

- I. $R_1 = H_2$, $R_2 = OH$
 II. $R_1 = OCOCH_3$, $R_2 = OCOCH_3$
 III. $R_1 = R_2 = H$

The PMR spectra were taken on a JNM-100/100-4H instrument (100 MHz; 0 — HMDS), and the mass spectra on an MKh-1303 instrument.

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AN INVESTIGATION OF *Seseli peucedanoides*

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From the total extractive substances of the roots of *Seseli peucedanoides* collected in the period of fruit-bearing in the Batabat area of the Shakhbuz region of the Nakhichevan ASSR by adsorption chromatography on silic gel (40/100 μ) a crystalline compound (I) has been isolated with the composition $C_{20}H_{24}O_{10}$, mp 257-259°C (acetone), $[\alpha]_D^{20} -24.58^\circ$ (c 3.2; pyridine). Substance (I) is new, not having been described in the literature, and we have called it seseloside.

The IR spectrum of (I) has absorption bands at (cm^{-1}) 3600-3100 (hydroxy group), 1715 (α -pyrone CO), 1630 and 1590 (aromatic ring), and 1380 (gem-dimethyl group). The 1H NMR spectrum of seseloside (Fig. 1) shows the signals of the protons of a gem-dimethyl group (1.45 ppm, 6 H, singlet), of a β -anomeric proton (5.05 ppm, 1 H, doublet, $J = 6.0$ Hz), the protons of a glucose residue (3.65-4.25 ppm, 6 H), and also the protons of a coumarin nucleus (6.20 ppm, 1 H, doublet, $J = 10.0$ Hz; 6.70 ppm, 1 H, broadened singlet; 7.60 ppm, 1 H, doublet, $J = 10.0$ Hz).

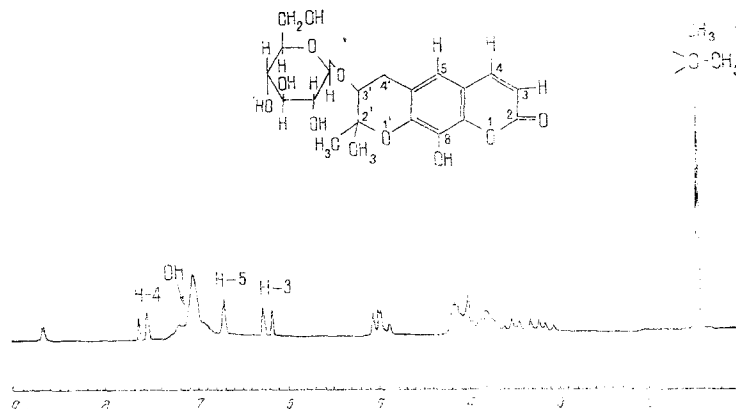


Fig. 1. 1H NMR spectrum of seseloside in D-pyridine; Varian HA-100D.

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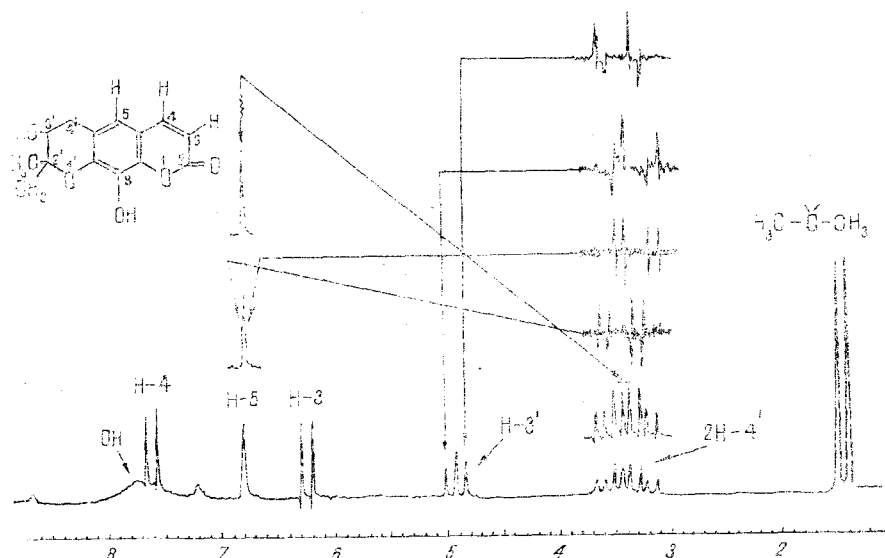


Fig. 2. ^1H NMR spectrum of the aglycone of seseloside in D-pyridine) Varian HA-100D.

It follows from a comparison of the elementary composition and the results of spectral analysis that seseloside is a monoglycoside. The acid hydrolysis of seseloside with a 4% solution of sulfuric acid formed D-glucose, which we identified on the basis of paper chromatography with a marker and its IR spectrum. The hydrolysate was also found to contain an aglycone with the composition $\text{C}_{14}\text{H}_{14}\text{O}_5$ (II), M^+ with m/z 262, mp 193–195°C (water), $[\alpha]_D^{20} -52.71^\circ$ (c 2.8; pyridine). The IR spectra of compound of (II) contained absorption bands at (cm^{-1}) 3600–3100 (hydroxy group), 1670 (α -pyrone CO), 1630, 1610, and 1580 (aromatic ring), and 1385 and 1370 (gem-dimethyl group of a chromane ring). The ^1H NMR spectrum of the aglycone (Fig. 2) showed the signals of the protons of a gem-dimethyl group (1.40 and 1.50 ppm, 3 H each, singlets), the protons of a $-\text{CH}-\text{CH}_2-$ fragment of a chromane ring (4.90 ppm, 1 H, quartet, $J = 8$ Hz and $J = 9.5$ Hz; 3.30 and 3.60 ppm, 1 H each, quartets, $J_{\text{gem}} = 16.0$ Hz, $J_{\text{vic}} = 8.0$ Hz and $J_{\text{vic}} = 9.5$ Hz), and also the protons of a coumarin nucleus (6.25 ppm, 1 H, doublet, $J = 7.0$ Hz; 6.80 ppm, 1 H, triplet, $J = 1.5$ Hz; 7.63 ppm, 1 H, doublet, $J = 10.0$ Hz). The appearance of the signals of the protons of the gem-dimethyl group in the aglycone in the form of two singlets, in contrast to the singlet signal of the same group in seseloside indicates that the glucose residue is present in the C-3' position of the chromane ring.

Under double-resonance conditions with irradiation by means of an additional radio frequency of the H-5 proton we observed a contraction of the lines of the signals of the protons of the methylene group of the chromane ring [1]. Analysis of the structure of the INDOR signals (see Fig. 2) obtained on the extreme lines of the H-5 proton also shows that this proton interacts only with the methylene protons of the chromane ring. These facts confirm that the 3',4'-dihydropyran ring is condensed with the coumarin nucleus in the C₆-C₇ position. The INDOR spectrum (see Fig. 2) also shows well the signals of the interaction of the protons of the methine and methylene groups of the 3',4'-dihydropyran ring. According to the facts given, seseloside is a monoglycoside and has the structure of 3'-O- β -D-glucopyranosyloxy-8-hydroxy-2',2'-dimethyl-3',4'-dihydropyrano-5',6':6,7-coumarin.

LITERATURE CITED

1. M. E. Perel'son, Yu. I. Sheinker, and A. A. Savina, The Spectra and Structure of Coumarins, Chromones, and Xanthenes [in Russian], Moscow (1965), p. 161.