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Characterization of the Aromatic Profile in Aqueous Essence and Fruit Juice of Yellow Passion Fruit (*Passiflora edulis* Sims F. *Flavicarpa degner*) by GC−MS and GC/O

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Chemical characterization by gas chromatography−mass spectometry (GC−MS) of the aromatic profile of yellow passion fruit essence and the juice of the fruit yielded a total of 62 and 34 components, respectively. Four new components have been identified and quantified for the first time in this fruit: 3-methyl-2-butanone; ethyl lactate (quantified only in the fruit juice); diethyl malonate (quantified only in the essence); and 3-penten-2-ol (quantified in both samples). Analysis of these samples by gas chromatography/olfactometry (GC/O) yielded a total of 66 components which appear to contribute to the aroma of passion fruit juice and its aqueous essence. Of these, four could not be quantified by GC−MS: acetic acid, ethyl propionate, ethyl 3-oxobutyrate, and propyl hexanoate. New components were described for the first time as constituents of the aromatic profile in this fruit including acetal, 1,3-dimethyl benzene, and 2-methylbutyl hexanoate. Aroma extract dilution analysis (AEDA) allowed for the detection of the most potent odorants in the commercial essence (2-methylbutyl hexanoate and hexyl hexanoate) and in the fresh juice (1,3-dimethyl benzene and 2-methylbutyl hexanoate). 2-Methylbutyl hexanoate, considered as one of the most potent odorants in this fruit, has been described for the first time as an aromatic constituent of yellow passion fruit.

KEYWORDS: GC−MS; GC/O; AEDA; yellow passion fruit; aqueous essence; fruit juice

INTRODUCTION

The term passion fruit represents the species *Passiflora edulis* Sims of which there are two forms: purple fruit and yellow fruit. Because of its more desirable flavor, the purple passion fruit is preferred for consumption as fresh juice, whereas the yellow passion fruit is considered better suited for processing (*1*). Yellow passion fruit is one of the most popular and best known tropical fruits, having a floral, estery aroma with an exotic tropical sulfur note (*2*). Because of their unique and delicate flavor, *P. edulis* varieties have been the subject of intensive research which has resulted in the characterization of a broad spectrum of volatile constituents (*3*). So far more than 200 components have been described as components of the flavor of this fruit. One class of the components stands out of this diverse mixture of compounds, namely volatile sulfur compounds. Of these, 3-(methylthio) hexanol, a mixture of (*Z*) and (*E*)-2-methyl-4-propyl-1,3-oxathiane, and (*Z*) and (*E*)-2-methyl-4-propyl-1,3-oxathiane-3-oxide, have been described as key odorants in the aroma of the yellow passion fruit by Winter et al. (*4*, *5*). The presence of these components, which impact the aromatic character in the fruit, has been reported by several researchers. Engel and Tressl (*6*) described for the first time the presence of 3-mercaptohexanol and the acetates, butanoates, and hexanoates of both 3-mercaptohexanol and 3-(methylthio) hexanol. Later, Werkhoff et al. (*2*) reported about 180 components for the first time in this fruit and declared that the attractive tropical flavor note of the ripe yellow passion fruits is associated with trace levels of sulfur compounds. These sulfur-containing components possess high odor intensities and low threshold values. The authors reported the presence of 47 new sulfur components in this fruit.

Recently Jordán et al. (*7*) studied the aromatic profile of yellow passion fruit aqueous essence. These authors reported a total of 51 compounds and concluded that the four most abundant compounds identified in order of relative abundance were linalool, octanol, ethyl hexanoate, and ethyl butanoate. A more in-depth study is necessary to accurately determine the aromatic profile of the aqueous essence and the juice of this fruit. More importantly, the real contribution of each component to the aromatic quality of the fruit can be known only by studying the aroma activity of each component. Gas chromatography/olfactometry (GC/O) has proven to be a powerful method to determine key aroma compounds in food (*8*). At the present time, olfactometric techniques can be classified into three categories: dilution methods; intensity methods; and detection frequency method (*9*). Aroma extract dilution analysis (AEDA) (*10*) is commonly applied and suitable to perceive the impact odorants in food. So far no research involving the aromatically active components in yellow passion fruit by GC/O has been

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accomplished. An integrated approach involving the joint determination of the volatile compounds in the passion fruit paste and passion fruit essence by GC−MS and the GC/O profile would provide useful information about the most important active contributors to these fruits.

