Hindawi
Journal of Food Quality
Volume 2021, Article ID 9958414, 15 pages
https://doi.org/10.1155/2021/9958414

Research Article

Volatile Profile Characterization of Winter Jujube from Different Regions via HS-SPME-GC/MS and GC-IMS

Yening Qiao,[1,2] **Jinfeng Bi**,[1] **Qinqin Chen**,[1] **Xinye Wu**,[1,2] **Min Gou**,[1,2] **Haonan Hou**,[1] **Xinwen Jin**,[3] **and Giorgia Purcaro**[2]

[1]*Institute of Food Science and Technology, Chinese Academy of Agricultural Sciences (CAAS)/ Key Laboratory of Agro-Products Processing, Ministry of Agriculture and Rural Affairs, 100193 Beijing, China*
[2]*Gembloux Agro-Bio Tech Department, University of Liége, 5030 Gembloux, Belgium*
[3]*Institute of Agro-Products Processing Science and Technology, Xinjiang Academy of Agricultural and Reclamation Science, 832000 Shihezi, China*

Correspondence should be addressed to Jinfeng Bi; bjfcaas@126.com and Qinqin Chen; celerylc@163.com

Received 13 March 2021; Revised 2 July 2021; Accepted 22 July 2021; Published 31 August 2021

Academic Editor: Luca Campone

Copyright © 2021 Yening Qiao et al. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

A combined untargeted and targeted approach was established for fingerprinting volatile organic compounds in winter jujubes from eight regions of China. Volatiles, including alcohols, aldehydes, acids, esters, and alkenes, were identified by gas chromatography-ion mobility spectrometry (GC-IMS). Benzyl alcohol, octanoic acid, 2-hexenal, linalool, 2-nonenal, and ethyl decanoate were the most common compounds present in all jujubes. Principal component analysis (PCA) from GC-IMS and untargeted E-nose showed that the main volatile organic compounds (VOCs) of most jujubes were similar. The volatile organic compounds of winter jujubes from Yuncheng city, Shanxi province, and Aksu region, Xinjiang province, were significantly different from those from other regions. 1-Penten-3-ol, ethyl hexanoate, methyl laurate, and 2-formyltoluene were the markers of XJAKS with green and fruity aroma, and SXYC could be labeled by acetone and 2-methoxyphenol with woody and pungent aroma. GC-IMS was an effective method for volatile fingerprinting of jujubes with high sensitivity and accuracy.

1. Introduction

Winter jujube (*Ziziphus jujuba* Mill. *cv.* Dongzao) is a unique late-ripening jujube cultivar which originated in China [1]. It is widely distributed in China, including Hebei, Shandong, Shaanxi, Shanxi, and Xinjiang provinces after years of domestication and cultivation [2]. As a representative variety of fresh jujube, it is recognized by its delicious taste and pleasant aroma [1, 3]. As a vital factor considered by consumers, sensory quality can be affected by aroma characteristics, which was correlated with VOCs. The VOCs of fresh winter jujube were composed by alkanes, alcohols, esters, and amines [4]. Geographic region and variety will cause the change of VOCs as reported for different varieties of red jujube [5, 6]. There were significant differences in contents of alcohols, acids, and aromatic compounds among different red jujube varieties [6]. However, there is no systematic study on the geographical differentiation of winter jujube, especially on the VOCs.

At present, headspace solid phase microextraction gas chromatography-mass spectrometry (HS-SPME-GC/MS) and electronic nose (E-nose) are widely applied for the analysis of VOCs in jujube [4, 6]. HS-SPME-GC/MS combines the high separation ability of SPME and the superior identification ability of MS for VOCs [7]. E-nose distinguishes samples via the values of VOCs on different metal-oxide sensors. It defects in the identification of differential components [8]. In contrast to these analytical methods, IMS is a complementary way to detect compounds with low concentration (ppbv levels) with an advantage of fast response [9]. In IMS, vapors from the sample are firstly transferred into the ionization region by carrier gas. Secondly, the product ions formed from the interaction between neutral sample molecules and buffer gas, or bath gas

molecules in the drift tube will be transported by the electric field into the separation region. Thirdly, the product ions with different drift velocities will reach the detector with different times. At last, the drift time will be used for the qualitative analysis [9]. GC-IMS combines the separation characteristics of GC and the fast response of IMS [10]. GC-IMS has been proved successful in regional identification and varieties classification based on differentiation of VOCs [11–13]. GC-IMS was also used to monitor the changes of VOCs in winter jujube during cold storage [14]. Besides, the combined analysis of GC-IMS and GC-MS has been successfully applied in the differentiation of VOCs from food matrices [15–17]. However, few investigations on the fingerprinting of volatile profiles in winter jujubes from different regions have been done by GC-IMS.

Principal component analysis (PCA) is an effective way to classify samples using unsupervised statics and has been widely employed in chemometrics and bioinformatics today [18]. Variable influence on projection (VIP) (greater than 1.0) has been applied to identify primary and specialized metabolites that are responsible for the discrimination of fruit and vegetables [19]. PCA and VIP scores would be effective for differentiation and selection of potential aroma maker of winter jujubes.

In this study, the geographic differentiation of winter jujubes was investigated by GC-IMS and E-nose based on VOCs. Furthermore, the potential markers of winter jujube from each specific region were identified and quantified by GC-IMS and GC-MS.

2. Material and Methods

2.1. Winter Jujube Preparation and Chemicals. Winter jujubes from eight different regions were purchased from China's famous jujube trading market (Beiyuanchun Jujube Market in Xinjiang, Xinzheng Jujube Market in Henan, and Cuierzhuang Jujube Market in Hebei). The information of jujube samples is shown in Table 1. 50 kg of winter jujube samples was collected from each region. Fresh fruits free from pests and diseases were washed, and pits were removed, sliced, and frozen by liquid nitrogen and then stored at −40°C for testing as soon as possible.

The reagent of C4–C20 alkanes was purchased from O2si Smart Solution (Charleston, West Virginia, USA), cyclohexanone was purchased from Genenode Trading Co., Ltd. (Beijing, China), and n-hexane was purchased from Hushi Co., Ltd. (Shanghai, China). Standards used in this project were as follows: benzyl alcohol, octanoic acid, 2-hexenal, 2-heptenal, linalool, methyl myristoleate, 2-nonenal, styrene, hexanoic acid, hexanal, ethyl decanoate, pentanoic acid, 1-penten-3-ol, 1-octen-3-ol, E-2-hexen-1-ol, butanoic acid, heptanoic acid, (E)-3-hexanoic acid, nonanoic acid, acetone, 3-pentanone, 2-hexanone, acetoin, 6-methyl-5-hepten-2-one, (E)-4-undecenal, butanal, E-2-heptanal, heptanal, 2,4-heptadienal, 2-decenal, 3-buten-2-one, ethyl hexanoate, methyl decanoate, methyl laurate, limonene, 2-formyltoluene, 2-formylphenol, 2-nitrophenetole, 2-nitrophenol, 2-methoxyphenol, and 2-pentylfuran were all purchased from MilliporeSigma (St. Louis, MO, USA).

2.2. Sample Preparation. About 100 g of frozen winter jujube slices was ground for 60 s with Joyoung juicer (JYL-CO20, Joyoung Co., Ltd., Shandong, China). Accurate 2.0 g of winter jujube pulp was put into a 20 mL vial sealed with a magnetic screw cap and septum before testing.

2.3. GC-IMS Analysis. A FlavourSpec instrument (G.A.S. Gesellschaft für analytische Sensorsysteme mbH Dortmund, Germany) was used for GC-IMS analysis. Procedures were referred to previous studies with small modifications [20]. The sample vial was incubated at 50°C for 20 min, and then 500 μL of headspace was injected at 85°C in splitless mode. Tritium (6.5 keV) was used as the ionization source in this project. A FS-SE-54-CB-1 (15 m × 0.53 mm ID) column was used for separation at 60°C. Linear pressure program of the column was as follows: 2 mL/min for 2 min, ramped up to 10 mL/min over 8 min, then reached to 100 mL/min over 10 min, and at last got to 150 mL/min over 5 min. Nitrogen of 99.99% purity was the drift gas at a flow rate of 150 mL/min and the drift tube was operated at 45°C. All standards were run under the same test procedure to supplement GC × IMS Library Search for qualitative analysis.

The spectrogram was analyzed by Laboratory Analytical Viewer (LAV), where retention time and drift time were analyzed for the qualification of VOCs. Reporter plug-in was used to compare spectrogram differences among samples from the two-dimensional and three-dimensional view. Gallery Plot plug-in was used to compare the differences of volatile fingerprints visually. PCA plug-in was used for classification analysis.

2.4. E-Nose Analysis. A commercial PEN 3.5 E-Nose (Airsense Analytics, GmBH, Schwerin, Germany) containing ten metal-oxide semiconductors was used to distinguish the overall flavor perception of winter jujubes from eight regions. The detailed procedure of sample preparation was referred to Chen et al. [6]. Sample preparation was the same as that in GC-IMS analysis.

2.5. HS-SPME-GC/MS Analysis. HS-SPME conditions and GC-MS analysis were referred to Chen et al. with small modifications [6]. The vials (the same as those in GC-IMS analysis) were equilibrated at 50°C for 40 min. Polydimethylsiloxane/divinylbenzene (PDMS/DVB) fiber was used for extraction and desorbed at 250°C for 3 min in splitless mode. DB-WAX capillary column (30 m × 0.25 mm × 0.25 μm) was used for separation. The oven temperature program was as follows: 40°C for 3 min, heating to 120°C (5°C/min), then rising to 200°C (10°C/min), and holding at 200°C for 5 min. Helium was the carrier gas at a flow rate of 1.0 mL/min. Electron Impact mode with the ion source temperature set at 200°C and the ionization energy of 70 eV was performed in the MS detector. The acquisition was full-scan mode and mass acquisition range was 35–550 m/z.

The standards were qualitatively analyzed under HS-SPME-GC/MS analysis. Retention index (RI) of the

Table 1: Geographical distribution information of winter jujubes from eight regions.

