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Characterization of volatile compounds profiles and identification of key volatile and odor-active compounds in 40 sweetpotato (*Ipomoea Batatas* L.) varieties

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ABSTRACT

Sweetpotato with different flesh colors exhibits significant differences in flavor. Nevertheless, research on the identification of the key aromatic compounds in sweetpotato is scarce. Therefore, 40 primary sweetpotato varieties with different flesh colors were analyzed by HS-SPME/GC–MS to characterize the volatile compounds. A total of 121 volatile compounds were detected, with aldehydes, furans and terpenes being the most abundant components. Additionally, 35 compounds were identified as the key aromatic compounds by OAV > 1, of which 17 were found in all varieties and hence considered as the major components of sweetpotato aroma. Further analysis demonstrated that the yellow-fleshed sweetpotato had the strongest aroma, which was presumed due to the aldehydes like (E,E)-2,4-heptadienal, nonanal, (E,E)-2,4-decadienal,etc. that were produced during the degradation of unsaturated fatty acids. The unique sweety and floral aroma of orange-fleshed sweetpotato might be attributed to apocarotenoid volatiles (trans-beta-ionone, β-ionone, geranylacetone, etc.), the derivates of carotenoids. The purple-fleshed sweetpotato exhibited weak aroma with a significantly high terpenoids concentration. Overall, these findings may be the main reason for the different aromas of different colored sweetpotatoes and provides insights into sweetpotato aroma and a theoretical basis for improving sweetpotato aroma.

1. Introduction

Sweetpotato (*Ipomoea batatas* [L.] Lam) is produced worldwide in 114 countries, accounting for 0.6 % of all global caloric intake. It is ranked as the eighth most consumed staples food in the world due to its resilience and adaptability (Kwak, 2019; WorldAltas, 2024). Additionally, sweetpotato boasts a relatively short growing period with a high yield potential even in poor terrain and a noteworthy nutritional contribution. Therefore, it is considered as one of the most economically important crops for addressing the concerns related to global food security and climate change (CIP, 2022). In the late 1980s, the primary breeding objectives of sweetpotao breeders were high dry matter and yield stability (Lindqvist-Kreuze et al., 2023). However, with the shifting of societal demographics, lifestyles, and general market demands, the importance of taste, including texture and flavor, has become the second most sought-after traits by farmers and consumers in selecting sweetpotato varieties (Ojwang et al., 2023). The texture and flavor of cooked sweetpotato are the critical characteristics of sweetpotato quality traits, which must be addressed by modern breeding programs.

Aroma plays an indispensable role in assessing the quality and flavor of sweetpotato. The composition and content of volatile organic compounds (VOCs) are mainly responsible for the aroma perceived (Klee & Tieman, 2018). Previous research on sweetpotato aroma mainly focused on the production mechanism of baked sweetpotato aroma, including the key aroma compounds and the impact of heating methods on aroma. Wang and Kays (2000a); Wang and Kays (2000b) identified 37 odor-active VOCs in baked sweetpotato, including maltol, phenylacetaldehyde, methyl-geranate, 2-pentyl furan, β-ionone, etc. The baked sweetpotato had more attractive aroma, which might be attributed to the increased contents of furans and terpenes (Zhang et al., 2023). Although numerous sweetpotato varieties have been selected and cultivated by farmers to assess their adaptability and flavor, whether in Latin America, Africa and other regions where sweetpotatoes are a staple, or in China, which is the largest producers of sweetpotato in the

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world (FAOSTAT, 2023), most research on sweetpotato aroma is restricted to a few varieties.Additionally, research on the compositional characteristics of VOCs across various sweetpotato varieties at the genetic level is scarce. This lack research on aroma diversity in sweetpotato varieties significantly hinders the selection of suitable aroma parents in sweetpotato breeding, thereby impeding the enhancement of sweetpotato aroma quality.

Flesh color is one of the most prominent characteristics of sweetpotato classification, and there are mainly four colors of sweetpotato flesh: white, yellow, orange, and purple (Amoanimaa-Dede et al., 2020). Flesh color significantly affects the quality traits and taste of sweetpotato. The white-fleshed sweetpotato (WFSP), typically with high dry matter, reduced sweetness, drier texture and reduced flavor, is dominated in Africa for both table-stock and starch extraction in China (Kays et al., 2005).The yellow-fleshed sweetpotato (YFSP) is distinguished by smooth texture, sweet taste, and flavor of brown sugar and dried apricot (Leksrisompong et al., 2012), and is the traditional predominant edible sweetpotato in both Africa and Asia (Tomlins et al., 2007; Y. Xie et al., 2018). The orange-fleshed sweetpotato (OFSP), characterized by fibrousness, moistness and residual fiber texture, carrot and flowery flavor, visually moist, high color homogeneity, and sour taste, is recognized as one of the affordable sources of vitamin A, playing a crucial role in addressing vitamin A deficiency through biofortification in sub-Sagaran Africa (Girard et al., 2021). The purple-fleshed sweetpotatoes (PFSP) have attracted consumers' attention duo to their high anthocyanin contents, which are generally regarded as beneficial phytonutrients. However, its texture is chalky, dense, and firm, with a flavor of white baked potato and aroma of vanilla (Huang et al., 2021). Previous studies have revealed significant differences between sweetpotato with different flesh colors, particularly the flavor, but the impact of aroma compounds on flavor has not yet been thoroughly investigated.

In this study, the aroma compounds in 40 sweetpotato varieties with different flesh colors were detected using headspace solid-phase microextraction (HS-SPME) combined with gas chromatography-mass spectrophotometry (GC–MS). The key aromatic compounds of sweetpotatoes were identified by odor activity value (OAV) >1. Furthermore, the differences in the VOCs and the aroma of sweetpotato with different flesh colors were analyzed. In summary, the present study was designed to fill a gap in research on the aroma across various sweetpotato varieties at the genetic level and aimed to provide a comprehensive analysis of the aroma profiles of various sweetpotato germplasm resources to comprehend their quality variations and lay the foundation for further research on the mechanism of aroma formation. The experimental results provide a theoretical basis for future advancements in enhancing the flavor of sweetpotato.

2. Materials and methods

2.1. Plant materials

A total of 40 sweetpotato varieties (Fig.1, Table S1) were used in this study, including 11 WFSP, 10 YFSP, 10 OFSP and nine PFSP varieties, which were supplied by the National Sweetpotato Germplasm Resources Nursery (Guangzhou) and planted on July in 2021 using the standard production practices at the Baiyun Experimental Station (23°23′N, 113°26′ E; 20 m above sea level) of Guangdong Academy of Agricultural Sciences, Guangzhou, China. The experiment was arranged in a randomized complete block design with three replications. All the sweetpotatoes were harvested after 130 days of planting.

