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Effects of *S. cerevisiae* strains on the sensory characteristics and flavor profile of kiwi wine based on E-tongue, GC-IMS and ^{1}H-NMR

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ABSTRACT

The fermentation of kiwifruit into kiwi wine (KW) can represent a strategy to reduce the economic losses linked to fruits imperfections, spoilage, over production and seasonality. In the study, Pujiang kiwifruit, a China National Geographical Indication Product, was used as raw material to produce KW fermented by four commercial *S. cerevisiae* strains, namely Drop Acid Yeast, DV10, SY and RW. The sensory characteristics and flavor profile of KW were assessed by means of sensory evaluation, E-tongue, GC-IMS and ^{1}H-NMR. KW fermented by RW strain obtained the higher sensory evaluation score. E-tongue could clearly distinguish the taste differences of KW fermented by distinct *S. cerevisiae* strains. A total of 128 molecules were characterized by GC-IMS and ^{1}H-NMR, indicating that the combinations of multiple technologies could provide a comprehensive flavor profile of KW. The main flavor compounds in KW pertained to the classes of esters and alcohols. Several pathways were found to be differently altered by the fermentation with the different yeast strains, namely butanoate metabolism, glycerolipid metabolism, alanine, aspartate and glutamate metabolism, arginine biosynthesis, arginine and proline metabolism. The present study will facilitate screening suitable S. cerevisiae strains for KW production and provide a theoretical basis for large-scale production of KW.

1. Introduction

Kiwifruit, native to southwestern China (Wang et al., 2021), is popular among consumers due to its high nutritional value and unique flavor (Sanz et al., 2021). In recent years, from the perspective of cultivation area and production amounts, China holds the top position globally (Baglieri et al., 2023), with inherently associated risks such as economic losses linked to over production, seasonality or below standards fruits (Kumarihami et al., 2022). Therefore, the development of innovative kiwifruit-based products should be considered of primary importance to increase its economic value, and in turn counterbalance economic losses (Lan et al., 2022).

As one of the main kiwifruit-related products, kiwi wine (KW) is a low-alcoholic beverage produced by *S. cerevisiae* fermentation of kiwifruit. It has been confirmed that KW could retain a high portion of vitamin C and polyphenols of the fresh kiwifruit, leading to a bioactivity higher than other kiwifruit products (Ma et al., 2019). Furthermore, its low alcohol content caters to the preferences of consumers seeking low-alcohol beverages, thereby presenting a wide range of market opportunities. (Varela & Varela, 2019).

Till now, numerous researchers have mainly investigated the consequences of kiwifruit varieties and fermentation parameters on the quality of KW. For instance, recent studies found that kiwifruit varieties could affect KW's antioxidant properties, enzymatic activity and volatile compounds (VOCs) (Huang et al., 2021; Zhao et al., 2020). Moreover, adding glutathione-enriched inactive dry yeast could improve the nutritional properties, color and VOCs of KW (Q. Liu, D., Xu, et al., 2020; X. Liu, D., Xu, et al., 2020).

It is worth to notice that yeasts' metabolism is crucial in determining the quality of the final product (Maicas, 2020; Zhao et al., 2020; Zhong et al., 2020, p. 25), so that the replacement of spontaneous yeasts with commercial counterparts seems appropriate in order to obtain products with consistent and efficiently reproducible characteristics (Molinet & Cubillos, 2020). A confirmation comes from the observation that

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commercial yeasts are now widely used for the fermentation of wines from fruits such as apple (Maslov Bandić et al., 2019), pear (Yang et al., 2019) and pomegranate (Kokkinomagoulos et al., 2020) wines. Indeed, several remarkable studies suggested that different yeast strains could shape the flavor of wine, in connection to numerous molecules produced by yeast metabolism (Sgouros et al., 2020; Sherman et al., 2020). Despite the importance of yeasts, studies have been rarely devoted to the selection of suitable commercial strains for KW fermentation, in particular from a flavor profile point of view.

Flavor (the combination of taste, aroma and chemical composition) is one of the most important features of wine, which is an essential driver of the consumers' preferences (Wu et al., 2023). Owing to the complexity of wine flavor profile, it is not possible to obtain a comprehensive fingerprint of KW flavor profile through single technique. Gas chromatography-ion mobility spectrometry (GC-IMS) is able to optimally reflect the flavor status of samples, compared to gas chromatography-mass spectrometry (GC-MS) (Martín-Gómez et al., 2019), which is another frequently applied technique to analyze the flavor profile of wines (Li et al., 2022; Zhang et al., 2023). At present, GC-IMS has been widely used for the study of the wine flavor (Xiao et al., 2020), such as yellow wine (Peng et al., 2022), yellow-fleshed peach wine (Liu et al., 2022) and cherry wine (Niu et al., 2019). Proton nuclear magnetic resonance spectroscopy (^{1}H-NMR) has enriched the study possibilities in the field of wine science, by granting pieces of information about yeasts metabolism (Le Mao et al., 2021; Perruchon et al., 2021) and wine chemistry (Bambina et al., 2022; Le Mao et al., 2023). Sensory evaluations by trained panelists could be conveniently integrated by the objective evaluation granted by E-tongue, a type of artificial sensory technology that simulates human taste mechanisms. It can grab the overall taste features of the samples and distinguish subtle differences in taste among samples (Lan et al., 2017; Yuan et al., 2023). However, despite the potentialities of the above-mentioned techniques, they have been rarely applied to the study of kiwi wine's flavor profile.

