# **Characterization of Volatiles in Strawberry Guava** (*Psidium cattleianum* Sabine) Fruit

Jorge A. Pino,\*,<sup>†</sup> Rolando Marbot,<sup>‡</sup> and Carlos Vázquez<sup>§</sup>

Food Industry Research Institute, Carretera del Guatao km 3<sup>1</sup>/<sub>2</sub>, La Habana 19200, Cuba; National Center for Scientific Research, La Habana, Cuba, and National Botanical Garden, La Habana, Cuba

Volatile compounds were isolated from strawberry guava fruit by simultaneous steam distillation– solvent extraction according to Likens–Nickerson. Compounds were identified by capillary GC-MS and sensorially characterized by sniffing GC. Two hundred and four compounds were identified in the aroma concentrate, of which ethanol,  $\alpha$ -pinene, (*Z*)-3-hexenol, (*E*)- $\beta$ -caryophyllene, and hexadecanoic acid were found to be the major constituents. The presence of many aliphatic esters and terpenic compounds is thought to contribute to the unique flavor of the strawberry guava fruit.

**Keywords:** Volatiles; strawberry guava; aliphatic esters; terpenic compounds

### INTRODUCTION

Among the many attractive and desirable attributes that create demand for fruits from the tropics and subtropics, their characteristic flavor is the most noticeable to consumers. In addition, these fruits are often inexpensive, extremely rich in vitamins, and can be used in a wide range of food products.

Probably native to, at least, the coastal scrubs and forests of eastern Brazil, strawberry guava (*Psidium cattleianum* Sabine) belongs in the same botanical family (Mytaceae) as guava and is often described as being more aromatic than that fruit. There are two known cultivars, the properly strawberry guava which is red and the yellow fruit (var. Lucidum Hort.).

The chemical composition of strawberry fruit has been published elsewhere (1, 2), but there is little quantitative information about its volatile flavor constituents and their sensory significance (3, 4). This is the subject of the present study.

#### EXPERIMENTAL PROCEDURES

**Materials.** Fruits from the red cultivar were collected mature from the National Botanical Garden near Havana and immediately processed. Diethyl ether was purchased from Merck (Darmstadt, Germany).

**Sample Preparation.** After addition of an internal standard (methyl undecanoate, 2 mng), pulp (200 g) was blended with distilled water (800 mL), adjusted to pH 7, and simultaneously distilled and extracted for 90 min in a Likens-Nickerson microapparatus with 25 mL of diethyl ether (previously redistilled and checked as to purity). The volatile concentrate was dried over anhydrous sulfate and concentrated to 0.6 mL in a Kuderna-Danish evaporator with a 12 cm Vigreux column and then to 0.2 mL with a gentle nitrogen stream.

GC and GC-MS Analyses. A Konik 2000 GC equipped with a 30 m  $\times$  0.25 mm (0.25  $\mu m$  film thickness) DB-1 fused-silica capillary column and a flame ionization detector (FID) was used. Injector and detector temperatures were both 250 °C. Oven temperature was held at 60 °C for 10 min and then

raised to 280 °C at 2 °C/min and held for 40 min. Carrier gas (hydrogen) flow rate was I mL/min. These conditions were used for quantitative analysis, by the internal standard method. The recovery of the method was determined by the standard addition technique applied to a sample. The analytes ( $\alpha$ -pinene, limonene, ethyl hexanoate, 1- hexanol, (Z)-3-hexenol, ethyl octanoate, (E)- $\beta$ -caryophyllene and  $\alpha$ -terpineol) were added at two different concentrations. The average recoveries were about 89–102% and their relative standard-deviations were lower than 10%.

GC-MS analyses were performed on a Hewlett-Packard model 5890 series II or model 6890 series IIGC coupled to an HP 5972 or HP 5973 mass spectrometer. They were fitted with a CP-SIL-5CB Chrompack fused silica column (50 m  $\times$  0.32 mm, 0.4  $\mu$ m film thickness) or an AT-WAX Alltech fused silica column (60 m  $\times$  0.32 mm, 0.25  $\mu$ m film thickness). Temperature programming was as follows: from 60 °C (10 min) to 280 °C at 3 °C/min and held for 60 min in the apolar column and from 65 °C (10 min) to 250 °C at 2 °C/min and held for 60 min in the polar column; injector temperature was 250 °C; transfer line temperature, 250 °C and carrier gas (helium) flow rate, 1 mL/min. Mass spectra were obtained at 70 eV. Linear retention indices were calculated against those of n-paraffins (5). Components identification was carried out by comparing the relative retention indices and mass spectra of 3 reference compounds in both columns. Mass spectra of published data were also compared (6, 7).