For each cultivar, five medium-sized (100–150 g) intact sweetpotato tubers were cleaned and cut into shreds. Then the tubers were combined, blended, and then frozen immediately in liquid nitrogen. All the samples were separately ground in a liquid nitrogen grinder (A10 basic, IKA, Staufen, Germany) and stored at −80 °C prior to GC–MS analysis.

2.2. Determination of volatile compounds by GC–MS

The volatile compounds were determined according to the methods reported by (Zhang et al., 2021), with minor modifications. Precisely, one gram of frozen sweetpotato tuber sample powder was put in a 20 mL headspace vial, and then 2 mL of saturated NaCl solution and 5 μL of 1-heptanol solution (internal standard, 0.137 μg mL^{-1}, CAS: 111–70-6) were added, followed by homogenization. The vial was then capped with a crimp type cap and a PTFE/silicone septum (CNW, Shanghai,

Fig. 1. 40 sweetpotato varieties with different flesh color (white-fleshed: 11, yellow-fleshed: 10, orange-fleshed: 10, purple-fleshed: 9). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

China) to prevent the leakage of volatile compounds. All analyses were performed in triplicates.

Afterward, the sample was heated in a water bath with a magnetic stirrer at 100 °C for 30 min and then incubate at 80 °C for 30 min. The volatile compounds were then extracted by an SPME device using a DVB/CAR/PDMS fiber for 30 min at the same temperature. Later, the extracted volatile components trapped by the SPME fiber were desorbed in the GC injection port for 3 min at 250 °C in splitless mode. The GC–MS analysis was performed using an Aglient 7890B gas chromatography system coupled to a 5977B mass spectrometer (Agilent Technologies, CA, USA) and equipped with an HP-5 ms column (30 m, 250 μm, 0.25 μm) (Agilent Technologies, CA, USA). A constant helium flow of one mL min^{-1} was used for chromatographic separation. The oven temperature program was as follows: an initial 35 °C for 2 min, 5 °C min^{-1} ramp up to 190 °C, hold for 1 min, 20 °C min^{-1} ramp up to 250 °C, hold for 2 min, and solvent delay 1 min. The detector was operated in an electron impact (EI) ionization mode at 70 eV and 230 °C in a full scan mode, and the mass/charge ratio (m z^{-1}) range was set between 35 and 450.

2.3. Identification and quantification of volatile compounds

The acquired data from the GC–MS analysis were pre-processed using Enhanced ChemStation software (Agilent Technologies, CA, USA) for peak picking and mass spectral deconvolution. Subsequently, the raw data were exported using Agilent's raw data (.D) and then converted to "ABF" format for further processing by MS-Dial software for metabolite annotations (ver4.92) (Tsugawa et al., 2015). Then, the ABF files were uploaded on the MS-Dial software with the subsequent parameters: mass range from 35 to 450 Da; retention time from 0 to 36 min; only one number of threads; peak height min = 50,000 amplitude; mass slice width and mass accuracy for centroiding default to 0.5 Da; smoothing method was linear weighted moving average; the smoothing level was set at 3 scan and the average peak width was 10 scans; the sigma window value was 0.5 and El spectra cut off was 10 amplitudes. The identification method was defined to use retention index and Alkanes for the Index type. The volatile compounds were identified by matching the mass spectra and retention index (RI) with the National Institute of Standards and Technology (NIST17) database. The RI value was calculated from the retention time (RT) of n-alkane series (C7-C30) (Supelco, Sigma-Aldrich, PA, USA) (Bianchi et al., 2007). The alignment parameters were as follows: retention index tolerance = 20; retention time tolerance = 0.5 min; *m/z* tolerance = 0.5 Da; EI similarity cut off = 70 %; Identification score cut off = 70 % and was set the use of compulsion gap filtering. The filtering parameters were as follows: peak count filter = 0 %; N% detected in at least one group = 10. The peak list information of each sample, including average retention time (RT), m/z values, MS spectra information, and peak intensity (area) were exported by MS-Dial before proceeding to further statistical analysis.

The VOCs were semi-quantitated using 1-heptanol as an internal standard (Sun et al., 2024). The VOC content was calculated using Eq. (1):

$$C_V = \frac{S_v}{S_a} \times C_a \tag{1}$$

where S_a and S_v represent the area of 1-heptanol and VOC, respectively. C_a represents the 1-heptanol content.

2.4. Identification of OAV

The odor activity value (OAV) is commonly used to evaluate the contribution of aroma compounds, and aroma compounds with OAV >1 are generally considered to contribute significantly to the overall aroma characteristics (Xu et al., 2023). The OAV was determined as the ratios of the contents to their odor thresholds of each volatile compound in water (Jiang et al., 2023).

2.5. Statistical analysis

Significant differences between the volatile compound profiles of sweetpotatoes from different fleshed color groups were assessed using multivariate and univariate statistical analysis. The variables were normalized through cubic root transformation and scaled by the Pareto scaling method before data analysis. The multivariate statistic plots were performed using the Metware Cloud (https://cloud.metware.cn), such as the principal component analysis (PCA) for data overview and outlier detection, and the orthogonal partial least squares-discriminant analysis (OPLS-DA) to determine the metabolic differences between experimental groups. The predictive quality of the OPLS-DA models was evaluated by the cumulative modeled variation in the X and Y matrix (R^2 X and R^2 Y) and the cross-validated predictive ability Q^2 (cum) values. The significantly regulated volatile compounds between groups were determined by variable importance in the projection (VIP) ≥ 1 and absolute $\log_2$Foldchange ≥ 1.The VIP values were extracted from the OPLS-DA results.

3. Results and discussion

3.1. Profiling of VOCs in 40 sweetpotato varieties

A total of 121 VOCs were identified in 40 sweetpotato varieties, and which were classified into 12 distinct chemical classes based on their chemical compositions: monoterpenoids (28), sesquiterpenoids (20), aldehydes (20), ketones (12), alcohols (9), esters (8), benzene derivatives (7), alkanes (4), phenols (3), acids (2), furans (2) and others (6) (Fig. 2A). Of these, terpenoids (monoterpenoids and sesquiterpenoids) were the most abundant compounds in all sweetpotato varieties, accounting for 39.6 % of all VOCs, followed by aldehydes with 16.5 % of the total VOCs. In terms of number of compounds, terpenoids and aldehydes were the main components of volatile compounds in sweetpotato. This result is in consistent with a previous study on VOCs using a few varieties of sweetpotato (Wang & Kays, 2000b; Zhang et al., 2023).

