The results obtained permitted the position of attachment of the two monomeric lactones to be established unambiguously and the conformation of anabsin to be determined. The conformation of the molecule as projected on the XZ plane is shown in Fig. 1.

The five-membered rings A, C, D, and H have the envelope conformation, while the fivemembered ring F is plane. The seven-membered ring G has the chair conformation and ring B a distorted twisted chair. The ring linkages are: A/B and G/H, trans; E/F, cis. The bond lengths and valence angles are the usual ones.

## LITERATURE CITED

- Sh. Z. Kasymov, N. D. Abdullaev, G. P. Sidyakin, and M. R. Yagudaev, Abstracts of the Second International Symposium on the Chemistry of Natural Compounds, Bulgaria (1978). p. 421.
- 2. V. I. Andrianov, Z. Sh. Safina, and B. L. Tarnopol'skii, Zh. Strukt. Khim., <u>15</u>, 911 (1974).

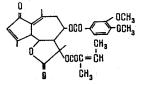
FEGVOLIDE - A LACTONE FROM THE ROOTS OF Ferula gigantea

A. A. Savina, L. I. Dukhovlinova, Yu. E. Sklyar, D. A. Fesenko, and M. G. Pimenov

A series of sesquiterpene lactones has been isolated from *Ferula gigantea* B. Fedtsch. F. latifolia Korov has also been assigned to F. gigantea [2]. From an acetone extract of giant fennel roots collected at the classical find site of F. latifolia (environs of the village of Shuroabad, TadzhSSR), by chromatographing three times on a column of silica gel L40/100  $\mu$  we have isolated three sesquiterpene lactones: C<sub>29</sub>H<sub>32</sub>O<sub>9</sub> (I), mp 210-212°; C<sub>26</sub>H<sub>28</sub>O<sub>9</sub> (II), mp 213-215°C; and C<sub>29</sub>H<sub>32</sub>O<sub>9</sub> (III), mp 218-220°C.

On the basis of the agreement of their melting points and the identity of their IR and PMR spectra, compounds (I) and (II) were identified as malaphyll and malaphyllin, respectively. Substance (III) proved to be new not previously described in the literature, and we have called it fegvolide. The parameters of its IR spectrum are close to those of the IR spectra of malaphyll and malaphyllin and show that (III) is a diacyloxyguaianolide; 1790 cm<sup>-1</sup> ( $\gamma$ lactone C=0); 1710 cm<sup>-1</sup> (C=O of an acyloxy group); 1690 (C=O of an  $\alpha,\beta$ -unsaturated cyclopentanone); 1640, 1620, 1650 cm<sup>-1</sup> (C=C). The PMR spectrum of compound (III) (CDCl<sub>3</sub>, TMS, Varian HA-100D) is characteristic for 6,11-diacyloxy-1-oxoguai-2,8-dien-4,5-olides and differs from the PMR spectra of malaphyll and malaphyllin by the parameters of only one acyloxy group — an angelic acid residue: 6.21 us,  $W_{1/2} = 4$  Hz, 1H(H-2); 4.76, q, J<sub>4,5</sub> = 10 Hz, J<sub>4,10</sub> = 11.0 Hz, 1H(H-4); 3.73, q, J<sub>4,5</sub> = 10.0 Hz, J<sub>3,6</sub> = 11.0 Hz, 1H(H-5); 5.78 sx, J<sub>6,72</sub> = 4.0 Hz, J<sub>5,6</sub> = J<sub>6,72</sub> = 11.0 Hz, 1H(H-6); 2.96, q, J<sub>72,72</sub> = 18 Hz; J<sub>72,6</sub> = 4.0 Hz, 1H(H-7e); 2.56, q, J<sub>72,72</sub> = 18 Hz, J<sub>72,6</sub> = 11.0 Hz; 3.66, d, J<sub>4,10</sub> = 10.2 Hz, 1H(H-10); 2.25, s, 6H(CH<sub>3</sub>-14, CH<sub>3</sub>-15); 1.64, s, 3H(CH<sub>3</sub>-13); veratroy1: 7.64, q, J<sub>1</sub> = 8.0 Hz, J<sub>2</sub> = 2.5 Hz, 1H(H-6'); 7.49, d, J = 2.5 Hz, 1H(H-2'); 6.84, d, J = 8.0 Hz, 1H(H-5'); 3.93, s, (OCH<sub>3</sub>); 3.89, s, (OCH<sub>3</sub>); angeloy1: 6.24, q, 1H(CH=); 1.96, d, 3H(CH<sub>3</sub>-CH=); 1.88 us, (CH<sub>3</sub>-C=C-CH<sub>3</sub>).

