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VOLATILE FLAVOUR COMPONENTS OF GUAVA

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Abstract—An essence of fresh guava fruit obtained by well-established procedures possessed the characteristic aroma of the fruit. It was analysed by GC/MS using both EI and CI techniques. Esters comprised over 55% of the essence and an extensive series of ethyl esters of the even carbon-numbered carboxylic acids was observed (over 52% of the sample). Two monoterpene hydrocarbons and five sesquiterpene hydrocarbons were also identified, myrcene being the major terpene. Evaluation at an odour port during GC showed eight peaks with significant guava aroma characteristics. The components concerned consisted of three esters, four sesquiterpene hydrocarbons and myrcene. It is considered that these are important contributors to fresh guava flavour and should be retained as far as possible in processed products.

INTRODUCTION

Guava is the fruit of *Psidium guajava* L., a small tree native to the American tropics. The fruit is green, but turns light yellow when ripe, and although it can be consumed fresh it has rather a sharp flavour when raw. In recent years the fruit and its various products have assumed increasing economic importance but relatively little attention has been devoted to the identification of the desirable flavour components.

As long ago as 1961, Kunishi and Seale isolated an essential oil from guava but made no specific identification of any components [1]. Similarly, Pattabhiraman *et al.* studied appropriate extracts, and although not identifying any constituents they came to the conclusion that carbonyl compounds and/or esters were significant to the characteristic flavour [2, 3]. Polyphenols in the fruit have been studied [4] and several sesquiterpene hydrocarbons and alcohols have been determined in the leaves of the tree [5]. However, it was not until 1970 that Stevens *et al.* reported the identification of 22 aroma components in a volatile essence of guava puree [6]. These included alcohols, aldehydes, esters, monoterpenenes and sesquiterpenes. No specific conclusions were reached concerning the importance of the various constituents to guava flavour. More recently, Wilson and Shaw studied the terpene hydrocarbons in guava puree [7]. They found that β-caryophyllene was the major component (*ca* 95% of the hydrocarbon fraction) and suggested it might be important to guava aroma. Here we report a more broadly based examination of the aroma volatiles of the fresh fruit. Apart from supplementing the relatively limited data for guava, the aim is to pinpoint any aroma components which might be particularly significant to the characteristic flavour of the fresh fruit and which should therefore be retained in any processed product.

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RESULTS AND DISCUSSION

An extract of fresh guava possessing the characteristic aroma of the fruit was obtained by standard procedures [8, 9] using the solvent 2-methylbutane (*iso*-pentane), which has been shown to be suitable for similar fruits [10, 11] and to be an efficient extractant [12]. The extract was concentrated [9], and the resultant essence retained the aroma qualities of the original extract. The essence was examined by routine temperature-programmed GC, and constituents were then identified as far as possible by GC/MS, using both electron impact ionization and chemical ionization techniques.

Table 1 lists the volatile components of fresh guava fruit, GC retention data, quantitative data and odour qualities of the various GC peaks. In all instances where positive identities are given, mass spectra agreed with those in the literature within instrumental variability. All spectra have been published previously [13, 14]. Sesquiterpene spectra agreed well with those compiled by Moshonas and Lund [15]. Literature [13, 16] Kovats retention indices of some important components are also included in the Table. These values were determined on the same GC phase as employed in this project and they serve as useful, but limited, confirmation of identity, particularly with regard to some sequiterpenes.

In total, just over 200 μg of aroma components were obtained per kg fresh fruit. This is a relatively modest concentration, and in our previous analyses of other tropical fruits using similar techniques greater amounts of aroma components were obtained for soursop, *Anona muricata* (1.2 mg/kg) [10] and for the strongly flavoured wood apple, *Feronia limonia* (80 mg/kg) [17]. However, the delicately flavoured mangosteen (*Garcinia mangostana*) provided only about 3 μg/kg [11].

