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Effects of pretreatment methods on the flavor profile and sensory characteristics of Kiwi wine based on ^{1}H NMR, GC-IMS and E-tongue

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ABSTRACT

The pretreatment method of fruit before fermentation is a crucial step in fruit wine production, exerting a considerable influence on its overall quality, particularly on sensory characteristics and flavor profile. In this study, Pujiang kiwifruits as raw material, four pretreatment methods were employed in kiwi wine (KW) production, namely kiwi fruit crushing with peel (KCP), crushing without peel (KCW), kiwi fruit squeezing juice with peel (KJP), and squeezing juice without peel (KJW). The sensory characteristics and flavor profile of KW were evaluated using sensory evaluation, E-tongue, GC-IMS, and ^{1}H NMR. KW produced through KCP method achieved the highest sensory evaluation score, compared to the others. E-tongue could effectively differentiate the taste features among KW produced by different pretreatment methods. A total of 137 compounds were characterized by the combination of GC-IMS and ^{1}H NMR. Moreover, among the molecules quantified by GC-IMS and ^{1}H NMR, the concentrations of 52 and 58 compounds, respectively, exhibited significant differences among the four groups, primarily comprising esters, organic acids and alcohols. Furthermore, enrichment analysis indicated that several metabolic pathways could be altered by different pretreatment methods. This study serves as a theoretical reference and application basis for the quality improvement of KW and offers insights on the reduction and utilization of winemaking by-products.

1. Introduction

Kiwifruit, originating from south-west China (Wang et al., 2021), has garnered widespread consumer appeal owing to its nutritional richness and distinctive flavor (Sanz, López-Hortas, Torres, & Domínguez, 2021). Among the diverse range of kiwifruit-derived products, kiwi wine (KW) is notable for preserving a significant portion of the polyphenols and vitamin C present in fresh kiwifruit, exhibiting greater biological activity compared to other kiwifruit products (Ma et al., 2019). Furthermore, its reduced alcohol content aligns with the preferences of consumers seeking beverages with lower alcohol content, thereby presenting considerable market opportunities to mitigate economic losses stemming from overproduction, seasonal fluctuations, or substandard fruit (Varela & Varela, 2019).

The pretreatment methods of fruit before fermentation constitute a critical step in the production of high-quality fruit wine. Currently, a common pretreatment method utilized in KW production involves fermenting the fruit after removing the peel and pomace (Huang et al., 2021). However, discarded pomace and peel (accounting for 20–40% of the whole fruit's weight), usually considered as by-products in KW production, have been found to contain several phenolic antioxidants (Guthrie et al., 2020). Moreover, peel dietary fibers and pomace polysaccharides of kiwifruit have exhibited their potential as prebiotic components to improve host health and alleviate chronic diseases (Chen et al., 2023; Soquetta et al., 2016).

Flavor, encompassing taste, aroma and chemical composition, plays

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a crucial role in shaping consumer preferences for fruit wine (Wu et al., 2023). Gas chromatography-ion mobility spectrometry (GC-IMS) is considered a key method for flavor analysis, for its ability to offer a detailed insight into the flavor profile of fruit wine (Liu et al., 2022; Peng et al., 2022; Niu et al., 2019). a part from volatile compounds, it is worth to note that nonvolatile components of wine matrix may interact with volatiles, thereby influencing the sensory characteristics of wine. Among the techniques suitable for the characterization of nonvolatile components of wine matrix, proton nuclear magnetic resonance spectroscopy (^{1}H NMR) has been successfully utilized to expand the understanding of wine flavor profiles (Zhu et al., 2023). In addition, E-tongue, an artificial sensory technology mimicking human taste, serves as a convenient adjunct to sensory evaluations by trained panelists, effectively capturing overall taste characteristics and subtle differences among samples (Yuan et al., 2023). Our previous studies have demonstrated the feasibility of obtaining comprehensive sensory characteristics and flavor profile of KW through the combined of the above techniques (Zhang et al., 2023).

Considering kiwifruit peel's edible and nutritive properties, we hypothesize that KW fermented by kiwifruit with pomace and peel could be appealing, to reduce the production of wastes and, at the same time, to increase the sensory quality of KW. Nonetheless, how sensory characteristics and flavor profile are affected by KW fermentation with pomace and peels has rarely been systematically explored. To address this knowledge gap, we investigated four types of pretreatment methods, namely kiwi fruit crushing with peel (KCP), crushing without peel (KCW), kiwi fruit squeezing juice with peel (KJP), and squeezing juice without peel (KJW) on the effects of sensory characteristics and flavor profile of KW by means of a portfolio of complementary techniques. The findings of this study have the potential to provide valuable insights into comprehending the influence and underlying mechanisms that affect the sensory characteristics and flavor profile of KW under various pretreatment methods. Furthermore, the present study could shed lights on the utilization of the whole fruit for KW production, and in turn alleviate waste management challenges in the KW industry.

2. Materials and methods

2.1. Materials

For the present study, Pujiang kiwifruits (approximately 100 g weight for each) were collected among those harvested in September 2023 at a plantation of Pujiang, Sichuan, China. The initial sugar content of kiwifruit was 10 °Brix and the juice yield was 75%. As a yeast strain, we used *S. cerevisiae* strain RW, purchased from Angel Yeast CO., LTD (China), recognized to have good fermentation effects in a previous study (Zhang et al., 2023).

2.2. KW samples

All kiwifruits collected for the study were quickly transported to the laboratory after being freshly picked. The detailed KW production process is shown in Fig. 1. After cleaning, all kiwifruits were randomly separated into four groups, subjected to the following pretreatment methods.

(1) KCP: Cleaned kiwifruits crushed with peel, with a ratio of kiwifruit juice, pomace and peel of approximately 7:2:1 (w/w/w).
(2) KCW: Cleaned kiwifruits crushed without peel, with a ratio of kiwifruit juice and pomace of approximately 4:1 (w/w).
(3) KJP: Cleaned kiwifruits crushed with peel, followed by pomace removal through three layers of sterile gauze.
(4) KJW: Cleaned kiwifruits crushed without peel, followed by pomace removal through three layers of sterile gauze.

Once the pretreatment was completed, an enzymatical digestion was performed with pectinase (0.02 g/L, 100,000 U/g, SAS SOFRALAB, France) at 40 °C for 2 h. Subsequently, potassium metabisulphite (70 mg/L) was added to prevent browning, and sucrose was added to adjust the initial sugar content to 23 °Brix. Finally, activated yeast (0.2 g/L, *Saccharomyces cerevisiae* RW, Angel Yeast Co., Ltd, China) was added, and the total volume of fermentation was set to 200 mL. Fermentation process was carried out at 25 ± 1 °C for 30 d. Each pretreatment was subjected to five replicate fermentations, while all other fermentation conditions remained constant. After the fermentation process, the KW samples were filtered through a triple layer of sterile gauze and stored at −80 °C until further analysis.

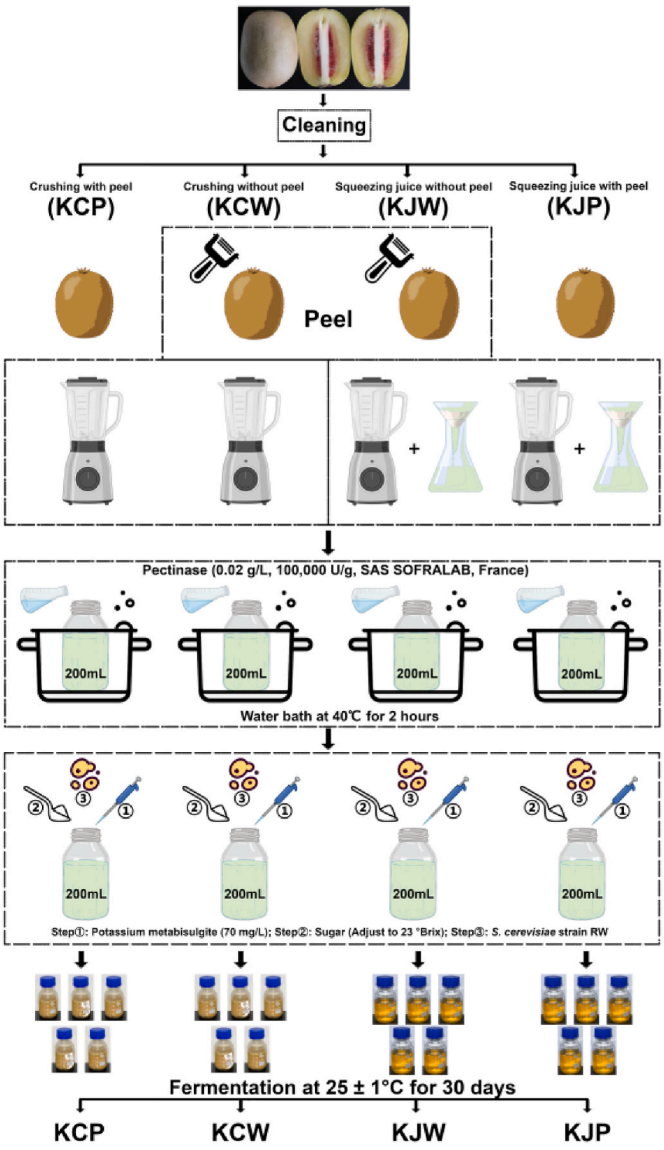

Fig. 1. KW production process chart.

2.3. Sensory evaluation

Sensory evaluation was performed as previously described (Zhang et al., 2023). In brief, the sensory assessment of KW samples enlisted a panel comprising 10 trained adults (5 females and 5 males). Samples were presented randomly in disposable paper cups. The evaluators rated the samples on attributes such as color, taste, aroma, flavor persistence, and overall acceptability, using a nine-point scale. To cleanse their palate, the testers rinsed with drinking water after each evaluation.

2.4. E-tongue analysis

E-tongue analysis was performed by an α-Astree E-tongue (Alpha MOS, France), equipped with seven potentiometric chemical sensors. The sensors were specifically sensitive to sweetness (ANS), saltiness (CTS), umami (NMS), sourness (AHS), bitterness (SCS) and two reference electrodes (PKS and CPS) (Zhao et al., 2023).

For each analysis, 80 mL of KW sample were transferred into a dedicated beaker designed for E-tongue analysis. The parameters for data acquisition time, stirring rate, and analysis duration were set to 120 s, 60 rpm/min, and 3 min, respectively. Post-analysis, the sensors underwent a thorough wash with deionized water for 30 s. The output values were recorded between 100 and 120 s. Each sample was tested eight times, and the mean value of the last five stable measurements were selected for the subsequent data analysis.

