STRUCTURE OF FERKUHININ

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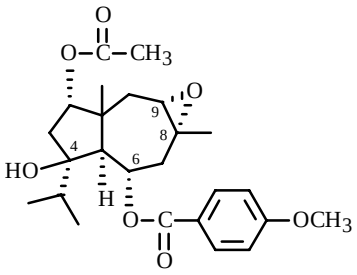
Plants of the *Ferula* genus (Apiaceae) are rich in terpenoid esters with aliphatic and aromatic acids [1]. In continuation of systematic studies of this type of terpenoids, we isolated a new compound of composition $C_{25}H_{34}O_7$, mp 118-119°C, $[\alpha]_D^{22}$ +105° (*c* 1.0, $CHCl_3$), from the neutral fraction of the total extracted substances of *F. kuhistanica* Korov. roots and called it ferkuhinin (**1**).



1

The UV spectrum exhibits a maximum at 262 nm (log ε 4.1), which is characteristic of *p*-hydroxysubstituted benzoyl derivatives [1]. The IR spectrum of **1** is typical of terpenoid esters with absorption bands at 3540 cm^{-1} (OH), 1730 and 1710 (ester), and 1590 and 1520 (aromatic ring).

The composition and IR spectrum indicate that ferkuhinin is a diester of a sesquiterpene alcohol with aromatic and aliphatic acids.

The PMR of ferkuhinin (taken on a Tesla BS 567 instrument, 100 MHz, $CDCl_3$, 0 = HMDS, δ, ppm, J/Hz): 0.81 and 0.93 (3H, d, J = 7, C_{11}-$2CH_3$), 1.3 (3H, s, CH_3-1), 1.4 (3H, s, CH_3-8), 2.40 (1H, d, J = 10, H-5), 2.70 (1H, t, J = 7, H-9), 4.78 (1H, d, J = 5, H-2), 5.32 (1H, sext, J = 10, 10, 2, H-6), 2.05 (3H, s, CH_3-1′), 6.8 (2H, d, J = 8, H-2″, H-6″), 7.8 (2H, d, J = 8, H-3″, H-5″), 3.86 (3H, s, OCH_3).

The PMR spectrum of ferkuhinin suggests that the compound is a carotane diester with acetic and anisic acids.

In fact, a sesquiterpene alcohol of composition $C_{15}H_{26}O_4$ with mp 194-195°C was isolated from the neutral portion of the alkaline hydrolysate. This was identified as the previously known lapiferinol, which was prepared by hydrolysis of lapiferinin [2]. The acidic part of the hydrolysate gave an acid of composition $C_8H_8O_3$ with mp 183-184°C, which was identified as anisic acid. Thus, ferkuhinin is a diester of lapiferinol with acetic and anisic acids.

The positions of the acid groups of **1** were determined as follows. The PMR spectrum of ferkuhinin contains signals for isopropyl methyls as two doublets at 0.81 and 0.93 ppm, i.e., the difference in the chemical shifts is 0.12 ppm. Such a large difference is observed in carotane esters of alcohols with aromatic acids on C_6 and is explained by the anisotropic effect of the aromatic ring on the proximal isopropyl group. The difference in the chemical shifts of these groups with an aliphatic moiety on C_6 is only 0.03-0.04 ppm [3]. Therefore, the anisic acid in ferkuhinin is located on C_6; the acetic acid, on C_2.

The positions of the acids in ferkuhinin were unambiguously determined by mild hydrolysis by 5% Na_2CO_3 in aqueous alcohol. This produced lapiferinol $C_{17}H_{28}O_5$ with mp 115-116°C. Its PMR spectrum lacks signals for anisic protons and exhibits a diamagnetic shift of the C_6–H signal by 1.27 ppm compared with the starting compound.

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Based on the investigation, we propose a ferkuhinin structure and the relative configuration as 2-α-acetoxy-6-α-anisoyloxy-4β-hydroxy-8α,9α-epoxy-*trans*-carotane (**1**).

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