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The Construction of Volatile Profiles of Eight Popular Peach Cultivars Produced in Shanghai Using GC-MS and GC-IMS

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Abstract: Peach (*Prunus persica* L.) is an economically important fruit crop worldwide due to its pleasant flavor. Volatile organic compounds (VOCs) are vital factors for assessing fruit quality. Here, we constructed the VOC profiles for the top eight popular commercial peach cultivars produced in Shanghai by combining gas chromatography-mass spectrometry (GC-MS), odor activity value and gas chromatograph-ion mobility spectrometry (GC-IMS). Seventy VOCs were detected using GC-MS, of which twenty-three were commonly found in eight peach cultivars, including hexanal, nonanal, benzaldehyde, 2-hexenal, butyl acetate, hexyl acetate, (*Z*)-3-hexen-1-yl acetate, linalool, β-myrcene, D-limonene, 1-hexanol, 3-hexenol, 2-hexenol, 2-ethyl-1-hexanol, γ-octalactone, δ-decalactone, γ-hexalactone, γ-decalactone, γ-dodecalactone, β-ionone, 2-octanone, 2-ethyl furan and 2,4-ditert-butyl phenol. A total of 17 VOCs were screened on the basis of OAV $\geq$ 1 and the top 5 of this contribution were γ-decalactone, β-ionone, hexanal, 2-hexenal and linalool. Lactones had the highest OAV in HJML and terpenoids had the highest OAV in JC. JXIU had the lowest OAV of lactones and terpenoids. Based on the range of their OAV values, the flavor evaluation standard of Shanghai high-quality peach cultivars can be established, which is also a reference for breeding excellent offspring. Twenty-six VOCs were detected using GC-IMS, and the largest proportion were aldehydes. Principal component analysis (PCA) showed that Hikawa Hakuho (HH) and Jinchun (JC) were distant from the other samples, indicating that their volatiles were more distinct. These results provide a foundation for improving our understanding of aroma compositions in these high-quality peach cultivars, which might also provide a reference for future design breeding to improve fruit flavor.

Keywords: peach; commercial cultivars; VOCs; GC-MS; GC-IMS; OAV

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1. Introduction

The peach (*Prunus persica* (L.) Batsch) has become an important economic crop due to its soft and juicy flesh, attractive aroma and enriched nutrition, and it has been grown extensively at home and abroad [1]. As the originating country of the peach, China holds a large number of wild relatives and landraces [2]. 'Chinese Cling', the most influential founder in peach-breeding history, has derived many excellent cultivars such as 'Elberta', 'J.H. Hale', 'Okubo' and 'Hakuho' [3]. The elite commercial peach cultivars planted in Shanghai, such as 'Hujingmilu' (HJML), 'Xinfengmilu' (XFML) and 'Jinxiu' (JX), are also excellent offspring of 'Chinese Cling'. These cultivars are popular in Shanghai for their high quality and were cultivated in 3100 hectares in 2021, accounting for approximately 82% of the total peach-cultivated area in Shanghai (data source: Shanghai Agricultural Technology Extension Service Center).

Aroma is an essential factor to determine consumers' preference, which has received great attention from geneticists and breeders in recent years [4,5]. The aroma profiles in

fruit result from the interactions of many volatiles. Currently, more than 100 volatiles have been identified in peaches, mainly including aldehydes, alcohols, esters, lactones, terpenes and ketones [6,7]. However, the compositions and content of volatiles are influenced by genetic backgrounds, fruit maturity and cultivation conditions. For instance, aldehydes and alcohols are the major contributors of VOCs in immature fruits and their contents decrease gradually during maturation, while the contents of lactones increase with peach fruit maturation [8]. Studies on several varieties have shown many differences in the composition and content of volatiles. Wang et al. have reported that the Chinese wild peach 'Wutao' has the highest content of total volatiles, while 'Ruipan 14' and 'Babygold 7' show high contents of lactones, and cultivars of American and European origin mainly contain high levels of linalool [7]. Several studies have also shown that cultivation conditions can also influence the composition and content of volatiles, such as fertilization and bagging [9–11]. Although more than 100 VOCs can be detected in peaches, only around 25 of them significantly contribute to flavor quality, and these are recognized as characteristic compounds [12]. The odor activity value (OAV) is commonly used to evaluate the contribution of a compound to the overall aroma, and it represents the ratio of the actual concentration in the sample to the threshold value in water, and was first proposed by Rothe [13]. Compounds with OAV ≥ 1 are not only considered major contributors to flavor, but also good indicators for the breeding of good-quality peaches.

Gas chromatography-mass spectrometry (GC-MS) is a commonly used technique that takes advantage of the high separation ability of GC and the superiority of mass spectrometry in the identification of substances, which allows it to be applied with high sensitivity and precision in the qualitative and quantitative analysis of VOCs in samples [14]. However, due to the complexity of most sample matrices, this method requires tedious and time-consuming sample pretreatment before analysis while working under vacuum conditions, making it unsuitable for rapid characterization studies of VOCs in complex samples [15,16]. Ion mobility spectrometry (IMS) is an atmospheric analytical chemistry method for the detection and identification of different types of substances based on the mobility of gas-phase ions in a weak electric field [15]. GC-IMS integrates the high separation ability of GC with the high sensitivity and fast response of IMS. Compared to GC-MS, it has the advantages of having a lower detection limit, no pre-treatment, convenience and can be operated at atmospheric pressure, which can maximize the authenticity of flavor in samples and reflect the original flavor information [16,17]. The method of combining various techniques to study VOCs in foods has become a hot topic, which can establish a more comprehensive and scientific aroma fingerprint. As far as we know, comparison analysis of volatiles in different commercial peach cultivars based on GC-MS and GC-IMS is rarely reported.

In the present study, the volatiles of eight commercial peach cultivars from Shanghai were analyzed by GC-MS, OAV and GC-IMS to comprehensively investigate their volatile compounds and aroma profiles. The results could improve our understanding of aroma compositions in these high-quality peach cultivars, which might also provide a reference for future design breeding to improve fruit flavor.

2. Materials and Methods

2.1. Plant Materials

Eight elite peach cultivars derived from 'Chinese Cling' were selected in this study, and all of them had a melting texture and displayed strong aromas. The characteristic information of each cultivar is listed in Figure 1 and Table 1. All trees were planted in the Peach Germplasm Repository of the Shanghai Academy of Agricultural Sciences, China (30°89′ N, 121°39′ E), and the orchard management procedures such as irrigation, pruning, disease control and fertilization were the same for all cultivars. Thirty fruits of each cultivar were picked at the commercial harvest stage in the summer of 2022 according to grounded skin color, fruit firmness and recorded maturity time. The fruits were picked from three trees and immediately transported to the laboratory. Fifteen fruits of each cultivar with

uniform size were selected in each biological replicate. The mesocarp was cut into pieces, frozen immediately in liquid nitrogen, grounded into powder and stored at −80 °C for use.

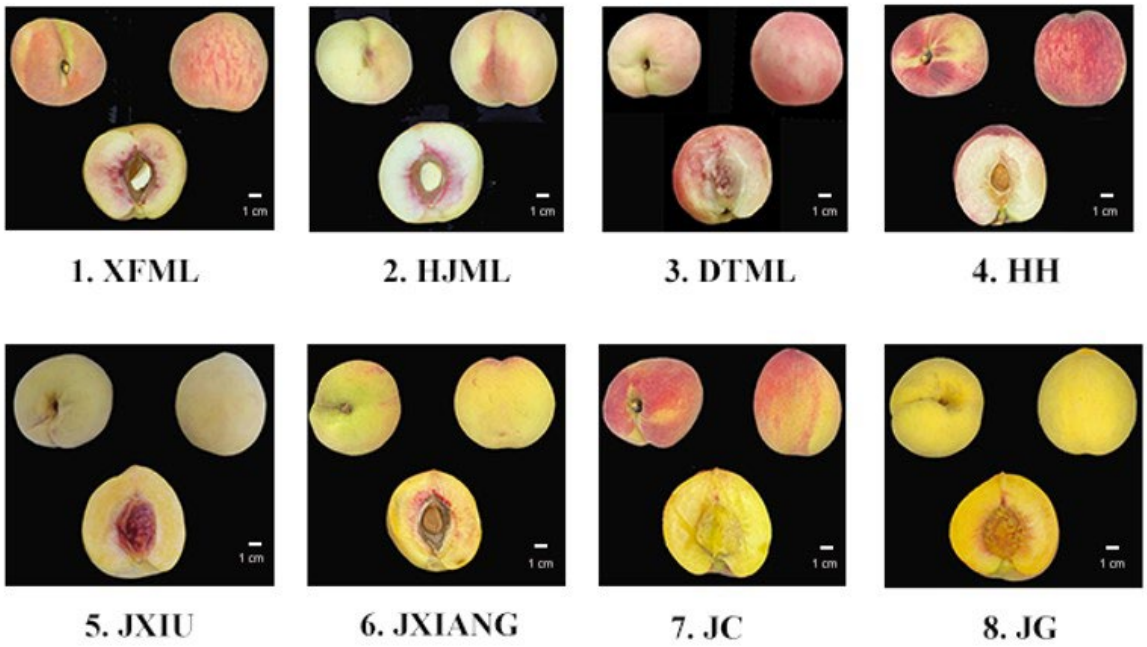


Figure 1. Representative images of eight peach cultivars used in this study. The codes under each image are the abbreviation names for each cultivar.

Table 1. The characteristic information of peach materials.

No.	Cultivar Name	Abbreviation Code	Origin	Flesh Color	Fruit Texture	Brix (%)	Acid	Harvest Date
1	Xinfengmilu	XFML	Shanghai, China	White	Soft-melting	14.9	Sub-acid	Mid-July
2	Hujingmilu	HJML	Jiangsu, China	White	Soft-melting	13.2	Sub-acid	Mid-July
3	Datuanmilu	DTML	Shanghai, China	White	Soft -melting	14.3	Sub-acid	Early-July
4	Hikawa Hakuho	HH	Japan	White	Soft-melting	10.2	Sub-acid	Mid-June
5	Jinxiu	JXIU	Shanghai, China	Yellow	Hard-melting	18.5	Sub-acid	Mid-August
6	Jinxiang	JXIANG	Shanghai, China	Yellow	Hard-melting	10.1	Sub-acid	Early-July
7	Jinchun	JC	Shanghai, China	Yellow	Hard-melting	11.0	Sub-acid	Early-June
8	Jinguan	JG	Shanghai, China	Yellow	Hard-melting	14.6	Sub-acid	Mid-July

2.2. Chemicals

All qualification and quantitative standards were purchased from Sigma Aldrich (Shanghai, China), and their purity was above 95%.