2.5. GC-IMS analysis

GC-IMS analysis was conducted by GC-IMS (Flavorspec®, G.A.S. Instrument, Germany) and MXT-WAX capillary column (30 m × 0.53 mm × 1 μm) (Restek, United States) according to our previous report (Zhang et al., 2023). An aliquot of 1.5 mL of each sample was introduced in a headspace vial with an internal volume of 20 mL, sealed with a magnetic screw cap, and incubated for 10 min at 60 °C. Subsequently, 100 μL of the headspace were automatically introduced into the injector (operated in no split mode) using a syringe at 85 °C. The temperature of column was set to 60 °C, while the drift tube was conditioned at 45 °C. The flow rate of the drift gas was set to 150 mL/min. A high-purity nitrogen carrier gas (99.999% purity) was used, and the GC column flow rate was adjusted as follows: 2 mL/min for 5 min, 10 mL/min for 10 min, 15 mL/min for 5 min, 50 mL/min for 10 min and 100 mL/min for 10 min. N-ketone C4–C9 was used as a reference to calculate for the retention index (RI) of VOCs. The identification of VOCs was performed by comparing their ions' drift time and RI with those of the standards in the GC-IMS library. One assay was performed for each sample and relative quantification of each VOC was performed based on peak intensity. Using the Laboratory Analysis Viewer and Reporter provided by the GC-IMS instrument, three-dimensional (3D) topographic, two-dimensional (2D) discrepancy, and fingerprint were created.

2.6. ^{1}H NMR analysis

Fig. S1 offers a pictorial representation of the main steps of ^{1}H NMR analysis, conducted according to Zhu et al. (Zhu et al., 2023). Briefly, solid residues were removed by centrifuging 0.5 mL of each sample at 18630 g and 4 °**C** for 15 min. Subsequently, the supernatant (0.35 mL), bi-distilled water (0.35 mL) and a solution for NMR analysis (100 μL) were mixed and centrifuged once more.

A 600.13 MHz AVANCE III spectrometer (Bruker, Wuhan, China), set at 298 K and equipped with the software Topspin 4.2, was used to obtain ^{1}H NMR spectra of KW samples. The main conditions of analysis are shown in Fig. S1 (c). In agreement with Zhu et al. (Zhu et al., 2022), the phase of each spectrum was adjusted in Topspin and subsequent processing of spectra and quantification of molecules were performed by custom R language scripts. As displayed in Fig. S1 (b). the residual water signal was removed, then the spectra baseline was adjusted via peak detection, through the "rolling ball" algorithm, part of the R baseline package. The whole spectral array was subjected to probabilistic quotient normalization (PQN), to compensate for protein and water content differences among samples. For molecules' identification multiplicity and chemical shift of the peaks were compared with the standard compound spectra of Chenomx library (Chenomx Inc., Canada, ver 10.1). For each molecule, the signals were integrated using rectangular integration.

2.7. Statistical analysis

Data mining was applied with the help of R language. To achieve normality, data distribution was transformed using Box and Cox's method (Box & Cox, 1964), before conducting univariate analyses. ANOVA, followed by Tukey HSD post hoc test ($p < 0.05$), was utilized to identify significant differences among groups in terms of E-tongue sensor responses and flavor profiles, respectively. To explore the overall trends in sample flavor profiles, rPCA models were employed and corresponding scoreplot and Pearson correlation plots based on the loadings were calculated. The online platform MetaboAnalyst 5.0 was utilized to perform pathway analysis. Moreover, the online platform Omicstudio was utilized to set up Mantel test in order to find out correlations between ^{1}H NMR and E-tongue.

3. Results

3.1. Sensory evaluation and E-tongue analysis of KW

Based on the sensory analysis, the KW produced by KCP pretreatment method yielded the highest overall sensory evaluation score, scoring well in aroma, mouthfeel, and overall acceptability, as illustrated in Fig. S2.

E-tongue was used to obtain an overall difference in taste characteristics among groups dominated by non-volatile compounds. To capture the overall trend of the data, an rPCA model was constructed using the response values of the sensors, as shown in Fig. S3. In Fig. S3 (a), PC 1 accounted for 87.6% of the samples set's variance, effectively summarizing the overall features of the samples. Notably, samples from different groups exhibited significant positional variations along PC 1 and PC 2 ($p < 0.05$). Samples fermented with/without pomace could be well distinguished along PC 1, while the differences linked to fermentation with/without peel could be visualized along PC 2. In detail, KW fermented without pomace (KJW and KJP) had higher SCS response values and lower response values of PKS, NMS and CPS sensors. KW fermented without peel (KJW and KCW) had higher NMS and PKS response values and lower response value of SCS.

3.2. GC-IMS analysis

Information on GC-IMS of VOCs in KW produced through different pretreatment methods is shown in Fig. 2 and Table S1.

The three-dimensional topographic plot, illustrated in Fig. 2 (a), conveniently visualizes the differences in the various parts of the GC-IMS spectra of KWs produced by different pretreatment methods. The detailed differences between the four groups of samples are shown in Fig. 2 (b). The main differences are in the retention time range from 200 to 1200 s. Taking the KJP group as a reference, red and blue dots indicate higher and lower concentrations of specific substances, respectively. Fig. 2 (c) shows that the VOCs of KW produced by different pretreatment methods mainly belong to esters and aldehydes. Overall, 58 VOCs were quantified, including esters (22), alcohols (8), aldehydes (8), acids (8), ketones (3), and others (9), as shown in Table 1. The concentrations of 52 VOCs exhibited significant differences ($p < 0.05$) among groups. To elucidate the overall view of different groups, an rPCA model was constructed based on their peak intensities, as illustrated in Fig. 3.

As depicted in Fig. 3 (a), PC 1 accounted for a substantial 72.3% of the overall variability in the sample set, effectively capturing the peculiarities of the groups. The main driver of the distribution of samples along PC 1 is the presence of peel, with samples pertaining to the KCP and KCW groups that exhibited positive PC 1 scores and samples pertaining to the KJP and KJW groups exhibiting negative PC 1 scores. PC 2 mainly catches the differences associated with the presence of pomace, with KCP and KJP samples appearing at positive PC 2 scores and KCW and KJW samples appearing negative PC 2 scores. In further detail,

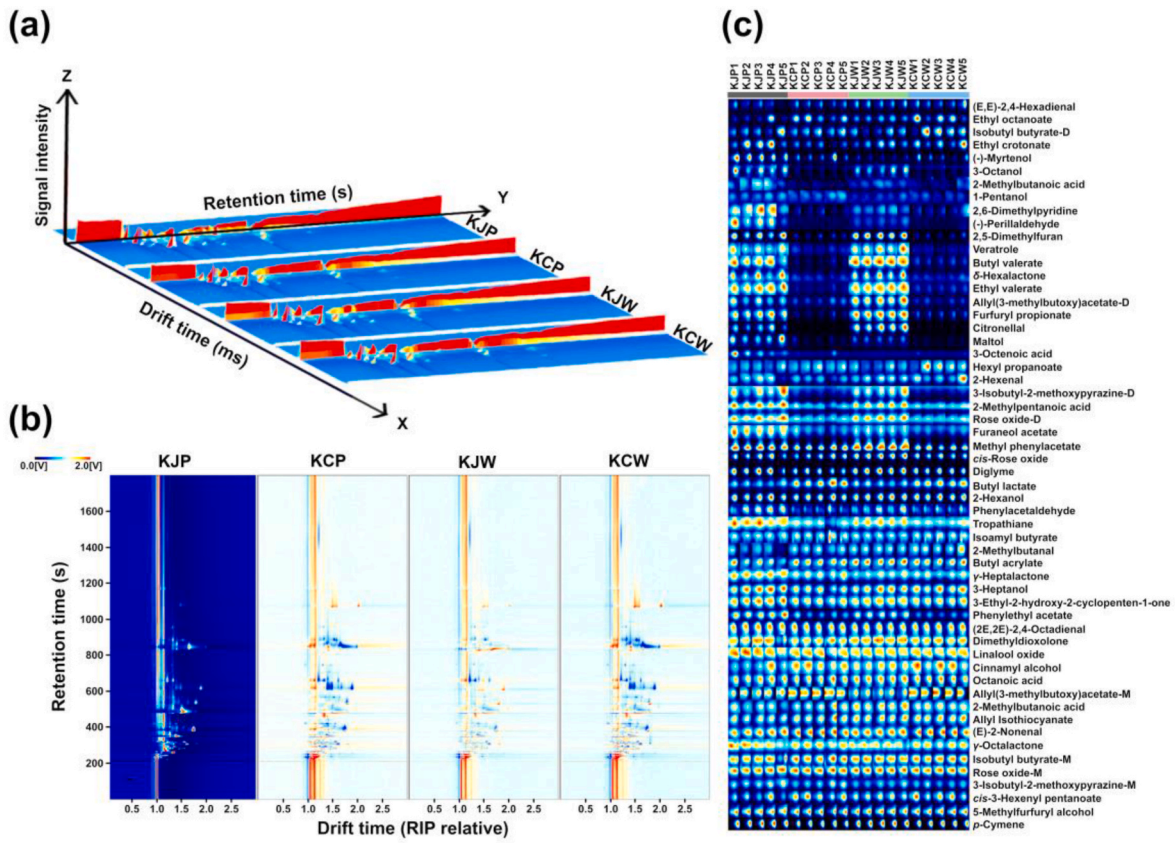

Fig. 2. Results of GC-IMS for KW produced by different pretreatment methods. (a) three-dimensional topographic plot; (b) two-dimensional difference plots using the spectra of the KJP group as a reference; (c) fingerprint plot representing the variation of VOCs concentrations among the four groups.

group KCP exhibited higher levels of 1-pentanol, γ-octalactone and (2E,2E)-2,4-octadienal in both PC 1 and PC 2 dimensions, compared to group KJW.

3.3. ^{1}H NMR analysis

A representative ^{1}H NMR spectrum of KW is depicted in Fig. S4. Seventy-nine molecules were unambiguously characterized in KW, including amino acids, peptides and analogues (23), carbohydrates and derivatives (11), organic acids and derivatives (13), nucleosides, nucleotides and analogues (4), as well as alcohols (4), as detailed in Table S2. Taking advantage of ANOVA, significant differences ($p < 0.05$) in the concentrations of 58 molecules were observed among the four groups, as outlined in Table 2. Among them, the concentrations of 15 amino acids showed significant differences among the four groups, with higher levels of 4-aminobutyrate, asparagine, carnosine, betaine, creatinine and threonine in KCP group, compared to the other groups. Meanwhile, the levels of seven carbohydrates resulted as significantly higher in KCP group, namely 1,3-dihydroxyacetone, arabinose, fructose, glucose, lactose, N-acetylglucosamine and xylose. Similarly to GC-IMS, an rPCA model was developed based on the concentrations of all molecules that showed significant differences among four groups, in order to get a bird-eye view of the samples' groups, as shown in Fig. 4.

