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Chemical composition of the essential oil from *Microlicia graveolens* growing wild in Minas Gerais

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Abstract: The chemical composition of the essential oil of the aerial parts of *Microlicia graveolens* DC., Melastomataceae, growing wild in the mountains of Minas Gerais, Brazil, was investigated for the first time. A pale orange to colourless oil was obtained in a yield of 4.8%. The oil was analyzed by GC-MS. The main components were (+)-*trans*-pinocarvyl acetate (78.9%), (-)-*trans*-pinocarvyl acetate (5.5%) and β-pinene (3.8%).

Introduction

The genus *Microlicia* comprises approximately 100 species and is native to Brazil. The genus occurs typically as herbs or shrubs in an altitudinal ecosystem characterized by sandy or rocky soils predominantly covered by open vegetation (campos rupestres) (Bomfim-Patrício et al., 2001). *Microlicia graveolens* DC., Melastomataceae, is native to Minas Gerais and is abundant in the area around Ouro Preto. It is an herbaceous perennial plant found in the mountains.

The purpose of this study was to examine the chemical composition of the essential oil isolated by hydrodistillation from the aerial parts of *M. graveolens*.

Materials and Methods

The aerial parts of *Microlicia graveolens* DC., Melastomataceae, were collected in the beginning of October 2009 in the mountains at Ouro Preto-MG, Brazil. The plant material was identified by Maria C. T. B. Messias and a voucher specimen (nº OUPR-5731) was deposited at the Herbarium of Department of Botany, Institute of Biological Sciences, Federal University of Ouro Preto-MG, Brazil.

The essential oil was obtained from dried aerial parts by steam distillation for 5 h. The oil was analyzed by GC-MS on an Agilent 6890N Network GC system coupled to a 5973 Network Mass Selective Detector. GC conditions: injector temperature: 150 ºC; temperature programme: start 50 ºC, 20 ºC/min to 300 ºC; column: HP5MS. A NIST library was used for comparison of MS data. Retention indices were determined relative to *n*-alkanes (Fluka).

In order to isolate the main component, *trans*-pinocarvyl acetate, 1 mL of the essential oil was applied to a Merck Silica gel column (600 x 16 mm) and eluted with toluene:ethyl acetate (93:7). Fractions were analysed by TLC on Merck Silica gel 60 F_{254} plates eluted with toluene:ethyl acetate (93:7), and fractions containing *trans*-pinocarvyl acetate were combined. Solvent was removed by rotational evaporation under reduced pressure. Optical rotation was measured in EtOH on a Jas.Co DJP-370 Digital Polarimeter. ^{1}H-NMR was recorded in $CDCl_3$ on a Varian Mercury 300 MHz instrument: δ 5.68, 1H, *t*; δ 4.84, 1H, *q*; δ 4.77, 1H, *d*; δ 2.56 1H, multiplet; δ 2.49, 1H, *quint*; δ 2.31, 1H, *quint-d;* δ 2.1, 1H, *q*; δ 2.14, 3H, *s*; δ1.70, 1H, *q-t*; δ 1.48, 1H, *d*; δ 1.26, 3H, *s*; δ 0.79, 3H, *s*.

Results and Discussion

After steam distillation of the aerial parts of *Microlicia graveolens* DC., Melastomataceae, a pale orange to colourless oil was obtained in a yield of 48

mL/kg. This is a very high yield, making the species a candidate for commercial production. The oil had a very pleasant, clean smell, which could have commercial value as a fragrant in hand soaps or household cleaning products.

The detailed chemical composition of the essential oil is presented in Table 1. In total thirteen compounds were identified, representing 99.8% of the oil composition. The oil was mainly composed of (+)-*trans*-pinocarvyl acetate as the major component (78.9%) followed by (-)-*trans*-pinocarvyl acetate (5.5%) and β-pinene (3.8%). *Trans*-pinocarvyl acetate is a chiral compound. To determine optical rotation of the major compound, it was isolated from the oil by column chromatography. *Trans*-pinocarvyl acetate isolated from *M. graveolens* had an optical rotation of $[\alpha]^{28}_{589} = +31.9º$. NMR data were recorded, and largely matched those reported for *trans*-pinocarvyl acetate (Agarwal et al., 2005; Corbet et al., 2008).

Table 1. Chemical composition of the essential oil of *Microlicia graveolens*.

Rt (min)	RI	Compound	Percent
6.674	890	β-pinene	3.8
6.831	909	β-myrcene	1.4
7.353	971	D-limonene	1.3
7.901	1035	1-methyl-4(1-acetoxy-1-methylethyl)-cyclohex-2-enol	0.7
8.974	1162	pinocarvone	0.4
9.114	1179	4-terpineol	0.7
9.220	1191	L-pinocarveol	2.1
9.256	1195	α-terpineol	3.4
10.353	1325	(-)-*trans*-pinocarvyl acetate	5.5
10.532	1346	(+)-*trans*-pinocarvyl acetate	78.9
10.605	1355	(+)-myrtenyl acetate	0.8
12.193	1542	β-bisabolene	0.3
12.727	1605	verbenyl propyl ether	0.5

Trans-pinocarvyl acetate has previously been detected in *Dracocephalum speciosum*, a Lamiaceae species from Himalaya, where it constituted 60.5% of the essential oil (Agarwal et al., 2005), and in flower heads of *Egletes viscosa*, Asteraceae, where it constituted 51.7% of the oil (Lima et al., 1996) and in *Salvia euphratica*, Lamiaceae, where it constituted 16.8% of the oil (Baser et al., 1998). It was at the time claimed that *D. speciosum* essential oil appeared to be the only major source of natural *trans*-pinocarvyl acetate. However, with the findings of this study, the essential oil of *M. graveolens* must now be regarded as the major natural source of *trans*-pinocarvyl acetate.

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