AROMATIC COMPOUNDS OF *Peucedanum pauciradiatum*

V. Yu. Bagirov, M. B. Belyi, F. A. Rasulov,
and N. M. Ismailov

UDC 547.587

The adsorption chromatography on neutral alumina of the total extractive substances of the roots of *Peucedanum pauciradiatum* collected in the Nakhichevan ASSR, Ordubad district, village of Anaband, in June, 1979, have enabled us to isolate two aromatic compounds corresponding to the compositions $C_{13}H_{16}O_5$ (I), M^+ with m/z 252, oil, and $C_{11}H_{12}O_4$ (II), M^+ with m/z 208, mp 85-86°C. On the basis of physicochemical characteristics, compound (II) has been identified as crocatone [1]. Compound (I) proved to be new and undescribed in the literature, and we have called it radiatinin. Its IR spectrum has characteristic absorption bands at 3010, 1645, 1620, 780, and 735 cm^{-1} (aromatic ring), 3085 and 890 cm^{-1} ($-CH=CH_2$), 1055 and 920 cm^{-1} ($-O-CH_2-O-$). The ^1H NMR spectrum of radiatinin (Fig. 1a) shows the signals of the protons of three methoxy groups, of a methylenedioxy group, and of an allyl group. These facts indicate that (I) is a completely substituted aromatic compound. It must also be mentioned that the methylenedioxy group in the radiatinin molecule may be present at C_5-C_6 or

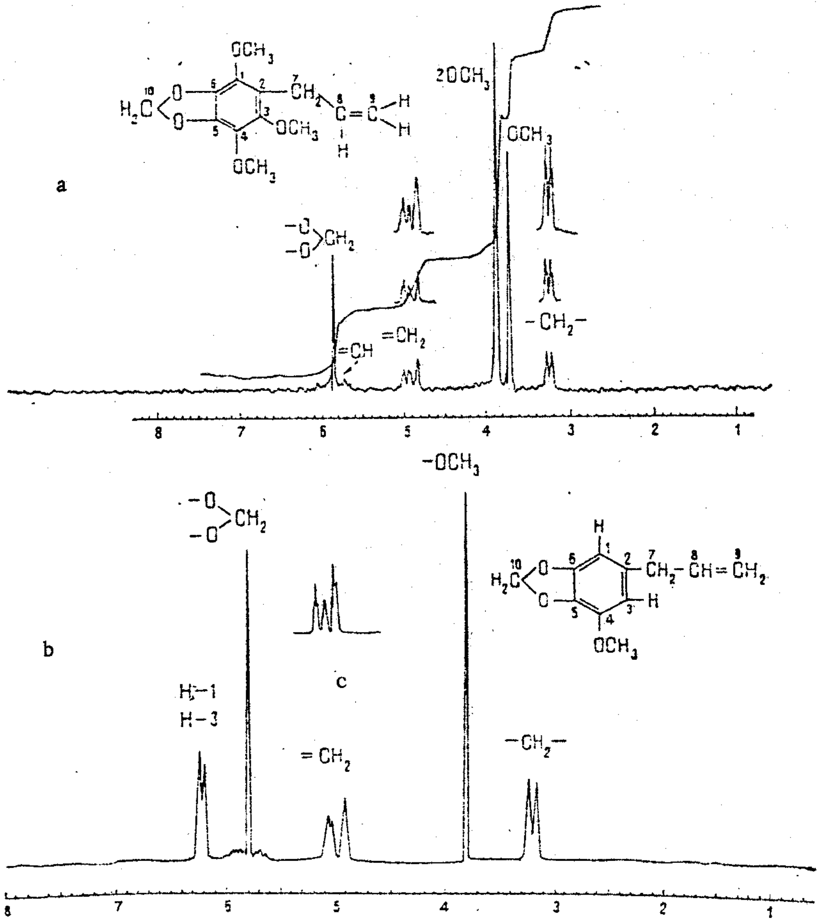

Fig. 1. NMR spectra of radiatinin (a) and myristicin (b) in $CDCl_3$; c) fragment spectra of myristicin in D-acetone.

V. L. Komarov Institute of Botany of the Academy of Sciences of the Azerbaidzhan SSR, Baku. Translated from Khimiya Prirodnykh Soedinenii, No. I, pp. 127-129, January-February, 1982. Original article submitted June 20, 1981.

0009-3130/82/1801-0123$07.50

C_6-C_1. The choice in favor of the C_5-C_6 position was made on the basis of a comparative study of the spectra of radiatinin in $CDCl_3$ and C_6D_6 solutions [2]. Thus, on passing from $CDCl_3$ solution to C_6D_6 solution a considerable upfield shift of the signal of the protons of the methylenedioxy group was observed in the ^1H NMR spectrum of radiatinin ($\Delta\delta$ 0.65 ppm). This shows that the benzene ring of the solvent is located above the methylenedioxy group. An upfield shift of the signals of the protons of the two methoxy groups was also observed ($\Delta\delta$ 0.14 ppm), while the position of the signals of a third methoxy group was practically unchanged [3]. The upfield shift of the signals of only two of the methoxy groups showed that these methoxyls falls into the region of screening of the benzene ring, i.e., they occupy positions adjacent to the methylenedioxy group. If the methylenedioxy group were present at C_6-C_1, the screening of the signals of only one methoxyl and of the methylene group of the $-CH_2-CH=CH_2$ fragment would be observed. A comparative study of the ^1H NMR spectra of radiatinin and myristicin (Fig. 1b), which we isolated from Lipskii's giant fennel and from *Ferula equisetacea* [4] showed that radiatinin and myristicin have the identical arrangement of the methylenedioxy and allyl groups and of one methoxy group. Thus, according to the spectral characteristics, radiatinin has the structure of 2-allyl-1,3,4-trimethoxy-5,6-methylenedioxybenzene.

IR spectra (mulls in paraffin oil) were taken on a UR-20 spectrophotometer NMR spectra in $CDCl_3$ and C_6D_6, 0 — TMS, δ scale) on a Varian HA 100 D spectrometer, and mass spectra on a Varian CH-8 spectrometer, and melting points were determined on a Kofler block.

LITERATURE CITED

1. M. Plat, J. Le Menet, M.-M. Janot, Bull. Soc. Chim. Biol., 45, 1119 (1963).
2. N. S. Bhacca and D. H. Williams, Applications of NMR Spectroscopy in Organic Chemistry, Holden-Day, San Francisco (1964) [Russian translation], Moscow (1966), p. 199.
3. R. G. Wilson, D. E. A. Rivett, and D. H. Williams, Chem. Ind. (London), 109 (1969).
4. V. N. Borisov, A. I. Ban'kovskii, V. I. Sheichenko, and M. G. Pimenov, Khim. Prir. Soedin., 275 (1973).