In the previous studies, the application of SPME in analyzing the VOCs of sweetpotato was limited and around 70 VOCs were identified by GC–MS in baked sweetpotato (Nakamura et al., 2013; Shen et al., 2024). The detected aldehydes (such as hexenal, benzeneacetaldehyde and benzaldehydes), furans (2-allylfuran and 2-pentylfuran), and terpenoids (including linalool, terpinen-4-ol, trans-beta-Ionone) in sweetpotato were consistent with the volatile profiling of previous studies (Yan & Kays, 2000; Zhang et al., 2021). Some compounds were discovered for the first time in sweetpotato, like (*Z*)-4-heptenal, acetophenone, (−)-cis-rose oxide, etc.

In addition to the classification, the content of VOCs in sweetpotato was determined. The average content of the total VOCs in 40 sweetpotato varieties was 1.86 ± 0.81 mg/kg FW, ranging from 0.78 mg/kg ('Zheshu 13') to 3.55 mg/kg ('Colo'). Notably, the average content of aldehydes was 0.94 ± 0.58 mg/kg, ranging from 0.33 mg/kg in 'Menglazihongpi' to 2.53 mg/kg in 'Colo' (Fig. 2B), which was the highest content among all VOCs. The 20 aldehydes in sweetpotato could be divided into two groups: (1) phenylalanine derivatives, like benzeneacetaldehyde and benzaldehydes; (2) saturated and unsaturated C6-C9 compounds or their derivatives and they were obtained during the oxidation of linoleic acid and linolenic acid (Dudareva et al., 2013). Thereinto, hexanal, (*E,E*)-2,4-decadienal, benzeneacetaldehyde, benzaldehydes and (*E,Z*)-2,4-decadienal were the main aldehydes in sweetpotato and their contents accounted for more than 70 % of the total aldehydes contents. This result was partially consistent with a previous study, reporting that benzeneacetaldehyde and benzaldehyde were the main aldehydes in sweetpotato (Shen et al., 2024; Zhang et al., 2021) Furans were the second major components of VOCs and their average content was 0.24 ± 0.15 mg/kg. The two furans (2-allylfuran and 2-pentylfuran) were identified in all the samples and almost all furan content was contributed by 2-pentyfuran in all samples assayed. The content of

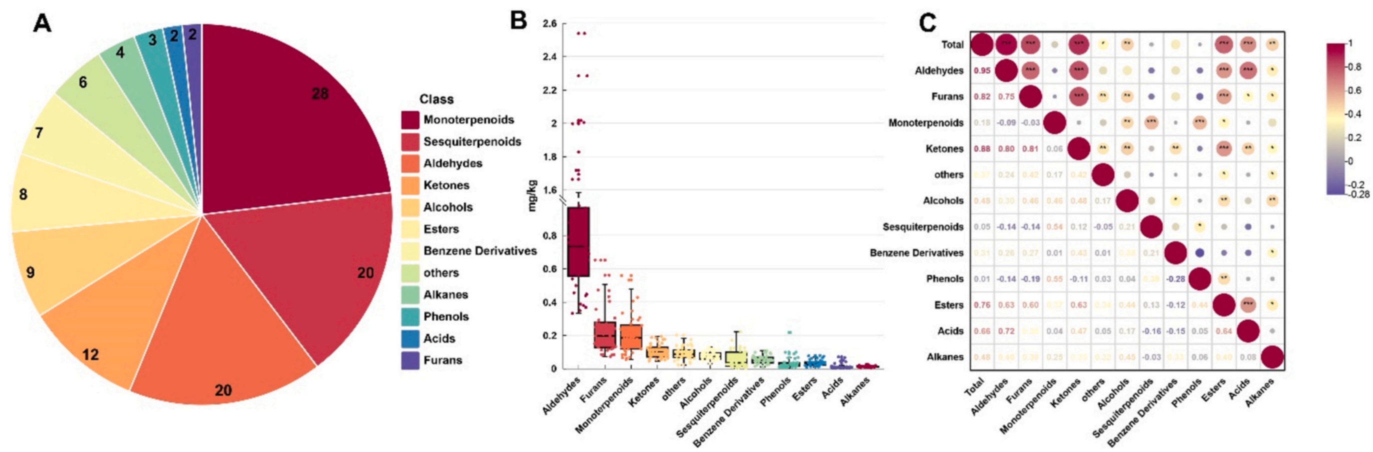

Fig. 2. Volatile compounds classes and contents in 40 sweetpotato varieties. A: Categories of determined volatile compounds in sweetpotato. B: Range and distribution of volatile compounds relative contents in 40 sweetpotato varieties. C: Correlation analysis of 12 volatile classes contents and total volatile contents of 20 sweetpotato vatieties. * indicates significance at $P < 0.05$, ** significance at $P < 0.01$, *** significance at $P < 0.001$. Color depth indicates Pearson correlation coefficient values.

2-pentyfuran ranged from 0.07 mg/kg in 'Heigui' to 0.65 mg/kg in 'Yuanji'. 2-pentyfuran, responsible for fruity, green and earthy nuances, is a typical compound produced by the oxidative decomposition of linoleic acid (de Sousa Fontes et al., 2024) and is probably produced during the heating process in sweetpotato.

Monoterpenes were the third most abundant VOCs with a total content ranging from 0.05 mg/kg in 'Baipisu' to 0.55 mg/kg in 'Hanzi'. Although the number of monoterpenes was high, the individual content was relatively low, with nearly all less than 0.01 mg/kg. Among these 40 sweetpotato varieties, nerol had the highest average content (0.023 ± 0.024 mg/kg), followed by linalool (0.02 ± 0.03 mg/kg), geraniol (0.02 ± 0.02 mg/kg), β-Ionone (0.019 ± 0.036 mg/kg) and citral (0.014 ± 0.009 mg/kg). Previously, nerol, linalool, and geraniol were recognized as the key floral aroma component of teas and fruits (Liu et al., 2022; Tan et al., 2022; M. Wang et al., 2020). The high concentration of these compounds in this study indicated that they were probably the key floral and sweet aroma contributors in sweetpotato. β-Ionone was remarkably high in the orange fleshed varieties and low in other varieties. It is reported that the violet flower aroma and plays a significant role in the aroma composition of baked sweetpotato, particularly in orange-fleshed sweetpotato, which had the highest content in baked Yanshu 25 (orange-fleshed) (Shen et al., 2024; Wang & Kays, 2000b). Some other compounds, such as nerol oxide, camphene, (−)-myrtenol and alpha-cyclocitral also presented a relative high accumulation in sweetpotatoes, with an average content more than 0.01 mg/kg.

