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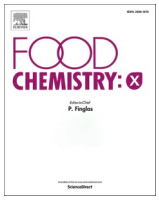

Sensory omics combined with mathematical modeling for integrated analysis of retronasal Muscat flavor in table grapes

Xiaomiao Zhou [a,b,c,e,1], Bingqi Shan [c,g,1], Songyu Liu [c], Wenping Gao [c], Xiaoyue Wang [e,f], Huiling Wang [e,f], Haiying Xu [a,d], Lei Sun [a,d,*], Baoqing Zhu [b,c,*]

[a] Institute of Forestry and Pomology, Beijing Academy of Agriculture and Forestry Sciences, Beijing 100093, China
[b] State Key Laboratory of Tree Genetics and Breeding, Bejing Forestry University, Beijing 100083, China
[c] Beiing Key Laboratory of Forestry Food Processing and Safety, Department of Food Science, Beijing Forestry University, Beijing 100083, China
[d] Key Laboratory of Biology and Genetic Improvement of Horticultural Crops (North China), Ministry of Agriculture and Rural Affairs, Beijing 100093, China
[e] Beijing Engineering Research Center for Deciduous Fruit Trees, Beijing 100093, China
[f] Key Laboratory of Urban Agriculture (North China), Ministry of Agriculture and Rural Affairs, China
[g] Heilongjiang Feihe Dairy Co., Ltd., Beijing 100015, China

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ABSTRACT

This study focused on analyzing the aroma formation mechanism of retronasal muscat flavor in table grapes. The sensory characteristics and fragrance components of table grape juice with different intensities of Muscat were investigated using GC-Quadrupole-MS, quantitative descriptive analysis and three-alternate forced choice. Free monoterpenoids were the main contributors to the retronasal Muscat flavor. The contribution of Muscat compounds to this flavor was quantified by Stevens coefficient, the most and the least sensitive compounds to concentration changes were citronellol and linalool, respectively. To predict the Muscat flavor intensity by mathematical modeling, established a model between Muscat flavor intensity and monoterpenoids concentration, and an optimal partial least squares regression model with a linear relationship between natural logarithms was obtained. These findings provide reference for understanding the formation mechanism of specific aromas in fruits and provide a basis for the development and quality control of processed products such as Muscat flavor grape juice.

1. Introduction

Grapes (*Vitis vinifera L.*) are one of the world's longest cultivated and most productive fruits and are mainly divided into table grapes and wine grapes. Chinese grape cultivation is dominated by table grapes, which account for 80 % of the total grape production in the country (Zhou et al.,2022). Secondary metabolites are widely distributed across various plants and play an important role (Tiwari et al., 2023; Panghal et al., 2021). Various aromatic compounds have been identified in grapes, including terpenoids, norisoprenoids, methoxypyrazines, esters, and alcohols. These components have different contents and aroma thresholds in the fruit and collectively contribute to the aroma and flavor of the fruit (Zhang et al., 2016). Aroma is an important sensory indicator of grapes. In recent years, there has been a growing popularity in the market for berries that have distinct flavors. Certain monoterpenoids can release a floral aroma, commonly known as Muscat, that is readily detected by the human sense of smell (Zhou et al.,2022). Currently, there is increasing interest in the quality of table grapes; therefore, it is important to explore the aroma quality of table grapes to improve the fruit aroma and to increase consumer preference and market acceptance.

At present, the analysis of aroma components in table grapes is mainly performed by gas chromatography and mass spectrometry (GC–MS) (Maoz et al., 2020). Headspace solid-phase microextraction is

* Corresponding authors at: Institute of Forestry and Pomology, Beijing Academy of Agriculture and Forestry Sciences, Beijing 100093, China (L. Sun); State Key Laboratory of Tree Genetics and Breeding, Bejing Forestry University, Beijing 100083, China (B. Zhu).

E-mail addresses: zhouxiaomiao123@163.com (X. Zhou), shanbingqi@feihe.com (B. Shan), l19970202@163.com (S. Liu), gaowenping2022@163.com (W. Gao), wangxiaoyue1988@163.com (X. Wang), whlhappy@aliyun.com (H. Wang), xuhaiying@baafs.net.cn (H. Xu), sunlei@baafs.net.cn (L. Sun), zhubaoqing@bjfu.edu.cn (B. Zhu).

[1] The two authors contributed equally.

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widely used in the sample pretreatment (Lin et al., 2021; Qian et al., 2019). The different classes of compounds can contribute to different aroma types. Terpenoids are typical aroma components in roses and their products (such as rose essential oil) due to their strong aroma and low sensory threshold (Zhao et al., 2016); furthermore, in other fruits, such as mango (Xiao et al., 2019) and orange (Deterre et al., 2011), they are also major aroma contributing components. Terpenoids, such as geraniol, nerol, linalool, and rose oxide, contribute to the floral, sweet, and Muscat aromas and are the main components of Muscat grapes (Mateo & Jiménez, 2000).

Aroma can reach the olfactory epithelium through orthonasal and retronasal routes (Bojanowski & Hummel, 2012). The detection of retronasal aroma is closely related to the release process of aroma substances in the oral cavity. The pH value of saliva, enzyme activity, chewing style, oral temperature, and other conditions have been shown to affect the results of retronasal perception of aroma substances (Roberts & Acree, 1995). Pittari et al. (2022) showed that the perception of oxidative molecular markers in wine was influenced by nonvolatile matrix components and saliva; however, it was unclear whether aroma compounds released from table grapes during oral processing were affected by saliva.

With the rapid development of the food processing industry, sensory analysis is becoming more widely used in food. Quantitative descriptive analysis (QDA) is often used in the sensory evaluation of table grapes. For example, in the studies by Wu et al. (2019) a trained panel of 36 assessors evaluated the odor intensity of three aroma types of table grapes. The results revealed typical aroma features among different grape varieties. In the study conducted by Maoz et al. (2020), a trained panel of 10–25 assessors performed quantitative descriptive analysis on the flavor intensity of different varieties of table grapes, and found a significant correlation between flavor impressions and berry preferences. In the study by Aubert and Chalot (2018), quantitative descriptive analysis of six table grapes varieties was assessed by eight trained assessors in terms of crispness, juiciness, hardness, sweetness, acidity, aroma intensity, and skin astringency. This study clarified the fruit characteristics of the varieties. The 3-AFC method is widely used for the determination of olfaction, taste, and flavor thresholds of volatile aroma substances. (Wang et al., 2021a; Zhao et al., 2019).

Previous studies indicated that the intensity of sensory attributes can be characterized by mathematical models. For example, Erdem et al. (2023) modeling of relate sweetness perception and sugar concentration based on sensory analysis to predict the intensity of sweetness in cookies. Stevens et al. showed that the relationship between the perceived intensity and physical stimuli could be represented via mathematical models, which was known as Stevens law (Stevens, 1957), and later, an improved version of Stevens law was proposed by Chen et al. (2021). The law indicates that there is a power index relationship between the intensity and concentration of flavor compounds. The sensitivity to the perception of the compound can be determined by the size of the power index, and a higher Stevens coefficient correlates to a higher sensitivity. Therefore, exploring the Stevens coefficients of compounds can help quantify the contribution of compounds in perceived intensity, and developing mathematical models is of great importance for predicting perceived intensity.

In this study, GC-Quadrupole-MS was used to investigate the differences in monoterpenoid components of different progenies of grapes from the same hybridization and to identify the key aroma components, in addition to investigate which forms of monoterpenoid components mainly contribute to the Muscat released from table grapes in the mouth. The intensity of Muscat of table grapes was quantified via QDA, and the retronasal odor threshold of key aroma components in aqueous solution was determined by the 3-AFC method. Stevens law was used to investigate the Stevens coefficients of Muscat compounds such as geraniol, citronellol, nerol and linalool, and the flavor intensity of the compounds at different concentrations. The prediction model between Muscat and monoterpenoid components was investigated via a mathematical modeling method to obtain the scientific prediction of Muscat intensity through the aroma components. This study provides a scientific basis to select high-quality, highly preferred Muscat flavor table grape varieties and supplies data support for the study of the flavor chemistry of table grapes.

2. Material and methods

2.1. Sample

2.1.1. Preparation of the grape juice samples

In this study, 14 grape juices with different degrees of Muscat flavor were selected as the experimental materials. MixA indicates a mixture of R23 and R62, mixB indicates a mixture of R9 and R149, and mixC indicates a mixture of R54, R81, and R87. The grapes were F1 progenies of the Muscat table grapes 'Italia' and 'Tamina' (*V. vinifera L.*) grown under a rain shelter with 2.5 m row spacing and 0.75 m plant spacing; they were planted at the Institute of Forestry and Pomology, Beijing Academy of Forestry and Agricultural Sciences vineyard (39°58′ N and 116°13′ E, Beijing, China). The samples were collected at (E-L38) in 2019 according to the phenological period of the E-L system (Coombe, 1995). Fifty berries without damage, pests or diseases were randomly collected from the bunches of grapes at the shoulder, middle and top positions on the plant. Then, a portion of the berries was immediately used for sensory analysis and physicochemical analyses (Table S1), and the remaining berries were frozen in liquid nitrogen and stored at −80 °C for subsequent volatile compound analysis.