**GC Sniffing Analysis.** Odor assessments were carried out using a Hewlett-Packard model 5890 series II GC equipped with a thermal conductivity detector (TCD). Separations were done with a methyl siloxane HP-1 fused silica column (30 cm  $\times$  0.53 mm, 2.65  $\mu$ m film thickness). An injector temperature of 250 °C, a detector temperature of 280 °C, and an oven temperature program of 60 °C to 280 °C at 3 °C/min were used. Sample size for each injection was approximately 0.5–1  $\mu$ L.

## RESULTS AND DISCUSSION

The volatile constituents of strawberry guava fruit were obtained by simultaneous steam distillation solvent extraction and analyzed by GC and GC-MS using fused silica capillary columns.

Table 1 shows the identified compounds and the sensory description of the corresponding peaks at the sniffing port of the GC. Two hundred and four compounds were identified in the aroma concentrate. Shiota et al. (*3*) identified 35 compounds in the fruits of red

<sup>&</sup>lt;sup>†</sup> Food Industry Research Institute.

<sup>&</sup>lt;sup>‡</sup> National Center for Scientific Research.

<sup>§</sup> National Botanical Garden.

# Table 1: Volatile Compounds of Strawberry Guava

compound	retention $RI_1$	index <sup><math>a</math></sup> RI <sub>2</sub>	concentration (ppm)	odor description
acetaldehyde	669	381	t <sup>b</sup>	
nethyl acetatec	724	511	0.03	
putanal <sup>c</sup>	813	600	0.09	overripe, somewhat fruity
ethyl acetate	825	581	2.91	estery, fruity
ethanol	854	377	9.70	
sopentanal <sup>c</sup>	864	617	t	
ethyl propanoatec	925	681	0.03	
ethyl isobutanoate	930	726	t	fruity
propyl acetate <sup>c</sup>	941	686	t	ethereal-fruity
2-pentanone	944	653	0.39	ethereal-fruity
pentanal <sup>c</sup>	950	657	t	
methyl butanoate <sup>c</sup>	955	696	0.02	
4-methyl-3-penten-2-one <sup>c</sup>	970	_	t	
isobutyl acetate <sup>c</sup>	986	741	0.03	fruity
x-pinene	1012	925	6.44	pine-like
ethyl butanoate	1025	781	0.98	fruity
3-hexanone <sup>c</sup>	1037	756	t	
α-fenchene <sup>c</sup>	1045	937	0.03	
camphene <sup>c</sup>	1052	940	0.04	
butyl acetate <sup>c</sup>	1052	791	0.04	ethereal-fruity
hexanal	1062	772	0.66	fatty-green
sobutanol	1064	592	0.14	sweet
ethyl carbonate <sup>c</sup>	1083	747	0.03	
2-pinene <sup>c</sup>	1091	965	0.36	woody
2-pentanol <sup>c</sup>	1094	664 855	0.19	winy-ethereal
