Journal of Essential Oil Research

ISSN: 1041-2905 (Print) 2163-8152 (Online) Journal homepage: http://www.tandfonline.com/loi/tjeo20

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To cite this article: Rafael F. Silva, Claudia M. Rezende, João B. Pereira, Roberto F. Vieira, Marcelly C.S. Santos & Humberto R. Bizzo (2015) Scents from Brazilian Cerrado: chemical composition of the essential oil from *Pseudobrickellia brasiliensis* (Asteraceae), Journal of Essential Oil Research, 27:5, 417-420, DOI: 10.1080/10412905.2015.1037021

To link to this article: https://doi.org/10.1080/10412905.2015.1037021

Published online: 27 Apr 2015.

Journal of Essential Oil Research, 2015
Vol. 27, No. 5, 417–420, http://dx.doi.org/10.1080/10412905.2015.1037021

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Scents from Brazilian Cerrado: chemical composition of the essential oil from *Pseudobrickellia brasiliensis* (Asteraceae)[±]

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(*Received 5 November 2014; accepted 28 March 2015*)

The chemical composition of the essential oil from the leaves of *Pseudobrickellia brasiliensis* (Asteraceae) from the Brazilian Cerrado was analyzed by GC/FID and GC/MS. Thirty-four out of thirty-eight components detected were identified. Major compounds in the oil were terpinen-4-ol (38.6%), γ-terpinene (19.5%), α-terpinene (7.8%) and α-terpineol (4.5%).

Keywords: *Pseudobrickellia brasiliensis*; Astereaceae; essential oil; Cerrado; terpinen-4-ol; arnica

1. Introduction

Brazilian biodiversity, which comprises *circa* one-sixth of the total plant species is divided into important biomes such as the Amazon rainforest, the Atlantic Forest and a savanna area in Central Brazil, known as Cerrado (1). Cerrado is the second largest Brazilian biome, but the most threaten by anthropic pressure. Only a small fraction of the 12,000 known botanical species were chemically investigated, making Cerrado a very promising source for flavor and fragrance applications (2).

Pseudobrickellia brasiliensis (Spreng.) R.M. King & H.Rob. (Asteraceae) is a shrub 1 to 1.5 m tall, largely distributed in Central Brazil at Cerrado vegetation (3). It is commonly known as 'arnica-do-mato' and used in traditional medicine to treat pain and as anti-inflammatory.

Previous investigation on the ethyl ether – petroleum ether extract from the aerial parts of *P. brasiliensis* lead to the isolation of a new compound, 4-hydroxygermacra-1(10),5-diene, as well as other sesquiterpenes and triterpenes (4). An essential oil containing 32.6% of α-pinene and 17.2% of α-thujene was reported in a phytochemical investigation on this species (5). Ethanol and ethyl acetate extracts from the leaves showed to be cytotoxic to human peripheral blood mononuclear cells, but not the aqueous extract, which was then observed to reduce the expression of interferon-gamma and tumor necrosis factor, cytokines related to cell inflammatory process (6). To the best of our knowledge, no peer-reviewed data on *P. brasiliensis*, besides ref. 4, appeared in the literature.

Herein, we report the results of the analysis of the essential oil from *P. brasiliensis* collected in the Cerrado biome.

2. Experimental part

2.1. Plant material

Leaf samples were collected at Araçuai, Minas Gerais State, and a voucher specimen (CEN 87608) was deposited at the herbarium of Embrapa Genetic Resources and Biotechnology, Brasilia DF. According to Brazilian law, collection and access were authorized by the Ministry of Environment (process IBAMA 02001.003166/2013-26).

2.2. Extraction of the essential oil

Dried leaves (212 g) from a representative sample of the individuals collected were subjected to hydrodistillation in a modified Clevenger-type apparatus for 2 hours. After distillation the oil was collected, dried with anhydrous sodium sulfate (Na_2SO_4) and stored in a freezer at -8°C for later analysis.

2.3. Analysis of the essential oil

The essential oil was diluted in dichloromethane in the proportion of 1%, and then 1.0 μL of the solution was injected (split 1:20) into an Agilent 6890N gas chromatograph equipped with a flame ionization detector (GC/FID) and a HP-5MS (5% phenyl-methylpolysiloxane)

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[±]Presented in part as a poster at the 44th International Symposium on Essential Oils.

Table 1. Chemical composition of the essential oil from *Pseudobrickellia brasiliensis*.

Peak	Compound	LRI[a] calc.	LRI[b] lit.	%
1	α-thujene	925	924	0.4
2	α-pinene	932	932	2.6
3	β-pinene	976	974	0.5
4	myrcene	990	988	0.7
5	α-phellandrene	1004	1002	0.2
6	α-terpinene	1016	1014	7.8
7	p-cymene	1023	1020	2.4
8	limonene	1027	1024	1.4
9	1,8-cineole	1029	1026	3.2
10	γ-terpinene	1056	1054	19.5
11	terpinolene	1086	1086	3.2
12	(*Z*)-p-menth-2-en-1-ol	1123	1118	0.3
13	(*E*)-p-menth-2-en-1-ol	1143	1136	0.2
14	terpinen-4-ol	1176	1174	38.6
15	α-terpineol	1189	1186	4.5
16	α-gurjunene	1406	1409	0.2
17	(*E*)-β-caryophyllene	1416	1417	0.4
18	aromadendrene	1436	1439	0.8
19	n.i.	1440	–	0.2
20	*cis*-muurola-3,5-diene	1447	1448	0.1
21	α-humulene	1450	1452	0.1
22	*allo*-aromadendrene	1457	1458	0.1
23	dauca-5,8-diene	1470	1471	0.1
24	n.i.	1488	–	0.1
25	viridiflorene	1492	1496	0.9
26	α-muurolene	1497	1500	0.2
27	δ-cadinene	1520	1522	1.3
28	*trans*-cadina-1,4-diene	1529	1533	0.2
29	n.i.	1564	–	0.2
30	spathulenol	1574	1577	0.4
31	globulol	1581	1590	1.8
32	viridiflorol	1588	1592	1.3
33	cubeban-11-ol	1591	1595	0.7
34	rosifoliol	1599	1600	0.1
35	n.i.	1620	–	0.5
36	1-*epi*-cubenol	1625	1627	1.3
37	*epi*-α-cadinol	1639	1638	0.7
38	α-muurolol	1644	1644	0.5
	Total identified:	**96.7**		
	Monoterpenes:	38.7		
	Oxygenated monoterpenes:	46.8		
	Sesquiterpenes:	4.7		
	Oxygenated sesquiterpenes:	7.3		

