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## Infraspecific chemical variability in the essential oils of *Pimenta pseudocaryophyllus* (Gomes) L.R. Landrum (Myrtaceae)

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### ABSTRACT

Leaf essential oils of *Pimenta pseudocaryophyllus* from the central Brazilian Cerrado were obtained by hydrodistillation and investigated by GC and GC–MS. A total of 57 constituents were identified, accounting for 96–100% of the volatile constituents. Principal component and cluster analysis identified three chemotypes: cluster I, characterized by high percentages of geranial (41.2 ± 3.9%), neral (26.8 ± 1.3%), caryophyllene oxide (3.8 ± 2.5%), and spathulenol (3.7 ± 1.8%); cluster II, with high contents of (E)-asarone (21.8 ± 30.9%), (E)-caryophyllene (16.2 ± 7.7%), and elemicin (8.8 ± 2.4%); and cluster III, with high amounts of (E)-methyl isoeugenol (93.2 ± 1%). The occurrence of these chemotypes at the same site indicates that chemovariation is genetically determined.

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### 1. Introduction

The Myrtaceae family, which consists of approximately 130 genera and 4000 species, is distributed throughout pantropical and subtropical regions. In Brazil, 23 genera with about 1000 species are known (Landrum and Kawasaki, 1997; Souza and Lorenzi, 2005). Among the representatives of this family include species of the *Pimenta* genus, mostly native to the Caribbean and Central America, which are well known because of the economic importance of “allspice”, *Pimenta dioica* (L.) Merrill (Suárez et al., 1997).

*Pimenta pseudocaryophyllus* (Gomes) L.R. Landrum is the only species of the *Pimenta* genus native to Brazil (Landrum, 1986; Landrum and Kawasaki, 1997). It consists of three varieties, *P. pseudocaryophyllus* var. *pseudocaryophyllus* (Gomes) Landrum, *P. pseudocaryophyllus* var. *fulvescens* (DC.) Landrum, and *P. pseudocaryophyllus* var. *hoehnei* (Burret) Landrum. This plant is found in high-altitude regions of the Atlantic forests and Cerrado regions in Brazil (Landrum, 1986; Landrum and Kawasaki, 1997). It is popularly known as “pau-cravo”, “louro-cravo”, “louro”, “craveiro”, “craveiro-do-mato”, “chá-de-bugre”, and “cataia”. In folk medicine, the leaf tea has been used to produce a refreshing drink with sedative, diuretic, and aphrodisiac properties, and to treat colds as well as digestive and menstrual problems (Landrum, 1986; Nakaoka-Sakita et al., 1994; Landrum and Kawasaki, 1997; Lima et al., 2006; Paula et al., 2008; Santos et al., 2009). Previous studies have demonstrated the antimicrobial activities of crude ethanol extract (Paula et al., 2009) and essential oils from *P. pseudocaryophyllus* leaves (Lima et al., 2006).

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**Table 1**Percentages and yields of volatiles of twelve specimens of *P. pseudocaryophyllus* from the Brazilian Cerrado.

