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B R I E F C O M M U N I C A T I O N S

STRUCTURE OF KUHFERININE

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In continuation of research on esters of *Ferula kuhistanica* (Apiaceae) [1], we isolated a new compound of composition $C_{20}H_{34}O_4$, mp 129-130°C, which we called kuhferinine, from the neutral part of the total extract of the roots.

The IR spectrum of this compound contains absorption bands at 3678-3652 cm^{-1} (hydroxyl), 1692 cm^{-1} (ester carbonyl), and 1656 cm^{-1} (double bond). The mass spectrum exhibits peaks for ions with *m*/*z* 338, 320, 238, 154, 136, 121, 97, and 83, which are characteristic of terpenoid esters with aliphatic acids [2, 3].

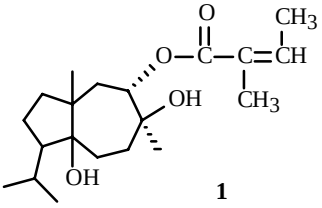
The PMR spectrum (Tesla BS 567 A/100 MHz in $CDCl_3$ with HMDS as internal standard) has doublets at 0.82 and 0.92 ppm (3H each, J = 7 Hz, C_{11}–$2CH_3$), singlets at 1.07 and 1.40 ppm (C_1–CH_3, C_8–CH_3), a singlet at 1.80 ppm and a doublet at 1.87 ppm (C_2'–CH_3, C_3'–CH_3), a doublet at 5.50 ppm (1H, J = 10 Hz, C_9–H) and a quartet 5.85 ppm (1H, J_1 = 12.5 Hz, J_2 = 2.5 Hz, C_4'–H), and a singlet at 4.40 ppm (2OH).

A sesquiterpene alcohol of composition $C_{15}H_{28}O_3$, mp 73-73.5°C, was isolated from the neutral part of the hydrolysate after alkaline hydrolysis of kuhferinine. It was identified by its IR spectrum and mixed melting point as pallitriol, which was isolated by hydrolysis of pallidin. The PMR spectrum contains doublets at 0.72 and 0.95 ppm (3H each, J = 7 Hz, C_{11}–CH_3), singlets at 1.24 and 1.45 ppm (3H each, C_1–CH_3, C_8–CH_3), a doublet at 4.05 ppm (1H, J = 10 Hz, C_9–H), and a singlet at 4.85 ppm (1H, OH).

The acid part of the hydrolysate yielded angelic acid $C_5H_8O_2$, mp 44-45°C. Thus, kuhferinine is an ester of pallitriol and angelic acid.

The position of angelic acid in kuhferinine was determined by comparing the chemical shifts of the signals for the gemacyl (kuhferinine, 5.50 ppm, J = 10 Hz, C_9–H) and gemhydroxyl protons (pallitriol, 4.05 ppm, J = 10 Hz, C_9–H) in their PMR spectra.

Therefore, kuhferinine is 9-angeloyloxypallitriol (**1**). We propose the relative configuration 9α-angeloyloxy-5β,8β-dihydroxy-*cis*-carotane for kuhferinine because the three-dimensional structure of pallitriol was proven by an x-ray analysis as 5β,8β-dihydroxy-9α-oxo-*cis*-carotane [4].



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