2.1.2. Collection of saliva and the preparation of samples for testing

To investigate whether the release of aroma compounds during oral processing is influenced by saliva. Following the method of Wang et al. (Wang et al., 2020; Wang et al., 2021b), six healthy participants (2 males and 4 females, average age ranges 24–27), who have provided explicit consent for the utilization of their personal information in the scope of this research, underwent saliva collection. All participants were vaccinated against hepatitis B and were not at risk of infection. Saliva stimulated by 1 % citric acid was collected from the 6 participants at 10 am. The participants were required to refrain from eating or drinking water for 2 h prior to saliva collection. Prior to collection, the oral cavity was rinsed with pure water. Citric acid (200 μL) was dropped to the back of the oral cavity to stimulate salivation. The first 30 s of secreted saliva was discarded, and the collection was continued for 5 s in a 50 mL centrifuge tube placed on ice. The saliva was filtered through a 40 μm cell sieve for 10 min, and the supernatant was stored for subsequent analysis (-80 °C). The average time needed to swallow a medium-sized grape (6 s) by the six participants was used as the reaction time for the saliva acting with the juice. Participants held 5 mL of grape juice in their mouth for 6 s (without swallowing) and then spit it out into a dixie cup. The ratio of secreted saliva to grape juice was calculated. The average secreted saliva from the 6 participants was 1.01 mL, resulting in a volume ratio of saliva to juice of 1:5.

According to previous laboratory research (unpublished), two terpenoid-rich grape juices, 'Aishenmeigui' and 'Ruiduhongmei', were selected as materials to be mixed with saliva. The process for the control group is as follows: After the addition of 1.00 g NaCl to the 15 mL sample vial, a total of 5 mL of clarified saliva and grape juice were added separately (V saliva: V juice = 1:5), and then 10 μL of internal standard (4-methyl-2-pentanol, 1.0388 g/L) was added. The process for the experimental group is as follows: A total of 5 mL of clarified saliva and grape juice (V saliva: V juice = 1:5) were initially added to a 15 mL sample vial, and then 1.00 g NaCl and 10 μL of internal standard were added after 6 s of interaction between saliva and juice. The samples were analyzed via GC–MS, and each sample was analyzed three times.

2.2. Reagents and standards

All analytical reagent grade chemicals of sodium hydroxide (NaOH), sodium chloride (NaCl), glucose, tartaric acid and distilled water were purchased from Beijing Chemical Works (Beijing, China). HPLC-grade ethanol was purchased from ANPEL Laboratory Technologies (Shanghai) Inc. D-gluconic acid lactone, polyvinylpolypyrrolidone (PVPP) and an *n*-alkane solution, C7 to C40, were obtained from Sigma–Aldrich (St. Louis, MO, USA). Food grade citric acid monohydrate was obtained from BOLINE Biotechnology (Shandong, China). γ-Terpinene (95 %), linalool (98 %), neral (>98 %) and geranial (>98 %) were purchased from Shanghai Macklin Biochemical Co., Ltd. (Shanghai, China). β-Myrcene (>90 %) was obtained from Sigma–Aldrich (St. Louis, MO, USA). β-Phellandrene (>99 %) was purchased from EA (French). Terpinolene was obtained from Tokyo Chemical Industry Co. Ltd. (Tokyo Japan). D-limonene (>99 %), α-terpineol (>95 %) and geraniol (99 %) were purchased from Aladdin Bio-Chem Technology (Shanghai, China). Rose oxide (mixture of *cis* and *trans*, >99 %) and linalool oxide (mixture of isomers, 97 %) were purchased from Supelco (Bellefonte, Pennsylvania, USA). 4-Terpineol (>98 %) and citronellol (>98 %) were obtained from Shanghai Yuanye Bio-Technology Co., Ltd. (Shanghai, China). Nerol (97 %), geranic acid (98 %) and 4-methyl-2-pentanol (>98 %) were purchased from Adamas Reagent, Ltd. (Shanghai, China), Alfa Aesar (China) Chemical Co., Ltd. (Shanghai, China) and CNW Technologies GmbH (Duesseldorf, Germany). All chemicals of food grade, including geraniol, citronellol, nerol, and linalool, were purchased from Dongguan Qiyi Spice Co., Ltd. (Dongguan, China).

2.3. HS-SPME-GC-Quadrupole MS analysis

Qualitative and quantitative analysis of monoterpenoids in 14 grape juice samples was performed based on the HS-SPME-GC-Quadrupole-MS technique. The SPME extraction head is connected to the CTC CombiPAL autosampler (CTC Analytics, Zwingen, Switzerland) for automated headspace solid-phase microextraction. The sample vial was moved to a heated stirrer device and agitated at 40 °C for 30 min at an agitation speed of 500 rpm. The activated SPME fiber was inserted into the headspace portion of the sample vial, and the sample was stirred at 40 °C for 30 min. After the SPME fiber was removed, it was immediately inserted into the GC injection port, and desorbed at 250 °C for 8 min to extract volatile compounds. The capillary column used for separating volatile compounds is an HP-Innowax with dimensions of 60 m × 0.25 mm × 0.25 μm (J&W Scientific, Folsom, CA, USA). The GC–MS conditions were set to enable the separation of the volatile compounds following published methods in our laboratory (Liu et al., 2018; Wang et al., 2018). Carrier gas: High-purity helium gas with a flow rate of 1 mL/min; the headspace solid-phase microextraction non-split mode was used for automatic injection. The temperature program was set as follows: 40℃ for 5 min, followed by an increase at a rate of 3℃/min to 180℃, then an increase at a rate of 30℃/min to 250℃, with a 10 min hold. The temperature of the mass spectrometry interface was set to 280℃, the ion source temperature to 230℃, and the ionization mode to electron ionization (EI) with an ionization energy of 70 eV. The mass scanning range was set from 29 to 350 *m/z*, and each sample was determined twice.

2.4. Qualitative and quantitative analysis of the monoterpenoids

The retention indices (RIs) of each component were calculated based on the analysis of *n*-alkanes under the same chromatographic conditions. Volatile compounds were identified by comparing their RIs and mass spectra with those of standard substances and the NIST11 library. Quantitative of volatile compounds was performed according to the previously published methods (Liu et al., 2018; Wang et al., 2018). According to the average sugar content (200 g/L) and acidity (7 g/L) in grape juices, a synthetic grape berry juice matrix was prepared by combining glucose and tartaric acid, and the pH of the synthetic grape berry juice matrix was adjusted to 3.4. Prepare in advance all the monoterpenoid standards and mix them with the synthetic matrix to create the standard solution. Then, dilute the resultant solutions into 15 levels in a sequential manner. Analyze the standard solutions extracted using the same method employed for the grape samples. Compounds with standards were completely quantified using the standard curve of the standards. Compounds without standards were relatively quantified according to the principle of a similar number of carbon atoms and similar chemical structures.

2.5. Sensory analysis

2.5.1. Quantitative descriptive analysis of grape juice

In table grapes, the Muscat flavor was perceived retronasally. Therefore, in this study, the visual scale for Muscat and retronasal odor thresholds were determined via retronasal sensory evaluation. The retronasal sensory evaluation method (Fig. 1A) was slightly modified with reference to the study by Zhao et al. (2018). The Muscat reference scale was developed according to Atanasova et al. (2004) and de-la-Fuente-Blanco et al. (2020) by slightly modifying their reference scale for *n*-butanol, the reference scales for sweet and sour by reference to the single solution reference sample of the national standard GB/T 29604–2013 (Sensory analysis-General guidance for establishing references for sensory attributes) set up by the China National Institute of Standardization (CNIS) for the intensity of sweet and sour (Fig. 1B). The specific concentrations of the reference sample solutions corresponding to each intensity listed in Table S2. When using the Muscat reference scale, it is necessary to feel it through the retronasal sensory evaluation method, while when using the Sweet and Sour reference scales, it is sufficient to taste the solution directly.

