AURAPTENE FROM Ferula microloba

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In the course of a systematic study of the roots of plants of the genus Ferula, we have isolated (by chromatography) from Ferula microloba Boiss [1] an optically inactive compound with the composition $C_{19}H_{22}O_3$, mp 67°C, M^+ 298, R_f 0.65 [TLC; benzene–chloroform–ethyl acetate (5:4:1)].

The UV spectrum of this compound [λ_{max}^{EtOH} 220, 243, 254, 295, 325 nm (log ε 4.15; 3.68, 3.41; 3.93; 4.2)] corresponds to the chromophore of 7-hydroxycoumarin.

IR spectrum, cm^{-1}: 1725 (C=O of an α-pyrone), 1620, 1510, 1460 (Ar), 3085, 3050, 850, 830 (>C=CH–), 1350, 1210, 1130, 640 [$(CH_3)_2$ C=C<].

The NMR spectrum of the compound (Varian, HA-100D, $CDCl_3$, 0 – HMDS) has signals at: 1.52, 1.58, and 1.69 ppm (3H, singlets) corresponding to three methyl groups on a double bond; a doublet at 4.48 ppm (J = 5 Hz) belonging to the protons of the methylene of a $-CH_2-O-Ar$ group; and the signal of a proton geminal to this group at 5.36 ppm (triplet, ΣJ = 13 Hz). Another olefinic proton appears in the form of a broadened singlet at 4.96 ppm. A signal at 2.0 ppm is due to two methylene groups present between double bonds. In the 6.03-7.42-ppm region, the signals correspond to the protons of a coumarin with an O–Alk substituent in position 7. The characteristics of the NMR spectrum and the composition of the compound show that the alkyl substituent is an alicyclic monoterpene with the structure of the 2,6-dimethyloctane type.

The mass spectrum (Varian CH-8.75 eV, 75°C) shows peaks with m/e 41(41%), 53(11.4), 55(7), 67(15), 68(14), 69(100), 77(13), 81(41), 89(6.6), 93(28), 95(11), 105(10), 107(3.5), 121(8), 134(26), 136(25), 137(20), 162(58), 163(38), 175(1), 187(1), 229(0.8), 298 – M^+(1.1).

The peaks of the ions with m/e 162, 163, and 175 additionally confirm the presence of an umbelliferone moiety in the compound under investigation. The terpene moiety of the molecule forms ions with m/e 137 ($M^+ - 161$), 136 ($M^+ - 162$), 121 ($M^+ - 162 - 15$), 93 (136 – 43), 81 ($CH_2 = C - C(CH_3) = C - C^+$), 69 ($CH_3 - C(CH_3) = C - CH_2^+$). The ions with m/e 229, 187, and 175 relate to both the coumarin and the terpenoid moieties of the molecule.

On the basis of the melting point and the IR, UV, NMR, and mass spectra, this compound was identified as auraptene, which is an ether of umbelliferone and geraniol [2]. Auraptene has been isolated previously from the family Rutaceae [2, 3]. This is the first time that it has been found in the genus Ferula.

LITERATURE CITED

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