PC 1, as depicted in Fig. 4 (a), accounts for 79.6% of the variance of the entire sample set and effectively summarizes the differences among the groups. KW fermented with/without pomace could be well distinguished along PC 1, while the differences linked to fermentation with/without peel could followed along PC 2. In detail, higher concentrations of tartrate, fructose, methanol, N-acetylglucosamine, hydroxyacetone, 1,3-dihydroxyacetone, arabinose, glucose, threonine, pantothenate, carnosine, galactarate, creatinine, betaine, acetate, 4-aminobutyrate, formate, pyroglutamate and aspartate were found in KW produced by KCP method. In contrast, higher amounts of oxypurinol, ethanolamine, *sn-glycero*-3-phosphocholine, guanosine, *myo*-Inositol, cytidine, 4-hydroxyphenylacetate, lactulose, xanthine, malate, propylene, fucose, N-acetylglycine, uridine and sarcosine were detected in KW produced by KJW method.

3.4. Correlation between E-tongue and ^{1}H NMR

To elucidate the impact of specific molecules on taste attributes, a correlation analysis was conducted using E-tongue response values and the molecules characterized by ^{1}H NMR whose concentrations showed significant differences among groups, as depicted in Fig. 5. The SCS sensor response value was positively associated with threonine, *sn-glycero*-3-phosphocholine, pyroglutamate, N-acetylglycine, methanol, galactose, arabinose and 1,3-dihydroxyacetone. The ANS sensor response values were positively associated with N-acetylglycine and galactose.

3.5. Pathway analysis

Pathway enrichment analysis was performed to identify the key pathways altered by different pretreatment methods, as illustrated in Fig. 6. Significant results were obtained for pyruvate metabolism, alanine, aspartate and glutamate metabolism, glycerolipid metabolism and butanoate metabolism.

4. Discussion

Flavor, as a crucial sensory attribute, significantly influences consumer perception and acceptance of fruit wines. However, in the fruit

Table 1
Peak intensity (mean ± sd) of VOCs in KW fermented by different pretreatment methods characterized by GC-IMS.

Compounds	CAS	Descriptor	Peak Intensity			
			KJP	KCP	KJW	KCW
Esters						
cis-3-Hexenyl pentanoate	35852-46-1	/	$3.43 \times 10^{-2} \pm 1.16 \times 10^{-2\ b}$	$7.61 \times 10^{-2} \pm 1.60 \times 10^{-2\ a}$	$4.15 \times 10^{-2} \pm 4.82 \times 10^{-3\ b}$	$7.89 \times 10^{-2} \pm 1.87 \times 10^{-2\ a}$
2-Methylbutanol acetate	624-41-9	/	$5.10 \times 10^{-3} \pm 8.52 \times 10^{-4\ c}$	$8.85 \times 10^{-3} \pm 8.92 \times 10^{-4\ b}$	$6.25 \times 10^{-3} \pm 4.68 \times 10^{-4\ c}$	$1.08 \times 10^{-2} \pm 1.51 \times 10^{-3\ a}$
Allyl(3-methylbutoxy)acetate-D	67634-00-8	/	$1.67 \times 10^{-2} \pm 3.07 \times 10^{-3\ b}$	$1.42 \times 10^{-2} \pm 8.29 \times 10^{-4\ b}$	$2.54 \times 10^{-2} \pm 2.55 \times 10^{-3\ a}$	$1.28 \times 10^{-2} \pm 1.57 \times 10^{-3\ b}$
Allyl(3-methylbutoxy)acetate-M	67634-00-8	/	$5.47 \times 10^{-2} \pm 7.72 \times 10^{-3\ b}$	$1.05 \times 10^{-1} \pm 7.12 \times 10^{-3\ a}$	$4.88 \times 10^{-2} \pm 5.51 \times 10^{-3\ b}$	$1.00 \times 10^{-1} \pm 9.44 \times 10^{-3\ a}$
Allyl Isothiocyanate	57-06-7	/	$6.40 \times 10^{-3} \pm 2.12 \times 10^{-4\ c}$	$1.03 \times 10^{-2} \pm 7.99 \times 10^{-4\ a}$	$7.08 \times 10^{-3} \pm 4.98 \times 10^{-4\ b}$	$1.17 \times 10^{-2} \pm 1.08 \times 10^{-3\ a}$
Butyl acrylate	141-32-2	/	$2.23 \times 10^{-2} \pm 1.95 \times 10^{-3\ b}$	$3.88 \times 10^{-2} \pm 4.84 \times 10^{-3\ a}$	$2.73 \times 10^{-2} \pm 9.49 \times 10^{-4\ b}$	$4.16 \times 10^{-2} \pm 2.75 \times 10^{-3\ a}$
Butyl lactate	138-22-7	/	$2.13 \times 10^{-2} \pm 2.62 \times 10^{-3\ b}$	$5.07 \times 10^{-2} \pm 4.15 \times 10^{-3\ a}$	$2.17 \times 10^{-2} \pm 1.94 \times 10^{-3\ b}$	$5.03 \times 10^{-2} \pm 6.03 \times 10^{-3\ a}$
Butyl valerate	591-68-4	/	$3.61 \times 10^{-2} \pm 8.27 \times 10^{-3\ a}$	$1.08 \times 10^{-2} \pm 9.02 \times 10^{-4\ c}$	$4.44 \times 10^{-2} \pm 1.86 \times 10^{-3\ a}$	$1.69 \times 10^{-2} \pm 1.33 \times 10^{-3\ b}$
Ethyl octanoate	106-32-1	apricot, banana, pear	$1.14 \times 10^{-2} \pm 8.30 \times 10^{-3\ b}$	$3.30 \times 10^{-2} \pm 1.14 \times 10^{-2\ a}$	$1.58 \times 10^{-2} \pm 2.65 \times 10^{-3\ ab}$	$3.64 \times 10^{-2} \pm 1.69 \times 10^{-2\ a}$
Ethyl valerate	539-82-2	fruity, green apple, brandy	$1.34 \times 10^{-2} \pm 8.84 \times 10^{-4\ a}$	$4.42 \times 10^{-3} \pm 5.16 \times 10^{-4\ c}$	$1.32 \times 10^{-2} \pm 3.05 \times 10^{-4\ a}$	$6.56 \times 10^{-3} \pm 5.36 \times 10^{-4\ b}$
Ethyl crotonate	623-70-1	/	$1.48 \times 10^{-2} \pm 7.10 \times 10^{-3\ a}$	$9.38 \times 10^{-3} \pm 3.64 \times 10^{-3\ a}$	$9.46 \times 10^{-3} \pm 3.02 \times 10^{-3\ a}$	$1.96 \times 10^{-2} \pm 1.03 \times 10^{-2\ a}$
Furaneol acetate	4166-20-5	/	$1.55 \times 10^{-2} \pm 1.34 \times 10^{-3\ a}$	$1.48 \times 10^{-2} \pm 2.35 \times 10^{-3\ a}$	$1.17 \times 10^{-2} \pm 8.63 \times 10^{-4\ b}$	$1.47 \times 10^{-2} \pm 8.60 \times 10^{-4\ a}$
Furfuryl propionate	623-19-8	/	$5.63 \times 10^{-2} \pm 6.90 \times 10^{-3\ b}$	$1.77 \times 10^{-2} \pm 1.96 \times 10^{-3\ d}$	$6.80 \times 10^{-2} \pm 1.86 \times 10^{-3\ a}$	$2.84 \times 10^{-2} \pm 1.99 \times 10^{-3\ c}$
Hexyl propanoate	2445-76-3	/	$1.51 \times 10^{-2} \pm 2.71 \times 10^{-3\ bc}$	$2.47 \times 10^{-2} \pm 5.03 \times 10^{-3\ ab}$	$1.41 \times 10^{-2} \pm 3.40 \times 10^{-3\ c}$	$3.18 \times 10^{-2} \pm 1.02 \times 10^{-2\ a}$
Isoamyl butyrate	106-27-4	sweet, pineapple, banana	$4.76 \times 10^{-2} \pm 2.99 \times 10^{-3\ b}$	$8.23 \times 10^{-2} \pm 4.46 \times 10^{-3\ a}$	$4.59 \times 10^{-2} \pm 3.56 \times 10^{-3\ b}$	$8.44 \times 10^{-2} \pm 7.31 \times 10^{-3\ a}$
Isobutyl butyrate-D	539-90-2	sweet fruity, apple, pineapple	$3.28 \times 10^{-2} \pm 5.05 \times 10^{-3\ b}$	$4.92 \times 10^{-2} \pm 4.37 \times 10^{-3\ a}$	$3.40 \times 10^{-2} \pm 2.10 \times 10^{-3\ b}$	$5.28 \times 10^{-2} \pm 4.56 \times 10^{-3\ a}$
Isobutyl butyrate-M	539-90-2	sweet fruity, apple, pineapple	$1.48 \times 10^{-2} \pm 6.61 \times 10^{-3\ ab}$	$2.42 \times 10^{-2} \pm 5.08 \times 10^{-3\ ab}$	$1.27 \times 10^{-2} \pm 4.17 \times 10^{-3\ b}$	$3.20 \times 10^{-2} \pm 1.42 \times 10^{-2\ a}$
Methyl phenylacetate	101-41-7	/	$2.39 \times 10^{-1} \pm 1.78 \times 10^{-2\ b}$	$2.29 \times 10^{-1} \pm 1.40 \times 10^{-2\ b}$	$3.01 \times 10^{-1} \pm 9.51 \times 10^{-3\ a}$	$2.08 \times 10^{-1} \pm 2.54 \times 10^{-2\ b}$
Phenylethyl acetate	103-45-7	sweet, floral, honey	$7.73 \times 10^{-2} \pm 8.74 \times 10^{-3\ a}$	$6.70 \times 10^{-2} \pm 8.60 \times 10^{-3\ ab}$	$5.74 \times 10^{-2} \pm 3.56 \times 10^{-3\ b}$	$6.36 \times 10^{-2} \pm 5.32 \times 10^{-3\ b}$
γ-Heptalactone	105-21-5	coconut	$9.25 \times 10^{-3} \pm 4.49 \times 10^{-4\ b}$	$1.20 \times 10^{-2} \pm 1.73 \times 10^{-3\ a}$	$7.17 \times 10^{-3} \pm 2.42 \times 10^{-4\ c}$	$1.19 \times 10^{-2} \pm 9.73 \times 10^{-4\ a}$
γ-Octalactone	104-50-7	/	$4.44 \times 10^{-2} \pm 9.45 \times 10^{-3\ b}$	$6.94 \times 10^{-2} \pm 7.95 \times 10^{-3\ a}$	$3.76 \times 10^{-2} \pm 5.89 \times 10^{-3\ b}$	$6.86 \times 10^{-2} \pm 6.81 \times 10^{-3\ a}$
δ-Hexalactone	823-22-3	/	$1.32 \times 10^{-2} \pm 3.10 \times 10^{-3\ a}$	$9.66 \times 10^{-3} \pm 1.82 \times 10^{-3\ a}$	$1.27 \times 10^{-2} \pm 9.97 \times 10^{-4\ a}$	$1.02 \times 10^{-2} \pm 1.43 \times 10^{-3\ a}$
Aldehydes						
(2E,2E)-2,4-Octadienal	30361-28-5	/	$2.99 \times 10^{-2} \pm 2.43 \times 10^{-3\ b}$	$4.23 \times 10^{-2} \pm 3.90 \times 10^{-3\ a}$	$2.68 \times 10^{-2} \pm 2.00 \times 10^{-3\ b}$	$4.48 \times 10^{-2} \pm 2.89 \times 10^{-3\ a}$
(−)-Perillaldehyde	18031-40-8	/	$5.37 \times 10^{-3} \pm 1.68 \times 10^{-3\ a}$	$1.86 \times 10^{-3} \pm 1.39 \times 10^{-4\ c}$	$2.72 \times 10^{-3} \pm 2.91 \times 10^{-4\ b}$	$1.99 \times 10^{-3} \pm 2.40 \times 10^{-4\ c}$
(E)-2-Nonenal	18829-56-6	/	$7.54 \times 10^{-2} \pm 7.76 \times 10^{-3\ b}$	$1.06 \times 10^{-1} \pm 5.29 \times 10^{-3\ a}$	$7.44 \times 10^{-2} \pm 5.53 \times 10^{-3\ b}$	$1.16 \times 10^{-1} \pm 8.73 \times 10^{-3\ a}$
(E,E)-2,4-Hexadienal	142-83-6	/	$8.67 \times 10^{-3} \pm 2.97 \times 10^{-3\ b}$	$1.39 \times 10^{-2} \pm 3.05 \times 10^{-3\ ab}$	$1.09 \times 10^{-2} \pm 5.27 \times 10^{-4\ b}$	$1.85 \times 10^{-2} \pm 5.12 \times 10^{-3\ a}$
2-Hexenal	505-57-7	/	$5.36 \times 10^{-3} \pm 2.08 \times 10^{-3\ a}$	$5.37 \times 10^{-3} \pm 1.55 \times 10^{-3\ a}$	$4.85 \times 10^{-3} \pm 6.42 \times 10^{-4\ a}$	$8.84 \times 10^{-3} \pm 3.83 \times 10^{-3\ a}$
2-Methylbutanal	96-17-3	cherry	$2.02 \times 10^{-3} \pm 5.89 \times 10^{-4\ b}$	$3.85 \times 10^{-3} \pm 7.92 \times 10^{-4\ a}$	$2.59 \times 10^{-3} \pm 1.65 \times 10^{-4\ b}$	$4.63 \times 10^{-3} \pm 7.54 \times 10^{-4\ a}$
Citronellal	106-23-0	/	$6.53 \times 10^{-2} \pm 2.20 \times 10^{-2\ b}$	$6.82 \times 10^{-3} \pm 3.25 \times 10^{-4\ d}$	$1.24 \times 10^{-1} \pm 1.73 \times 10^{-2\ a}$	$9.69 \times 10^{-3} \pm 7.72 \times 10^{-4\ c}$
Phenylacetaldehyde	122-78-1	floral, honey, rose	$3.06 \times 10^{-2} \pm 5.37 \times 10^{-3\ ab}$	$3.06 \times 10^{-2} \pm 2.89 \times 10^{-3\ ab}$	$2.60 \times 10^{-2} \pm 1.79 \times 10^{-3\ b}$	$3.60 \times 10^{-2} \pm 5.01 \times 10^{-3\ a}$
Ketones						
3-Ethyl-2-hydroxy-2-cyclopenten-1-one	21835-01-8	/	$3.03 \times 10^{-2} \pm 2.26 \times 10^{-3\ b}$	$3.95 \times 10^{-2} \pm 5.15 \times 10^{-3\ a}$	$2.88 \times 10^{-2} \pm 1.94 \times 10^{-3\ b}$	$4.30 \times 10^{-2} \pm 3.12 \times 10^{-3\ a}$
Dimethyldioxolone	37830-90-3	/	$9.33 \times 10^{-3} \pm 1.88 \times 10^{-3\ b}$	$1.25 \times 10^{-2} \pm 1.45 \times 10^{-3\ a}$	$9.66 \times 10^{-3} \pm 3.30 \times 10^{-4\ b}$	$1.38 \times 10^{-2} \pm 1.30 \times 10^{-3\ a}$
Maltol	118-71-8	/	$2.72 \times 10^{-2} \pm 8.67 \times 10^{-3\ a}$	$1.04 \times 10^{-2} \pm 3.34 \times 10^{-3\ bc}$	$1.52 \times 10^{-2} \pm 3.65 \times 10^{-4\ b}$	$8.35 \times 10^{-3} \pm 1.01 \times 10^{-3\ c}$
Alcohols						
(−)-Myrtenol	19894-97-4	/	$1.03 \times 10^{-1} \pm 1.75 \times 10^{-2\ a}$	$8.24 \times 10^{-2} \pm 3.03 \times 10^{-2\ a}$	$3.06 \times 10^{-2} \pm 2.37 \times 10^{-3\ b}$	$7.42 \times 10^{-2} \pm 1.81 \times 10^{-2\ a}$

