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F. Tateo [a], M. Mariotti [a] & M. Bononi [a]

[a] DIFCA, Università degli Studi di Milano, Via Celoria 2, 20133, Milano, Italy

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RESEARCH REPORT

Essential Oil Composition and Enantiomeric Distribution of Some Monoterpenoid Components of *Coridothymus capitatus* (L.) Rchb. Grown on the Island of Kos (Greece)

F. Tateo,* M. Mariotti and M. Bononi
DIFCA, Università degli Studi di Milano, Via Celoria 2, 20133 Milano, Italy

Abstract

An oil produced from *Coridothymus capitatus* (L.) Rchb. grown in island of Kos (Greece) has been analyzed by GC/MS and by chiral GC. The principal component of this oil was carvacrol (66.7%). The enantiomeric distribution of α-pinene, camphene, β-pinene, limonene, 1-octen-3-ol, linalool, terpinen-4-ol and α-terpineol in *C. capitatus* oil is presented for the first time.

Key Word Index

Coridothymus capitatus, Labiatae, essential oil composition, enantiomeric distribution, carvacrol, chiral analysis.

Introduction

The oils of more than 80 *Thymus* species from different countries all over the world have been the subject of previous studies that have been recently reviewed (1,2). It is generally accepted that the genus *Thymus* is divided into two subgenera, the monotypic subgenus *Coridothymus* and the subgenus *Thymus*. *Coridothymus capitatus* (L.) Reichenb. fil. [syn. *Thymus capitatus* (L.) Hoffm. & Link.] is native to the Iberian peninsula. This work is related to the GC/MS characterization and chiral investigation on plants of *C. capitatus* grown in island of Kos (Greece).

With specific reference to Thymus oils, Tateo et al. (3-5) have recently identified the existence of commercial adulterated Thymus oils using GC/MS and NMR. Another analytical control technique of genuineness is that of enantiomeric distribution of optically active oil components. Furthermore the significance of chirality for flavor and fragrance quality and for flavor and fragrance intensity can be demonstrated for many components. A survey of the literature reveals that little information is known about the enantiomeric distribution of components of *C. capitatus* oil except that Ravid et al. (6-8) reported the enantiomeric distribution of α-terpineol, borneol and terpinen-4-ol. The present study contains the results of an examination of the enantiomeric distribution of components in an oil of *C. capitatus*.

Experimental

Identification of Oil Components: Oil isolation was realized by infusion of the plant in 96% EtOH.

*Address for correspondence
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Table I. Composition of *Coridothymus capitatus* grown in island of Kos (Greece)

Peak no.	Compound	Percentage	Peak No.	Compound	Percentage
1.	α-thujene	0.7	15.	linalool	0.4
2.	α-pinene	0.7	16.	camphor	t
3.	camphene	0.1	17.	borneol	t
4.	1-octen-3-ol	0.4	18.	terpinen-4-ol	0.5
5.	β-pinene	0.1	19.	α-terpineol	0.1
6.	myrcene	1.6	20.	n.i.	0.8
7.	3-octanol	0.3	21.	n.i.	0.5
8.	α-phellandrene	0.1	22.	bornyl acetate	t
9.	δ-3-carene	0.1	23.	thymol	0.3
10.	α-terpinene	<0.1	24.	carvacrol	66.7
11.	p-cymene	6.6	25.	β-caryophyllene	4.8
12.	limonene	0.8	26.	n.i.	3.1
13.	γ-terpinene	6.4	27.	caryophyllene oxide	0.7
14.	terpinolene	0.4			

20: M=136: m/z (rel. int.): 43(67), 55(9), 77(36), 79(11), 92(2), 93(72), 94(7), 109(8), 119(21), 121(100), 136(65)
21: M=164: m/z (rel. int.): 53(38), 67(1), 68(21), 91(42), 93(68), 107(8), 108(18), 121(69), 136(54), 149(52), 164(100)
26: M=166: m/z (rel. int.): 65(5), 77(10), 78(5), 79(7), 105(18), 123(3), 151(100), 152(10), 166(35), 167(5);
t = trace

Table II. Enantiomeric distribution of some monoterpenoid components of *Coridothymus capitatus* grown in island of Kos (Greece)

Peak no.	Component			
		S(−)	R(+)	ee
1.	α-pinene	16.7%	83.3%	R(+) 66.6
		R(−)	S(+)	ee
2.	camphene	57.0%	43.0%	R(−) 14.0
		R(+)	S(−)	ee
3.	β-pinene	68.7%	31.3%	R(+) 37.4
		S(−)	R(+)	ee
4.	limonene	17.7%	82.3%	R(+) 64.6
		S(+)	R(−)	ee
5.	1-octen-3-ol	0.1%	99.9%	R(−) 99.8
		R(−)	S(+)	ee
6.	linalool	83.3%	16.7%	R(−) 66.6
		R(+)	S(−)	ee
7.	terpinen-4-ol	69.6%	30.4%	R(+) 39.2
		S(−)	R(+)	ee
8.	α-terpineol	24.4%	75.6%	R(+) 51.2

GC analyses were performed on a fused silica capillary column SPB-5 (30 m x 0.32 mm, 0.25 μm film thickness). The oven temperature was programmed as follows: 80°C (10 min), 80°-120°C at 1°C/min, 120°C (10 min), 120°-230°C at 3°C/min. The GC/MS analyses were carried out on an HP 5971A MSD, equipped with an HP 5890 Series II GC unit, under conditions analogous to those stated for the GC analyses.

