NEW PHENOLIC COMPOUNDS OF THE ROOTS OF Ferula tschimganica

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Continuing a study of the phenolic compounds of Ferula tschimganica Lipsky, in addition to chimganin and chimgin [1] we have found two other esters with R_f 0.55 and 0.49 (petroleum ether–ethyl acetate system chromogenic agent a 1% solution of vanillin in concentrated sulfuric acid)[2]. By column chromatography on silica gel with elution by chloroform and chloroform–ethyl acetate (9 : 1) we have isolated colorless crystalline substances with the composition $C_{23}H_{32}O_5$ (I), mp 140-141°C, $[\alpha]_D^{20}$ $-97.9°$ (c 1.2; $CHCl_3$), which we have called chimganidin, and $C_{22}H_{30}O_4$ (II), with mp 191-192°C, $[\alpha]_D^{20}$ $-90.2°$ (c 1.1; $CHCl_3$). The compounds are soluble in caustic alkalis and give a weak color reaction with diazotized sulfanilamide. The UV spectrum of (I) has maxima at 267 and 298 nm (log ε 4.10, 3.96, and that of (II) has a maximum at 262 nm (log ε 4.18). In an alkaline medium, the long-wave maxima undergo bathochromic shifts of 24 and 45 nm, respectively, which shows that the two substances belong to the phenol group.

The IR spectrum of (I) has absorption bands at (cm^{-1}) 1690 (carbonyl group of an ester of an unsaturated acid), 1680, 1610, 1590 (aromatic nucleus), and 3180-3450 (hydroxy group). On saponification with 5% aqueous alkali, substance (I) underwent cleavage, forming a hydroxy acid with the composition $C_8H_8O_4$, mp 205-206°C, which was identified by a mixed melting point and by IR spectroscopy as 4-hydroxy-3-methoxybenzoic acid.

The neutral part of the hydrolyzate yielded a sesquiterpene diol with the composition $C_{15}H_{26}O_2$, mp 135-136°C, $[\alpha]_D^{20}$ $-67.5°$, (1.2; ethanol), corresponding in composition, melting point, and optical activity with angrendiol, isolated previously from Ferula angrenii, F. Ceratophylla, F. prangifolia, and F. karategina [3]. For identification, the alcohol was subjected to catalytic hydrogenation, giving a dihydro derivative with mp 214-216°C corresponding to dihydroangrendiol.

On the basis of these facts it may be concluded that chimganidin is an ester of angrendiol and 4-hydroxy-3-methoxybenzoic acid. In the NMR spectrum of angrendiol, the signal of the methine proton appears at 3.6 ppm (δ), and in the NMR spectrum of chimganidin it appears at 4.40 ppm. The paramagnetic shift of the methine proton due to the influence of the ester grouping shows that the angrendiol is esterified with the 4-hydroxy-3-methoxybenzoic acid at the secondary hydroxy group.

The IR spectrum of (II) greatly resembles that of (I), which shows the structural similarity of the two compounds isolated. The alkaline saponification of (II) also gave angrendiol and an acid $C_7H_6O_3$ which was identified as p-hydroxybenzoic acid. Consequently, substance (II) is identical with the ferulin which we isolated previously from Ferula pallida [4].

According to thin-layer chromatography, the plants investigated do not contain angrendiol in the free state. It may be assumed that the angrendiol discovered previously in other species of Ferula [3] was an artefact.

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