THE COUMARIN COMPOSITION OF THE ROOTS OF *Prangos uloptera*

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We have previously reported the isolation from the resin of the roots of Prangos uloptera D.C. of a number of known coumarin derivatives and of a new compound ulopterol [1, 2].

Continuing a study of the coumarin composition of the plant under investigation, we have isolated another four crystalline substances with properties characteristic for compounds of the coumarin group – $C_{15}H_{18}O_5$ (I), mp 126-128°C; $C_{12}H_8O_4$ (II), mp 144°C; $C_{12}H_8O_4$ (III), mp 194°C; and $C_{16}H_{16}O_6$ (IV), mp 126.5-128°C.

From their chemical compositions, R_f values, IR spectra, and mixed melting points with authentic samples, (I) and (II) were identified, respectively, as meranzin hydrate and xanthotoxin [3-5].

From their melting points and IR spectra, compounds (III) and (IV) correspond to bergapten and to prangenin hydrate [6]. For their complete identification, we made use of their NMR spectra and some chemical reactions.

Thus, in the NMR spectrum of (III) in the region of aromatic protons there are four doublets with chemical shifts of δ 6.25 and 8.18 ppm (J 10 Hz) and 7.02 and 7.60 ppm (J 2 Hz), due to the 3,4 protons of the coumarin nucleus and the 4',5' protons of the furan ring. A singlet at δ 7.13 ppm relates to a proton in position 8. A three-proton singlet at δ 4.20 ppm is due to the protons of a $-OCH_3$ group present in position 5. These facts confirm the identity of (III) as bergapten.

In the NMR spectrum of (IV) in the region of aliphatic protons there are the signals of methyl groups with δ 1.35 ppm (resolved singlet, 6 H), of a $O-CH_2-\underset{|}{CH}-$ grouping in the δ 3.85-4.55-ppm range (complex multiplet, 3 H). A signal at δ 2.73 ppm corresponds to the protons of hydroxy groups (resolved singlet, 2 H). In the region of aromatic protons doublets appear with δ 6.39 and 7.80 ppm (J 10 Hz) and 6.96 and 7.75 ppm (J 2 Hz), which are due to the protons in the 3,4 position of the coumarin ring and the 4',5' positions of the furan ring, respectively. A singlet at δ 7.41 ppm is due to the proton in position 5. It follows from the features of the NMR spectrum that (IV) is 8-(2'',3''-dihydroxy-3''-methylbutoxy)furo-2',3':7,6-coumarin, which corresponds to the structure of prangenin hydrate [6].

The acetylation of (IV) with acetic anhydride in pyridine led to the formation of a diacetate (V), $C_{20}H_{20}O_8$, mp 85-87°C, the IR spectrum of which lacked the absorption band of hydroxy groups.

When (IV) was treated with 10% sulfuric acid, an isomer of prangenin hydrate was obtained – (VI), $C_{16}H_{14}O_5$, mp 134.5-135.5°C.

Thus, the roots of Prangos uloptera D.C. contain, in addition to the coumarin derivatives found previously [1, 2], meranzin hydrate, xanthotoxin, bergapten, and prangenin hydrate.

The NMR spectra were taken on a JNM-C-60-HL spectrometer in deuterochloroform (with HMDS as internal standard), and the melting points were determined on a Kofler block.

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