A new tetracyclic phenol and other constituents from the roots of Bauhinia racemosa

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The roots of Bauhinia racemosa Lamk. (Fam. Caesalpinioideae) afford lupeol, betulin and β-sitosterol along with a novel tetracyclic phenol. The latter has been identified as 3-hydroxy-de-O-methyl racemosol by comparative spectral studies with racemosol and de-O-methyl racemosol isolated earlier from this plant.

Bauhinia racemosa Lamk. (Fam. Caesalpinioideae), a small deciduous tree, is found in tropical parts of the world and grows throughout India. The bark and leaves are known to cure skin diseases, throat troubles, tumors, chronic dysentery, headache and malaria. The alcoholic extract of stem bark of B. racemosa was found to exhibit anticancer activity against human epidermal carcinoma of the nasopharynx in tissue culture, CNS depressant activity and hypothermia in mice whereas its seed extract exhibited specific de-aggregating properties. Phytochemical investigations on this plant species have revealed the isolation of resveratrol, pacharin, racemosol and β-sitosterol from the heartwood along with a novel tetracyclic phenol derivative which is being reported for the first time. The l3C NMR spectrum of compound 1 further confirmed the proposed structure. The assignments were made by comparison with the spectra of related compounds.

Experimental Section

Melting points are uncorrected. IR spectra were recorded (as KBr pellets) on a Perkin-Elmer model 557 spectrophotometer. 1H NMR and 13C NMR spectra on model Jeol FX 90Q at 89.55 MHz and 22.49 MHz respectively, using CDCl3 and DMSO-d6 as solvents and TMS as an internal standard were recorded on a Hitachi Model RMU 6E Mass Spectrometer.

Column chromatography was carried out using silica gel (60-120 mesh). TLC was carried out on silica gel G chromatoplates and 2% ceric ammonium sulphate was used as spraying agent.
The roots of *B. racemosa* Lamk. were collected from the Campus of the University of Rajasthan, Jaipur and were identified for authenticity in the Herbarium, Department of Botany. The air-dried and finely powdered roots (1.5 kg) were exhaustively extracted with 95% C₂H₅OH and the concentrate (80 g) was fractionated into pet. ether (0.5 g), benzene (30.5 g) and ether (7 g) solubles. The benzene fraction on CC (silica gel) afforded lupeol (0.72 g, m.p. 210-13°C, pet. ether - C₆H₆, 1:4); β-sitosterol (0.86 g, m.p. 135-36°C, C₂H₆H); racemosol (0.52 g, m.p. 200°C, C₆H₆); betulin (0.87 g, m.p. 245-48°C, C₆H₆-CHCl₃, 1:1) and de-O-methyl racemosol (0.68 g, m.p. 215-18°C, CHCl₃-MeOH, 1:1).

The ether fraction on CC (silica gel) afforded the new tetracyclic phenol compound 1, 0.97 g (C₆H₆ - EtOAc, 3:1), yellowish-brown crystals, m.p. 240-45°C (CH₃OH - CHCl₃). It dissolved in NaOH solution and gave blue-green colour with neutral FeCl₃. IR (KBr) : 3450 (broad), 3010, 2900, 2870, 1590, 1520, 1380, 1360, 1230, 1200, 1180, 975 and 850 cm⁻¹; ¹H NMR (89.55 MHz, DMSO-d₆) : δ 7.82 (1H, s), 7.48 (1H, s), 6.95 (1H, d, J=8Hz), 6.63 (1H, d, J=8Hz), 6.62 (1H, s), 5.94 (1H, s), 4.97 (1H, d, J=6.3Hz), 3.92 (1H, d, J=6.3Hz), 3.12-2.12 (5H, m), 1.99 (3H, s), 1.56 (3H, s) and 1.36 (3H, s); EIMS (m/z) : 342 (M⁺), 327, 271, 270, 225, 195, 181, 167, 161, 134, 129, 105, 91, etc; ¹³C NMR (22.49 MHz, DMSO-d₆) : δ 82.86 (C-2), 86.24 (C-3), 41.27 (C-4), 125.48 (C-5), 115.02 (C-6), 112.50 (C-7), 144.15 (C-8), 141.67 (C-9), 114.23 (C-10), 127.22 (C-11), 34.15 (C-12), 133.88 (C-13), 109.10 (C-14), 152.44 (C-15), 109.37 (C-16), 153.63 (C-16a), 131.00 (C-16), 26.83 and 20.35 (gem-Me) and 8.98 (Me-Ar); tetraacetate : brown crystals, m.p. 182-85°C (CH₂OH).

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References