Ten assessors (2 males and 8 females, average age ranges 24–27), who have provided explicit consent for the utilization of their personal information in the scope of this research, were selected for training. A total of 8 training sessions were organized, each lasting 1.5 to 2 h. Training sessions 1 to 3 used the ranking method to familiarize each assessor with the process of olfactory sensory evaluation and the strength differences among reference solutions. Training sessions 4 to 8 used the intensity method to ensure that each assessor became familiar with and memorized the corresponding intensities of the reference solutions. Finally, these 10 assessors who completed the training formed the Sensory Panel of Preferred Assessors.

The 14 samples of grape juice (10 mL each) to be accessed in terms of strength were added separately to lidded tasting cups. The tested samples were labeled with random three-digit codes and presented to the preferred assessors in a randomized order. The juice samples were tasted in turn, and the intensity of the different sensory attributes of the grape juice was assessed using the reference scale (0–15 cm). When tasting different samples, the tasters rinsed their mouths and then rest for a period of time; the experiment was repeated twice.

2.5.2. Retronasal odor thresholds of terpene alcohols in an aqueous solution

According to the research of Wang et al. and Zhao et al., the retronasal thresholds of the three terpene alcohols of geraniol, citronellol, and nerol were determined in aqueous solutions using 3-AFC (Wang et al., 2021a; Zhao et al., 2018; Zhao et al., 2019). The assessors are the Sensory Panel of Preferred Assessors for the completion of the training.

Initially, two samples were provided to the assessors, a known characteristic sample (target compound added to pure water) and a blank sample (pure water). The concentration of the characteristic sample was not too high or too low, which caused the target compound to be perceptible to all assessors. Then, 10 concentration gradients of the target compounds were prepared in a twofold concentration gradient, and a set of three samples were provided to the assessor each time in increasing order of concentration gradient; one of these samples was an

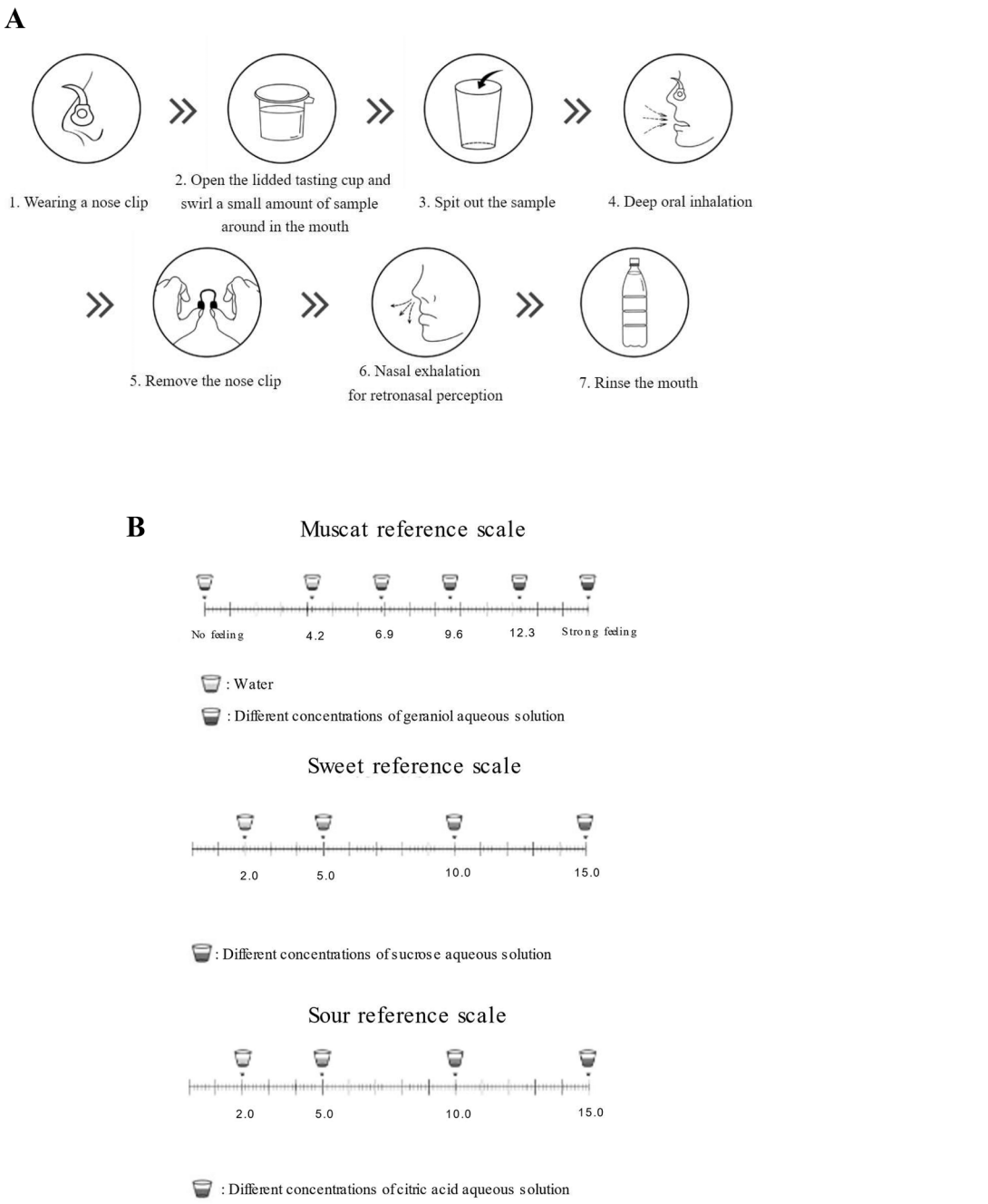

Fig. 1. Establishment of the sensory evaluation method and scale. (A) Visualized steps for retronasal sensory evaluation. (B) Visualized scales for Muscat, sweet and sour.

additive sample (target compound added to pure water) and the other two were blanks, and each were presented to the assessor in random order. The assessors were asked to select the sample with the target compound from the three samples using the retronasal sensory evaluation; mouth rinsing and resting occurred between tasting different samples.

After the evaluation, the results of the sensory panel under each gradient were counted, and the probability of being able to correctly select the target compound at that gradient (p) could be calculated. Then the corrected probability of detection (P) was calculated using the chance factor (P=(3*p-1)/2), the chance probability in the 3-AFC test is 1/3. The correspondence between sample concentration and detection probability can be fitted by sigmoid curve ($P = 1/(1 + e^{(-(x-x0)/b)}$, where X = concentration value after log10 conversion, X0 = logarithmic value of the threshold concentration and b = slope). The threshold concentration of a substance is defined as the minimum concentration of the sample when the probability of detection reaches 50 % (Lytra et al., 2012).

2.6. Determination of the retronasal intensity of the Muscat compounds

The flavor intensities of four Muscat compounds of geraniol, citronellol, nerol and linalool were determined at their corresponding concentrations of different dose over threshold (DoT) factors by the Sensory Panel of Preferred Assessors. Each standard (food grade) was dissolved in purified water, five corresponding concentration points were selected according to the distribution range of the DoT factors in grape samples, and a target compound solution of the corresponding concentration was

