COUMARINS FROM THE ROOTS OF Ferula Pseudooreoselinum

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By chromatography on Al_2O_3, from an acetone extract of the roots of Ferula pseudooreoselinum (Rgl. et Schmalh.) K. Pol., in addition to samarcandin acetate and isosamarcandin angelate [1], we have isolated three umbelliferone derivatives with a bicyclic terpenoid side chain: (I) – $C_{24}H_{30}O_4$ (M^+ 382), mp 116.5-117.5°C, $[\alpha]_D^{20}$ −98.5° (c 0.22; ethanol), which has been called feselol [additional purification of the coumarin was performed by preparing the acetate $C_{26}H_{32}O_5$ (M^+ 424), mp 163-165°C, $[\alpha]_D^{20}$ −119.1° (c 0.9; ethanol) and its subsequent saponification]; (II) – $C_{24}H_{30}O_4$ (M^+ 382), mp 136.5-137.5°C, $[\alpha]_D^{20}$ −82.8° (c 5.2; ethanol) – a stereoisomer of feselol; and (III) – $C_{24}H_{28}O_4$ (M^+ 380), mp 141-142°C, $[\alpha]_D^{20}$ −49.8° (c 0.23; ethanol). Compounds (I), (II), and (III) have UV and IR spectra typical for derivatives of 7-hydroxycoumarin. The IR spectra of (I) and (II) have the absorption bands of OH groups at ν 3350 and 3620 cm^{-1}, respectively. The oxidation of these compounds with chromium trioxide in acetone forms the same product, a ketone $C_{24}H_{28}O_4$, mp 141-142°C, which was identical in melting point and IR spectrum with the coumarin (III). The NMR spectra of (I) and (II) have the signals of protons geminal to hydroxy groups with δ, ppm, 3.20 (1H), a triplet (ΣJ = 15 Hz), and 3.41 (1H) (half-width of the signal ~ 8 Hz), respectively. It follows from this that the hydroxy group has the equatorial orientation in feselol and the axial orientation in its stereoisomer. In the NMR

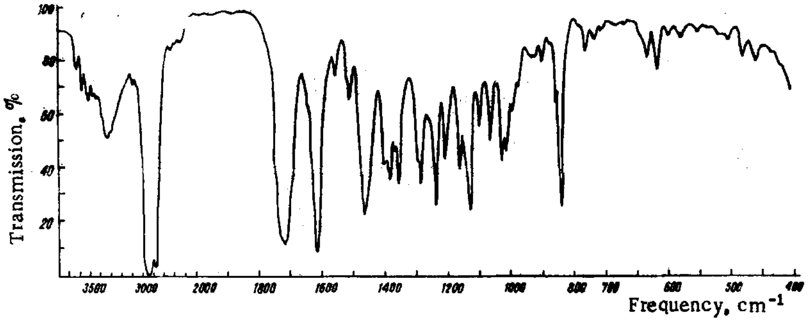

Fig. 1. IR spectrum of feselol (paraffin oil, UR-10).

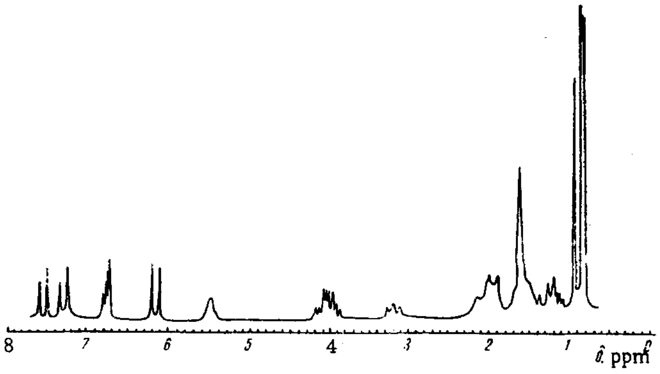

Fig. 2. NMR spectrum of feselol ($CDCl_3$, Varian HA-100).

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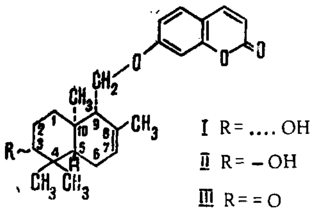
spectra of (I), (II), and (III), the signals of an olefinic proton at δ, ppm, 5.48-5.54 (1H) (broadened singlet) and of a vinylmethyl group at δ 1.62-1.66 (3H) (broadened singlet) show the presence of the fragment $H-\underset{|}{C}=\underset{|}{C}-CH_3$ in the molecule.

The hydrogenation of (II) with PtO_2 by Adams' method in ethanol formed a product $C_{24}H_{32}O_4$ (M^+ 384), mp 195.5-196°C, $[\alpha]_D^{20}$ −71.7° (c 1.4; ethanol), identified by its melting point and IR spectrum as the substance that we obtained by the hydrogenation of badrakemin [2].

On the basis of what has been said above and available literature information on the stereochemistry of related compounds [2, 3], the new coumarin feselol may be ascribed structural formula (I).



I R= ....OH
II R= −OH
III R= =O

Compounds (II) and (III) proved to be identical with conferol and conferone [4, 5], respectively, to which, on the basis of the identification of hydrogenated conferol with hydrogenated badrakemin, the spatial formulas (II) and (III), respectively, have been ascribed.

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