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Comprehensive comparison of flavor and metabolomic profiles in kiwi wine fermented by kiwifruit flesh with different colors

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ABSTRACT

The objective of the study was to comprehensively assess flavor and metabolomic disparities in the aroma and taste profiles of kiwi wine (KW) derived from kiwifruits with green (Hayward), red (Donghong), and yellow (Jinshi) flesh. The findings revealed that Hayward wine exhibited the most "floral, fruity and pleasant" aromas, while Donghong wine demonstrated the most "sweet, fullness and balanced" tastes. In KW, a total of 106 compounds were characterized using a flavor-directed research strategy and metabolomics. PCA and PLS-DA effectively differentiated the three types of KW based on their aroma and taste characteristics. Ten volatile compounds (ethyl isovalerate, ethyl hexanoate, isoamyl acetate-D, acetone, hexyl acetate-M, hexyl acetate-D, ethyl isobutyrate, 2-butylfuran, 2-pentylfuran and 2-methylbutanal) and ten non-volatile compounds (malate, lactate, hydroxyacetone, pyroglutamate, succinate, 2-oxoglutarate, galactarate, acetoin, pyruvate and proline) were identified through multivariate analysis as key discriminators of flavor and metabolomic differences among the three types of KW. Furthermore, several metabolic pathways were investigated to distinguish the KW fermented with the three flesh-colored kiwifruits, mainly pertaining to glycerolipid, amino acid, sucrose, butanoate and pyruvate metabolism. This study could offer valuable insights into the effect of flesh colors on the flavor and metabolomic characteristics of KW.

1. Introduction

A constant growth in the adoption of health-conscious habits brought in recent years a notable surge in consumer's interest towards leisure beverages associated with beneficial properties (Chen et al., 2019). Kiwi wine (KW), a low-alcohol beverage fermented from kiwifruit, is renowned for its distinct flavor profiles, rendering it a favored choice among consumers (Zhou et al., 2023). This appeal stems from the rich nutritional composition of kiwifruit, encompassing dietary fiber, vitamin C, and phenols, along with its prebiotic properties, which confer anti-inflammatory, blood pressure-lowering, and immune-boosting benefits (Pinto et al., 2020). Furthermore, KW, in contrast to other processed kiwifruit derivatives (such as dried fruit and jam), not only retains a wide portion of the nutritional constituents inherent to kiwifruit but also enriches its flavor profile (Ma et al., 2019).

The pivotal factor influencing KW's quality is represented by the color of the flesh, that can be green, yellow or red. The color, in fact, depends on the variety, so that divergent colors are associated with marked differences in nutritional composition and flavor profiles. In detail, comparative studies indicated that yellow-fleshed and red-fleshed kiwifruit exhibit elevated levels of nutrients, such as vitamin C, polyphenols, and minerals, accompanied by superior antioxidant properties, compared to green-fleshed kiwifruit (Yuan, Chi, et al., 2023). Furthermore, while green-fleshed kiwifruit is highly acid (Richardson et al., 2018), yellow-fleshed kiwifruit presents tropical fruits notes (Singletary, 2012), and red-fleshed kiwifruit have a sweet flavor profile, given by the elevated sugar-to-acid ratio, accentuated by aroma compounds such as 1-pentanol (Yuan, Chi, et al., 2023). Regrettably, while

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KW from the three kinds of kiwifruits have been compared focusing on physicochemical properties, nutritional attributes, and aroma profiles, a limited attention has been paid to flavor, on one side, and to the overall metabolome's profile (Wen et al., 2023; Zhou et al., 2023).

As a blend of aroma and taste, flavor serves as a pivotal evaluative metric for assessing wine quality, predominantly determined by volatile and non-volatile compounds (Chen, Wang, et al., 2023). Gas chromatography-ion mobility spectrometry (GC-IMS) is an emerging analytical technique that has gained widespread application because it does not require sample's pre-treatment and it has low limits of detection (Wang et al., 2020). An example of its successful applications to KW can be traced in the work by Wen et al. who identified 14 volatile compounds, such as butyl acetate and ethyl butyrate, that allowed distinguishing KW fermented from whole pulp and clear juice (Wen et al., 2024). Metabolomics serves as an effective tool for characterizing the overall non-volatile metabolites of fermented foods, offering novel insights into the variations in metabolic activity linked to different treatments (Chen, Wang, et al., 2023). Among the prominent platforms for metabolomic investigation, proton nuclear magnetic resonance spectroscopy (^{1}H NMR) has demonstrated potential in capturing quantitative information on non-volatile compounds in KW, owing to its easy sample preparation and high reproducibility features (Zhang et al., 2023). Besides, several designed softwares (such as Chenomx, Chenomx inc., Edmonton, Canada) could enable the users to automatically match the studied spectra with those of pure compounds in the library, thereby enhancing the number of compounds identified and quantified by ^{1}H NMR. E-tongue, an artificial sensory technology mimicking human taste mechanisms, comprises a series of chemical sensors that effectively portray the overall taste profiles of samples (Yuan, Chi, et al., 2023). Combined with sensory evaluations, these techniques could not only give key pieces of information about the overall acceptability of a food from subjective and objective points of view, but they can also provide valuable insights into the metabolic mechanisms altered by the different treatments (Ruiz-Capillas et al., 2021; Zhang et al., 2023).

Consequently, this study aimed to provide a comprehensive evaluation of flavor and metabolome's profiles of KW fermented from Hayward (green), Jinshi (yellow) and Donghong (red) fleshed kiwifruit, employing sensory evaluation, E-tongue, GC-IMS and ^{1}H NMR techniques. To identify the key volatile and non-volatile compounds that discriminate the flavor differences among the three types of KW, multivariate statistical analysis (PCA and PLS-DA) combined with ROAV analysis were applied. The present study has the potential to offer valuable insights into the unique flavor profiles and metabolomic characteristics of KW obtained from varieties with different flesh colors. Furthermore, it may shed light on the strategic selection of kiwifruit flesh colors to enhance KW quality.

2. Materials and methods

2.1. Materials and reagents

Three varieties of kiwifruit were utilized, namely Hayward, Donghong, and Jinshi, with flesh colors of green, yellow, and red, respectively. All these kiwifruits were harvested in Qionglai, Sichuan, China (N 30°12′ to 30°33′, E 103°04′ to 103°45'). *S. cerevisiae* strain RW was bought from Angel Yeast Co., LTD (China).

