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Composition of the Floral Essential Oil of *Brugmansia suaveolens*

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Abstract: The floral essential oils of *Brugmansia suaveolens*, from Monteverde, Costa Rica, were collected at three different times of the day by hydrodistillation and the oils analyzed by gas chromatography-mass spectrometry (GC-MS). The floral essential oil showed a dramatic change in composition between the freshly opened night (white) blossoms and the rose-colored senescent blossoms the following day. The white blossoms were dominated by 1,8-cineole (72.1%), (*E*)-nerolidol (11.7%), α-terpineol (5.3%), and phenethyl alcohol (3.2%), notably different from headspace analyses of *B. suaveolens* reported previously. The floral essential oil from "rose-colored" senescent blossoms of *B. suaveolens* showed dramatic decreases in 1,8-cineole (2.0%), (*E*)-nerolidol (1.9%), and phenethyl alcohol (not detected), with concomitant increases in heptanal (10.2%), nonanal (17.4%), terpinen-4-ol (10.5%), and megastigmatrienones (35.5%).

Keywords: *Brugmansia suaveolens*; essential oil composition; temporal variation; 1,8-cineole; nerolidol; heptanal; nonanal; megastigmatrienone

1. Introduction

Brugmansia suaveolens (Humb. & Bonpl. ex Willd.) Bercht. & C. Presl ("reina de la noche"), Solanaceae, is a small tree, often 3 m tall. The leaves are generally oval in shape and average 20 cm long. The large pendulous flowers are pale yellow before opening, open at night to reveal white flaring corollas that are sweetly fragrant [1]. The following day the flowers turn a rose color (see Figure 1). This plant occurs naturally in South America (eastern slopes of the Andes and western Amazonia) [2]. In Costa Rica it is grown as an ornamental and has escaped cultivation. *B. suaveolens* is known to be toxic and hallucinogenic [3]. In this work we have collected and determined the chemical

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compositions of the night-blooming "white" and day-after "rose" floral essential oils of *B. suaveolens* growing in Monteverde, Costa Rica.

"yellow" before opening "white" night-opened "rose" following day

Figure 1. *Brugmansia suaveolens* temporal floral color variation.

2. Materials and Methods

2.1. Plant Material

Flowers of *B. suaveolens* were collected from lower montane moist forest at ca. 1350 m above sea level at Monteverde, Costa Rica (10°18'N, 84°28'W). The plant was identified by W. Zuchowski. A voucher specimen has been deposited with the Missouri Botanical Garden (Pennys 264). Fresh white flowers (73.5 g) were collected at night, 21:00, on 12 May, 2008, and were hydrodistilled using a Likens-Nickerson apparatus with continuous extraction of the distillate with chloroform to give a clear colorless floral essential oil (9.2 mg; 0.013% yield). The floral essential oil of the rose-colored flowers (84.4 g), collected in the daytime, 16:00, on 13 May, 2008, yielded 2.3 mg (0.0027% yield) essential oil. Attempts to obtain the floral essential oil from the yellow pre-opened flowers resulted in no essential oil yield.

2.2 Gas Chromatography-Mass Spectrometry

The floral essential oils of *B. suaveolens* were subjected to gas chromatographic-mass spectral analysis using an Agilent 6890 GC with Agilent 5973 mass selective detector, fused silica capillary column (HP 5ms, 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. Each sample was dissolved in $CHCl_3$ to give a 1% w/v solution; 1-μL 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 [4] and stored on the MS library [NIST database (G1036A, revision D.01.00)/ChemStation data system (G1701CA, version C.00.01.08)]. The chemical compositions of *B. suaveolens* floral essential oils are summarized in Table 1.

Table 1. Chemical compositions of the floral essential oil of *Brugmansia suaveolens*.

