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Received for review February 8, 1988. Accepted June 21, 1988.

Volatile Constituents of Guava Fruits (*Psidium guajava* L.) and Canned Puree

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Essences of fresh guava (*Psidium guajava* L.) with white and pink flesh, respectively, were obtained by direct extraction of flesh juices with dichloromethane. Commercial canned puree of guava was water distilled, and the distillate was extracted with dichloromethane. The three essences were analyzed by fused silica capillary gas chromatography and gas chromatography/mass spectroscopy. A total of 122 volatile components were identified: 13 aldehydes, 17 ketones, 31 alcohols, 10 acids, 28 esters, 10 hydrocarbons, and 13 miscellaneous compounds. Quantitatively, the major constituents of fresh fruits were C_6 compounds. The total amount of C_6 aldehydes, alcohols, and acids comprised 20% of the essence of fresh white and 44% of the essence of fresh pink. The canned puree contained acetoin, which comprised 81% of the essence, as the major constituent.

The guava (*Psidium guajava* L.), which has an unique quince- and banana-like odor, is native to Central America. It was distributed into other parts of tropical and subtropical areas such as Asia, South Africa, Egypt, and Brazil by the early 17th century and is now cultivated in nearly 60 countries. The production of guava in the world is still much less than those of other major tropical fruits, but it is economically important in certain countries. In addition to consumption as fresh fruit, guava has been processed into many different foods: jellies, jams, cheese, ketchup, puree, juice powder, nectar, and juices.

A pioneer study on volatile components in guava was done in the early 1960s (Kunishi and Seale, 1961). The aroma constituents of guava were not, however, reported until Stevens et al. (1970) identified 22 aroma components of Hawaiian guava. They suggested that β-ionone, which has a low odor threshold and intense violet aroma, contributed floral flavor to the fruit. Wilson and Shaw (1978), who identified 12 terpenes in an extract of guava puree, described that β-caryophyllene plays an important role in guava aroma. Later, MacLeod and de Troconis (1982) reported that 2-methylpropyl acetate, hexyl acetate, and benzaldehyde had a guava-like odor among 40 volatiles identified in guava from Venezuela. Most recently, Idstein and Schreier (1985) identified 154 compounds in guava from Brazil including 115 compounds described for the first time. In the present study, volatile components of fresh guava fruit from Amami Island, Japan, and canned guava puree from South Africa were identified.

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EXPERIMENTAL SECTION

Materials. Fresh ripe guava fruits (pink and white) were obtained from Amami Island located 300 miles south of the mainland of Japan. Canned guava puree was purchased from the Potona Canning and Production Co., Ltd. Authentic chemicals for gas chromatographic analysis were purchased from reliable commercial sources or were donated by Ogawa & Co., Ltd., Tokyo, Japan.

Sample Preparations. Fresh guava with white flesh (white) and fresh guava with pink flesh (pink) were treated and analyzed separately. The fruit flesh (1.5 kg) was separated from peel and seeds, sliced into small pieces (3 cm), and homogenized with an electric blender. The homogenized sample was mixed with 1.5 L of deionized water, and stone cells were removed with a centrifuge. The fresh juice (2 L) was extracted with 150 mL of dichloromethane with use of a liquid–liquid continuous extractor for 12 h. After the extract was dried over anhydrous sodium sulfate, the solvent was removed on a Vigreux column at 42 °C. The solvent was further removed with a purified nitrogen stream, and approximately 0.3 mL of a fresh fruit essence was obtained.

Canned puree (1.5 kg) was also homogenized with 1.5 L of deionized water and was water-distilled under reduced pressure (40 mmHg) in a nitrogen stream at 40 °C. The distillation was continued until 1.5 L of distillate was obtained. The distillate was extracted with 150 mL of dichloromethane with use of a liquid–liquid continuous extractor for 12 h. The extract was treated in the same manner as the one from fresh fruit, and approximately 0.5 mL of essence was obtained.

Analysis of Volatiles. Identification of volatile constituents of the guava samples was made by comparison of their Kovats gas chromatographic retention indices and mass spectra to those of authentic compounds.