2.2. KW preparation

Kiwifruits were transported to the laboratory right after harvesting. Wines were prepared as schematized in Fig. 1, consistent with our previous study (Zhang et al., 2023). After fermentation, KW samples were filtered through a sterile gauze and subsequently preserved at a temperature of −80 °C for subsequent analysis.

2.3. Sensory evaluation

Quantitative descriptive analysis (QDA) was conducted, as described in previous publications (Cao et al., 2022; Liu, Li, et al., 2022), involving a screening process of a panel consisting of 12 members (comprising 8 females and 4 males, average age of 25 years) with relevant professional backgrounds. Three in-depth discussions (2 h each) were held to determine the descriptions of KW in order to fully and accurately describe the differences among the three groups of KW samples (aroma profile: floral, fruity, sweet, green and pleasant; taste profile: acid, sweet, alcoholic, balanced and fullness). Briefly, approximately 30 mL of

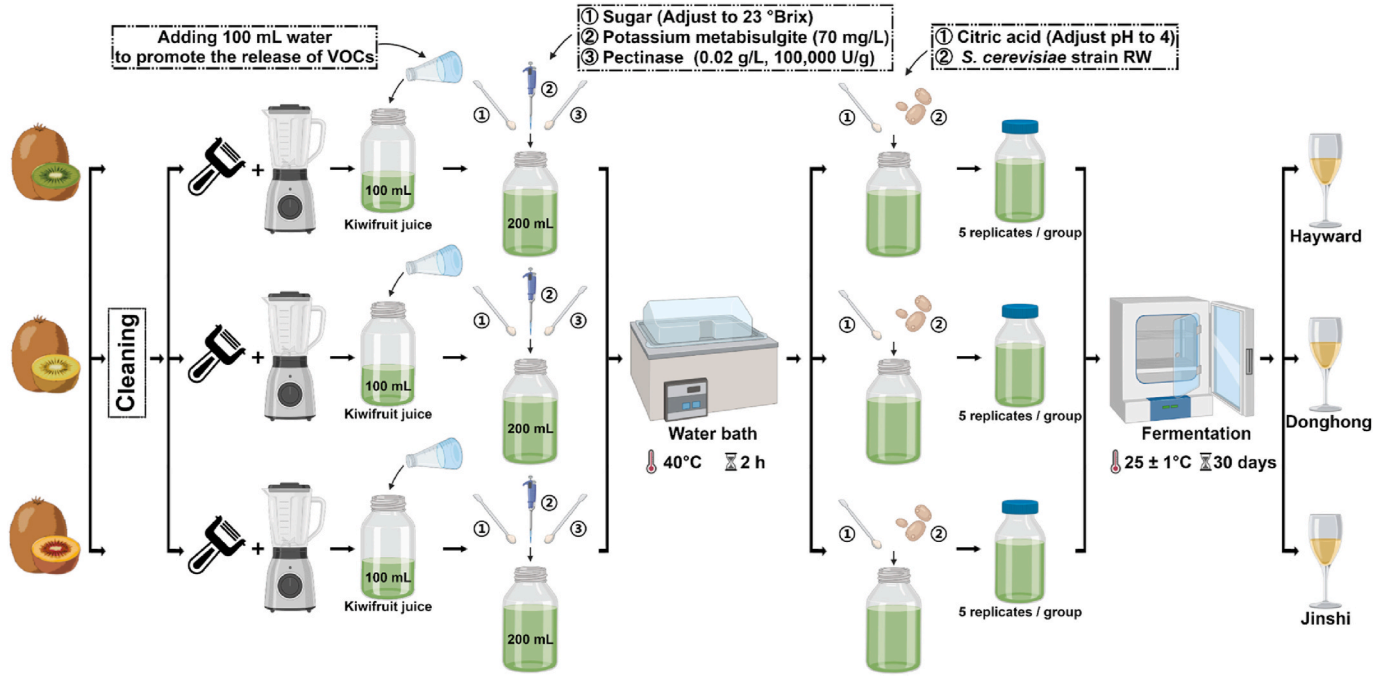

Fig. 1. Graphic design of the workflow for KW preparation.

KW sample were placed in a clear tasting glass, labeled with a random three-digit code, and presented to panelists in a randomized order. Panelists expressed their judgments by quantifying each sensory description on a scale that spanning from 1 to 9, indicating low to high intensity, respectively.

2.4. E-tongue analysis

Following our previous study for E-tongue analysis (Zhang et al., 2023), each KW sample (80 mL) was transferred to a dedicated beaker and analyzed by means of an α-Astree E-tongue (Alpha MOS, France). The E-tongue system is equipped with seven sensors, namely AHS, CTS, NMS, ANS, SCS, PKS and CPS. The performance description of E-tongue sensors is listed in Table S1. The data acquisition time, period, delay and stirring rate for E-tongue were set to 120 s, 1.0 s, 10 s and 60 rpm, respectively. Post to each measurement, sensors were cleaned with deionized water. To get stable data, each KW sample was tested 10 times in parallel, the last five stable measured data were preserved and the mean value of the aforementioned data was taken for further analysis. Five repeated samples were tested for each group.

2.5. GC-IMS analysis

Following our previously reported method (Zhang et al., 2024), volatile compounds in KW samples were characterized via GC-IMS (Flavorspec®, G.A.S. Instruments, Germany). Each KW sample (1.5 mL) was moved into a 20 mL headspace vial and incubated (60 °C) for 10 min. Post to the incubation, a fully automated headspace sampling technique was employed, with injection volume and injection needle temperature set to 100 μL and 85 °C, respectively. The MXT-WAX capillary column (30 m × 0.53 mm × 1 μm) was carried out for the gas chromatography separation process, conducted at a temperature of 60 °C. To achieve the desired separation efficiency, the flow rate of the carrier gas, nitrogen with a purity of 99.999%, was strategically regulated. the initial flow rate of 2 mL/min was increased to 10 mL/min after 5 min, to 15 mL/min after 10 min, to 50 mL/min after 5 min and finally to 100 mL/min after 10 min. GC, effectively integrated with the IMS system, was maintained at a constant temperature (45 °C). Additionally, the IMS drift gas flow rate was configured to 150 L/min to ensure optimal performance.