2.3. GC-MS Analysis of Volatile Compounds

The method of sample pretreatment referred to a previous study [4], with the difference that each headspace vial in this study contained three grams of sample. A fiber (65 μm, PDMS/DVB, Supelco, Bellefonte, PA, USA) was inserted into the headspace of a vial to extract the volatile compounds at 40 °C for 30 min. At the end of extraction, the fiber was desorbed into the injection port of the GC for 5 min. The time of solvent delay was 3 min. The samples were analyzed using the Agilent gas chromatography mass spectrometry (GC-MS) instrument (7890–5975) with a DB-WAX (60 m × 250 μm × 0.25 μm, Agilent

122–7062) under splitless injection mode. Helium (99.999%) was used as a carrier gas at a constant flow (1 mL/min).

The GC oven temperature was initially held at 40 °C for 2 min, increased to 100 °C at 3 °C/min and then increased to 230 °C at 5 °C/min and held for 5 min. The mass detector was used in an electron impact mode at 70 eV, an ion source temperature of 230 °C and a mass spectrometry scan range of m/z 30–350. According to the NIST 08 (National Institute of Standards and Technology) mass spectrometry database, the volatile compound was identified by matching degree, retention time, retention index (RI) and standard chemicals. Compounds with matching degrees greater than 80% were selected as effective aroma components. In order to quantify the components, semi-quantification was performed using an internal standard method to calculate the relative concentration of volatile compounds in the samples. Measurements were repeated three times for each sample.

2.4. GC-IMS Analysis of Volatile Compounds

The VOCs of different peach cultivars were detected using HS-GC-IMS (FlavorSpec ®, G.A.S, Dortmund, Germany). Two grams of grounded sample from each cultivar were transferred into 20 mL headspace bottles. The headspace injection condition was set at the following parameters: incubation time was 15 min, incubation temperature was 40 °C, injection needle temperature was 85 °C and injection volume was 500 µL. The GC conditions were as follows: the chromatographic column was MXT-5 (15 m × 0.53 mm, 1 µm, Agilent Technology, Palo Alto, CA, USA)). Nitrogen of 99.99% purity was used as a carrier gas at a programmed flow as follows: 2 mL/min for 2 min, 10 mL/min for 8 min and 100 mL/min for 10 min. The IMS conditions were as follows: the drift tube temperature was 45 °C, and the drift gas velocity was 150 mL/min. All tests were repeated three times. Volatile compounds were preliminarily identified by comparing the RI and ion drift times (the time in milliseconds it takes for an ion to reach the collector through the drift tube) of standards in the GC-IMS library and the NIST database.

2.5. Identification of Characteristic Aroma Compounds in Samples by the Odor Activity Value Method

The OAVs of compounds were calculated using the following formula: $OAV = C_i/OT_i$, where C_i indicates the concentration of a compound and OT_i indicates the odor threshold. The odor thresholds of all compounds were obtained from the published literature [18]. For a compound with multiple thresholds, the standard we chose was its threshold in water and the most recent data.

2.6. Statistical Analysis

The experimental data derived from GC-MS were analyzed using Origin 2021 software (Microcal Software, Inc., Northampton, MA, USA). Analysis of variance (ANOVA) and Duncan's multiple range test ($p < 0.05$) were used to analyze the significant differences among samples. Cluster analysis was performed using TB tools software (versions v1.1043). For the data obtained using GC-IMS, four software programs from the instrument were used for analyzing: (1) VOCal was used for viewing analytical spectra and qualitative and quantitative data; the NIST database and IMS database built into the application software can be used for qualitative analysis of compounds. (2) The Reporter plug-in for directly comparing the spectral differences between samples. (3) The Gallery Plot plug-in was used for fingerprint profile comparison. (4) The Dynamic PCA plug-in was used for dynamic principal component analysis.

3. Results and Discussion

3.1. Volatile Profile of Different Peach Cultivars Using GC-MS

3.1.1. The Construction of VOCs Profiling for Eight Peach Cultivars

By searching the NIST database and the chemical standard, a total of seventy VOCs were tentatively identified and quantified for eight peach cultivars using GC-MS. They were categorized into ten groups, including nine aldehydes, ten esters, eleven terpenoids, nine

alcohols, six lactones, five ketones, five alkanes, eleven aromatic hydrocarbons, two furans and two other compounds (Figure 2, Table 2). Twenty-three VOCs were commonly identified in all cultivars, including hexanal, nonanal, benzaldehyde, 2-hexenal, butyl acetate, hexyl acetate, linalool, β-myrcene, D-limonene, 1-hexanol, 3-hexenol, 2-hexenol, 2-ethyl-1-hexanol, γ-octalactone, δ-decalactone, γ-hexalactone, γ-decalactone, γ-dodecalactone, β-ionone, 2-octanone, 2-ethyl furan and 2,4-ditert-butyl phenol. More than 40 VOCs were identified in HJML (44), DTML (42), HH (42) and JC (43). Fewer than 35 volatile compounds were identified in XFML (35), JXIU (29), JXIANG (35) and JG (32). Seventeen unique compounds were identified only in one cultivar. Differences were observed in the total content of volatile compounds among the eight peach cultivars (Table 2 and Figure 2).

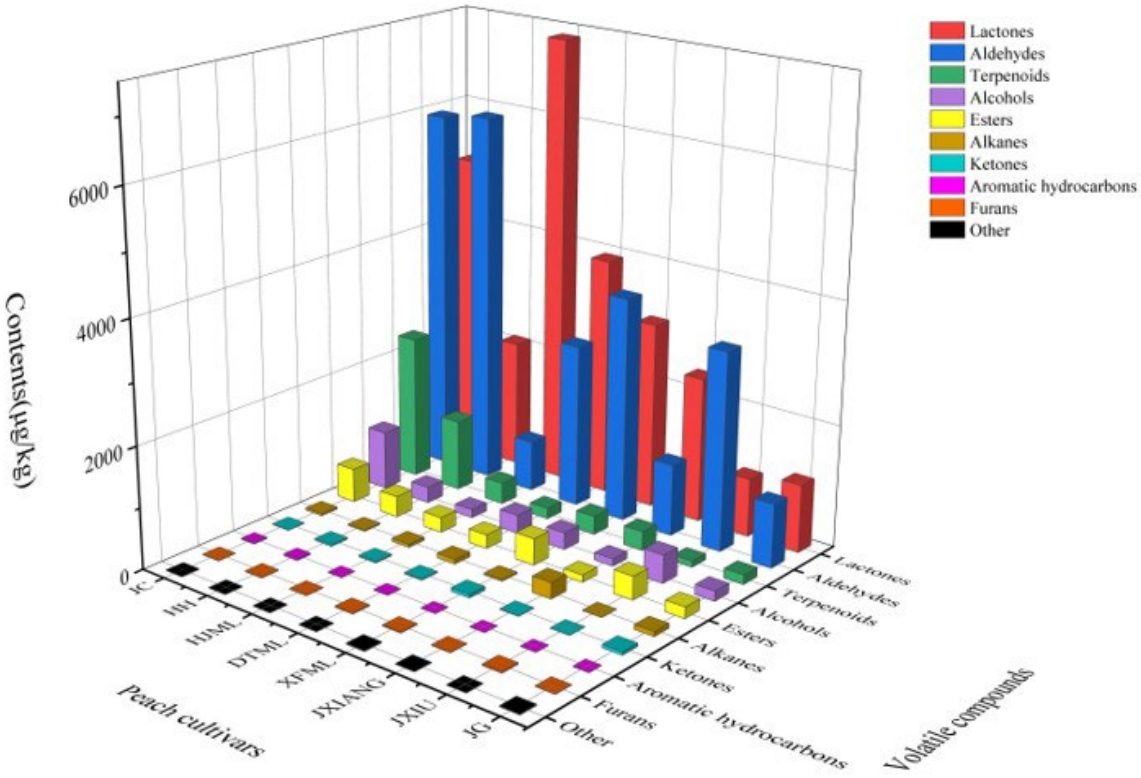


Figure 2. The total contents of each category of VOCs in eight peach cultivars. 3.1.2 Cluster Analysis of VOCs of eight peach cultivars.

Aldehydes were regarded as one of the most significant contributors to the peaches' green and grassy flavor, and have been reported to exist widely in immature plums, apples and pears [19,20]. The aldehydes detected in this experiment include hexanal, nonanal, benzaldehyde, 2-hexenal, 3-hexenal, (E)-2-nonenal, (E)-2-hexenal, (E)-2-heptenal and heptanal (Table 1). Among these, hexanal, nonanal, 2-hexenal and benzaldehyde were identified as major components and were detected in all the samples, which is consistent with previous studies [20,21]. Notably, the highest content of 2-hexenal among all samples was 5132.24 μg/kg in HH, while the lowest was 589.96 μg/kg in HJML; therefore, this compound may be the most important factor responsible for the differences in aldehydes among the samples. It is also clear from Figure 2 that the total content of aldehydes is highest in HH and lowest in HJML.

Alcohols are a group of compounds other than aldehydes that give peach fruit a green aroma. In this study, nine alcohols were found, namely 2-ethyl-1-hexanol, 3-methyl-3-nonanol, carbitol, 3-hexenol, hexanol, 2-hexenol, 3-methyl-3-buten-1-ol, α-terpineol and geraniol. Among them, 3-hexenol, hexanol, 2-hexenol and 2-ethyl-1-hexanol were detected in all samples at high levels (Table 2). JC had the highest level of alcohols and JXIANG had the lowest (Figure 2).

Table 2. The absolute and relative contents of VOCs in eight peach cultivars tested using GC-MS.