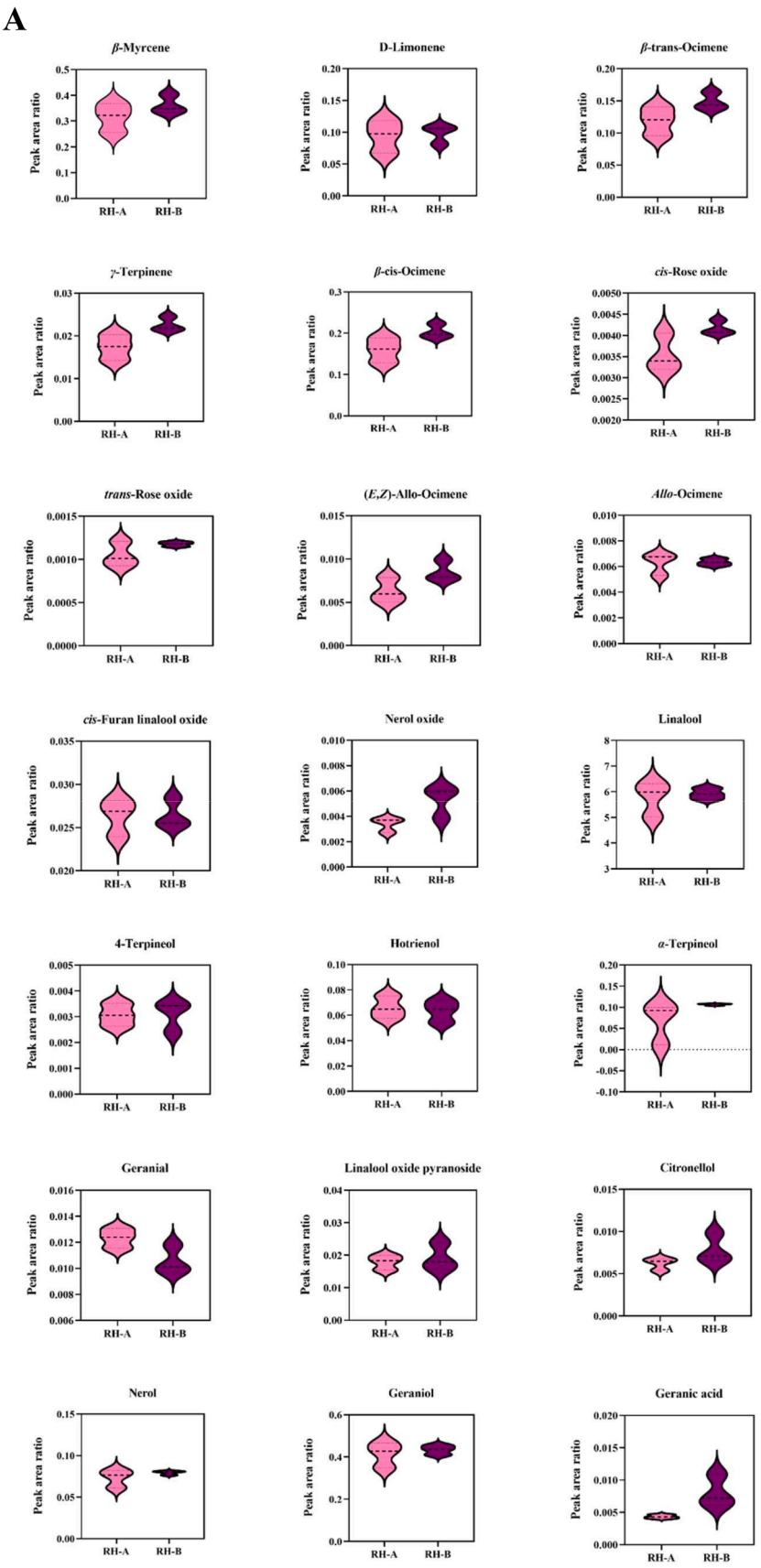

Fig. 2. Violin diagram of the monoterpenoids in Ruidu Hongmei and Aishen Rose. (A) Violin diagram of the monoterpenoids in Ruidu Hongmei. (RH-A is the control group, and RH-B is the treatment group) (B) Violin diagram of the monoterpenoids in Aishen Rose. (AM-A is the control group, and AM-B is the treatment group).

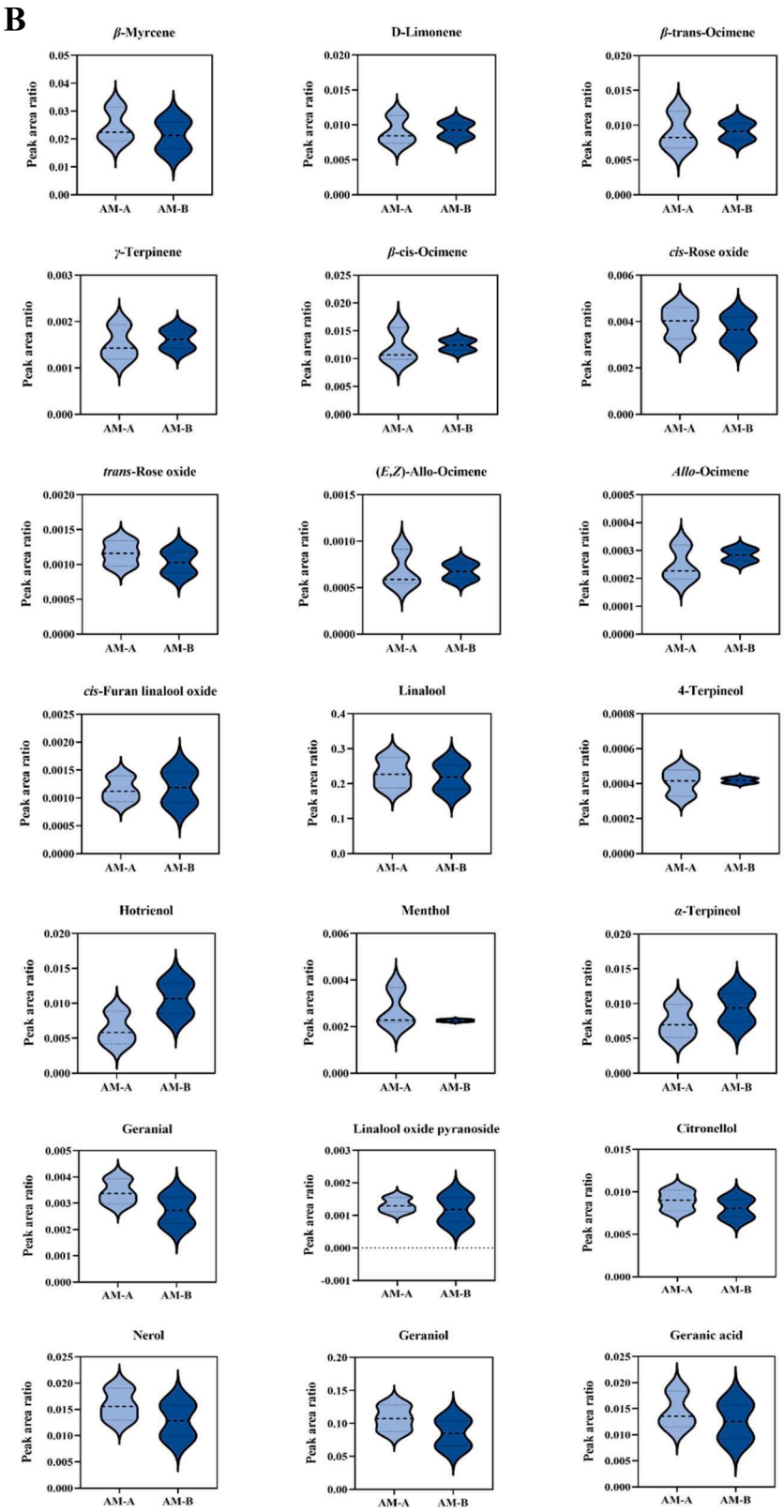

Fig. 2. (*continued*).

prepared.

The retronasal odor of linalool in aqueous solution was 3.8 μg/L (Ahmed et al., 1978), and the corresponding concentrations with DoT factors of 1, 10, 100, 1000, and 2000 were selected to prepare the solution. The retronasal odors of citronellol and nerol in aqueous solution were 5.4 μg/L (Fig. 4A) and 35.9 μg/L (Fig. 4B), respectively, and the corresponding concentrations with DoT factors of 1, 5, 10, 25, and 50 were selected to prepare the solutions. The retronasal odor of geraniol in aqueous solution was 4.5 μg/L (Fig. 4C), and the corresponding concentrations with DoT factors of 1, 10, 100, 250, and 500 were selected to

prepare the solution. The solutions of the target compounds were randomly coded with three digits and presented to the assessors in a random order. The retronasal sensory evaluation was used to determine the retronasal flavor intensity, and the sensory panel used the Muscat reference scale to evaluate the flavor intensity of the target compounds. Mouth rinsing and resting were needed between assessments of different samples, the experiment was repeated twice, and the average value was taken as the result.

2.7. Statistical analysis

GraphPad Prism 9.0.0 was used to create the violin diagrams and score charts of sensory attribute intensity. A sensory panel ability check was performed by PanelCheck 1.4.2. Bubble plots, stepwise regression, and one-way ANOVA were performed using R 3.6.3. SIMCA 14.1 (Umetrics, Umea, Sweden) was used to perform principal component analysis (PCA). The heatmap was generated via MetaboAnalyst 5.0 (https://www.metaboanalyst.ca/). Partial least squares regression