Based on previous studies, the retention indices (RI) of volatile compounds were calculated utilizing a series of *n*-ketone (ranging from C_4 to C_9) as referential standard compounds. To identify volatile compounds, their RI and drift time were cross-referenced against the established standards within the GC-IMS database. A single measurement was taken for each KW sample and relative quantifications were obtained by relying on the intensity of the corresponding peak from per volatile compound. Finally, a Gallery Plot software provided with GC-IMS instrument was used to generate gallery plots. The relative content of each volatile compound in KW was calculated using peak area normalization, according to the following formula:

$$\text{Relative content}\ (\%) = \frac{M}{N} \times 100$$

In such formula, M and N represent the peak area of an individual volatile compound and whole volatile compounds, respectively.

In agreement with Xu et al. (Xu et al., 2024), the relative odor activity value (ROAV) of each volatile compound present in KW was computed according to the following formula:

$$ROAV_x \approx \frac{C_x}{C_{max}} \times \frac{T_{max}}{T_x} \times 100$$

In such formula, T_X and C_X are the thresholds of the volatile compounds and their respective content, while T_{max} and C_{max} are the thresholds and respective content of the volatile compounds that mainly contribute to the overall aroma.

2.6. ^1H NMR analysis

The preparation of KW samples for ^1H NMR analysis adhered to our previously described protocol (Zhang et al., 2023), as visually depicted in Fig. S1 (a). In brief, to eliminate solid impurities, KW sample (0.5 mL) was centrifuged (18630 g, 4 °C) for 15 min. Next, 0.35 mL of the supernatant was added to equal amount of bi-distilled water and 100 μL of NMR analysis solution, followed by a second centrifugation under the above conditions.

^1H NMR analysis of KW samples was carried out at 298 K using a 600.13 MHz AVANCE III spectrometer (Bruker Wuhan, China), with the key parameters detailed in Fig. S1 (b). In accordance with our previously described approach (Zhang et al., 2023), each spectrum underwent phase adjustment by means of Topspin software (version 4.2). Subsequent spectral processing and compound quantification were carried out using custom R scripts. As depicted in Fig. S1 (c), the baseline of each spectrum was adjusted through peak detection following the removal of the residual water signal, utilizing the "rolling ball" algorithm provided in R. The identification of compound was conducted by comparing their multiplicity and chemical shifts with the reference spectra of standard pure compound available in the Chenomx software (version 8.4). To eliminate the interference caused by variations in protein and water content among the KW samples, probabilistic quotient normalization (PQN) was applied to the entire spectral dataset. The quantification of compound was conducted using 3-(trimethylsilyl)-propionic-2,2,3,3-d_4 acid sodium salt (TSP) as an internal standard. The area of the representative signal for each compound was integrated using rectangular integration.

2.7. Statistical analysis

Data presented in this study are represented as mean ± standard deviation (SD). Statistical analyses were executed utilizing R programming language. Prior to univariate analysis, non-normally distributed data were converted to normal distribution according to Box and Cox (Box & Cox, 1964). Data normalization was performed using PQN. Significant differences in E-tongue sensor responses, volatile and non-volatile compound contents among the three groups were investigated by ANOVA, followed by Tukey HSD test ($p < 0.05$), respectively. The PCA and PLS-DA models were calculated utilizing the MetaboAnalyst 6.0 tool (https://www.metaboanalyst.ca), accessed on March 15, 2024. Network and Mantel tests, along with a correlation analysis, were performed utilizing the OmicStudio platform (https://www.omicstudio.cn/tool., accessed on March 25, 2024). Partial least squares regression (PLSR) analysis was executed utilizing the Unscrambler X 10.4 software, provided by CAMO ASA in Oslo, Norway.

3. Results and discussion

3.1. Sensory evaluation

QDA was conducted to acquire a holistic perspective encompassing the aroma and taste characteristics of KW fermented from kiwifruit with distinct flesh colors, as shown in Fig. 2.

In terms of aroma profile, Hayward showed the highest "floral, fruity and pleasant" aromas, while Donghong presented the highest "green and sweet" aromas. Regarding taste, Donghong showed the highest "sweet, fullness and balanced" notes, while "acid and alcoholic" notes were the lowest. The high sweetness and low acidity of Donghong kiwifruit may be due to its high sugar-to-acid ratio (Yuan, Chi, et al., 2023). Moreover, it is worth noting that a high "sweet" feature could be beneficial for reducing the typical harshness connected to alcohol, therefore yielding to a balanced and full-bodied taste of KW (Li, Jia, et al., 2023).

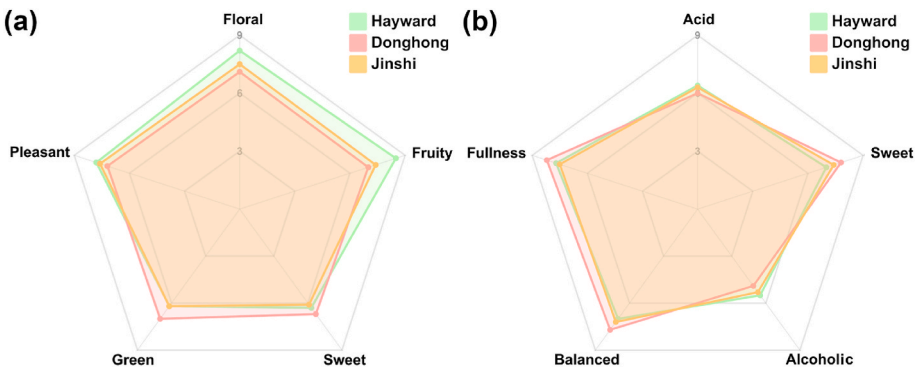

Fig. 2. Radar charts for QDA of KW, indicating aroma profile (a) and taste profile (b).

3.2. GC-IMS analysis

GC-IMS was employed to obtain information on the volatile characteristics of KW, to investigate the aroma profile changes among different groups, as depicted in Fig. 3.

A total of 42 volatile compounds was characterized in the three types of KW samples, including esters (22), alcohols (7), ketones (6), aldehydes (3), furans (3) and others (1), as detailed in Table S2. As shown in Fig. 3(d) and (e), esters constituted the greatest proportion of volatile compounds in all KW samples, succeeded by alcohols, which aligns with previous researches (Qi et al., 2019; Zhang et al., 2023). The contents of ester, alcohols and aldehydes varied among the three types of KW, with Hayward showing the highest contents and Donghong the lowest. In addition, the highest relative content of ketones was found in KW fermented from red-fleshed kiwifruit compared to the others.

In the analysis of volatile compounds using GC-IMS, significant variations in the concentrations of 36 volatile compounds were observed across the three distinct groups.