0021-8561/89/1437-0139$01.50/0

Table I. Volatile Compounds Identified in Guava

	I_k (CW20M)	GC peak area,[a] % white	pink	puree		I_k (CW20M)	GC peak area,[a] % white	pink	puree
Aldehydes									
acetaldehyde	690	b	0.14	b	furfural	1440	b	b	1.03
hexanal	1084	3.03	6.71	c	(*E*,*E*)-2,4-heptadienal	1455	b	b	c
4-pentenal	1134	b	0.20	c	benzaldehyde	1494	0.53	0.42	0.13
(*E*)-3-hexenal	1138	0.39	2.11	c	5-methylfurfural	1559	c	c	b
(*Z*)-3-hexenal	1142	1.04	7.83	c	*m*-hydroxybenzaldehyde	1637	c	b	c
(*Z*)-2-hexenal	1203	0.11	0.56	c	cinnamic aldehyde	1986	b	0.16	c
(*E*)-2-hexenal	1222	3.56	16.86	c					
Ketones									
acetone	820	c	b	c	*p*-methylacetophenone	1746	c	b	c
3-pentanone	958	0.91	0.36	c	furfuryl pentyl ketone	1822	c	0.13	c
2,3-butanedione	961	c	c	0.10	furfuryl hexyl ketone	1913	c	2.05	c
2,4-dimethyl-3-pentanone	997	c	c	b	*β*-ionone	1922	b	c	b
2-acetylfuran	1475	c	c	b	2,5-dimethyl-4-hydroxy-3(2*H*)-furanone	1960	6.32	1.13	c
2-propionylfuran	1565	c	c	b					
3,3,5-trimethyl-2-cyclohexanone	1584	0.19	0.23	c	dihydromethylionone	1967	c	c	b
methyl benzyl ketone	1637	c	c	b	5,6-epoxy-*β*-ionone	1968	c	b	c
5-ethyl-2(5*H*)-furanone	1716	0.10	0.20	c	*p*-methoxyacetophenone	2144	b	b	c
Alcohols									
isobutyl alcohol	1048	c	c	0.11	*α*-terpineol	1679	b	b	c
isopentyl alcohol	1180	b	b	c	decanol	1746	c	b	c
pentanol	1230	0.10	0.21	c	6-mercaptohexanol	1798	3.14	0.56	c
acetoin	1255	3.67	8.78	80.98	benzyl alcohol	1822	0.43	0.35	0.56
acetol	1266	b	b	0.75	phenylethyl alcohol	1858	0.11	0.15	b
cyclopentanol	1283	0.30	0.83	c	methyleugenol	1962	c	c	b
hexanol	1323	1.64	2.52	0.99	3-phenylpropyl alcohol	1989	5.53	1.51	2.60
(*E*)-3-hexenol	1334	0.65	0.44	0.13	*β*-nerolidol	2003	b	b	c
(*Z*)-3-hexenol	1362	5.50	4.98	1.85	eugenol	2103	b	c	b
(*E*)-2-hexenol	1388	0.19	0.24	b	*γ*-cadinol	2125	c	c	b
2,3-butanediol	1494	0.70	c	0.10	*T*-cadinol	2139	c	c	b
octanol	1523	c	c	0.10	*δ*-cadinol	2150	c	c	b
linalool	1529	b	0.11	c	isoeugenol	2180	b	b	c
2-decanol	1613	c	0.55	c	*α*-cadinol	2201	c	c	0.10
menthol	1619	0.34	0.62	c	cinnamyl alcohol	2300	28.31	12.27	1.71
furfuryl alcohol	1623	c	c	0.10					
