A NEW SESQUITERPENE HYDROXYLACTONE FROM *Ferula oopoda*

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From the roots of *Ferula oopoda* (Boiss. et Buhse) Boiss., besides ferulin [1, 2] and ferulidin [3], we have isolated a substance with the composition $C_{15}H_{20}O_4$, mp 212-214°C (decomp.). The IR spectrum of the compound shows absorption bands at 3540 cm^{-1} (OH group), 1775 cm^{-1} (γ-lactone), and 1660 cm^{-1} (double bond).

The NMR spectrum (Fig. 1) has the singlet of an angular group at 0.72 ppm ($CH_3-\overset{|}{\underset{|}{C}}-$, 3H), and the doublet of a secondary methyl group with its center at 1.21 ppm (J = 6 Hz, $CH_3-CH<$, 3H). The singlet of the $CH_3-\overset{|}{\underset{|}{C}}-$ group permits the assumption that the lactone under investigation has a bicyclic carbon skeleton. According to the NMR spectrum, the substance contains one double bond, this being present in an exocyclic methylene group. Two doublets with centers at 5.44 ppm (J = 2 Hz, 1 H) and 5.54 ppm (J = 2 Hz, 1H) are similar in the value of their chemical shifts (CSs) and the nature of their splitting to the signals of the exocyclic methylene group of badkhysinin, which is located adjacent to an oxide ring. The chemical shift of the methylene group is apparently caused by its propinquity to an ethoxide function. Signals in the 3.4-3.8 ppm region possibly relate to protons in an oxide ring (2H) and in an OH group (1H).

Consequently, two of the oxygen atoms of the molecule participate in the formation of a lactone ring and the third belongs to an OH group and the fourth to an oxide ring. A direct comparison of the NMR spectra of the lactone under investigation (I) and of saponified badkhysinin (II) shows their similarity. The NMR spectrum of (I) lacks the doublets of an exocyclic methylene group on a lactone ring which is present in (II). In return, the doublet of a $CH_3-CH<$ group is formed (1.21 ppm, J = 6 Hz) while in the spectrum of (II) an isolated singlet of a $CH_3-\overset{|}{\underset{|}{C}}-$ group is found in the methyl group region at 0.72 ppm.

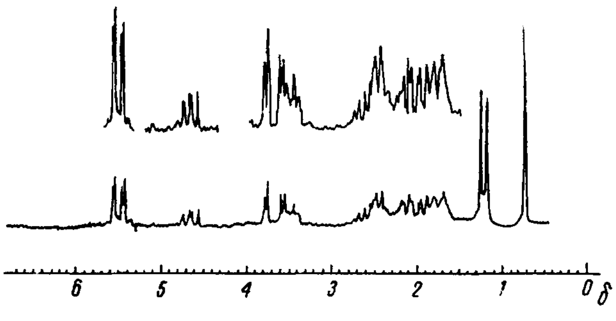

Fig. 1. NMR spectrum of the hydroxylactone.

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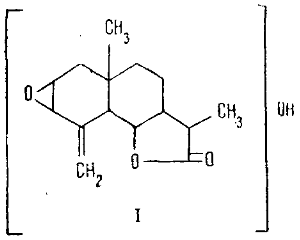
This suggests that (I) apparently has the structure of a dihydro derivative of (II) and, in addition, differs from the latter by the position of the OH group.

The lactone proton in the spectrum of (I) appears in the form of a quartet with its center at 4.65 ppm ($J_1=10$ Hz, $J_2=7$ Hz), which shows its interaction only with two neighboring protons. The singlet of the $CH_3-\overset{|}{\underset{|}{C}}-$ group excludes the presence of a guaiane carbon skeleton in the molecule of (I). The nature of the splitting of the lactone proton also excludes the presence of a pseudoguaiane carbon skeleton. Consequently, the compound isolated most probably belongs to the sesquiterpene lactones of the eudesmane series. Thus, we propose for it the structure I.



I

The IR spectrum was recorded on a UR-20 spectrophotometer (paraffin oil), and the NMR spectrum on a Varian HA-100D spectrometer [in $CDCl_3$ solution with $(CH_3)_4Si$ as the standard, the chemical shifts being given in the δ scale].

LITERATURE CITED

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