STRUCTURE OF MOGOLTACIN

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UDC 547.913.55:668.5+587.51

Continuing a study of the coumarins of Ferula mogoltavica collected in the Tadzhik SSR (village of Chashma, Leninabad oblast), by chromatographing a methanolic extract of the roots on a column of silica gel we have isolated a new coumarin $C_{24}H_{30}O_4$ (M^+ 382) with mp 155-156°C, $[\alpha]_D^{23}-55°$ (c 1.00; chloroform), which we have called mogoltacin (I).

The UV spectrum of (I) has maxima at 218, 244, 290, and 326 nm ($\log \varepsilon$ 4.25, 3.80, 4.00, 4.24), which are characteristic for a 7-hydroxy-substituted coumarin nucleus, and the IR spectrum has absorption bands at 3350-3600 cm^{-1} (hydroxy group), 1720 cm^{-1} (carbonyl of an α-pyrone), 1660 cm^{-1} (inflection; double bond), and 1620, 1560, and 1520 cm^{-1} (aromatic nucleus).

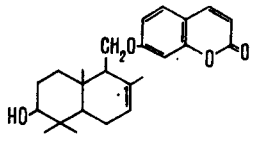
The acid hydrolysis of (I) with a mixture of acetic and sulfuric acids gave umbelliferone, $C_9H_6O_3$ (II), mp 231-232°C, and dehydrogenation with selenium at 220-250°C gave 1,2,5,6-tetramethylnaphthalene $C_{14}H_{16}$ (III), with mp 113-114°C.

In this way, it was established that (I) is an ether of umbelliferone and a bicyclic sesquiterpene alcohol with composition $C_{15}H_{26}O_2$. The mass spectrum of (I) has the peaks of ions with m/e 382 (M^+), 367 $(M-CH_3)^+$, 364 $(M-H_2O)^+$, 220 $(M-ArOH)^+$, 203 $(M-ArO-H_2O)^+$, 162 $(ArOH)^+$, which are characteristic for terpenoid coumarins of the iresane group [1, 2].

The NMR spectrum of (I) (JNM-4H-100/100 MHz, solutions in $CDCl_3$, 0 – HMDS) showed the signals from the protons of tertiary methyl and vinyl methyl groups – singlets at (ppm) 0.80, 0.90, 0.94, and 1.68 pp (3H each), broadened signals at 3.42 ($W_{1/2}$ = 6 Hz) and 5.51 ($W_{1/2}$ = 11 Hz) due to hemihydroxyl and olefinic protons, and a multiplet at 4.11 (2 H) relating to the methylene proton in an $ArOCH_2$ grouping. In addition, in the 6.22-7.55 ppm region there were the signals from the five protons of a 7-hydroxy-substituted coumarin.

A comparison of the characteristics of the IR, mass, and NMR spectra of (I) with those of conferol (IV) showed their similarity, but the melting point of (I) was 155-156°C and that of (IV) 137-138°C. A mixture of (I) and (IV) gave a depression of the melting point, melting at 115-116°C. To confirm the proposed structure, we performed a transition from mogoltavin (V) [4] to mogoltacin (I). The dehydration of (V) with 10% sulfuric acid in ethanol for 30 min yielded a substance with the composition $C_{24}H_{30}O_4$, mp 155-156°C, which was identified by its spectra and by a mixed melting point as mogoltacin.

On the basis of the information given, for mogoltacin we propose the most probable structure (I):



The study of the stereochemistry of (I) is continuing.

LITERATURE CITED

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