soamyl acetate	1107	855	0.19	banana, fruity
p-xylene	1117	852	t +	othered further
ethyl pentanoate <sup>c</sup>	1125	881	t 0.18	ethereal-fruity
I-butanol	1126 1132	619 847	0.18	chemical
<i>m</i> -xylene			0.05	
δ-3-carene <sup>c</sup>	1138 1141	1001	0.08 0.09	
1-penten-3-ol <sup>c</sup>	1141	981	4.01	sweet-balsamic
myrcene	1155	993	4.01 t	Sweet-Daisainit
α-phellandrene <sup>c</sup> 1(7),8- <i>p</i> -menthene <sup>c</sup>	1157	993	0.02	
l-pentyl acetate <sup>c</sup>	1158	893	0.02 t	
x-terpinene	1167	1006	t	
2-heptanone	1172	859	0.37	fruity-spicy
<i>p</i> -xylene	1172	863	0.05	if unty-spicy
methyl hexanoate <sup><math>c</math></sup>	1175	904	0.07	
limonene	1187	1016	2.06	citrus
sopentanol	1187	700	0.67	fruity-winey
1.8-cineole <sup>c</sup>	1193	1022	0.47	camphoraceous
$\beta$ -phellandrene <sup>c</sup>	1196	1016	0.10	cumpnoraceous
cis-anhydro linalool oxide <sup>c</sup>	1199	979	t	
2-methylbutanol <sup>c</sup>	1204	708	t	
( <i>E</i> )-2-hexenal	1206	817	0.27	fruity, green
ethyl hexanoate	1225	981	2.63	fruity-winey
$(Z)$ - $\beta$ -ocimene	1228	1026	3.45	floral, herbaceous
<i>trans</i> -anhydro linalool oxide <sup>c</sup>	1233	993	t.40	nor al, nor baccoub
v-terpinene	1235	1046	0.73	herbaceous-citrus
$(E)$ - $\beta$ -ocimene	1244	1037	1.36	floral, herbaceous
styrene <sup>c</sup>	1245	871	t	
2-heptyl acetate <sup>c</sup>	1255	1022	ť	
sopentyl butanoate <sup><math>c</math></sup>	1255	1041	0.05	
o-cymene	1259	1007	0.24	citrus
nexyl acetate	1265	993	0.58	sweet fruity
acetoin	1273	667	0.48	buttery
erpinolene	274	1076	1.77	pine-like
octanal <sup>c</sup>	1276	981	t	1
sopentyl pentanoate <sup>c</sup>	1288	1090	ť	
ethyl ( $E$ )-3-hexenoate <sup>c</sup>	1291	981	0.11	pineapple, fruity
ethyl (Z)-3-hexenoate <sup><math>c</math></sup>	1295	982	0.01	fruity
<i>(E)</i> -3-hexenyl acetate	1298	983	0.03	fruity, green
2-heptanol <sup>c</sup>	1301	887	t	
(Z)-2-pentenol <sup>c</sup>	1302	734	ť	
(Z)-3-hexenyl acetate	1307	984	0.91	fruity, green
( <i>E</i> )-2-heptenal <sup>c</sup>	1326	930	t	
(Z)-2-hexenyl acetate	1327	993	0.02	
2-methyl-2-hepten-6-one <sup>c</sup>	1330	962	0.01	
ethyl lactate <sup>c</sup>	1333	787	0.34	ethereal-buttery
I-hexanol	1343	849	3.58	fatty, fruity
sobutyl hexanoate <sup>c</sup>	1346	1137	t	Luce, many
(E)-3-hexenol	1364	823	0.13	grassy, green
isoprenyl pentanoate <sup>c</sup>	1365	1113	t.13	5-100J, 510011
	2000		•	