Enantioselective GC: GC chiral analyses were performed on a fused silica capillary column Beta-Dex 120 (30 m x 0.25 mm, 0.25 μm film thickness). The oven temperature was programmed as follows: 60°C (10 min), 60°-120°C at 1.5°C/min, 120°-220°C at 3°C/min.

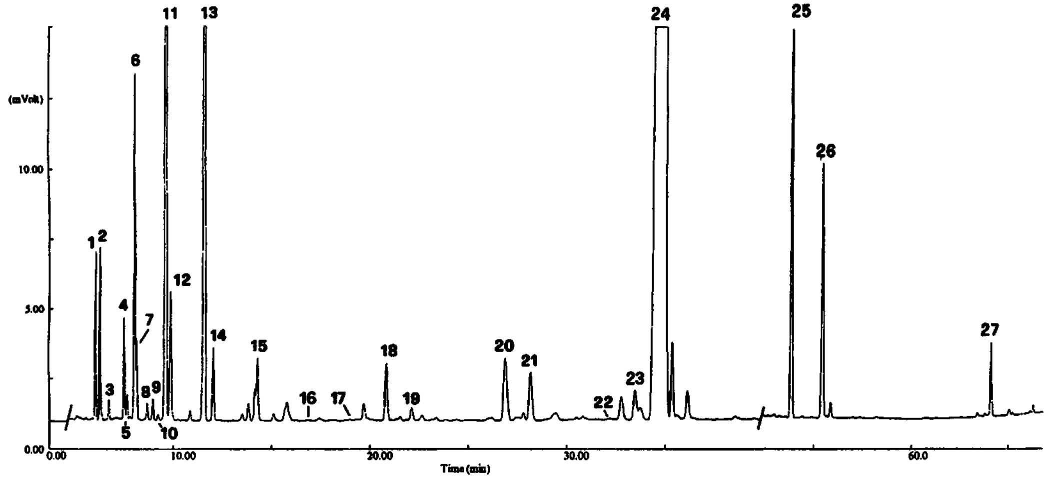

Figure 1. Gas chromatogram (column SPB-5) of the volatile components of *Coridothymus capitatus*. Peak numbers refer to Table I

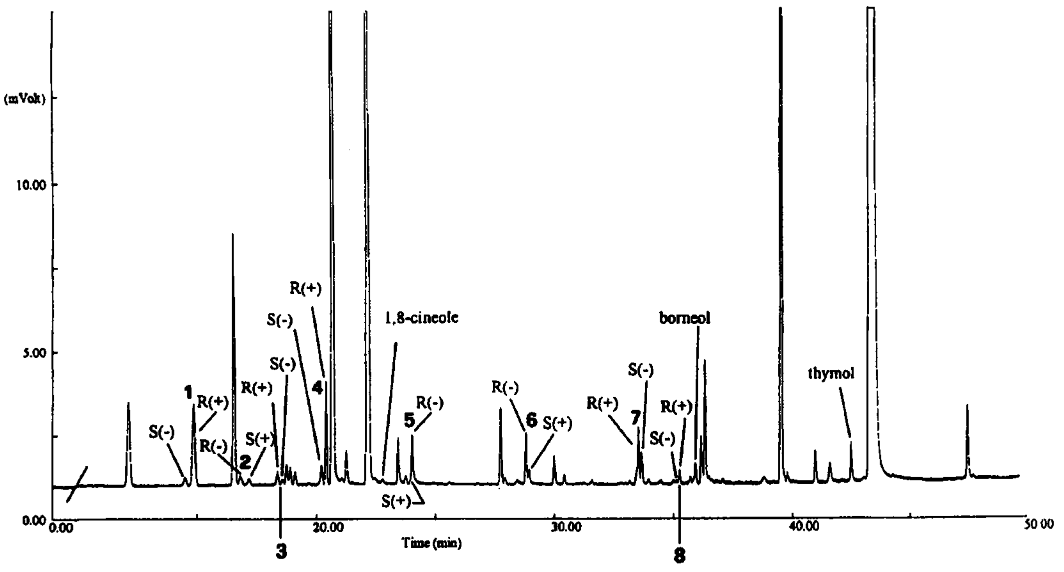

Figure 2. Gas chromatogram (column Beta-Dex-120, Heptakis 2,3,6-tri-O-methyl-β-cyclodextrin) showing the enantiomeric distribution of some volatile components of *Coridothymus capitatus*. Peak numbers refer to Table II

Results and Discussion

The compounds identified in *C. capitatus* oil are listed in Table I, and Figure 1 shows the corresponding gas chromatogram. The chemical composition data appear to be similar to those reported by Sendra and Cunat (9) for two lab-distilled oils from *C. capitatus* of Portuguese and Greek origin. It is particularly interesting to note that, in our sample, camphor, borneol and bornyl acetate were present only in trace amounts. The same was true for 1,8-cineole as confirmed by the Beta-Dex column.

Enantiomeric distribution of some monoterpenoids (α-pinene, β-pinene, camphene, limonene, 1-octen-3-ol, linalool, terpinen-4-ol, α-terpineol) is reported in Table II as deduced from the gas chromatogram presented in Figure 2.

For a statistically significant number of samples of *Thymus*, the enantiomeric distribution of the optically active components could prove most useful in controlling the genuineness of *C. capitatus* oil as well as that of other commercially important Labiatae oils.

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