MATERIALS AND METHODS

Yellow Passion Fruit Samples. Unpasteurized yellow passion fruit juice and aqueous essence were obtained from a local manufacturer of aqueous essences located in Florida. Both the essence and the juice were derived from the same fruit source. The aqueous essence was manufactured by a proprietary process that utilizes low temperature, short time, and steam distillation.

Extraction of Volatile Compounds. *Yellow Passion Fruit Juice.* Isolation of volatile compounds was made using a liquid extraction technique. Cyclohexanone (10 ppm) was added to 120 g of juice. The volatile components in the juice were then extracted with 80 mL of methylene chloride (Sigma Chemical Co., St. Louis, MO) by stirring for 1 h with a magnetic stirrer at approximately 2 °C. The resulting mixture was centrifuged for 10 min (5000 rpm, approx. 3000*g*),and the organic layer was dried with sodium sulfate and concentrated to approximately 1 mL using a distillation−rectification system, followed by further concentration to 0.1 mL by a flow of nitrogen.

Yellow Passion Fruit Essence. Essence (3 mL) with 10 ppm added cyclohexanone was extracted twice with 2 mL of methylene chloride for each extraction using two glass syringes connected by a stainless steel luer lock adaptor and combined. The final emulsion was centrifuged as above, and the organic layer was recovered. This fraction was concentrated to 0.1 mL using a flow of nitrogen. The extraction efficiencies for the yellow passion fruit essence and yellow passion fruit juice were 98%. Extraction efficiency was determined by considering the relative concentrations of all components recovered from three serial extractions for the essence and two for the juice.

GC−MS Analysis. The qualitative and quantitative analyses of the volatile compounds were made using an Agilent model 5973N MSD mass spectrometer (MS) with a 7683 autosampler and model 6890 gas chromatograph (GC) equipped with a 30 m × 0.25 mm i.d. HP-5 (cross-linked phenyl-methyl siloxane) column with 0.25 mm film thickness (Agilent, Palo Alto, CA). The initial oven temperature was held at 40 °C for 6 min. It was then increased at 2.5 °C/min to 150 °C, and finally at 90 °C/min to 250 °C. The injection port and ionizing source were kept at 250 °C and 280 °C, respectively. The split ratio was 10:1 with 2 μL of sample injected. There was a solvent delay of 2 min after which the mass spectrum was collected from *m*/*z* 35−350 generating 5.27 scans/s. Compound identifications were made by comparison of the mass spectra and retention times with those of corresponding reference standards (Aldrich Chemical Co., St. Louis, MO and Bedoukian Research, Inc., Danbury, CT) for all compounds except 2-methyl-3-buten-2-ol, propyl propionate, isobutyl propionate, 2-methyl-1-butanol acetate, propyl butyrate, butyl propionate, isoamyl propionate, 3-(methylthio)-1-propanol, ethyl 3-(methylthio) propionate, (*Z*)-6-nonen-1-ol, (*Z*)-3-octen-1-ol acetate, and methyl 3-phenylpropanoate which were identified by the NIST98 library (NIST, Gaithersburg, MD) and previously reported retention indices.

Quantification. For the purpose of quantifying identified components, linear regression models were determined using standard dilution techniques with cyclohexanone as internal standard. Target ions were used in the identification and quantification of each component by the mass spectrometer. Standard reference compounds were used in all cases if commercially available. For the quantification of the three compounds that were not available, linear regressions of similar components were used. The substitutions were: 3-methyl-2-butanone by 3-methyl-butanal, ethyl 3-(methylthio) propanoate by methyl 3-(methylthio) propanoate, and (*Z*)-3-hexenyl hexanoate by hexyl hexanoate. Two different extractions of the volatile components were made for the essence and the juice, respectively. Three runs were made for each extraction, and six values were compiled for determining the standard deviations values.