Acids									
acetic acid	1408	0.16	0.81	0.10	pentanoic acid	1685	0.12	0.14	c
isobutanoic acid	1519	c	b	0.19	hexanoic acid	1789	1.88	1.17	0.69
butanoic acid	1576	c	c	0.48	5-hexenoic acid	1885	2.30	0.98	c
isopentanoic acid	1627	0.12	0.15	0.11	octanoic acid	1998	0.46	0.45	0.32
2-ethylbutanoic acid	1658	3.78	0.81	0.20	benzoic acid	2350	1.76	2.28	0.26
Esters									
ethyl acetate	874	0.95	0.53	0.11	ethylphenyl acetate	1763	c	c	b
ethyl propionate	955	b	0.10	c	phenylethyl acetate	1785	b	c	c
methyl butanoate	980	c	b	c	ethylphenyl propanoate	1846	c	c	0.87
ethyl butanoate	1010	b	b	0.13	*γ*-octalactone	1880	b	b	b
ethyl hexanoate	1241	c	0.10	c	3-phenylpropyl acetae	1930	7.51	6.25	0.87
(*Z*)-3-hexenyl acetate	1311	0.90	0.65	b	hexyl decanoate	2017	b	c	c
ethyl octanoate	1426	c	c	b	(*Z*)-9-tetradecyl acetate	2049	0.37	0.25	c
octyl acetate	1461	c	c	b	ethyl cinnamate	2081	c	c	b
ethyl *β*-hydroxybutanoate	1484	c	c	b	*γ*-decalactone	2098	0.19	0.14	c
methyl benzoate	1608	b	0.47	b	cinnamyl acetate	2100	2.13	1.02	0.13
ethyl benzoate	1658	c	c	0.12	*δ*-decalactone	2153	0.11	0.12	c
γ-hexalactone	1671	0.30	0.47	0.21	(*Z*)-5-(2-pentenylpentanolide-5,1)	2196	0.20	0.24	c
benzyl acetate	1695	c	0.15	c	diethyl phthalate	2311	b	c	c
(*Z*)-3-hexenyl heptanoate	1730	c	c	b	*γ*-dodecalactone	2317	c	c	b
Hydrocarbons									
toluene	1019	c	0.14	c	limonene	1200	c	c	b
ethyl benzene	1098	0.13	0.21	c	*γ*-terpinene	1213	c	c	b
o-xylene	1145	c	0.20	b	*β*-caryophyllene	1617	b	0.20	b
m-xylene	1149	0.11	0.21	b	*α*-humulene	1685	c	b	c
p-xylene	1180	b	b	c	*β*-bisabolene	1735	b	b	c
Miscellaneous Compounds									
isobutyl mercaptan	1054	b	c	c	diethylene glycol monoethyl ether	1589	1.50	1.95	0.26
2-methyl 5-propylfuran	1102	b	c	c	*N*-methylpyrrolidone	1646	b	b	c
2-pentylfuran	1241	b	b	c	diethylene glycol monobutyl ether	1760	b	c	c
N,*N*-dimethylformamide	1304	b	b	0.21	dimethyl sulfone	1833	b	b	c
(*Z*)-linalool oxide	1433	b	b	c	phenol	1933	b	b	c
(*E*)-linalool oxide	1473	b	b	c	diethylene glycol monophenyl ether	2072	0.45	0.36	c
diethylene glycol monomethyl ether	1553	0.16	0.24	c					