The average content of ketones was 0.10 ± 0.04 mg/kg with 'Carver' having the highest content of 0.19 mg/kg. In contrast, 'zheshu 13' had the lowest content of 0.04 mg/kg. 2-Hetanone, 2-methyloctan, and 3-nonen-2-one were the main ketones in all varieties. The content of 6-methyl-5-heptone-2-one in the yellow fleshed varieties was higher than other groups. The average content of alcohols was 0.09 ± 0.03 mg/kg, followed by ketones, with a maximum content of 0.17 mg/kg ('heigui') and a minimal content of 0.04 mg/kg ('zheshu 13'). 1-Hexenol and 1-octen-3-ol made up over half of the alcohols content, making them the dominant type. Sesquiterpenes were the second largest components of VOCs in sweetpotato, but their average content was only 0.05 ± 0.05 mg/kg, which varied greatly among sweetpotato varieties (0.002 mg/kg in 'Baipishu' and 0.22 mg/kg in 'Hanzi'). The contents of most of individual sesquiterpenes were less than 0.001 mg/kg in most sweetpotato varieties. Finally, phenols, acids, and alkanes had low contents, accounting for 0.07 mg/kg.

The contribution of these components to the total volatiles was explored using the correlation analysis between them. As shown in Fig.2C, the total VOCs content was significantly and positively related with the content of aldehydes ($r = 0.95$***), furans ($r = 0.82$***), ketones ($r = 0.88$***) and esters ($r = 0.76$***). Meanwhile, the content of alcohols, acids and alkanes were positively but weakly correlated with the total content of VOCs. Therefore, based on the components content and correlation analysis, we concluded that aldehydes, furans and ketones were found to be the primary volatile compounds for sweetpotato.

3.2. Identification of key aromatic compounds in sweetpotato

There are various types of volatile compounds in sweetpotato, but only a few, i.e., the key aroma compounds with concentrations above their threshold that can be considered as significant odors. Among 121 VOCs, the OAV of 69 VOCs could be calculated taking the odor threshold in the water as the reference. A total of 35 odorants with OAV > 1 were identified as the key aromatic compounds in 40 sweetpotato varieties and their threshold values, odor descriptions and OAV are listed in Table 1 and Table S3. The 35 compounds with OAV > 1 comprised of 12 aldehydes, 10 monoterpenoids and 5 ketones, accounting for 77.14 % of the total compounds. This result indicated that aldehydes, monoterpenoids, and ketones are the primary contributor of sweetpotato aroma. Notably, 17 compounds had the OAV above one in all varieties, including eight aldehydes ((*E*,*E*)-2,4-Decadienal, (*E*,*E*)-2,4-Nonadienal, (*E*)-2-Nonenal, (*Z*)-4-Heptenal, Heptanal, Hexanal, Benzeneacetaldehyde, Benzaldehyde), three monoterpenoids (Damascenone, β-Ionone, Linalool), one ester (Benzoic acid methyl ester), one alcohol (1-Octen-3-ol), two ketones (1-Octen-3-one, 2-Heptanone), one furan (2-Pentylfuran) and one phenol (guaiacol). These compounds were considered as the dominated contributors to general sweetpotato aroma. Among them, benzeneacetaldehyde, 2-pentylfuran, β-ionone, linalool, (*E*,*E*)-2,4-Decadienal have been reported as the important contributors to the aroma of baked sweetpotato (Y. Wang & S. Kays, 2000).

In this study, 1-octen-3-one and (*E*,*E*)-2,4-decadienal with mushroom and fried and wax aromas were the key contributors to sweetpotato aroma due to their higher OAV, with an average OAV of 4831 and 10,641, respectively. (*E*,*E*)-2,4-decadienal with chicken flavor, has been reported as an important compound contributing to the formation of all meat flavors (Cui et al., 2023). The high content and OAV of (*E*,*E*)-2,4-decadienal in sweetpotato significantly contributed to the fatty aroma. Damascenone is a key flavor of various food and drinks, especially the sweetpotato shochu, a Japanese traditional spirit (Kaneshima et al., 2023). Damascenone probably contributed to the sweet and fruity aroma of sweetpotato and its OAV ranged from 76 in 'Sanjiaoning' to 6915 in 'Hanzi'. β-ionone, derived from carotenoid, is considered as an important volatile compound, contributing to a complex woody and

Table 1
The volatile compounds with relative odor active values (OAV) >1 in 40 sweetpotato varieties.

Name	Class	Flavor[1]	OTV (mg/kg) [2]	Average OAV	Min OAV	Max OAV
(*E*,*E*)-2,4-Decadienal	Aldehydes	fried, wax, fat	0.00003	10,614.05	286.89	49,090.55
1-Octen-3-one	Ketones	mushroom, metal	0.000003	4831.07	1669.30	11,589.07
β-Ionone	Monoterpenoids	floral woody sweet fruity	0.0000104	1867.79	50.98	16,117.34
Damascenone	Monoterpenoids	sweet fruity rose	0.00000495	756.32	76.24	6915.12
(*E*,*E*)-2,4-Nonadienal	Aldehydes	fat, wax, green	0.00006	314.78	52.28	802.74
Heptanal	Aldehydes	green, citrus, rancid	0.00018	191.14	49.03	442.63
(*E*)-2-Nonenal	Aldehydes	cucumber, fat, green	0.000065	181.83	36.52	416.95
guaiacol	Phenols	smoke, sweet, medicine	0.00017	134.25	3.54	1259.81
Octanoic acid	Acids	sweet, cheese	0.0001	67.48	0.02	641.70
2-Pentylfuran	Furans	green bean, butter	0.0048	49.46	14.78	135.84
Octanoic acid, ethyl ester	Esters	fruit, fat	0.0001	49.39	0.63	340.74
(*Z*)-4-heptenal	Aldehydes	biscuit, cream	0.00004	46.69	13.65	147.16
1-Octen-3-ol	Alcohols	mushroom	0.001	30.94	9.78	74.21
Geraniol	Monoterpenoids	rose, geranium	0.0007	28.80	0.28	170.02
Benzeneacetaldehyde	Aldehydes	honey, sweet	0.0063	27.16	10.06	55.57
Hexanal	Aldehydes	grass, tallow, green	0.005	24.74	10.51	49.35
(*E*,*Z*)-2,4-Decadienal	Aldehydes	fried, fat	0.004	16.73	0.32	93.25
Linalool	Monoterpenoids	flower, lavender	0.0015	13.50	1.89	113.07
3,5-Octadien-2-one	Ketones	fruity green grassy	0.0005	8.15	0.21	29.44
Benzoic acid, methyl ester	Esters	prune, lettuce, herb, sweet	0.00052	8.08	1.57	30.30
1-Hexanol	Alcohols	resin, flower, green	0.006	4.80	0.86	12.84
alpha-Cyclocitral	Monoterpenoids		0.003	3.38	0.02	42.00
Benzaldehyde	Aldehydes	almond, burnt sugar	0.024	3.32	1.01	8.37
2-Heptanone	Ketones	soap	0.0068	2.89	1.12	6.11
Citral	Monoterpenoids	lemon	0.005	2.83	0.62	7.65
trans-beta-Ionone	Monoterpenoids	seaweed, violet, flower	0.000461	2.81	0.12	19.91
(*E*,*E*)-2,4-Heptadienal	Aldehydes	nut, fat	0.01	2.33	0.53	4.69
Nonanal	Aldehydes	fat, citrus, green	0.0035	2.27	0.79	4.45
3-Octanone	Ketones	herb, butter, resin	0.005	0.96	0.10	3.53
Decanal	Aldehydes	soap, orange peel, tallow	0.007	0.80	0.21	1.81
p-Cymene	Monoterpenoids	Mild, pleasant; aromatic	0.0062	0.69	0.10	1.66
Styrene	Benzene Derivatives	balsamic, gasoline	0.0036	0.55	0.11	1.23
Geranylacetone	Monoterpenoids	rose leaf floral	0.01	0.47	0.07	1.88
nerol	Monoterpenoids	sweet	0.08	0.29	0.03	1.93
2-Nonanone	Ketones	fresh sweet green weedy	0.025	0.19	0.02	3.42