GC/Olfactometry. The analysis was carried out using a Hewlett-Packard 5890 Series II plus chromatograph equipped with a 30 m × 0.25 mm i.d. HP-5 (cross-linked phenyl-methyl siloxane) column with 0.25 mm film thickness (Palo Alto, CA) directly connected to a Hewlett-Packard 5970 series mass selective detector and a sniffing port (Gerstel, Inc., Baltimore, MD). The GC effluent was split 1/1 between the mass spectrometer and the sniffing port. The injector and detector temperatures were maintained at 250 °C and 280 °C, respectively. The transfer line to the GC/O sniffing port was held at 300 °C. The volume of extract analyzed and oven program temperatures were the same as those described above for the GC−MS. Humidified air was added in the sniffing port at 100 mL/min. Compound identifications were made by comparison of the mass spectra, retention times, and the Kovat's index (as determined relative to alkanes from pentane to pentadecane) of the volatile components in both extracts with those of corresponding reference standards. The mass spectrometer retention times were compared with the retention times measured in the olfactometry runs, and both were compared to reference standards. Data were collected using the ChemStation G1701AA data system (Hewlett-Packard, Palo Alto, CA).

Olfactometry Global Analysis (Frequency Response). GC/O frequency analysis was performed by using a modified version of the method reported by Pollien et al. (*11*). Three panelists analyzing each sample in triplicate were used for the detection of aromatically active compounds, and verbal descriptors of the odor active components were recorded for both extracts. Aromatically active components were those that were detected and described using identical terms by at least one panelist three times.

AEDA. This technique was performed according to the method defined by Grosch (*12*). Serial dilutions of the extracts were made in a proportion of 1:3 in dichloromethane and sniffed until no components could be perceived by any of the panelists. The results are expressed as a flavor dilution factor (FD factor = 3^{n-1}, with n = number of coincident responses.

RESULTS AND DISCUSSION

Volatile Components in Yellow Passion Fruit Essence and Juice. Analysis of the aromatic profile by GC−MS in the commercial essence and the fresh juice resulted in a total of 62 and 34 components quantified, respectively (**Table 1**). The aromatic fraction of the commercial essence consists of 32 esters, 17 alcohols, 5 ketones, 3 terpenic hydrocarbons, 2 acids, 1 sulfur compound, and 1 furan. 2-Methyl-propanol, ethyl propionate, ethyl butyrate, ethyl hexanoate, octanol, and hexyl hexanoate were the components found in greatest concentrations. For the juice extracts 14 esters, 7 alcohols, 5 ketones, 3 aldehydes, 3 terpenic hydrocarbons, and 2 acids comprise the aromatic profile. Among these components, 3-hydroxy-2-butanone, ethyl 3-hydroxy butyrate, ethyl hexanoate, benzyl alcohol, octanoic acid, and hexyl hexanoate were the most abundant compounds.

In both samples almost half the compounds are esters and are the components found in the biggest concentrations. These results agree with those found by Chen et al. (*13*), who reported a total of 60 components in the headspace of passion fruit juice and that ethyl acetate, ethyl butanoate, ethyl hexanoate, hexyl butanoate, and hexyl hexanoate were among the major esters identified. Werkhoff et al. (*2*) completed an extensive study about the flavor chemistry of yellow passion fruit, and they reported 180 new components identified for the first time in this fruit. We can now add new components found in the present study not previously reported by these researchers. Among these are 3-methyl-2-butanone, ethyl lactate, 5-hydroxymethyl furfural (found only in the juice of the fruit), diethyl malonate (found only in the essence), and 3-penten-2-ol (found in both samples).

The comparative study between the aromatic profile of the commercial essence and the juice reveal that esters with the highest volatility were not detected in the juice. Ethyl butyrate, followed by ethyl hexanoate and hexyl hexanoate, were the esters found in greatest concentration in the essence. In the juice,

Table 1. Volatile Components Quantified in Yellow Passion Fruit Essence and Yellow Passion Fruit Juice by GC–MS