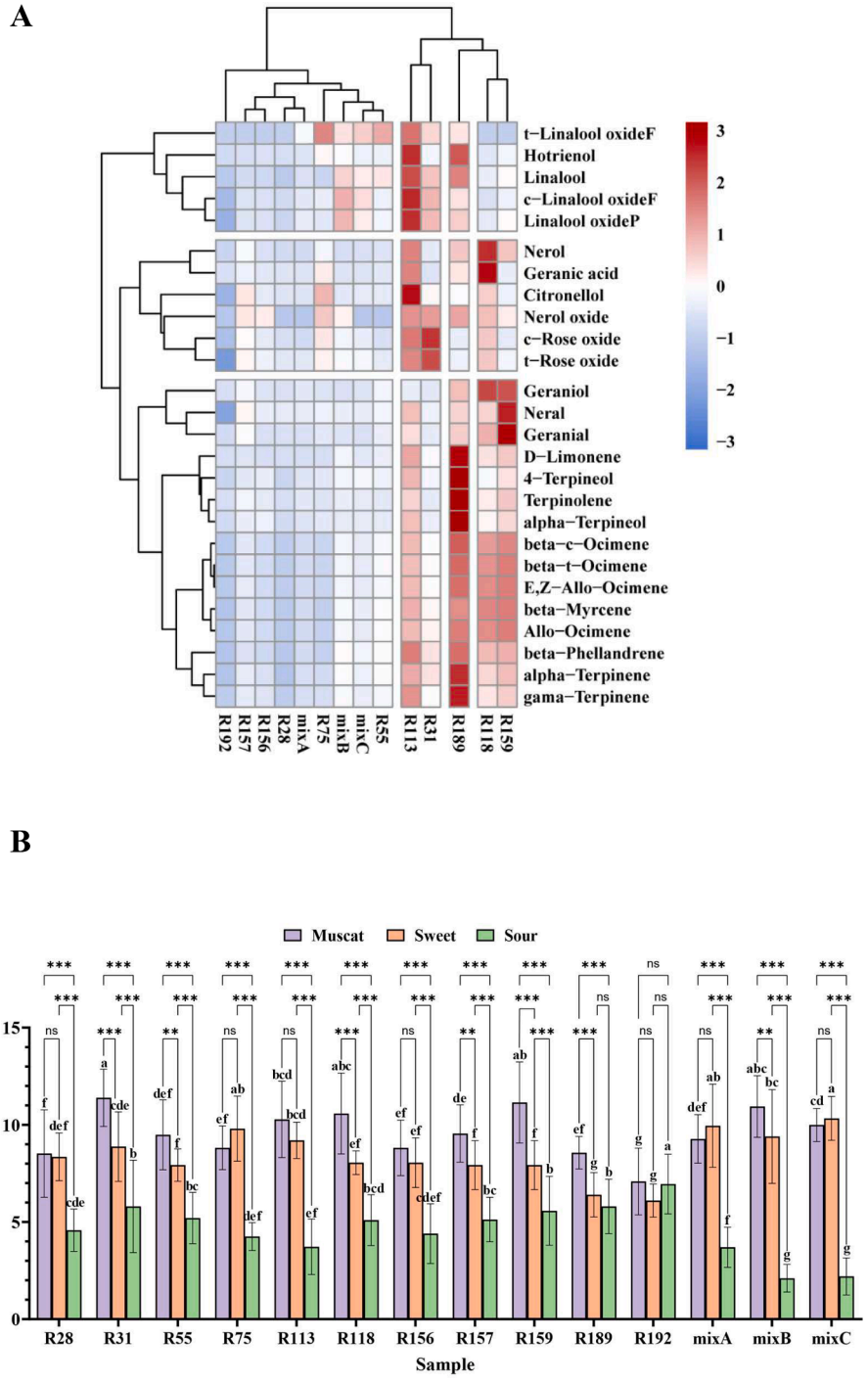

Fig. 3. Contents of the volatile compounds and the intensity of the sensory properties in 14 grape juice samples. (A) Heatmap based on the contents of the volatile compounds (all the data were standardized). (B) Score chart of the different sensory attribute intensities of the grape juice samples (different letters indicate significant differences in the intensity of certain sensory properties among the fourteen samples, significant levels of intensity of different sensory attributes of the same grape juice sample: **, $p < 0.01$; ***, $p < 0.001$; ns, not significance).

analysis (PLSR) was conducted using XLSTAT 2019.

3. Results and discussion

3.1. Effect of saliva on the content of the monoterpenoids in juice

Two grape juices ('Aishenmeigui' and 'Ruiduhongmei') with strong Muscat flavor were selected to investigate whether glucoside-binding substances were hydrolyzed via salivary α-amylase during the oral processing of table grapes. A total of 22 monoterpenoids were detected in the two juice samples (Table S3); these included *β*-myrcene, D-limonene, *β-trans*-ocimene, *γ*-terpinene, *β-cis*-ocimene, *cis*-rose oxide, *trans*-rose oxide, *(E,Z)-allo*-ocimene, *allo*-ocimene, *cis*-furan linalool oxide, nerol oxide, linalool, 4-terpineol, hotrienol, menthol, *α*-terpineol, geranial, linalool oxide pyranoside, citronellol, nerol, geraniol, and geranic acid. Among them, menthol was not detected in 'Ruiduhongmei', and nerol oxide ether was not detected in 'Aishenmeigui'.

Compared with the control group, there was no significant difference in the contents of the 22 monoterpenoids in the experimental group, and the distribution of monoterpenoids was similar between the control group and the experimental group (Fig. 2); this result indicated that after salivary action, the substances without the glycoside-bound state in grape juice were hydrolyzed by salivary *α*-amylase. The Muscat flavor perceived in the mouth of table grapes was likely caused by the free monoterpenoids rather than the glycoside-bound monoterpenoids.

3.2. Qualitative and quantitative analysis of the monoterpenoids

14 grape juices from the F1 progenies of the 'Italia' and 'Tamina' hybrids were selected to investigate the differences in the free monoterpenoids. A total of 26 monoterpenoids were identified (Table S4), and the total amount of monoterpenoids in different samples varied (Table S5). Among them, the total amount of monoterpenoids in R189 was the highest, and the total amount of monoterpenoids in R192 was the lowest.

The 26 monoterpenoids were divided into three groups (Fig. 3A). The first group was *trans*-furan linalool oxide, hotrienol, linalool, *cis*-furan linalool oxide, and linalool oxide pyranoside; these were linalool and its derivatives. The second group was nerol, geranic acid, citronellol, nerol oxide, *cis*-rose oxide, and *trans*-rose oxide; these were all geraniol derivatives. The third group consisted of geraniol, neral, geranial, D-limonene, 4-terpineol, terpinolene, *α*-terpineol, *β-cis*-ocimene, *β-trans*-ocimene, *(E,Z)-allo*-ocimene, *β*-myrcene, *allo*-ocimene, *β*-phellandrene, *α*-terpinene, and *γ*-terpinene; these included geraniol and its derivatives and the cyclic and chain monoterpenoids.

Clustering heat map analysis of terpenoids and grape juice samples revealed that the 14 samples were divided into 4 groups (Fig. 3A): R159 and R118 as Group 1; R189 as Group 2; R113 and R31 as Group 3; and R28, R55, R75, R156, R157, R192, mixA, mixB, and mixC as Group 4. The contents of geraniol and its derivatives, chain monoterpenoids, and cyclic monoterpenoids were higher in Group 1, while the contents of linalool and its derivatives were lower. The monoterpenoid content of Group 2 was overall higher than that of the other samples, and only a few monoterpenoids, such as *cis*-rose oxide and *trans*-rose oxide, were significantly lower than those of the other samples. In Group 3, the contents of linalool and its derivatives, as well as geraniol derivatives, such as nerol oxide, *cis*-rose oxide, and *trans*-rose oxide, were higher. Group 4 showed lower contents of monoterpenoids. Based on the determination of free monoterpenoids, it was found that the distribution of monoterpenoids in the different lines of grapes from the same hybrid population varied.

3.3. Sensory analysis

The flavor of fruits is primarily determined by the sugars, acids, and aroma (Tieman et al., 2017). Therefore, the intensity of sweet, sour, and retronasal Muscat of the 14 table grape juice samples were assessed via QDA using the established reference scales. To assess the consensus of the sensory panel and the repeatability and discrimination ability of each assessor for the samples, PanelCheck software (Tomic et al., 2013; Tomic et al., 2007) was used to assess the QDA results from the 10 assessors (Fig. S1). The dots in the Tukey-1 (Fig. S1A) analysis chart represent each assessor, and the degree of aggregation between the dots represents the consistency of the sensory panel. A closer distance between dots correlates to a higher consistency level between sensory panels (Tomic et al., 2009), the results showed that the sensory panel showed good consistency in the attributes of sweet, sour, and retronasal Muscat. The F value (Fig. S1B) can be used to demonstrate an assessor's ability to differentiate samples and is the ratio of the between-group variation to the within-group variation. Larger F values indicate that the assessor is better at differentiating the relevant attributes (Li et al., 2019), different color lines represent different sensory attributes, and the results show that the ten assessors have high F-values for the attributes of sweet, sour, and retronasal Muscat and all of them are at or close to the significant level of 5 %, which means that the ten assessors have a good ability to differentiate the samples. The mean square error (MSE) value (Fig. S1C) can be used to show the repeatability of the samples evaluated by the assessor, which is the within-group variance. A lower MSE value correlates to a better repeatability of the individual assessor (Tomic et al., 2009), different color lines represent different sensory attributes, and the results showed that the MSE values of the ten assessors for the attributes of sweet, sour, and retronasal Muscat, were all less than 2, which means that the ten assessors had a good repeatability.