PCA was conducted to visually discern the main variations in KW fermented from the three types of kiwifruits (Fig. 4 (a)). The primary two principal components collectively accounted for 93.8% of the overall variance observed in the KW samples, thus nicely summarizing the differences among the three groups in terms of aroma profile. Moreover, PLS-DA was used to develop a correlation model between the contents of volatile compounds and groups, as illustrated in Fig. 4(b) and (c). Three types of KW could be effectively differentiated according to component 1 (55.6%) and component 2 (37.7%), with an accumulated variance contribution totaling 93.3%. Besides, the model fit parameters, namely R^2Y, R^2X and Q^2 were 0.941, 1.0 and 0.823, respectively, which indicated a good predictive ability. The VIP score, which represents a weighted summation of the squared PLS-DA loadings, served as a metric to evaluate the contribution of individual variables to the overall classification performance (Zhao et al., 2023). According to Figs. 4 (c), 18 volatile compounds (VIP>1) were identified as mainly contributing to the variations in the aroma profile of KW subjected to the three groups. Furthermore, ROAV analysis was used to select the key volatile compounds by considering their threshold values (Su et al., 2022). Ten substances were identified as key volatile compounds, namely ethyl isovalerate, ethyl hexanoate, isoamyl acetate-D, acetone, hexyl acetate-M, hexyl acetate-D, ethyl isobutyrate, 2-butylfuran, 2-pentylfuran, 2-methylbutanal, as presented in Fig. 4 (d) and (e) and Table S3.

Ethyl hexanoate is a pivotal aroma-active compound, imparting fruity and wine-like aromas (Li, Jia, et al., 2023) and enhancing the perception of sweet aroma in fermented kiwifruit products (Zhao et al., 2021). Among the three types of KW, Donghong exhibited the highest contents of ethyl hexanoate and 2-butylfuran, which partly explain the highest rating in terms of "sweety" in the aroma profile, compared to the other groups. In this respect, 2-butylfuran may play a particularly important role, due to its low perception threshold.

2-Methylbutanal is stemming from the Strecker degradation pathway of isoleucine and is mainly generated during the wine-making process. It could interact synergistically with other aromas to enhance fruity and nutty notes (Li, Jia, et al., 2023). Together with ethyl isovalerate and ethyl isobutyrate, these compounds could exert crucial influence on the ultimate flavor characteristics of wine, with particular reference to fruity aroma, as suggested by previous studies (Chen, Wang, et al., 2023; Kalogiouri et al., 2024; Wen et al., 2023).

Methyl acetate is a signature compound of fruit-aromatic wine. Liu et al. b. found that different cherry varieties had distinct methyl acetate contents, which in turn led to the diverse aroma profiles of cherry wines (Liu, Li, et al., 2022). Hexyl acetate, a key aroma compound in apple and banana, has been previously identified in red wine (Cao et al., 2022). In our study, compared to the other groups, the higher ROAV of hexyl acetate in KW fermented from Hayward indicated its superior fruity aroma, which agreed with our sensory evaluation. Isoamyl acetate, formed by the reaction of isoamyl alcohol and acetate, is one of the esters that contribute significantly to the wine's aroma, imparting a strong fruity aroma (Chen, Wang, et al., 2023). The present study observed that isoamyl acetate contents of KW fermented from Hayward and Jinshi were significantly higher than that of Donghong, suggesting that KW fermented from green and yellow fleshed kiwifruit had stronger fruity aroma.

Produced through Maillard reaction and oxidative breakdown of lipids, 2-Pentylfuran possesses distinctive green and nutty aromas (Li et al., 2022). In line with our study, 2-pentylfuran has been identified as a volatile compound distinguishing wine fermented from different cultivars of muscadine grapes utilizing gas chromatography-mass spectrometry coupled with multivariate statistical analysis (Deng et al., 2021). The difference concentrations of 2-pentylfuran could also be at the base of the "green" aromas of KW fermented from Donghong and Hayward, that resulted superior to that of Jinshi through sensory evaluation.

Acetone exhibits stimulating and solvent-like aromas that could negatively impact the overall aroma profile of wine (Campbell-Sills et al., 2016). This study found that acetone, as a key volatile compound, constituents specifically in KW fermented from Donghong, suggesting that the aroma quality of KW fermented from Donghong might be less desirable compared to that of Hayward and Jinshi.

3.3. E-tongue analysis

E-tongue has the advantages of simplicity, speed and efficiency, compared to traditional sensory evaluation. Equipped with electronic sensors that emulate human taste perception, it could offer an objective assessment of the taste profile of food samples. (Zhao et al., 2023). PCA was performed to gain an overall understanding of the differences in the taste profiles of three types of KW, based on the response values measured by E-tongue sensors.

As depicted in Fig. 5 (a), the first two principal components explained as much as 96.4% of the variability in the KW samples, thus

