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Chemical Composition of the Essential Oils of *Cymbopogon citratus* (DC.) Stapf Cultivated in North of Brazil

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Abstract: The essential oils obtained from blades, sheaths and rhizomes of *Cymbopogon citratus* were obtained by hydrodistillation and analyzed by GC-FID and GC-MS. The essential oils from aerial parts (blades and sheaths) from three other specimens also were studied. Neral and geranial were major in blades (30.1 % and 39.9 %, respectively), and sheats (27.8 % and 50.0 %, respectively). Rhizome oils showed a different chemical profile and was characterized by a high amount of selina-6-en-4-ol (27.8 %), followed by α-cadinol (8.2 %), neointermediol (7.2 %) and eudesma-7(11)-en-4-ol (5.3 %).

Key Words: Cymbopogon citratus, neral, geranial, selina-6-en-4-ol, α-cadinol, neointermediol, eudesma-7(11)-en-4-ol, essential oil composition.

Introduction: *Cymbopogon citratus* (DC.) Stapf [Syn.: *Andropogon ceriferus* Hack., *A. citratus* DC. ex Nees, *A. citratus* DC., *A. citriodorum* Hort. ex Desf., *A. nardus* subsp. *ceriferus* (Hack.) Hack., *A. roxburghii* Nees ex Steud., *A.schoenanthus* L., *Cymbopogon nardus* subvar. *citratus* (DC.) Roberty], belonging the family Poaceae, probably originated in India [1]. It is now widespread in the tropics and in Brazil is frequently cultivated in gardens and along pathsides. This plant has been studied extensively because of the importance of its oil for the numerous varieties of industrial application. Most oils contained 40-90 % of citral [2-4], except for plants grown in Ethiopia (13 %) [5]. Two chemotypes of *C. citratus* have been found in Congo: a citral-type and a geraniol-type [6]. The majority studies were made using the aerial parts of the *C. citratus*. However, Li *et al*.[7], when studied the allelopathic effects of the volatiles of *C. citratus* reported the occurrence of selina-6-en-4-ol (20.0 %) and longifolene (56.7 %) in their rhizomes. In Brazil *C. citratus* were known

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as “capim-limão” and “capim-santo” and has been used against many diseases [8-10]. Although the chemical composition of the essential oils from plant material of *C. citratus* from many countries are well documented, little effort has been spent on investigation of the chemical composition from these species cultivated in North of Brazil. We therefore, report the chemical composition of the volatile oils of *C. citratus* cultivated in States of Pará, Brazil.

Material and Methods

Plant Material: The samples of *C. citratus* were collected from cultivated plants in the open market called Ver-o-Peso, in the city of Belém (Sample A), in the campus of Museu Paraense Emílio Goeldi (Sample B), and in the campus of Universidade Federal Rural da Amazônia (Samples C and D). A voucher specimen (MG 167,632) has been deposited in the Herbarium of MPEG.

Oil distillation: The samples were dried in a room under air-conditioned for 7 days, grounded and hydrodistilled (3h) using a Clevenger-type apparatus. The oils obtained were dried over anhydrous sodium sulphate, and immediately submitted to GC-FID and GC-MS analysis. The total oil yields were expressed as mL/100g of the dried material.

GC-MS: The oils were analyzed by EI on a Hewlett Packard-6890 system equipped with a HP-5MS fused capillary column (30 m x 0.25 mm; 0.25 µm film thickness), directly coupled to a selective mass detector Hewllet Packard-5973. Helium (1mL/min.) was used as carrier gas; oven temperature program: 60°C-300°C at 3°C/min; splitless during 1.50 min; sample volume 2 µL of the oil solution in CH_2Cl_2 (2:1000). Injector and detector temperature was 240°C. EIMS: electron energy, 70 eV; ion source temperature and connection parts: 180°C. Identifications were made by matching of their mass spectra and retention times with those recorded in the MS library and by comparison of retention indices and mass spectra with literature data [11]. GC-FID were performed on a HP5890-II instrument, equipped with a DB-5MS (30 m x 0.25 mm; 0.25 µm film thickness) fused silica capillary column. Hydrogen was used as carrier gas adjusted to a linear velocity of 32 cm/s (measured at 100°C). Split flow was adjusted to give a 20:1 ratio and septum sweep was a constant 10 mL/min. The oven was programmed as follows: 60°C-240°C at 3°C/min. The samples were injected using the splitless technique: 2 µL of the oil solution in hexane (2:1000). Injector and detector temperature was 250°C. The GC was equipped with FID and connected with an electronic integrator HP 5896 Series II. The percentage composition of the oil samples were computed from the GC peak areas without using correction for response factors.