Abbreviation	Geographical origin	Longitude and latitude
HBHH	Hebei province, Huanghua city	E 117.30, N 41.03
SDZH	Shandong province, Zhanhua city	E 118.14, N 37.7
SDYT	Shandong province, Yantai city	E 121.17, N 36.76
SXYC	Shanxi province, Yuncheng city	E 110.15, N 34.35
SXLY	Shanxi province, Linyi city	E 110.77, N 35.15
SNXDL	Shaanxi province, Dali city	E 109.93, N 34.80
XJKEL	Xinjiang Uygur Autonomous Region, Kuerle city	E 86.06, N 41.68
XJAKS	Xinjiang Uygur Autonomous Region, Aksu	E 80.29, N 41.15

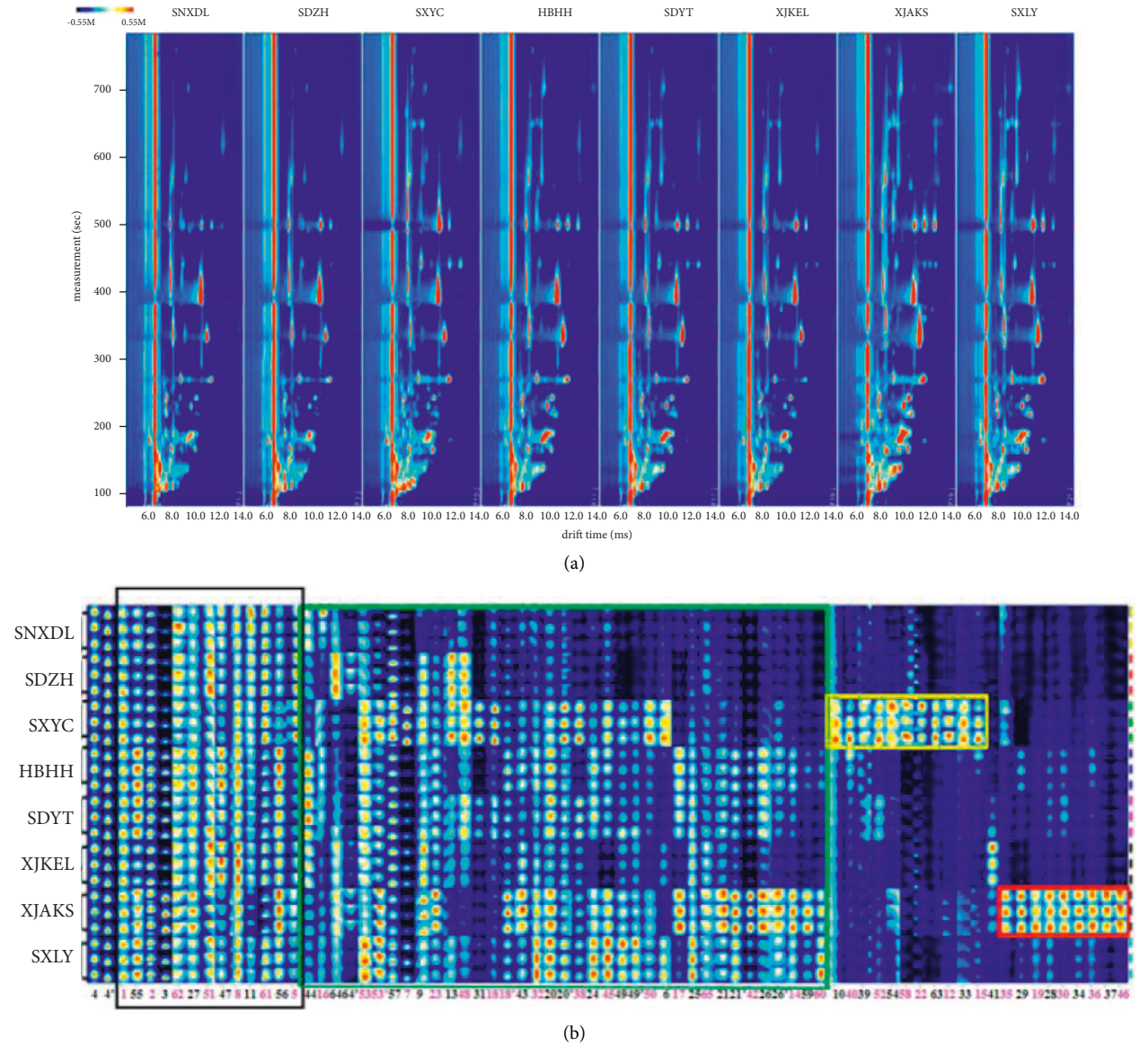

Figure 1: (a) 2D topographic plots of VOCs from eight regions of winter jujube. (b) VOCs qualitative comparisons of eight regions of winter jujube by GC-IMS.

compounds was calculated based on the retention time of C4–C20 alkanes mixture and used as additional support for the identification of compounds. A 2 mg/L solution of cyclohexanone as the optimized internal standard was used for the relative quantitative analysis of VOCs. NIST 17 database was used for identification of the compounds.

Table 2: Volatile organic compounds identified by GC-IMS.

No.	Compound	Cas	Formula	Molecular weight	RI	Rt [sec]	Dt [RIPrel]	Identification approach
1	Benzyl alcohol (monomer)	100-51-6	C_7H_8O	108	1090	758.55	1.21	RI, DT, Std
2	Unknown (monomer)	—	—	—	987	568.62	1.17	RI, DT
3	Hexanoic acid (monomer)	142-62-1	$C_6H_{12}O_2$	116	989	573.49	1.30	RI, DT, Std
4	Cyclohexanone (monomer)	108-94-1	$C_6H_{10}O$	98	904	410.86	1.15	RI, DT, Std
4′	Cyclohexanone (dimer)	108-94-1	$C_6H_{10}O$	98	904	402.28	1.45	RI, DT, Std
5	Hexanal (monomer)	66-25-1	$C_6H_{12}O$	100	796	269.29	1.56	RI, DT, Std
6	Unknown (monomer)	—	—	—	768	242.96	1.11	RI, DT
7	2,4-Heptadienal (monomer)	5910-85-0	$C_7H_{10}O$	110	1427	242.38	1.41	RI, DT, Std
8	2-Nonenal (monomer)	2463-53-8	$C_9H_{16}O$	140	687	181.34	1.07	RI, DT, Std
9	3-Buten-2-one (monomer)	79-77-6	$C_{13}H_{20}O$	192	1914	179.98	1.30	RI, DT, Std
10	Acetone (monomer)	67-64-1	C_3H_6O	58	814	110.75	1.11	RI, DT, Std
11	Styrene (monomer)	100-42-5	C_8H_8	104	602	140.40	1.05	RI, DT, Std
12	Unknown (monomer)	—	—	—	596	137.86	1.32	RI, DT
13	E-2-heptenal (monomer)	18829-55-5	$C_7H_{12}O$	112	570	127.33	1.04	RI, DT, Std
14	Unknown (monomer)	—	—	—	629	152.29	1.16	RI, DT
15	Unknown (monomer)	—	—	—	739	218.98	1.22	RI, DT
16	1-Octen-3-ol (monomer)	3391-86-4	$C_8H_{16}O$	128	1349	226.98	1.15	RI, DT, Std
17	Unknown (monomer)	—	—	—	1042	664.75	1.14	RI, DT
18	Limonene (monomer)	138-86-3	$C_{10}H_{16}$	136	1032	647.98	1.21	RI, DT, Std
18′	Limonene (dimer)	138-86-3	$C_{10}H_{17}$	136	1032	647.00	1.30	RI, DT, Std
19	Ethyl hexanoate (monomer)	123-66-0	$C_8H_{16}O_2$	144	1405	600.99	1.39	RI, DT, Std
20	Unknown (monomer)	—	—	—	961	513.04	1.15	RI, DT
20′	Unknown (dimer)	—	—	—	958	507.19	1.47	RI, DT
21	Unknown (monomer)	—	—	—	924	443.23	1.28	RI, DT
21′	Unknown (dimer)	—	—	—	922	440.50	1.67	RI, DT
22	Unknown (monomer)	—	—	—	786	259.34	1.09	RI, DT
23	Nonanoic acid (monomer)	112-05-0	$C_9H_{18}O_2$	158	2083	256.62	1.36	RI, DT, Std
24	Butanoic acid (monomer)	107-92-6	$C_4H_8O_2$	88	1538	218.01	1.12	RI, DT, Std
25	Unknown (monomer)	—	—	—	737	217.42	1.43	RI, DT
26	Unknown (monomer)	—	—	—	654	164.18	1.17	RI, DT
26′	Unknown (dimer)	—	—	—	655	164.97	1.40	RI, DT
27	2-Heptenal (monomer)	2463-63-0	$C_7H_{12}O$	112	663	169.06	1.15	RI, DT, Std
28	2-Formyltoluene (monomer)	529-20-4	C_8H_8O	120	1555	121.67	1.19	RI, DT, Std
29	1-Penten-3-ol (monomer)	616-25-1	$C_5H_{10}O$	86	1134	122.26	1.03	RI, DT, Std
30	2-Formylphenol (monomer)	90-02-8	$C_7H_6O_2$	122	1542	116.99	1.22	RI, DT, Std
31	Unknown (monomer)	—	—	—	740	219.37	1.40	RI, DT
32	Unknown (monomer)	—	—	—	780	254.27	1.16	RI, DT
33	Unknown (monomer)	—	—	—	721	205.33	1.14	RI, DT
34	(E)-4-Undecenal (monomer)	68820-35-9	$C_{11}H_{20}O$	168	2719	203.77	1.43	RI, DT, Std
35	3-Hexenoic acid, (E)-(monomer)	1577-18-0	$C_6H_{10}O_2$	114	1876	730.66	1.19	RI, DT, Std
36	Methyl laurate (monomer)	111-82-0	$C_{13}H_{26}O_2$	214	1765	709.01	1.21	RI, DT, Std
37	2-Pentylfuran (monomer)	3777-69-3	$C_9H_{14}O$	138	1218	317.26	1.21	RI, DT, Std
38	Unknown (monomer)	—	—	—	503	104.13	1.04	RI, DT
39	6-Methyl-5-hepten-2-one	110-93-0	$C_8H_{14}O$	126	1335	652.47	1.26	RI, DT, Std
40	Unknown (monomer)	—	—	—	953	498.41	1.66	RI, DT
41	Unknown (monomer)	—	—	—	699	189.54	1.39	RI, DT
42′	Unknown (dimer)	—	—	—	699	189.54	1.42	RI, DT
43	Methyl decanoate (monomer)	110-42-9	$C_{11}H_{22}O_2$	186	1613	185.05	1.33	RI, DT, Std
44	2-Hexanone (monomer)	591-78-6	$C_6H_{12}O$	100	1087	260.91	1.18	RI, DT,Std
45	Unknown (monomer)	—	—	—	954	499.97	1.56	RI, DT
46	Heptanal (monomer)	111-71-7	$C_7H_{14}O$	114	1280	373.42	1.32	RI, DT, Std
47	Methyl myristoleate (monomer)	56219-06-8	$C_{15}H_{28}O_2$	240	670	172.37	1.08	RI, DT, Std
48	2-Decenal (monomer)	3913-71-1	$C_{10}H_{18}O$	154	1638	171.40	1.36	RI, DT, Std
49	Unknown (monomer)	—	—	—	1062	702.38	1.33	RI, DT
49′	Unknown (dimer)	—	—	—	1061	701.22	1.81	RI, DT
50	Unknown (monomer)	—	—	—	988	571.74	1.25	RI, DT
51	Linalool (monomer)	78-70-6	$C_{10}H_{18}O$	154	981	556.52	1.42	RI, DT, Std
52	Phenol, 2-nitro-(monomer)	88-75-5	$C_6H_5NO_3$	139	1810	359.18	1.57	RI, DT, Std

Table 2: Continued.