RI	Compound	Percent Composition	
		"white"	"rose"
900	Heptanal	0.1	10.2
997	Octanal	---	1.0
1031	1,8-Cineole	72.1	2.0
1045	Phenylacetaldehyde	0.9	---
1050	(*E*)-β-Ocimene	2.6	4.2
1059	γ-Terpinene	1.1	1.6
1099	Linalool	---	0.4
1106	Nonanal	1.8	17.4
1116	Phenethyl alcohol	3.2	---
1178	Terpinen-4-ol	1.3	10.5
1182	2-Isobutyl-3-methoxypyrazine	---	0.5
1193	α-Terpineol	5.3	1.1
1283	unidentified	---	1.7
1288	Theaspirane A	t	1.4
1302	Theaspirane B	t	1.1
1560	Megastigmatrienone I	---	1.7
1565	(*E*)-Nerolidol	11.7	1.9
1579	Megastigmatrienone II	---	24.5
1610	Megastigmatrienone III	---	0.8
1624	Megastigmatrienone IV	t	8.5
2500	Pentacosane	t	1.5
2700	Heptacosane	t	6.4
2900	Nonacosane	t	1.1
3100	Hentriacontane	t	0.4

3. Results and Discussion

The chemical composition of the floral essential oil of *B. suaveolens* changed remarkably from the freshly opened "white, night" form to the day-following "rose" form. The freshly-opened blossoms were dominated by 1,8-cineole (72.1%), (*E*)-nerolidol (11.7%), and α-terpineol (5.3%). After blooming for about 19 hours, the concentration of 1,8-cineole and (*E*)-nerolidol dropped dramatically while megastigmatrienones (total of 35.5%), aliphatic aldehydes (total = 28.6%), and *n*-alkanes (total = 9.4%) increased.

The theaspiranes and megastigmatrienones are C_{13} nor-isoprenoids derived from carotenoids [5,6] and are notable components of tobacco [7-11] and other members of the Solanaceae [12,13]. Theaspiranes have also been found in relatively abundant quantities in the essential oil of *Pterospartum tridentatum* (Fabaceae) [14] while megastigatrienones were found in *Stachys palustris* (Lamiaceae) [15] and *Bidens pilosa* (Asteraceae) essential oils [16]. The C_{13} nor-isoprenoids are presumably bound as glycosides [9,13,17], which are enzymatically released as flavor and aroma components of the flowers. The aliphatic aldehydes, heptanal, octanal, and nonanal, have been found in other floral essential oils, including *Gossypium hirsutum* [18], *Narcissus* spp. [19], *Pourouma*

guianensis [20], *Anthemis altissima* [21], *Zizyphus mauritiana* [22], and *Pterospartum tridentatum* [14]. Long-chain alkanes have also been found to dominate some floral essential oils such as *Clusia* spp. [23], *Lamium* spp. [24], *Staphylea* spp. [25], or *Centaurea* spp. [26].

The chemical composition of the floral essential oil *B. suaveolens* collected at night (the "white" flowers) is qualitatively similar to *Brugmansia* × *candida* that was collected by headspace sampling [27]. Thus, *Brugmansia* × *candida* floral volatiles were rich in (*E*)-β-ocimene (38-52%) and 1,8-cineole (5-19%) with smaller amounts of phenethyl alcohol (1-3%) and (*E*)-nerolidol (5-6%). Although the floral volatiles were collected over 30 h, apparently aliphatic aldehydes, long-chain alkanes, and megastigmatrienones were not detected from this species of *Brugmansia*. A headspace analysis of *Brugmansia suaveolens* reported previously revealed the sample to be dominated by benzenoids, predominantly methyl benzoate (18.7%), as well as 1,8-cineole (25.5%), and geraniol (17.9%) [28]. McGee and Purzycki had previously investigated the temporal variation in the headspace volatiles of *B. suaveolens* and demonstrated that geraniol, methyl benzoate, and nerolidol floral emissions peaked between midnight and 4:00 am [29]. It is notable that neither methyl benzoate nor geraniol were detected in the floral essential oil from Costa Rica. Additionally, neither theaspiranes nor megastigmatrienones were detected in the headspace analyses previously reported. Temporal variation of floral volatiles has been much studied [30-33] and *Brugmansia* is another example whereby the volatile emissions change dramatically as the flower opens in the evening and senesces the following day.

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