(*continued on next page*)

Table 1 (*continued*)

Compounds	CAS	Descriptor	Peak Intensity			
			KJP	KCP	KJW	KCW
1-Pentanol	71-41-0	bitter almond, fatty	$4.55 \times 10^{-3} \pm 6.42 \times 10^{-4\ b}$	$7.89 \times 10^{-3} \pm 1.05 \times 10^{-3\ a}$	$3.53 \times 10^{-3} \pm 3.58 \times 10^{-4\ c}$	$6.82 \times 10^{-3} \pm 9.09 \times 10^{-4\ a}$
5-Methylfurfuryl alcohol	3857-25-8	/	$1.22 \times 10^{-1} \pm 9.78 \times 10^{-3\ b}$	$1.58 \times 10^{-1} \pm 2.48 \times 10^{-2\ a}$	$1.12 \times 10^{-1} \pm 5.88 \times 10^{-3\ b}$	$1.83 \times 10^{-1} \pm 1.31 \times 10^{-2\ a}$
2-Hexanol	626-93-7	banana, floral, grass	$5.02 \times 10^{-2} \pm 8.62 \times 10^{-3\ b}$	$6.68 \times 10^{-2} \pm 6.18 \times 10^{-3\ a}$	$4.81 \times 10^{-2} \pm 5.28 \times 10^{-3\ b}$	$7.61 \times 10^{-2} \pm 8.55 \times 10^{-3\ a}$
3-Heptanol	589-82-2	fruity, musty	$1.89 \times 10^{-2} \pm 3.43 \times 10^{-3\ ab}$	$1.97 \times 10^{-2} \pm 4.31 \times 10^{-3\ ab}$	$1.52 \times 10^{-2} \pm 1.78 \times 10^{-3\ b}$	$2.55 \times 10^{-2} \pm 4.71 \times 10^{-3\ a}$
3-Octanol	589-98-0	/	$1.36 \times 10^{-2} \pm 1.92 \times 10^{-3\ a}$	$6.35 \times 10^{-3} \pm 7.06 \times 10^{-4\ c}$	$1.11 \times 10^{-2} \pm 1.45 \times 10^{-3\ b}$	$7.89 \times 10^{-3} \pm 1.17 \times 10^{-3\ c}$
Cinnamyl alcohol	104-54-1	/	$9.15 \times 10^{-3} \pm 2.66 \times 10^{-3\ b}$	$1.84 \times 10^{-2} \pm 2.34 \times 10^{-3\ a}$	$1.10 \times 10^{-2} \pm 5.59 \times 10^{-4\ b}$	$2.02 \times 10^{-2} \pm 4.21 \times 10^{-3\ a}$
Linalool oxide	60047-17-8	floral	$3.32 \times 10^{-2} \pm 4.82 \times 10^{-3\ b}$	$4.92 \times 10^{-2} \pm 8.44 \times 10^{-3\ a}$	$3.20 \times 10^{-2} \pm 2.85 \times 10^{-3\ b}$	$5.24 \times 10^{-2} \pm 1.30 \times 10^{-3\ a}$
Acids						
2-Methylbutanoic acid	116-53-0	/	$8.38 \times 10^{-4} \pm 1.50 \times 10^{-4\ a}$	$4.83 \times 10^{-4} \pm 1.40 \times 10^{-4\ b}$	$6.78 \times 10^{-4} \pm 7.71 \times 10^{-5\ ab}$	$6.62 \times 10^{-4} \pm 1.43 \times 10^{-4\ ab}$
2-Methylpentanoic acid	97-61-0	/	$2.05 \times 10^{-2} \pm 1.48 \times 10^{-3\ ab}$	$2.08 \times 10^{-2} \pm 3.66 \times 10^{-3\ ab}$	$1.86 \times 10^{-2} \pm 1.28 \times 10^{-3\ b}$	$2.33 \times 10^{-2} \pm 1.88 \times 10^{-3\ a}$
3-Octenoic acid	1577-19-1	/	$5.15 \times 10^{-2} \pm 1.37 \times 10^{-2\ a}$	$4.28 \times 10^{-2} \pm 2.55 \times 10^{-3\ a}$	$2.50 \times 10^{-2} \pm 1.88 \times 10^{-3\ b}$	$4.41 \times 10^{-2} \pm 3.20 \times 10^{-3\ a}$
Octanoic acid	124-07-2	cheese, fatty	$4.37 \times 10^{-2} \pm 3.81 \times 10^{-3\ b}$	$6.47 \times 10^{-2} \pm 3.84 \times 10^{-3\ a}$	$4.57 \times 10^{-2} \pm 1.35 \times 10^{-3\ b}$	$6.75 \times 10^{-2} \pm 6.68 \times 10^{-3\ a}$
Ethers						
Diglyme	111-96-6	/	$6.71 \times 10^{-2} \pm 1.85 \times 10^{-2\ a}$	$6.87 \times 10^{-2} \pm 1.21 \times 10^{-2\ a}$	$6.96 \times 10^{-2} \pm 6.29 \times 10^{-3\ a}$	$8.29 \times 10^{-2} \pm 1.10 \times 10^{-2\ a}$
Veratrole	91-16-7	/	$1.40 \times 10^{-2} \pm 2.11 \times 10^{-3\ a}$	$8.26 \times 10^{-3} \pm 7.58 \times 10^{-4\ b}$	$1.57 \times 10^{-2} \pm 1.10 \times 10^{-3\ a}$	$7.55 \times 10^{-3} \pm 7.99 \times 10^{-4\ b}$
Others						
Rose oxide-D	16409-43-1	rose	$1.39 \times 10^{-1} \pm 1.10 \times 10^{-2\ b}$	$2.18 \times 10^{-1} \pm 1.27 \times 10^{-2\ a}$	$1.38 \times 10^{-1} \pm 6.93 \times 10^{-3\ b}$	$2.25 \times 10^{-1} \pm 1.35 \times 10^{-2\ a}$
Rose oxide-M	16409-43-1	rose	$5.64 \times 10^{-2} \pm 5.22 \times 10^{-3\ bc}$	$6.61 \times 10^{-2} \pm 7.69 \times 10^{-3\ ab}$	$5.24 \times 10^{-2} \pm 2.63 \times 10^{-3\ c}$	$7.11 \times 10^{-2} \pm 4.76 \times 10^{-3\ a}$
cis-Rose oxide	3033-23-6	rose	$1.15 \times 10^{-1} \pm 2.68 \times 10^{-2\ b}$	$1.55 \times 10^{-1} \pm 1.80 \times 10^{-2\ a}$	$1.50 \times 10^{-1} \pm 8.84 \times 10^{-3\ ab}$	$1.69 \times 10^{-1} \pm 2.81 \times 10^{-2\ a}$
2,6-Dimethylpyridine	108-48-5	/	$1.58 \times 10^{-3} \pm 3.50 \times 10^{-4\ a}$	$5.31 \times 10^{-4} \pm 1.55 \times 10^{-4\ b}$	$7.98 \times 10^{-4} \pm 1.27 \times 10^{-4\ b}$	$8.93 \times 10^{-4} \pm 4.07 \times 10^{-4\ b}$
2,5-Dimethylfuran	625-86-5	/	$5.08 \times 10^{-2} \pm 1.22 \times 10^{-2\ a}$	$1.93 \times 10^{-2} \pm 3.04 \times 10^{-3\ b}$	$5.67 \times 10^{-2} \pm 4.04 \times 10^{-3\ a}$	$2.15 \times 10^{-2} \pm 6.05 \times 10^{-3\ b}$
3-Isobutyl-2-methoxypyrazine-D	24683-00-9	/	$2.80 \times 10^{-2} \pm 4.84 \times 10^{-3\ b}$	$3.81 \times 10^{-2} \pm 3.27 \times 10^{-3\ a}$	$2.23 \times 10^{-2} \pm 1.64 \times 10^{-3\ b}$	$3.50 \times 10^{-2} \pm 2.88 \times 10^{-3\ a}$
3-Isobutyl-2-methoxypyrazine-M	24683-00-9	/	$9.90 \times 10^{-3} \pm 2.06 \times 10^{-3\ a}$	$7.77 \times 10^{-3} \pm 1.13 \times 10^{-3\ ab}$	$9.34 \times 10^{-3} \pm 7.52 \times 10^{-4\ ab}$	$7.23 \times 10^{-3} \pm 5.28 \times 10^{-4\ b}$
Tropathiane	67715-80-4	/	$1.35 \times 10^{-2} \pm 1.50 \times 10^{-3\ b}$	$1.50 \times 10^{-2} \pm 2.62 \times 10^{-3\ ab}$	$1.23 \times 10^{-2} \pm 6.20 \times 10^{-4\ b}$	$1.74 \times 10^{-2} \pm 7.80 \times 10^{-4\ a}$
p-Cymene	99-87-6	/	$3.24 \times 10^{-1} \pm 3.00 \times 10^{-2\ b}$	$3.31 \times 10^{-1} \pm 2.87 \times 10^{-2\ b}$	$3.03 \times 10^{-1} \pm 1.82 \times 10^{-2\ b}$	$4.23 \times 10^{-1} \pm 4.36 \times 10^{-2\ a}$