Table 1 shows that the guava fruit essence contained 52 main components, of which 39 (comprising over 93% of the sample) have been positively

Table 1. Volatile flavour components of guava

Peak no.	Component	R_t (min)	Kovats index (literature)*	% relative abundance	μg/kg fruit	Odour quality
1.	Acetaldehyde	3.3	690	0.2	0.5	—
2.	Octane	3.8	800	1.4	2.8	—
3.	Acetone	4.3	814	0.8	1.6	Sour, yeasty, fruity
4.	2-Methylpropan-2-ol	4.8	830	1.0	2.1	—
5.	Ethyl acetate	5.7	872	26.2	53.9	Fruity, ester
6.	Ethyl alcohol plus unknown	6.6	900	25.8	53.1	Sweet, yeasty
7.	Butanone	7.2	908	2.2	4.5	Chemical solvent
8.	Butanedione	7.8	963	2.0	4.1	Diacetyl, buttery
9.	Unknown	8.7	—	0.2	0.4	Toffee-like, pentanone
10.	2-Methylpropyl acetate	8.9	1000	0.5	1.1	Guava
11.	Ethyl butanoate	9.5	1025	8.7	17.8	Ester, buttery, sweat
12.	Toluene	9.8	—	0.2	0.4	—
13.	Butyl acetate	10.3	1059	0.1	0.3	—
14.	Hexanal	10.6	1084	3.2	6.6	Green grass, hexanal
15.	Unknown	11.0	—	tr	tr	Green, buttery
16.	3-Methylbutyl acetate	11.5	1110	0.1	0.2	Pears
17.	Myrcene	12.0	1156	2.7	5.6	Green grass, guava
18.	Methyl hexanoate plus 3-methylbutan-1-ol	12.3	1177 1184	0.3	0.6	Green grass
19.	Limonene	13.2	1206	0.1	0.2	—
20.	Ethyl hexanoate	13.6	1228	15.5	31.8	Fruity, ester, almonds
21.	Unknown	14.2	—	tr	tr	Unpleasant, rancid
22.	Hexyl acetate	14.4	1307	0.3	0.5	Guava
23.	Unknown	14.8	—	tr	tr	Burnt, roasted
24.	*cis*-Hex-3-en-1-yl acetate	15.1	1300	0.5	1.0	Pears, fruity
25.	*cis*-Hex-3-en-1-ol	15.4	1351	1.0	2.0	Fruity, green, buttery
26.	Unknown	15.6	—	0.1	0.2	Slightly burnt
27.	Ethyl octanoate	15.9	1423	1.9	3.9	Slightly nutty
28.	2-Furfural	17.0	1449	0.7	1.4	Smoking bonfires
29.	Octyl acetate	17.5	1459	0.8	1.7	Fruity, fermented
30.	Acetylfuran	18.1	1491	tr	tr	—
31.	Octan-1-ol	18.6	1519	0.1	0.2	Sweet, slightly buttery
32.	Benzaldehyde plus α-copaene	18.9	1502 1530	0.1	0.2	Green guava
33.	5-Methyl-2-furfural	19.4	1563	0.2	0.3	Rubbery, peanuts
34.	Unknown	20.1	—	tr	tr	—
35.	Ethyl decanoate	20.5	1624	0.1	0.2	Guava
36.	β-Caryophyllene	21.0	1618	0.4	0.9	Guava, slightly burnt
37.	Unknown	21.4	—	0.1	0.2	Mouldy fruit
38.	α-Humulene	22.9	1682	0.6	1.3	Fresh green guava
39.	β-Bisabolene	24.0	1726	0.2	0.3	Dandelion leaves
40.	α-Selinene	25.4	—	0.1	0.2	Fruity, guava
41.	Unknown	25.9	—	0.1	0.2	Sweet, ester, oily
42.	2-Phenethylacetate	26.9	1785	0.2	0.5	Rotten apples, oily, fruity (banana)
43.	Ethyl dodecanoate	29.0	—	tr	tr	Mango
44.	Unknown	30.3	—	0.2	0.4	Mango
45.	Unknown	31.0	—	0.1	0.2	Sweet, fruity
46.	?*p*-Methylstyrene	31.5	—	0.3	0.5	—
47.	Ethyl tetradecanoate	36.8	2027	0.2	0.4	—
48.	Unknown	37.3	—	0.3	0.6	—
49.	Ethyl hexadecanoate	56.0	2217	tr	tr	—

*Literature = [13, 16], tr = trace.

identified and one (0.3%) partially characterized. The doubt with regard to *p*-methylstyrene is its unexpected occurrence in this system, but the mass spectrum of the component was near perfect. Although styrene itself has been reported among volatiles, derivatives are comparatively rare.

Of the identified components, just over 55% are esters, with ethyl acetate (*ca.* 26%), ethyl hexanoate (15.5%) and ethyl butanoate (8.7%) being the major representatives. Amongst the esters, only ethyl acetate and 2-phenethyl acetate have been previously reported in guava [6]. Clearly, however, esters must have considerable importance with regard to the fresh fruit flavour, and it is interesting that there are two main series. First, all the ethyl esters of the even carbon-numbered carboxylic acids were detected from the lowest member up to ethyl hexadecanoate (making eight in total). This group comprised over 52% of the aroma volatiles of guava, but these esters do commonly occur in aroma volatiles of many other foods. The other series of esters is more limited, but includes the acetates of all the even carbon-numbered alcohols from the lowest member up to octyl acetate.