component	RT (min)	Kovat's index[b]	concentration: ppm (SD)[a]	
			passion fruit essence	passion fruit juice
ethyl acetate	2.14	613	n.c.	n.c.
2-methyl-propanol	2.30	619	109.81 (7.52)	n.d.
3-methyl-2-butanone	2.50	707	n.d.	1.56 (0.11)
1-butanol	2.71	653	10.22 (0.60)	n.d.
2-pentanone	2.92	687	3.53 (0.19)	n.d.
3-penten-2-ol	3.06	774	1.47 (0.15)	0.75 (0.04)
2-pentanol	3.25	706	5.30 (0.46)	n.d.
ethyl propionate	3.30	709	43.22 (2.23)	n.d.
propyl acetate	3.35	716	1.19 (0.07)	n.d.
3-hydroxy-2-butanone	3.44	711	2.50 (0.11)	27.87 (0.85)
methyl butyrate	3.52	723	2.65 (0.41)	n.d.
3-methyl-1-butanol	4.08	737	17.30 (0.76)	0.33 (0.03)
isobutyl acetate	4.90	753	1.12 (0.03)	n.d.
3-hexanone	5.30	787	0.62 (0.09)	n.d.
diethyl carbonate	5.41	765	3.87 (0.12)	n.d.
cyclopentanone	5.54	766	10.74 (0.22)	0.54 (0.03)
ethyl butyrate	5.99	771	215.40 (8.49)	3.86 (0.31)
butyl acetate	6.54	816	2.35 (0.11)	n.d.
2,3-butanediol	6.74	782	n.d.	0.55 (0.07)
ethyl lactate	6.81	788	4.77 (0.18)	0.33 (0.09)
2-cyclopenten-1-one	7.63	802	0.50 (0.04)	n.d.
furfural	7.75	852	n.d.	0.42 (0.06)
ethyl crotonate	8.15	812	4.41 (0.10)	0.03 (0.01)
(*E*)-3-hexen-1-ol	9.05	828	6.98 (2.16)	n.d.
(*Z*)-3-hexen-1-ol	9.31	852	1.70 (0.10)	n.d.
isoamyl acetate	9.78	880	28.92 (2.69)	n.d.
hexanol	10.27	865	9.78 (1.30)	1.56 (0.06)
2-heptanol	12.01	974	1.87 (0.15)	n.d.
γ-butyrolactone	12.57	891	n.d.	1.26 (0.18)
methyl hexanoate	12.64	934	0.69 (0.01)	n.d.
ethyl 3-hydroxybutyrate	13.82	914	9.89 (0.29)	6.62 (0.16)
ethyl acetoacetate	14.71	930	4.34 (0.48)	n.d.
benzaldehyde	15.13	962	25.35 (2.36)	3.06 (0.46)
myrcene	16.64	989	4.37 (0.82)	0.58 (0.08)
butyl butyrate	17.00	993	0.48 (0.02)	n.d.
ethyl hexanoate	17.42	997	183.21 (13.48)	5.08 (0.28)
(*Z*)-3-hexenyl acetate	17.79	985	6.63 (0.33)	n.d.
hexyl acetate	18.24	1008	21.10 (1.57)	0.98 (0.03)
limonene	18.85	1031	6.59 (1.58)	0.5 (0.05)
(*E*)-β-ocimene	19.73	1048	1.06 (0.25)	0.69 (0.65)
hexanoic acid	19.95	970	26.78 (2.75)	tr
ethyl 2-hexenoate	20.23	1030	3.61 (0.25)	n.d.
ethyl 2-furoate	21.10	1045	0.73 (0.10)	n.d.
benzyl alcohol	21.40	1033	1.35 (0.09)	4.74 (0.05)
(*Z*)-linalool oxide	21.95	1060	3.42 (0.20)	n.d.
diethyl malonate	22.13	1064	0.43 (0.11)	n.d.
1-octanol	22.76	1075	67.47 (4.82)	n.d.
ethyl 3-(methylthio) propanoate	23.81	1094	1.97 (0.08)	n.d.
furaneol	24.28	1090	n.d.	tr
linalool	24.30	1101	18.18 (1.84)	n.d.
2-phenylethanol	25.64	1116	1.28 (0.41)	1.57 (0.37)
ethyl 3-hydroxyhexanoate	25.84	1130	5.04 (0.33)	2.63 (0.22)
isobutyl hexanoate	26.54	1143	0.56 (0.13)	n.d.
benzyl acetate	27.83	1163	5.64 (0.35)	0.23 (0.05)
terpinen-4-ol	28.67	1182	1.60 (0.27)	n.d.
diethyl succinate	28.70	1179	n.d.	0.8 (0.08)
hexyl butyrate	29.03	1191	20.55 (4.07)	1.17 (0.19)
ethyl octanoate	29.38	1195	18.84 (3.28)	1.01 (0.18)
propyl acetate	29.86	1203	3.21 (0.36)	0.98 (0.07)
octyl acetate	30.24	1200	3.35 (0.59)	0.24 (0.01)
octanoic acid	31.22	1179	1.98 (0.28)	5.0 (0.43)
2-methylhexyl butyric acid	31.45	1234	0.58 (0.09)	n.d.
citronellol	31.91	1228	2.24 (0.54)	n.d.
isoamyl hexanoate	32.29	1247	2.70 (0.35)	n.d.
2-phenylethyl acetate	33.02	1260	1.09 (0.06)	n.d.
5-hydroxymethyl furfural	34.43	1285	n.d.	tr
geraniol	33.37	1240	18.14 (2.99)	n.d.
benzyl butyrate	37.91	1345	1.37 (0.08)	n.d.
(*Z*)-3-hexenyl hexanoate	39.44	1375	11.91 (1.49)	1.25 (0.30)
hexyl hexanoate	39.75	1383	77.64 (11.36)	9.90 (1.75)