Odor description found in the literature with database (Flavornet; The LRI and Odor Database).
OTV: odor threshold value, all OTV were obtained from (Guo et al., 2022; Van Gemert, 2003; Yue et al., 2023)

fruity odor and its OAV varied greatly in different varieties from 51 to 16,117. The high OAV of β-ionone contributed to the rich wood-like flavor and increased the sweetness of sweetpotato, as the odor-taste interaction of β-ionone could enhance the sweetness of foods in sensory evaluation similar to the enhanced sweetness by some sweet odors (Yu et al., 2021). Heptanal (OAV = 49–442), (*E*,*E*)-2,4-nonadienal (OAV = 52–802), (*E*)-2-Nonenal (OAV = 36–416), 2-pentylfuran (OAV = 14–135), and hexanal (OAV = 10–49) produced during the oxidation of the oleic acid precursors and palmitoleic have the aroma of green, cucumber, grass or green beans, respectively, which easily affected the aroma characteristics of sweetpotato (Xi et al., 2024). Guaiacol is a compound with smoke and sweet aroma, has been previously reported in sweetpotato and its OAV ranged from 3 to 1259. Therefore, it was inferred that guaiacol might have different impacts on the aroma of sweetpotato. (*Z*)-4-heptenal has the aroma of biscuit and cream, while benzeneacetaldehyde has honey and sweet odor, which were identified as other important aldehydes in sweetpotato (Xiao et al., 2022). Both provided attractive flavor to sweetpotato with 10 < OAVs <150. 1-Octen-3-ol is an alcohol with mushroom aroma, contributing to the unpleasant odor to some extent. Linalool, benzoic acid methyl ester, and benzaldehyde with the aroma of flower, herb, sweet and almond, and burnt sugar had significant effects on the overall aroma of sweetpotato, which might be due to their relatively low OAV (〈10). These compounds with OAV ≥1 in all samples indicated that they were the main key aroma active compounds in all samples and played important roles in the composition of sweetpotato aroma.

Furthermore, octanoic acid ethyl ester, 3,5-octadien-2-one, (*E*,*Z*)-2,4-decadienal and 1-hexanol had OAV lower than 1 in only one variety and geraniol, (*E*,*E*)-2,4-heptadienal and nonanal in three varieties. These compounds contributed to the fruity, green, fried, flower, nut, and other aromas of most varieties. In addition, some compounds like citral, octanic acid, alpha-cyclocitral and trans-beta-ionone exhibited OAVs greater than 1 in more than 20 varieties. Therefore, it was suspected that they had significant effect on modification of the aroma among these varieties. Especially the OAV of trans-beta-ionone, an iconic floral fragrance, was greater than one in all yellow and orange fleshed sweetpotatoes, but lower than one in all white and purple fleshed varieties. This could be related to the carotenoids content as trans-beta-ionone is a representative volatile compound obtained through carotenoids degradation (Wang et al., 2022). In the contrast to compounds described above, 3-octanone, styrene, geranylacetone, and nerol had OAVgreater than 1 in few varieties, potentially contributing to some special odor to these varieties, such as herb, balsamic, rose, and sweet (Yao et al., 2023).

3.3. Comparison of VOCs in sweetpotato with different flesh colors

Based on the flesh color, the 40 sweetpotato varieties were divided into four groups: 11 WFSP, 10 YFSP, 10 OFSP and 9 PFSP. The similarities and differences in the VOCs of sweetpotato with different flesh colors were evaluated by the principal component analysis (PCA) was performed. As shown in Fig. 3A, the OFSP group was in the center and the other fleshed groups could be separated around it. A total of 41.1 % variances were explained by the principal component 1 (27.61 %) and principal component 2 (13.5 %). The PCA analysis confirmed that the VOCs of sweetpotatoes with different flesh colors were largely distinct. Furthermore, their accumulation differences were explored by plotting a heatmap of VOCs content in 40 sweetpotato varieties (Fig. 3B). These 40 varieties were clearly clustered into four groups, Cluster I to IV. All sweetpotatoes in Cluster I had yellow flesh, except for 'Hanzi' with

