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STRUCTURE OF SAMFERINE

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In continuation of systematic research on terpenoids of plants in the *Ferula* L. genus (Apiaceae, Carrot) [1], we isolated from roots of *F. samarcandica* Korov. by chromatographic separation over KSK silica gel with elution by benzine:ethylacetate (6:1) a new compound of formula $C_{22}H_{30}O_5$ called samferine.

Its IR spectrum has absorption bands for hydroxyl (3356 cm^{-1}), ester carbonyl (1704 cm^{-1}), and aromatic rings (1688, 1683, 1609, and 1593 cm^{-1}). Its mass spectrum is typical of terpenoid esters with peaks at *m/z* 314, 274, 234, 193, 177, 157, 148, 121, 93, 81, and 69 [2].

The PMR spectrum of samferine exhibits signals (δ, ppm, J/Hz) at 0.93 and 0.99 (d, 3H each, J = 6, C_{11}-2CH_3), 1.10 (s, 3H, C_1-CH_3), 1.70 (br.s, 3H, C_8-CH_3), 3.90 (t, 1H, $J_1 = J_2 = 6$, C_2-H), 5.40 (m, 2H, C_6-H, C_9-H), 6.95 (d, 2H, J = 9, C_3'-, C_5'-H), 7.95 (d, 2H, J = 9, C_2'-, C_6'-H).

Comparison of spectral data with the literature [2-4] led to the conclusion that samferine is an ester of a sesquiterpene alcohol of the carotane type with *p*-hydroxybenzoic acid. Alkaline hydrolysis by aqueous-alcoholic KOH (5%) produced from the neutral part of the hydrolysate a sesquiterpene alcohol of formula $C_{15}H_{26}O_3$ with mp 144-145°C that we called samferol.

We isolated *p*-hydroxybenzoic acid, $C_7H_6O_3$, mp 212-213°C, from the acidic part of the hydrolysate.

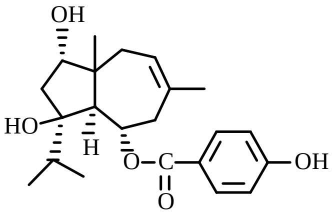
The PMR spectrum of samferol contains signals (δ, ppm, J/Hz) at 0.84 (t, 6H, $J_1 = J_2 = 6.5$, C_{11}-2CH_3), 0.98 (s, 3H, C_1-CH_3), 1.64 (s, 3H, C_8-CH_3), 3.85 (t, 1H, $J_1 = J_2 = 6$, C_2-H), 4.45 (sext., 1H, $J_1 = J_2 = 10.5$, $J_3 = 2,5$, C_6-H), 5.30 (t, 1H, $J_1 = J_2 = 6$, C_9-H).

Comparison of spectral data for samferine and samferol with those for the esters ferutinol, akichenol, lapidol, lapiferol, and lapidolinol [5] provides a basis to propose that samferol is a sesquiterpene alcohol of the carotane type with one hydroxyl located on C_6 and a double bond at C_8–C_9.

Signals of two geminal OH protons at 3.85 and 4.45 ppm in the PMR of samferol indicate that two of the three OH groups are secondary and one is tertiary. Considering the multiplicity of the C_6-proton, the only possible position for the tertiary OH is C_4.

The position of the second secondary OH in samferine follows from the chemical shift of the angular methyl. The signal for C_1-CH_3 in carotane esters without a C_2-OH appears at 0.75-0.85 ppm [5]. The second secondary OH in samferine is thought to reside on C_2 according to the chemical shift of C_1-CH_3 in the spectra of samferine and samferol at 1.10 and 0.98 ppm, respectively.

A sesquiterpene ester isolated from *F. communis* subsp. *communis* has been described [6]. Comparison of it and samferine indicates that the compound isolated by us is an isomer with a different orientation of the C_2-OH for which we propose the following structure as most probable.



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