Data are displayed as mean ± standard deviation (n = 5). For each molecule, sd values followed by a common superscript identify no significant differences. RI, RT, and DT stand for retention index, retention time, and drift time, respectively. Aroma descriptors mainly refer to previous study (Cai et al., 2020; Huang et al., 2021; Yiman et al., 2019)./: not found.

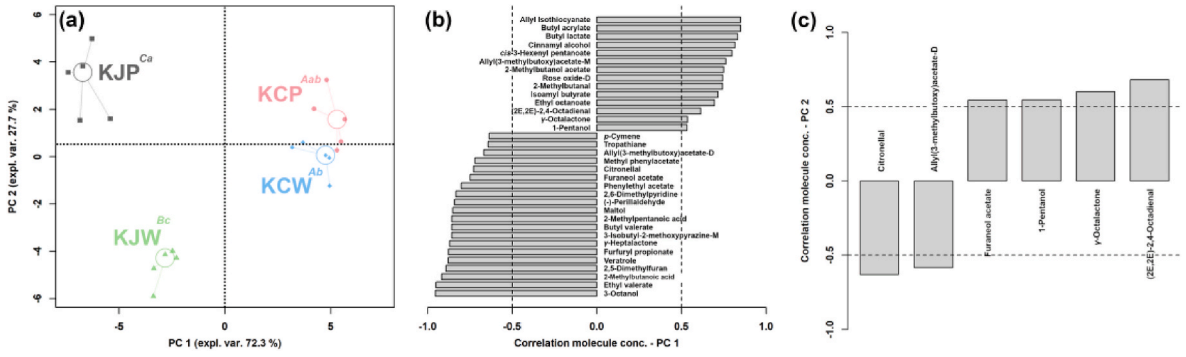

Fig. 3. RPCA model calculated on the basis of VOCs' concentrations showing significant differences in peak intensities among groups, represented as Scoreplot (a) and Loading plot (b and c). The median of each group is denoted by a wide and empty circle. Superscript capital and lowercase letters indicate significant differences along PC 1 and PC 2, respectively.

Table 2
Concentrations (mmol/L, mean ± sd) of molecules that showed significant differences among the four groups.