Thus, fegvolide corresponds to the following structure:



All-Union Scientific-Research Institute of Medicinal Plants, Moscow. Translated from Khimiya Prirodnykh Soedinenii, No. 5, p. 733, September-October, 1979. Original article submitted May 28, 1979.

649

UDC 547.9:582.89

## LITERATURE CITED

1. V. Yu. Bagirov, B. I. Sheichenko, R. Yu. Gasanova, and M. G. Pimenov, Khim. Prir. Soedin., 445 (1978).

2. M. G. Pimenov and Yu. V. Baranova, Byull. MOIP, 84, No. 3 (1979).

STRUCTURE OF AJADIN

M. I. Yusupov, Sh. Z. Kasymov, and G. P. Sidyakin UDC 547.314+582.998

We have continued the study of the new sesquiterpene lactone ajadin (I) [1].

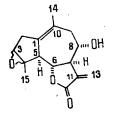
In the PMR spectrum of (I) (JNM-4H-100 MHz instrument, deuterochloroform,  $\delta$  scale, internal standard HMDS) the following signals were observed: three-proton singlets at 1.58 ppm (methyl on a carbon atom attached to an oxygen atom) and 1.63 ppm (methyl on a double bond). A one-proton singlet at 3.32 ppm was due to a methine proton connected with an oxygen atom. The signal of a lactone proton appeared in the form of a triplet with its center at 3.58 ppm (J = 10 Hz). The signals of exomethylene protons were superposed on one another and appeared in the form of a doublet with its center at 6.1 ppm (J = 3 Hz). This behavior of the signals of the exomethylene protons is observed in cases where a hydroxy group is present in the  $\beta$ position [2, 3].

With the composition  $C_{15}H_{18}O_4$  and the presence of the functional groups described above, ajadin can have only a guaiane skeleton. The absence of the signal of an olefinic proton and the triplet nature of the lactone proton make it obvious that a double bond is present at  $C_1-C_{10}$ . The nature of the splitting of the signal of the lactone proton and the magnitude of the spin-spin coupling constant show that the lactone ring is attached at  $C_6-C_7$  and has a trans linkage.

With acetic anhydride in pyridine, ajadin gave a monoacetyl derivative (II) with the composition  $C_{17}H_{20}O_{5}$ ,mp 202-203°C (ether-hexane),  $[\alpha]D^{20}$  +112°(c 0.8; chloroform). Its IR spectrum showed absorption bands at (cm<sup>-1</sup>) 1765 ( $\gamma$ -lactone ring), 1740 and 1245 (ester group), and 1668 and 1625 (C=C bond). The formation of a monoacetate showed the secondary nature of the hydroxy group.

Thus, the functions of all the oxygen atoms in the ajadin molecule have been determined. The absence from the IR spectrum of (II) of the absorption band of the hydroxy group and also the presence in the PMR spectrum of (I) of the signal of a methine proton shows that the fourth oxygen atom is present in an epoxide ring. The presence in the PMR spectrum of ajadin of the signal of the protons of a methyl group at 1.58 ppm determines the position of the epoxide group at  $C_3-C_4$ .

In the PMR spectrum of (II) three-proton singlets were observed at 1.63 ppm (CH<sub>3</sub>-C-O) and 1.69 ppm (C=C-CH<sub>3</sub>). The signal of the protons of the methyl group of an acetyl residue appeared at 2.07 ppm; and a broadened one-proton singlet at 3.34 ppm was due to a gem-epoxide proton. The lactone proton appeared in the form of a triplet at 3.66 ppm (J = 10 Hz). A one-proton sextet with its center at 4.71 ppm (J<sub>1</sub>= J<sub>2</sub> = 10, J<sub>3</sub> = 3 Hz) was due to a gem-acyl proton. The signals of the protons of an exomethylene group appeared in the form of two doublets



Institute of the Chemistry of Plant Substances, Academy of Sciences of the Uzbek SSR, Tashkent. Translated from Khimiya Prirodnykh Soedinenii, No. 5, pp. 733-734, September-October, 1979.

650