The scores of each sample on each attribute were calculated, and the score chart of sensory attributes was plotted (Fig. 3B). The 14 juice samples showed significant differences in the three sensory attributes. The intensity of the retronasal Muscat flavor attribute ranged from 7.08 to 11.39 points; the intensity of the Muscat flavor of R31 was significantly higher than those of the other samples, while that of R192 was significantly lower than those of the other samples. For the sweet attribute, the intensity of sweet of the 14 grape juices ranged from 6.10 to 10.32 points; the sweet of mixC was significantly higher than those of the other samples, while the sweet of R192 was significantly lower than those of the other samples. In terms of the intensity of the sour attribute, the sour intensity of the 14 grape juices ranged from 2.20 to 6.95 points; the sour of R192 was significantly higher than those of the other samples, while the sour of mixC was significantly lower than those of the other samples. According to the results of the analysis, among the 14 grape juices in the same cross group, the intensity of the Muscat flavor varied significantly, with grape samples with stronger Muscat flavor usually having weaker sour and stronger sweet, and grape samples with stronger sour having weaker Muscat flavor and sweet.

3.4. Fitted curve of the retronasal odor thresholds and analysis of the odor activity values (OAVs) and DoT values

3.4.1. Analysis of the retronasal odor

To assess the flavor contribution of monoterpenoid compounds in samples, the retronasal odor, also known as the flavor threshold value (FTV), of the key Muscat flavor compounds of geraniol, citronellol and nerol was determined in an aqueous solution. To improve the accuracy of the calculated results, an S-curve was used to fit the obtained data, and the retronasal odors of geraniol (Fig. 4A), citronella (Fig. 4B), and nerol (Fig. 4C) in an aqueous solution (Table S6) were 4.5 μg/L, 5.4 μg/L, and 35.9 μg/L, respectively. Plotto et al. (2004) found that the odor threshold value (OTV) of aroma compounds was usually higher than those of the retronasal odor. In this study, the OTVs of geraniol, citronellol and nerol in an aqueous solution were 40 μg/L, 40 μg/L and 300 μg/L, respectively (Fenol et al., 2009), which were all higher than the retronasal odor and consistent with other reported studies.

The retronasal odor of other monoterpenoid compounds in aqueous solutions has been determined previously. For example, Buettner and

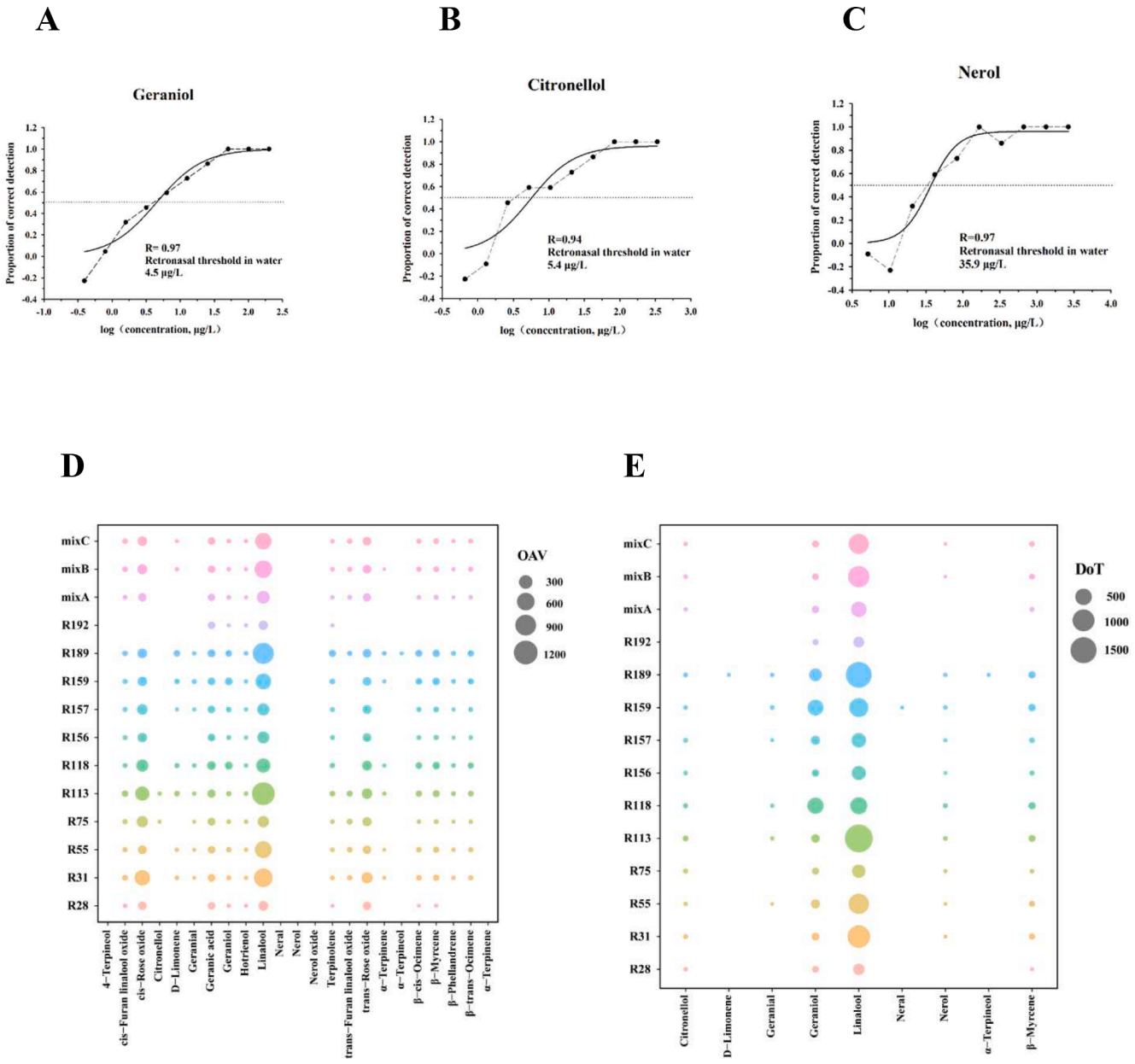

Fig. 4. Evaluation of the flavor contribution of the monoterpenoids in the samples. (A) Detection probability of geraniol in an aqueous solution. (B) Detection probability of citronellol in an aqueous solution. (C) Detection probability of nerol in an aqueous solution. (D) Bubble plots based on OAVs of the monoterpenoids in the grape juice samples. (E) Bubble plots based on DoTs of the monoterpenoids in the grape juice samples.

Schieberle (2001) determined that the retronasal odor of (R)-limonene in aqueous solution was 34 μg/L. Ahmed et al. (1978) determined retronasal odors of 1014 μg/L for α-pinene, 42 μg/L for myrcene, 210 μg/L for limonene, 300 μg/L for α-terpineol, 3.8 μg/L for linalool, and 41.4 μg/L for citral (isomer mixture) in an aqueous solution. The results of this study can provide a supplement for the retronasal odor of monoterpenoids in an aqueous solution.

3.4.2. *Analysis of the OAV and DoT values*

The OAV is the ratio of the concentration of the aroma substance to its odor threshold value, and the DoT is the ratio of the concentration of the aroma substance to its retronasal odor (Wang et al., 2021a). The aroma activity and flavor contribution of the monoterpenoids in the samples were evaluated by calculating the OAV values and DoT factors (Table S7) for the 26 monoterpenoids in all samples. The OAV values for *(E,Z)-allo*-ocimene, *allo*-ocimene, and linalool oxide pyranoside could not be calculated because the odor threshold value was not found. The DoT factor was calculated for *β*-myrcene, D-limonene, linalool, neral, *α*-terpineol, geranial, citronellol, nerol, and geraniol; however, it could not be calculated for the other compounds because their retronasal odors could not be found.

The results of the analysis of OAV values showed that linalool has a high OAV value; the highest OAV value of 1111.28 was in the R113 sample, and high OAV values of over 500 were in the R189, R31, mixB, R55, and mixC samples. The *cis*-rose oxide and *trans*-rose oxide also showed higher OAV values in the samples. The *cis*-rose oxide had the highest OAV values in the three samples of R31, R113, and R118, which were all greater than 200, and high OAV values in the samples of R75, R157, mixB, mixC, R189, R156, and R159, which were all greater than 100. The *trans*-rose oxide had the highest OAV values in the R31, R113, and R118 samples, which were all greater than 100 (Fig. 4D).