	KJP	KCP	KJW	KCW
Amino Acids, Peptides and Analogues				
4-Aminobutyrate	$1.23 \times 10^{-3} \pm 1.95 \times 10^{-4}$ ^{a}	$1.45 \times 10^{-3} \pm 1.45 \times 10^{-4}$ ^{a}	$8.56 \times 10^{-4} \pm 2.29 \times 10^{-4}$ ^{b}	$1.32 \times 10^{-3} \pm 1.05 \times 10^{-4}$ ^{a}
Asparagine	$2.13 \times 10^{-4} \pm 1.52 \times 10^{-5}$ ^{b}	$2.76 \times 10^{-4} \pm 4.08 \times 10^{-5}$ ^{a}	$2.25 \times 10^{-4} \pm 1.67 \times 10^{-5}$ ^{ab}	$2.44 \times 10^{-4} \pm 5.95 \times 10^{-5}$ ^{a}
Carnosine	$1.99 \times 10^{-4} \pm 5.85 \times 10^{-5}$ ^{bc}	$3.36 \times 10^{-4} \pm 3.73 \times 10^{-5}$ ^{a}	$1.50 \times 10^{-4} \pm 2.03 \times 10^{-5}$ ^{c}	$2.81 \times 10^{-4} \pm 5.03 \times 10^{-5}$ ^{ab}
Phenylalanine	$6.18 \times 10^{-4} \pm 4.94 \times 10^{-5}$ ^{b}	$6.60 \times 10^{-4} \pm 9.12 \times 10^{-5}$ ^{ab}	$7.07 \times 10^{-4} \pm 1.57 \times 10^{-5}$ ^{a}	$5.88 \times 10^{-4} \pm 1.33 \times 10^{-4}$ ^{ab}
Methylamine	$6.08 \times 10^{-5} \pm 6.39 \times 10^{-6}$ ^{a}	$4.29 \times 10^{-5} \pm 1.08 \times 10^{-5}$ ^{b}	$4.79 \times 10^{-5} \pm 3.29 \times 10^{-6}$ ^{ab}	$4.99 \times 10^{-5} \pm 6.91 \times 10^{-6}$ ^{ab}
Aspartate	$4.49 \times 10^{-4} \pm 4.48 \times 10^{-5}$ ^{b}	$5.55 \times 10^{-4} \pm 5.26 \times 10^{-5}$ ^{a}	$4.58 \times 10^{-4} \pm 4.26 \times 10^{-5}$ ^{b}	$6.74 \times 10^{-4} \pm 2.10 \times 10^{-4}$ ^{a}
Betaine	$5.75 \times 10^{-5} \pm 8.15 \times 10^{-6}$ ^{ab}	$7.03 \times 10^{-5} \pm 1.06 \times 10^{-5}$ ^{a}	$4.81 \times 10^{-5} \pm 2.06 \times 10^{-6}$ ^{c}	$5.22 \times 10^{-5} \pm 3.88 \times 10^{-6}$ ^{b}
Creatinine	$4.09 \times 10^{-4} \pm 3.75 \times 10^{-5}$ ^{b}	$5.10 \times 10^{-4} \pm 1.85 \times 10^{-5}$ ^{a}	$3.89 \times 10^{-4} \pm 3.31 \times 10^{-5}$ ^{b}	$4.39 \times 10^{-4} \pm 5.10 \times 10^{-5}$ ^{b}
Leucine	$1.02 \times 10^{-3} \pm 1.06 \times 10^{-4}$ ^{b}	$1.04 \times 10^{-3} \pm 1.31 \times 10^{-4}$ ^{b}	$1.20 \times 10^{-3} \pm 6.79 \times 10^{-5}$ ^{a}	$1.01 \times 10^{-3} \pm 2.07 \times 10^{-4}$ ^{ab}
N,N-Dimethylglycine	$8.76 \times 10^{-5} \pm 6.34 \times 10^{-6}$ ^{ab}	$8.59 \times 10^{-5} \pm 1.67 \times 10^{-6}$ ^{ab}	$9.28 \times 10^{-5} \pm 7.15 \times 10^{-6}$ ^{a}	$7.72 \times 10^{-5} \pm 9.42 \times 10^{-6}$ ^{b}
N-Acetylglycine	$7.26 \times 10^{-3} \pm 6.26 \times 10^{-4}$ ^{a}	$4.37 \times 10^{-3} \pm 2.19 \times 10^{-4}$ ^{c}	$6.17 \times 10^{-3} \pm 4.66 \times 10^{-4}$ ^{b}	$3.72 \times 10^{-3} \pm 2.88 \times 10^{-4}$ ^{d}
Pyroglutamate	$9.87 \times 10^{-5} \pm 2.43 \times 10^{-5}$ ^{b}	$1.54 \times 10^{-4} \pm 4.96 \times 10^{-5}$ ^{ab}	$1.28 \times 10^{-4} \pm 2.39 \times 10^{-5}$ ^{ab}	$1.71 \times 10^{-4} \pm 3.51 \times 10^{-5}$ ^{a}
Sarcosine	$1.09 \times 10^{-4} \pm 2.07 \times 10^{-5}$ ^{a}	$7.02 \times 10^{-5} \pm 7.80 \times 10^{-6}$ ^{b}	$1.15 \times 10^{-4} \pm 9.60 \times 10^{-6}$ ^{a}	$7.70 \times 10^{-5} \pm 1.39 \times 10^{-5}$ ^{b}
Threonine	$1.77 \times 10^{-3} \pm 5.64 \times 10^{-4}$ ^{c}	$1.82 \times 10^{-2} \pm 2.38 \times 10^{-3}$ ^{a}	$2.97 \times 10^{-3} \pm 8.43 \times 10^{-4}$ ^{b}	$1.40 \times 10^{-2} \pm 2.77 \times 10^{-3}$ ^{a}
Valine	$3.24 \times 10^{-4} \pm 3.37 \times 10^{-5}$ ^{b}	$3.43 \times 10^{-4} \pm 5.13 \times 10^{-5}$ ^{b}	$4.56 \times 10^{-4} \pm 4.01 \times 10^{-5}$ ^{a}	$3.53 \times 10^{-4} \pm 9.65 \times 10^{-5}$ ^{b}
Carbohydrates				
1,3-Dihydroxyacetone	$2.47 \times 10^{-4} \pm 8.16 \times 10^{-5}$ ^{c}	$2.11 \times 10^{-3} \pm 3.59 \times 10^{-4}$ ^{a}	$3.29 \times 10^{-4} \pm 1.16 \times 10^{-4}$ ^{c}	$1.34 \times 10^{-3} \pm 1.30 \times 10^{-4}$ ^{b}
Arabinose	$1.03 \times 10^{-3} \pm 1.11 \times 10^{-4}$ ^{d}	$3.87 \times 10^{-3} \pm 5.52 \times 10^{-4}$ ^{a}	$1.27 \times 10^{-3} \pm 1.18 \times 10^{-4}$ ^{c}	$2.88 \times 10^{-3} \pm 1.28 \times 10^{-4}$ ^{b}
Fructose	$4.26 \times 10^{-3} \pm 3.94 \times 10^{-4}$ ^{c}	$1.49 \times 10^{-2} \pm 2.23 \times 10^{-3}$ ^{a}	$4.27 \times 10^{-3} \pm 7.27 \times 10^{-4}$ ^{c}	$1.08 \times 10^{-2} \pm 8.65 \times 10^{-4}$ ^{b}
Fucose	$3.78 \times 10^{-4} \pm 1.31 \times 10^{-4}$ ^{b}	$1.34 \times 10^{-4} \pm 9.02 \times 10^{-5}$ ^{c}	$6.55 \times 10^{-4} \pm 8.75 \times 10^{-5}$ ^{a}	$5.03 \times 10^{-4} \pm 1.36 \times 10^{-4}$ ^{ab}
Galactose	$1.11 \times 10^{-2} \pm 5.83 \times 10^{-3}$ ^{a}	$6.69 \times 10^{-3} \pm 2.43 \times 10^{-3}$ ^{ab}	$3.60 \times 10^{-3} \pm 2.59 \times 10^{-3}$ ^{b}	$6.61 \times 10^{-3} \pm 3.95 \times 10^{-3}$ ^{b}
Glucose	$1.09 \times 10^{-3} \pm 4.67 \times 10^{-5}$ ^{c}	$4.06 \times 10^{-3} \pm 6.14 \times 10^{-4}$ ^{a}	$1.15 \times 10^{-3} \pm 8.57 \times 10^{-5}$ ^{c}	$2.70 \times 10^{-3} \pm 2.81 \times 10^{-4}$ ^{b}
Lactose	$1.62 \times 10^{-4} \pm 1.10 \times 10^{-4}$ ^{ab}	$1.79 \times 10^{-4} \pm 5.55 \times 10^{-5}$ ^{a}	$1.13 \times 10^{-4} \pm 5.24 \times 10^{-5}$ ^{bc}	$9.82 \times 10^{-5} \pm 7.20 \times 10^{-5}$ ^{c}
Lactulose	$7.31 \times 10^{-4} \pm 3.83 \times 10^{-5}$ ^{b}	$6.73 \times 10^{-4} \pm 4.68 \times 10^{-5}$ ^{b}	$8.45 \times 10^{-4} \pm 6.54 \times 10^{-5}$ ^{a}	$7.58 \times 10^{-4} \pm 7.95 \times 10^{-5}$ ^{ab}
N-Acetylglucosamine	$4.48 \times 10^{-4} \pm 5.18 \times 10^{-5}$ ^{c}	$3.16 \times 10^{-3} \pm 3.90 \times 10^{-4}$ ^{a}	$4.06 \times 10^{-4} \pm 4.14 \times 10^{-5}$ ^{c}	$1.59 \times 10^{-3} \pm 2.83 \times 10^{-4}$ ^{b}
Xylose	$2.53 \times 10^{-3} \pm 2.64 \times 10^{-3}$ ^{b}	$3.74 \times 10^{-3} \pm 1.32 \times 10^{-3}$ ^{a}	$1.61 \times 10^{-3} \pm 1.17 \times 10^{-3}$ ^{b}	$1.97 \times 10^{-3} \pm 1.58 \times 10^{-3}$ ^{b}
Organic Acids and Derivates				
2-Oxoglutarate	$4.45 \times 10^{-3} \pm 1.31 \times 10^{-3}$ ^{ab}	$4.73 \times 10^{-3} \pm 6.95 \times 10^{-4}$ ^{a}	$3.29 \times 10^{-3} \pm 6.59 \times 10^{-4}$ ^{b}	$3.77 \times 10^{-3} \pm 6.21 \times 10^{-4}$ ^{ab}
Acetate	$1.06 \times 10^{-2} \pm 1.38 \times 10^{-3}$ ^{b}	$1.50 \times 10^{-2} \pm 3.91 \times 10^{-3}$ ^{a}	$9.15 \times 10^{-3} \pm 1.19 \times 10^{-3}$ ^{b}	$1.47 \times 10^{-2} \pm 1.53 \times 10^{-3}$ ^{a}
Acetoacetate	$2.17 \times 10^{-4} \pm 8.57 \times 10^{-6}$ ^{b}	$2.53 \times 10^{-4} \pm 1.93 \times 10^{-5}$ ^{a}	$2.63 \times 10^{-4} \pm 2.24 \times 10^{-5}$ ^{a}	$2.56 \times 10^{-4} \pm 2.31 \times 10^{-5}$ ^{a}
2-Hydroxyisobutyrate	$1.35 \times 10^{-4} \pm 7.39 \times 10^{-5}$ ^{a}	$4.62 \times 10^{-5} \pm 1.43 \times 10^{-5}$ ^{c}	$4.35 \times 10^{-5} \pm 5.26 \times 10^{-6}$ ^{bc}	$1.12 \times 10^{-4} \pm 8.93 \times 10^{-5}$ ^{ab}
Formate	$2.33 \times 10^{-4} \pm 7.00 \times 10^{-5}$ ^{ab}	$2.89 \times 10^{-4} \pm 4.49 \times 10^{-5}$ ^{a}	$1.79 \times 10^{-4} \pm 1.32 \times 10^{-5}$ ^{b}	$3.08 \times 10^{-4} \pm 4.71 \times 10^{-5}$ ^{a}
Malate	$5.37 \times 10^{-3} \pm 1.02 \times 10^{-3}$ ^{ab}	$4.33 \times 10^{-3} \pm 2.73 \times 10^{-4}$ ^{b}	$5.61 \times 10^{-3} \pm 4.28 \times 10^{-4}$ ^{a}	$4.28 \times 10^{-3} \pm 3.35 \times 10^{-4}$ ^{b}
Syringate	$3.62 \times 10^{-4} \pm 3.50 \times 10^{-5}$ ^{ab}	$3.82 \times 10^{-4} \pm 5.26 \times 10^{-5}$ ^{a}	$3.17 \times 10^{-4} \pm 6.70 \times 10^{-6}$ ^{b}	$3.48 \times 10^{-4} \pm 4.08 \times 10^{-5}$ ^{ab}
trans-Aconitate	$1.30 \times 10^{-4} \pm 1.14 \times 10^{-5}$ ^{b}	$1.51 \times 10^{-4} \pm 6.77 \times 10^{-6}$ ^{a}	$1.32 \times 10^{-4} \pm 1.51 \times 10^{-5}$ ^{ab}	$1.45 \times 10^{-4} \pm 1.16 \times 10^{-5}$ ^{ab}
Nucleotides				
Cytidine	$6.89 \times 10^{-5} \pm 1.12 \times 10^{-5}$ ^{b}	$5.01 \times 10^{-5} \pm 1.14 \times 10^{-5}$ ^{c}	$1.04 \times 10^{-4} \pm 2.60 \times 10^{-5}$ ^{a}	$5.87 \times 10^{-5} \pm 1.81 \times 10^{-5}$ ^{bc}
Guanosine	$4.29 \times 10^{-5} \pm 8.18 \times 10^{-6}$ ^{ab}	$3.44 \times 10^{-5} \pm 5.79 \times 10^{-6}$ ^{b}	$8.43 \times 10^{-5} \pm 3.19 \times 10^{-5}$ ^{a}	$4.04 \times 10^{-5} \pm 1.35 \times 10^{-5}$ ^{ab}
Uracil	$3.20 \times 10^{-4} \pm 1.12 \times 10^{-4}$ ^{ab}	$2.90 \times 10^{-4} \pm 5.42 \times 10^{-5}$ ^{b}	$3.84 \times 10^{-4} \pm 1.05 \times 10^{-5}$ ^{a}	$2.66 \times 10^{-4} \pm 8.02 \times 10^{-5}$ ^{b}
Uridine	$8.52 \times 10^{-4} \pm 2.03 \times 10^{-4}$ ^{b}	$4.39 \times 10^{-4} \pm 5.22 \times 10^{-5}$ ^{d}	$1.40 \times 10^{-3} \pm 3.24 \times 10^{-4}$ ^{a}	$6.13 \times 10^{-4} \pm 2.22 \times 10^{-4}$ ^{c}
Alcohols				
Ethanol	$4.23 \pm 5.46 \times 10^{-2}$ ^{ab}	$4.58 \pm 2.60 \times 10^{-2}$ ^{a}	$3.96 \pm 3.13 \times 10^{-2}$ ^{b}	$4.26 \pm 9.75 \times 10^{-2}$ ^{b}
Glycerol	$1.33 \times 10^{-1} \pm 2.23 \times 10^{-2}$ ^{ab}	$1.40 \times 10^{-1} \pm 9.15 \times 10^{-3}$ ^{a}	$1.16 \times 10^{-1} \pm 1.09 \times 10^{-2}$ ^{b}	$1.24 \times 10^{-1} \pm 2.77 \times 10^{-2}$ ^{ab}
Methanol	$3.89 \times 10^{-3} \pm 1.06 \times 10^{-3}$ ^{d}	$5.82 \times 10^{-2} \pm 7.64 \times 10^{-3}$ ^{a}	$5.56 \times 10^{-3} \pm 1.80 \times 10^{-3}$ ^{c}	$3.52 \times 10^{-2} \pm 4.33 \times 10^{-3}$ ^{b}
myo-Inositol	$2.35 \times 10^{-2} \pm 1.51 \times 10^{-3}$ ^{a}	$2.08 \times 10^{-2} \pm 1.45 \times 10^{-3}$ ^{b}	$2.36 \times 10^{-2} \pm 2.05 \times 10^{-3}$ ^{a}	$1.98 \times 10^{-2} \pm 1.58 \times 10^{-3}$ ^{b}
Miscellaneous				
4-Hydroxy-3-methoxymandelate	$2.90 \times 10^{-4} \pm 1.78 \times 10^{-5}$ ^{a}	$2.23 \times 10^{-4} \pm 3.13 \times 10^{-5}$ ^{b}	$1.77 \times 10^{-4} \pm 3.79 \times 10^{-5}$ ^{c}	$1.56 \times 10^{-4} \pm 2.28 \times 10^{-5}$ ^{c}
4-Hydroxyphenylacetate	$8.21 \times 10^{-4} \pm 9.09 \times 10^{-5}$ ^{a}	$6.70 \times 10^{-4} \pm 4.87 \times 10^{-5}$ ^{b}	$8.09 \times 10^{-4} \pm 6.39 \times 10^{-5}$ ^{a}	$7.37 \times 10^{-4} \pm 9.83 \times 10^{-5}$ ^{ab}
Acetoin	$4.77 \times 10^{-4} \pm 3.74 \times 10^{-4}$ ^{a}	$6.81 \times 10^{-5} \pm 4.99 \times 10^{-5}$ ^{b}	$7.14 \times 10^{-5} \pm 7.71 \times 10^{-6}$ ^{ab}	$3.81 \times 10^{-4} \pm 4.33 \times 10^{-4}$ ^{a}
Dimethyl sulfone	$6.62 \times 10^{-5} \pm 6.18 \times 10^{-6}$ ^{ab}	$6.62 \times 10^{-5} \pm 5.91 \times 10^{-6}$ ^{ab}	$7.60 \times 10^{-5} \pm 5.90 \times 10^{-6}$ ^{a}	$6.54 \times 10^{-5} \pm 3.51 \times 10^{-6}$ ^{b}
Epicatechin	$9.40 \times 10^{-5} \pm 3.16 \times 10^{-5}$ ^{a}	$1.02 \times 10^{-4} \pm 1.54 \times 10^{-5}$ ^{a}	$6.61 \times 10^{-5} \pm 1.42 \times 10^{-5}$ ^{b}	$6.29 \times 10^{-5} \pm 4.20 \times 10^{-6}$ ^{b}
Ethanolamine	$5.13 \times 10^{-4} \pm 4.25 \times 10^{-5}$ ^{ab}	$5.04 \times 10^{-4} \pm 1.64 \times 10^{-5}$ ^{ab}	$5.64 \times 10^{-4} \pm 3.59 \times 10^{-5}$ ^{a}	$4.89 \times 10^{-4} \pm 1.60 \times 10^{-5}$ ^{b}
Fumarate	$4.62 \times 10^{-5} \pm 9.41 \times 10^{-6}$ ^{ab}	$4.62 \times 10^{-5} \pm 6.10 \times 10^{-6}$ ^{a}	$4.13 \times 10^{-5} \pm 2.23 \times 10^{-6}$ ^{ab}	$4.48 \times 10^{-5} \pm 1.82 \times 10^{-5}$ ^{b}
Hydroxyacetone	$5.49 \times 10^{-5} \pm 6.32 \times 10^{-6}$ ^{c}	$1.58 \times 10^{-4} \pm 3.08 \times 10^{-5}$ ^{a}	$6.40 \times 10^{-5} \pm 4.68 \times 10^{-6}$ ^{c}	$1.15 \times 10^{-4} \pm 2.03 \times 10^{-5}$ ^{b}
Hypoxanthine	$1.10 \times 10^{-4} \pm 1.39 \times 10^{-4}$ ^{b}	$7.18 \times 10^{-5} \pm 3.25 \times 10^{-5}$ ^{ab}	$2.00 \times 10^{-4} \pm 1.37 \times 10^{-4}$ ^{a}	$7.53 \times 10^{-5} \pm 2.63 \times 10^{-5}$ ^{ab}
Pantothenate	$7.21 \times 10^{-4} \pm 1.37 \times 10^{-4}$ ^{b}	$2.29 \times 10^{-3} \pm 6.95 \times 10^{-4}$ ^{a}	$5.61 \times 10^{-4} \pm 8.57 \times 10^{-5}$ ^{b}	$1.53 \times 10^{-3} \pm 3.69 \times 10^{-4}$ ^{a}
N-Acetylserotonin	$1.19 \times 10^{-4} \pm 3.39 \times 10^{-5}$ ^{a}	$1.00 \times 10^{-4} \pm 2.11 \times 10^{-5}$ ^{ab}	$7.97 \times 10^{-5} \pm 2.46 \times 10^{-5}$ ^{b}	$8.16 \times 10^{-5} \pm 1.89 \times 10^{-5}$ ^{b}
N-Nitrosodimethylamine	$8.07 \times 10^{-6} \pm 2.52 \times 10^{-6}$ ^{c}	$7.98 \times 10^{-6} \pm 2.02 \times 10^{-6}$ ^{bc}	$1.17 \times 10^{-5} \pm 1.67 \times 10^{-6}$ ^{a}	$9.88 \times 10^{-6} \pm 3.05 \times 10^{-6}$ ^{ab}
Oxypurinol	$1.02 \times 10^{-4} \pm 1.30 \times 10^{-4}$ ^{b}	$6.05 \times 10^{-5} \pm 2.70 \times 10^{-5}$ ^{b}	$2.06 \times 10^{-4} \pm 1.00 \times 10^{-4}$ ^{a}	$7.27 \times 10^{-5} \pm 1.99 \times 10^{-5}$ ^{ab}
Propylene	$8.73 \times 10^{-3} \pm 1.85 \times 10^{-3}$ ^{ab}	$5.75 \times 10^{-3} \pm 1.07 \times 10^{-3}$ ^{c}	$1.07 \times 10^{-2} \pm 1.15 \times 10^{-3}$ ^{a}	$7.48 \times 10^{-3} \pm 2.30 \times 10^{-3}$ ^{bc}
sn-Glycero-3-phosphocholine	$8.21 \times 10^{-5} \pm 1.86 \times 10^{-5}$ ^{a}	$5.45 \times 10^{-5} \pm 8.69 \times 10^{-6}$ ^{bc}	$6.81 \times 10^{-5} \pm 1.69 \times 10^{-5}$ ^{ab}	$4.78 \times 10^{-5} \pm 4.60 \times 10^{-6}$ ^{c}
Tartrate	$1.49 \times 10^{-5} \pm 4.69 \times 10^{-6}$ ^{b}	$1.82 \times 10^{-4} \pm 5.00 \times 10^{-5}$ ^{a}	$1.28 \times 10^{-5} \pm 3.10 \times 10^{-6}$ ^{b}	$8.71 \times 10^{-5} \pm 2.36 \times 10^{-5}$ ^{a}
Xanthine	$1.13 \times 10^{-4} \pm 2.15 \times 10^{-5}$ ^{ab}	$7.09 \times 10^{-5} \pm 1.38 \times 10^{-5}$ ^{c}	$1.79 \times 10^{-4} \pm 3.87 \times 10^{-5}$ ^{a}	$9.90 \times 10^{-5} \pm 2.97 \times 10^{-5}$ ^{bc}

