

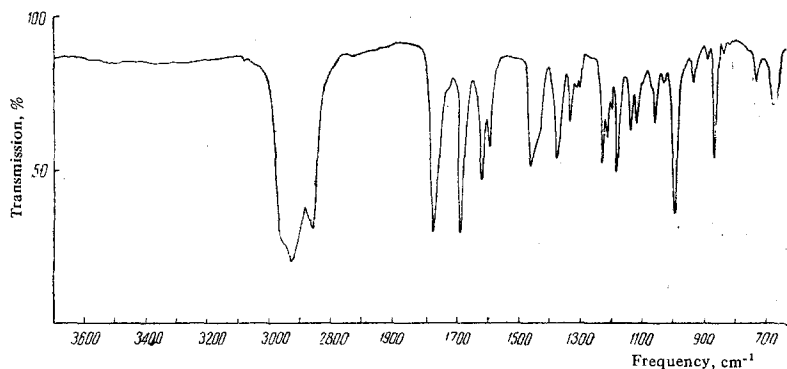
THE SESQUITERPENE LACTONE FERULIN FROM THE ROOTS OF FERULA OPODA

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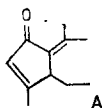
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From the roots of Ferula oopoda (Boiss. et Buhse) Boiss. we have isolated a substance with the composition $C_{15}H_{16}O_3^*$, mp 176-178° C. Yield 0.01%. Chromatography in a thin layer of alumina gave a single spot with R_f 0.84 (activity grade II; solvent, chloroform). The IR spectrum of the substance (figure) shows absorption bands at, cm^{-1} : 1775 (CO of a γ -lactone ring), 1690 (CO-keto group of a five-membered ring conjugated with double bonds), 1620 and 1610 (double bonds). We have named the substance "ferulin."



IR spectrum of ferulin.

The presence of a lactone ring in the molecule of ferulin was shown by its solubility in alkaline solutions on heating. Similar maxima are found in the IR spectra of the sesquiterpene lactones lactucin [1], leucodin (leucomisin) [2, 3], austriacin [2], jacquinelin [4], badkhyisin [5], and others. On the basis of these facts, it may be considered that ferulin has the partial structure A.

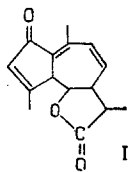


The IR spectrum of the lactone also has strong bands at 870 and 995 cm^{-1} which are characteristic, respectively, for $-CH=C<$ and $-CH=CH$ groupings. It is known that a strong band in the 990 cm^{-1} region generally appears in trienes and polyenes and shows the presence in them of a trans double bond [6]. Furthermore, the UV spectra of all the lactones mentioned above that contain a similar structural fragment show a single maximum (254-256 $m\mu$, $\log \epsilon$ 4.12). However, the UV spectrum of the compound under investigation shows the presence of three maxima, at λ 310, 258, and 244 $m\mu$ ($\log \epsilon$ 3.83, 4.45, and 4.42), apparently due to an extension of conjugation. Similar maxima have been found in the spectrum of anhydroaustriacin [2] with mp 207-258° C (λ_{max} 305, 255, and 245 $m\mu$; $\log \epsilon$ 3.66, 4.33, and 4.35).

Thus, the substance contains three conjugated double bonds and three oxygen atoms, two of which participate in the formation of the lactone ring while the third is present in the form of a ketone group.

Taking into account the fact that ferulin belongs to the group of sesquiterpene lactones and the features of its IR and UV spectra, it may be suggested that it probably has structure I, anhydroaustriacin. It differs from the latter stereochemically.

*The elementary composition was calculated on the basis of the IR and UV spectra.



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