[a] n.d., not detected; tr, trace; n.c., not calculated. [b] Directly from, or interpolated from, values obtained from Kondjoyan and Berdagué (*14*).

the order of abundance was hexyl hexanoate, followed by ethyl 3-hydroxy-butyrate, ethyl hexanoate, and ethyl butyrate. These differences can be explained by the affinity of these compounds to water. Moreover, as was to be expected, compounds with high volatility were extracted in greatest concentration during the distillation process.

Similar results were observed for the alcohols, but in this case the components found in greatest concentration in the essence (2-methyl-1-propanol, octanol, linalool, and geraniol) were not detected in the juice of the fruit. Only benzyl alcohol and 2-phenylethanol were quantified in greater concentrations in the juice than in the essence.

With respect to the rest of the components identified, it is interesting to note that only one sulfur component has been identified and quantified in the commercial essence of this fruit. According to Engel and Tressl (*6*) and Werkhoff et al. (*2*), sulfur-bearing molecules are organoleptically by far the most interesting components in yellow passion fruits. These researchers identified a total of 47 sulfur components in the fruit. These differences can be explained on the basis that a flame photometric detector specific for the detection of these components was used.

Three furan compounds were identified only in the juice of the yellow passion fruit. Among them 5-hydroxymethyl furfural is described for the first time in this fruit. It is possible that the distillation−rectification device used during the concentration process may be responsible for the formation of these furan compounds as artifacts.

GC/O. *Olfactometric Global Analysis (Frequency of Detections).* To study the aromatic profile of yellow passion fruit juice and essence the determination of those components responsible for the quality of the aroma of this fruit was necessary, and for this purpose gas chromatography/olfactometry was used. The aromatic descriptors for all volatile components perceived by panelists in commercial essence and fruit juice of yellow passion fruit are shown in **Table 2**. All the descriptors listed were described at least three times.

As a result of the different aroma thresholds of each component, not all of the compounds quantified contribute to the aroma in the passion fruit essence and juice. However, olfactometric analysis allows for the detection of components which were not quantified by GC−MS (acetic acid, heptane, 3-methyl-2-buten-1-ol, ethyl pentanoate, ethyl 3-oxobutyrate, 6-methyl-5-hepten-2-one, 5-methyl furfural, γ-hexalactone, heptanoic acid, propyl hexanoate, and eugenol), and even the identification of new components described for the first time as constituents of the aromatic profile in this fruit including acetal, 1,3-dimethyl benzene, and 2-methylbutyl hexanoate.

Regarding yellow passion fruit essence, 54 components appear to contribute to the overall aroma. Among them, acetal, isobutyl acetate, ethyl butyrate, ethyl lactate, ethyl hexanoate, hexanoic acid, octanol, linalool, benzyl acetate, and 2-methylbutyl hexanoate define the aroma of this commercial essence because they were perceived by all the panelists in all the replications. However, it is important to include the contributions of other components that have not been recognized in all the replications but that have been perceived by all the panelists including heptane, 3-methyl-1-butanol, 1,3-dimethyl benzene, ethyl pentanoate, ethyl-3-hydroxy butyrate, 6-methyl-5-hepten-2-one, ocimene, benzyl alcohol, and propyl hexanoate.