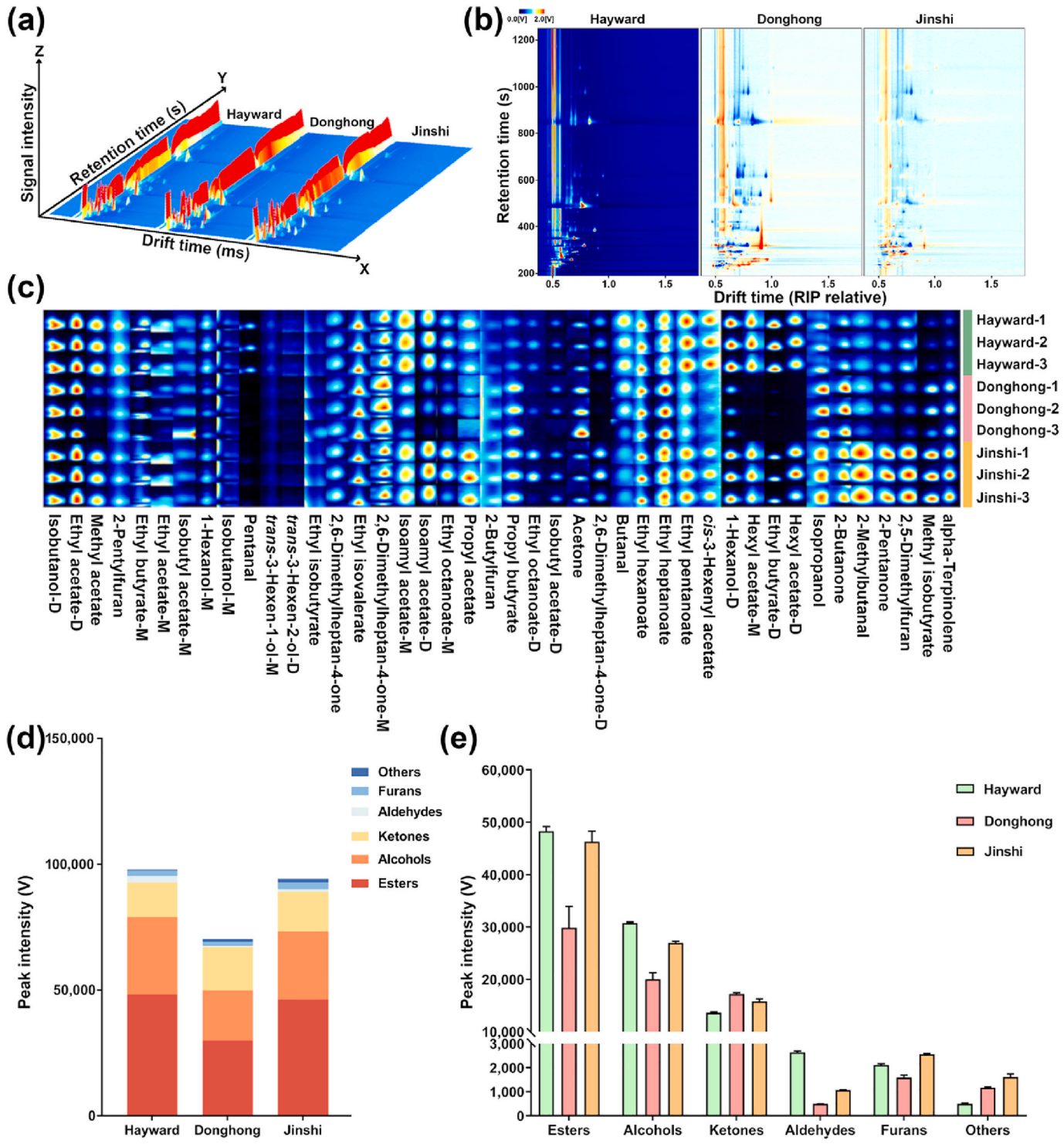

Fig. 3. Volatile compounds observed by GC-IMS, including 3D topographic map (a), 2D difference map (b) and gallery map (c). Peak intensities of total volatile compounds (d) and each category of volatile compounds (e) for the three groups.

effectively summarizing the taste profile differences among the three groups. Fig. 5 (b) shows that the response values of ANS and NMS sensors to KW fermented from Donghong were significantly elevated compared to those of the other groups ($p < 0.05$), which indicates that it exhibited greater intensities of sweetness and umami. Compared to yellow-fleshed and green-fleshed kiwifruit, red-fleshed kiwifruit possessed a higher sugar content, resulting in a sweeter taste generally favored by consumers (Yuan, Chi, et al., 2023). In our study, such findings fitted with the high sweetness of KW fermented from red-fleshed kiwifruit, a further proof of the advantages of red-fleshed kiwifruit as raw material for winemaking.

3.4. ^{1}H NMR analysis

Utilizing ^{1}H NMR spectroscopy, a comprehensive characterization of 64 non-volatile compounds was achieved in KW, mainly pertaining to the classes of organic acids (21), amino acids (18), carbohydrates (6), alcohols (5) and others (14), as shown in Table S4.

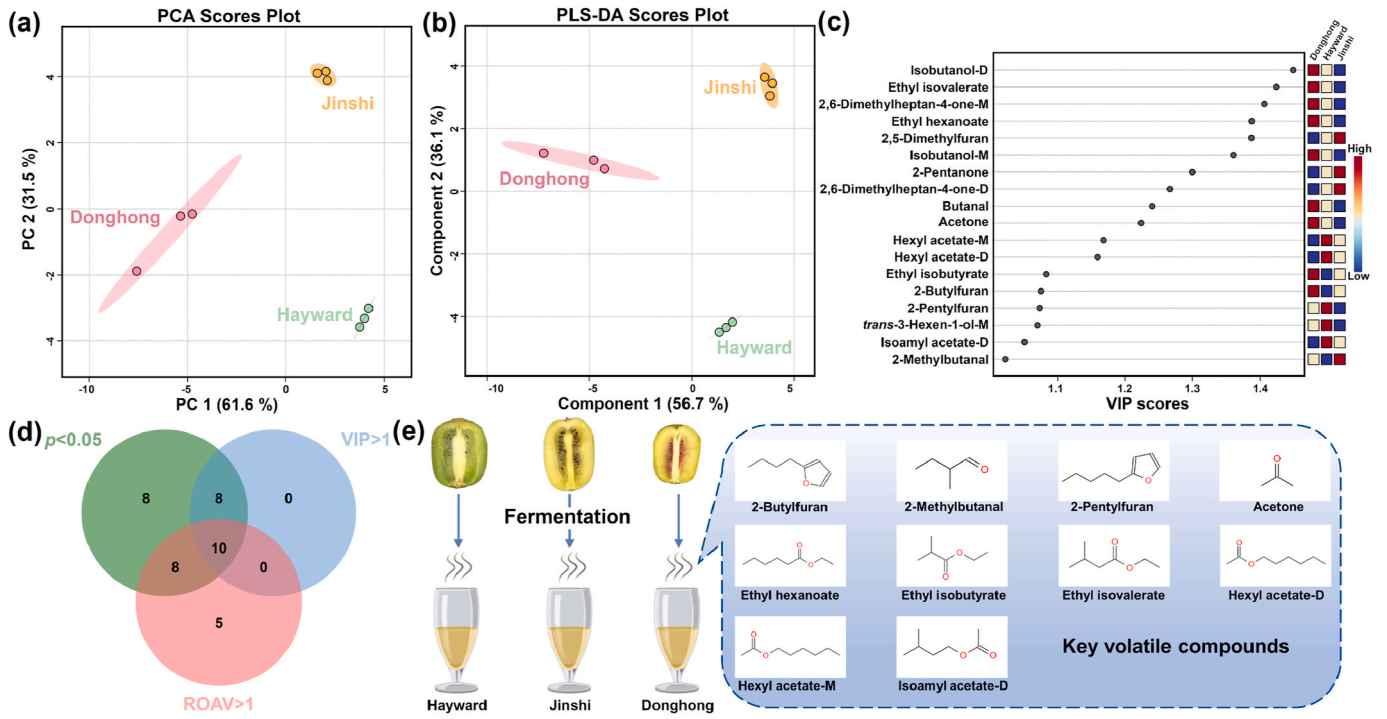

Fig. 4. PCA scores plot (a) PLS-DA scores plot (b) and variable importance projection (VIP) scores of the volatile compounds in KW sample (c). Venn plot of *p*-value, ROAV, and VIP values of the volatile compounds among three groups of KW (d). Key volatile compounds for KW (e).