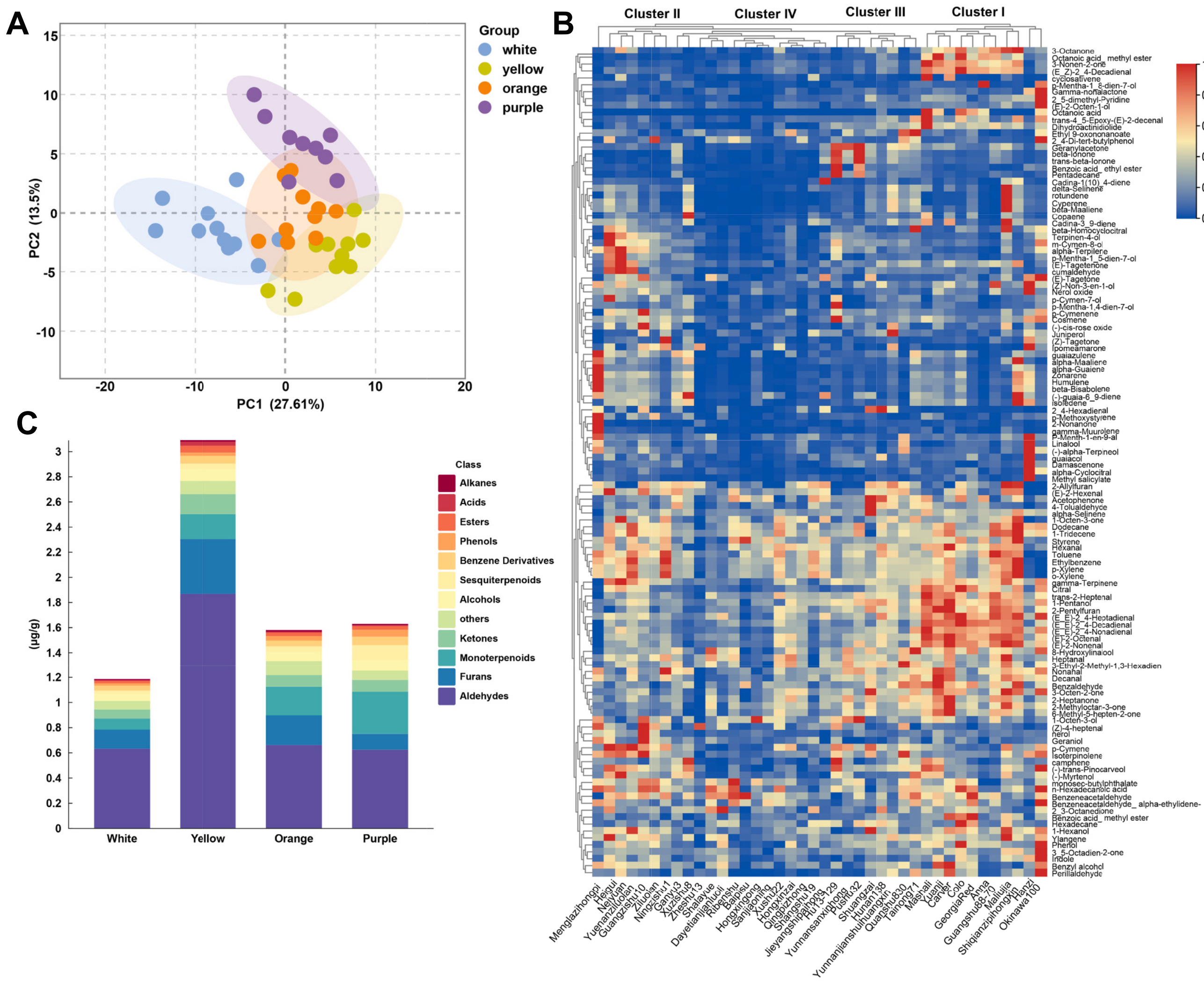

Fig. 3. The multivariate statistical analysis of volatile compounds in 40 sweetpotato varieties. A: The PCA score plots, each dot represents an independent variety. B: Heatmap visualization of all the volatile compounds. The red blocks indicate the up-regulated metabolites, blue blocks indicate down-regulated metabolites, yellow blocks represent the average relative expressed intensity of all metabolites. C: Category statistics for volatile compounds in each sweetpotato group with different flesh color. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

purple flesh. The PFSPs were practically all clustered into Cluster II, and ‘Ganshu 3’, an orange-fleshed variety, was clustered with them, exhibiting a strong resemblance to ‘Xuzi 8’. All other OFSP and WFSP varieties were clustered in Cluster IV and Cluster III respectively. This result was consistent with the PCA results, indicating that sweetpotatoes with different flesh colors have quite distinct aromas.

Later, the differences in components were analyzed preliminarily to explore the relationship between the flesh color and aroma of sweetpotato. Notably, the YFSP had the largest level of volatile compounds and the total VOCs content of YFSP was twice than other groups (Fig. 3C). Its aldehydes content (0.63 ± 0.18 mg/kg) was approximately three times higher than that of other groups, and the contents of furans and ketones were at least twice as high. The higher accumulations of aldehydes were primary contributed by (*E*,*Z*)-2,4-decadienal, trans-2-heptenal, 1-pentanol, (*E*,*E*)-2,4-heptadienal, (*E*,*E*)-2,4-decadienal, (*E*, *E*)-2,4-nodadienal, (*E*)-2-octenal, (*E*)-2-nonenal and benzaldehydes (Fig. 3B, Table S2), especially in the varieties ‘Mashali’, ‘Yuanji’ and ‘Carver’. Most aldehydes were mainly produced by the oxidation reaction using the unsaturated fatty acids like linoleic acid and linolenic acid (Yao et al., 2024). Therefore, it was speculated that the lipid components in YFSP were probably different from other flesh sweetpotato varieties, demanding further study. Moreover, the ketones, such as 3-octanone, 3-nonen-2-one, 3-octen-2-one, 2-heptanone, 2-methyloctan-3-one and 6-methyl-5-hepten-2-one were also enriched in the yellow-fleshed varieties, particularly in ‘Yuanji’, ‘Carver’, and ‘Maliujia’ (Fig. 3B). The YFSP had the highest concentration of 2-pentyfuran among all varieties (Fig. 3B, Table S2). Compared to other groups, PFSP had the lowest furan content, but they had much high concentrations of monoterpenoids and sesquiterpenoids (Fig. 3C). Some monoterpenoids like terpinene-4-ol, m-cymen-8-ol, and alpha-terpilene showed a higher level in PFSP, specifically ‘Heigui’ and ‘Neiyuan’. Sesquiterpenoids, such as guaiazulene and alpha-maalinene, were mostly detected in the purple-fleshed varieties at significantly higher concentrations than in other groups. This was especially evident in the variety named ‘Menglazipihong’ (Fig. 3B, Table S2). The high content of terpenoids in PFSP was consistent with the previous study, which might relate to the biological resistance of PFSP, as many terpenoids played important roles in the interactions and defense reactions between plants, microorganisms, and animals (Li et al., 2023).

3.4. Multivariate analysis of differential accumulated VOCs between sweetpotato with different flesh colors

The WFSP had the lowest VOCs concentration with the lightest aroma (Zhang et al., 2023). Thus, it was selected as the control group to identify the differentially accumulated VOCs associated with different sweetpotato flesh colors. Firstly, the OPLS-DA analysis was performed between other fleshed-color sweetpotatoes and white groups (Fig. 4A-C). Based on the OPLS-DA models, the VOCs of sweetpotatoes with different flesh colors could be divided into distinct groups, which were easily distinguished and had a goodness of fit and prediction with $R^2X > 0.8$ and $Q^2 > 0.8$ (Fig. 4A-C). Then, the variable influence on the projection (VIP) score was calculated for each VOC to delve deeper into the specific factors contributing to the difference between two groups. The significantly different VOCs between two groups were screened using the following criteria: $Log_2(\text{fold change}) \geq 1$ or $Log_2(\text{fold change}) \leq -1$, VIP ≥ 1, and $p < 0.05$.