From the analysis of the DoT factor results, both linalool and geraniol showed higher DoT factors in the samples. Linalool had the highest DoT factors in the three samples of R113, R189, and R31, which were all

higher than 1000. The DoT factors were also higher in the five samples of mixB, R55, mixC, R159, and R118, which were all greater than 500. Geraniol had the highest DoT factor of over 200 in the three samples of R118, R159 and R189 (Fig. 4E).

According to the results of retronasal odor, OAV values and DoT factor analysis, linalool, *cis*-rose oxide, *trans*-rose oxide, and geraniol were found to be the important compounds contributing to the table grape flavor.

3.5. Analysis of the concentration-intensity relationships of the Muscat compounds

According to the modified Stevens law (Chen et al., 2021), $S = k(I/I0)^n$, it can be obtained that there is a power exponential relationship between the perceived intensity of a compound and the concentration threshold ratio, and n denotes the Stevens coefficient of a compound, the higher the value of n, the more sensitive is the perception of the compound. To investigate the relationship between the concentration of Muscat flavor compounds and flavor sensitivity, the Muscat reference scale was used to determine the flavor intensity of the Muscat flavor compounds, such as geraniol, citronellol, nerol, and linalool at different concentrations, and calculated the Stevens coefficient. The natural logarithm of the concentration of the target compound was used as the x-axis, and the natural logarithm of the flavor intensity of the compound was used as the y-axis to plot the concentration-intensity relationship diagram (Fig. 5A). The DoT factor of the compound was used as the x-axis, and the flavor intensity value was used as the y-axis to plot the DoT-intensity relationship diagram of the compound (Fig. 5B). These relationships were plotted to determine the relationship between concentration or DoT factor and flavor intensity in Muscat flavor compounds.

According to the analysis results, the Stevens coefficient for geraniol was 0.2577, which was close to the standard Stevens coefficient of 0.26 reported by Patte et al. (1975) for geraniol. The Stevens coefficient of citronellol was 0.4581, the Stevens coefficient of nerol was 0.4029, and the Stevens coefficient of linalool was 0.1676. By comparing the results of the four compounds, the intensity of the Muscat flavor of the Muscat compounds varied at the same concentration level, and the Stevens coefficients of the four compounds in the order from high to low was as follows: citronellol > nerol > geraniol > linalool. The flavor perception of citronellol was the most sensitive to changes in concentration, while that of linalool was the least sensitive to changes in concentration. These results quantify the contribution of geraniol, citronellol, nerol, and linalool to the Muscat flavor.

3.6. Development of a regression model between the Muscat and monoterpenoids and an assessment of the predictive ability

The current research on table grapes primarily focuses on cultivation treatments, taste variation, and metabolomic analysis of flavor components, while studies on predicting the intensity of flavor in table grapes through mathematical modeling are less common (Zhou et al., 2022; Maoz et al., 2020; Wu et al., 2019). To predict the intensity of Muscat flavor in the table grapes via mathematical modeling, this study conducted mathematical modeling based on the data from 11 single grape juices samples, including R28, R31, R55, R75, R113, R118, R156, R157, R159, R189, and R192. Three blended grape juice samples were utilized to validate the predictive performance of the models. Regression analysis can accurately measure the degree of correlation between factors and the extent of regression fit to improve prediction. Stepwise regression analysis is often used to establish optimal or appropriate regression models that allow for a more in-depth study of the dependencies between variables. Partial least squares regression analysis is a prediction-oriented statistical analysis method that can be used to accurately predict the response variable that may result from a given explanatory variable, and has great advantages in terms of better model performance and prediction accuracy. Two models were used to develop the regression models between the Muscat flavor and the aroma components and to evaluate the prediction ability of the models under different data transformations. The data of mixA, mixB and mixC were substituted into the obtained model equations to obtain the predicted values of the Muscat flavor intensity compared with the actual values, and the paired *t* test p value and Pearson correlation coefficient between the predictive value and the actual value were calculated to verify the predictive effect of the model.

For the 9 monoterpenoid compounds that could calculate the DoT factors, stepwise regression modeling was performed with Muscat flavor intensity using three different data transformations. In the first model, the DoT factors of the compounds were used as X variables and the intensity of Muscat flavor as Y variables. In the second model, the natural logarithm of the DoT factors of the compounds were used as X variables and the intensity of Muscat flavor as Y variables. In the third model, the natural logarithm of the DoT factors of the compounds were used as X variables and the natural logarithm of the intensity of Muscat flavor as Y variables. The parameters and validation results of the obtained stepwise regression models are shown in Table S8. It was found that all three models showed relatively poor prediction performance.

Partial least squares regression (PLSR) modeling was performed between the quantified results of terpenoid compounds and Muscat flavor intensity using six different data transformations. In the first model, the concentrations of all monoterpenoids were used as X variables and the intensity of Muscat flavor as Y variables. In the second model, the DoT factors of 9 compounds were used as X variables and the intensity of Muscat flavor as Y variables. In the third model, the natural logarithm of the DoT factors of 9 compounds were used as X variables and the intensity of Muscat flavor as Y variables. In the fourth model, the natural logarithm of the DoT factors of 9 compounds were used as X variables and the natural logarithm of the intensity of Muscat flavor as Y variables. In the fifth model, the natural logarithm of the concentrations of all monoterpenoids were used as X variables and the intensity of Muscat flavor as Y variables. In the sixth model, the natural logarithm of the concentrations of all monoterpenoids were used as X variables and the natural logarithm of the intensity of Muscat flavor as Y variables. The parameters and validation results of the PLSR models are shown in Table S9. It was found that the fourth and sixth models showed better prediction performance.

After comparing the quality parameters and the predictive ability of the model, the natural logarithm of the concentration of the compound was selected as the X variable, and the natural logarithm of the intensity of Muscat flavor was selected as the Y variable to establish a PLSR model as the optimal model for predicting the Muscat flavor of the table grapes. The model covered all the monoterpenoids that were quantified in the grape juice, and a linear relationship was found between the natural logarithm of the intensity of the Muscat flavor and the natural logarithm of the concentration of the aroma components. The regression model equation is shown as follows:

$$\ln(I_{Muscat}) = 2.782 + 0.008 \times \ln(C_{\beta\text{-myrcene}}) + 0.002 \times \ln(C_{\alpha\text{-terpinene}}) + 0.001 \times \ln(C_{\text{D-limonene}}) + 0.009 \times \ln(C_{\beta\text{-phellandrene}}) + 0.007 \times \ln(C_{\beta\text{-}trans\text{-ocimene}}) + 0.001 \times \ln(C_{\gamma\text{-terpinene}}) + 0.006 \times \ln(C_{\beta\text{-}cis\text{-ocimene}})\text{-}0.01 \times \ln(C_{\text{terpinolene}}) + 0.06 \times \ln(C_{cis\text{-rose oxide}}) + 0.06 \times \ln(C_{trans\text{-rose oxide}}) + 0.008 \times \ln(C_{(E,Z)\text{-allo-ocimene}}) + 0.012 \times \ln(C_{allo\text{-ocimene}}) + 0.005 \times \ln(C_{cis\text{-furan linalool oxide}})\text{-}0.001 \times \ln(C_{trans\text{-furan linalool oxide}}) + 0.002 \times \ln(C_{\text{nerol oxide}}) + 0.006 \times \ln(C_{\text{linalool}})\text{-}0.123 \times \ln(C_{\text{4-terpineol}})\ 0.097 \times \ln(C_{\text{hotrienol}}) + 0.005 \times \ln(C_{\text{neral}})\text{-}0.019 \times \ln(C_{\alpha\text{-terpineol}}) + 0.013 \times (\ln C_{\text{geranial}}) + 0.005 \times \ln(C_{\text{linalool oxide pyranoside}}) + 0.005 \times \ln(C_{\text{citronellol}}) + 0.007 \times \ln(C_{\text{nerol}}) + 0.005 \times \ln(C_{\text{geraniol}})\text{-}0.006 \times \ln(C_{\text{geranic acid}}).$$

Studies by Stevens (1957) and Chen et al. (2021) showed a linear relationship between the natural logarithm of perceived intensity and the natural logarithm of physical stimulus concentration, which was consistent with the findings of the optimal model obtained in our study.