Compound	CAS	Identification	Concentration (μg/kg)							
			XFML	HJML	DTML	HH	JXIU	JXIANG	JC	JG
Aldehydes										
Benzaldehyde	100-52-7	MS, RI, Std	46.70 ± 34.23a	29.62 ± 1.96a	14.33 ± 2.70a	17.66 ± 0.32a	20.14 ± 7.80a	37.13 ± 35.21a	10.64 ± 2.87a	11.74 ± 0.77a
2-Hexenal	505-57-7	MS, RI, Std	3127.39 ± 512.19b	589.96 ± 109.27d	2228.96 ± 151.92bc	5132.24 ± 276.90a	2713.64 ± 1240.09b	882.17 ± 142.51cd	4782.91 ± 1407.01a	816.73 ± 193.16cd
Hexanal	66-25-1	MS, RI, Std	484.13 ± 173.46b	148.91 ± 21.65c	420.23 ± 42.53bc	891.07 ± 52.4a	490.39 ± 277.91b	240.58 ± 40.05bc	1134 ± 328.54a	123.66 ± 13.28c
Nonanal	124-19-6	MS, RI	19.62 ± 4.07b	37.81 ± 8.21a	19.55 ± 0.59b	34.23 ± 1.26a	32.82 ± 1.81a	17.42 ± 0.91b	23.84 ± 2.93b	37.69 ± 1.1a
3-Hexenal	4440-65-7	MS, RI	ND	ND	1.34 ± 0.12a	ND	ND	ND	ND	ND
(E)-2-Nonenal	18829-56-6	MS, RI	3.60 ± 0.50ab	ND	ND	ND	ND	ND	4.36 ± 0.19a	3.5 ± 0.33b
(E)-2-Hexenal	6728-26-3	MS, RI	ND	22.15 ± 3.52b	ND	ND	ND	ND	ND	52.82 ± 13.12a
(E)-2-Heptenal	18829-55-5	MS, RI	ND	ND	ND	2.85 ± 0.10a	ND	ND	2 ± 0.3	ND
Heptanal	111-71-7	MS, RI	ND	ND	ND	3.64 ± 0.12a	ND	ND	ND	ND
Esters										
Butyl acetate	123-86-4	MS, RI, Std	151.68 ± 54.97b	1.49 ± 0.09c	132.75 ± 15.77b	274.47 ± 18.42a	153.13 ± 86.01b	53.1 ± 46.12bc	353.26 ± 107.81a	1.0 ± 0.1c
Isopentyl acetate	123-92-2	MS, RI, Std	ND	ND	ND	5.49 ± 0.52ab	ND	6.29 ± 1.09a	3.61 ± 1.04b	ND
Hexyl acetate	142-92-7	MS, RI, Std	3.25 ± 0.69d	14.9 ± 0.37d	30.49 ± 2.28c	5.05 ± 0.16d	72.28 ± 11.88b	5.43 ± 0.39d	91.17 ± 17.61a	1.56 ± 0.14d
Heptyl acetate	112-06-1	MS, RI, Std	ND	ND	1.47 ± 1.10a	ND	ND	ND	ND	ND
(Z)-3-Hexen-1-yl acetate	3681-71-8	MS, RI, Std	274.56 ± 28a	223.62 ± 11.88b	37.06 ± 2.32de	58.64 ± 11.23d	156.08 ± 31.53c	7.9 ± 0.48e	9.78 ± 0.68e	180.94 ± 30.04c
2-Ethyl hexyl acetate	103-09-3	MS, RI	ND	1.22 ± 0.03cd	0.89 ± 0.12e	1.52 ± 0.03b	1.07 ± 0.02d	1.32 ± 0.16cd	1.97 ± 0.02a	ND
(E)-2-Hexen-1-yl acetate	2497-18-9	MS, RI	6.73 ± 0.72d	ND	19.47 ± 1.30c	ND	ND	45.06 ± 3.44b	99.57 ± 10.23a	2.86 ± 0.2d
(Z)-2-Penten-1-yl acetate	42125-10-0	MS, RI	ND	5.00 ± 0.07b	5.82 ± 0.73a	ND	ND	ND	ND	ND
Nonyl acetate	143-13-5	MS, RI	ND	1.5 ± 0.12	ND	ND	ND	ND	ND	ND
(Z)-3-Nonen-1-yl acetate	13049-88-2	MS, RI	ND	ND	ND	ND	2.47 ± 0.42 d	ND	ND	ND
Terpenoids										
Linalool	78-70-6	MS, RI, Std	57.66 ± 3.46d	128.13 ± 7.35c	4.03 ± 0.38d	339.26 ± 3.37b	3.76 ± 0.50 d	181.32 ± 3.05c	820.73 ± 88.58a	3.81 ± 0.18d
β-Myrcene	123-35-3	MS, RI, Std	5.84 ± 1.95d	9.86 ± 6.78d	3.64 ± 1.5d	42.55 ± 3.51b	3 ± 0.92d	31.8 ± 3.4c	112.76 ± 5.6a	3.42 ± 0.62d
D-Limonene	5989-27-5	MS, RI, Std	225.5 ± 18.37c	209.86 ± 2.36c	155.22 ± 15.7c	772.21 ± 17.36b	93.57 ± 16.62c	100.17 ± 122.38c	1427.32 ± 390.57a	150.66 ± 8.18c
(Z)-2-Dodecene	7206-26-0	MS, RI	ND	ND	2.81 ± 2.79a	1.58 ± 0.08a	ND	ND	4.37 ± 0.25a	ND
1-Dodecene	112-41-4	MS, RI	4.95 ± 0.68	ND	ND	ND	ND	ND	ND	ND
1-Tetradecene	1120-36-1	MS, RI	9.07 ± 9.07a	ND	8.32 ± 8.32a	9.42 ± 9.42a	ND	ND	ND	ND
(E)-3-Dodecene	7206-14-6	MS, RI	ND	ND	1.61 ± 0.16a	2.32 ± 0.9a	ND	ND	ND	ND
(Z)-β-Ocimene	3338-55-4	MS, RI	ND	1.37 ± 0.09	ND	ND	ND	ND	ND	ND
2-Carene	554-61-0	MS, RI	ND	2.19 ± 0.08	ND	ND	ND	ND	ND	ND
(E)-β-Ocimene	3779-61-1	MS, RI	ND	ND	ND	ND	ND	1.53 ± 0.02b	4.8 ± 0.68a	ND
Terpinolene	586-62-9	MS, RI	ND	ND	ND	3.58 ± 0.85	ND	ND	ND	ND
Alcohols										
1-Hexanol	111-27-3	MS, RI, Std	46.55 ± 24.93bcd	14.19 ± 1.38d	36.18 ± 4.16bcd	63.73 ± 7.92bc	73.98 ± 15.75b	20.85 ± 4.51cd	263.24 ± 57.24a	9.72 ± 0.61d
3-Hexenol	928-96-1	MS, RI, Std	60.97 ± 13.64c	45.55 ± 1.6cd	91.23 ± 8.47b	33.9 ± 17.32de	120.7 ± 20.7a	14.4 ± 2.75e	72.08 ± 20.03bc	46.99 ± 0.51cd
2-Hexenol	928-95-0	MS, RI, Std	28.52 ± 3.98c	23.22 ± 1.44c	60.43 ± 16.52c	110.88 ± 13.45bc	215.88 ± 45.15b	33.27 ± 22.51c	556.7 ± 157.73a	22.63 ± 4.48c
3-Methyl-3-buten-1-ol	763-32-6	MS, RI, Std	45.26 ± 11.06a	ND	67.79 ± 26.14a	ND	ND	ND	ND	ND
2-Ethyl-1-hexanol	104-76-7	MS, RI	71.51 ± 0.5a	43.33 ± 0.73c	43.39 ± 1.07c	46.44 ± 1.14b	41.71 ± 1.00c	43.01 ± 1.48c	38.93 ± 0.95d	73.3 ± 0.59a
3-Methyl-3-nonanol	21078-72-8	MS, RI	9.67 ± 0.36a	8.28 ± 0.08a	ND	8.89 ± 0.17a	8.02 ± 0.11cd	7.86 ± 0.19d	ND	ND
Carbitol	111-90-0	MS, RI	16.26 ± 1.70a	ND	3.68 ± 0.25c	ND	1.86 ± 0.08c	ND	ND	12.54 ± 0.92b
α-Terpineol	98-55-5	MS, RI	ND	ND	ND	ND	ND	ND	15.4 ± 0.98	ND
Geraniol	106-24-1	MS, RI	ND	ND	ND	ND	ND	ND	3.45 ± 0.35	ND