[a] Solvent excluded. [b] Area percent less than 0.01. [c] Not detected.

Instruments. A Hewlett-Packard Model 5710-A gas chromatograph equipped with a flame ionization detector (FID) was used for routine gas chromatographic analysis. Two types of wall coated open tubular (WCOT) fused silica capillary columns were used: 50 m × 0.22 mm (i.d.) coated with Carbowax 20M and 60 m × 0.22 mm (i.d.) coated with

OV-101. The oven temperature was programmed from 80 to 200 °C at 2 °C/min. A Hewlett-Packard Model 3385-A integrator was used to determine the GC peak area.

A Hitachi Model M-80 combination mass spectrometer/gas chromatograph (Hewlett-Packard Model 5710A) equipped with Hitachi Model M-6010 and 10 II/A data system was used under the following conditions: ionization voltage, 70 eV; emission current, 80 mA; ion accelerator voltage, 3100/V; ion source temperature, 200 °C.

RESULTS AND DISCUSSION

The volatile compounds identified in the three samples are shown in Table I along with their Kovats indices on a Carbowax 20M (I_K).

The major volatile constituents of guava fresh were C_6 compounds in the present study. The total GC peak area percents of C_6 aldehydes hexanal, (*E*)-3-hexenal, (*Z*)-3-hexenal, (*Z*)-2-hexenal, and (*E*)-2-hexenal were 8% in fresh white and 34% in fresh pink. The C_6 alcohols comprised 8% of the essence from both fresh white and fresh pink. The C_6 acids comprised 4% and 2% of the essence from white and pink, respectively. Therefore, the total amount of C_6 compounds (aldehydes, alcohols, acids) comprised 20% of the essence of fresh white and 44% of the essence of fresh pink in the present study. Idstein and Schreier (1985) reported that 50% of the total volatiles from Brazilian guava were aldehydes. They identified hexanal and (*E*)-2-hexenal as major components and suggested that the presence of high amounts of C_6 aldehydes and alcohols involved enzymic oxidation and reduction of C_6 compounds. The presence of C_6 acids agrees with this hypothesis.

3-Phenylpropyl acetate was found as one of the main components in fresh fruits, but it was detected in only a small amount in canned puree in the present study. Shiota (1978) reported 3-phenylpropyl acetate as one of the minor constituents of puree from Taiwan. Idstein and Schreier (1985) identified it in the fruit pulp from Brazil and listed it in a second major group of guava constituents. Cinnamyl alcohol was the major component (28.3%) of fresh white, and it was the second major component of fresh pink (12.0%) after (*E*)-2-hexenal (16.9%) in the present study but it was found in only trace amount in the fruit pulp from Brazil (Idstein and Schreier, 1985). These aromatic compounds may play an important role in the characteristic sweet flavor of ripening guavas from Amami Island.

It is rather surprising that canned puree contained acetoin in a large amount (81% of the total GC area of the essence). Acetoin has not been reported in guavas prior to the present study, but it was found in other tropical fruits such as mango (Hunter et al., 1974; Engel and Tressl, 1983), papaya (Yamaguchi et al., 1983), and passion fruit (Yamaguchi et al., 1983). The origin of acetoin is not understood, but it may be produced from a sugar degradation reaction (Hodge, 1967) during the canning process. Furanones, the other possible sugar degradation products, were also found in fresh fruits in relatively large quantities. 2,5-Dimethyl-4-hydroxy-3(2*H*)-furanone, which was reported by Idstein and Schreier (1985) for the first time as a guava fruit constituent and comprised 6.3% of the essence from fresh white. On the other hand, it was not detected in canned puree, suggesting a biogenetic origin.

(*Z*)-5-(2-Pentenylpentanolide-5,1), so-called jasmine lactone, is reported here as a fresh guava constituent for the first time. This δ-lactone was found in jasmine oil (Winter et al., 1962) and is characterized as having a peach- or apricot-like note (Arctander, 1969).

Wilson and Shaw (1978) reported that β-caryophyllene was by far the largest single component among the 11 terpene hydrocarbons identified in guava puree from Florida. β-Caryophyllene and limonene comprised over 95% of the hydrocarbon fraction. MacLeod and de Troconis (1982) found slightly more α-humulene than β-caryophyllene, but neither of them was a major component of Venezuelan guava. Only trace amounts of β-caryophyllene and α-humulene were detected in the present study. Limonene, which has been found in many varieties of guavas, was not detected in the fresh fruits and detected only trace amount in canned puree in the present study. On the other hand, bisabolene, which has also been reported in many varieties, was found in fresh fruits but not in canned puree in the present study.

A unique sulfur-containing compound 6-mercaptohexanol was found in fresh fruits for the first time. It was more in fresh white (3.1%) than in fresh pink (0.6%). The difference of flavor characteristics between white and pink guavas may be partially due to the presence of this compound. 3-Pentanethiol is the only thiol compound reported in guava (idstein and Schreier, 1985) prior to the present study. Idstein and Schreier (1985) also reported many S- and N-containing heterocyclic compounds such as thiophenes, thiazoles, and pyrazines for the first time in guava. The origin of these compounds is not clearly known because they form readily from amino acids or protein by heat treatment (Waller and Feather, 1983).