Two monoterpene hydrocarbons were identified but only one of these (limonene) has been previously reported in guava [6, 7]. However, the other (myrcene) was present in much greater amounts and made up nearly 3% of the sample. Moreover, the GC peak due to myrcene was described by assessors during odour evaluation to possess significant guava character, so this compound is presumably important to the flavour. Myrcene is not one of the more widely-occurring monoterpene hydrocarbons.

Only five sesquiterpene hydrocarbons were detected and they constituted only *ca* 1.5% of the essence. Except for α-copaene, all of these had previously been identified in guava puree by Wilson and Shaw [7], who did, however, detect β-copaene and four others in addition to those listed here. Particular efforts were made to detect these other compounds in our samples, but they were not found. The major sequiterpene hydrocarbon identified in previous work on guava puree was β-caryophyllene [6, 7], but we found slightly more α-humulene, and neither compound was found as a major component of the essence.

On assessment at an odour port during GC, a surprisingly large number of peaks (eight) were described as possessing significant guava character. However, these descriptions were confirmed in a number of replicate runs. Of the eight GC peaks, one consisted of two unresolved components (benzaldehyde and α-copaene). This peak was particularly described as having green (unripe) guava aroma, but whether one compound or both was responsible is not known. Myrcene has already been mentioned as an important contributor to guava flavour on this basis, and it was the major peak of those described as having guava aroma (2.7% of a total of 5.0% for the eight peaks). The six other compounds whose GC peaks were given guava odour descriptions comprised three esters (2-methylpropyl acetate, hexyl acetate and ethyl decanoate) and three sesquiterpene hydrocarbons (β-caryophyllene, α-humulene and α-selinene). All nine compounds are fairly common components of food volatiles, except for myrcene, so therefore none can be considered to be particularly characteristic of guava. However, it would seem that these compounds are the most important constituents of guava flavour and that therefore they should be retained to the greatest possible extent in any processed guava product.

EXPERIMENTAL

Fresh ripe guava fruits were transported by air from Venezuela and were analysed the day after arrival.

Sample preparation. Fruit pulp (520 g) was mixed with H_2O (400 ml) and extracted for 4.5 hr in a Likens and Nickerson apparatus [8] as modified by MacLeod and Cave [9] using 2-methylbutane (25 ml) as solvent. Extracts were concd to 4.5 ml using a low temp.–high vacuum distillation procedure [9].

Gas chromatography. Essences were examined by GC with heated FID. A 5.5 m × 4 mm i.d. glass column packed with 10% Carbowax 20 M coated on 100–120 BSS mesh acid-washed Diatomite C was used, with a carrier gas (N_2) flow rate of 60 ml/min. The temp. programme adopted was 60° for 5 min followed by an increase at 12°/min to 200°. The detector and injection point heaters were at 250° and typically 2 μl of essence was injected.

GC/MS. The same GC conditions as described above were used, but with He as carrier gas. The single-stage, all-glass jet separator was operated at 250°. Both electron impact (EI) and chemical ionization (CI) MS were performed. Significant operating parameters of the MS during EI work were: ionization potential, 70 eV; ionization current, 100 μA; source temp., 230°; accelerating voltage, 1.5 kV; resolution, 600; scan speed, 1 sec/decade (repetitive throughout run). Identical conditions were employed during CI work except for the following : reagent gas, methane; ionization potential, 100–110 eV; emission current, 5 mA.

Quantitative assessment. Samples were prepared in such a manner that a known aliquot of the fruit sample was analysed. Quantitative data were then derived both from the trace obtained from the TIC monitor during GC/MS and from the FID trace during routine GC. Known amounts of a selection of identified compounds (butanone, ethyl butanoate, hexanal, limonene, hexyl acetate and *cis*-hex-3-en-1-ol) were injected under the same analytical conditions in order to enable calculation of absolute amounts of components in the essence.

Odour assessment. Aromas of the separated components of the essence were assessed at an odour port following GC. An outlet splitter set at 10:1 diverted the major fraction of the eluent through a heated line to the outside of the GC oven for aroma assessment by three subjects, all of whom were familiar with guava flavour.

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