ISOC YNAROSIDE - A NEW FLAVONE GLYCOSIDE

FROM Sonchus arvensis

V. G. Bondarenko, V. I. Glyzin, A. I. Ban'kovskii, and V. L. Shelyuto

We have previously reported the isolation from the flowers of <u>Sonchus arvensis</u> L. (field sowthistle) of luteolin and luteolin 7-glycoside (cynaroside) [1]. Continuing an investigation of the flavonoids of the field sowthistle, we have isolated a substance $C_{21}H_{20}O_{11}$ with mp 180-182°C, $[\alpha]^{20}$ -148.6° (c 0.5; formamide). On acid and enzymatic hydrolyses with glucodelemarin this substance formed luteolin, $C_{15}H_{10}O_6$, mp 327°C (ace-tate with mp 228°C) and glucose. The glucose in the compound under investigation is in position 7: $\lambda CH_{3}OH_{max}$

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255, 268 (shoulder) 350; $\lambda_{\max}^{CH_3ONa+H_3BO_3}$ 272, 416; $\lambda_{\max}^{AlCl_3}$ 272, 432.

The NMR spectrum of the glycoside showed the following signals: multiplet at 7.24 ppm, 2H (H-2', 6'); doublet at 6.80 ppm, 1H, J=8Hz (H-5'); doublet at 6.56 ppm, 1 H, J=2.5 Hz (H-8); doublet at 6.24 ppm (H-6) superposed on a singlet from H-3; doublet at 4.86 ppm, 1H, J=7 Hz - the signal of the glucosidic center of β -glucose; signals in the 3.2-3.8-ppm region corresponding to the six glucose protons. The NMR and UV spectra are identical with those of luteolin 7-glucoside.

However, from its physicochemical properties the substance isolated differs from cynaroside: it dissolves in water, is readily hydrolyzed by acids, has a larger angle of rotation, and is more mobile on chromatograms, and it differs in its melting point and in the IR spectrum in the $1000-1100-cm^{-1}$ region, where bands appear at 1020 and 1050 cm⁻¹.

In an analysis of the NMR spectra of the acetates of cynaroside and of the substance under investigation, differences were found in the nature of the signals of the aliphatic acetyl groups. The differences can be connected only with differences in the size of the oxide rings of the glucose residue. The results of a calculation of the values of molecular rotations of cynaroside ($M_D = -381.9^\circ$) and of the substance under consideration ($M_D = -650.86^\circ$) show that in the latter the glucose possesses a furan ring [2]. This agrees well with the rate of acid hydrolysis.

Thus, the compound that we have isolated is an isomer of cynaroside. For it we propose the name isocynaroside; it has the structure of $7-\beta$ -D-glucofuranosyloxy-3',4',5-trihydroxyflavone.



Fig. 1. NMR spectrum of isocynaroside acetate (CDCl₃).

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The nature of the signals of the aliphatic acetyl groups contradicts the information for the acetates of isoquercetin and hirsutrin [3].

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