The VOCs of YFSP, OFSP, and PFSP were compared with WFSP, and 43, 31, and 31 VOCs were identified as differentially accumulated VOCs (DAVs), respectively (Table S4–6). Five DAVs (cosmene, (−)-trans-pinocarveol, cumaldehyde, alpha-guaiene, and humulene) were found to be common among three compared groups and most of them were terpenoids. This result indicated that terpenoid is an important factor contributing to the difference in flavor between white and other flesh sweetpotatoes. Meanwhile, most of DAVs were exclusive to each sweetpotato with specific flesh color (Fig. 4D). This result demonstrated that sweetpotatoes with different flesh color really have distinct aromas of their own. Afterward, the DAVs of sweetpotatoes with various flesh colors were investigated, and the results showed that all DAVs were upregulated compared to the WFSP. The DAVs of the YFSP group are shown in Fig. 4E, and aldehydes made up most of the DAVs that differed noticeably. Among them, (*E*,*E*)-2,4-heptadienal, nonanal, benzaldehydes, (*E*,*E*)-2,4-decadienal, (*E*,*E*)-2,4-nonadienal, (*E*)-2-Nonenal and (*E*,*Z*)-2,4-Decadienal were key aromatic compounds of sweetpotato and contributed to fried, fat, green, and burnt sugar aroma. Except for benzaldehydes, all were formed from the degradation of unsaturated fatty acid under the heating or enzymatic actions (Li et al., 2021). Therefore, it was inferred that the primary cause of the aroma differences between the yellow- and white-fleshed sweetpotatoes is most likely the unsaturated fatty acid degradation products.

The DAVs of OFSP compared to WFSP were analyzed and almost all were identified as terpenoids (Fig. 4F). VIP is a crucial indicator for assessing the importance of the variables in differentiating groups. Among these DAVs, the VOCs with the highest VIP value (VIP > 1.7) were trans-beta-ionone, β-ionone, geranylacetone, pentadecane, and dihydroactinidiolide. Besides pentadecane, other compounds included apocarotenoid volatiles, which are the derivatives or metabolites of carotenoids (Simkin et al., 2004) and they have the aroma like sweet, floral, and fruity. Moreover, apocarotenoid volatile have a significant impact on the perception of sweetness (Tieman et al., 2017). It has been reported that the contents of apocarotenoid volatiles are proportional to their carotenoid precursor contents in fruits (Lewinsohn et al., 2005).

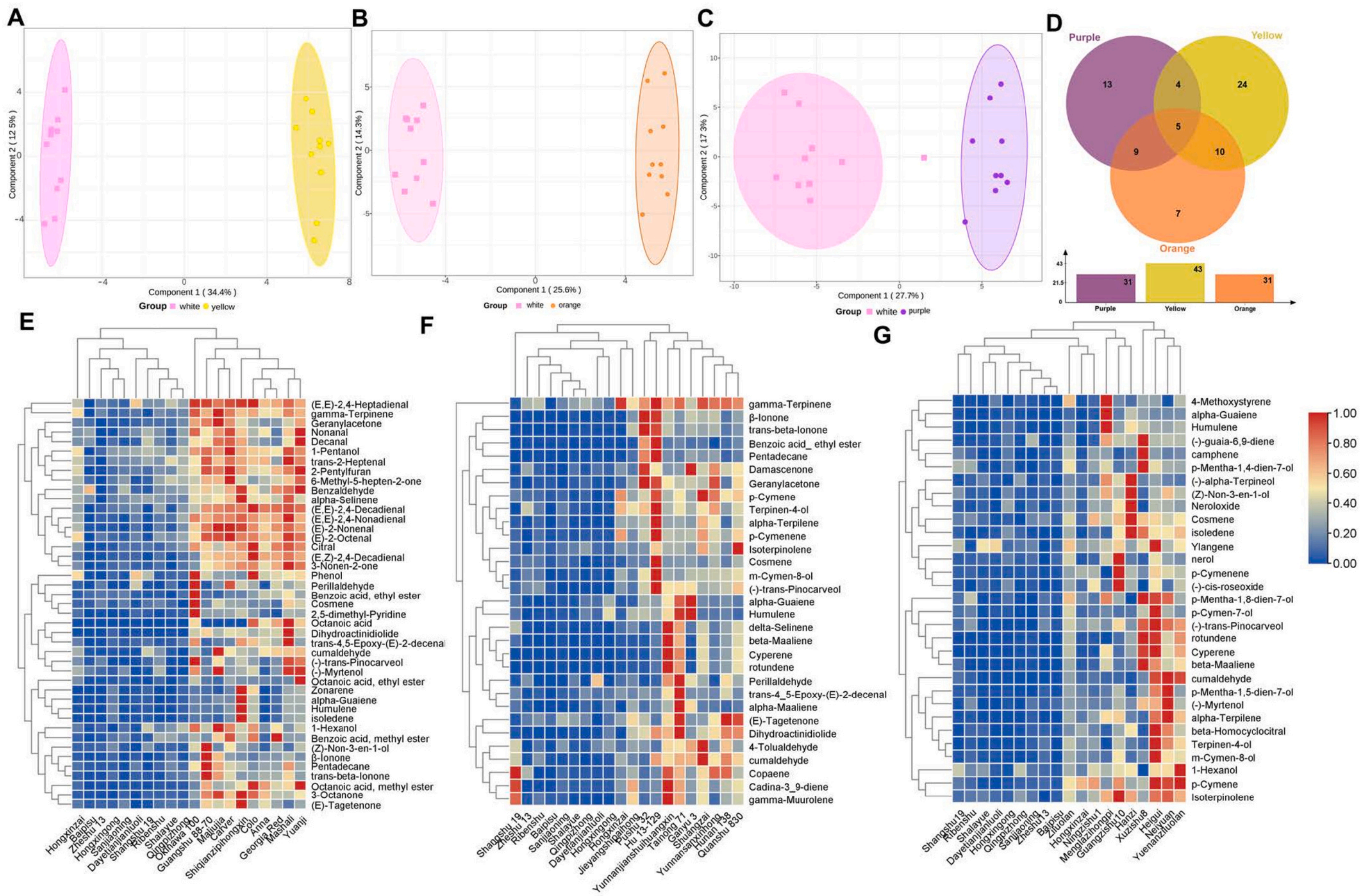

Fig. 4. Analysis of the differentially accumulated volatile compounds of four different flesh color groups. A, B, C: The OPLS-DA score plot for yellow-fleshed, orange-fleshed, purple-fleshed sweetpotato compared with white-fleshed sweetpotato. D: Venn diagram showing the distribution of differential volatile compounds. E, F, G: Cluster heatmap analysis of volatile compounds with variable importance in the projection (VIP) values above one in the comparisons of yellow-fleshed, orange-fleshed, purple-fleshed sweetpotato and white-fleshed sweetpotato. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Compared to other sweetpotatoes, OFSP had a noticeably higher total carotenoids content (Jia et al., 2022). The high content of apocarotenoid volatiles in OFSP might be attributed to the high content of carotenoids, which is also a major contributing element to their distinctive flavor.