Table 2. *Cont.*

Compound	CAS	Identification	Concentration (μg/kg)							
			XFML	HJML	DTML	HH	JXIU	JXIANG	JC	JG
Lactones										
γ-Octalactone	104-50-7	MS, RI, Std	31.82 ± 2.90cd	152.72 ± 5.82a	57.2 ± 23.84b	30.87 ± 1.43cd	14.66 ± 1.60d	43.03 ± 3.20bc	55.31 ± 2.45b	27.07 ± 2.77cd
γ-Decalactone	706-14-9	MS, RI, Std	566.29 ± 25.71c	1878.4 ± 101.12a	847.91 ± 57.66b	335.06 ± 12.00d	111.9 ± 7.80e	361.77 ± 17.98d	811.07 ± 22.98b	149.08 ± 17.74e
δ-Decalactone	705-86-2	MS, RI, Std	2125.73 ± 422.74c	4334.12 ± 517.04a	2203.62 ± 211.66c	1097.68 ± 119.79d	254.40 ± 37.91e	981.25 ± 65.47d	3060.85 ± 107.94b	276.04 ± 54.89e
γ-Hexalactone	695-0-7	MS, RI, Std	272.53 ± 28.29e	891.48 ± 37.54b	760.62 ± 50.23c	633.98 ± 29.58cd	575.32 ± 62.65d	958.80 ± 69.18b	1099.58 ± 122.39a	647.4 ± 48.79cd
γ-Heptalactone	105-21	MS, RI, Std	ND	17.03 ± 2.98b	7.91 ± 2.06c	6.07 ± 1.70c	ND	28.54 ± 2.62a	15.07 ± 1.97b	ND
γ-Dodecalactone	2305-05-7	MS, RI, Std	67.77 ± 1.13b	83.76 ± 5.08a	43.17 ± 2.88c	1.48 ± 0.77g	4.27 ± 0.25g	10.27 ± 0.23f	35.05 ± 0.85d	14.8 ± 0.57e
Ketones										
β-Ionone	79-77-6	MS, RI, Std	0.43 ± 0.07e	1.95 ± 0.14a	0.90 ± 0.05c	2.03 ± 0.15a	0.67 ± 0.06d	0.65 ± 0.07d	1.16 ± 0.11b	0.64 ± 0.06d
2-Octanone	111-13-7	MS, RI	44.97 ± 1.75b	2.49 ± 0.02c	3.06 ± 0.42c	3.63 ± 0.22c	2.80 ± 0.68c	6.67 ± 6.09c	2.64 ± 0.32c	50.81 ± 1.23a
Dihydro-beta-ionone	17283-81-7	MS, RI	11.79 ± 1.1c	16.01 ± 0.07b	11.64 ± 0.06c	24.22 ± 1.33a	ND	ND	ND	ND
2-Nonanone	821-55-6	MS, RI	ND	0.87 ± 0.07	ND	ND	ND	ND	ND	ND
Geranylacetone	3796-70-1	MS, RI	ND	ND	ND	ND	ND	ND	3.93 ± 0.64	ND
Alkanes										
Tridecane	629-50-5	MS, RI, Std	ND	11.39 ± 7.91b	43.06 ± 34.94b	17.53 ± 9.64b	ND	227.41 ± 102.94a	ND	36.73 ± 12.76b
Dibromochloro-methane	124-48-1	MS, RI	ND	2.38 ± 0.41a	2.90 ± 1.12a	2.15 ± 0.60a	2.27 ± 0.98a	2.13 ± 0.34a	1.96 ± 0.37a	ND
Octamethyl cyclotetrasiloxane	556-67-2	MS, RI	20.64 ± 16.52a	26.63 ± 4.95a	24.87 ± 3.86a	ND	ND	33.00 ± 8.39a	27.25 ± 10.18a	35.70 ± 3.37a
Bromoform	75-25-2	MS, RI	ND	4.17 ± 0.06a	4.37 ± 0.37a	ND	2.88 ± 0.77c	ND	3.68 ± 0.49b	ND
Dodecane	112-40-3	MS, RI	ND	3.82 ± 0.16b	ND	ND	ND	5.36 ± 3.04a	2.29 ± 0.26c	ND
Aromatic hydrocarbons										
Styrene	100-42-5	MS, RI, Std	1.04 ± 0.46a	1.82 ± 0.19a	1.45 ± 0.28a	ND	4.52 ± 4.45a	2.65 ± 0.35a	ND	ND
Ethylbenzene	100-41-4	MS, RI	ND	2.75 ± 0.03bc	1.85 ± 0.28c	5.54 ± 0.81a	ND	ND	2.96 ± 0.42b	ND
Toluene	108-88-3	MS, RI	3.13 ± 0.58b	ND	ND	5.36 ± 0.64a	ND	ND	5.99 ± 1.13a	1.82 ± 0.11b
Meta-xylene	108-38-3	MS, RI	ND	1.99 ± 0.11b	3.51 ± 0.81a	ND	ND	ND	ND	2.35 ± 0.29b
Ortho-cymene	527-84-4	MS, RI	ND	0.50 ± 0.10	ND	ND	ND	ND	ND	ND
Hemimellitene	526-73-8	MS, RI	ND	1.13 ± 0.09	ND	ND	ND	ND	ND	ND
α-Ionene	475-03-6	MS, RI	ND	ND	ND	2.53 ± 0.34b	ND	ND	2.76 ± 0.03a	ND
Edulan	41678-29-9	MS, RI	ND	ND	ND	ND	ND	ND	3.78 ± 0.23	ND
p-Xylene	106-42-3	MS, RI	ND	ND	ND	7.47 ± 5.84	ND	ND	ND	ND
o-Xylene	95-47-6	MS, RI	ND	ND	ND	6.13 ± 1.64	ND	ND	ND	ND
1-Methyl naphthalene	90-12-0	MS, RI	ND	ND	ND	0.94 ± 0.08	ND	ND	ND	ND
Furans										
2-ethyl furan	3208-16-0	MS, RI, Std	15.22 ± 2.83ab	5.85 ± 2.32c	18.17 ± 2.66ab	9.16 ± 3.85ab	20.89 ± 17.51a	5.39 ± 1.28c	5.89 ± 3.46c	5.16 ± 3.86c
2-Pentyl furan	3777-69-3	MS, RI	ND	ND	ND	ND	ND	2.12 ± 0.09	ND	ND
Other										
2,4-Ditert-butyl phenol	96-76-4	MS, RI	14.09 ± 0.57a	3.32 ± 0.15e	3.62 ± 0.25de	4.34 ± 0.39cd	3.82 ± 0.22cde	4.71 ± 0.49cde	4.12 ± 0.51cde	13.03 ± 0.76b
Neroloxide	1786-08-9	MS, RI	ND	ND	ND	ND	ND	2.93 ± 0.41a	1.50 ± 0.06b	ND

ND represents not detected; the meanings of a–e in the same row with different superscripts represent significant differences ($p < 0.05$). The "Std" in the identification column indicates that these compounds were quantified by a chemical standard.

Esters are the main flavor components of most ripe fruits and provide the fruity notes, and particularly (Z)-3-hexen-1-yl acetate and hexyl acetate are considered to contribute significantly to the aroma characteristics of peaches [6,22,23]. A total of ten esters were detected in the eight peach cultivars. Among these, butyl acetate, (Z)-3-hexen-1-yl acetate and hexyl acetate was detected in all samples and the levels were significantly different between samples. (E)-2-hexen-1-yl acetate was also detected at high levels in most cultivars. The remaining unmentioned esters were present at less than 10 μg/kg in each sample, so these components were not the focus of this study.

A total of 11 terpenoids were identified, of which linalool, β-myrcene and D-limonene were detected in all peach cultivars with significant differences. Horvat et al. [24] identified linalool as one of the key aroma compounds of peach fruit that increased significantly with fruit ripening and has floral aroma properties [25,26]. The order of linalool content in all samples was as follows: JC > HH > JXIANG > HJML > XFML> DTML > JG > JXIU. Surprisingly, the linalool content in JC was more than twice that of HH. Previous studies have shown that nectarines contain higher levels of linalool than peaches [7]. Although the material in this study did not include nectarines, JC was derived from peach Jinxiu and nectarine Huyou 018, which may be the reason for its highest linalool content among the eight cultivars. β-myrcene is reported as a precursor of linalool and is one of the common terpenoids in peaches and nectarines [27,28]. Here, the content of β-myrcene ranked consistently with linalool in the eight cultivars.

More than 10 lactones have been found in peaches [6,27,29]. Here, we identified six lactones: γ-hexalactone, γ-decalactone, γ-octalactone, γ-dodecalactone, γ-heptalactone and δ-decalactone. Consistent with previous studies [7], γ-decalactone, δ-decalactone and γ-hexalactone were the leading lactones with the highest content in these elite cultivars, with the difference that δ-decalactone was the most abundant in the present study. As reported, mid- and later-ripening cultivars have higher lactone content than early-ripening cultivars [30]. However, in this study, some early- and mid-maturing cultivars such as HJML and JC had the highest total lactone content, while the late-maturing cultivar JXIU had the lowest content (Figure 2), which might be related to its genetic background and cultivation conditions.

Five ketones were detected, and β-ionone and 2-octanone were detected in all samples. The content of total ketone was highest in 'XFML' and lowest in 'JX' (Figure 2). Interestingly, dihydro-β-ionone was detected in all white flesh peaches, but not in all yellow flesh peaches; this result is similar to that of several researchers [31]. This is due to the fact that C-13-norisoprenoids such as dihydro-β-ionone in peach fruit are mainly synthesized via the isoprenoid pathway, and carotenoids are precursors for their synthesis. Carotenoids in white-flesh peaches are cleaved to disubstituted carotenoids via the action of carotenoid cleavage dioxygenase (CCD4), which in turn forms the volatile compounds such as dihydro-β-ionone, while the CCD4 enzyme gene in yellow-flesh peaches is mutated and cannot degrade carotenoids, so less dihydro-β-ionone is synthesized than in white-fleshed peaches [32,33].

To further understand the differences of volatiles in different peach cultivars, a cluster analysis heat map was constructed (Figure 3). The vertical axis of the figure represents different volatiles and the horizontal axis represents different peach cultivars. The red-to-blue and large-to-small circles indicate the abundance of volatiles from highest to lowest. According to the content of each of the VOCs, cluster analysis clustered JXIU, DTML, JG and XFML into one group. This indicates that the composition and content of their volatiles are similar. Horizontally, the numerous volatiles were roughly divided into three clusters. Cluster 1 covers most of the aldehydes and alcohols. In general, this cluster of compounds is relatively higher in XFML and JG. The substances in cluster 2 mainly include esters and lactones, and the HH and HJML shows a high abundance in this cluster. The most abundant compounds in cluster 3 are terpenoids and aromatic hydrocarbons, and JC shows the highest abundance in this cluster. Cluster analysis plots visually show the abundance of various substances in the sample.

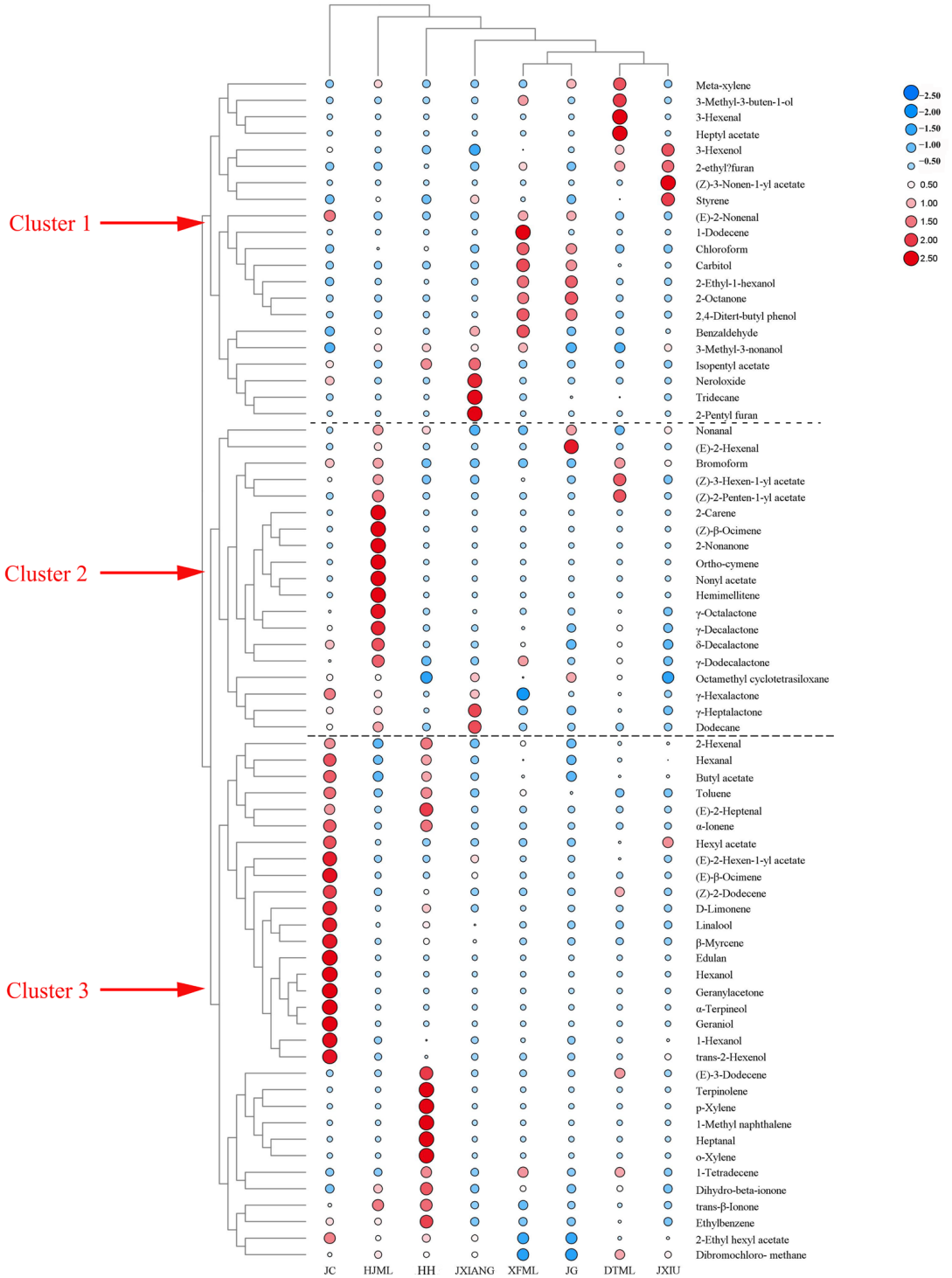


Figure 3. A clustered heatmap of VOCs among eight peach cultivars.