Results and Discussion: Table 1 contains the chemical composition and yield oils of the different samples of *C. citratus*. The oil content varied greatly according the parts of the plant: the maximum oil yield was obtained from the rhizome (2.7 %) and blades (1.9 %). Minimum oil was obtained from sheaths (0.9 %). Aerial parts furnish oils between 1.1 % and 1.3 %. The compositions found for each of the different parts of the plant revealed that blades and sheaths showed similar chemical profile, with a high amount of neral (blades: 30.1 %, sheath: 27.8 %), than compared with rhizomes (5.0 %). In the same way geranial was major in blades (39.9 %), and in sheaths (50.0 %), when compared with rhizomes (9.6 %). The major compound identified in the rhizome oils was selina-6-en-4-ol (27.8 %). Essential oils from aerial parts and blades had similar chemical profile: rich in myrcene and citral. The oil from aerial parts *C. citratus* cultivated in the city of Manaus, State of Amazonas, also contains neral (30.8 %) and geranial (53.9 %) as major components (M. da Paz, data not published). Myrcene was major in blades (17.8 %) than compared to those of sheaths (5.8 %). Comparison of our results with the data obtained by Li *et al*. reveals that the oils from rhizomes studied showed similar amount of selina-6-en-4-ol. However we could not detect the presence of longifolene. This is the first report on the rhizome oils from *C. citratus* cultivated in the North of Brazil.

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Table 1. Volatiles (%) identified in the oils of *Cymbopogon citratus*

		Yield oil (%)					
		A	B	C		D	
Components	RI		aerial part		blade	sheath	rhizome
		1.2	1.3	1.1	1.9	0.9	2.7
α-Thujene	917	0.3	-	-	-	0.1	0.2
α-Pinene	929	0.3	0.1	-	-	0.1	0.5
6-Methyl-5-hepten-2-one	986	1.2	1.3	0.7	0.4	0.2	0.1
Myrcene	990	14.2	10.7	13.1	18.2	6.0	1.0
Limonene	1030	0.3	0.2	0.4	0.4	1.1	0.1
(Z)-β-Ocimene	1038	0.3	-	-	0.4	0.5	0.9
(E)-β-Ocimene	1046	0.1	0.1	0.3	0.3	0.5	0.3
6,7-Epoxy-myrcene	1092	0.2	-	0.2	0.2	0.1	tr
Linalool	1097	1.1	1.0	0.9	1.4	1.0	0.4
Citronellal	1151	0.2	0.2	0.1	0.3	0.1	0.1
β-Pinene oxide	1163	1.7	1.1	1.7	1.4	1.0	0.1
α-Terpineol	1181	0.2	0.2	-	0.1	0.1	0.2
M = 152	1183	2.3	1.6	2.3	1.8	1.4	0.3
Citronellol	1232	0.1	0.1	0.3	0.2	0.6	0.1
Neral	1244	31.5	31.5	32,1	30.1	27.8	5.0
Geraniol	1258	3.3	3.1	3.1	2.4	2.4	0.4
Geranial	1275	39.9	40.2	41.3	39.9	50.0	9.6
Undecan-2-one	1294	-	0.1	0.1	0.1	0.1	-
Geranyl methyl	1324	0.2	0.3	0.3	0.1	tr	-
Geranyl formate	1298	-	-	-	-	0.1	0.1
Geranyl acetate	1383	0.4	0.6	0.6	0.4	0.1	tr
β-Caryophyllene	1419	0.2	0.2	0.2	0.2	0.1	1.7
trans-α-Bergamotene	1438	0.1	0.1	0.1	0.1	tr	0.7
α-Humulene	1449	-	-	-	0.1	tr	0.5
Germacrene D	1482	0.1	0.1	0.1	-	0.1	1.3
α-Muurolene	1497	0.1	0.2	-	0.2	0.1	0.8
δ-Cadinene	1521	0.2	-	0.2	0.2	0.4	2.0
Caryophyllene oxide	1578	-	-	0.1	-	0.5	0.6
Selina-6-en-4-ol	1615	0.1	0.1	0.2	0.1	2.9	27.8
epi-α-Muurolol	1642	-	-	-	-	0.1	1.0

table 1. (continued).

Components	RI	Yield oil (%) A 1.2	B aerial part 1.3	C 1.1	D blade 1.9	D sheath 0.9	D rhizome 2.7
α-Muurolol	1646	-	-	-	-	0.5	5.0
α-Cadinol	1652	0.4	-	0.1	-	0.9	8.2
Neointermediol	1658	-	tr	0.1	-	0.7	7.2
Eudesm-7(11)-en-4-ol	1692	-	tr	0.1	tr	0.5	5.3
Opoplanone	1735	-	-	-	-	0.1	0.2

*Retention indices on DB-5MS
A = Ver-o-Peso open market
B = campus of MPEG
C = campus of UFRA
RI = 1183, m/z (rel. int.): 152[M^+](4), 137(8), 119(16), 109(64), 94(56), 81(97), 77(27), 67(76), 55(44), 41(100).