For the fruit juice, 55 components appear to contribute to the overall aroma. 2-Pentanone, isobutyl acetate, ethyl butyrate, ethyl lactate, 1,3-dimethyl benzene, ethyl hexanoate, benzyl alcohol, octanol, ethyl 3-hydroxy hexanoate, and 2-methylbutyl hexanoate define the aroma of the fresh juice because they were perceived by all the panelists in all the replications. Components which should be considered as important contributors to the aroma of this juice and which have been described by all the panelists, although not in all nine runs, include heptane, 3-methyl-1-butanol, 6-methyl-5-hepten-2-one, ethyl-3-(methylthio) propanoate, benzyl acetate, hexyl butyrate, isoamyl hexanoate, and two unknown components. Components which may contribute to the aromatic differences between the commercial essence and the fruit juice include those components perceived by all the panelists and only detected in the commercial essence or in the juice samples. Among these, 2-pentanone**,** ethyl 3-(methylthio)propanoate, furaneol, and four unknown components have been perceived only in the juice. Acetal, (*Z*)-3-hexen-1-ol, (*Z*)-3-hexenyl acetate, ocimene, one not-positively-identified component, and hexyl hexanoate were described as aromatic components of only the commercial essence by the three panelists.

Werkhoff et al. (*2*) studied the aromatic profile of yellow passion fruit and reported that this fruit is characterized by an exotic estery aroma with a sharp sulfury note. At the same time, these authors declared that these sulfur components, because of their high odor values and their olfactive profiles, are expected to be key ingredients of the yellow variety. In this study, ethyl 3-(methylthio)propanoate was the only sulfur compound identified, and it contributed a menthol, caramel, and medicinal aroma. For this reason the next step in the present study was the determination of the key aroma components of this juice and its corresponded commercial essence by AEDA.

AEDA. The results obtained by using aroma extract dilution analysis in commercial essence and fresh juice are shown in **Table 2**. In the development of this study two judges were utilized, and values of AEDA are reported as FD factor $= 3^{n-1}$ where n corresponds to the number of dilutions in which the compound was detected.

In the commercial essence, two components appear to be the most intense odorants (FD values of 2187): 2-methylbutyl hexanoate which contributes to a sharp sweat odor and hexyl hexanoate which contributes to a peach and plum odor. Other components that need to be considered as impact odorants were 2-hepatanol, ethyl hexanoate, and linalool. Regarding the fresh juice, two components appear to be the most intense odorants, one of them coinciding with that found in the commercial essence, 2-methylbutyl hexanoate, and the other one being 1,3-dimethyl benzene, which is described for the first time as a contributor to the aromatic profile in this fruit.

It should be noted that hexyl hexanoate was found to be one of the strongest odorants in the essence, but it was not perceived in the juice by the panelists. This might be due to the extraction efficiency of the essence, from which this component was recovered in a higher concentration (**Table 1**), and its presence in the juice at a concentration lower than its aromatic threshold. Other components which have been perceived in high dilution include ethyl butyrate, ethyl lactate, ethyl pentanoate, 2-heptanol, furfural, 6-methyl-5-hepten-2-one, ethyl hexanoate, hexanoic acid, octanol, propyl hexanoate, linalool, furaneol, phenylethyl alcohol, isobutyl hexanoate, diethyl succinate, hexyl butyrate, and isoamyl hexanoate. These differences among the components detected in the highest dilutions in commercial essence and the fresh juice, might be the cause of the different aroma perceived in both samples.

In general, the components that have been perceived by all the panelists also have the highest dilution factors, except for low-boiling-point components such as 2-pentanone, heptane,

Table 2. Odor Active Components in Yellow Passion Fruit Essence and Yellow Passion Fruit Juice by GC/O