Notes: (a) on a HP-5MS column; (b) references 10 and 11; n.i.: not identified.

fused silica capillary column (30 m × 0.25 mm × 0.25 μm). Hydrogen was used as carrier gas at a flow rate of 1.0 mL/minute. The oven temperature was programmed from 60 to 240°C at 3°C/minute. Injector temperature was kept at 250°C and detector temperature at 280°C. The percentage composition was obtained by normalization. Samples were injected in triplicate.

Analyses by GC/MS were performed on an Agilent 5973N mass selective detector coupled to an Agilent 6890 gas chromatograph fitted with a HP-5MS fused silica capillary column (30 m × 0.25 mm × 0.25 μm). Helium was used as carrier gas at 1.0 mL/minute. The mass detector was operated in electronic ionization mode (70 eV), at 3.15 scans/second, with mass range from 40 to 450 u. Transfer line was kept at 260°C, ion source at 230°C and analyzer at 150°C. Oven temperature program and injection procedure were the same as above.

The identification of the oil components was performed by comparison of their mass spectra with those from the Wiley Registry of Mass Spectral Data (7) or NIST databases (8), as well as their linear retention indices (LRI), calculated according to Van Den Dool and Kratz (9), after the injection of a homologous series of hydrocarbons (C_7-C_{26}) in the same conditions as above, and compared to literature data (10, 11). Authentic

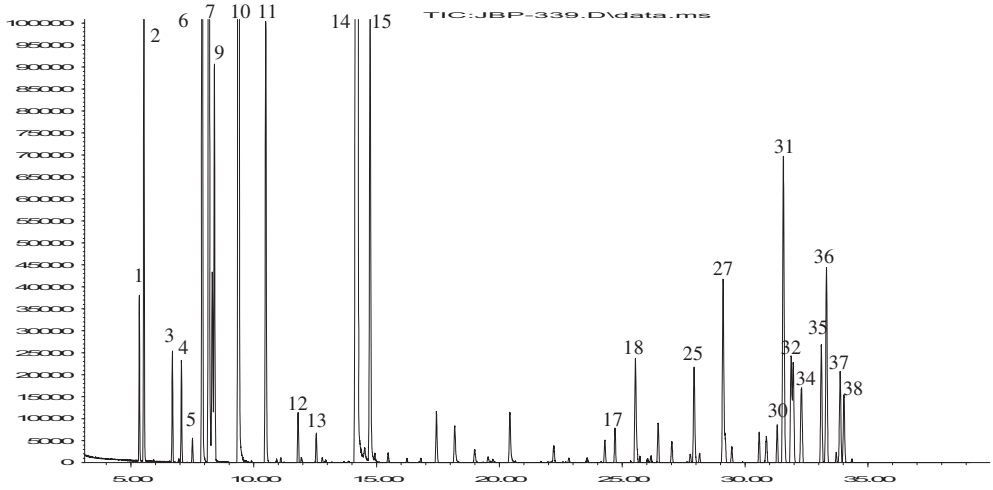

Figure 1. TIC of the essential oil from *Pseudobrickellia brasiliensis*.

standards (Aldrich Co.) of terpinen-4-ol, α-terpineol and γ-terpinene were injected for confirmation.

3. Results and discussions

The essential oil yield was 0.4% and thirty-four out of thirty-eight compounds were identified in the oil. Terpinen-4-ol (38.6%), γ-terpinene (19.5%), α-terpinene (7.8%) and α-terpineol (4.5%) were the major components (Table 1). A representative chromatogram is presented in Figure 1.

Only one previous investigation on the essential oil of the same species was found, as a Master of Science thesis (5). A very low oil yield, 0.02%, and a quite different chemical composition, with α-pinene (32.6%), α-thujene (17.9%), α-phellandrene (8.9%), β-pinene (7.6%) as major compounds were reported (5).

Although both materials came from the same geographical area, some differences between samples were observed: our material was collected in July (winter), during the beginning of bloom at an altitude of 568 m, while samples for ref. 5 were picked in April (fall) at 1348 m in vegetative stage. It is worth note to mention the two oils are rich in different cyclic monoterpenoids, but these compounds share a common precursor, the terpinyl cation (12). Therefore, the environment and phenological differences registered could explain the variation in oil yield and composition, but further investigation is needed in order to exclude other possible modulating factors.

Acknowledgements

The authors are grateful to CNPq, Faperj, Capes and Embrapa for financial support.

Disclosure statement

No potential conflict of interest was reported by the authors.

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