*Data are displayed as mean ± standard deviation (n = 5). For each molecule, sd values followed by a common superscript identify no significant differences.

processing industry, such as fruit wine production, peels are often discarded or utilized as animal feed without harnessing their rich aromatic components and bioactive compounds (Liang, Zhang, & Fang, 2022). In this respect, the current study not only sheds lights on the KW process optimization, but also presents innovative approaches for the reduction and utilization of winemaking by-products.

Sensory evaluation revealed that KW produced through KCP method received the highest total score, primarily attributed to its superior overall acceptability and color. Conversely, KW produced through KJW method obtained the lowest scores for aroma and mouthfeel indicators, mainly due to higher perceived sourness and bitterness. Both of these taste characteristics have been reported to have a negative impact on wine quality (Bi, Li, & Wang, 2019; Cosme, Filipe-Ribeiro, & M. Nunes, 2021). In this study, the various pretreatment methods of KW were

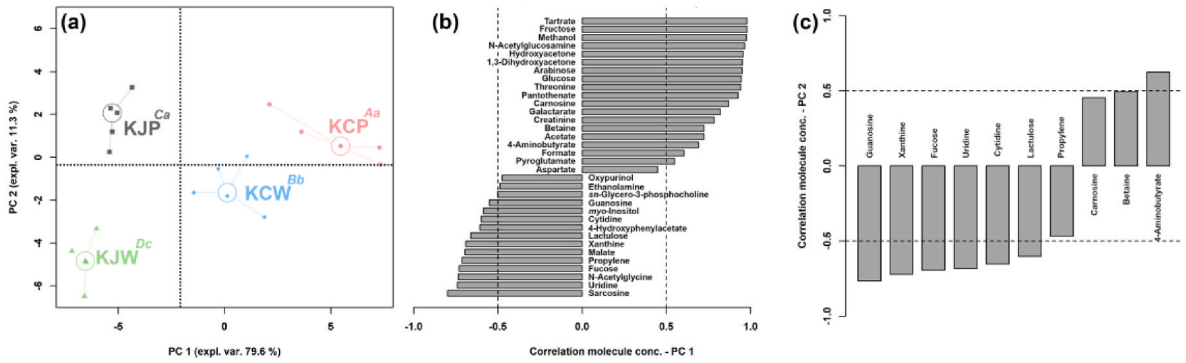

Fig. 4. RPCA model calculated on the basis of molecules' concentrations showing significant differences characterized by ^{1}H NMR among groups representing Scoreplot (a) and Loading plot (b and c). The median of each group is denoted by a wide and empty circle. Superscript capital and lowercase letters indicate significant differences along PC 1 and PC 2, respectively.

