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Chaerophyllum coloratum L.: Essential Oils of Ripe Fruits and Umbels

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ABSTRACT: Essential oils of ripe fruits and umbels of *Chaerophyllum coloratum* L. (Apiaceae) were found by GC and GC/MS to contain very high percentage of (E)-β-farnesene (79.21% and 68.40% respectively).

KEY WORD INDEX: *Chaerophyllum coloratum*, Apiaceae, essential oil composition, (E)-β-farnesene.

INTRODUCTION: The *Chaerophyllum* genus (ca. 40 species) occurs commonly throughout Europe, Asia and northern America (1). *Chaerophyllum coloratum* L. is a species which is endemic in the Adriatic countries where it can be found in the rocky submediterranean areas, such as mountain Prokletije (Kosovo, Serbia), Croatia, Herzegovina, Montenegro and Albania (1,2). Analysis of essential oils of ripe fruits and umbels of this species is reported in this paper.

EXPERIMENTAL: Ripe fruit and umbels of *Chaerophyllum coloratum* were collected from the vicinity of Herceg Novi (Montenegro) in July 1994. A voucher specimen of the plant is kept at the Faculty of Pharmacy, Belgrade University, Yugoslavia.

Isolation Procedure—The essential oil samples were isolated from 100 g of air-dried ground ripe fruits and umbels of *C. coloratum*, using the standard hydrodistillation Clevenger-type procedure (3). The oils were analyzed on a capillary GC and GC/MS, and

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Table I. Percentage composition of essential oils of *Chaerophyllum coloratum*

	Plant part	
Compound	Ripe fruits	Umbels
α-pinene	1.21	0.36
β-pinene	6.95	1.51
(Z)-β-ocimene*	4.29	5.51
(E)-β-ocimene	1.62	1.81
p-cymene	0.35	0.78
α-terpinolene	0.42	0.73
β-caryophyllene	1.04	1.04
(E)-β-farnesene*	79.21	68.46
Total	95.09	80.20

*Isolated by preparative GC and the identification confirmed by IR and ^{1}H-NMR

most constituents were identified by comparison of their mass spectra to those from the MS library (4), taking into account the relative retention times. The structures of the main compounds were also verified by ^{1}H-NMR and IR data of the samples isolated by preparative GC.

Analytical GC—A Varian model 3400 gas chromatograph equipped with a split/splitless injector (250°C) and a 30 m x 0.32 mm DB-Wax fused silica capillary column and FID (300°C), was used for GC and GC/MS measurements. The column was temperature programmed as follows: 50°C (3 min) and then 50°-200°C at 10°C/min; carrier gas 3 mL H_2/min. Peak areas were calculated electronically by a Varian DS-604 data station.

GC/MS—The gas chromatograph was connected via an open split interface and a fused silica capillary (at 250°C) to the ion source of a Finnigan MAT 8230 mass spectrometer, equipped with a PDP 11/74 computer. Working conditions: carrier gas 2 mL He/min; other GC conditions as above. MS: ion source (electron impact), 170°C, 70 eV.

Preparative GC—All preparative separations were performed using a Varian Aerograph 920 instrument, equipped with TCD (210°C) and a 2 m x 4 mm glass column packed with 10% Carbowax 20M on Chromosorb W (60-80 mesh). Working conditions: Injector temperature 220°C; oven temperature 120°C and 140°C (isothermal conditions); carrier gas, 25 mL H_2/min. Samples (ca. 50 μL) were repeatedly injected and fractions were collected at the outlet of the detector in ice-cooled U-tubes.

^{1}H-NMR spectra of the isolated compounds were measured in $CDCl_3$ on a Varian FT 80A NMR spectrometer (at 80 MHz). IR spectra were recorded in the form of liquid films on a Perkin-Elmer 457 grating spectrometer.

RESULTS AND DISCUSSION: The essential oils (pale yellow) were isolated from ripe fruits and umbels in yields of 1.1% and 1.0% (calculated per weight of dried plant material), respectively. Both samples exhibited very similar chemical composition (Table I), i.e. mono- and sesquiterpene hydrocarbons with (E)-β-farnesene as dominating constituent (79.21% and 68.46% in fruits and umbels, respectively). This compound was positively identified by comparison of its mass, IR and ^{1}H-NMR spectra to those reported for (E)-β-farnesene (5,6). Among the monoterpenes, the major constituents were β-pinene (6.95%) and (Z)-β-ocimene (5.51%) in fruits and umbels, respectively. Since, according to the available GC/MS data, the identity of (Z)-β-ocimene could not be firmly established, it was isolated from the oils by preparative GC and identified by comparison of its ^{1}H-NMR and IR spectra to those previously published (7). The oil originating from umbels showed higher content of (not identified) high-boiling fractions, eluting after (E)-β-farnesene.

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