PLSR analysis was performed for the optimal model (Fig. 6), and the standard regression coefficients for each terpenoid compound in the

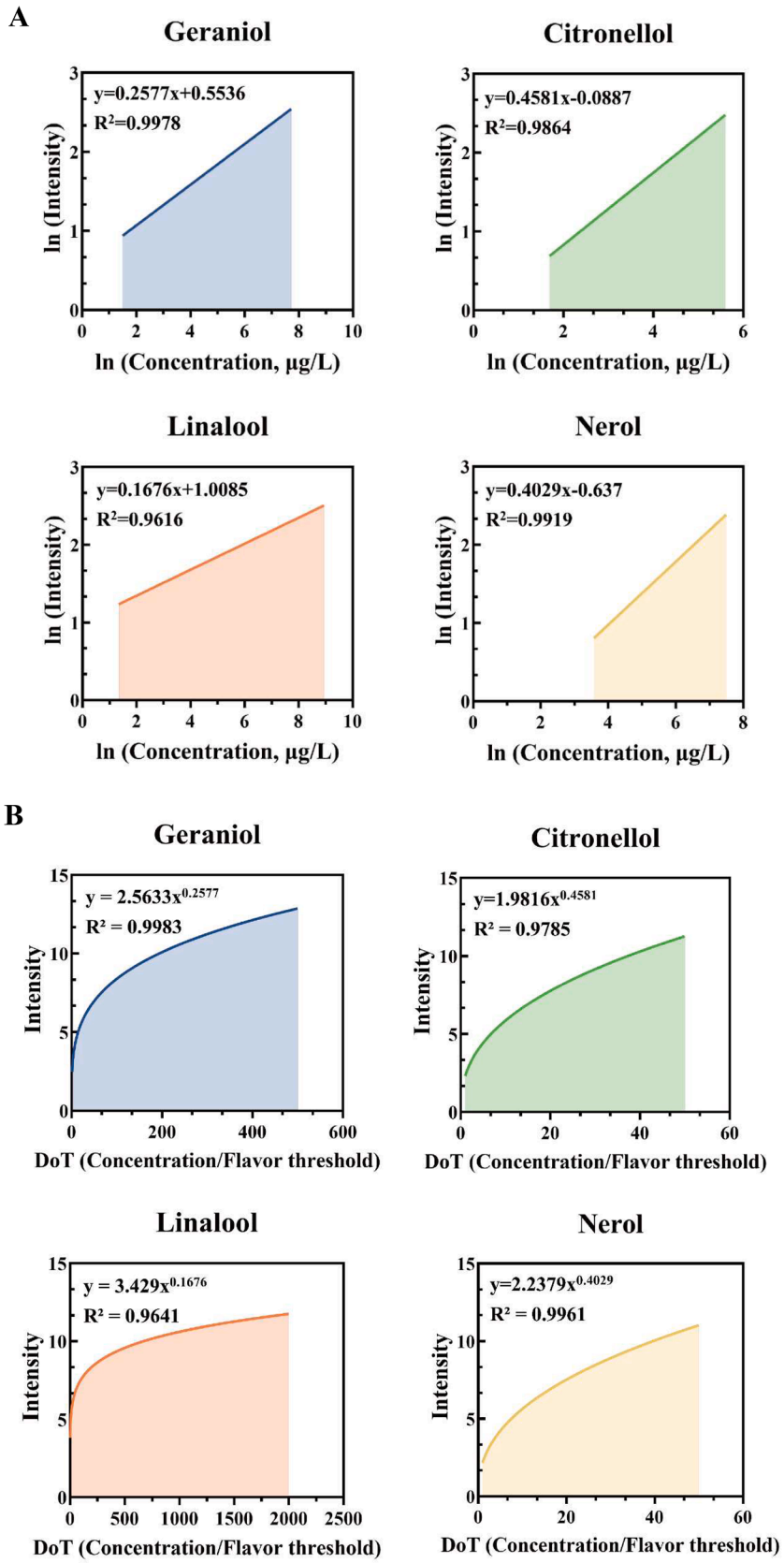

Fig. 5. The relationship between the concentration of the Muscat compounds and flavor intensity. (A) Concentration-intensity relationship diagram of geraniol, citronellol, nerol and linalool in an aqueous solution. (B) DoT-intensity relationship diagram of geraniol, citronellol, nerol and linalool in an aqueous solution.

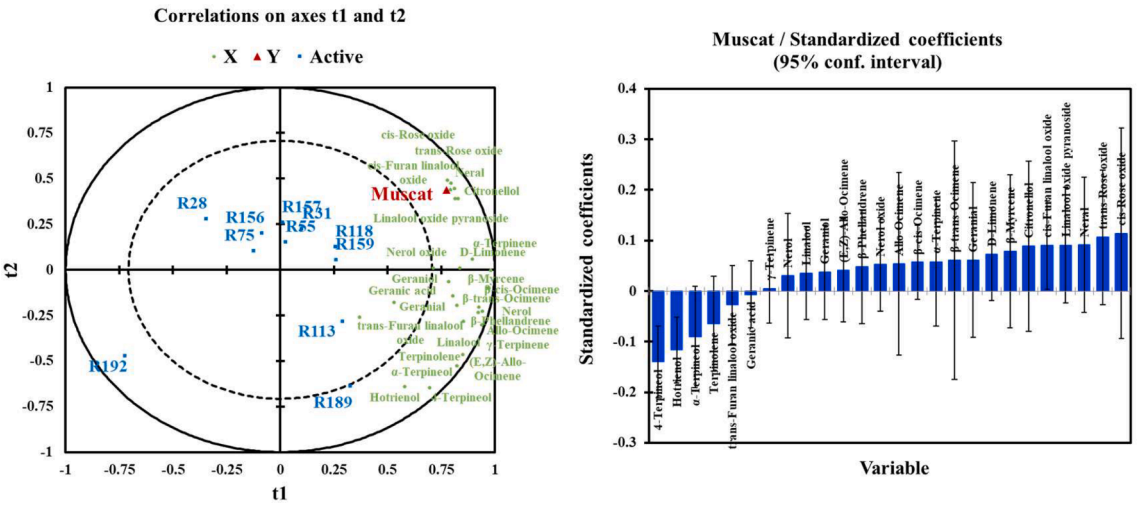

Fig. 6. Optimal PLSR model between the content of the monoterpenoids and the intensity of the Muscat for the different grape juice samples.

model are listed in Table S10. The model contained 26 monoterpenoids, and there were 20 monoterpenoids positively and 6 monoterpenoids negatively correlated with the Muscat flavor. The five Muscat compounds of citronellol, nerol, geraniol, linalool, and *cis*-rose oxide showed a positive correlation with Muscat flavor.

4. Conclusions

In this study, flavor sensoryomics was carried out to analyze the mechanism of aroma formation in the retronasal muscat flavor of table grapes. Firstly, by investigating whether saliva processing affects the content of terpenoids, it was clarified that the retronasal Muscat flavor perceived in the mouth was mainly caused by free monoterpenoids rather than glycoside-bound monoterpenoids. Among them, linalool, *cis*-rose oxide, *trans*-rose oxide, and geraniol were important compounds contributing to the Muscat flavor of 14 table grape juices from different lines of the same hybrid population. Retronasal odor and Steven's coefficient analyses quantified the contribution of Muscat compounds to the retronasal Muscat flavor, and provide a supplement for the retronasal odor of monoterpenoids in an aqueous solution. Results indicated that citronellol had the highest concentration sensitivity and linalool had the lowest sensitivity; with the contribution of linalool to the retronasal Muscat flavor depended on the concentration level of the monoterpenoids in the grape samples and showed a strong positive correlation with the Muscat flavor at higher monoterpenoids concentration. The optimal PLSR model for predicting the intensity of Muscat from monoterpenoid concentration was obtained by comparing the model quality and predictive ability of two mathematical models, stepwise regression and partial least squares regression, under different data transformations. A reference scale was established for the assessment of retronasal Muscat flavor in this study, and it could be used to scientifically quantify the intensity of the Muscat flavor of table grapes. These results provide a reference for analyzing the formation mechanism of other specific flavor in future studies. The results of this study provide a basis for grape breeders to select high-quality Muscat flavor table grape varieties and improve the grape flavor.

Ethical Statement.

The experimental samples were meet national food safety standards and are not hazardous to human health. This study was approved by the Ethics Committee of the College of Humanities and Social Sciences of Beijing Forestry University.

CRediT authorship contribution statement

Xiaomiao Zhou: Conceptualization, Formal analysis, Investigation, Methodology, Writing – original draft. **Bingqi Shan:** Data curation, Investigation, Validation. **Songyu Liu:** Data curation, Formal analysis. **Wenping Gao:** Data curation, Validation. **Xiaoyue Wang:** Project administration, Writing – review & editing. **Huiling Wang:** Project administration, Resources. **Haiying Xu:** Project administration, Resources. **Lei Sun:** Funding acquisition, Project administration, Resources, Writing – review & editing. **Baoqing Zhu:** Conceptualization, Project administration, Supervision, Writing – review & editing.

Declaration of competing 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.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.fochx.2024.101198.

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