Registry No. Acetaldehyde, 75-07-0; hexanal, 66-25-1; 4-pentenal, 2100-17-6; (*E*)-3-hexenal, 69112-21-6; (*Z*)-3-hexenal, 6789-80-6; (*Z*)-2-hexenal, 16635-54-4; (*E*)-2-hexenal, 6728-26-3; furfural, 98-01-1; (*E*,*E*)-2,4-heptadienal, 4313-03-5; benzaldehyde, 100-52-7; 5-methylfurfural, 620-02-0; *m*-hydroxybenzaldehyde, 100-83-4; cinnamic aldehyde, 104-55-2; acetone, 67-64-1; 3-pentanone, 96-22-0; 2,3-butanedione, 431-03-8; 2,4-dimethyl-3-pentanone, 565-80-0; 2-acetylfuran, 1192-62-7; 2-propionylfuran, 3194-15-8; 3,3,5-trimethyl-2-cyclohexanone, 35413-38-8; methyl benzyl ketone, 103-79-7; 5-ethyl-2(5*H*)-furanone, 2407-43-4; *p*-methylacetophenone, 100-06-1; furfuryl pentyl ketone, 55107-03-4; furfuryl hexyl ketone, 87487-99-8; β-ionone, 79-77-6; 2,5-dimethyl-4-hydroxy-3(2*H*)-furanone, 3658-77-3; 5,6-epoxy-β-ionone, 23267-57-4; isobutyl alcohol, 78-83-1; isopentyl alcohol, 123-51-3; pentanol, 71-41-0; acetoin, 513-86-0; acetol, 116-09-6; cyclopentanol, 96-41-3; hexanol, 111-27-3; (*E*)-3-hexenol, 928-97-2; (*Z*)-3-hexenol, 928-96-1; (*E*)-2-hexenol, 928-95-0; 2,3-butanediol, 513-85-9; octanol, 111-87-5; linalool, 78-70-6; 2-decanol, 1120-06-5; menthol, 89-78-1; furfuryl alcohol, 98-00-0; α-terpineol, 98-55-5; decanol, 112-30-1; ethyl acetate, 141-78-6; ethyl propionate, 105-37-3; methyl butanoate, 623-42-7; ethyl butanoate, 105-54-4; ethyl hexanoate, 123-66-0; (*Z*)-3-hexenyl acetate, 3681-71-8; ethyl octanoate, 106-32-1; octyl acetate, 112-14-1; ethyl β-hydroxybutanoate, 5405-41-4; methyl benzoate, 93-58-3; ethyl benzoate, 93-89-0; γ-hexalactone, 695-06-7; benzyl acetate, 140-11-4; (*Z*)-3-hexenyl heptanoate, 61444-39-1; ethylphenyl acetate, 101-97-3; phenylethyl acetate, 103-45-7; γ-octalactone, 104-50-7; 3-phenyl propyl acetate, 122-72-5; hexyl decanoate, 10448-26-7; (*Z*)-9-tetradecyl acetate, 16725-53-4; ethyl cinnamate, 103-36-6; γ-decalactone, 706-14-9; cinnamyl acetate, 103-54-8; δ-decalactone, 705-86-2; (*Z*)-5-(2-pentenylpentanolide-5,1), 100428-67-9; 6-mercaptohexanol, 1633-78-9; benzyl alcohol, 100-51-6; phenylethyl alcohol, 60-12-8; methyleugenol, 93-15-2; 3-phenylpropyl alcohol, 122-97-4; β-nerolidol, 108911-07-5; eugenol, 97-53-0; γ-cadinol, 50895-55-1; *T*-cadinol, 5937-11-1; δ-cadinol, 19435-97-3; isoeugenol, 97-54-1; α-cadinol, 481-34-5; cinnamyl alcohol, 104-54-1; acetic acid, 64-19-7; isobutanoic acid, 79-31-2; butanoic acid, 107-92-6; isopentanoic acid, 503-74-2; 2-ethylbutanoic acid, 88-09-5; pentanoic acid, 109-52-4; hexanoic acid, 142-62-1; 5-hexenoic acid, 1577-22-6; octanoic acid, 124-07-2; benzoic acid, 65-85-0; diethyl phthalate, 84-66-2; γ-dodecalactone, 2305-05-7; toluene, 108-88-3; ethylbenzene, 100-41-4; *o*-xylene, 95-47-6; *m*-xylene, 108-38-3; *p*-xylene, 106-42-3; limonene, 138-86-3; γ-terpinene, 99-85-4; β-caryophyllene, 87-44-5; α-humulene, 6753-98-6; β-bisabolene, 495-61-4; isobutyl mercaptan, 513-44-0; 2-methyl-5-propylfuran, 1456-16-2; 2-pentylfuran, 3777-69-3; *N*,*N*-dimethylformamide, 68-12-2; diethylene glycol monomethyl ether, 111-77-3; diethylene glycol monoethyl ether, 111-90-0; *N*-methylpyrrolidone, 872-50-4; diethylene glycol monobutyl ether, 112-34-5; dimethyl sulfone, 67-71-0; phenol, 108-95-2; diethylene glycol monophenyl ether, 104-68-7.