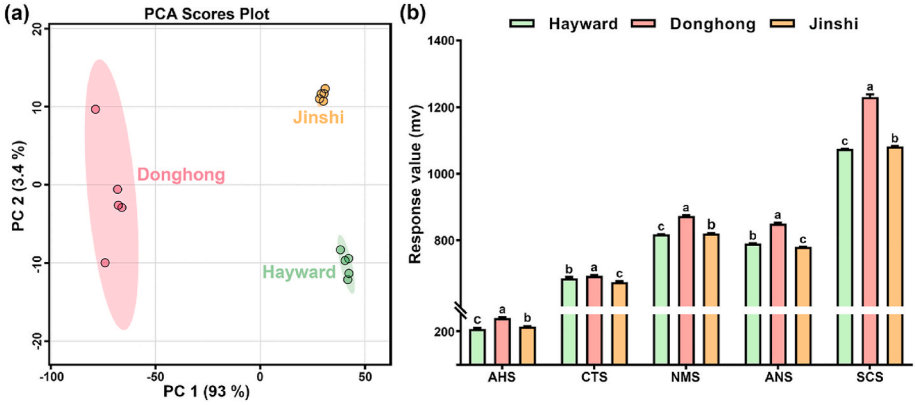

Fig. 5. Overall taste profile of KW fermented from kiwifruit with distinct flesh colors. PCA scores plot of response values for all sensors (a) and response values for specific taste sensors (b). Different lowercase letters indicate statistically significant variations among groups ($p < 0.05$). (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

As shown in Fig. 6 (a), in all KW samples, alcohols accounted for the highest concentration of non-volatile compounds, followed by organic acids. The concentrations of alcohols, carbohydrates and organic acids varied among the three types of KW, with Hayward being the highest. In addition, higher concentration of amino acids was found in Donghong compared to the others.

Among all the non-volatile compounds quantified by ^{1}H NMR, the concentrations of 61 non-volatile compounds showed significant differences. Similar to the above issue, PCA and PLS-DA were carried out on the basis of these differential non-volatile compounds' concentrations, respectively. Overall, Hayward, Donghong and Jinshi formed separate clusters reflecting different taste profile among the three groups, as depicted in Fig. 6(b) and (c). A total of 10 key non-volatile compounds ($p < 0.05$ and VIP>1) were identified that contributed to the differences in taste profile among KW samples, namely malate, lactate, hydroxyacetone, pyroglutamate, succinate, 2-oxoglutarate, galactarate, acetoin, pyruvate and proline, as evidenced in Fig. 6 (d). Fig. 6 (e) and (f) offer a visual representation of the variations in the aforementioned key non-volatile compounds' concentrations, along with the correlations between the response outputs of the E-tongue sensors and the concentrations of the key non-volatile compounds in KW, respectively. Besides, Fig. S2 shows five key pathways that distinguish the KW fermented from three flesh-colored kiwifruits, namely alanine, aspartate and glutamate metabolism, glycerolipid metabolism, starch and sucrose metabolism, butanoate metabolism and pyruvate metabolism.

During wine production, low levels of nitrogen compounds, key components of the juice, can increase the risk of slow or stagnant fermentation of the juice (Heit et al., 2018). Amino acids, as the primary nitrogen source that can be utilized by yeast, are influenced by the type of raw material and fermentation process (Yang et al., 2019). Moreover, amino acids play a pivotal role in shaping the sweet, sour, and bitter tastes of wine, while also can interact with sugars, organic acids and