No.	Compound	Cas	Formula	Molecular weight	RI	Rt [sec]	Dt [RIPrel]	Identification approach
53	E-2-Hexen-1-ol (monomer)	928-95-0	$C_6H_{12}O$	100	1361	346.71	1.18	RI, DT, Std
53′	E-2-Hexen-1-ol (dimer)	928-95-0	$C_6H_{12}O$	100	1361	344.37	1.51	RI, DT, Std
54	2-Methoxyphenol (monomer)	90-05-1	$C_7H_8O_2$	124	1831	309.46	1.25	RI, DT, Std
55	Octanoic acid (monomer)	124-07-2	$C_8H_{16}O_2$	144	756	232.43	1.10	RI, DT, Std
56	Pentanoic acid (monomer)	109-52-4	$C_5H_{10}O_2$	102	754	231.26	1.35	RI, DT, Std
57	3-Pentanone (monomer)	96-22-0	$C_5H_{10}O$	86	898	188.76	1.35	RI, DT, Std
58	2-Nitrophenetole (monomer)	610-67-3	$C_8H_9NO_3$	167	1651	162.82	1.19	RI, DT, Std
59	Unknown (monomer)	—	—	164	652	163.40	1.31	RI, DT
60	Acetoin (monomer)	513-86-0	$C_4H_8O_2$	88	1120	204.55	1.05	RI, DT, Std
61	Ethyl decanoate (monomer)	110-38-3	$C_{12}H_{24}O_2$	200	682	179.01	0.94	RI, DT, Std
62	2-Hexenal (monomer)	505-57-7	$C_6H_{10}O$	98	633	154.04	1.02	RI, DT, Std
63	Unknown (monomer)	—	—	—	525	111.14	1.17	RI, DT
64	Butanal (monomer)	123-72-8	C_4H_8O	72	568	126.55	1.10	RI, DT, Std
64′	Butanal (dimer)	123-72-9	C_4H_9O	72	864	124.99	1.28	RI, DT, Std
65	Unknown (monomer)	—	—	—	537	115.24	1.15	RI, DT

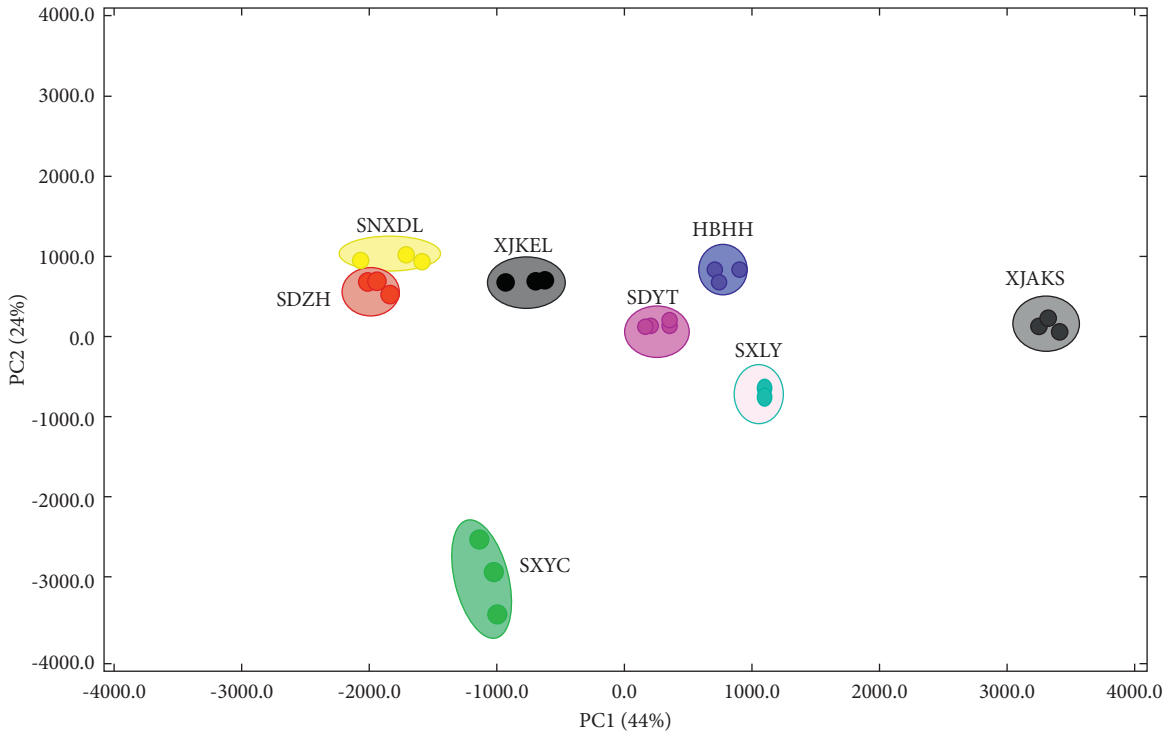

Figure 2: PCA plot of eight regions of winter jujube.

2.6. Statistical Procedures. Data standardization was performed using SPSS 13.0 software (SPSS Inc, Chicago, IL). MetaboAnalyst was used for biplot and calculation of LDA analysis and VIP scores (https://www.metaboanalyst.ca/MetaboAnalyst/home.xhtml). Morpheus was applied for the correlation analysis by heatmap (https://software.broadinstitute.org/morpheus/). Each sample was repeated in triplicate.

3. Results and Discussion

3.1. Determination of VOCs from Eight Regions of Winter Jujube by GC-IMS. VOCs of winter jujube samples from eight regions of China were analyzed by GC-IMS, and the result is shown in Figure 1(a). The red baseline on the left is the reaction ion peak (RIP). RIP represents the total number of ions in the ionization chamber, described as $H^+(H_2O)n$ (n represents the number of water molecules) [17]. The points on the right of RIP represent the signal (monomer, dimer, and even trimer) of volatiles extracted from the samples. Most of the signals appeared in the retention time of 100–600 s and the drift time of 6.0–14.0 ms. The red color represents the higher signal intensity (higher concentration) of the substance, while the white color indicated weaker intensity (lower concentration) [21]. In IMS, the formation of product ions mainly depends on the affinity of analytes to

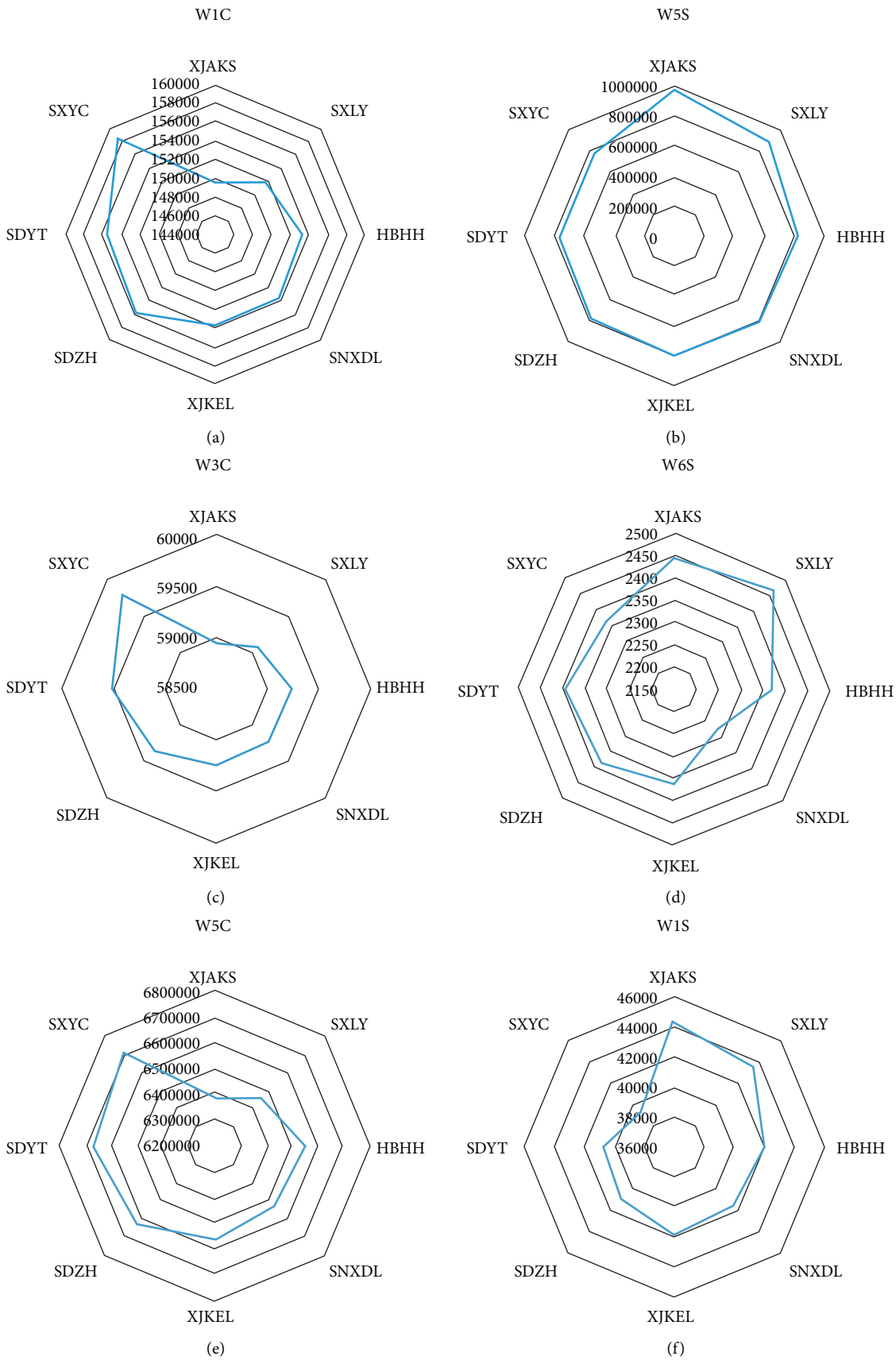

Figure 3: Continued.