3.1.2. Analysis of Odor Activity Values of VOCs in Eight Peach Cultivars

OAV is the main method of aroma characterization and it is also an indicator of whether human can perceive VOCs in samples by olfactory. Here, by calculating the OAV for each compound, we grasped the compounds that contribute to the peaches. The sensory thresholds of each compound and their OAV in the samples are listed in Table 3, and considering that OAV ≥ 1 is required to have a contribution to flavor, we only analyzed this part of the data.

Table 3. Comparison of odor activity values of different VOCs.

Compound	Aroma Description [1]	Threshold	XFML	HJML	DTML	HH	JXIU	JXIANG	JC	JG	Range of OAV
Aldehydes											
2-Hexenal	fruity, vegetable	30	104.25	19.67	74.3	171.07	90.45	29.41	159.43	27.22	19.67–171.07
Hexanal	green, grassy	5	96.83	29.78	84.05	178.21	98.08	48.12	226.8	24.73	24.73–226.8
Nonanal	cucumber	1.1	17.84	34.37	17.77	31.12	29.84	15.84	21.67	34.26	15.84–34.37
Octanal	orange peel, green	0.587	ND	15.03	11.31	15.47	13.37	8.18	9.86	22.37	8.18–22.37
Esters											
Butyl acetate	sweet, ripe banana	58	2.62	0.03	2.29	4.73	2.64	0.92	6.09	0.02	0.02–6.09
Isopentyl acetate	sweet, fruity	0.15	ND	ND	ND	36.6	ND	41.93	24.07	ND	24.07–41.93
(Z)-3-Hexen-1-yl acetate	fruity, apple and pear	31	8.86	7.21	1.2	1.89	5.03	0.25	0.32	5.84	0.25–8.86
Terpenoids											
Linalool	floral, woody	0.22	262.09	582.41	18.32	1542.09	17.09	824.18	3730.59	17.32	17.09–3730.59
β-Myrcene	woody, vegetative	1.2	4.87	8.22	3.03	35.46	2.5	26.5	93.97	2.85	2.5–93.97
D-Limonene	sweet, orange, citrus	34	6.63	6.17	4.57	22.71	2.75	2.95	41.98	4.43	2.75–41.98
Alcohols											
1-Hexanol	green, fruity	5.6	8.31	2.53	6.46	11.38	13.21	3.72	47.01	1.74	1.74–47.01
3-Hexenol	fresh, green	1.9	32.09	23.97	48.02	17.84	63.53	7.58	37.94	24.73	7.58–63.53
Lactones											
γ-Octalactone	fruity, creamy	12	2.65	12.73	4.77	2.57	1.22	3.59	4.61	2.26	1.22–12.73
γ-Decalactone	fruity, peach	1.1	514.81	1707.64	770.83	304.6	101.73	328.88	737.34	135.53	101.73–1707.64
δ-Decalactone	creamy, fatty, buttery	66	32.21	65.67	33.39	16.63	3.85	14.87	46.38	4.18	3.85–65.67
γ-Dodecalactone	fruity, peach	2	33.89	41.88	21.59	0.74	2.14	5.14	17.53	7.4	0.74–41.88
Ketones											
β-Ionone	floral, violet	0.007	61.43	278.57	128.57	290	95.71	92.86	165.71	91.43	61.43–290

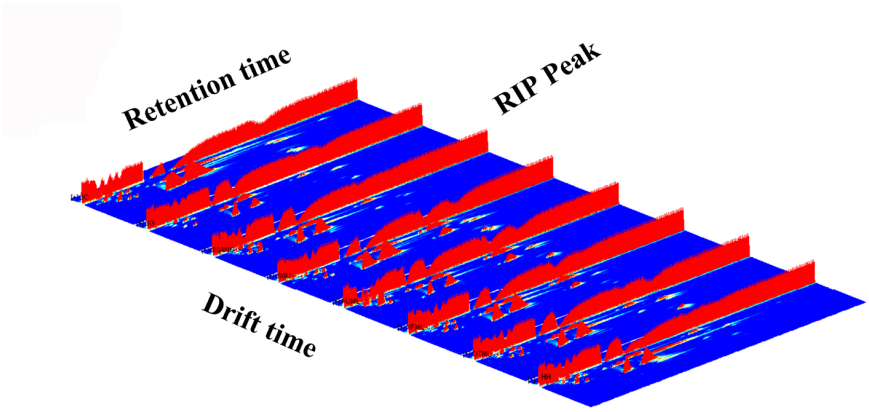
[1] The aroma description of the compounds come from the website: http://www.thegoodscentscompany.com/ (accessed on 12 January 2023).

By statistical analysis, only 17 volatiles with OAV ≥ 1 were retained, including 4 aldehydes, 3 esters, 3 terpenoids, 1 ketones, 2 alcohols and 4 lactones. The importance of these compounds was determined by ranking them according to the minimum OAV in each of the eight cultivars: γ-decalactone > β-ionone > hexanal > 2-hexenal > linalool > nonanal > 3-hexenol > δ-decalactone > D-limonene > β-myrcene > 1-hexanol > γ-octalactone > γ-dodecalactone > (Z)-3-hexen-1-yl acetate > butyl acetate > isopentyl acetate > octanal. Although γ-decalactone was not the most abundant in quantity, it showed the highest OAV due to the low threshold value. As the main contributor of peach-like aroma, it is also an essential factor that distinguishes peaches from other fruits [34,35]. The OAV of γ-decalactone was highest in HJML. β-ionone and linalool are the two most dominant floral compounds in peach fruits with extremely low-threshold values. They can exhibit rose and violet flavor despite their low content. In our result, both the amount and OAV of linalool were high in the eight peaches. The OAV ranged from 17.09 to 3730.59, and the highest value was present in JC. Due to the 0.007 μg/kg threshold value, the range of OAV of β-ionone was from 61.43 to 290, and the highest value exhibited in HH. Regarding the grass/green-notes aldehydes and C6 alcohols, hexanal and 3-hexenol were the most active flavor compounds in most investigated cultivars. Their OAV ranged from 24.73 to 226.8 and 7.58 to 63.53. The highest value of these two compounds was observed in JC and JXIU, respectively.

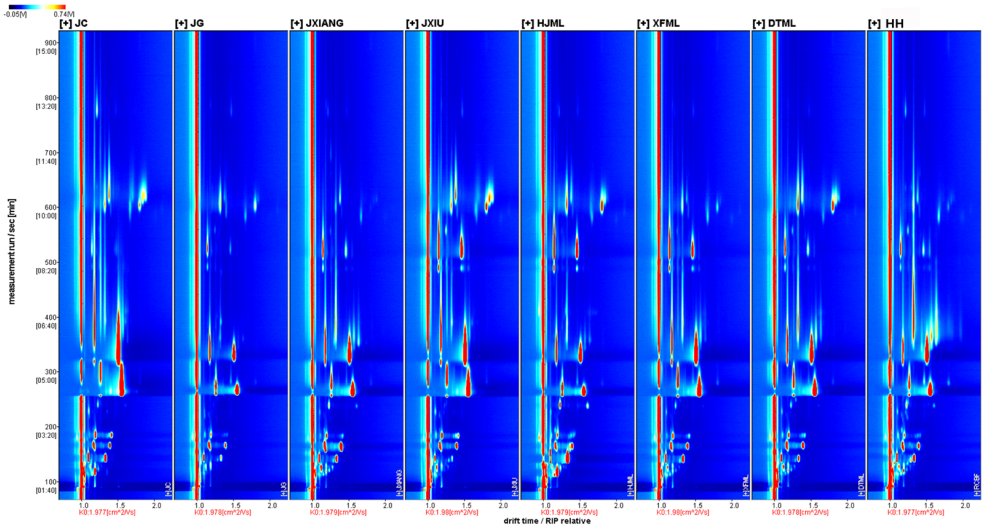
3.2. Volatile Profile of Different Peach Cultivars Using GC-IMS

3.2.1. Differential Analysis of the Topographic Plots of VOCs in Eight Cultivars Using GC-IMS

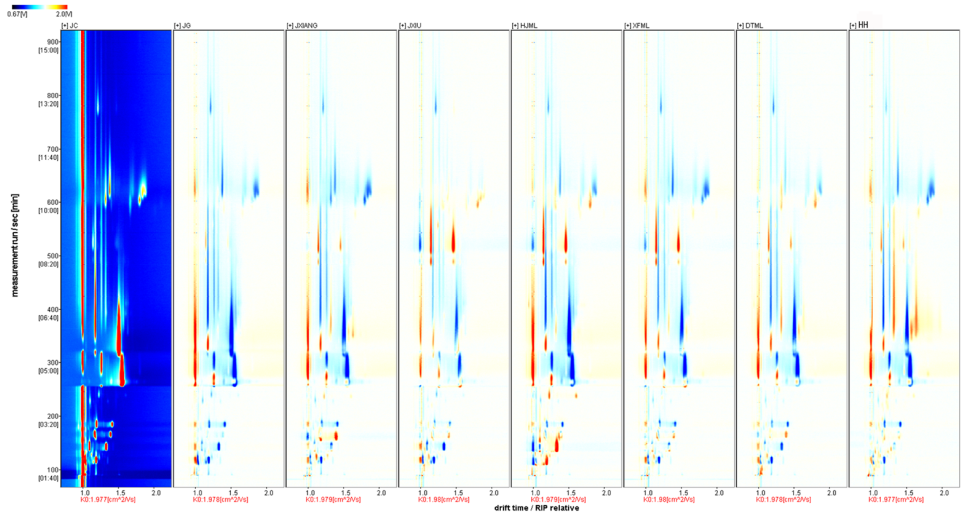
The VOC profiles of eight peaches were also constructed using GC-IMS. The 3D topographic plot of the peach volatiles showed that the composition and signal intensities of VOCs varied considerably between different peach cultivars (Figure 4a). To observe the data more conveniently and intuitively, we normalized the ion migration time and the reaction ion peak, and obtained a two-dimensional top-view plot of the ion migration spectrum (Figure 4b). The red line at the horizontal coordinate 1.0 in the graph is the RIP peak. Each point to the right of the RIP peak represents a volatile and the color of the point represents the concentration of the compound, with white to red indicating low-to-high concentrations [36]. Most of the signal is concentrated between drift times of 1.0–1.9 ms and retention times of 100–700 s. It is clear from the graph that the signal intensity of VOCs appearing between retention times of 500–700 s varies considerably between samples. To compare the differences more obviously between samples, a difference comparison model can be used, where the spectrum of JC is selected as a reference and the spectra of the other samples are deducted from the reference. If the VOCs of both are the same, the background after deduction is white, while red means that the concentration of the substance is higher than the reference, and blue means that the concentration of the substance is lower than the reference [37]. JXIU, HJML and XFML showed significantly higher concentrations of VOCs in the retention time range of 500–600 s than the other samples. It is clearly seen that VOCs in the retention time range of 350–450 s and ion drift times of 1.6 ms are specific in the HH. The substances in the green-dotted box are significantly more concentrated in the HJML than in the other samples. The location and quantities of VOC peaks in the samples are approximately the same in the spectra, but there are differences in peak strength, indicating that the content of VOCs is determined by the peach cultivars.



