FEKROL — A TERPENOID COUMARIN FROM *Ferula krylovii*

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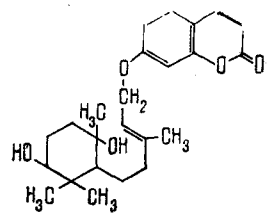
From an acetone extract of the roots of *Ferula krylovii* Korov. by chromatography on alumina followed rechromatography on silica gel L 40/100 in petroleum ether–ethyl acetate we have isolated a new terpenoid coumarin, fekrol (I), $C_{24}H_{32}O_5$, M^+ 400, mp 172-174°C (ethyl acetate–petroleum ether).

The IR spectrum of (I) shows a broad absorption band with its center at 3330 cm^{-1} which is characteristic for bound hydroxy groups, and also bands at 1725 cm^{-1} (C=O of an α-pyrone) and 1620, 1560, and 1510 cm^{-1} (vibrations of an α-pyrone and of a benzene ring).

The PMR spectrum of fekrol (Varian HA-100D; δ, ppm; $CDCl_3$, TMS) showed, in addition to the signals of a 7-substituted coumarin, the following structural elements: $3CH_3-\overset{|}{\underset{|}{C}}-$ (0.7, 0.98, 1.01, all s, 3 H each), $CH_3-C=C-$ (1.73, s, 3 H); CH–OH (3.38, s, 1 H), $-CH_2-O-Ar$ (4.57, d, 2 H, J = 7.0 Hz), and $H-C=C-$ (5.48, t, 1 H). The molecule of (I) contains the $-C=CH-$ (CH_3) CH_2-OAr grouping, as was shown by the double-resonance method.

The closeness of the parameters of the PMR spectra of fekrol and of kopeolin [1] permit us to assume that their structures are similar with the exception of the orientation of the secondary hydroxy group.

When fekrol was acetylated with acetic anhydride in pyridine, a monoacetate $C_{26}H_{34}O_6$ was obtained with mp 128-130°C, δ, 4.61 ppm ($CH-OCOCH_3$), ν 3510 cm^{-1} (tert-OH). The value of the half-width of the H–C–OH signal ($W_{1/2}$ ≈ 6.0 Hz) in the spectrum of (I) and the sum of the constants of the $H-C-OCOCH_3$ signal in the spectrum of the acetate (I) (ΣJ ≈ 6.0 Hz) show that the hydroxyl is axial and only one methylene group is adjacent to the H–C–OH grouping.



I

Thus, fekrol is a stereoisomer of kopeolin with the axial orientation of the secondary hydroxy group.

LITERATURE CITED

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