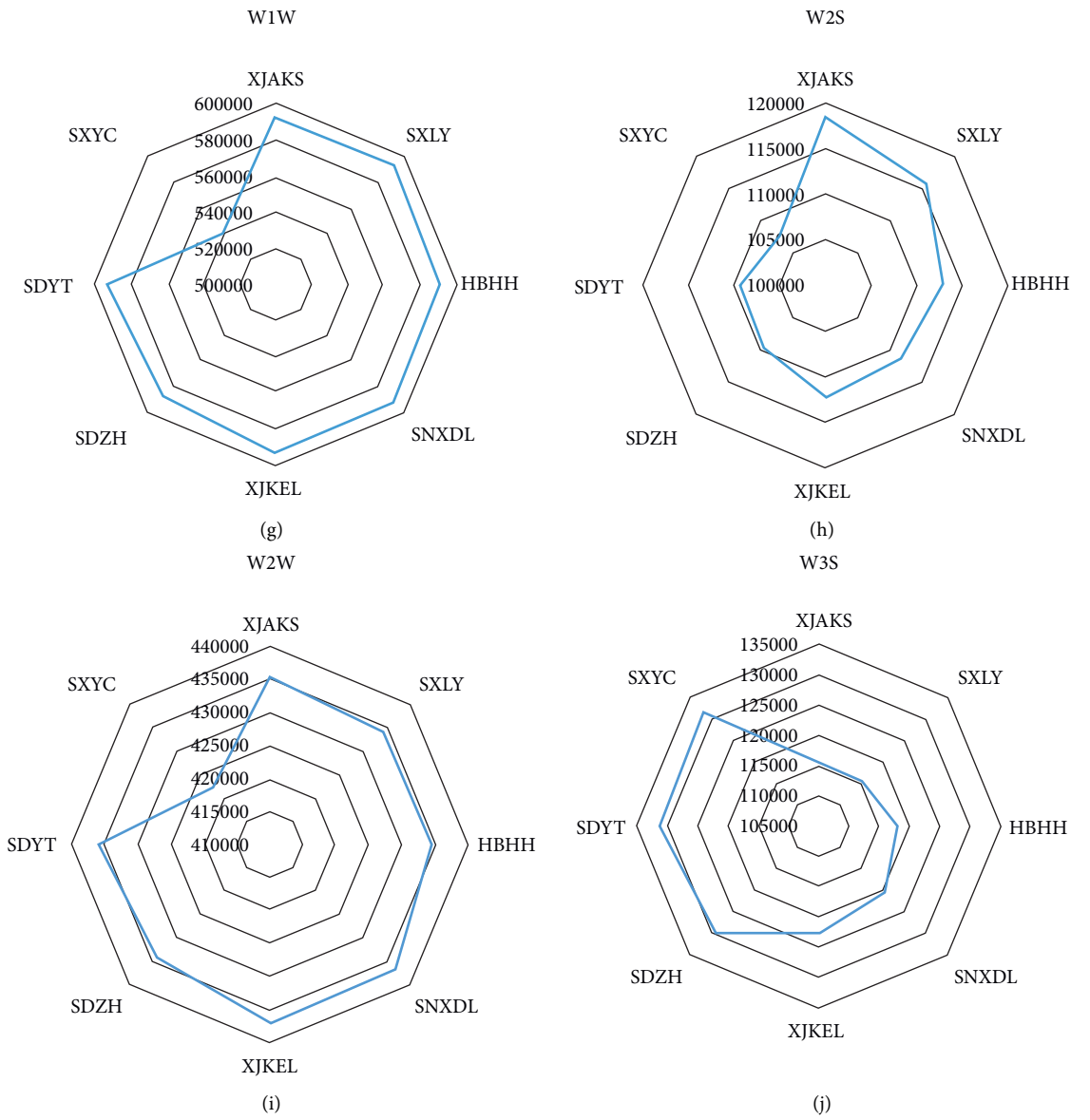

Figure 3: Response intensities of different sensors to aroma characteristics of different regions of winter jujube. (a–j) response on different sensors.

protons. Product ions could also be affected by the concentration of the analyte, the chemical properties, and the temperature of the drift tube [20].

Varieties of fruits have distinct aroma depending on the composition, concentration, aroma description, and odor threshold of VOCs [22]. The composition of VOCs varied in winter jujubes from different regions. In order to identify the specific differences and make a quantitative comparison, all peaks were identified and numbered for fingerprint comparison. The direct comparison of the components in each sample was shown in Figure 1(b). VOCs in the black frame were the common components among eight regions of winter jujubes. VOCs in the yellow and red frame were the ones present only in SXYC and XJAKS. VOCs in the green frame were the differential ones in eight regions of winter jujube. The corresponding data of retention time (RT) and drift time (DT) are presented in Table 2.

The *X*-axis represented the code of the compound, corresponding to the information in Table 2.

Common compounds included alcohols, aldehydes, acids, esters, and alkenes (Figure 1(b)). In particular, benzyl alcohol, octanoic acid, 2-hexenal, 2-heptenal, linalool, methyl myristoleate, 2-nonenal, styrene, hexanoic acid, hexanal, ethyl decanoate, and pentanoic acid presented small concentration difference (Figure 1(b)). These identified volatiles, as well as their aroma characteristics, would be important for the whole aroma of winter jujube.

Alcohols were formed by sugar catabolism and/or acid degradation in the food matrix [23]. Benzyl alcohol contributes to a slightly fruity aroma, while linalool, a

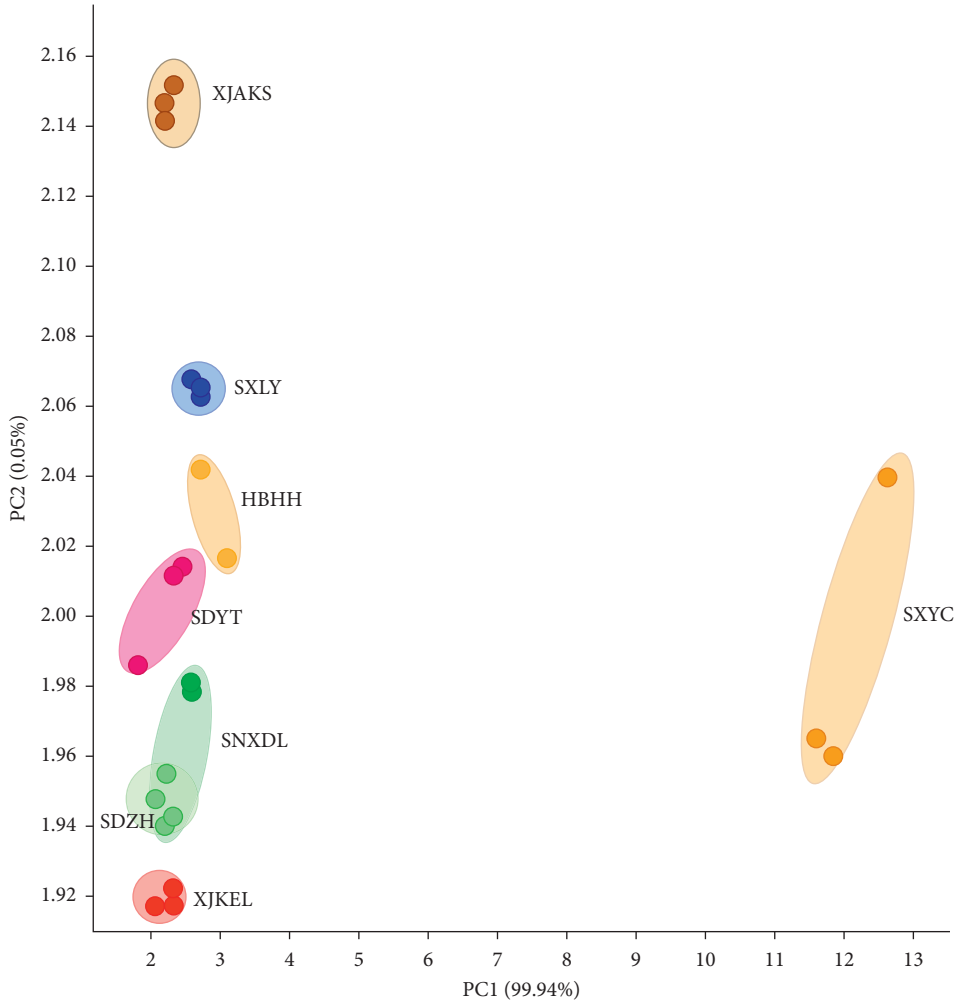

Figure 4: PCA results of eight regions of winter jujubes differentiated by E-nose.

Table 3: Sensors and response characteristics of E-nose.

Number	Sensors	Response characteristics
1	W1C	Aromatic compounds
2	W5S	Nitroxide
3	W3C	Ammonia and aromatic components
4	W6S	Hydrogen selective
5	W5C	Alkanes and aromatic components
6	W1S	Methane
7	W1W	Sulfides
8	W2S	Ethyl alcohol
9	W2W	Aromatic components and organic sulfide
10	W3S	Alkanes

monoterpenoid, contributes to floral, lavender, lemon, and rose flavor [23, 24]. Aldehydes were thought to be mainly produced via lipid oxidation and decomposition, contributing most to the overall aroma among all categories because of relatively low odor thresholds. Hexanal derived from linoleic acid contributes to flavor of fruity, grass, and green, with a low odor threshold of 1.1 ng/L [25]. 2-Nonenal is a plant metabolite and derives from linoleate decomposition, with flavor of paper [25]. 2-Heptenal is a plant metabolite with soapy and fatty aroma and existed in white pomelo peel [26]. Acids like octanoic acid, hexanoic acid, and pentanoic acid might be related to cheese aroma [27]. Ethyl decanoate is present in fruits like cherry and pineapple with fruity aroma [26]. Styrene was reported to have sweet, balsamic, and almost floral odor that was extremely penetrating [28]. Esters endow fruity aroma for fruits and methyl myristoleate

Table 4: Volatile organic compounds of winter jujubes quantified by HS-SPME-GC/MS.

