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## Leaf and Bark Essential Oil Compositions of *Bursera simaruba* from Monteverde, Costa Rica

**William N. Setzer****Abstract**

The leaf and bark essential oils of *Bursera simaruba* (L.) Sarg. from Monteverde, Costa Rica were obtained by hydrodistillation and analyzed by gas chromatography – mass spectrometry. The leaf oil was dominated by the monoterpene *o*-cymene (65.2%), while the bark oil had  $\alpha$ -phellandrene (29.1%), (*E*)-caryophyllene (19.3%), *o*-cymene (13.1%), and  $\alpha$ -thujene (11.9%) as major components. The essential oil compositions of *B. simaruba* from Monteverde, Costa Rica, were markedly different from those previously reported from Jamaica or Guadeloupe.

**Keywords:** Essential oil composition, *o*-cymene,  $\alpha$ -phellandrene, (*E*)-caryophyllene,  $\alpha$ -thujene.

**1. Introduction**

*Bursera simaruba* (L.) Sarg. ranges from south Florida, the Florida Keys and the Bahamas, throughout the West Indies, and Central America from southern Mexico to Colombia, from sea level to 1800 m<sup>[1, 2]</sup>. The bark, gum, and leaves of this tree are used as traditional medicines throughout its range<sup>[1, 3]</sup>. For example, the plant is used in Belize to treat wounds, insect bites, and skin sores<sup>[4]</sup>, leaves are used as a bath by the Yucatec Maya to treat fever<sup>[5]</sup>, a leaf decoction is taken in Cuba as a carminative<sup>[6]</sup>, and the leaf decoction is used in the Bahamas to treat poisonwood (*Metopium toxiferum*) dermatitis<sup>[7]</sup>. The tree is commonly used as living fence posts in Costa Rica<sup>[8]</sup>.

**2. Materials and Methods****2.1 Plant Materials**

Leaves and bark of *B. simaruba* were collected from several living fence posts in the Monteverde region of northwestern Costa Rica (10° 16' 26" N, 84° 50' 24" W) on 14 May, 2009. The plant was identified by William A. Haber, and a voucher specimen has been deposited in the herbarium of the Missouri Botanical Garden (Haber 9988). The fresh leaves (175.6 g) were chopped and hydrodistilled using a Likens-Nickerson apparatus with continuous extraction with chloroform for 4 h to give a pale yellow essential oil (216.0 mg). The bark (410.8 g) was chopped and hydrodistilled as above to give a colorless essential oil (55.5 mg). The essential oils were stored at -5 °C until analyzed.

**2.2 Gas Chromatography – Mass Spectrometry**

The essential oils of *B. simaruba* were subjected to gas chromatographic-mass spectral analysis using an Agilent 6890 GC with Agilent 5973 mass selective detector, fused silica capillary column (HP 5 ms, 30 m × 0.25 mm), helium carrier gas, 1 mL/min flow rate; injection temperature 200 °C, oven temperature program: 40 °C initial temperature, hold for 10 min; increased at 3 °C/min to 200 °C; increased 2°/min to 220 °C, and interface temp 280 °C; EIMS, electron energy, 70 eV. The sample was dissolved in CHCl<sub>3</sub> to give a 1% w/v solution; 1- $\mu$ L injections using a splitless injection technique were used. Identification of oil components was achieved based on their retention indices (determined with reference to a homologous series of normal alkanes), and by comparison of their mass spectral fragmentation patterns with those reported in the literature<sup>[9]</sup> and stored on the MS library [NIST database (G1036A, revision D.01.00)/ChemStation data system (G1701CA, version C.00.01.08)].

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### 3. Results and Discussion

A total of 39 compounds were identified in the leaf and bark essential oils of *Bursera simaruba* from Monteverde, Costa Rica, accounting for 100% of the compositions (Table 1). The leaf oil of *B. simaruba* was dominated by *o*-cymene (65.2%), while the bark oil had  $\alpha$ -phellandrene (29.1%), (*E*)-caryophyllene (19.3%), *o*-cymene (13.1%), and  $\alpha$ -thujene (11.9%) as the major components. Two previous studies on the leaf essential oils of *B. simaruba* reveal very different compositions. The leaf oil of *B. simaruba* from Jamaica was rich in sesquiterpenes [*trans*-cadinane-1(6),4-diene (9.7%) (*E*)-caryophyllene (9.0%),  $\alpha$ -humulene (6.2%),  $\beta$ -elemene (5.6%)  $\alpha$ -cadinol (4.7%),  $\alpha$ -selin-11-en-4-ol (4.2%), caryophyllene oxide (3.2%) and  $\delta$ -selinene (3.1%)], along with monoterpene hydrocarbons [ $\alpha$ -pinene (10.2%), myrcene (5.2%) and  $\beta$ -pinene (3.4%)]<sup>[10]</sup>, while the leaf oil from Guadeloupe was rich in limonene (46.7%), (*E*)-caryophyllene (14.7%),  $\alpha$ -humulene

