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Chemical composition of *Pourouma guianensis* Aublet essential oils

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ABSTRACT: The essential oils from leaves, stem barks and pistillate flowers of *Pourouma guianensis* Aublet (Moraceae) were isolated by hydrodistillation and the volatile constituents were determined by HRGC and HRGC–MS. Methyl salicylate was the major compound identified in all oils studied and was present in yields of 20.8% (leaves), 31.2% (stem bark) and 62.2% (pistillate flowers). Altogether, 50 constituents have been identified in the essential oil obtained from leaves, representing 76.6% of the total oil. Aliphatic C_6 alcohols and esters were, in number and in quantity, the principal constituents (29.5%). Oxygenated monoterpenes were found to be an important group of compounds and the most representative compound was linalol (2.4%). Thirty-eight components were identified in the essential oil from stem barks, representing 79.3% of the total oil. Among the monoterpenes identified, linalol was the principal compound (0.8%). The total content of fatty acids amounted to 40.0%. Analysis of the essential oil from pistillate flowers allowed the identification of 36 compounds, representing 88.5% of the oil. Ten oxygenated monoterpenes were identified, whereas linalol and its furan derivatives (9.7%), nerol (0.4%) and geraniol (1.3%) were the most abundant. Five aromatic derivatives were identified in the pistillate flower essential oil: methyl salicylate (62.2%), ethyl salicylate (0.1%), benzyl salicylate (0.2%), benzyl benzoate (0.3%) and benzaldehyde (0.1%).

KEY WORDS: *Pourouma guianensis* Aublet; Moraceae; essential oil; pistillate flower; stem bark; leaf; methyl salicylate; fatty acids

Introduction

Pourouma species are small to medium-sized trees occurring in the rain forest areas of South and Central America. *Pourouma guianensis* Aublet (Moraceae) is a dioic tree, ca. 30 m tall, which is found throughout the Amazon Basin, extending to eastern Colombia and to the Guiana region. In Brazil, *P. guianensis* Aublet also occurs in eastern region, from Pernambuco to Santa Catarina, where it is locally know as 'embaúba da mata', 'mapati', 'amapati', 'imbaubarana', 'itararanga' and 'tararanga branca'. The fruits of this species are edible and are appreciated among the natives. The fruit shape and the taste of the fleshy mesocarp strongly resembles that of grapes.[1] Unripe fruits of *P. guianensis* Aublet are used in traditional medicine to cure wounds and a stem bark infusion is used as a remedy for the treatment of dysentery.[1,2] The wood and other vegetative parts of *P. guianensis* Aublet emit a peculiar and strong odour, resembling spearmint and wintergreen.[1]

Up to now there has been no report concerning the chemical composition of *P. guianensis* Aublet. The present study deals with the investigation of the volatile components of leaves, stem barks and pistillate flowers of this species.

Experimental

Plant Material

Leaves, stem barks and pistillate flowers of *Pourouma guianensis* Aublet were collected from a specimen growing in Tropical Pluvial Forest, Mangaratiba District, Rio de Janeiro, in November 1995. A voucher sample (No. 6303) is deposited at Herbarium Alberto Castellanos (GUA).

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Table 1. Volatile components from leaves, stem barks and pistillate flowers of *Pourouma guianensis* Aublet