	Compound	CAS	RI cal	RI lit	Concentration (mg/kg)								Aroma description
					SNXDL	SDZH	XJAKS	HBHH	SDYT	XJKEL	SXYC	SXLY	
Alcohols (3)	1-Penten-3-ol*	616-25-1	1162	1148	6.11 ± 0.33^{c}	2.28 ± 0.23^{c}	52.08 ± 5.74^{a}	3.45 ± 0.65^{c}	1.75 ± 0.20^{c}	2.03 ± 0.50^{c}	30.7 ± 3.12^{b}	5.21 ± 0.14^{c}	Grassy, green
	1-Octen-3-ol	3391-86-4	1455	1449	8.06 ± 0.13^{c}	10.85 ± 1.13^{b}	0.12 ± 0.02^{e}	4.34 ± 0.14^{d}	0.44 ± 0.01^{e}	18.63 ± 2.01^{a}	nd.	0.45 ± 0.02^{e}	Cucumber, earth, fat, floral, mushroom
	E-2-hexen-1-ol	928-95-0	1420	1409	8.98 ± 0.45^{a}	7.46 ± 0.45^{ab}	nd.	nd.	5.64 ± 0.22^{b}	8.76 ± 3.26^{a}	8.70 ± 1.34^{c}	nd.	Blue cheese, vegetable
	Total				23.15 ± 0.91	20.59 ± 1.81	52.20 ± 5.76	7.79 ± 0.79	7.83 ± 0.43	29.42 ± 5.77	39.40 ± 4.46	5.66 ± 0.16	
Acids (3)	Butanoic acid	107-92-6	1634	1623	nd.	3.98 ± 0.22^{c}	16.56 ± 2.23^{a}	5.65 ± 1.21^{b}	1.03 ± 0.02^{d}	0.45 ± 0.02^{d}	nd.	nd.	Butter, cheese, sour
	3-Hexenoic acid, (E)-	1577-18-0	1929	1948	0.70 ± 0.11^{d}	0.78 ± 0.11^{d}	5.19 ± 0.11^{bc}	nd.	3.00 ± 0.23^{bc}	36.11 ± 7.89^{a}	8.28 ± 2.33^{b}	nd.	Fruit
	nonanoic acid	112-05-0	2174	2171	3.45 ± 0.06^{c}	0.22 ± 0.01^{d}	9.43 ± 1.01^{b}	0.43 ± 0.01^{d}	4.88 ± 0.12^{c}	7.70 ± 2.12^{b}	9.34 ± 1.30^{b}	20.43 ± 3.23^{a}	Fat, green, sour
	Total				4.15 ± 0.17	4.98 ± 0.34	31.18 ± 3.35	6.08 ± 1.22	8.91 ± 0.37	44.26 ± 10.03	17.62 ± 1.02	20.43 ± 3.23	
Ketones (6)	Acetone*	67-64-1	825	816	1.39 ± 0.32^{c}	nd.	nd.	5.45 ± 0.12^{b}	7.99 ± 0.43^{b}	2.02 ± 0.11^{c}	30.78 ± 4.78^{a}	nd.	Pungent
	3-Pentanone*	96-22-0	975	956	25.43 ± 2.45^{b}	38.80 ± 3.15^{a}	0.34 ± 0.02^{d}	nd.	1.60 ± 0.05^{d}	13.95 ± 3.14^{c}	10.84 ± 1.23^{d}	nd.	Acetone-like
	2-Hexanone	591-78-6	1124	1100	4.56 ± 0.82^{b}	4.34 ± 0.82^{b}	nd.	nd.	nd.	nd.	4.45 ± 0.21^{b}	19.16 ± 3.02^{a}	—
	Acetoin	513-86-0	1272	1291	5.45 ± 0.90^{b}	2.22 ± 0.20^{c}	9.43 ± 0.20^{a}	nd.	4.88 ± 0.32	nd.	nd.	nd.	Butter, creamy, green pepper
	6-Methyl-5-hepten-2-one	110-93-0	1548	1341	nd.	nd.	nd.	nd.	1.60 ± 0.12^{b}	nd.	3.84 ± 0.22	nd.	Citrus, mushroom, pepper, rubber, strawberry
	3-Buten-2-one	79-77-6	1947	1958	1.39 ± 0.12^{cd}	6.10 ± 0.12^{b}	nd.	5.45 ± 0.12^{b}	8.99 ± 1.11^{a}	2.02 ± 0.34^{c}	0.88 ± 0.09^{d}	nd.	Pungent odor
	Total				38.22 ± 4.61	51.46 ± 4.29	9.77 ± 0.22	10.9 ± 0.24	25.06 ± 2.03	17.99 ± 3.59	50.79 ± 6.53	19.16 ± 3.02	
Aldehydes (5)	Butanal	123-72-8	898	867	1.39 ± 0.22^{bc}	1.11 ± 0.22^{bc}	1.37 ± 0.22^{bc}	nd.	8.99 ± 1.52^{ab}	2.02 ± 0.52^{c}	0.88 ± 0.09^{d}	nd.	Pungent odor
	Heptanal	111-71-7	1194	1327	0.97 ± 0.11^{d}	nd.	3.43 ± 0.21^{c}	nd.	nd.	9.43 ± 0.21^{b}	16.43 ± 2.11^{a}	nd.	Citrus, fat, green, nut
	2,4-Heptadienal	5910-85-0	1490	1468	2.45 ± 0.04^{d}	nd.	2.17 ± 0.04^{d}	9.36 ± 2.04^{bc}	9.87 ± 1.23^{ab}	7.70 ± 1.23^{c}	11.39 ± 1.12^{a}	nd.	—
	2-Decenal	3913-71-1	1645	1659	0.23 ± 0.01^{d}	4.34 ± 0.11^{c}	6.70 ± 0.31^{b}	0.54 ± 0.11^{d}	nd.	nd.	4.45 ± 0.32^{c}	19.16 ± 1.52^{a}	Fat, fish, orange
	(E)-4-undecenal	68820-35-9	2992	—	0.87 ± 0.02^{d}	1.70 ± 0.02^{c}	4.34 ± 0.02^{b}	nd.	5.65 ± 0.34^{a}	1.03 ± 0.31^{d}	0.45 ± 0.02^{e}	nd.	—
	Total				5.91 ± 0.4	7.15 ± 0.35	18.01 ± 0.8	9.9 ± 2.15	24.51 ± 3.09	20.18 ± 2.27	33.6 ± 3.66	19.16 ± 1.52	
Esters (3)	Ethyl hexanoate	123-66-0	1435	1240	7.03 ± 1.01^{c}	1.84 ± 0.41^{f}	33.22 ± 0.41^{a}	4.56 ± 0.52^{d}	nd.	3.58 ± 0.37^{e}	8.67 ± 0.69^{b}	4.49 ± 0.21^{de}	Apple peel, overripe fruit, pineapple
	Methyl decanoate	110-42-9	1640	1633	16.34 ± 1.23^{c}	0.11 ± 0.01^{e}	0.09 ± 0.01^{e}	7.98 ± 2.01^{d}	30.47 ± 3.23^{a}	23.52 ± 2.89^{b}	5.51 ± 2.11^{d}	0.34 ± 0.04^{e}	A constituent of many plants
	Methyl laurate*	111-82-0	1805	1805	1.03 ± 0.01^{c}	0.45 ± 0.01^{c}	34.43 ± 3.01^{b}	9.43 ± 2.32^{a}	0.43 ± 0.01^{c}	nd.	7.70 ± 0.21^{a}	9.34 ± 2.33^{b}	Exists in melon, pineapple and other fruits
	Total				24.4 ± 2.4	2.4 ± 0.43	67.74 ± 3.43	21.97 ± 4.85	30.9 ± 3.24	27.1 ± 3.26	21.88 ± 3.01	14.17 ± 2.58	

Table 4: Continued.

Compound		CAS	RI cal	RI lit	Concentration (mg/kg)								Aroma description
					SNXDL	SDZH	XJAKS	HBHH	SDYT	XJKEL	SXYC	SXLY	
Alkenes (1), benzenes (5)	Limonene	138-86-3	1192	1189	0.98 ± 0.05^{cd}	18.80 ± 2.05^{a}	0.34 ± 0.05^{d}	4.34 ± 0.35^{c}	$1.60 \pm 0.32c^{d}$	13.95 ± 4.34^{b}	10.84 ± 1.87^{b}	1.45 ± 0.05^{cd}	Lemon-like aroma
	2-Formyltoluene*	529-20-4	1646	1621	nd.	nd.	19.02 ± 2.02^{a}	0.12 ± 0.02^{c}	nd.	0.44 ± 0.09^{c}	8.63 ± 1.98^{b}	nd.	Cherries and bitter almond
	2-Formylphenol	90-02-8	1679	1636	0.44 ± 0.02^{d}	nd.	7.70 ± 1.01^{b}	2.17 ± 0.03^{c}	9.36 ± 1.23^{a}	nd.	2.43 ± 0.10^{c}	nd.	Almond, pungent, spice
	2-Nitrophenetole	610-67-3	1816	—	4.56 ± 0.21^{b}	4.34 ± 0.21^{b}	nd.	nd.	nd.	nd.	17.70 ± 0.23^{a}	nd.	—
	2-Nitro-phenol	88-75-5	1819	1812	0.34 ± 0.01^{e}	nd.	nd.	7.98 ± 0.10^{c}	10.47 ± 0.02^{a}	3.52 ± 0.04^{d}	8.67 ± 0.21^{b}	nd.	Peculiar sweet smell
	2-Methoxyphenol*	90-05-1	1866	1862	5.45 ± 0.32^{b}	2.22 ± 0.30^{cd}	1.43 ± 0.21^{d}	nd.	4.88 ± 1.31^{b}	nd.	28.63 ± 1.31^{a}	2.89 ± 0.14^{c}	Burnt, phenol, wood
	Total				10.79 ± 0.56	6.56 ± 0.51	4.88 ± 2.27	10.27 ± 0.15	24.71 ± 2.56	3.96 ± 0.13	81.33 ± 3.83	2.89 ± 0.14	
Furans (1)	2-Pentylfuran	3777-69-3	1229	1249	nd.	nd.	1.75 ± 0.11^{b}	nd.	0.54 ± 0.08^{c}	nd.	nd.	4.45 ± 1.29^{a}	Butter, floral, fruit, green bean

"RI cal" means RI calculated by the retention time of alkanes. "RI lit" means RI listed in the literature. Compounds with "*" mean variables with VIP score >1. "nd." means not detected.

