

an aromatic nucleus. In the PMR spectrum of the acetate, one of the singlets at δ 2.24 and 2.38 ppm corresponded to it. The second singlet was due to an acetyl group. The empirical formula of the aglycone, $C_8H_{10}O_3$, was calculated on the basis of a molecular-weight determination and the results of elementary analysis. The structure of 2-methoxy-6-methylhydroquinone β -D-glucopyranoside is proposed for substance (8). We have found no information on such a substance in the literature. We have previously isolated the substances mentioned above, apart from substance (8), from the leaves of *A. frutescens* in fairly similar quantitative ratios [1, 2]. Substance (8) was detected in trace amounts. Thus, in its chemical composition *A. muschketovii* corresponds to *A. frutescens* and not to *A. pyrifolia* as reported previously [5]. The species studied previously was probably a hybrid.

By two-dimensional paper chromatography using qualitative reactions in comparison with the species studied we made a qualitative evaluation of ten species of *Atraphaxis*, samples of which were kindly provided by the Institute of Botany and the Main Botanical Garden of the Academy of Sciences of the Kazakh SSR: *A. pungens* (M. B.) Jaub. et Sp., *A. virgata*, *A. laetevirens* (Ldb) Jaub. et Sp., *A. spinosa*, *A. replicata*, *A. compacta*, *A. karataviensis*, *A. caucasica*, *A. seravschanica*, *A. teretifolia*. According to their chemical compositions, they can be divided into two groups: the first includes *A. pungens* and *A. laetevirens*, the flavonoid complex of which is identical with the complex of the leaves of *A. pyrifolia*, and the second includes the other species mentioned above, the flavonoid complexes of which are similar to the complex on the leaves of *A. muschketovii* and *A. frutescens*. The differences in the quantitative ratios were slight.

LITERATURE CITED

1. T. K. Chumbalov and V. B. Omurkaminova, *Khim. Prirodn. Soedin.*, 120 (1971).
2. T. K. Chumbalov and V. B. Omurkaminova, *Khim. Prirodn. Soedin.*, 424 (1975).
3. T. K. Chumbalov, M. M. Mukhamed'yarova, I. S. Chanysheva, L. P. Smirnova, and V. B. Omurkaminova, *Khim. Prirodn. Soedin.*, 658, 660 (1976).
4. T. K. Chumbalov, M. M. Mukhamed'yarova, and V. B. Omurkaminova, *Khim. Prirodn. Soedin.*, 793 (1974).
5. T. K. Chumbalov and V. B. Omurkaminova, *Khim. Prirodn. Soedin.*, 815 (1976).

THE STRUCTURE OF FEXERIN

K. Buzhanova, A. I. Saidkhodzhaev,
and V. M. Malikov

UDC 547.913.2.668.5:547.39

Continuing a study of the esters of plants of the genus *Ferula*, from the roots of *F. xeromorpha* Eug. Kor. collected in the Chimkent oblast of KazSSR, by column chromatography on KSK silica gel with elution by hexane-ether (9:1), we have isolated three esters (I-III).

Substance (I), composition $C_{20}H_{32}O_3$ (M^+ 320), R_f 0.26 [hexane-ether (3:2) system], n_D^{20} 1.5095, $[\alpha]_D^{20}$ -24° (c 1.0; chloroform) had a neutral character and was rapidly soluble in organic solvents and insoluble in water.

The IR spectrum of (I) had bands at (cm^{-1}) 3300-3600 (hydroxy group), 1240, 1710 (ester group), and 1660 (double bond), and the mass spectrum had the peaks of ions with m/e 320 (M^+), 237 ($M - 83$) $^+$, 220 ($M - 100$) $^+$, 205 ($M - 100 - 15$) $^+$, 202 ($M - 100 - 18$) $^+$, which are characteristic for esters of sesquiterpene alcohols with aliphatic acids. The substance proved to be a new one and we have called it fexerin.

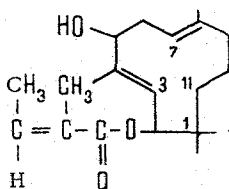
When fexerin was subjected to alkaline hydrolysis by being heated with a 5% aqueous methanolic solution of caustic potash, from the neutral part of the hydrolyzate we isolated a sesquiterpene alcohol with the composition $C_{15}H_{26}O_2$ (IV), mp 135-136°C (from ether), which, from its IR and PMR spectra and a direct mixed melting point, was identified as juniferol [1].

Institute of the Chemistry of Plant Substances, Academy of Sciences of the Uzbek SSR, Tashkent. Translated from *Khimiya Prirodnikh Soedinenii*, No. 3, pp. 407-408, May-June, 1978. Original article submitted January 20, 1978.

From the acid part of the hydrolyzate we obtained an acid with the composition $C_5H_8O_2$ (V) (M^+ 100), mp 65-65.5°C, which was identified as tiglic acid. This was also confirmed by the value of the CS of the signal of the olefinic proton of the acid residue (6.66 ppm, m, 1H) in the PMR spectrum of (I) [2, 3].

Thus, fexerin is an ester of juniferol and tiglic acid. The position of the acid residue in fexerin follows from the following facts. As is well known, juniferol contains two secondary groups, the geminal protons of which differ from one another by their CS values and multiplicities [3]. A comparison of the PMR spectra of fexerin and juniferol showed that the signals in the form of a doublet underwent a paramagnetic shift (C_2-H , $\Delta\delta$ 1.15 ppm), while the quartet signal (C_5-H , $\Delta\delta$ 0.25 ppm) shifted only slightly.

The acetylation of fexerin with acetic anhydride in pyridine led to a monoacetate of (I), $C_{22}H_{34}O_4$ (VI), in the PMR spectrum of which the signal in the form of a quartet had shifted downfield by 0.7 ppm. These facts unambiguously show that in fexerin the hydroxy group at C_5 is free and the acid residue is present at C_2 . Consequently, fexerin has the structure (I)



Substance (II), with the composition $C_{23}H_{32}O_5$, mp 85-86°C, $[\alpha]_D -1.5^\circ$ (c 5.8; ethanol) and substance (III), $C_{23}H_{30}O_4$, mp 107-108°C, $[\alpha]_D -195^\circ$ (c 1.0; ethanol) were identified by a comparison of IR and NMR spectra and direct mixed melting points with authentic samples as juniferin [1] and ferocinin [4], respectively. It must be mentioned that pyranocoumarins have been isolated previously from *F. xeromorpha* [5]. However, we found no coumarin derivatives in our sample, which was collected in the same region.

LITERATURE CITED

1. G. V. Sagitdinova and A. I. Saidkhodzhaev, *Khim. Prirodn. Soedin.*, 790 (1977).
2. M. E. Perel'son, Yu. N. Sheinker, and A. A. Savina, *The Spectra and Structure of Coumarins, Chromones, and Xanthenes* [in Russian], Moscow (1975).
3. R. R. Fraser, *Can. J. Chem.*, 38, 549 (1960).
4. L. A. Golovina and A. I. Saidkhodzhaev, *Khim. Prirodn. Soedin.*, 796 (1977).
5. A. A. Aminov and S. S. Kasymova, *Khim. Prirodn. Soedin.*, 283 (1977).