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Volatile Components of Oiti Fruit (*Licania tomentosa* Benth.)

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Abstract: The fresh fruits from *Licania tomentosa* Benth. (Chrysobalanaceae), were submitted to hydrodistillation in a modified Clevenger-type apparatus. Analysis of volatile oil were performed by GC and GC-MS. Comparison of results with literature data allowed the chemical characterization of 83% of compounds of mixture. Thirteen compounds were identified, three monoterpenes, five aliphatic esters, two alcohols, two ketones and one aldehyde. The alcohols were the major compounds (35.6%), but the esters showed great diversity.

Keywords: *Licania tomentosa; Chrysobalanaceae;* Oiti; hexanol.

1. Plant Source

The Chrysobalanaceae family encompasses 17 genera and about 450 species represented by trees and shrubs growing in tropical and subtropical lowlands [1]. The dispersal of plants this family is in the Amazon, where 120 representatives occurs [2]. Some of Chrysobalanaceae species have been used in the tropics as fruit trees and many of them are used popularly as medicine in several countries, mainly for the treatment of dysentery, diarrhea, and leucorrhea [3, 4]. In Brazil species of *Licania*, are known popularly as Oiti and the oil extracted from its seeds is used as a substitute for "tung" oil. *Licania tomentosa* Benth. is widely used in the ornamentation of Brazilian cities [5].

The fruits of *L. tomentosa* Benth. (Chrysobalanaceae) were collected in Rio de Janeiro State, Brazil and identified by the botanist Dr. Rosa Fuks from the Rio de Janeiro Botanical Garden. A

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voucher specimen has been deposited in the Museu Nacional Herbarium, Universidade Federal do Rio de Janeiro, UFRJ, under number R195.941.

2. Previous Studies

The chemical constituents or pharmacological action of *Licania tomentosa* has been poorly investigated. From the extracts of its leaves and fruits the following compounds were isolated: betulinic acid; oleanolic acid, tormentic acid, ursolic acid, lupeol, licanolide, a new triterpene lactone, palmitoleic and hexadecanoic acid; stigmasterol and sitosterol [6, 7]. The crude extract of the seeds of *L. tomentosa* was reported to possess inhibitory activity against acyclovir-resistant herpes simplex virus type 1 (ACVr-HSV1) [8]. The triterpenes isolated from a methanolic extract of leaves from *L. tomentosa* was reported to possess cytotoxicity activity on multidrug resistant and sensitive leukemia cell lines [9]. The aim of this paper was to determine the composition of the volatile oil from fresh fruits of *L. tomentosa.* To the best of our knowledge, no previous studies have been reported on the composition of the volatile oil of this plant.

3. Present Study

The fresh fruits (500 g) from *L. tomentosa* were submitted to hydrodistillation for two hours in a modified Clevenger-type apparatus. The oil was extracted from distilled water with dichloromethane, dried over anhydrous sodium sulfate and stored at -18 ^{o}C until analysis in sealed vials [10].

GC analysis was performed using a Varian Star 3400 CX gas chromatograph, fused silica capillary column (DB-5, 30 m x 0.20 mm), flame-ionization detector (FID), hydrogen as carrier gas at a flow rate 1 mL/min in the split mode 1:50, with an injection volume of 0.2 μL and temperature programming from 60-240 ^{o}C (3 ^{o}C/min), injector and detector at 250 ^{o}C. Retention times (RT) were measured in minutes and the relative amount in percent values of each compound in the mixture was obtained directly from the GC data. GC/MS analysis was performed using a HP5890 SII gas chromatograph coupled to a VG Autospec mass spectrometer at 70 eV, fused silica capillary column (DB-1, 30 m x 0.20 mm), helium as carrier gas at a flow rate of 1 mL/min, injector heater 250 ^{o}C and temperature programming from 60-240 ^{o}C (3 ^{o}C/min). Scanning speed was 1.0 scan/s from *m/z* 40 to 300. Retention indices (RI) were calculated using GC data of a saturated aliphatic hydrocarbon homologous series within C8 to C22, performed in the same column and conditions as used in the GC analysis for the volatile oil.

Identification of the substances was carried out primarily by comparing the mass spectra with a computer databank (National Institute for Standard Technology–NIST–62,235 compounds). Further visual comparison of the mass spectra with literature records and comparison of the RI permitted identification of the major compounds [11, 12].

The qualitative and quantitative composition of the volatile oil from *Licania tomentosa* is presented in Table 1. The thirteen compounds identified are listed in order of their elution on apolar (DB-5) column. GC/MS analyses and comparison of their MS and RI values with those in the literature permitted records allowed the identification of 83% of the oil. Components were categorized in monoterpenes, alcohols, carbonyls (aldehyde and ketone), and aliphatic esters. The oil was characterized by a high percentage of alcohols (35.6%), aldehyde (16.7%), aliphatic esters (12.0%), monoterpenes (3.9%) and ketone (22.4%). The main constituents in *L. tomentosa* were hexanol (33.5%), followed by 3-hexanone-2-ol (21.0%) and hexanal (16.7%). The three monoterpenes identified are: myrcene (2.1%), terpinen-4-ol (1.0%) and α-terpineol (0.8%), one aliphatic and two oxygenated. The aliphatic alcohols are the major compounds, but the esters showed great diversity: ethyl butyrate, butyl butyrate, amyl butyrate, hexyl butyrate and vinyl butyrate.

Some fruits volatile oils, apple and cashew, are rich in aliphatic esters, alcohols and ketones. The main volatile compounds in apple are esters 2-methyl buthyl acetate, buthyl acetate, hexyl acetate and ∝-farnesen (71%) [13]. Analysis of alcoholic fermentation of cashew apple juice revealed that the esters methyl 3-methyl butyrate, ethyl 3-methyl butyrate, methyl butyrate, ethyl butyrate, trans-ethyl crotonate and methyl 3-methyl pentanoate were important to the cashew-like aroma of the beverage [14]. The esters are formed mainly at the stage of ripening of fruit, from the bark and they are important for the sweet and fruity aroma [15].

Table 1. Volatile oil composition of fruits *Licania tomentosa* Benth. from GC-MS anlaysis.

RI	Compounds	%
804	Hexanal	16.7
805	Ethyl butyrate	2.1
835	3-Hexene-1-ol	2.1
844	Hexanol	33.5
856	3-Hexanone-2-ol	21.0
913	Cyclopentyl ethanone	1.4
950	Butyl butyrate	6.4
956	Myrcene	2.1
1024	Amyl butyrate	2.2
1168	Terpinen-4-ol	1.0
1186	α-Terpineol	0.8
1195	Hexyl butyrate	1.0
1250	Vinyl butyrate	2.3
	Total	**92.6**

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