Constituent	RI <sup>a</sup>	Origins											
		SGA1 <sup>b</sup>	SGA2 <sup>b</sup>	SGA3 <sup>b</sup>	SGA4 <sup>b</sup>	SGA5 <sup>b</sup>	SGA6 <sup>b</sup>	SGA7 <sup>b</sup>	SGA8 <sup>b</sup>	SJB1 <sup>c</sup>	SJB2 <sup>c</sup>	SJB3 <sup>c</sup>	BRA <sup>d</sup>
$\alpha$ -Thujene	930						0.8						
$\beta$ -Pinene	973	0.9		0.8		1.3	1.9		1.0				
6-Methyl-5-hepten-2-one	980						0.2		0.4				
Dehydro-1,8-cineole	987								0.2				
Limonene	1024				0.2					0.3	0.3		
1,8-Cineole	1028									0.2	0.1	0.1	
(E)- $\beta$ -Ocimene	1042			0.7		1.2			0.2			0.3	
Linalool	1096	0.4	0.2	1.3		1.4	6.6	1.1	0.5	0.6	0.8	4.9	
n-Nonanal	1100		0.1	0.8									
2-Methylbutyl-2-methylbutyrate	1100											0.1	
exo-Isocitral	1139								0.3				
(Z)-Isocitral	1160	0.6					0.8		1.0				
(E)-Isocitral	1178	1.0					1.3		1.8				
$\alpha$ -Terpineol	1188								0.2			0.1	
Citronellol	1224							0.4					
Nerol	1225	0.9					1.0		0.9				
Neral	1237	25.9					25.8	0.8	28.7			0.1	
Geraniol	1251	2.3					2.8		2.2			0.1	
Geranial	1267	46.6					39.6	1.0	37.3			0.1	
Methyl geranate	1320								0.1				
$\alpha$ -Cubebene	1347					0.8							
$\alpha$ -Copaene	1373	0.6	0.1		0.3	5.7	1.8	0.2	0.6			0.3	0.4
Geranyl acetate	1379						0.3						
$\beta$ -Bourbonene	1382								0.2				
$\beta$ -Elemene	1389								0.2		0.3		
Methyleugenol	1399		2.4		1.3			1.8			0.2		3.1
$\alpha$ -Gurjunene	1406			1.0									
(E)-Caryophyllene	1416	1.7	0.6	13.3	1.3	26.6	0.7	1.7	8.0	1.9	2.2	8.5	1.6
$\beta$ -Copaene	1426					1.2			0.3			0.1	
Aromadendrene	1436			3.9					0.3				
(Z)-Methyl isoeugenol	1451		2.5	2.2	3.3			1.4		2.3	1.8		0.9
$\alpha$ -Humulene	1451	0.8				4.9			1.5			1.4	
9- <i>epi</i> -(E)-Caryophyllene	1458						0.3						
allo-Aromadendrene	1458			1.8					0.5				
trans-cadina-1(6),4-diene	1470					0.6							
$\gamma$ -Muurolene	1473					4.5	0.3		4.2			1.6	
trans-Muurolo-4(14),5-diene	1477					4.7							
$\gamma$ -Himachalene	1482									0.5	0.5		
(E)-Methyl isoeugenol	1492	1.8	93.7	61.3	92.5	22.7	0.4	91.5		94.3	93.8	5.0	93.6
Bicyclogermacrene	1494								5.7				
$\alpha$ -Muurolene	1497					1.4			0.2			0.2	
$\gamma$ -Cadinene	1510					1.9			0.2			0.2	
$\delta$ -Cadinene	1520	0.5	0.2	1.1	0.4	9.2	0.6		0.9			0.9	0.4
Elemicin	1550			11.7		8.8						5.8	
Spathulenol	1574	6.1	0.3		0.4		3.0		1.9			0.3	
Caryophyllene oxide	1580	5.5					5.5		0.3			0.8	
Globulol	1589											0.3	
(Z)-Asarone	1595											1.3	
Humulene epoxide II	1606	0.8					0.8						
5- <i>epi</i> -7- <i>epi</i> - $\alpha$ -Eudesmol	1619											0.1	
1- <i>epi</i> -Cubenol	1624											0.1	
1,10-di- <i>epi</i> -Cubenol	1628											0.1	
Muurolo-4,10(14)-dien-1- $\beta$ -ol	1634	0.7						0.3					
<i>epi</i> - $\alpha$ -Muurolo	1638											0.7	
$\alpha$ -Muurolo	1650							0.3				0.2	
14-hydroxy-(Z)-Caryophyllene	1667	0.4						0.7					
(E)-Asarone	1671											65.5	
Monoterpene hydrocarbons		1.0		1.5	0.2	2.5	2.7		1.4	0.3	0.3	0.3	
Oxygenated monoterpenes		77.7	0.2	1.3		1.4	77.9	3.4	73.0	0.8	0.9	5.4	
Sesquiterpene hydrocarbons		3.6	0.9	21.2	2.0	61.6	3.8	1.9	22.3	2.4	3.0	13.3	2.4
Oxygenated sesquiterpenes		13.6	0.3		0.4		10.7		2.2			2.5	
Phenols		1.9	98.5	75.2	97.1	31.5	0.4	94.8		96.6	95.9	77.6	97.6
Others			0.1	0.8			0.6		0.5			0.1	
Yield (% v/w)		1.4	1.2	0.3	1.2	0.6	1.6	0.8	1.3	1.1	1.5	0.8	0.8

<sup>a</sup> Calculated linear retention indices.<sup>b</sup> São Gonçalo do Abaeté.<sup>c</sup> São José do Barreiro.<sup>d</sup> Brasília.

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