## Table 1 (Continued)

compound	retention RI <sub>1</sub>	index <sup>a</sup> RI <sub>2</sub>	concentration (ppm)	odor description
(Z)-3-hexenol	1368	828	6.55	grassy, green
2-nonanone	1379	1077	0.14	fruity-floral
methyl octanoate <sup>c</sup>	1381	1109	0.07	
nonanal	1381	1089	0.14	fatty-floral
(E,E)-2,4-hexadienal	1400	877	t	
(Z)-2-hexenol	1402	847	0.04	grassy
butyl hexanoate <sup>c</sup>	1404	1176	0.04	
hexyl butanoate	1406	1173	0.12	fruity
ethyl octanoate	1425	1181	1.38	fruity-winey, sweet
1,3,8- <i>p</i> -menthatriene <sup>c</sup>	1429	-	0.05	
1-heptanol <sup>c</sup>	1443	949	t	1-1
acetic acid	1443	547	0.11	acid
isopentyl hexanoate <sup>c</sup>	1447	1238	0.03	anne at ann an
(Z)-3-hexenyl butanoate	1448	1166	0.11	sweet-green
furfural cis-linalool oxide (furanoid)	$1448\\1449$	795 1068	0.09 0.11	burnt flored woody
	1449	1217		floral-woody
( <i>Z</i> )-3-hexenyl 2-methylbutanoate <sup><i>c</i></sup> 1-octyl acetate <sup><i>c</i></sup>			t	
	1464	1189	t 0.14	
α-ylangene <sup>c</sup>	1467	1371		d
$\alpha$ -copaene	1476	1374	0.60	woody
ethyl (E)-3-octenoate <sup>c</sup>	1483	1177 892	t	
2-acetylfuran	1488		0.05	
ethyl sorbate <sup>c</sup>	1490	694 007	t 0.10	torm
ethyl 3-hydroxybutanoate <sup>c</sup>	1501 1505	907	0.10	tarry
2-nonanol		1084	0.05	
benzaldehyde	1508	923	0.05	
(E)-2-nonenal <sup>c</sup>	1509	1135	t	
$\alpha$ -gurjunene <sup>c</sup>	1516	1405	t 0.03	
4-undecanone <sup>c</sup>	1518			flowel
linalool	1530	1083	0.92	floral
1-octanol	1544	1054	0.03	florel
linalyl acetate	1545	1243	0.03	floral
isobutanoic acid <sup>c</sup>	1556	732	t	buttery
<i>cis</i> -2- <i>p</i> -menthene-1-ol <sup>c</sup>	1560	1104	t	
$\beta$ -longipinene <sup>c</sup>	1561		0.07	
bomyl acetate <sup>c</sup>	1562	1274	0.09	
endo-fenchol	1565	1094	0.09	
terpinen-4-ol	1571	1157	0.27	spicy
cisα-bergamotene <sup>c</sup>	1573	1414	t	
$(E)$ - $\beta$ -caryophyllene	1576	1410	10.25	woody-spicy
aromadendrene <sup>c</sup>	1589	1437	0.07	
1-hexyl hexanoate	1597	1371	0.33	fruity-grassy
phenylacetaldehyde	1612	1009	t	
isopentanoic acid <sup>c</sup>	1642	816	0.04	sweet, oily
ethyl decanoate	1625	1382	1.04	
$\delta$ -patchoulene <sup>c</sup>	1627	1452	t	
(E)-2-decenal <sup>c</sup>	1637	1242	t	
(Z)-3-hexenyl hexanoate	1642	1364	0.38	fruity-green
$\gamma$ -patchoulene <sup>c</sup>	1648	1483	0.30	
α-humulene	1651	1443	1.72	woody
allo-9-aromadendrene <sup>c</sup>	1653	1490	t	
4,11-selinadiene <sup>c</sup>	1656	1410	0.21	woody
limonene-4-ol <sup>c</sup>	1664	1157	0.34	woody
$\alpha$ -terpenyl acetate <sup>c</sup>	1673	1335	0.17	herbaceous, sweet
$\gamma$ -muurolene <sup>c</sup>	1673	_	0.45	woody
α-terpineol	1679	1171	2.48	floral, sweet
borneol <sup>c</sup>	1680	1151	0.09	, ,
germacrene-D <sup>c</sup>	1684	1476	0.43	dry-woody
eremophilene <sup>c</sup>	1697	1486	0.71	woody
α-selinene <sup>c</sup>	1699	1491	0.38	woody
α-muurolene <sup>c</sup>	1704	1491	0.17	woody
$\beta$ -bisabolene <sup>c</sup>	1716	1505	0.09	
cadinene <sup>c</sup>	1727	1508	0.30	dry-woody, spicy
$\delta$ -cadinene <sup>c</sup>	1741	1511	1.21	dry-woody, spicy
$\beta$ -maaliene <sup>c</sup>	1750	_	0.23	woody
(Z)-3-hexenyl heptanoate <sup>c</sup>	1755	1462	0.08	_
3,7(1 1)-selinadiene <sup>c</sup>	1760	1530	0.98	woody
cubenene <sup>c</sup>	1761	1531	0.09	
$\alpha$ -cadinene <sup>c</sup>	1766	1527	0.04	
<i>trans</i> -chrysanthenyl acetate <sup>c</sup>	1785	-	0.04	
2-tridecanone	1791	1480	0.79	spicy, herbaceous
phenylethyl acetate	1795	1221	0.23	rosy-fruity
5-decenyl acetate <sup>c</sup>	1805	_	0.06	J J
<i>trans</i> -calamenene <sup>c</sup>	1812	1515	0.03	
ethyl dodecanoate <sup><math>c</math></sup>	1824	1581	0.23	fatty-fruity
hexanoic acid	1825	988	0.74	acrid-acid