(a)



(b)



(c)

Figure 4. VOCs of eight peach cultivars determined by GC-IMS. (**a**) The 3D topographic plot of the peach VOCs. (**b**) The 2D topographic plots. (**c**) The difference comparison topographic plots.

3.2.2. The Volatile Fingerprints of Eight Cultivars Using GC-IMS

The results of the qualitative analysis of the VOCs of the sample using GC-IMS are shown in Table 4. According to the NIST gas phase retention index database and the IMS migration time database built into the flavor analyzer (FlavourSpec®) software, 53 signal peaks were detected and 26 typical volatiles were identified, including 11 aldehydes, 5 esters, 4 alcohols, 2 ketones, 2 terpenes and 2 furans. There are 12 substances that were not identified. The most abundant substances detected in peach fruit using GC-IMS in this study were aldehydes, while other researchers [31,38] have detected esters, which are closely related to factors such as peach ripeness and variety selection. The compounds of 2-hexenal, 1-hexanal, acetic acid ethyl ester, benzaldehyde, 1-hexanol, methyl acetate, 2-butanone, pentanal, 2-methylbutanal, 3-methyl butanal, (Z)-3-hexenyl acetate, 2-methylpropyl acetate and (E)-2-pentenal exhibited more than two peaks. This is due to the fact that during ionic drift, when the concentration of a substance increases, two or more molecules will share a proton or electron, forming a dimer or monomers [14,39]. The 53 signals obtained were used to draw fingerprint profiles based on peak intensities to compare the differences in volatiles between samples, which can give clearer results (Figure 5). Each row of the figure indicates the signal peaks of all volatiles in the same sample, and each column indicates the signal intensity of the same compounds in different samples. The areas where the signal is more pronounced are boxed out for easier analysis.

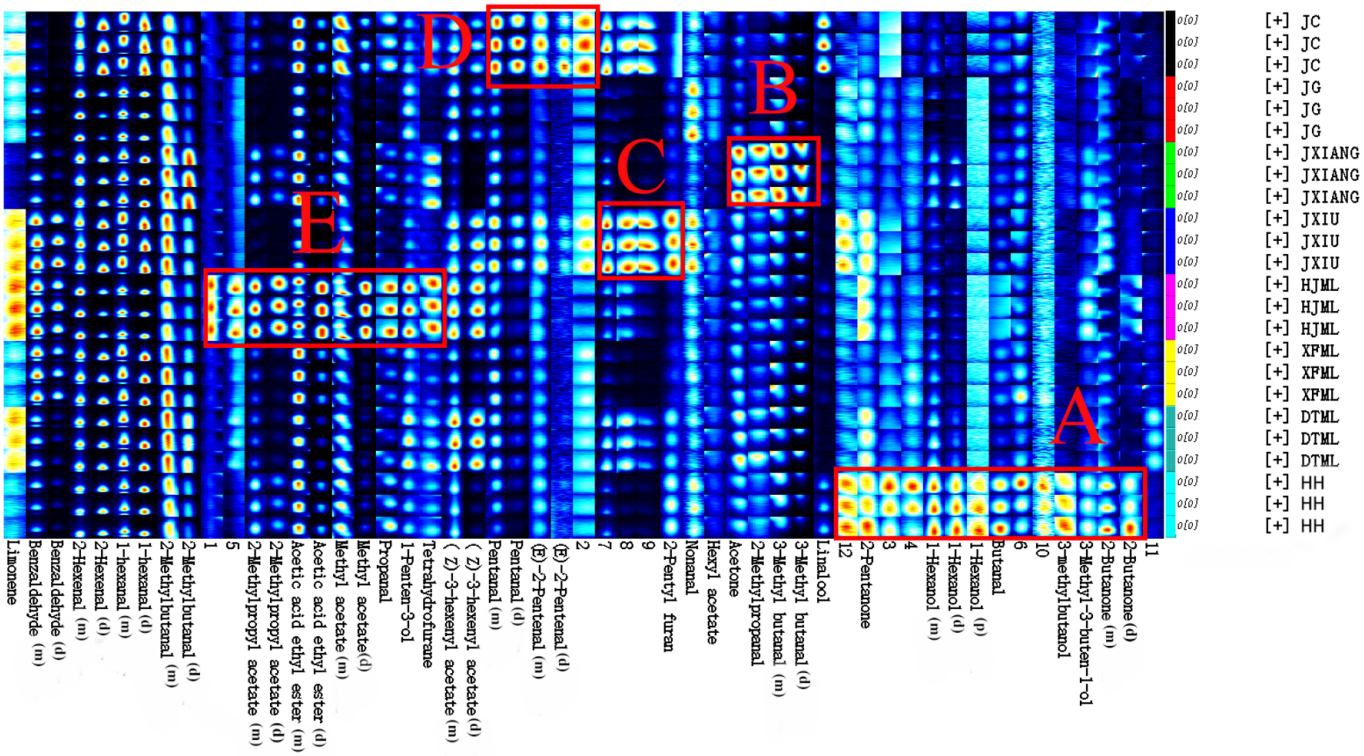


Figure 5. The VOCs fingerprints of different peach cultivars using GC-IMS. Box (A) 14 compounds highly accumulated in cv. 'HH'; Box (B) four compounds highly accumulated in 'JXIANG'; Box (C) four compounds highly accumulated in 'JXIIU'; Box (D) five compounds highly accumulated in cv. 'JC'; Box (E) eleven compounds highly accumulated in 'HJML'.

Table 4. Identification of VOCs in eight peach cultivars using GC-IMS.