Peak no.	Compound	RI (HP-1)	Leaf	Flower	Stem bark	Methods	Reference
			Peak area (%)				
1	*n*-Hexanal	776	0.8	t	0.3	MS	5
2	(*E*)-Hex-2-enal	829	0.3	–	–	MS	6
3	(*Z*)-Hex-3-en-1-ol	842	12.4	0.2	–	MS	5
4	(*E*)-Hex-2-en-1-ol	849	14.5*	–	–	MS	5
5	*n*-Hexanol	855	–	0.1	–	MS	5
6	*n*-Heptanal	879	0.6	0.1	t	MS	5
7	(*Z*)-Hex-3-enyl formate	904	0.2	–	–	MS	5
8	Benzaldehyde	927	–	0.1	–	MS	6
9	Oct-1-en-3-ol	965	1.0	0.3	t	MS	5
10	*n*-Octanal	981	0.07	0.2	0.09	MS	5
11	Octan-3-ol	986	0.6	–	0.2	MS	7
12	(*Z*)-Hex-3-enyl acetate	989	0.1	–	0.2	MS	5
13	Hexyl acetate	1002	0.1	–	–	MS	5
14	*p*-Cymene	1005	0.2	t	t	MS, Co	9
15	1,8-Cineole	1008	0.3	0.2	0.2	MS, Co	5
16	Limonene	1012	0.4	0.2	0.2	MS, Co	9
17	(*E*)-β-Ocimene	1038	0.2	0.1	t	MS, Co	5
18	*cis*-Linalol oxide (furan isomer)	1055	0.3	0.5	0.09	MS	10
19	Fenchone	1058	0.6	–	0.2	MS	11
20	*trans*-Linalol oxide (furan isomer)	1073	0.5	0.8	0.09	MS	10
21	*n*-Nonanal	1082	1.9	2.6	1.3	MS, Co	5
22	Linalol	1084	2.4	8.4	0.8	MS, Co	6
23	Menthone	1125	0.4	0.2	0.3	MS	5
24	Isomenthone	1132	0.3	0.2	0.2	MS	9
25	Terpinen-4-ol	1160	0.2	0.2	0.2	MS	11
26	**Methyl salicylate**	**1172**	**20.8**	**62.2**	**31.2**	**MS, Co**	**5**
27	α-Terpineol	1174	0.4	–	–	MS, Co	11
28	(*Z*)-Hex-3-enyl butanoate	1176	0.3	–	–	MS	5
29	Hexyl butanoate	1182	0.5	–	–	MS	5
30	β-Cyclocitral	1187	0.1	0.07	0.2	MS	4
31	Nerol	1209	–	0.4	–	MS	11
32	(*E*)-Dec-2-enal	1232	–	–	0.3	MS	6
33	Geraniol	1234	–	1.3	–	MS	11
34	Ethyl salicylate	1240	0.4	0.09	0.6	MS	5
35	Hex-3-enyl 2-methylbutanoate	1254	1.4	–	–	MS	–
36	Safrole	1267	0.2	–	–	MS	12
37	(*E,E*)-Deca-2,4-dienal	1284	0.06	0.07	0.4	MS, Co	6
38	(*E*)-Undec-2-enal	1338	t	–	0.1	MS	6
39	α-Copaene	1365	0.3	0.09	0.3	MS, Co	8
40	Not identified	1370	–	0.6	–	–	–
41	α-Cedrene	1393	–	0.3	–	MS	5
42	α-Ionone	1399	0.7	–	–	MS	5
43	β-Caryophyllene	1401	–	t	0.06	MS, Co	13
44	α-Bergamotene	1422	0.1	–	0.2	MS	6
45	Not identified	1426	0.3	1.4	–	–	–
46	β-Ionone	1466	0.8	0.1	–	MS	5
47	α-Muurolene	1478	–	–	0.1	MS	13
48	Calamenene	1502	0.1	t	0.2	MS	13
49	δ-Cadinene	1506	0.09	–	0.1	MS	9
50	α-Calacorene	1519	0.08	t	0.2	MS	9
51	(*E*)-Nerolidol	1549	0.5	0.1	–	MS, Co	4
52	Not identified	1630	–	2.3	–	–	–
53	Cadalene	1641	0.4	–	0.5	MS	4
54	Benzyl benzoate	1742	–	0.3	–	MS	5
55	Tetradecanoic acid	1751	0.6	–	1.9	MS	10
56	Benzyl salicylate	1840	–	0.2	–	MS	10
57	Pentadecanoic acid	1848	0.3	–	0.9	MS	–
58	**Hexadecanoic acid**	**1946**	**6.3**	**5.8**	**20.6**	**MS**	**10**
59	Heptadecanoic acid	2047	0.1	–	0.8	MS	–
60	Phytol	2091	2.4	0.4	0.7	MS	13
61	**(*Z,Z*)-Octadeca-9, 12-dienoic acid**	**2107**	**0.8**	**2.7**	**14.9**	**MS**	**–**
62	Octadecanoic acid	2152	0.5	–	0.9	MS	–
	Total		76.6	88.5	79.3		

* (*E*)-hex-2-en-1-ol plus *n*-hexanol.
RI = Retention index on non-polar HP-1 column.
MS = Identification based on the mass spectrum.
Co = Identity confirmed by co-chromatography with authentic sample.
t = trace, <0.05%.

Isolation of Volatile Compounds

Leaves (2.0 kg), stem barks (958 g) and pistillate flowers (293 g) were comminuted and submitted to hydrodistillation for 6 h using a Clevenger-type apparatus.[3] The oils were obtained from the aqueous phase by extraction with dichloromethane (spectroscopic grade), dried over anhydrous sodium sulphate and stored at 5°C.