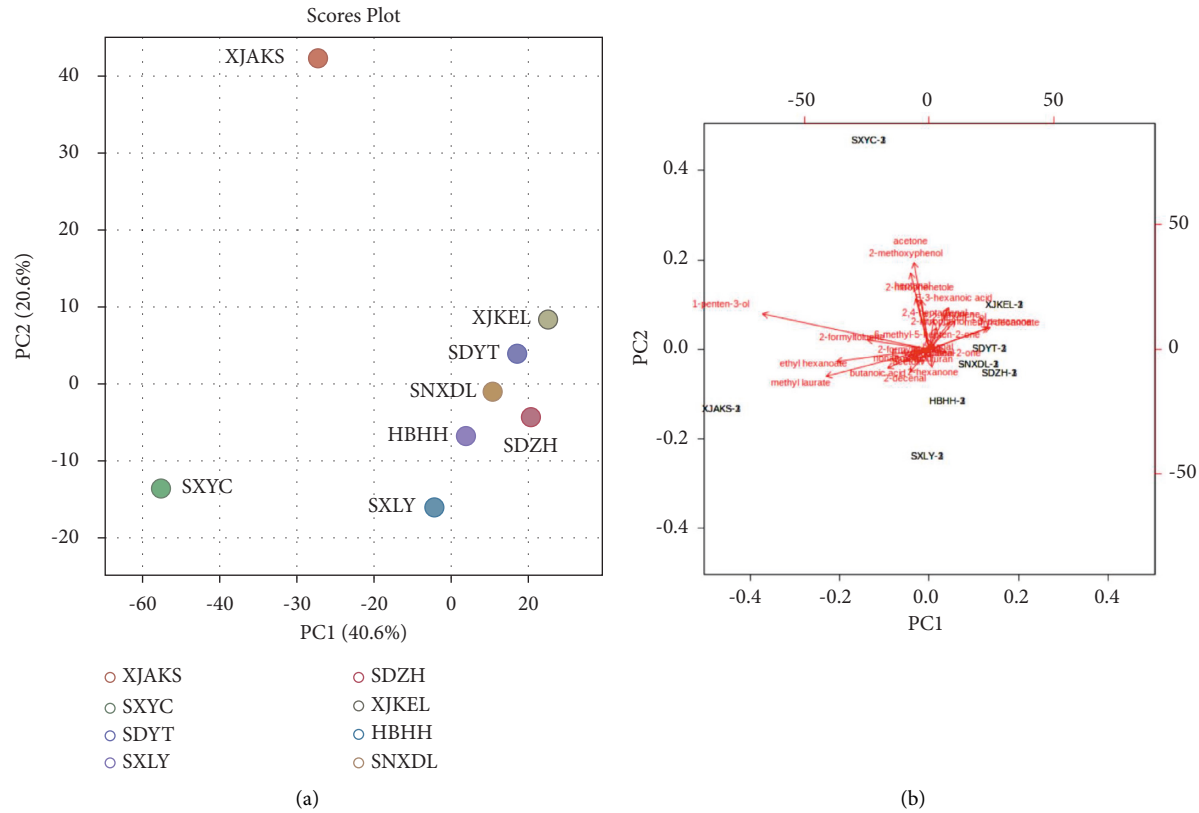

Figure 5: (a) PLS-DA analysis of the different cultivars of winter jujubes based on differential compounds. (b) Biplot analysis of the differential compounds in winter jujubes.

was found to be with aroma of honey and iris [29]. Mutual comprehensive effect of VOCs is the basis of the formation of the overall aroma of winter jujubes. Most of these common volatiles were found to be aroma attributes of fruity, grass, or green, which was in agreement with Pu et al. [4].

As is shown in Figure 2, PCA of GC-IMS data showed that SXYC and XJAKS were individually apart from the other winter jujubes. All the jujubes studied in this study were distributed in the middle latitude of the northern hemisphere, among which SXYC had the smallest latitude and XJAKS has the smallest longitude (Table 1). The special geographical location and associated climatic factors of SXYC and XJAKS might be the reason why the jujube aroma of these two regions was different from others. SXYC and XJAKS had their own specific VOCs that are framed with yellow and red color separately in Figure 1(b). The substances identified in the yellow frame, including acetone, 6-methyl-5-hepten-2-one, 2-nitrophenol, 2-methoxyphenol, and 2-nitrophenetole, were the specific chemicals in SXYC. XJAKS was characterized by compounds in the red frame, including (E)-3-hexenoic acid, 1-penten-3-ol, ethyl hexanoate, 2-methyl-benzaldehyde, 2-hydroxy-benzaldehyde, trans-4-undecenal, methyl laurate, 2-pentylfuran, and heptanal. The volatile markers of SXYC and XJAKS would be confirmed by the correlation analysis between E-nose and the relative quantitative results of GC-MS for the discriminating components in the following parts.

3.2. E-Nose Analysis. Aroma characteristics and PCA results based on E-nose of winter jujubes are shown in Figures 3 and 4. Sensors and response characteristics of E-nose are shown in Table 3. E-nose results were not specific information on sample composition but rather a simple fingerprint through pattern recognition.

Figures 3(b), 3(g), and 3(i) show that VOCs of SNXDL, SDZH, HBHH, SDYT, XJKEL, and SXLY responded almost the same tendency on sensors W5S, W1W, and W2W. Aroma of SXYC had the highest response value on sensors of W1C, W3C, and W5C (Figures 3(a), 3(c), and 3(e)). XJAKS had the highest response value on sensors W5S, W1S, and W2S inferred from Figures 3(b), 3(f), and 3(h). PCA results (Figure 4) based on Figure 3 showed that SNXDL, SDZH, HBHH, SDYT, XJKEL, and SXLY relatively clustered. SXYC and XJAKS were far away from others. The classification results of aroma characteristics obtained by E-nose (Figure 4) showed the same trend as those obtained by GC-IMS (Figure 2). The classification results of the two technologies strongly indicated that GC-IMS and E-nose had advantages in rapid classification and accuracy. Although targeted and qualitative analysis of winter jujubes was performed well by GC-IMS, the identification and quantitation of potential contributed markers in different winter jujubes were further combined with GC-MS analysis.

3.3. Potential Markers Analysis. HS-SPME-GC/MS was performed targeting the different VOCs (volatiles in the

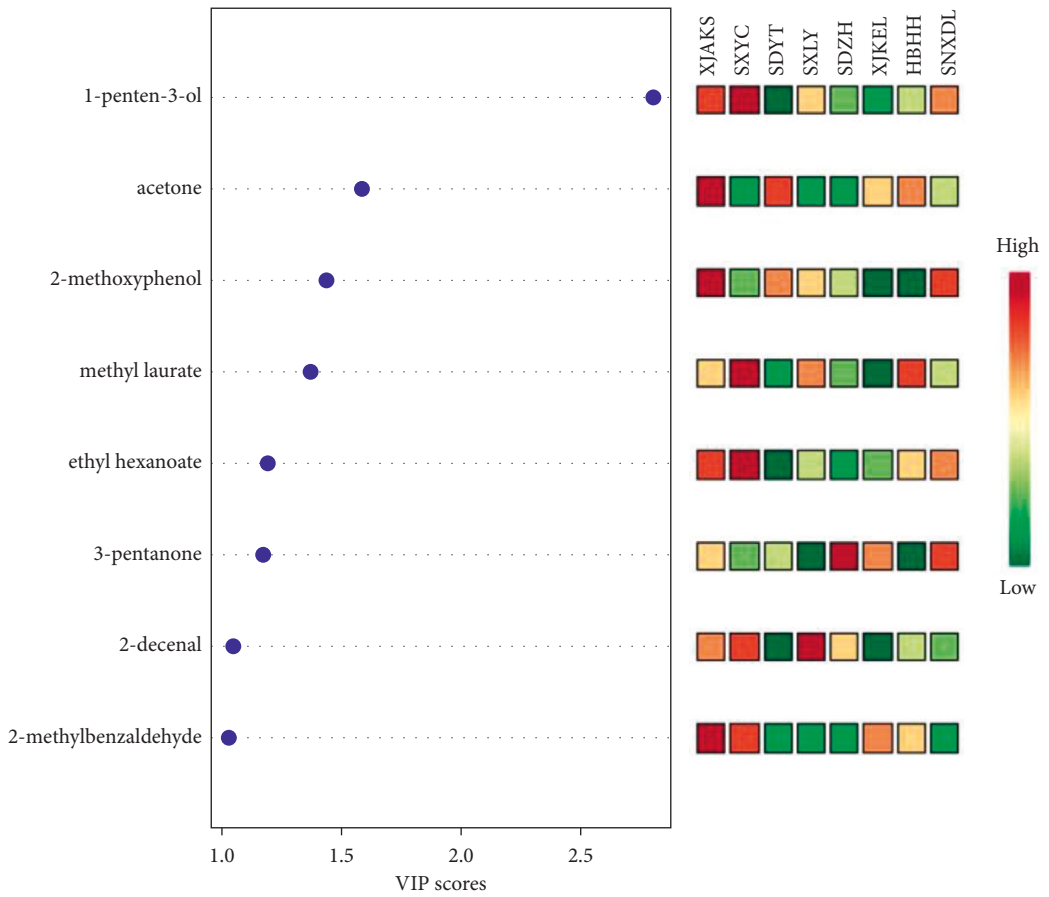

Figure 6: VIP scores of the differential compounds in winter jujubes.