component	RI	descriptors	frequency of detection		AEDA FD Factor			
					essence		juice	
			essence	juice	J-1	J-2	J-1	J-2
ethyl acetate	664	fruity, acid	6	6	3	3	3	1
acetic acid	677	acid, fruity, plastic	4	4	3	1	3	1
2-pentanone	679	burnt plastic, pungent	0	9			3	3
heptane	698	burnt matches, plastic, floral	8	8	27	1	9	1
acetal	719	tropical fruit, sweet	9	0	9	1		
methyl butyrate	726	fruity, floral, roasted nut	3	4	3	1	1	1
3-methyl-1-butanol	742	onion, gasoline, rubber, burnt oil	7	7	3	1	9	1
isobutyl acetate	758	herbal, plastic, solvent	9	9	27	9	81	9
3-methyl-2-buten-1-ol	763	cooked nut	0	3			9	1
2,3-butanediol	778	faint herbal	0	4			1	1
ethyl butyrate	781	fruit, sweet, strawberry candy	9	9	81	81	243	9
ethyl lactate	798	onion, pungent, rubbery	9	9	3	3	243	9
ethyl crotonate	835	faint tropical fruit	3	5	1	1	3	1
(*Z*)-3-hexen-1-ol	841	green, herbal, unripe banana	5	0	3	1		
1,3-dimethyl benzene	852	nut, medicinal, oily, fried	7	9	3	9	2187	243
hexanol	863	herbal, fruity	4	0	1	1		
ethyl pentanoate	885	dry fish, nutty, herbal	7	6	81	1	243	1
2-heptanol	894	mush potato, fried, oily	6	5	243	3	243	9
NPI	895	burnt matches, cooked meat, fried chicken	0	6			1	3
furfural	899	fresh garlic, rubber, moldy	3	3	27	1	729	1
γ-butyrolactone	910	toasted nut, cheesy	3	5	3	1	1	9
ethyl 3-hydroxy-butyrate	931	pesticide, roasted nut, medicinal	7	6	3	1	9	1
ethyl 3-oxo-butyrate	943	ripe onion, pesticide, medicinal	3	3	1		3	1
benzaldehyde	954	roasted pepper, green almond	0	3			9	
NPI	956	spicy, plastic, mushroom	0	8			1	1
6-methyl-5-hepten-2-one	970	plastic, mushroom	7	8	9	1	243	9
5-methyl furfural	976	roasted garlic, spicy, metallic	4	4	9	1	81	1
β-myrcene	982	fruity, herbal, spicy	3	0		3		
ethyl hexanoate	995	anise, fruit over ripe	9	9	243	27	243	81
(*Z*)-3-hexenyl acetate	1002	fruity, candy, banana	6	0	3	3		
hexyl acetate	1010	banana, fruity, cherry	5	4	3	1	1	1
limonene	1022	herbal, mild fruit, pesticide	4	5	27	1	1	1
hexanoic acid	1036	pesticide, pungent, oily	9	3	81	1	729	
ocimene	1043	floral, rose, spicy, carnation	7	0	9	9		
benzyl alcohol	1051	sunflower seeds, herbal, moldy, roasted bread	8	9	27	1	81	3
γ-hexalactone	1059	ripe onion, pesticide	5	5	3	3	3	1
heptanoic acid	1067	liquorice fruit, floral, apricot	5	0	3	1		
octanol	1077	skin potato, burnt matches, fatty, bitter almond	9	9	81	81	243	243
propyl hexanoate	1092	petrol, roasted garlic, skin potato, pesticide	8	3	27	3	243	1
ethyl 3-(methylthio) propionate	1102	eucaliptol, mentol, caramel, medicinal	0	7			81	9
linalool	1103	sweet, fruit, floral, lemon	9	5	729	27	243	1
NPI	1115	nutty, caramel, sweet potato	3	5	1		81	1
furaneol	1121	caramel, passion fruit	0	6			243	1
phenylethyl alcohol	1125	talc powder, fruity, floral	6	6	9	3	729	81
ethyl 3-hydroxy hexanoate	1136	floral, pasion fruit, sharp herbal, fruity	6	9	81	81	81	9
NPI	1146	basil leaves	3	0	9			
isobutyl hexanoate	1148	plastic, pesticide, spicy, green	6	5	81	81	243	3
NPI	1155	caramel, floral, fruity	6	3	81	1	1	
NPI	1157	herbal, fruity, celery	0	5			1	1
benzyl acetate	1161	menthol, woody, honey, rain	9	8	81	1	81	1
diethyl succinate	1166	fabric, floral, cotton	6	4	81	1	243	1
NPI	1174	celery leaves	0	5			9	1
hexyl butyrate	1192	toothpaste, fresh, medicinal, faint citrus-like	3	8	1		243	9
octyl acetate	1205	woody, tar, burnt plastic	0	4			1	1
isoamyl hexanoate	1243	anise, spicy, fruity	5	8	1	81	243	81
2-methylbutyl hexanoate	1246	sharp sweat	9	9	2187	2187	2187	729
geraniol	1257	tropical fruit, passion fruit, peach	3	3		3		1
NPI	1262	vanilla, aromatic herbs	0	3			27	
NPI	1270	spicy, cinnamon	0	4			81	9
NPI	1280	spicy, fruity, floral	3	3		1		9
NPI	1287	herbal, roses, carnation, balsamic, vanilla	3	3	1		9	
NPI	1308	pollen, floral, camphor	0	7				3
NPI	1320	moldy orange, spicy, woody	0	6			3	9
benzyl butyrate	1337	sweet, peachy	3	0	1			
eugenol	1351	spicy, fruity	6	0	1	1		
hexyl hexanoate	1370	peachy, plum	6	0	729	218	729	218

[a] NP, not positively identified.