#### **Table 1 (Continued)**

compound	retention RI <sub>1</sub>	index <sup><math>a</math></sup> RI <sub>2</sub>	concentration (ppm)	odor description
$\beta$ -vetivene <sup>c</sup>	1833	1546	0.13	
(Z)-3-hexenyl octanoate <sup>c</sup>	1837	1561	0.14	fruity-green
α-calacorene	1887	1531	0.87	dry-woody
2-phenylethanol	1888	1081	0.23	floral
$\beta$ -calacorene <sup>c</sup>	1893	1550	0.16	
2-tridecanol	1899	1490	0.92	sweet-fruity
3-phenylpropyl acetate	1917	1345	0.03	5
$\beta$ -caryophyllene epoxide	1954	1578	1.16	spicy
1,4,9-cadalatriene <sup>c</sup>	1962	1601	0.05	1 0
3-hydroxy-2-pyranone <sup>c</sup>	1967	_	0.17	
$\alpha$ -humulene epoxide I <sup>c</sup>	1986	1578	0.08	
2-pentadecanone	1997	1682	0.55	spicy, herbaceous
α-humulene epoxide II <sup>c</sup>	2009	_	0.27	1 57
(E)-nerolidol	2015	1549	0.25	
$\beta$ -caryophyllene hydrate <sup>c</sup>	2021	1553	0.70	spicy
cubenol	2030	1618	0.15	1 0
epi-cubenol <sup>c</sup>	2035	1621	0.62	sweet-woody
viridiflorol <sup>c</sup>	2053	1587	0.09	
(Z)-methyl isoeugenol	2059	1420	0.05	
(E)-methylisoeugenol	2062	1460	0.05	
cubebol <sup>c</sup>	2063	1500	0.15	
2-pentadecanol <sup>c</sup>	2097	1690	0.53	floral
ethyl ( <i>E</i> )-cinnamate	2103	1443	0.10	balsamic
$\gamma$ -eudesmol <sup>c</sup>	2136	1620	0.19	sweet-woody
T-cadinol	2139	1633	0.60	woody
T-muurolol <sup>c</sup>	2154	1622	0.86	spicy
$\delta$ -cadinol <sup>c</sup>	2167	1631	1.07	spicy
$\alpha$ -eudesmol <sup>c</sup>	2186	1613	0.42	sweet-woody
methyl hexadecanoate <sup>c</sup>	2191	-	0.11	Sweet woody
$\beta$ -eudesmol	2195	1590	0.29	sweet-woody
$\alpha$ -cadinol	2198	1628	1.04	spicy
2-hexadecanone <sup>c</sup>	2202	-	0.09	spicy
$\alpha$ -11-selinene-4-ol <sup>c</sup>	2216	1632	0.55	woody
ar-himachalene <sup>c</sup>	2220	1563	1.34	woody
ethyl hexadecanoate <sup>c</sup>	2224	1981	0.19	woody
decanoic acid <sup><math>c</math></sup>	2242	1360	0.14	
2-hexadecanol	2295	1794	0.08	
caryophyllenol <sup>c</sup>	2299	1614	0.95	spicy
( <i>E</i> )-isoeugenol	2309		t	spicy
undecanoic acid <sup>c</sup>	2346	1460	0.05	
methyl octadecanoate <sup>c</sup>	2010	1100	t	
2-octadecanone <sup>c</sup>	2402	_	t	
ethyl stearate <sup>c</sup>	2424	2181	t	
dodecanoic acid <sup>c</sup>	2448	1561	0.32	waxy
ethyl linoleate <sup>c</sup>	2491	2141	0.19	waxy
ethyl linolenate <sup><math>c</math></sup>	2555	2141	0.11	
phytol	2571	2066	0.02	
benzyl benzoate	2579	2000	0.02	
tetradecanoic acid <sup>c</sup>	2624	1743	1.22	
pentadecanoic $acid^c$	2756	1743	0.12	
hexadecanoic $acid^c$	2756 2862	1844	8.25	11/2 1/1
oleic acid <sup>c</sup>	2933	1932	0.12	waxy
oreit atiu-	2000	1920	0.12	