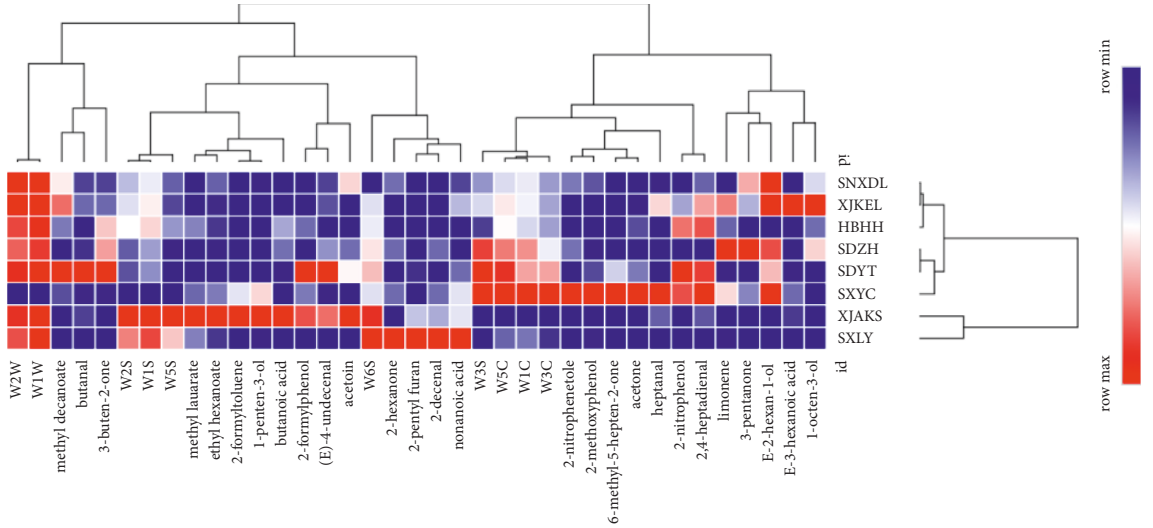

Figure 7: Correlation analysis between different components and sensors by heatmap.

green, yellow, and red frame in Figure 1(b) of winter jujubes). The results are shown in Table 4. Partial least squares discriminant analysis (PLS-DA) assesses the relationship between a descriptor matrix X and a response matrix Y in a supervised way [19]. The differential variations were amplified to illustrate the relationships between the groups in biplot. Identification of the most important variables for the prediction ability of the PLS-DA model is generally performed by analyzing the regression coefficients. VIP scores provide information about the importance of each

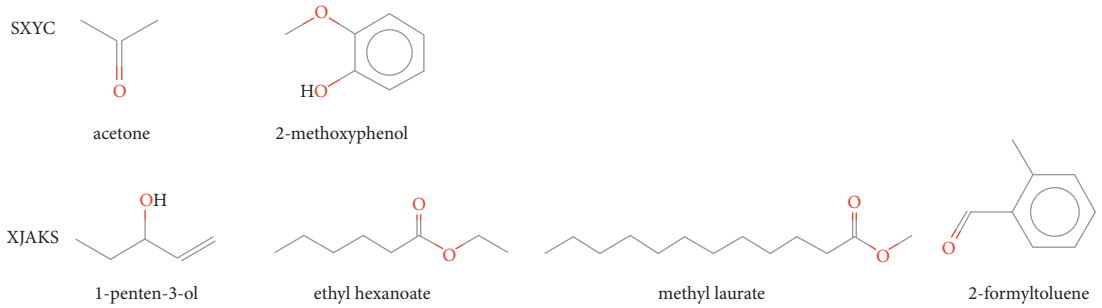

Figure 8: Potential markers in SXYC and XJAKS.

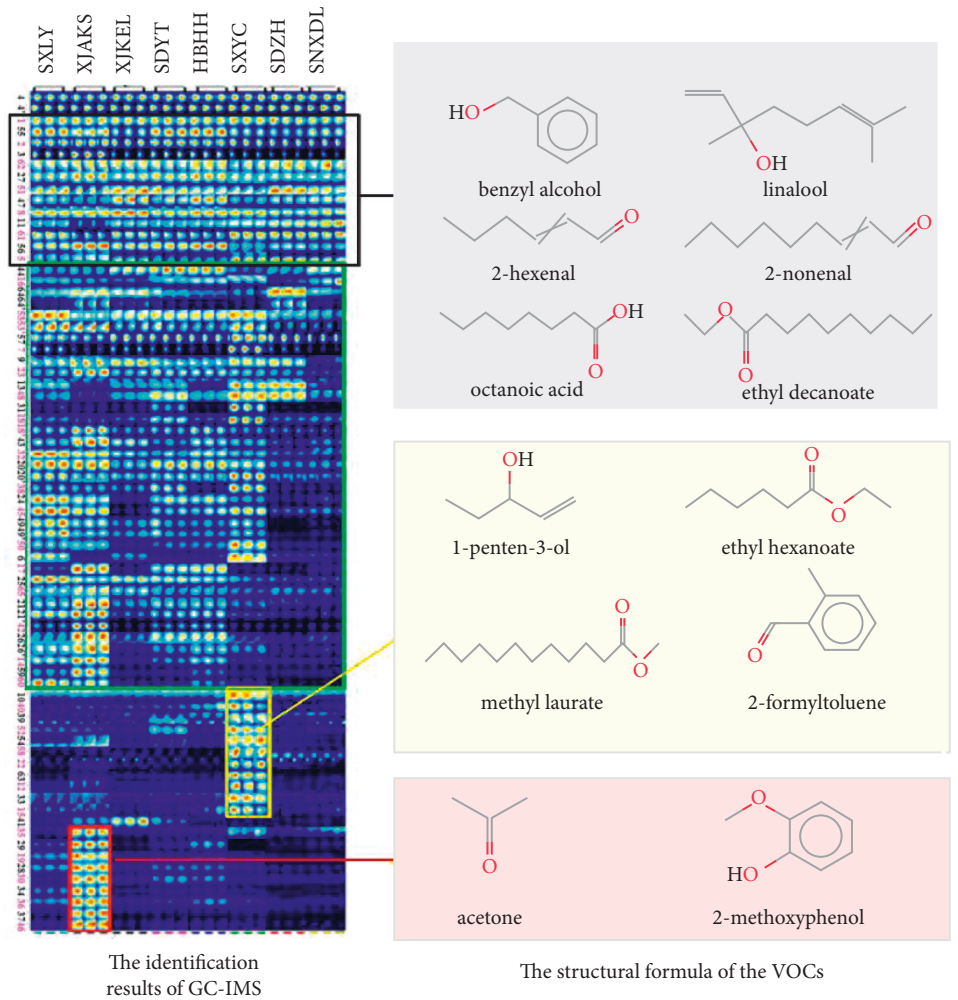

Figure 9: The common and specific VOCs for the eight cultivars of winter jujubes (SNXDL, SDZH, HBHH, SDYT, XJKEL, SXLY, SXYC, and XJAKS).

variable used in the grouping model of PLS-DA [30]. VIP scores greater than 1.0 are always treated as the discriminating factor. PLS-DA has been applied to identify primary and specialized metabolites that are responsible for the discrimination of fruits and vegetables [31].

PLS-DA and biplot (Figures 5(a) and 5(b)) got from Table 4 showed the same tendency as the PCA results got from GC-IMS and E-nose (Figures 2 and 4). SNXDL, SDZH, HBHH, SDYT, XJKEL, and SXLY relatively clustered, while SXYC and XJAKS were apart from others. As shown in Figure 6, 1-peten-3-ol, acetone, 2-methoxyphenol, methyl laurate, 3-pentanone, 2-formyltoluene, and ethyl hexanoate were the components with VIP scores >1, indicating that they were crucial components for the discrimination of

winter jujubes from eight regions. The relationship between the differential VOCs (Table 4) and sensors (Figure 3) was analyzed by heatmap (Figure 7). The potential markers for SXYC and XJAKS were analyzed according to the VIP scores and heatmap.

For SXYC, the sensors with higher response values (W1C, W3C, and W5C) were in close relationship with heptanal, acetone, 6-methyl-5-hepten-2-one, 2-methoxyphenol, and 2-nitrophenetole (Figure 7). However, only acetone and 2-methoxyphenol had VIP scores over 1. Research showed that 2-methoxyphenol was a product of pyrolysis of lignin with woody odor. Acetone existed naturally in plants with pungent odor [32]. The quantitative results in GC-MS showed that 2-methoxyphenol and acetone accounted for 31.67% of the differential VOCs in SXYC (Table 4). Their concentration in SXYC were several times higher than that in other jujubes (Table 4). Hence, 2-methoxyphenol and acetone might be the potential markers of SXYC with woody and pungent aroma.

For XJAKS, the sensors with higher response values (W5S, W1S, and W2S) were in close relationship with acetoin, (E)-4-undecenal, 2-formylphenol, butanoic acid, 1-penten-3-ol, 2-formyltoluene, ethyl hexanoate, and methyl laurate (Figure 7). However, 1-penten-3-ol, ethyl hexanoate, methyl laurate, and 2-formyltoluene were the ones with VIP scores >1, and their amount comprised 74.65% of the different VOCs in XJAKS. 1-Penten-3-ol was one of the secondary lipid oxidation products. It was once found in oolong tea infusions and it was responsible for butter and pungent odor [33]. Ethyl compounds like ethyl hexanoate exist in kinds of fruits [34]. Methyl laurate could effectively inhibit enzyme activities and thus could help to prevent the green color of fruits from fading away [35]. Methyl-benzaldehydes were present in tomato, cider, elderberry juice, tea, and so forth [36]. 2-Formyltoluene was found in winter jujube for the first time. Thus 1-penten-3-ol, ethyl hexanoate, methyl laurate, and 2-formyltoluene might be the potential markers for XJAKS with green and fruity-like aroma (Figure 8).

4. Conclusion

In conclusion, the difference and similarity in VOCs of winter jujube from eight regions of China were well analyzed by GC-IMS, E-nose, and GC-MS. All results showed that SNXDL, SDZH, HBHH, SDYT, XJKEL, and SXLY clustered together with the differentiation of SXYC and XJAKS. As is shown in Figure 9, benzyl alcohol, octanoic acid, 2-hexenal, linalool, 2-nonenal, and ethyl decanoate were the common volatiles of winter jujubes from eight regions of China. The combined analysis of VIP scores, heatmap, and aroma description indicated that 1-penten-3-ol, ethyl hexanoate, methyl laurate, and 2-formyltoluene were the potential markers for green and fruity aroma profile of SXYC, and XJAKS could be labeled by acetone and 2-methoxyphenol with wood-like and pungent aroma.

Data Availability

Data are contained within this article.

Conflicts of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Authors' Contributions

The authors' contributions are as follows: conceptualization, methodology, and formal analysis: Jinfeng Bi, Qinqin Chen, Giorgia Purcaro, Yening Qiao, and Xinye Wu; investigation, Yening Qiao; writing-original draft preparation: Yening Qiao; writing-review and editing: Jinfeng Bi, Qinqin Chen, and Giorgia Purcaro; supervision: Giorgia Purcaro, Min Gou, Haonan Hou, and Xinwen Jin. All authors have read and agreed to the published version of the manuscript.

