KARATAVICIN — A NEW COUMARIN FROM *Ferula karatavica*

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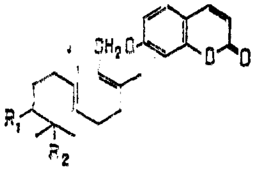
On studying the chemical composition of *Ferula karatavica* Rgl. et Schmalh., in addition to compounds reported previously [1, 2] we have isolated a new coumarin — karatavicin (I), $C_{26}H_{34}O_6$, M^+ 442, mp 60-62°C, $[\alpha]_D^{25}$ −21° (c 1.0; ethanol). The UV spectrum — $\lambda_{max}^{C_2H_5OH}$ 218, 243, 250, 325 nm (log ε 4.36; 3.65; 3.53; 4.19, respectively) — shows the absorption maxima of a o-substituted 7-hydroxycoumarin. The IR spectrum shows absorption bands at (cm^{-1}) 3450 (OH group); 1735, 1720 (C=O's of an α-pyrone and of an ester group); 1620, 1518, 1510 (aromatic nucleus).

In the NMR spectrum of (I) (JNM-4H-100 MHz, $CDCl_3$, 0 — HMDS) appear the signals of a gem-dimethyl group (1.13 ppm, s, 6 H) and of vinylmethyl groups (1.53, 1.69 br.s, 3 H, each), the broadening of the last-mentioned signals being due to their allyl interaction with olefinic protons. In addition, the signals can be seen of the methyl group of an acetyl residue (2.00 ppm, s, 3 H), of the methyl protons in an $Ar{-}O{-}CH_2{-}$ group (4.53 ppm, d, 2 H, J = 9 Hz), of a hemihydroxylic proton (3.28 ppm, q, 1 H, J_1 = 8 Hz, J_2 = 3 Hz), and of olefinic protons (5.05 ppm, m, 1 H, and 5.38 ppm, br. t, 1 H, $J_1 = J_2$ = 7 Hz). The signals of the protons of a 7-substituted coumarin nucleus are observed in the 6.13-7.50 ppm region.

The elementary composition and the spectral characteristics given above permit (I) to be assigned to the aliphatic sesquiterpenoid o-substituted 7-hydroxycoumarins [3].

The positions of the functional groups were determined in the following way. Since in the PMR spectrum of (I) the singlet signal from the gem-dimethyl group is located in the higher field at 1.13 ppm and the hydroxyl is secondary, the acetic acid residue can be present only at $C_{11'}$. The signal of the hemihydroxylic group is represented in the PMR spectrum in the form of a quartet at 4.64 ppm. Consequently, three positions are possible for it: $C_{4'}$, $C_{8'}$, and $C_{10'}$. We gave our preference to the $C_{10'}$ position by analogy with karatavikinol (II). In actual fact, alkaline hydrolysis of karatavicin led to (II). Furthermore, on the oxidation of (I) with chromium trioxide in acetone, we obtained a compound (III) with mp 70-72°C identical with karatavikin acetate. Thus, karatavicin is the monoacetate of karatavikinol at the tertiary hydroxy group. The study of the chemical composition of *Ferula karatavica* is continuing.



I $R_1 = OH$; $R_2 = OCOCH_3$

II $R_1 = OH$; $R_2 = OH$

III $R_1 = O$; $R_2 = OCOCH_3$

LITERATURE CITED

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