PHENOLIC COMPOUNDS OF Ononis arvensis. I

V. N. Kovalev, M. I. Borisov, and V. N. Spiridonov

UDC (547.56:547.52):633.88

Studying the chemical composition of the hypogeal organs of Ononis arvensis L. (family Leguminosae), we have found on chromatograms a series of substances which, from their fluorescence in UV light before and after treatment with various chromogenic reagents have been assigned to the polyphenolic compounds. By the separation of a purified aqueous extract we have isolated individual substances A, B, C, D, and E.

The comminuted roots were extracted with ethanol, the extracts were evaporated to an aqueous residue, and the lipophilic substance were eliminated with chloroform. On evaporation of the chloroform extract followed by crystallization from methanol, crystals were obtained in the form of thin white needles with mp 232-233°C and with the composition $C_{30}H_{50}O_2$. On the basis of qualitative reactions, IR spectroscopy, and its acetyl and benzoyl derivatives, this compound was characterized as the triterpene alcohol onocerin [1].

The purified aqueous extract was deposited on a column of polyamide and eluted with mixtures of water and ethanol. Analysis of the eluates obtained showed that they contained mixtures of substances. On rechromatography of the individual fractions on the same sorbent, using as eluents mixtures of chloroform and ethanol in various proportions, we obtained the substances mentioned above.

Substance B consists of crystals in the form of colorless needles with mp 210-212°C (from ethanol), λ_{max}^{MeOH} 257, 300 nm. Acid hydrolysis with 5% sulfuric acid gave an aglycone and a sugar component, which were identified as formononetin and D-glucose. By its physicochemical properties, the glycoside obtained was identified as formononetin 7-O-β-glucopyranoside (ononin). This is the first time that onocerin and ononin have been isolated from this species [2, 3].

Substance E, $C_{17}H_{14}O_6$, crystallizes from ethanol in the form of white acicular crystals with mp 213-214°C, $[\alpha]_D^{20} \pm 0$, M^+ 314. Analysis of the nature of the UV spectra [λ_{max}^{MeOH} 278, 308 nm (log ε 4.19; 4.15)] permits the assumption of an isoflavanone structure for this compound. The bathochromic shift of the maxima in the presence of sodium acetate by 8 nm in the presence of alkali by 32 nm shows that the hydroxy group is present in the C_7 position [5]. In the IR spectrum, absorption bands appear in the 3320 cm^{-1} region (phenolic hydroxyl) and at 2950, 2900, and 2845 cm^{-1} (=CH_2, $-OCH_3$, $\equiv$ CH at C_2-C_3), 1665 cm^{-1} (C=O of an isoflavanone), 1590, 1509, and 1489 cm^{-1} (skeletal vibrations of aromatic rings A and B), 1118 and 1038 cm^{-1} (OCH_3), and 810, 825, and 860 cm^{-1} (nonplanar CH deformation vibrations of aromatic rings). A strong band at 931 cm^{-1} and a medium-intensity band at 727 cm^{-1} are due to a methylenedioxy group of an aromatic system [6], the presence of which is also shown by qualitative reactions [7, 8].

On the basis of the results obtained, for substance E it is possible to suggest the structure of a 7-hydroxyisoflavanone containing methoxy and methylenedioxy groups. The complete structure of compound E has not yet been established.

Substance A consisted of crystals in the form of thin white needles with mp 152-154°C (from ethanol), $[\alpha]_D^{20} -18°$ (c 0.1; methanol); λ_{max}^{MeOH} 270-306 nm.

Substance D formed light pink crystals with mp 217-219°C (ethanol), $[\alpha]_D^{20} -34°$ (c 0.1; methanol), λ_{max}^{MeOH} 258-295 nm.

Substance C consists of crystals in the form of elongated white needles with mp 193-194°C (ethanol), $[\alpha]_D^{20} -158°$ (c 0.1; methanol), λ_{max}^{MeOH} 285, 310 nm. Substances A, D, and C are still being investigated.

Khar'kov Pharmaceutical Institute. Khar'kov Scientific-Research Institute of Pharmaceutical Chemistry. Translated from Khimiya Prirodnykh Soedinenii, No. 6, pp. 795-796, November-December, 1974. Original article submitted February 13, 1974.

LITERATURE CITED

1. R. Barton and K. H. Overton, J. Chem. Soc., 2639 (1955).
2. A. A. Felsberg and P. É. Rozentsveig, Aptechnoe Delo, 6, 26 (1965).
3. A. A. Felsberg and P. É. Rozentsveig, Aptechnoe Delo, 3, 25 (1965).
4. L. Jurd, Flavone Chemistry [Russian translation] (1963), p. 147.
5. R. M. Horowitz and L. Jurd, J. Org. Chem., 26, No. 7, 2446 (1961).
6. L. H. Briggs, L. D. Colebrook, H. M. Fales, and W. P. Wildman, Anal. Chem., 29, 904 (1957).
7. Houben-Weyl, Methoden der organischen Chemie [Russian translation], Moscow (1967), p. 416.
8. O. A. Stamen, H. Schmid, and J. Buchi, Helv. Chim. Acta, 41, No. 7, 2016 (1958).