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Note

A disubstituted pyrone from *Centella asiatica*

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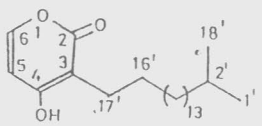
A new compound isolated from *Centella asiatica* has been characterized as 3-isooctadecanyl-4-hydroxy-α-pyrone by spectral evidence.

Centella asiatica (Umbelliferae) is found throughout India in marshy places upto an altitude of 6,000 ft[1]. The plant is reported to possess antileprotic[2], antitumor[3], antistress[4], wound healing[5], antifilarial[6], antifeedant[7], and antibacterial[8] properties and is used as a tonic in Ayurvedic formulations. Earlier work on this plant has led to the isolation of asiaticoside[9], hyperin[10], brahmic acid[11], sterols[7] and lipids[12] . The characterization of 3-isooctadecanyl-4-hydroxy-α-pyrone **1** is reported in this note.



Column chromatography of the hexane fraction over silica gel yielded a crystalline compound **1**. The IR spectrum of **1** showed absorption bands for OH (3340 cm^{-1}), α-pyrone (1720, 1680, 1656, 1627, 1547 cm^{-1})[13], double bond (840 cm^{-1}) and straight-chain functions (720 cm^{-1}). The UV spectrum had a maxima at 268 nm typical of a α,β-unsaturated ketone system having a hydroxyl group at β-position and a substituent at α-position[14]. An $[M]^+$ at m/z 364 in its mass spectrum was in agreement with the molecular formula $C_{23}H_{40}O_3$. The prominent ions at m/z 111 and 253 established the presence of hydroxypyrone and isooctadecanyl moieties in the molecule. An $[M-Me]^+$ at m/z 349 suggested the presence of a Me group as a substituent. The loss of a CO group was seen at m/z 336. The base peak obtained at m/z 81 could be due to the loss of a lactone group (44 mass units) from the ion m/z 125. In the ^1H NMR spectrum the protons at 5- and 6-positions appeared as doublets at δ 5.75 and 6.10 while the protons at 3- and 4-positions were absent as these positions were occupied by hydroxyl and isooctadecanyl substituents. Since hydrogen bonding was not seen in the IR spectrum (OH group at 3340 cm^{-1}), OH group was placed at 4-position and isooctadecanyl moiety at 3-position. The proposed structure was also corroborated by ^{13}C NMR spectrum (see Experimental).

Experimental

Melting points are uncorrected. The IR spectra were recorded in KBr and UV spectra in MeOH, ^1H NMR at 80 MHz and ^{13}C NMR at 100 MHz in $CDCl_3$ with TMS as internal standard. TLC analyses were carried out on silica gel and the spots visualized by exposure to I_2 vapours. The plant was collected from the local area and identified in our Botany Department, where a voucher specimen is maintained.

Isolation of compound 1. The air-dried and powdered plant (2 kg) was extracted with MeOH (8×4.5 L), the combined extract concentrated to 250 mL and H_2O (250 mL) was added to it. The aq. methanolic extract was then fractionated successively with *n*-hexane (8×500 mL, 66 g), EtOAc (6×500 mL, 70 g), and *n*-BuOH (10×250 mL, 105 g). Part of the hexane fraction (35 g) was chromatographed over silica gel (990 g), eluting with varying proportions of hexane, C_6H_6, $CHCl_3$ and MeOH. Fractions (100 mL) each were collected and monitored by TLC. The residue from $CHCl_3$-MeOH (9.5: 0.5) fractions afforded a solid (100 mg), m.p. 82°; IR: 3340, 2920, 2850, 1720, 1656, 1627, 1547, 1470, 1259, 997, 840, 720 cm^{-1}; UV: 268 nm; MS m/z (rel. int): 364 $[M]^+$ $[C_{23}H_{40}O_3]$(15), 349(16), 336(25), 321(35), 293(30), 265(12), 253(13), 181(10), 167(20), 153(12), 125(30), 113(70), 111(40), 99(60), 85(15), 81(100), 71(20), 57(85), 43(70); ^1H NMR: δ 0.95 (6H, d, *J*=8Hz, –CH $(CH_3)_2$), 1.25 (28H, br s. 14×CH_2), 5.75 (1H, d, *J*=10 Hz, H-5), 6.10 (1H,

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d, J=9 Hz, H-6), 3.15 (2H, t, J=6 Hz, H_2-17'), 2.15 (1H, m, H-2'); ^{13}C NMR: δ 166.37 (C-2), 121.66 (C-3), 142.66(C-4), 141.48(C-5), 128.23(C-6), 20.95 (C-1', 18'), 22.60 (C-2'), 29.6 (C-3'), 32.86 (C-4'), 31.86 (C-5'), 28.8(C-6'), 28.6(C-7'), 29.28 (C-8' to C-14'), 29.38 (C-15'), 29.13(C-16'), 46.94(C-17').

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