ESTERS OF Ferula leucographa STRUCTURE OF LEUCOFERIN

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Continuing investigations of the terpenoids from plants of the genus *Ferula* (*Ferula* L., fam. Apiaceae), from the roots of *Ferula leucographa* Korov., gathered in Chimkent province, Republic of Kazakhstan, by ethanolic extraction followed by column chromatography of the neutral fraction of the extractive substances we have isolated three compounds of ester nature, two of which have been identified as ugaferin $C_{25}H_{36}O_7$ (1), mp 125-126°C, $[\alpha]_D - 24.0^\circ$ (*c* 1.0, chloroform) and fekorin $C_{22}H_{34}O_5$ (2), $[\alpha]_D - 28^\circ$ (*c* 1.0; chloroform) [1, 2].

The third substance, new, we have named leucoferin, $C_{20}H_{32}O_4$ (3), mp 79-80°C, $[\alpha]_D - 66^\circ$ (c 1.0; chloroform); its IR spectrum had absorption bands at (cm⁻¹) 1660 (double bond), 1700 (ester carbonyl group) and 3300-3500 (hydroxy group).

In the PMR spectrum of compound (3) we observed the following resonance signals (CDCl₃, 0 – TMS, ppm): 0.96 and 1.12 (doublets 3H each, ${}^{3}J = 6.5$ Hz, H₃C-12, 13), 1.18 (singlet, 3H, H₃C-14), 1.79 (broadened singlet, 3H, H₃C-15), 1.91 (multiplet, 3H, ${}^{4}J = 1.5$ Hz, H₃C-4'), 2.03 (doublet with additional splittings, 3H, ${}^{3}J = 7.2$ and ${}^{5}J$ 1.5 Hz, 6H-3' and CH₃-4', respectively, H₃C-5'), 2.83 (doublet, 1H, ${}^{3}J = 8.0$ Hz, H-5), 3.51 (doublet of doublets, 1H, ${}^{3}J = 8.0$ and 1.5 Hz, H-6), 5.26 (multiplet, 2H, H-1 and H-8), 6.2 (quartet with additional splittings, 1H, ${}^{3}J = 7.5$ and ${}^{4}J = 1.5$ Hz, H-3').

The mass spectrum of leucoferin was typical for esters of sesquiterpene alcohols, with peaks of ions having m/z 236 $(M-100)^+$ (5), 218 $(M-100-18)^+$ (5), 193 $(M-100-43)^+$ (6), 175 $(M-100-43-18)^+$ (10), 136 (20), 83 $(C_5H_7O)^+$ (100).

When leucoferin was subjected to alkaline hydrolysis with a 5% aqueous alcoholic solution of caustic potash, the neutral part of the hydrolyzate yielded a sesquiterpene alcohol $C_{15}H_{26}O_3$ with mp 82-83°C, identified as ugamdiol (4), and the acid part gave angelic acid $C_5H_8O_2$ with mp 44-45°C. Thus, leucoferin is an ester of ugamdiol with angelic acid.

It follows from a comparative analysis of the characteristics of the PMR spectra of leucoferin and its acetyl derivative that on acetylation the greatest paramagnetic shift (by 1.44 ppm) was undergone by the H-6 signal, while the chemical shift of the H-8 signal decreased slightly. From this we drew the conclusion that the angeloyl residue was present at C-8, and leucoferin has the structure 8-angeloylugamdiol.

The relative configuration of the substituents in ugaferin – an ester of ugamdiol with 3,4,5-trimethoxybenzoic acid – has been established previously by x-ray structural analysis [3]. In the light of this information, we assume for leucoferin, also, the α -orientation of the substituents at C-4 and C-8 and β - at C-6 and C-7 as shown in the following structure for (3).



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REFERENCES

- 1. A. I. Saidkhodzhaev and V. M. Malikov, Khim. Prir. Soedin., 721 (1978).
- 2. A. Sh. Kadyrov, A. I. Saidkhodzhaev, and G. K. Nikonov, Khim. Prir. Soedin., 152 (1975).
- 3. M. K. Makhmudov, A. I. Tashkhozhaev, A. I. Saidkhodzhaev, and B. T. Ibragimov, Khim. Prir. Soedin., 198 (1990).