3-methyl-1-butanol, acetal, ethyl 3-hydroxy butyrate, and ocimene, which were detected by all the panelists in almost all the replications and have low dilutions factors, and furfural which was only detected three times and was present at a high dilution coefficient in the juice.

LITERATURE CITED

(1) Bora, P. S.; Narain, N. Passion fruit. In *Postharvest Physiology and Storage of Tropical and Subtropical Fruits*; Mitra, S., Ed.; CAB International: New York, 1997; pp 375−386.

(2) Werkhoff, P.; Guntert, M.; Krammer, H.; Sommer, H.; Kaulen, J. Vacuum headspace method in aroma research: Flavor chemistry in yellow passion fruits. *J. Agric. Food Chem*. **1998**, *46*, 1076−1093.

(3) Whitfield, F. B.; Last, J. H. The flavour of the passion fruit - a review. In *Progress in Essential Oil Research*; Brunke, E. J., Ed.; de Gruyter: Berlin, 1986; pp 3−48.

(4) Winter, M.; Furrer, A.; Willhalm, B.; Thommen, W. Identification and synthesis of two new organic sulfur compounds from the yellow passion fruit (*Passiflora edulis* f. *flavicarpa*). *Helv. Chim. Acta* **1976**, *59*, 1613−1620.

(5) Winter, M. Oxathiane and oxathiolane derivates as perfuming agents. U.S. Patent 4,220,561, 1980.

(6) Engel, K. H.; Tressl, R. Identification of new sulfur-containing volatiles in yellow passion fruits (*Passiflora edulis* f. *flavicarpa*). *J. Agric. Food Chem.* **1991**, *39*, 2249−2252.

(7) Jordán, M. J.; Goodner, K. L.; Shaw, P. E. Volatile components in tropical fruit essences: yellow passion fruit (*Passiflora edulis Sims* f. *flavicarpa* Degner) and banana (*Musa sapientum* L.). *Proc. Fla. State Hortic. Soc*. **2000**, *113*, 284−286.

(8) Priser, C.; Etiévant, P. X.; Nicklaus, S.; Brun, O. Representative champagne wine extracts for gas chromatography olfactometry analysis. *J. Agric. Food Chem*. **1997**, *45*, 3511−3514.

(9) Le Guen, S.; Prost, C.; Demaimay, M. Critical comparison of three olfactometry methods for the identification of the most potent odorants in cooked mussels (*Mytilus edulis*). *J. Agric. Food Chem*. **2000**, *48*, 1307−1314.

(10) Ulrish, F.; Grosch, W. Identification of most intense volatile flavour compounds formed during autoxidation of linoleic acid. *Z. Lebensm.-Unters. Forsch.* **1987**, *184*, 277−282.

(11) Pollien, P.; Ott, A.; Montignon, F.; Baumgartner, M.; Muñoz-Box, R.; Chaintreau, A. Hyphenated headspace gas chromatography-sniffing technique: Screening of impact odorants and quantitative aromagram comparison. *J. Agric. Food Chem.* **1997**, *45*, 2630−2637.

(12) Grosch, W. Review: Determination of potent odourants in foods by Aroma Extract Dilution Analysis (AEDA) and calculation of Odour Activity Values (OAVs). *Flavour Fragance J.* **1994**, *9*, 147−158.

(13) Chen, Ch. Ch.; Kuo, M. Ch.; Hwang, L. S.; Swi-Bea, J.; Wu, Ch. M. Headspace components of passion fruit juice. *J. Agric. Food Chem.* **1982**, *30*, 1211−1215.

(14) Kondjoyan, N.; Berdagué, J. L. *A Compilation of Relative Retention Indices for the Analysis of Aromatic Compounds*; Laboratoire Flavour: Theix, France, 1996.

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