A SESQUITERPENE HYDROCARBON OF *Ocimum gratissimum*

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In the investigation of the nonphenolic fraction of the essential oil of *Ocimum gratissimum* Lim. (East Indies basil) a substance was isolated by fractional distillation which consisted of a colorless readily polymerizing liquid with bp 97-98.5°C/5 mm, n_D^{20} 1.5112, d_{20}^{20} 0.8996, $[\alpha]_D^{20}$ −162.5°, composition $C_{15}H_{24}$, mol. wt. 204. Mass spectrum, m/z (%): M^+ 204(22), 189(7), 162(17), 161(100), 157(10), 134(12), 133(24), 121(13), 120(25), 119(46), 117(11), 107(17), 106(13), 93(43), 92(17), 81(46), 79(40), 77(34), 69(18), 67(23), 65(16), 55(34), 53(23), 43(30), 39(30).

The UV spectrum of the hydrocarbon has bands with $\lambda_{max}^{C_{16}H_{14}}$ 202 nm (17,000) and 256 nm (4900), showing the presence in the molecule of three conjugated multiple bonds [1]. According to the IR spectrum (Fig. 1) one of them is a $>CH=CH_2$ methylene bond (890, 3090 cm^{-1}) and another a trans-disubstituted CH=CH bond (976 cm^{-1}).

The addition of three molecules of hydrogen when the substance was hydrogenated over Adam's platinum oxide in acetic acid confirmed the presence of the third multiple bond. On exhaustive hydrogenation in this way, a compound was obtained with n_D^{20} 1.4591 the IR spectrum of which was identical with that of bisabolane [2]. The fact that the compound belonged to the bisabolane type of terpenoids quite obviously showed that the trans-disubstituted multiple bond was present in an aliphatic chain, and its position was determined by the following facts.

The mass spectrum of the compound has its strongest peak at m/z 161. In all probability, it is due to the splitting out of an isopropyl group and the localization of the charge on the remainder of the molecule. The presence of an isopropyl group was confirmed by the existence of bands at 1365 and 1387 cm^{-1} in the IR spectrum of the compound (see Fig. 1) [2, p. 173].

The existence of an isopropyl group determined the position of the $>C=CH_2$ methylenic bond and, consequently, the position of the trans-disubstituted multiple bond conjugated with it. The latter was confirmed by the oxidation of the hydrocarbon with potassium permanganate, as a result of which, together with formic acid, isovaleric (β-methylbutyric) acid (anilide with mp 109-110°C) was obtained.

According to its composition and chemical and spectral characteristics, the substance isolated was a monocyclic sesquiterpene hydrocarbon with the most probable structure of 9-(3'-methylbut-1'-ylidene)-p-mentha-3,8(10)-diene. We have given this compound the name of gratissimene. The presence of gratissimene in the essential oil of East Indies basil has obviously led research workers into error in relation to the presence of the strongly rotating *l*-cadinene [3, 4]. According to the literature, gratissimene is apparently present in the essential oil of *Artemisia taurica* and *A. Monogynus*, since the substance isolated from

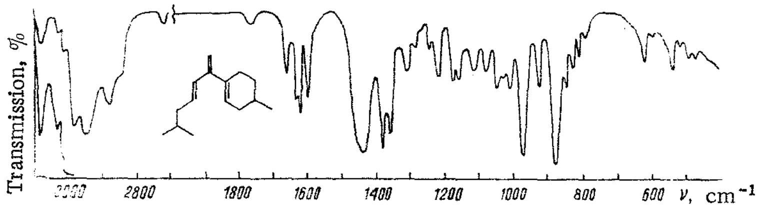

Fig. 1. Infrared spectrum of gratissimene (UR-20 spectrophotometer, layer thickness 0.032 mm).

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them had practically the same values of the constants as our compound: d_4^{20} 0.8948, n_D^{20} 1.5099, $[\alpha]_D$ −163.75 [5, 6].

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SESQUITERPENE LACTONES OF *Jurinea suffruticosa*

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The leaves and anthodia of *Jurinea suffruticosa* Rgl. [1] collected in the Chimkent province were exhaustively extracted with chloroform. The resin obtained was dissolved in small amount of ethanol and the solution was diluted with water to an ethanol concentration of 35%. The precipitate that deposited was filtered off, and the filtrate was extracted with chloroform. The material obtained after the evaporation of the chloroform was chromatographed on a column of alumina with elution successively by benzene and benzene—acetone (95:5, 9:1, and 8:2).

The fractions eluted by benzene—acetone (95:5) yielded a crystalline compound(I) with the composition $C_{19}H_{23}O_7Cl$ having mp 195-197°C (ethanol). The IR spectrum of (I) had absorption bands at (cm^{-1}) 1740 (γ-lactone carbonyl and ester group); 1665, 1650, 1630 (C=C bond), and 3460 (OH group). Elution with benzene—acetone (9:1) gave substance (II) with the composition $C_{15}H_{29}O_4$, mp 136-138°C (ethyl acetate—hexane). The IR spectrum of (II) showed absorption bands at (cm^{-1}) 1745 (γ-lactone carbonyl), 1650 (C=C bond), and 3250, 3560 (OH group).

From its composition, properties, the results of a comparison of IR and PMR spectra, and a mixed melting point, (I) was identified as acroptilin [2]. Substance (II) proved to salonitenolide [3]. This is the first time that acroptilin has been isolated from plants from the genus *Jurinea*.

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