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Received for review February 18, 1988. Accepted June 13, 1988.

Selection and Classification of Volatile Compounds of Apricot Using the RV Coefficient

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The RV coefficient is a measure of similarity between two sets of variables recorded from the same sample. If the number of variables in a principal-component analysis is high, the RV coefficient allows selection of a few variables without disturbing the relative location of individuals in the first sample plots. This selection is explained and improved by a classification of variables based on the RV coefficient to define proximities between variable clusters. The groups are then submitted to a principal-coordinate analysis and minimum spanning tree using the RV matrix among the groups in order to describe relations between variable cluster. This statistical approach appears to be a very useful tool for chromatographic data handling. An example is given in a study of 56 volatile compounds quantified in 18 samples of apricots. It shows that compounds are grouped according to the chemical classes.

Progress in gas chromatography allows the separation and quantification of a great number of volatile compounds in foods or beverages. Assume that n chromatograms have been processed and p compounds quantified in each. These data are customarily arranged into a $n \times p$ matrix $\mathbf{X}$, in which the ith row contains the p observations of variables (volatile compounds) recorded on the ith individual (chromatogram). The sample can be seen geometrically as a configuration of n points in a p-dimensional space.

Today, principal-component analysis (PCA) (Morrisson, 1976) is a classical tool in food science, as shown in the bibliography of Martens and Harries (1983) and in the methodological paper of Piggot and Sharman (1986). PCA gives an orthogonal system of principal directions of the variance of this configuration. The answer is given by the first eigenvectors of the $p \times p$ covariance matrix $\mathbf{C}$ of the compounds; if the variables have been previously autoscaled, $\mathbf{C}$ becomes the correlation matrix. Each eigenvector is defined by a linear combination of the p compounds. The interpretation of a principal component amounts to the comparison of the p coefficients of the associated linear combination.

A few problems appear when p is large (for instance higher than 30). On one hand, matrix $\mathbf{C}$ cannot be loaded in the memory of some microcomputers and the length of computing time would be prohibitive. On the other hand, and this is the main problem, the interpretation of a linear combination of so many variables would certainly be tiresome and not very convincing. In fact, a few compounds only are generally heavily loaded on the first principal axes, while the other ones only bring a background noise. However, it is often difficult to distinguish between that noise and main information and to decide which are the relevant correlations between variables and principal components. It would be of great interest to have previous knowledge of the relevant variables and then perform the PCA with these compounds only. Moreover, if p is greater than n, PCA can be performed, but $p-n$ dimensions of the sample configuration space are of course unnecessary.

The RV coefficient (Escoufier, 1970, 1973) is a measure of similarity, varying from 0 to 1, between p-dimensional and q-dimensional configurations of the same sample. It can be seen as a generalized correlation coefficient between

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0021-8561/89/1437-0142$01.50/0