 ${}^{a}$  RI<sub>1</sub> and RI<sub>2</sub> = retention indices on AT-WAX and CP–SIL-5CB capillary column.  ${}^{b}$  t = trace (<0.01 ppm).  ${}^{c}$  Reported for the first time.

and yellow strawberry guava, whereas Vernin et al. (4) identified 154 volatile compounds in both varieties. Many of the compounds identified herein are reported for the first time in this fruit. Although alkyl benzenes, acetals, and cinnamyl derivatives were reported in significant quantities in the fruits grown in Reunion (4), no evidence of this class of compounds was found in the fruit studied here, with the exception of ethyl (*E*)-cinnamate. Among the compounds found in this study, a greater number of terpenes and terpenic derivatives were identified.

A quantitative analysis of the volatile compounds of strawberry guava is shown also in Table 1 The yield of total volatiles, estimated by the addition of a measured amount of internal standard to the pulp, was 110 mg/ kg of fruit pulp. Major constituents were ethanol,  $\alpha$ -pinene, (*Z*)-3-hexenol, (*E*)- $\beta$ -caryophyllene, and hexadecanoic acid. The observed differences between com-

position figures given by other authors (3, 4) can be explained by the fact that different isolation methods were used. Besides, those papers report only percentage abundance, as determined from the TIC peak areas, but these data should be used as giving only a general indication of relative amounts, because extraction efficiencies were not considered.

The coincidence of an identified peak with some odor impression does not imply that this specific compound is solely responsible for the odor. The possibility of an underlying minor component strongly influencing the sensory results can never be ruled out.

The following compounds are thought to contribute to the complexity of the strawberry guava flavor. Fruity notes are due to the presence of many aliphatic esters, whereas floral notes can be attributed to (*Z*)- and (*E*)- $\beta$ -ocimene, linalool, and linalyl acetate. Spicy notes can be ascribed to (*E*)- $\beta$ -caryophyllene oxygenated derivatives, 2-tridepanone, and 2-pentadecanone, whereas green notes are due to (*Z*)-3-hexenol and its esters. The woody notes can be attributed to the presence of many sesquiterpenes, particularly (E)- $\beta$ -caryophyllene.

It can be concluded from the results that the aliphatic esters and terpenic compounds contribute much to the typical strawberry guava flavor. However, it was not possible to find one or more impact compounds.

### LITERATURE CITED

- (1) Clement, C. R.; Dasilva, D. F. Amazonian Small Fruits with Commercial Potential. *Fruit Var. J.* **1994**, *48* (3), 152–158.
- (2) Herrmann, K. Über die Inhaltsstoffe und die Verwendung wichtiger exotischer Obstarten. IX. Melonenbaumfrachte: Babaco, Berg-papaya, sowie Feijoa und Erdbeerguave. Ind. Obst.-Gemoseverwertung 1995, 83 (1), 7–10.
- (3) Shiota, H.; Minami, T.; Tsuneya T. Aroma constituents of guava-like fruits. *Koryo* **1980**, *128*, 35–39.

- (4) Vernin, G.; Vemin, C.; Pierisbattesti, J. C.; Roque, C. Analysis of the volatile compounds of *Psidium cattleianum* Sabine fruit from Reunion Island. *J. Essent. Oil Res.* **1998**, *10* (4), 353–362.
- (5) Majlat, P.; Erdos, Z.; Takacs, J. Calculation and application of retention indices in programmed temperature-gas chromatography. *J. Chromatogr.* **1974**, *91*, 89–110.
- (6) MacLafferty, F. W.; Staffer, D. B. The Wiley/NBS Registry of Mass Spectral Data. John Wiley & Sons: New York, 1989.
- (7) Adams, R. P. Identification of Essential Oil Components by Gas Chromatography/Mass Spectroscopy, Allured Publishing Corp., Carol Stream, 1995.

Received for review March 28, 2001. Revised manuscript received August 14, 2001. Accepted August 17, 2001.

JF010414R