THE STRUCTURE OF FEROPODIN

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Recently [1] a report has been given of a sesquiterpene lactone feropodin with the composition $C_{15}H_{20}O_2$ mp 140-141°C, for which two probable structures were suggested. As has been shown by the results of IR and UV spectra (ν_{max} 1645 and 1587 cm^{-1}, λ_{max} 264 nm, log ε 3.82), the substance contains a conjugated system of double bonds. The value of log ε shows that feropodin, like artabsin is a homoannular, and not a heteroannular, diene [2].

The NMR spectrum (Fig. 1) taken with integration of the areas of the signals, gives unambiguous information on the structure of feropodin. The spectrum has the singlet of an angular methyl group at 0.86 ppm $(CH_3{-}\overset{|}{\underset{|}{C}}{-}, 3\,H)$, the doublet of a secondary methyl group with a center at 1.16 ppm ($CH_3{-}CH<$, 3 H, J = 7 Hz), and the signal of a vinyl methyl group at 1.98 ppm $(CH_3{-}\overset{|}{C}{=}, 3H)$.

The NMR spectrum of feropodin has a one-proton doublet with its center at 2.42 ppm (J = 10 Hz). In the structures put forward previously, there was no proton which could interact with a spin–spin coupling constant of 10 Hz. In addition to this, the signal of the lactone proton appears in the form of a quartet at 4.63 ppm (J_1 = 10 Hz, J_2 = 6 Hz), showing interaction with only two neighboring protons (at C_{10} and C_7).

Consequently, in the molecule of the lactone under investigation, the lactone ring is at $C_7{-}C_8$, and an isopropyl group at C_7 participates in its formation. The one-proton doublet with its center at 2.42 ppm therefore relates to H-10 and is the result of interaction of this proton with the lactone proton (H-8). This shows that feropodin belongs to the group of sesquiterpene lactones of the eudesmane series.

In a discussion of the question of the position of the conjugated double bonds, it must be observed that according to the integration curve the area of the olefinic protons is equal to three units. A triplet with its

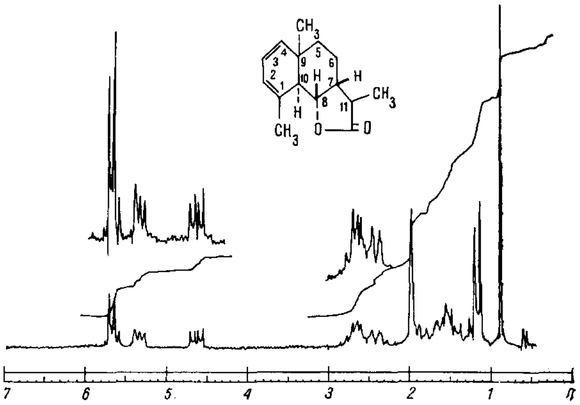

Fig. 1. NMR spectrum of feropodin.

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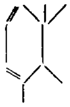
center at 5.35 ppm (1 H) and a signal at 5.67 ppm (2 H) together with the signal of the vinyl methyl group show the presence in the substance of the structural fragment



This position of the conjugated double bonds is also confirmed by the chemical shift and the nature of the splitting of the signal of the lactone proton. On the basis of the spin–spin splitting constants of the lactone proton it is possible to determine the stereochemistry at C_7, C_8, and C_{10}. The H-8 proton interacts with the two neighboring protons (H-10 and H-7) with constants of 10 and 6 Hz, respectively. In addition to this, H-10 also interacts with H-8 with a constant of 10 Hz. Consequently, H-8 and H-10 are in the trans position with respect to one another. The second constant (6 Hz) shows that H-8 and H-7 apparently occupy the cis position.

Thus, feropodin has the probable structure of eudesma-3,1-dien-8,12-olide.

The NMR spectrum was taken on a Varian HA-100D spectrometer in CCl_4 solution. Tetramethylsilane was used as internal standard, and the chemical shifts are given on the δ scale.

LITERATURE CITED

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2. M. Suchy, V. Herout, and F. Šorm, Collection Czech. Chem. Commun., 29, 1829 (1964).