ESTERS OF Ferula akitschkensis

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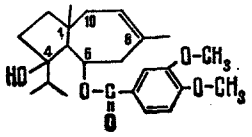
Continuing a study of the esters of plants of the genus Ferula, from a methanolic extract of the fruit of Ferula akitschkensis B. Fedtsch. ex K.-Pol. gathered in the Susamyr valley, Kirghiz SSR, in the fruit-bearing period, by separation on a column of KSK silica gel we have isolated a new ester with the composition $C_{24}H_{34}O_5$ (I) (M^+ 402) with mp 102-103°C, $[\alpha]_D^{22}$ + 69.1° (c 1.08; chloroform). Substance (I) is readily soluble in ethanol, chloroform, and acetone, sparingly soluble in ether, and insoluble in petroleum ether and water. The UV spectrum of (I) shows maxima at 260 and 295 nm (log ε 3.49, 3.36) which are characteristic for a 3,4-dihydroxybenzoyl residue, and the IR spectrum shows absorption bands at 1520, 1580, and 1620 cm^{-1} (aromatic nucleus), 1705 and 1250 cm^{-1} (ester group), and 3540 cm^{-1} (hydroxy group).

The NMR spectrum of (I) (Jeol 60 MHz, $CDCl_3$, 0 – HMDS) contains the following signals: doublets at 0.78 and 0.85 ppm (J = 6.5 Hz, 3 H each), singlets at 1.05 and 1.70 ppm (3 H each), 3.40 and 3.42 ppm (3 H each), sextet at 5.02 ppm (J_1 = 10 Hz, J_2 = 2.5 Hz, 1 H), multiplet at 5.32 ppm (1 H), doublet at 6.74 ppm (J = 10 Hz, 1 H), quartet at 7.5 ppm (J_1 = 10 Hz, J_2 = 2.5 Hz, 1 H), and doublet at 7.4 ppm (J = 2.5 Hz, 1 H). A comparison of the NMR spectra of (I) with those of ferutin, ferutinin [1], and teferin [2] showed that substance (I) is also an ester of ferutinol. When (I) was hydrolyzed with 5% aqueous methanolic caustic potash with heating for 4 h, the neutral fraction of the hydrolyzate yielded an alcohol $C_{15}H_{26}O_2$ [2] with mp 89-90°C, $[\alpha]_D^{20}$ + 38° (c 1.0, chloroform), identical with ferutinol [1], and the acid fraction yielded an acid $C_8H_8O_4$ (III) with mp 193°C. By a comparison of IR spectra and a mixed melting point with an authentic sample, the acid (III) was identified as veratric acid. The position of the acid residue in substance (I) follows from the value of the signal of its hemiacyl proton (5.05 ppm) in the NMR spectrum, and by analogy with ferutin and ferutinin, it is attached to the secondary hydroxy group at C_6.

Thus, substance (I), which we have called akiferin, is a new ester and has the structure of 6-O-veratroglyferutinol.



From the roots of the sample plant, in addition to akichenin [3], we have isolated another three substances: $C_{23}H_{32}O_5$ with mp 130-131°C (IV), $C_{22}H_{30}O_4$ with mp 121-122°C (V), and $C_{22}H_{32}O_4$ with mp 102-103°C (VI). On the basis of mixed melting points and IR spectra, they have been identified as ferutin, ferutinin [1], and ferutidin [4], respectively.

LITERATURE CITED

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