Acknowledgments

The funding support of the Science and Technology Project in Key of Xinjiang Production and Construction Corps (2019AB024), Financial Science and Technology Project of Xinjiang Production and Construction Corps (2020CB008), National Key R&D Program of China (2017YFD0400900 and 2017YFD0400904), and Agricultural Science and Technology Innovation Project (CAAS-ASTIP-2020-IFST-04) is greatly appreciated by the authors.

References

[1] Y. Zhao, C. Zhang, S. Zhu, Y. Li, Y. He, and F. Liu, "Shape induced reflectance correction for non-destructive determination and visualization of soluble solids content in winter jujubes using hyperspectral imaging in two different spectral ranges," *Postharvest Biology and Technology*, vol. 161, Article ID 111080, 2020.

[2] S. Zhou, X. Dong, and W. Guo, "Introduction to the nutrition and variety of winter jujube," *Special Economic Animal and Plant*, vol. 22, no. 2, pp. 45–48, 2019, in Chinese with English abstract.

[3] Y. Zhao, X. Zhu, Y. Hou, X. Wang, and X. Li, "Postharvest nitric oxide treatment delays the senescence of winter jujube (*Zizyphus jujuba* mill. cv. dongzao) fruit during cold storage by regulating reactive oxygen species metabolism," *Scientia Horticulturae*, vol. 261, Article ID 109009, 2020.

[4] Y. Pu, N. Zhang, and S. Li, "Analysis of nutrition and volatile components of Dongzao jujube in southern Xinjiang," *Anhui Agricultural Science*, vol. 39, no. 13, pp. 7715–7720, 2011, in Chinese with English abstract.

[5] A. Wojdyło, A. Figiel, P. Legua, K. Lech, Á. A. Carbonell-Barrachina, and F. Hernández, "Chemical composition, antioxidant capacity, and sensory quality of dried jujube fruits as affected by cultivar and drying method," *Food Chemistry*, vol. 207, pp. 170–179, 2016.

[6] Q. Chen, J. Song, J. Bi, X. Meng, and X. Wu, "Characterization of volatile profile from ten different varieties of Chinese jujubes by HS-SPME/GC-MS coupled with E-nose," *Food Research International*, vol. 105, pp. 605–615, 2018.

[7] R. D. C. M. Luisa, R. Monica, F. Gema, and B. G. Patricia, "New method based on solid phase microextraction and multidimensional gas chromatography-mass spectrometry to

determine pesticides in strawberry jam," *LWT-Food Science and Technology*, vol. 99, pp. 283–290, 2019.

[8] M. Mohd Ali, N. Hashim, S. Abd Aziz, and O. Lasekan, "Principles and recent advances in electronic nose for quality inspection of agricultural and food products," *Trends in Food Science & Technology*, vol. 99, pp. 1–10, 2020.

[9] Z. Karpas, "Applications of ion mobility spectrometry (IMS) in the field of foodomics," *Food Research International*, vol. 54, no. 1, pp. 1146–1151, 2013.

[10] S. Wang, H. Chen, and B. Sun, "Recent progress in food flavor analysis using gas chromatography-ion mobility spectrometry (GC-IMS)," *Food Chemistry*, vol. 315, Article ID 126158, 2020.

[11] X. Wang, S. Yang, J. He et al., "A green triple-locked strategy based on volatile-compound imaging, chemometrics, and markers to discriminate winter honey and sapium honey using headspace gas chromatography-ion mobility spectrometry," *Food Research International*, vol. 119, pp. 960–967, 2019.

[12] M. Li, R. Yang, H. Zhang, S. Wang, D. Chen, and S. Lin, "Development of a flavor fingerprint by HS-GC-IMS with PCA for volatile compounds of Tricholoma matsutake singer," *Food Chemistry*, vol. 290, pp. 32–39, 2019.

[13] D. Pu, W. Duan, Y. Huang et al., "Characterization of the key odorants contributing to retronasal olfaction during bread consumption," *Food Chemistry*, vol. 318, Article ID 126520, 2020.

[14] L. Yang, J. Liu, X. Wang et al., "Characterization of volatile component changes in jujube fruits during cold storage by using headspace-gas chromatography-ion mobility spectrometry," *Molecules*, vol. 24, no. 21, p. 3904, 2019.

[15] W. Li, Y. P. Chen, I. Blank, F. Li, C. Li, and Y. Liu, "GC × GC-ToF-MS and GC-IMS based volatile profile characterization of the Chinese dry-cured hams from different regions," *Food Research International*, vol. 142, Article ID 110222, 2021.

[16] Y. Chen, P. Li, L. Liao, Y. Qin, L. Jiang, and Y. Liu, "Characteristic fingerprints and volatile flavor compound variations in Liuyang Douchi during fermentation via HS-GC-IMS and HS-SPME-GC-MS," *Food Chemistry*, vol. 361, Article ID 130055, 2021.

[17] J. Chen, L. Tao, T. Zhang et al., "Effect of four types of thermal processing methods on the aroma profiles of acidity regulator-treated tilapia muscles using E-nose, HS-SPME-GC-MS, and HS-GC-IMS," *LWT*, vol. 147, Article ID 111585, 2021.

[18] S. Chatterjee, B. Singh, A. Diwan et al., "A perspective on two chemometrics tools: PCA and MCR, and introduction of a new one: pattern recognition entropy (PRE), as applied to XPS and ToF-SIMS depth profiles of organic and inorganic materials," *Applied Surface Science*, vol. 433, pp. 994–1017, 2018.

[19] J. F. Hoffmann, I. R. Carvalho, R. L. Barbieri, C. V. Rombaldi, and F. C. Chaves, "Butia spp. (arecaceae) LC-MS-based metabolomics for species and geographical origin discrimination," *Journal of Agricultural and Food Chemistry*, vol. 65, no. 2, pp. 523–532, 2017.

[20] N. Gerhardt, S. Schwolow, S. Rohn et al., "Quality assessment of olive oils based on temperature-ramped HS-GC-IMS and sensory evaluation: comparison of different processing approaches by LDA, kNN, and SVM," *Food Chemistry*, vol. 278, pp. 720–728, 2019.

[21] N. Arroyo-Manzanares, A. Martín-Gómez, N. Jurado-Campos, R. Garrido-Delgado, C. Arce, and L. Arce, "Target vs spectral fingerprint data analysis of Iberian ham samples for avoiding labelling fraud using headspace—gas chromatography-ion mobility spectrometry," *Food Chemistry*, vol. 246, pp. 65–73, 2018.

[22] M. El Hadi, F.-J. Zhang, F.-F. Wu, C.-H. Zhou, and J. Tao, "Advances in fruit aroma volatile research," *Molecules*, vol. 18, no. 7, pp. 8200–8229, 2013.

[23] H. Issa-Issa, G. Guclu, L. Noguera-Artiaga et al., "Aroma-active compounds, sensory profile, and phenolic composition of fondillón," *Food Chemistry*, vol. 316, Article ID 126353, 2020.

[24] F. Yuan, F. He, Y. Qian, J. Zheng, and M. C. Qian, "Aroma stability of lemon-flavored hard iced tea assessed by chirality and aroma extract dilution analysis," *Journal of Agricultural and Food Chemistry*, vol. 64, no. 28, pp. 5717–5723, 2016.

[25] X. Hu, L. Lu, Z. Guo, and Z. Zhu, "Volatile compounds, affecting factors and evaluation methods for rice aroma: a review," *Trends in Food Science & Technology*, vol. 97, pp. 136–146, 2020.

[26] B. Arancha and S. María-Pilar, "Fourteen ethyl esters of wine can be replaced by simpler ester vectors without compromising quality but at the expense of increasing aroma concentration," *Food Chemistry*, vol. 30, no. 71, pp. 55–53, 2020.

[27] H. Tian, X. Xu, C. Chen, and H. Yu, "Flavoromics approach to identifying the key aroma compounds in traditional Chinese milk fan," *Journal of Dairy Science*, vol. 102, no. 11, pp. 9639–9650, 2019.

[28] G. A. Burdock, *Fenaroli's Handbook of Flavor Ingredients*, CRC Press, Boca Raton, FL, USA, 6th edition, 2010.

[29] G.-H. Qin, X.-X. Qi, Y.-J. Qi et al., "Identification and expression patterns of alcohol dehydrogenase genes involving in ester volatile biosynthesis in pear fruit," *Journal of Integrative Agriculture*, vol. 16, no. 8, pp. 1742–1750, 2017.

[30] S. Wold, M. Sjöström, and L. Eriksson, "PLS-regression: a basic tool of chemometrics," *Chemometrics and Intelligent Laboratory Systems*, vol. 58, no. 2, pp. 109–130, 2001.

[31] J. E. L. Villa, N. R. Quiñones, and F. Fantinatti-Garboggini, "Fast discrimination of bacteria using a filter paased SERS platform and PLS-DA with uncertainty estimation," *Analytical and Bioanalytical Chemistry*, vol. 411, no. 3, pp. 1–9, 2018.

[32] M. Ishida, M. Hara, N. Fukino, T. Kakizaki, and Y. Morimitsu, "Glucosinolate metabolism, functionality and breeding for the improvement of brassicaceae vegetables," *Breeding Science*, vol. 64, no. 1, pp. 48–59, 2014.

[33] J. Zhu, F. Chen, L. Wang et al., "Comparison of aroma-active volatiles in oolong tea infusions using GC-olfactometry, GC-FPD, and GC-MS," *Journal of Agricultural and Food Chemistry*, vol. 63, no. 34, pp. 7499–7510, 2015.

[34] J. Shi, H. Wu, M. Xiong et al., "Comparative analysis of volatile compounds in thirty nine melon cultivars by headspace solid-phase microextraction and gas chromatography-mass spectrometry," *Food Chemistry*, vol. 316, Article ID 126342, 2020.

[35] N. Yamauchi, Y. Tokuhara, Y. Ohyama, and M. Shigyo, "Inhibitory effect of sucrose laurate ester on degreening in citrus nagato-yuzukichi fruit during storage," *Postharvest Biology and Technology*, vol. 47, no. 3, pp. 333–337, 2008.

[36] M. Miyazawa, S. Hashidume, T. Takahashi, and T. Kikuchi, "Aroma evaluation of gamazumi (*Viburnum dilatatum*) by aroma extract dilution analysis and odour activity value," *Phytochemical Analysis*, vol. 23, no. 3, pp. 208–213, 2011.