Identification of Oil Components

Capillary GC was carried out using a Hewlett-Packard 5890 Series II Chromatograph under the following conditions: hydrogen was used as carrier gas at 1 ml/min; split ratio, 100/1 and flame ionization detector; HP-1 fused-silica column (25 m × 0.32 mm, film thickness 0.17 μm); oven temperature was programmed from 40°C (5 min) to 260°C at 3°C/min; injector port temperature, 280°C; detector temperature, 300°C. Peak areas were computed by a Hewlett-Packard integrator.

GC–MS analyses were carried out on a Hewlett-Packard capillary GC-quadruple MS system (Model 5995C), using the same gas chromatographic parameters as above with helium as carrier gas at 1 ml/min; ionization voltage, 70 eV; ion source temperature, 180°C.

Identification of the oil components was obtained by comparison of retention indices (RIs)[4–13] and, whenever possible, by co-injection with an authentic sample. Comparison and interpretation of fragmentation patterns in mass spectra with those stored in the NIST computer database and published in reference books[5, 14] were also applied for the identification of the compounds.

Results and Discussion

The yields of the oils obtained from leaves, stem barks and pistillate flowers of *Pourouma guianensis* Aublet were low and amounted to 0.001%, 0.010% and 0.040% on dry basis, respectively. Methyl salicylate was the major compound identified in the three oils and it was present in percentages of 20.8%, 31.2% and 62.2%, respectively. The volatile compounds of *P. guianensis*, their percentages and RIs are shown in Table 1. Fifty compounds were identified in the leaf essential oil, representing 76.6% of the total oil. Aliphatic C_6 alcohols and esters comprised 29.5% of this oil. Among them, (*Z*)-hex-3-en-1-ol (12.4%) and *n*-hexanol plus (*E*)-hex-2-en-1-ol (14.5%) were the main components. The mixture of *n*-hexanol and (*E*)-hex-2-en-1-ol was resolved on a FFAP phase and *n*-hexanol was the predominant compound (9.2%). Aliphatic aldehydes C_6–C_{11} comprised 3.7% of the total oil. Oxygenated monoterpenes were found to be an important group of constituents and linalol (2.4%) was the principal component. Six sesquiterpene hydrocarbons (1.1%) were identified, of which α-copaene (0.3%) and cadalene (0.4%) occurred in higher quantities. One sesquiterpene alcohol was identified as (*E*)-nerolidol (0.5%) and two norterpenes (1.5%) as α-ionone and β-ionone. Safrole was obtained in low yield (0.2%). Fatty acids C_{14}–C_{18} were present in the leaf essential oil at a percentage of 8.6%.

Thirty-eight constituents were identified in the stem bark essential oil, representing 79.3% of the total oil. C_6 alcohols and esters were not found in this material; however, aliphatic aldehydes C_6–C_{11} accounted for 2.5%, where *n*-nonanal (1.3%) predominated. Nine oxygenated monoterpenes were found and linalol (0.8%) was the principal compound within this group. Among the sesquiterpenes, eight compounds were identified: α-copaene (0.3%), β-caryophyllene (0.1%), α-bergamotene (0.2%), α-muurolene (0.1%), calamenene (0.2%), δ-cadinene (0.1%), α-calacorene (0.2%) and cadalene (0.5%). Fatty acids C_{14}–C_{18} accounted for 40.0% of the stem bark oil.

Analysis of the flower essential oil led to the identification of 36 components, representing 88.5% of the oil. Oxygenated monoterpenes were also a significant group of compounds present in this essential oil. Ten oxygenated monoterpenes (12.2%) were identified, linalol and its furan derivatives (9.7%), nerol (0.4%) and geraniol (1.3%) being the most representative. Aromatic derivatives comprised 62.9% of the total oil and were represented by methyl salicylate (62.2%), ethyl salicylate (0.1%), benzyl salicylate (0.2%), benzyl benzoate (0.3%) and benzaldehyde (0.1%). One sesquiterpene alcohol was identified as (*E*)-nerolidol (0.1%) and the three major sesquiterpenes remained unidentified. Five sesquiterpene hydrocarbons were identified as α-copaene (0.1%), α-cedrene (0.3%), β-caryophyllene (trace), calamenene (trace) and calacorene (trace).

The similarity of *Pourouma guianensis* odour to spearmint and winter-green odours may be due to the presence of low amounts of menthone and isomenthone and the high quantity of methyl salicylate.

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