Similar to WFSP, PFSP had a relatively less aroma than other sweetpotatoes (Jiang et al., 2023). Almost all DAVs of PFSP were terpenoids (Fig. 4G). Among the 31 DAVs, only three compounds, 1-hexanol, p-cymene, and nerol were the key aromatic compounds in PFSP, contributing to green, sweet, and pleasant aromatic flavor. Although the VOCs content of purple-fleshed and white-fleshed sweetpotatoes differs significantly, no significant difference was observed for aroma variation. Though many terpenoids were detected in PFSP, the rate of contribution of these compounds to the aroma is still unclear due to their unknow odor threshold and aroma. The exploring their roles in sweetpotato, particularly in PFSP, has high significance.

To the best of our knowledge, this is the first analysis of the VOCs profile of sweetpotato with different flesh colors in germplasm level. In the present study, the volatile compounds of 40 sweetpotato varieties were quantified by HS-SPME/GC–MS and 121 VOCs were identified. In a previous study, the aroma volatile compounds of five different sweetpotatoes after baking were analyzed and 61 compounds were detected. Among them, benzaldehyde and acetaldehyde were the common components in all varieties and linalool, decaldehyde, 2-camphene, furfural, and α-terpineol were considered as the important aroma components of sweetpotato (Tian et al., 2020). This study detected more volatile compounds in sweetpotato than the previous study. Moreover, the overall VOCs contents of each variety were evaluated and their contents were compared across different classes. Consequently, aldehydes and terpenoids were detected as the main volatile compounds of sweetpotato. Among them, most of the aldehydes were derived from the oxidative degradation of fatty acids and some were the derivatives of phenylalanine. The terpenoids identified in this study surpassed the number determined in the previous study (Shen et al., 2024). Although the contents of terpenoids were relatively low, they contributed to a rich variety of flavors for sweetpotato.

Moreover, the key aromatic compounds in sweetpotatoes were identified by OAV > 1. In a previous study, nine compounds with OAV > 1 were identified as the odor-active compounds of sweetpotato essential oils in four cultivars (Nakamura et al., 2013). In this study, 35 compounds were identified, of them 17 compounds were confirmed as the common key aromatic compounds in 40 varieties. The OAVs of key aromatic compounds in different varieties have significant difference. For instance, the OAV of β-ionone in WFSP and PFSP ranged from 50 to 400, and in YFSP, the majority were in the 400 to 2000, while in OFSP, it was greater than 2000 and even more than 10,000. It means that β-ionone provided different levels of floral aroma in different flesh-colors sweetpotatoes. Therefore, the types of compounds in different varieties of sweet potato are similar, but due to the difference in content, the same compound contributes to different flavor degrees in different varieties, resulting in the flavor differences in different varieties.

Furthermore, the differentially accumulated VOCs in different fleshed sweetpotatoes were compared, which is also the first attempt in this field. The result demonstrated that the color of the flesh significantly affects the aroma of sweetpotato. The main difference between YFSP and WFSP was aldehydes, which is produced by the oxidative degradation of unsaturated fatty acids. However, for OFSP, there were with distinctive aroma flavor which was most probably due to its abundant carotenoids content as carotenoids are good precursors to many of the aroma compounds. Terpenoids played a major role in the aroma difference of PFSP and WFSP, and their function need to be further studied.

This study represents a basic investigation of the volatile compounds in sweetpotato. The results indicated that sweetpotatoes have a complicated volatile composition that mostly varies depending on the varieties and the color of flesh had a significant effect on its aromatic volatile composition. Future studies will fucus on improving the comprehension of sweetpotato aroma flavor, and analyzing the influence of geographical origin, growing area, environmental conditions, etc., on the effect of sweetpotato aroma flavor.

4. Conclusion

In this study, the aromatic characteristics, and VOCs of 40 sweetpotato varieties with white, yellow, orange, and purple flesh colors were identified and analyzed using HS-SPME/GC–MS. A total of 121 major VOCs belonging to 12 chemical classes were detected in sweetpotatoes. Terpenoids (monoterpenoids and sesquiterpenoids), aldehydes and furans were the most abundant compounds in all varieties. Among them, 35 compounds were identified as the key aromatic compounds by OAV > 1, of which 17 were found to be the common key aromatic compounds across 40 different sweetpotato varieties, suggesting that these compounds are the primary contributors to sweetpotato aroma. Significant differences were observed for the volatile components and contents among sweetpotatoes with different flesh colors. YFSP had the highest concentration of VOCs components, while WFSP had the lowest. The differentially accumulated VOCs of other fleshed sweetpotatoes were identified and compared with WFSP. The rich aroma of YFSP could be due to the aldehydes produced by the oxidation of unsaturated fatty acids, like (E,E)-2,4-heptadienal, nonanal, benzaldehydes, (E,E)-2,4-decadienal, (E,E)-2,4-nonadienal, etc. The apocarotenoid volatiles (trans-beta-ionone, β-ionone, geranylacetone, and dihydroactinidiolide.), produced from carotenoids contributed to the sweet and aromatic flavor of OFSP. Although PFSP had a rich terpene content but low concentration, it had a weak aroma. Nevertheless, the effect of terpenoids on the aroma needs further exploration. In conclusion, these results not only provided a comprehensive understanding of volatile compounds of sweetpotato with different flesh colors, and lay the foundation of future exploration of the causes of flavor differences that can be continued at the genetic level, but helped breeders select varieties with special aroma characteristics and promote the aroma quality improvement during sweetpotato breeding.

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CRediT authorship contribution statement

Rong Zhang: Writing – review & editing, Writing – original draft, Methodology, Formal analysis, Data curation, Conceptualization. **Chaochen Tang:** Resources. **Bingzhi Jiang:** Resources. **Xueying Mo:** Formal analysis. **Zhangying Wang:** Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Data availability

Data will be made available on request.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.

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