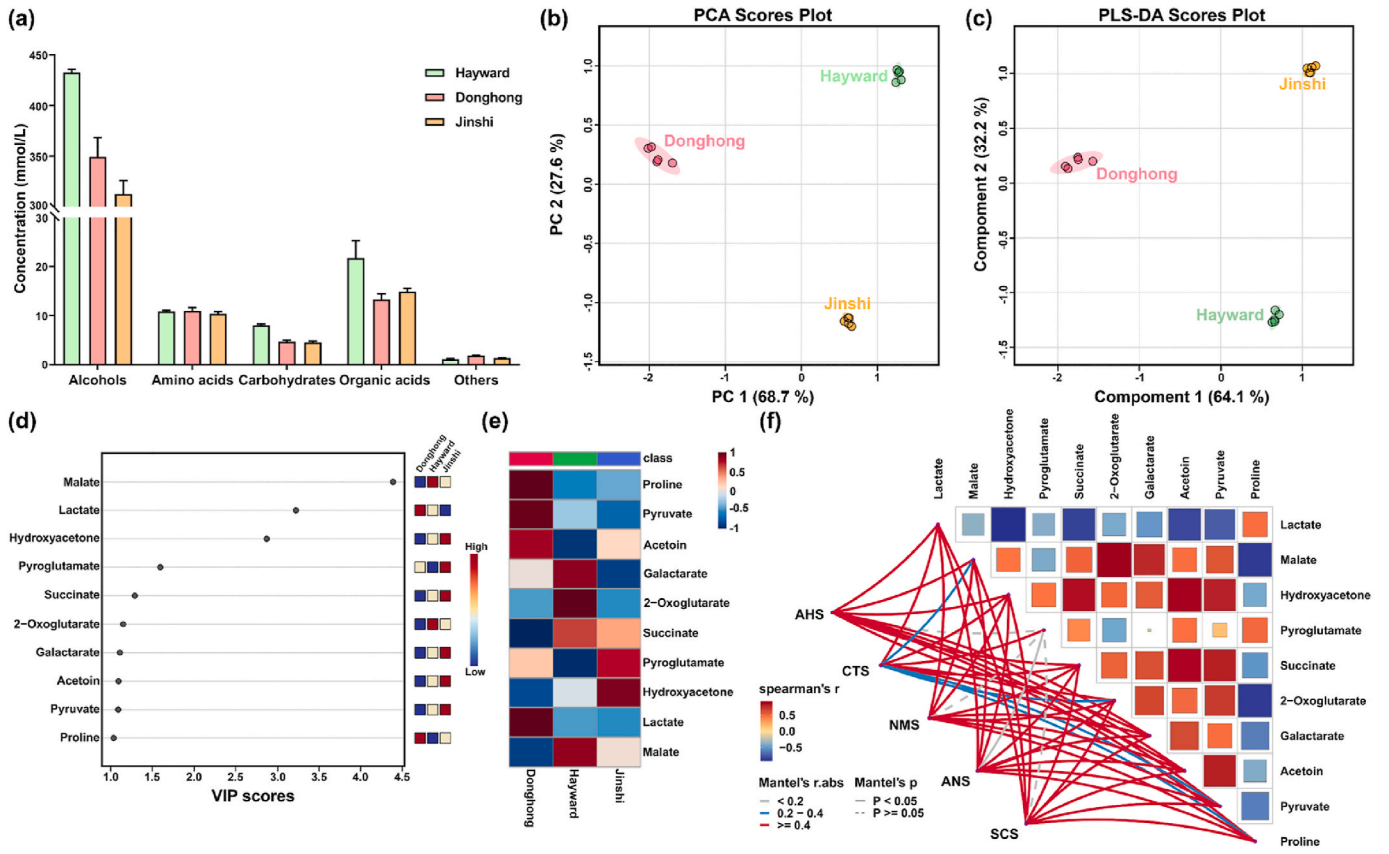

Fig. 6. Concentrations of each category of non-volatile compounds among the three groups (a). PCA scores plot (b), PLS-DA scores plot (c) and VIP scores (d) of the non-volatile compounds in KW samples. Heatmap of key non-volatile compounds (e). Correlations between response values of E-tongue sensors and key non-volatile compounds through Mantel test (f).

ethanol to give unique taste profiles (Zhang et al., 2018). In our study, variations in amino acid concentrations were observed among the three types of KW, with Donghong being the highest and Jinshi the lowest. This variance is likely to affect the fermentation rate of the yeast, ultimately leading to KW with distinct taste profiles. In the present study, the concentrations of 16 amino acids exhibited significant disparities among the distinct types of KW (Table S4). It is worth to note that several studies have successfully distinguished different types of wines from amino acids' levels (Tian et al., 2021; Yang et al., 2019). Therefore, amino acids occupy a pivotal position in investigating the taste profile differences for various types of KW. During the process of alcoholic fermentation, proline cannot be consumed by the yeasts, but it contributes to the conversion of amino acids and has a great impact in the perception of sweetness of wine (Cataldi & Nardiello, 2003; Tzachristas et al., 2021). It is reported that its high concentration is beneficial for the balance of the red wine taste, which could be linked to grape variety used for wine-making (Hu et al., 2020; Lee et al., 2009). In the current study, proline emerged as a key non-volatile compound in KW and its concentration was highest in Donghong, suggesting that KW fermented from red-flesh kiwifruit has a sweeter and more balanced taste. Besides, we found a correlation between proline concentration and the response value of the sweet taste sensor (ANS), in agreement with our previous study (Zhang et al., 2023). Pyroglutamate could diminish the notes of freshness and could bring bitterness to food (Aiello et al., 2023). Moreover, our study observed that a correlated correlation between the pyroglutamate level and the E-tongue sensor more sensitive to bitter taste (SCS). From this point of view the wine obtained from Jinshi showed the most unfavorable profile.

Organic acids, an indispensable class of compounds presented in wine, originating either inherently from the fruit or are generated by yeast during the winemaking process, resulting from the metabolism involving fatty acids and the tricarboxylic acid (TCA) cycle. They could greatly influence the sensory characteristics of wine, especially for the taste profile (Lima et al., 2022; Swiegers & Pretorius, 2005). Malate, mainly derived from fruits, contributes negatively to fruit's perceived quality, in turn imparting a sour taste to fruit wine (Reshef et al., 2022). Girelli et al. found by ^{1}H NMR that malate concentration was significantly different between the wine fermented from two varieties of pomegranates (Girelli et al., 2023).

During the yeast metabolism in wine fermentation, a part of malate is converted into lactate and succinate (Jin et al., 2021). Lactate confers elegance and roundness of tastes to wine. Hu et al. discovered that Cabernet Sauvignon wine possessed a notably higher lactate content compared to other types of wine, which in turn gave them a smooth taste (Hu et al., 2020). Besides, the reduced concentration of succinate could also soften the wine's taste. In this study, compared to the other groups, Donghong showed higher lactate levels and lower malate and succinate levels, suggesting that KW fermented from red-fleshed kiwifruit may have a more desirable and softer tastes, consistently with previous studies (Hu et al., 2020). 2-Oxoglutarate, a pivotal intermediate in the TCA cycle, could alter the wine's taste by affecting the content of certain sugars and amino acids (Xu et al., 2020). In our study, the highest amount of 2-oxoglutarate was detected in KW from Hayward kiwifruit.

Hydroxyacetone, detected recently in both kiwifruit and KW (He et al., 2023; Zhang et al., 2023), exhibits sweet and ethereal tastes. In the present study, hydroxyacetone showed the highest concentration in KW from Jinshi kiwifruit and its concentration was found to be related with the response value of the sweetness sensor (ANS). As a vital quality indicator for fermentation products, acetone gives wine a distinctive creamy flavor (Zhao et al., 2020). However, when the concentration of acetone exceeds 150 mg/L, it is considered to negatively impact on sensorial quality (Liu et al., 2023). In our study, acetone concentration

did not reach this level in any KW samples, with KW from Donghong variety showing the highest concentration, resulting in the attractive creamy taste.

3.5. Correlation analysis of sensory descriptions, key volatile and non-volatile compounds

In order to gain the deeper observation of the correlation between sensorial descriptors of aroma and taste, PLSR and network analysis were performed on key volatile and non-volatile compounds, as shown in Fig. 7.

In PLSR plot, two variables are positively correlated if they are located in the same quadrant, and their contribution is stronger if they are further away from the beginning of the axis (Yu et al., 2019). As shown in Fig. 7 (a), two principal components of the x-variable (key volatile compounds) explained 92% of the variance, while the y-variable (aroma descriptions) explained 94% of the variance. The contents of 2-methylbutanal, isoamyl acetate-D, hexyl acetate-D and hexyl acetate-M were found to have the strongest positive correlations with "pleasure" attribute. All the above volatile compounds impart favorable fruity aroma to KW, thus partially justifying this correlation (Cao et al., 2022). Both contents of 2-pentylfuran (fruity aroma) and ethyl hexanoate (pineapple, banana and sweet aromas) were positively correlated with "floral, sweety and fruity" attributes. Besides, a positive correlation was found between the contents of acetone and ethyl isovalerate and the "green" attribute.

