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VOLATILE COMPOUNDS EMITTED FROM FLOWERS AND LEAVES OF *BRUGMANSIA × CANDIDA* (SOLANACEAE)

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Key Word Index—*Brugmansia × candida*; Solanaceae; flower; leaf; volatile compounds; scent; odour.

Abstract—The volatile compounds emitted from flowers of *Brugmansia × candida* Pers. were characterized to investigate reports that the floral scent may have intoxicating effects. The dominant components were *trans*-ocimene (38–52%) and 1,8-cineole (5–19%), while the minor components consisted of various other terpenoids, benzenoids and indole. The floral scent was typical of many white flowers. The volatile compounds emitted from the leaves were also examined and were found to be mainly terpenoids. Perillene (14–25%) was the major component and its analogous furanoid sesquiterpenoid, dendrolasin, was also present. Volatile tropane alkaloids could not be detected in either the floral or foliar odours, and none of the compounds emitted by the flowers are likely to cause intoxicating effects at low exposures.

INTRODUCTION

In the U.K. there has been concern about the sale of toxic plants to the public [1], resulting in 1993–94 in a review being made of potentially hazardous plants throughout the U.K. horticultural trade and a code of practice for trade labelling being produced [2]. This paper is a product of that review.

Species of *Brugmansia* (Solanaceae) have become increasingly popular as houseplants because of their large showy flowers, even though they are known to contain toxic tropane alkaloids and there are many recorded cases of poisoning in humans [3]. The plant most widely documented for sale in the U.K. is *Brugmansia × candida* Pers. [synonym: *Datura candida* (Pers.) Saff.], a hybrid between *B. aurea* Lagerh. and *B. versicolor* Lagerh., although this is often mis-labelled as '*B. arborea*' in retail outlets [the true species *B. arborea* (L.) Lagerh. is rarely found in cultivation].

Poisoning by *B. × candida* usually arises when parts of the plant are deliberately eaten for their hallucinogenic effects [3]. However, there are also reports of symptoms of intoxication occurring when the scent of the flowers is unwittingly inhaled over a period of time in a confined space: a plant bearing one to three flowers has been thought responsible for causing hallucinations, while it is claimed that a plant with over six flowers can cause fits and paralysis [4]. The only reported scent analysis in *Brugmansia* has been from a plant named as *Datura arborea* (=*B. arborea*) and the major scent component was stated to be an unusual trienol [5]. Other scent components were not identified, and the trienol has since been found to be an analytical artefact derived from *trans*-ocimene, a common major constituent of flower scents [6].

Thus, it is not possible to substantiate the reports of intoxicating volatile compounds being emitted from flowers of *Brugmansia* using existing analytical data, and so in this paper we perform detailed analyses of both the floral and foliar odours of *B.×candida* to determine whether any of the compounds being produced present known hazards to health. In particular, we examine the compounds emitted in trace amounts to check for the presence of any tropane alkaloids, such as tropane itself, which have sufficient vapour pressures for them to form a detectable component of the odours.

RESULTS AND DISCUSSION

The floral scent of *B. × candida* was found to be composed of various terpenoids and benzenoids with the alkaloid indole also being present as a minor component (Table 1). No tropane alkaloids could be detected by single ion monitoring. All the compounds have been reported previously in floral scents [6]; indole, for example, is present in the scents of common garden plants like *Narcissus*, *Syringa* and *Philadelphus* [6]. The monoterpenoids *trans*-ocimene and 1,8-cineole were the dominant components of the scent, comprising 38–52% and 5–19%, respectively, of the total mass of volatile compounds produced. The high percentage of *trans*-ocimene is not unusual in flower scents: the orchid *Laelia anceps* produces scent containing 87% *trans*-ocimene [7] and it is also an important component (11%) of the scent of *Nicotiana otophora*, another member of the Solanaceae [8].