In order to fill such gaps, in the current study, we used Pujiang kiwifruit, a China National Geographic Indication product, as raw material to produce KW fermented by four commercial strains of *S. cerevisiae*, namely Drop Acid Yeast, DV10, SY and RW. The sensory characteristics and flavor profile were evaluated taking advantages of the combination of sensory evaluation, E-tongue, GC-IMS and ^{1}H-NMR. This study will facilitate screening suitable S. cerevisiae strains for KW production and provide a theoretical basis for large-scale production of KW.

2. Materials and methods

2.1. Materials and solvents

Pujiang Kiwifruit, harvested in October 2022 weighting about 100 g each, were purchased from a planting site in Pujiang, Sichuan China (30°05′-30°21′ N, 103°19′-103°41′ E), awarded with the China National Geographic Indication Product designation in 2010. *S. cerevisiae* strain SY (SY) and RW (RW) was purchased from Angel Yeast CO., LTD (China). *S. cerevisiae* strain Drop Acid Yeast (DB) and DV10 (LA) were purchased from Yantai Diboshi CO., LTD (China) and Lallemand CO., LTD (China), respectively. Analytical grade chemicals were used in the analysis.

2.2. KW samples

All freshly harvested kiwifruits selected for the study were promptly transported to the laboratory. Upon arrival, the kiwifruits underwent a series of procedures including washing, peeling, and pressing using a laboratory pilot press in order to extract the kiwifruit juice. According to the suggestion of Liang et al. (Liang et al., 2022, p. 604), we added equal proportions of deionized water to kiwifruit juice to promote the release of VOCs during fermentation. The total fermentation volume was 200 mL. As suggested by Zhou et al., to attain an initial sugar content of 23 °Brix, sucrose was added, and to prevent browning, potassium metabisulfite (70 mg/L) and citric acid were incorporated (Zhou et al., 2023). Following this, pectinase (0.02 g/L, 100,000 U/g, SAS SOFRALAB, France) was introduced to facilitate the release of cell contents. The mixture was then subjected to a 40 °C water bath for 2 h. Subsequently, the pH of the liquid was adjusted to 4 by adding citric acid and calcium carbonate. Finally, yeast (0.2 g/L, suitable fermentation temperature 25 °C) was added to the mixture, which was then maintained at 25 ± 1 °C for a duration of 30 days. Each yeast strain was subjected to five replicate fermentations, while all other fermentation conditions remained constant. Upon completion of the fermentation process, the KW samples were filtered using triple layer sterile gauze. All KW samples were stored at −80 °C until further analysis.

2.3. Sensory evaluation

Prior to sensory evaluation, the physicochemical features of KW were measured by pH meter (PHS-3E, Shanghai, China) and Calorie Answer™ (CA-HM, JWP, Japan). Sensory evaluation was performed following the method of Huang et al. (Huang et al., 2022). The sensory assessment panel consisted of 10 trained adults (5 males and 5 females). Samples were randomly placed in disposable paper cups. The participating testers evaluated KW samples based on color, aroma, taste, flavor persistence and overall acceptability. For each characteristic, a nine-point scale was applied. After each sensory assessment, the testers were required to rinse off with drinking water.

2.4. E-tongue analysis

All samples were analyzed using an α-Astree E-tongue (Alpha MOS, France) with seven potentiometric chemical sensors and an automatic sampler. The sensors were specifically sensitive to sweetness (ANS), saltiness (CTS), umami (NMS), sourness (AHS), bitterness (SCS) and two reference electrodes (PKS and CPS) respectively (Wang et al., 2021).

An 80 mL sample of KW was placed in a special beaker for E-tongue analysis. The signal acquisition time, stirring time rate and analysis time were set to 120 s, 60 rpm and 3 min, respectively. After each analysis, the sensors were washed thoroughly with deionized water for 30 s. The output value was obtained between 100 and 120 s. Following the suggestions of Zhao et al. (Zhao et al., 2023), with the aim of minimizing errors, each sample was replicated eight times and the last five stable measurements were chosen for data mining. The average value for each sample was used as a base for robust principal component analysis (rPCA) multivariate analysis.

