THE STRUCTURE OF PRANGEFEROL

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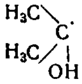
We have previously [1] reported the isolation of substance Zh [mp 176.5°C (from benzene), $[\alpha]_D^{20} \pm 0°$ (chloroform)] from the roots of *Prangos ferulacea* (L) Lindl., and we gave it the name *prangeferol*. The present paper gives the results of a study of its structure.

Prangeferol (I) possesses the properties characteristic for coumarin compounds. Its IR spectrum has absorption maxima at $\lambda_{max}^{C_2H_5OH}$ 332-336, 248, 224 nm (log ε 4.18; 3.69; 4.02, respectively) and λ_{min} 270 nm (log ε 3.19), which are characteristic of dihydrofurocoumarins.

The IR spectrum of (I), taken in paraffin oil on a UR-10 spectrometer, shows absorption bands at (cm^{-1}) 3455 (hydroxy group), 1710 (C=O α-pyrone), 1635, 1570, and 1495 (aromatic nucleus). The UV and IR spectra of (I) almost coincide with those for the known dihydrofurocoumarin marmesin. Only a slight difference in the IR spectrum of (I) can be seen.

The NMR spectrum of (I) in $CDCl_3$ (JNM-4H-100 MHz, 0 – TMS) shows the signals of the protons of a gem-dimethyl grouping (1.24 and 1.38 ppm, singlets, 3 H each), of a methyl group (4.81 ppm, triplet, 1 H), and of a methylene group adjacent to it (3.24 ppm, doublet, 2 H, J = 8 Hz), attached to an aromatic ring. The signal at δ 2.20 ppm is due to the proton of a hydroxy group. In the region of the signals of aromatic protons there are two doublets with chemical shifts of δ 6.22 and 7.60 ppm (J = 9.8 Hz) due to the protons in positions 3 and 4 of the coumarin ring. Two signals at δ 7.22 and 6.71 ppm relate to the protons in positions 5 and 8, respectively. Thus, the facts given above show that (I) has the structure of 5'-(hydroxyisopropyl)-4',5'-dihydrofuro-2',3' : 7,6-coumarin. This structure corresponds to two optical antipodes – marmesin (dextrorotatory form) and nodakenetin (levorotatory form). Consequently, (I) is the racemate of these substances. The results of study of the structure of (I) are also confirmed by its mass spectrum, in which the molecular ion M^+ 246 m/e and the peak of a fragment  $(H_3C)_2\dot{C}OH$ with m/e 59 clearly appear. A mixture of authentic samples of (I) and marmesin also gave no depression of the melting point.

LITERATURE CITED

1. A. Z. Abyshev, Author's Abstract of Candidate's Dissertation [in Russian], Leningrad (1967).

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