Table 1. Composition of scents collected from each of three flowers of *Brugmansia* × *candida*

id*	R_t (min)	Compound	Percentage composition 1	2	3
		Benzenoids			
1	10.2	Benzaldehyde	2.9	5.9	3.9
1	14.0	Methyl benzoate	1.4	1.4	1.4
1	14.7	Phenylethyl alcohol	2.2	1.2	3.1
1	15.4	Benzyl acetate	—	0.1	0.7
2	16.8	Methyl salicylate		3.8	
1	31.6	Benzyl benzoate	—	0.4	0.6
2	33.2	Benzyl salicylate	—	0.7	0.7
		Monoterpenoids			
1	8.6	α-Thujene	0.3	0.3	0.3
1	8.9	α-Pinene	0.5	<0.1	0.1
1	10.4	β-Pinene	1.4	3.4	2.4
1	11.5	Limonene	3.6	4.3	3.5
1	11.9	1,8-Cineole	16.5	18.9	4.8
1	12.5	*trans*-Ocimene	49.1	38.0	52.3
2	13.1	*trans*-Sabinene hydrate	1.0	0.5	1.3
2	13.4	Terpinolene	0.9	0.2	1.1
2	17.0	α-Terpineol	3.5	3.1	4.9
		Sesquiterpenoids			
2	23.0	β-Elemene			0.1
2	24.1	β-Cedrene	0.5	0.2	—
2	24.3	[*z*]-α-*trans*-Bergamotene	<0.1	0.1	0.1
2	26.4	α-Farnesene	<1.7	3.4	2.8
2	27.7	*trans*-Nerolidol	4.5	6.2	5.4
2	29.5	*cis,trans*-Farnesol	<0.1	0.1	0.2
2	30.1	*trans,trans*-Farnesol	<0.1	0.3	0.3
2	30.7	*trans,cis*-Farnesol	<0.1	1.3	0.9
		Alkaloid			
1	20.0	Indole	—	0.2	1.1

*Identification criteria as in Table 2.

Table 2. Volatile compounds emitted by leaves of *Brugmansia* ×*candida* in each of three analyses

id*	R_t (min)	Compound	Percentage composition A	B	C
		Benzenoids			
1	16.3	Ethyl benzoate	0.5	—	—
2	16.8	Methyl salicylate	5.3	2.7	6.3
		Monoterpenoids			
1	8.9	α-Pinene	1.5	1.3	2.9
1	12.5	*trans*-Ocimene	4.4	0.9	5.2
3	14.0	Perillene	20.6	13.9	25.3
		Sesquiterpenoids			
2	23.0	β-Elemene	1.9	—	2.4
2	23.7	[*z*]-α-*cis*-Bergamotene	2.8	2.2	2.5
2	23.9	α-Santalene	1.3	2.3	2.9
2	24.1	β-Caryophyllene	1.9	2.0	1.7
2	24.3	[*z*]-α-*trans*-Bergamotene	9.9	9.3	8.8
2	24.4	α-Guaiene	1.5	2.6	0.5
2	24.7	*cis*-β-Farnescene	4.9	4.4	4.8
2	26.0	γ-Gurjunene	7.5	10.9	2.3
2	26.3	β-Selinene	6.5	12.2	1.5
2	26.4	β-Bisabolene	—	—	2.5
2	26.8	β-Sesquiphellandrene	0.8	1.2	2.4
2	27.7	*trans*-Nerolidol	0.1	—	1.0
2	28.0	Dendrolasin	11.3	8.8	13.0
2	30.1	Santalol acetate	2.2	8.4	—

*Identification criteria: 1, comparison of MS and retention time with standard; 2, comparison of MS and relative retention time with published data; 3, comparison of MS with published data.

The presence of the acyclic sesquiterpenoid alcohols farnesol and nerolidol in the scent, together with benzenoid alcohols (e.g. phenylethyl alcohol) and esters, is typical of the 'white floral' class of fragrances [7]. This combination of scent constituents is common amongst white flowers, which tend to release their scent during the late evening or night and are pollinated by moths. The pollination biology of *Brugmansia* has not been studied in detail, but the American hawk moth (*Phlegethontius sexta*) has been seen visiting flowers of *D. meteloides* [9].

