpenoid saponin from leaves and seeds [3].

New isolated constituents. 3'-Prenylapigenine 7-O-rutinoside (1), 125 mg from 3 kg of air-dried, powdered stems.

3'-Prenylapigenine 7-O-rutinoside (1). Mp 128°C; UV max (MeOH): 270, 355 nm (bathochromic shift of 44 nm in band I with AlCl₃/MeOH showed free hydroxyl

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group C-5 [4]; bathochromic shift of 48 nm in band I with NaOMe/MeOH confirmed the presence of hydroxyl group at C-4' [5] with blocked C-7 position; IR bands (KBr): 1701 (>C=O), 1375, 1385 (gem-dimethyl) cm⁻¹; ²H-NMR (400 MHz, acetone-d₆): δ 1.77 (6H, s, 2×CH₃-13), 3.42 (2H, d, J 8 Hz, CH₂-11), 5.32 (1H, m, C-12), 6.22 (1H, d, J 2 Hz, H-6), 6.30 (1H, d, J 8.5 Hz, H-8), 6.52 (1H, s, H-3), 6.65 (1H, d, J 8 Hz, H-5’), 7.72 (1H, dd, J 2.0, 8.5 Hz, H-6’), 7.80 (1H, d, J 2 Hz, H-2), 5.90 (1H, d, J 7 Hz, H-1’); ¹³C-NMR [6] (DMSO-d₆): 164.5 (C-2), 103.3 (C-3), 181.8 (C-4), 161.2 (C-5), 100.2 (C-6), 162.8 (C-7), 95.1 (C-8), 95.1 (C-8), 157.1 (C-9), 105.6 (C-10), 21.4 (C-11), 122.5 (C-12), 130.4 (C-13), 25.5 (C-14), 17.7 (C-15), 123.6 (C-1’), 130.3 (C-2’), 118.7 (C-3’), 162.2 (C-4’), 118.7 (C-5’), 130.3 (C-6’), 99.0 (C-1”), 72.9 (C-2”), 76.0 (C-3”), 69.2 (C-4”), 75.8 (C-5”), 65.9 (C-6”), 100.1 (C-1””), 70.0 (C-2””), 70.2 (C-3””), 71.9 (C-4””), 68.4 (C-5””), 17.5 (C-6””) [7]; MS m/z: 646 (M⁺), 338, 310, 295, 185, 153.

Permethylation (MeI, DMF/Ag₂O) of 1 followed by acid hydrolysis, yielded tri-O-methyl-l-glucose, tri-O-methyl-l-rhamnose and 3’-prenylapigenine (2) [8].

Enzymatic hydrolysis of 1 with diastase gave 3’-prenylapigenine 7-O-β-D-glucopyranoside (3) and l-rhamnose. Enzymatic hydrolysis of 3 with almond emulsion yielded aglycone 2 and D-glucose.

3’-Prenylapigenine (2). Mp 102°C; M⁺ 338; IR (KBr): 1660, 1615, 1580 cm⁻¹; ³H-NMR (400 MHz, acetone-d₆): δ 1.75 (6H, s, 2×CH₃-13), 3.40 (2H, d, J 7.5 Hz, CH₂-11), 5.40 (1H, m, H-12), 6.25 (1H, d, J 2 Hz, H-6), 6.50 (1H, d, J 2 Hz, H-8), 6.60 (1H, s, H-3), 7.0 (1H, d, J 8.5 Hz, H-5), 7.75 (1H, dd, J 2.2 Hz, 8.5 Hz, H-6’), 7.80 (1H, d, J 2.2 Hz, H-2’).
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References