STRUCTURE OF JUNIFERDIN — AN ESTER OF *Ferula juniperina*

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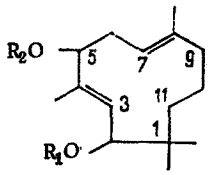
Continuing a study of the chemical composition of the roots of *Ferula juniperina* Eug. Kor. [1-3], by a method described previously we have isolated a new ester with the composition $C_{22}H_{30}O_4$, $[\alpha]_D$ −2.8° (c 0.53; methanol), mp 75-77°C, which we have called juniferdin [1]. UV spectrum (in ethanol): λ_{max} 211 nm (log ε 4.0), 260 nm (log ε 4.2), while a bathochromic shift of the long-wave maximum with an increase in the value of log ε when the spectrum was taken with the addition of alkali and also the good solubility of the substance in solutions of alkalis show the presence of a free phenolic hydroxyl in the molecule of the substance.

IR spectrum (tablets with KBr), λ_{max}, cm^{-1}: 1520, 1590, 1610 (aromatic nucleus), 1690 (carbonyl group), 3400-3500 (hydroxy group).

PMR spectrum (JNM-4H 100 MHz, $CDCl_3$, O — HMDS, δ scale, ppm): 0.89 and 0.93 (s, 3 H each), C_1-$2CH_3$; 1.67 (s, 6 H), C_4-CH_3 and C_8-CH_3; 4.2 ppm (d, J = 10 Hz, 1 H), C_2-H; 5.1 (t, $J_1 = J_2 = 7.5$ Hz), C_7-H; 5.59 (m, 2 H), C_3-H and C_5-H. In the weak-field region are observed the signals of the protons of an aromatic nucleus present in the ortho position relative to one another in the form of two doublets at 6.77 and 7.80 ppm with spin—spin coupling constants (SSCC) of J = 9.5 Hz. The alkaline hydrolysis of juniferdin with 5% KOH gave p-hydroxybenzoic acid (II), $C_7H_6O_3$, mp 208-210°C and the sesquiterpene diol juniferol (III), $C_{15}H_{26}O_2$, mp 135-136°C [1, 2], which were identified from their IR spectra and mixed melting points with an authentic sample; hence, juniferdin is a monoester of juniferol. The reaction of (I) with acetic anhydride in pyridine gave a diacetate (IV), $C_{26}H_{34}O_6$, $[\alpha]_D$ +18.6° (c 3.0; methanol), which proved to be identical with juniferinin acetate (V) [2] (according to IR and PMR spectra).

Thus, juniferdin is an ester of juniferol at C_5. A confirmation of the position of the acyl residue at C_5, suggested on the basis of chemical transformations, is a comparison of the PMR spectra of a known monoester of juniferol at C_5, juniferin (VI), and juniferdin. The closeness of the values of the coupling constants of the C_2—H signal (4.18 ppm in (VI) and 4.20 ppm in (I)) and the identical multiplicity (doublet) and SSCC (J = 10 Hz) in the spectra of the two monoesters indicate that in juniferdin, as in juniferin, the hydroxy group is located at C_2 and the acyl residue, consequently, at C_5. On the basis of the facts presented above, structure (I) is proposed for juniferdin



I. R_1=H, R_2=—C(=O)—C_6H_4—(OH)

III. R_1=R_2=H

IV, V. R_1=Ac, R_2=—C(=O)—C_6H_4(OAc)

VI. R_1=H, R_2=—C(=O)—C_6H_3(OCH_3)(OH)

LITERATURE CITED

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