The volatile compounds emitted from the leaves of *B.*×*candida* also consisted of terpenoids and benzenoids, like the flower scent (Table 2), but there was a greater structural diversity of sesquiterpenoids and fewer monoterpenoid and benzenoid structures. Indole was absent and, again, tropane alkaloids could not be detected in the analyses. The major component was identified as the furanoid monoterpenoid perillene, which comprised up to 25% of the total mass of volatile compounds; its sesquiterpenoid analogue, dendrolasin, was also present (comprising up to 13% of the volatile compounds). Perillene and dendrolasin are not frequently reported as volatile compounds from plants: the former is known mainly from perilla oil [10] whilst dendrolasin occurs in sweet potato [11]. Seeds of *Perilla* species, from which perilla oil is extracted, are routinely cooked in curry meals in north-east India [12] and thus, with dendrolasin also occurring in a foodstuff, these more unusual furanoid terpenoids are unlikely to cause poisoning by inhalation. However, both compounds do occur in the defence secretion of the ant *Lasius* (=*Dendrolasius*) *fuliginosus* [13], which suggests they do have some biological effects.

To assess whether the volatile chemicals produced by *B.*×*candida* present a significant risk to a person in close proximity to the plant, perhaps in a closed room for several hours, the level of exposure to the chemicals through inhalation must be considered. In perfumery it has been estimated that the level of exposure to perfume constituents by inhalation is well below the occupational exposure limits of all but the most toxic chemicals [14]. Thus, normal wearing of perfume presents minimal risk, even though many of the constituents have biological effects [15]. The quantity of volatile compounds being emitted by the leaves of *B.*×*candida* did not appear to be particularly great, as a long sampling period was required to capture sufficient quantities for analysis; however, considerably more volatile compounds were emitted by the flowers and they are also perceived to have a strong scent. As with other strongly scented flowers, some people may find the scent of *Brugmansia* 'overpowering' after a period of time, with the prolonged sensory stimulation by the terpenoids and benzenoid esters possibly causing headaches and nausea.

In conclusion, this study could not identify any volatile compounds produced by leaves or flowers of *B.* × *candida*, which, at low exposure levels, could cause intoxicating effects by inhalation, although, as with exposure to all chemicals, some individuals may show unexpected hypersensitive reactions. If there are further substantiated reports of people suffering ill effects from being in close proximity to species of *Brugmansia* or *Datura*, then it would be advisable to analyse the particular species or cultivar under suspicion.

EXPERIMENTAL

Plant material. A mature plant of *B.* × *candida* growing in the Temperate House of the Royal Botanic Gardens, Kew, was used for the analyses (Kew Accession No. 1965-57503).

Collection of volatiles. Flower volatiles were collected *in situ* by enclosing a recently opened flower in a glass dome and sampling the headspace at $50\,ml\,min^{-1}$ through a 3 mm diameter freshly desorbed sampling tube packed with 100 mg Tenax TA (60–80 mesh, Thames Chromatography). The sampling period was 18 h and began late in the afternoon. Leaf volatiles were collected *ex situ* by placing a sprig of foliage in water in a large desiccator and sucking air (filtered through Tenax) through the system into a sampling tube at $5\,ml\,min^{-1}$. The sampling period was 30 h during which time air from the laboratory was also sampled directly to identify background volatiles that had passed through the filter.

Analysis of volatiles. A sampling tube was inserted into a thermal desorption injector (set at 320°) of a GC/MS and, as the trap heated up in the flow of He, the volatiles were desorbed and passed directly on to the GC capillary column (25 m × 0.22 mm i.d. × 0.25 μm BPX5, SGE) where they were concd by means of a liquid CO_2 cryogenic cold trap; the GC oven temp. during desorption was 40°. After 5 min the cold trap was switched off and chromatography of the volatiles was achieved using an oven temp. programme of 40–180° ($5°\,min^{-1}$), 180–360° ($10°\,min^{-1}$), 360° (10 min) with a He carrier gas pressure of 20 psi. Detection was by FID and ion trap detector (70 eV; Finnigan-MAT) in parallel configuration. Compounds were identified by comparison of relative retention times and mass spectra with published data [16, 17] or, where possible, with purchased standards. The approximate percentage composition of each component was obained from the FID data. The MS data were screened for various tropanes alkaloid by single ion monitoring at m/z 82, 124 and 138.

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