(13.3%), and germacrene D (7.6%)<sup>[11]</sup>. Noge and Becerra<sup>[12]</sup> had found germacrene D to be a dominant sesquiterpene in several *Bursera* leaf oils and it did make up 5.3% of the composition of *B. simaruba* leaf oil from Monteverde.

In marked contrast to the bark essential oil of *B. simaruba* from Monteverde, Costa Rica, the bark oil from Jamaica was dominated by the monoterpenes  $\alpha$ -pinene (32.1%),  $\beta$ -pinene (13.5%) and isolimonene (5.6%) while the major sesquiterpenes were viridiflorol (7.1%),  $\beta$ -caryophyllene (4.9%),  $\beta$ -selinene (4.3%),  $\alpha$ -humulene (3.1%) and caryophyllene oxide (3.1%)<sup>[10]</sup>. Thus, the volatiles from *B. simaruba* show very different chemical compositions depending on geographical location. It would be interesting to compare additional essential oil compositions from other Caribbean and Central American locations for this popular medicinal plant.

**Table 1:** The leaf and bark essential oil compositions of *Bursera simaruba* from Monteverde, Costa Rica.

RI	Compound	Percent Composition	
		Leaf	Bark
692	1-Penten-3-ol	0.4	---
700	2-Ethylfuran	0.3	---
799	Hexanal	0.3	---
857	( <i>E</i> )-2-Hexenal	1.9	---
859	( <i>Z</i> )-3-Hexenol	3.3	---
864	( <i>E</i> )-2-Hexenol	0.4	---
865	<i>n</i> -Hexanol	0.3	---
933	$\alpha$ -Thujene	0.2	<b>11.9</b>
942	$\alpha$ -Pinene	3.7	4.5
954	3,5-Dimethylene-1,4,4-trimethylcyclopentene	---	7.0
969	Sabinene	tr	1.4
977	$\beta$ -Pinene	0.6	0.5
992	Myrcene	0.4	---
1003	$\alpha$ -Phellandrene	6.3	<b>29.1</b>
1020	$\alpha$ -Terpinene	---	3.7
1024	<i>p</i> -Cymene	1.2	1.7
1027	<i>o</i> -Cymene	<b>65.2</b>	<b>13.1</b>
1035	$\beta$ -Phellandrene	2.8	2.6
1038	( <i>Z</i> )- $\beta$ -Ocimene	tr	tr
1047	( <i>E</i> )- $\beta$ -Ocimene	0.1	0.2
1058	$\gamma$ -Terpinene	1.6	3.4
1238	( <i>Z</i> )-Ocimenone	---	tr
1278	Cumin aldehyde	---	tr
1337	$\delta$ -Elemene	tr	---
1392	$\beta$ -Elemene	0.5	---
1421	( <i>E</i> )-Caryophyllene	3.9	<b>19.3</b>
1433	$\gamma$ -Elemene	0.1	---
1453	$\alpha$ -Humulene	tr	0.4
1483	Germacrene D	5.3	0.4
1505	$\alpha$ -Muurolene	---	tr
1505	( <i>E,E</i> )- $\alpha$ -Farnesene	0.1	---
1509	Cuparene	---	tr
1523	$\delta$ -Cadinene	0.1	tr
1560	Germacrene B	1.2	tr
1566	( <i>E</i> )-Nerolidol	---	tr
1582	Caryophyllene oxide	---	0.7
1597	Humulene epoxide II	---	tr
1645	Caryophylla-4(12),8(13)-dien-5 $\beta$ -ol	---	tr
1966	(3 <i>Z</i> )-Cembrene A	---	tr

#### 4. Conclusions

The leaf and bark essential oil compositions of *Bursera simaruba* from Monteverde, Costa Rica, are markedly different from samples from either Jamaica or from Guadeloupe. The different chemical compositions may be important in considering the traditional uses of this medicinal plant.

#### 5. Acknowledgments

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