In Fig. 7 (b), the key non-volatile compounds were employed as x-variables, while taste descriptors were employed as y-variables. Malate, galactarate and 2-oxoglutayrate concentrations were positively correlated with "acid and alcohol" attributes. In particular, malate was proven to greatly influence the acid taste of KW (Yang et al., 2022). Proline, a sweet amino acid, was shown to facilitate taste balance in wine (Hu et al., 2020). This aligns with our study, which found the proline concentration was positively correlated with "sweet and balanced" attributes. Besides, a positive association was observed between lactate content and "fullness".

To explore the correlation between key volatile and non-volatile compounds in KW, a correlation network analysis was conducted, as depicted in Fig. 7 (c). Organic acids could promote the generation of volatile compounds, thereby enhancing the overall flavor of food (Nie et al., 2017). This study revealed that the contents of succinate and lactate correlated with the contents of isoamyl acetate-D, ethyl isovalerate and hexyl acetate-D, in agreement with Wu et al. (Wu et al., 2023). This indicated the potential influence of lactate and succinate on the production of key volatile compounds that contribute to the characteristic aroma profile of KW. Besides, the contents of most volatile compounds demonstrated both positive and negative correlations with the concentrations of non-volatile compounds, indicating that changes in these compounds are closely related.

4. Conclusion

This study attempted to provide a comprehensive evaluation of flavor and metabolomic profiles of KW fermented from green, yellow and red fleshed kiwifruit through sensory evaluation, E-tongue, GC-IMS and ^{1}H NMR, in conjunction with multivariate analysis. The combination of multiple approaches has been proven to provide a more comprehensive flavor and metabolomic fingerprint than single method. The outcomes indicated that Hayward wine exhibited the most pronounced aroma, while Donghong wine had the most favorable taste profile. However, it's worth to note that the exploration based on other analytical platforms (such as LC-MS), and the integration with other omics approaches, may help in setting up strategies toward further flavor and metabolomic investigations of KW. Anyway, this study could be helpful to evaluate the quality of wine-making in kiwifruit with the above three flesh colors and shed light on the selection of kiwifruit flesh colors to promote the flavor quality of KW.

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Data availability

None of the data were deposited in an official repository. The data that support the study findings are available upon request.

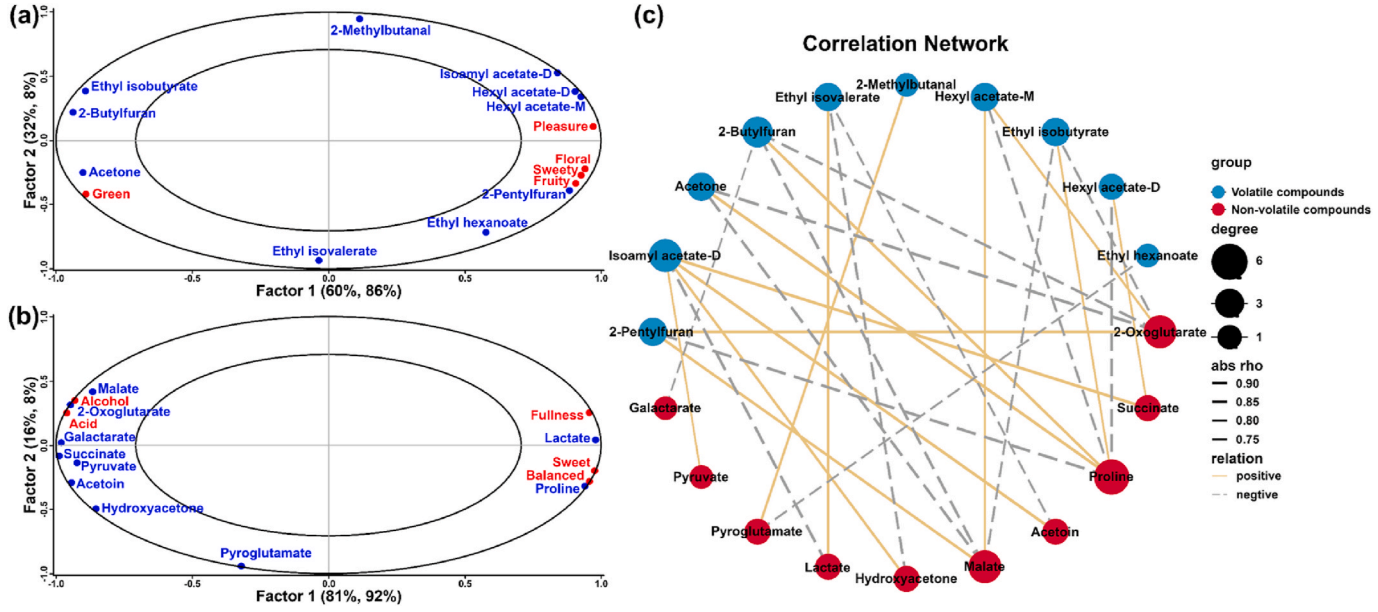

Fig. 7. PLSR correlation loading diagram, including the key volatile compounds with aroma profile descriptors (a) and key non-volatile compounds with taste profile descriptors (b). Spearman's correlation network of key volatile and non-volatile compounds in KW fermented from three types of flesh-colored kiwifruit (c).

CRediT authorship contribution statement

Qian Zhang: Writing – review & editing, Writing – original draft, Investigation, Formal analysis. **Yuyan Ma:** Writing – review & editing, Formal analysis. **Fang Wan:** Writing – review & editing, Formal analysis. **Zijian Cai:** Writing – review & editing. **Rui Zeng:** Writing – review & editing. **Junni Tang:** Writing – review & editing. **Xin Nie:** Writing – review & editing. **Xiaole Jiang:** Writing – review & editing. **Chenglin Zhu:** Writing – review & editing, Writing – original draft, Supervision, Methodology, Funding acquisition, Data curation, Conceptualization. **Luca Laghi:** Writing – review & editing, Writing – original draft, Methodology.

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.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.lwt.2024.116719.

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