Compound	CAS	RI [1]	Rt [2]	Dt [3]	Peak Volume							
					JC	JG	JXIANG	JXIU	HJML	XFML	DTML	HH
Aldehydes												
(E)-2-Pentenal(d)	C1576870	758.7	227.87	1.36	51.97 ± 4.05a	22.12 ± 0.50d	26.16 ± 3.97cd	38.57 ± 2.19b	24.88 ± 2.37cd	21.81 ± 3.64d	27.52 ± 1.39cd	31.11 ± 4.68c
(E)-2-Pentenal(m)	C1576870	758.9	227.98	1.10	336.98 ± 31.57a	139.48 ± 2.95f	157.38 ± 3.59ef	280.05 ± 6.04b	204.01 ± 5.93c	177.96 ± 1.76de	196.39 ± 2.51cd	191.34 ± 14.43cd
1-Hexanal(d)	C66251	801.9	268.96	1.55	30,604.71 ± 561.98a	8987.07 ± 662.56g	13,835.73 ± 88.57e	23,730.42 ± 141.44b	8637.36 ± 337.60g	18,301.17 ± 439.93c	16,176.68 ± 225.65d	11,927.3 ± 1846.66f
1-Hexanal(m)	C66251	796.4	263.50	1.27	7287.71 ± 346.03a	4782.78 ± 103.52e	5988.45 ± 81.33c	7405.57 ± 55.69a	4583.58 ± 65.67e	6670.8 ± 235.55b	6219.04 ± 48.74c	5230.7 ± 369.12d
2-Hexenal	C505577	854.7	326.70	1.51	43,619.63 ± 710.51a	9204.41 ± 2304.39g	19,841.39 ± 151.32e	32,700.99 ± 133.9b	11,936.95 ± 667.43f	25,817.46 ± 417.42c	22,247.55 ± 306.11d	20,911.24 ± 2001.96de
2-Hexenal(d)	C505577	865.5	339.97	1.18	1600.33 ± 144.88de	1606.4 ± 64.49de	1997.49 ± 29.93a	1837.04 ± 34.42b	1487.00 ± 16.23e	1765.89 ± 14.43bc	2010.28 ± 8.72a	1688.35 ± 74.85cd
2-Methylbutanal(d)	C96173	674.6	166.00	1.40	12,233.73 ± 215.63a	8206.57 ± 633.12de	9785.16 ± 187.90c	12,317.08 ± 220.07a	8804.16 ± 339.86d	11,064.99 ± 303.33b	9597.46 ± 161.29c	7740.01 ± 454.24e
2-Methylbutanal(m)	C96173	677.9	167.61	1.17	877.81 ± 221.07eg	796.89 ± 84.01g	2773.17 ± 85.98a	1423.53 ± 115.26c	1174.23 ± 19.75de	1292.4 ± 13.07cd	1987.4 ± 37.99b	1021.39 ± 135.35ef
2-Methylpropanal	C78842	577.4	125.97	1.28	42.23 ± 9.50de	33.31 ± 2.27e	152.23 ± 2.62a	74.87 ± 9.72c	68.22 ± 2.22c	49.41 ± 0.93d	91.89 ± 14.92b	72.12 ± 8.52c
Butanal	C123728	612.1	138.80	1.29	312.37 ± 12.32c	155.28 ± 12.96e	261.22 ± 10.32d	174.22 ± 6.66e	419.05 ± 7.74b	287.09 ± 25.66cd	195.58 ± 2.36e	546.85 ± 49.49a
Nonanal	C124196	1104.8	774.37	1.47	150.22 ± 18.46cd	230.37 ± 0.78a	122.16 ± 6.07d	223.34 ± 2.33a	160.43 ± 5.25c	155.95 ± 9.30c	149.23 ± 15.95cd	193.6 ± 29.89b
Pentanal(d)	C110623	705.2	184.54	1.42	968.25 ± 121.94a	130.00 ± 8.01e	244.36 ± 10.61cd	645.23 ± 32.61b	288.21 ± 5.09c	306.74 ± 12.17c	298.92 ± 2.21c	166.87 ± 44.9de
Pentanal(m)	C110623	704.5	184.00	1.20	1871.51 ± 76.8a	830.14 ± 36.13e	1113.94 ± 16.97cd	1557.64 ± 31.15b	1060.65 ± 16.75d	1189.49 ± 20.90c	1169.46 ± 10.15cd	843.09 ± 143.07e
3-Methyl butanal(d)	C590863	661.9	160.09	1.41	205.63 ± 79.89e	281.10 ± 71.31de	1761.39 ± 46.38a	541.67 ± 18.76b	471.98 ± 29.5bc	552.2 ± 117.72b	584.41 ± 62.46b	384.04 ± 58.43cd
3-Methyl butanal(m)	C590863	657.8	158.21	1.19	317.96 ± 87.56d	445.8 ± 75.54bc	1029.99 ± 21.67a	502.81 ± 12.27b	353.13 ± 17.07cd	466.57 ± 77.21b	470.14 ± 20.84b	529.67 ± 45.99b
Benzaldehyde(d)	C100527	968.7	501.50	1.47	578.38 ± 111.68d	619.73 ± 67.97d	1443.43 ± 126.43d	8603.64 ± 1495.6a	6885.61 ± 537.68b	5497.32 ± 225.66c	1555.85 ± 96.07d	1225.19 ± 314.58d
Benzaldehyde(m)	C100527	969.9	503.84	1.15	1757.8 ± 382.67f	2795.57 ± 223.01e	4466.92 ± 176.88cd	10,020.69 ± 940.46a	10,399.49 ± 241.07a	8684.41 ± 97.20b	4594.33 ± 211.88c	3617.75 ± 542.84de
Propanal	C123386	538.5	113.51	1.15	468.16 ± 30.05b	104.94 ± 23.59d	317.07 ± 8.66c	144.57 ± 1.8d	820.09 ± 9.05a	258.12 ± 2.33c	263.93 ± 73.16c	419.19 ± 84.39b
Esters												
(Z)-3-hexenyl acetate(d)	C3681718	1021.5	601.44	1.81	1714.33 ± 223.69c	1175.14 ± 118.31d	160.16 ± 24.78f	2639.57 ± 61.82b	3100.4 ± 36.46a	603.68 ± 86.84e	3106.75 ± 168.24a	361.33 ± 60.58f
(Z)-3-hexenyl acetate(m)	C3681718	1022.8	603.79	1.32	3152.18 ± 153.7d	2704.95 ± 176.68e	1068.08 ± 61.83g	3537.69 ± 43.29c	4131.79 ± 27.19b	2045.67 ± 146.72f	4537.70 ± 10.96a	2524.31 ± 44.88e
2-Methylpropyl acetate(d)	C110190	771.2	239.36	1.61	62.12 ± 9.66c	29.38 ± 3.92d	148.21 ± 18.50b	29.35 ± 8.12d	457.21 ± 6.19a	49.65 ± 7.83c	54.31 ± 2.84c	165.64 ± 4.44b
2-Methylpropyl acetate(m)	C110190	771.8	239.88	1.23	375.34 ± 21.76d	100.63 ± 7.69g	655.74 ± 31.80c	155.76 ± 12.85f	1207.12 ± 11.83a	336.15 ± 21.58e	374.42 ± 10.72d	742.15 ± 7.55b
Acetic acid ethyl ester(d)	C141786	627	144.89	1.34	3001.99 ± 89.14b	733.20 ± 31.31f	2266.37 ± 128.24d	476.77 ± 7.82g	11,109.44 ± 39.89a	2685.42 ± 63.79c	1226.58 ± 16.69e	2630.65 ± 67.8c
Acetic acid ethyl ester(m)	C141786	627	144.89	1.10	2598.11 ± 12.56b	1650.35 ± 66.16e	2382.52 ± 37.21c	1337.23 ± 26.8f	2697.34 ± 3.36a	2600.02 ± 61.28b	1984.03 ± 16.38d	2425.16 ± 24.8c
Hexyl acetate	C142927	1015.7	590.78	1.41	241.27 ± 5.73b	294.96 ± 7.52a	143.01 ± 6.74d	287.98 ± 19.06a	252.94 ± 5.62b	200.91 ± 23.16c	237.13 ± 6.59b	162.53 ± 9.66d
Methyl acetate(d)	C79209	545	115.50	1.19	2781.88 ± 273.34b	655.77 ± 121.18e	923.26 ± 23.47d	634.88 ± 46.62e	7076.44 ± 26.91a	771.28 ± 9.32de	957.98 ± 92.82d	1284.63 ± 126.41c
Methyl acetate(m)	C79209	543.2	114.96	1.04	3104.27 ± 93.55a	1188.14 ± 77.32e	1861.66 ± 27.21d	1826.83 ± 17.01d	2819.23 ± 22.61b	1724.07 ± 19.18d	2305.57 ± 124.32c	2298.63 ± 98.43c
Alcohols												
1-Hexanol(d)	C111273	887.6	368.84	1.64	1323.93 ± 140.84c	405.12 ± 88.78f	1594.08 ± 53.78b	850.42 ± 39.26de	757.35 ± 34.80e	1043.38 ± 68.98d	1637.77 ± 75.13b	4895.53 ± 264.62a
1-Hexanol(m)	C111273	893.2	376.65	1.33	3967.25 ± 553.26de	2153.19 ± 734.17f	5842.45 ± 443.38c	3288.28 ± 260.43e	3820.28 ± 51.39de	4707.34 ± 223.45d	7033.03 ± 370.91b	12,508.58 ± 521.32a
1-Hexanol(p)	C111273	889.8	371.96	1.98	434.94 ± 29.41b	244.16 ± 19.66d	331.93 ± 28.52c	418.18 ± 12.56b	253.31 ± 24.32d	350.39 ± 44.11c	322.64 ± 15.26c	538.73 ± 26.7a
1-Penten-3-ol	C616251	697.4	178.90	0.94	411.06 ± 57.52cd	489.01 ± 26.97b	379.93 ± 14.22d	364.81 ± 9.91d	677.31 ± 18.63a	446.93 ± 27.38bc	631.23 ± 7.78a	453.1 ± 10.38bc
3-Methyl-3-buten-1-ol	C763326	720.6	196.05	1.17	92.47 ± 16.12c	72.95 ± 6.08d	139.63 ± 2.58b	103.79 ± 4.23c	144.53 ± 5.64b	92.15 ± 7.96c	93.56 ± 3.21c	162.17 ± 2.94a
3-Methylbutanol	C123513	748	218.42	1.24	23.03 ± 1.93bc	25.77 ± 3.09bc	30.39 ± 0.98b	21.71 ± 3.07bc	18.91 ± 1.99c	20.93 ± 1.16c	20.66 ± 2.67c	90.71 ± 10.66a
Ketones												
2-Butanone(d)	C78933	599.2	133.77	1.25	31.98 ± 2.22c	19.15 ± 1.68c	24.05 ± 2.07c	27.19 ± 1.13c	87.91 ± 6.46b	28.79 ± 1.21c	21.3 ± 0.93c	110.06 ± 20.68a
2-Butanone(m)	C78933	598.5	133.50	1.06	319.61 ± 14.41d	360.83 ± 12.34c	321.68 ± 4.50d	482.58 ± 13.03b	160.1 ± 0.44e	336.18 ± 4.64cd	316.86 ± 2.98d	557.61 ± 41.51a
Acetone	C67641	575.8	125.42	1.12	364.17 ± 71.04e	389.55 ± 40.35e	1092.99 ± 8.34a	751.46 ± 46.56b	482.36 ± 5.97d	610.86 ± 28.07c	729.81 ± 54.62b	590.19 ± 24.6c
Terpenoids												
Limonene	C138863	1025.7	609.11	1.22	120.52 ± 18.56bc	105.33 ± 13.46c	63.63 ± 2.70d	117.98 ± 15.92bc	173.58 ± 9.04a	109.2 ± 11.04c	138.42 ± 9.07b	96.33 ± 13.65c
Linalool	C78706	1105.3	775.33	1.22	1186.93 ± 63.28a	187.44 ± 30.65e	360.36 ± 9.68c	181.43 ± 7.50e	348.96 ± 18.96c	262.68 ± 43.69d	172.45 ± 23.91e	606.47 ± 16.55b
Furans												
2-Pentyl furan	C3777693	996.7	557.68	1.25	230.71 ± 37.63b	136.53 ± 12.88c	119.58 ± 14.26cd	422.35 ± 7.37a	97.53 ± 5.06d	133.59 ± 14.86c	218.49 ± 15.8b	237.38 ± 12.38b
Tetrahydrofurane	C109999	574.9	125.13	1.23	142.53 ± 22.09bc	43.25 ± 3.04e	163.44 ± 1.57b	78.88 ± 6.29d	318.79 ± 2.48a	70.99 ± 2.85d	162.15 ± 18.57b	138.77 ± 10.35c
Unknown												
1	*	685.1	171.09	1.09	117.25 ± 5.5b	82.43 ± 4.12e	93.33 ± 11.25cde	104.67 ± 2.36bcd	375.05 ± 5.42a	105.09 ± 2.08bcd	107.42 ± 5.46bc	92.37 ± 12.96de
2	*	798.5	265.59	1.40	413.68 ± 65.07a	259.3 ± 62.85b	195.78 ± 11.76b	259.33 ± 9.99b	253.49 ± 14.52b	207.40 ± 3.70b	196.21 ± 17.12b	238.52 ± 17.63b
3	*	816.2	283.45	1.47	102.35 ± 2.7d	150.87 ± 7.31bc	127.98 ± 3.29cd	106.11 ± 5.90d	166.64 ± 18.91b	136.19 ± 13.21bcd	131.14 ± 11.05bcd	287.51 ± 46.04a
4	*	813.2	280.43	1.81	77.86 ± 5.71cd	69.75 ± 13.53d	92.80 ± 7.10bcd	115.27 ± 3.63bc	63.20 ± 4.48d	129.57 ± 6.95ab	115.98 ± 9.41bc	158.38 ± 52.02a
5	*	917	412.17	0.94	297.44 ± 31.73c	315.20 ± 25.56c	283.00 ± 7.370c	294.40 ± 21.60c	661.04 ± 12.12a	381.65 ± 32.88b	419.70 ± 25.18b	230.25 ± 6.78d
6	*	1012.2	584.68	1.67	470.66 ± 60.53b	464.72 ± 22.45b	478.73 ± 36.63b	554.72 ± 20.11b	521.88 ± 55.17b	655.55 ± 137.57ab	529.27 ± 62.05b	789.95 ± 210.28a
7	*	1034.5	625.61	1.39	3870.5 ± 210.86b	1001.12 ± 115.81f	1368.3 ± 87.42e	4268.32 ± 34.83a	1887.88 ± 51.23d	885.33 ± 51.50f	2823.64 ± 8.95c	1237.11 ± 73.81e
8	*	1033.5	623.68	1.85	2420.1 ± 342.75b	292.2 ± 44.66e	163.82 ± 17.50e	2841.04 ± 55.39a	1225.76 ± 54.02d	210.16 ± 19.39e	1774.59 ± 78.03c	269.1 ± 0.7e
9	*	1031.5	619.81	1.89	1184.83 ± 163.65b	102.19 ± 2.83e	135.6 ± 10.61e	1426.78 ± 56.07a	267.01 ± 15.53d	89.92 ± 8.87e	497.00 ± 22.86c	135.14 ± 19.9e
10	*	1155	901.20	1.80	125.8 ± 13.95c	137.23 ± 16.59bc	139.42 ± 17.29bc	147.90 ± 3.48bc	160.7 ± 32.14abc	168.21 ± 36.69ab	155.05 ± 7.89abc	193.68 ± 10.28a
11	*	780	247.77	1.29	31.42 ± 5.58cd	36.91 ± 2.77cd	30.15 ± 1.72d	40.15 ± 3.23c	49.24 ± 0.59b	55.47 ± 5.87b	101.64 ± 8.16a	38.82 ± 2.25cd
12	*	751.4	221.36	1.17	24.2 ± 5.97d	33.01 ± 7.70c	25.65 ± 2.22cd	42.27 ± 0.77b	20.35 ± 1.23d	21.52 ± 2.94d	25.50 ± 3.30cd	56.07 ± 4.55a