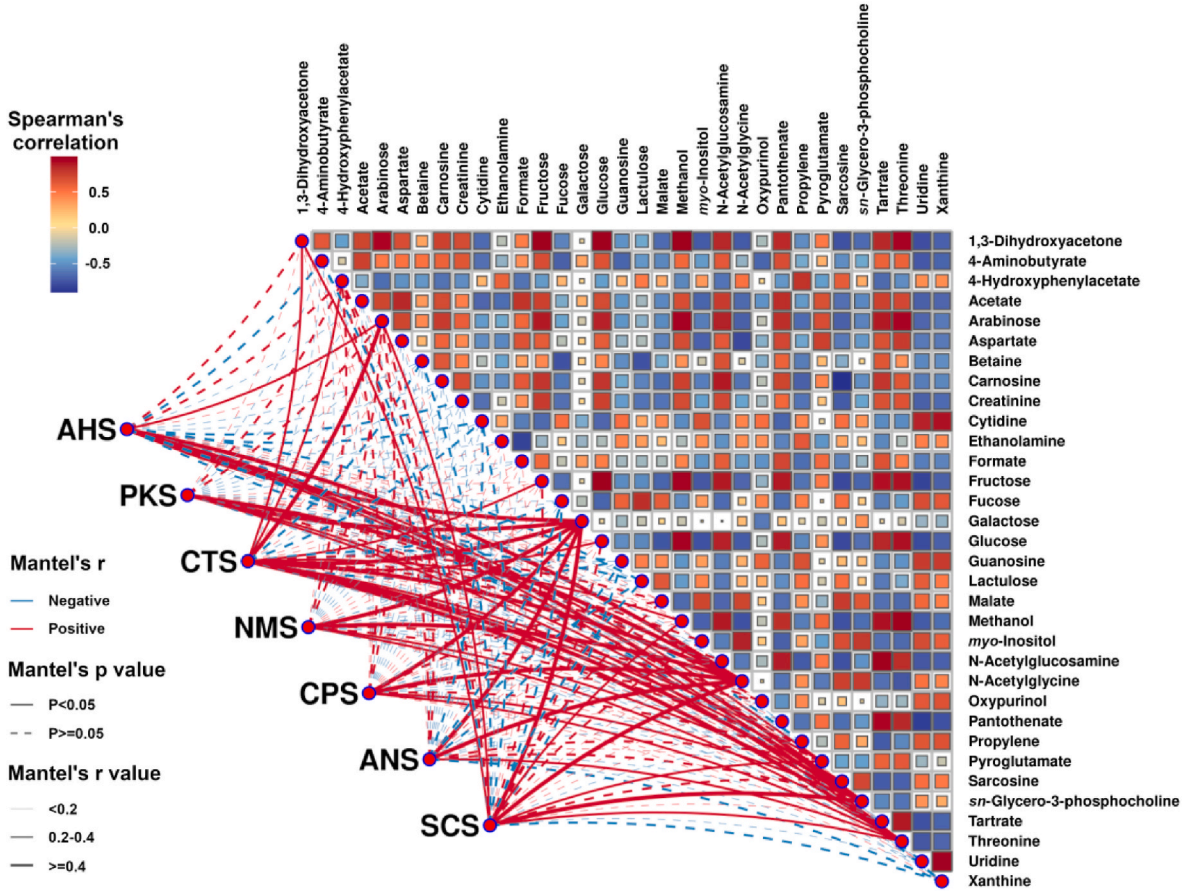

Fig. 5. Correlations between molecules quantified by ^{1}H NMR and E-tongue sensor responses in KW. Negative and positive correlations between molecules are indicated in blue and red in the upper triangular heat map. Width and type of line indicate *r* and *p* values of Mantel correlations between molecules' levels and E-tongue sensor responses, respectively. Blue and red colors of the lines indicate negative and positive correlations between E-tongue sensor responses and molecules' levels. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

effectively differentiated using E-tongue analysis. Moreover, its findings were consistent with these results, as KW produced through KJW method showed the highest response value for SCS, which is primarily sensitive to bitterness. On one side, such phenomenon could be linked to significantly higher levels of bitter amino acids (such as leucine, valine and phenylalanine) in KJW group. On the other side, it could also be related to synergistic effects among subthreshold bitter compounds, as suggested by Estier et al. (Estier & Marchal, 2024).

Sugars, as one of the extensively studied classes of compounds in fruit wines, not only influence yeast metabolism but also impact the sensory perception and flavor profile of fruit wines (Horváth, Sárdy, Kellner, & Magyar, 2020; Sirén, Sirén, & Sirén, 2015). In this study, a total of ten sugars were characterized using ^{1}H NMR. Among them, the concentrations of galactose and glucose exhibited significant variations among the groups. Glucose can originate from kiwifruit itself or be produced by hydrolysis of sucrose (Huang et al., 2022). The differences among four groups may be attributed to the effect of different fermentation substrates (with/without peel and pomace) that could have altered the metabolic ability of yeasts (Apolinar-Valiente et al., 2014).

Organic acids, which contribute to the sourness of fruit wine, can

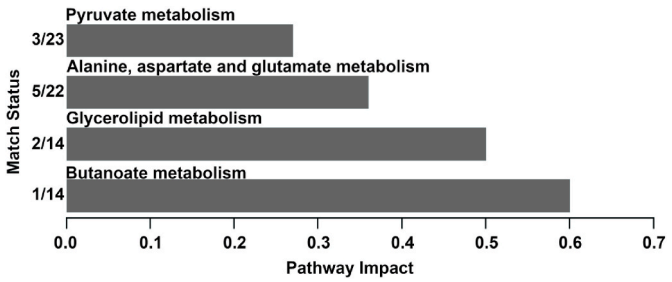

Fig. 6. Pathways of metabolism were assessed by enrichment analysis based on statistically significant quantified molecules (impact value > 0.2) in four groups of KW samples.

impact both its sensory quality and chemical properties (Loira et al., 2015). An increased organic acid content may enhance the stability of vitamin B and influence the interaction between organic acids and aroma compounds (Li et al., 2021). Acetate, a flavor-active compound commonly present in fruit wines, is synthesized via the acetate kinase pathway in the phosphogluconate pathway and through the metabolism of citric acid (Peng, Meng, Yue, Wang, & Gao, 2021). Moreover, Acetate is among the most important volatile acids produced by yeast, arising from the irreversible oxidation of acetaldehyde to acetic acid catalyzed by Ald6 (Peng et al., 2021). In this study, KW produced by KCP method exhibited the highest concentration of acetate, as determined by ^{1}H NMR. Variations in acetate concentration among different groups were linked to the presence of pomace, which affected yeast metabolism. On the other side, decanoic acid, octanoic acid and other medium-chain fatty acids may impart soapy and acidic notes to fermented beverages, and in turn potentially diminishing their sensory quality (Ye, Yue, & Yuan, 2014). Phenolic acids exhibited higher levels in peel compared to pomace (Beres et al., 2017; Soquetta et al., 2016). Their concentrations in fruit wine could be affect by several factors, such as destemming, pressing and maceration (Ky, Lorrain, Kolbas, Crozier, & Teissedre, 2014). Production with peel yielded more phenolic acids in KW, which was partly attributed to peel maceration facilitating the entry and retention of phenolic acids from the peel into KW.

Epicatechin, a flavonoid and monomeric form of flavanols, plays a role in stabilizing the color and organoleptic characteristics of wines, particularly astringency and bitterness. In this study, the content of epicatechin was higher in KW produced by KCP pretreatment, which is consistent with the findings of Zhu et al. (Zhu et al., 2019). Such differences could be linked to polymerization reactions, formation of oxidation products and to the formation of precipitate in distinct groups (Revilla & González-SanJosé, 2003).

Esters, known for imparting fruity aromas, are commonly formed during fruit wine fermentation, playing a pivotal role in the overall aroma profile. Their content and composition are primarily linked to enzymatic synthesis by yeast (Mencher, Morales, Curiel, Gonzalez, & Tronchoni, 2021) and by lactic acid bacteria's metabolism during malolactic fermentation (Antalick, Perello, & De Revel, 2012). In our study, esters were detected by GC-IMS as the predominant compounds in KW samples, in agreement with Qi et al. (Yiman, Miaomiao, Kun, & Mingtao, 2019). Even if esters are mainly derived from microorganisms' activity, a few could originate from kiwifruit itself, such as ethyl hexanoate (Zhao et al., 2021) and methyl acetate (Lan et al., 2021). KW produced via KCP method exhibited higher ester contents compared to the other groups. This is particularly true for ethyl octanoate, giving a desirably rich fruity aroma, therefore contributing to the high sensory score of the samples pertaining to the KCP group (Muñoz-Redondo et al., 2021; Zhao et al., 2020). Additionally, several esters, namely ethyl valerate, isoamyl butyrate and phenylethyl acetate were found to play crucial roles in distinguishing KW produced by different pretreatment methods, with isoamyl butyrate notably enhancing fruity and sweet aromas.

Alcohols, akin to esters, are another class of compounds known to contribute to the flavor profile of wines, which are primarily synthesized through yeast metabolism during fermentation (Lan et al., 2022; Varavuth, Jiraratananon, & Atchariyawut, 2009). Huang et al. identified 3-methyl-1-butanol and butanol in KW by means of GC-MS, which is in line with our results (Huang et al., 2022). In addition, it is worth noting that certain alcohols are negatively correlated with wine flavor. For instance, 1-propanol is characterized by a musty flavor and associated with lower-quality wines (Gambetta et al., 2017).

5. Conclusion

This study presents a comprehensive characterization of the sensory attributes and flavor profiles of KW produced by different pretreatment methods, employing a combination of sensory evaluation, E-tongue, GC-IMS and ^{1}H NMR. The integration of multiple techniques has been shown to yield a more comprehensive flavor fingerprint compared to single techniques. Our results of sensory evaluation and E-tongue analyses reveal distinctive flavor characteristics among KW produced by various pretreatment methods. Notably, KW produced via KCP method achieved the highest sensory scores, significantly higher levels of acetate, epicatechin, ethyl octanoate, ethyl valerate, isoamyl butyrate, phenylalanine, leucine and valine, positioning it as a potential contender for KW production. Further studies could pay attention to comprehensively evaluate the effects of different pretreatments on KW quality through multi-Omics approaches. Anyway, these findings not only shed lights on the KW process optimization, but also present innovative approaches for the reduction and utilization of winemaking by-products.

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CRediT authorship contribution statement

Zhibo Yang: Writing – review & editing, Writing – original draft, Investigation, Formal analysis. **Qiuyu Lan:** Writing – review & editing, Writing – original draft. **Xiaoyu Liu:** Writing – review & editing. **Zijian Cai:** Writing – review & editing. **Rui Zeng:** Writing – review & editing. **Junni Tang:** Writing – review & editing. **Xiaole Jiang:** Writing – review & editing. **Chenglin Zhu:** Writing – review & editing, Writing – original draft, Supervision, Methodology, Funding acquisition, Conceptualization. **Bin Hu:** Writing – review & editing. **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.2024.116375.

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