[1] indicates retention index; [2] denotes retention time; [3] denotes migration time; d, m and p following compounds represents dimer, monomer and polymer, respectively. * indicates unknown compounds without CAS number.

As shown in box A, some alcohols, ketones and unknown compounds were the most abundant in the HH, and these were the main reasons for the differences in the overall fingerprint profile of the HH compared to the other samples. Aldehydes, namely (E)-2-pentenal, 3-methyl butanal, 2-methylpropanal and pentanal, dominated in JC and JXIANG (box B and D), which differed from the GC-MS, where aldehydes were mainly dominated by 2-hexenal and hexanal. Among the overall peak signals of JXIU, box C had the strongest signals of substances that were not characterized; it is therefore necessary to characterize these unknown compounds in future research. Box E demonstrates that HJML had high concentrations of methyl acetate, acetic acid ethyl ester, 2-methylpropyl acetate, and the flavor of these compounds is discriminatingly fruity. None of these were found in GC-MS. As we can see, 12 unknown compounds have strong peak signals in the fingerprints, indicating that these compounds were present at high levels in the samples, and characterizing these substances is essential for the establishment of a complete GC-IMS-based peach fingerprint.

Combining Tables 2 and 4, the types of VOCs detected by the two techniques differed significantly, with GC-MS detecting more than GC-IMS. Lactones, typical VOCs in peaches, were not found in GC-IMS due to their high molecular weight, which makes them difficult to be detected. Although both techniques are used in conjunction with GC, their focus is dissimilar. GC-MS works under a vacuum and at a high temperature and focuses on the accuracy of qualitative and quantitative information, while GC-IMS performs detection at atmospheric pressure and normal temperature and focuses more on reflecting the authenticity of the sample flavor [40,41].

3.2.3. Similarity Analysis of Samples between Different Peach Cultivars Based on PCA

PCA was performed on the volatile compound content (signal peak volume) of different cultivars of peaches using the Dynamic PCA plug-in, and the data were visualized to obtain a spatial–dimensional plot containing three principal components, where the X, Y and Z axes indicate the first, second and third principal components, respectively (Figure 6). The cumulative contribution rate of PC1, PC2 and PC3 was 65.7%. The results show that the eight peach cultivars were clearly distinguished based on the identified VOCs using GC-IMS. JC and JXIU are located on the right side of the PC1-axis (Figure 6a), indicating that the content of characteristic aroma compounds in these two cultivars were more similar, which might be caused by the fact that JC was an F1 offspring of JXIU. DTML, XFML, JG and JXIANG are close together and can be grouped together, while HH and HJML are located at the ends of the PC3 and PC2 axes, which means that they are relatively different from the other samples based on the VOC performance (Figure 6a). The difference between samples in a group is small, while the differences between groups are more obvious. Overall, the aroma profiles of JC, HJML and HH are more specific compared to the other samples. This result is highly consistent with that of the cluster analysis in Figure 3. The PCA loading plot showed that (E)-2-pentenal, 2-hexenal and pentanal highly contributed to the JC's aroma, and 1-hexanol, 3-methylbutanol highly contributed to the HH aroma. These results are consistent with the GC-IMS fingerprints. These findings suggest that the aroma profiles of these eight popular peaches are quite different for selecting strong/specific aroma cultivars.

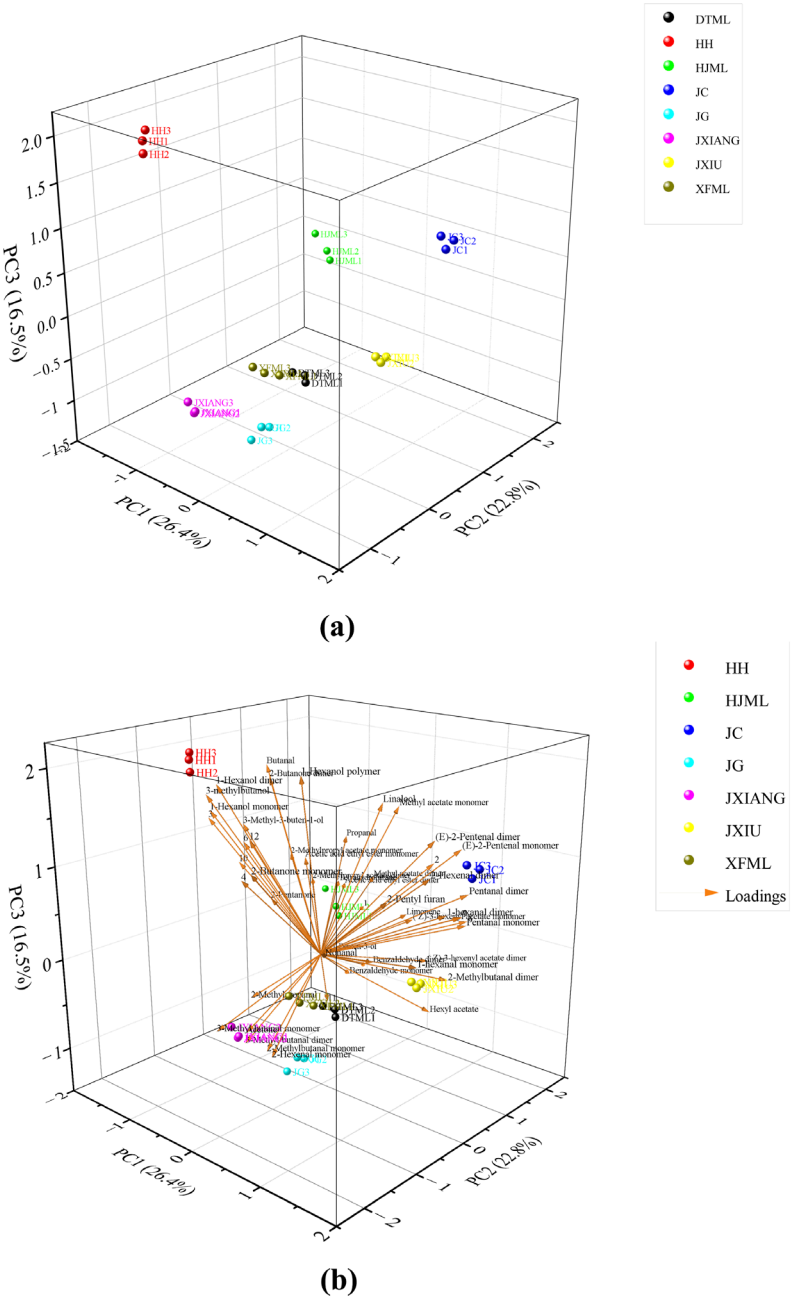


Figure 6. Principal component analysis (PCA) score plot (**a**) and PCA loading plot of different peach cultivars (**b**).

4. Conclusions

The aroma profiles of eight popular peach cultivars produced in Shanghai were comprehensively analyzed using GC–MS, OAV determination and GCIMS. Seventy VOCs were detected using GC-MS, including nine aldehydes, ten esters, eleven terpenoids, nine alcohols, six lactones, five ketones, five alkanes, eleven aromatic hydrocarbons, two furans and two other compounds, of which twenty-three VOCs were commonly identified in eight peach cultivars. The most VOCs were detected in HJML and the least in JG. Cluster analysis classified XFML, JG, DTML and JXIU into one cluster, which means that their aroma profiles are more similar.

In addition, based on an OAV $\geq$ 1, a total of 17 key aroma compounds were screened, and their contributions were ranked as follows: γ- decalactone> β- ionone > hexanal > 2-hexenal > linalool > nonanal > 3-hexenol > δ-decalactone > D-limonene > β-myrcene

> 1-hexanol > γ-octalactone > γ-dodecalactone > (Z)-3-hexen-1-yl acetate > butyl acetate > isopentyl acetate > octanal. The OAV of VOCs differed greatly among the cultivars. Lactones had the highest OAV in HJML, which indicates that HJML is the cultivar that contains the most fruity notes. Terpenoids had the highest OAV in JC, meaning that JC had the strongest floral notes. It is obvious that JXIU was the cultivar with the lightest aroma.

Furthermore, a total of twenty-six VOCs were detected using GC-IMS, among which aldehydes accounted for the largest proportion. GC-IMS has the advantage of data visualization, which can visualize the differences of volatiles among samples. It can be directly observed in the fingerprints that aldehydes have the strongest signals in samples. The PCA results showed that XFML, JG, DTML and JXIU were close to each other, whereas HJML, HH and JC were distant from other samples, which is similar to the results of the cluster analysis. The differences in focus and working conditions between GC-MS and GC-IMS led to significant differences in the composition of the VOCs detected by them. The combination of GC-MS and GC-IMS can capture relatively complete flavor information of samples, which is a hot research topic in the field of flavor at present and will be for a long time in the future.

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