2.5. GC-IMS analysis

GC-IMS analysis was performed following the method of Liu et al. (Liu et al., 2022). The VOCs of KW samples were characterized through a GC-IMS (Flavorspec®, G.A.S. Instrument, Germany) with an MXT-WAX capillary column (30 m × 0.53 mm × 1 μm) (Restek, United States). 1.5 mL of each KW sample were taken to a 20 mL headspace vial with a magnetic screw seal cover, and incubated at 60 °C for 10 min. Subsequently, 100 μL of the headspace sample were automatically injected into the injector (no split mode) using a heated syringe at 85 °C. The temperatures of column and drift tube were maintained at 60 °C and 45 °C, respectively. Drift gas flow rate was set to 150 mL/min. A high-purity nitrogen carrier gas (99.999% purity) was used, and the GC column flow rate was programmed in accordance with the following program: 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. In accordance with the previous studies (Liu et al., 2023; Wang et al., 2022), the retention index (RI) of VOCs were calculated using n-ketone C_4–C_9 as a reference. VOCs were identified by comparing their RI and ions' drift time with those of the standards in the GC-IMS library. Each sample was

tested once, and the relative quantification of each VOC was based on its peak intensity. The three-dimensional (3D) topographic plots, two-dimensional (2D) difference plots, and gallery plots were built using the Laboratory Analytical Viewer, Reporter and Gallery Plot provided by GC-IMS instrument.

2.6. ^{1}H-NMR analysis

The ^{1}H-NMR analysis was conducted using a method previously described (Zhu et al., 2023), pictorially represented in Fig. S1. Briefly, an amount of 0.5 mL of KW sample were centrifuged for 15 min (18630 g, 4 °C) to remove solid residues. Then, 0.35 mL of supernatant, 0.35 mL of bi-distilled water, and 100 μL of NMR analysis solution were mixed and centrifuged under the above conditions, as shown in Fig. S1 (a).

A 600.13 MHz AVANCE III spectrometer (Bruker, Wuhan, China) at 298 K was used in order to obtain ^{1}H-NMR spectra of KW samples. The main analysis conditions are shown in Fig. S1 (b). Following Zhu et al. (Zhu et al., 2022, p. 1536), phase adjustment was performed for each spectrum by Topspin software (version 4.2), and subsequent spectral processing and molecule quantification were performed by specialized R language scripts. As displayed in Fig. S1 (c), the baseline of the spectra was adjusted via peak detection after residual water signal removal, taking advantage of "rolling ball" algorithm included in the R baseline package. Probabilistic quotient normalization (PQN) was performed to the whole spectral array to eliminate protein and water content differences among samples. Molecule identifications were conducted by comparing their multiplicity and chemical shift with the standard compound spectra available in the Chenomx library (Chenomx Inc., Canada, ver 8.4). For each molecule, the signals were integrated using rectangular integration.

2.7. Statistical analysis

The statistical analysis was conducted using the R computational language. Prior to performing univariate analyses, the data distribution was transformed to achieve normality, following the method proposed by Box and Cox (Box & Cox, 2018). ANOVA was performed to find significant differences in the E-tongue sensors response and flavor profile from different groups, respectively, followed by Tukey HSD post hoc test ($p < 0.05$). rPCA models were used to obtain a holistic view of the trends in the flavor profile of the samples. For each rPCA model, we calculated a scoreplot and a Pearson correlation plot based on the loadings.

Pathway analysis was conducted by the online platform MetaboAnalyst 5.0 (https://www.metaboanalyst.ca). Spearman correlation analysis was setup using the online tool (https://www.omicstudio.cn) to determine correlations between E-tongue and ^{1}H-NMR.

3. Results

3.1. Sensory evaluation and E-tongue analysis of KW

The physicochemical values of KW were reported in Table S1. In terms of sensory analysis, the KW fermented by RW had the highest overall sensory evaluation score, with high scores for aroma, mouthfeel and overall acceptability, as shown in Fig. 1 (a). The lowest overall score was registered for KW fermented by SY strain. For the purpose of obtaining an overview of the taste characteristics of KW, an rPCA model was performed, as shown in Fig. 1 (b) and (c).

In Fig. 1 (b), the first PC accounted for 91% of the variance of the entire samples' set, thus nicely summarizing the overall features of the samples. Samples pertaining to different groups appeared at significantly different positions along PC 1 ($p < 0.05$), with KW fermented by SY showing the highest response values of AHS and SCS and the lowest values of ANS, PKS, CPS and CTS.

3.2. GC-IMS analysis

The processing's pipeline of GC-IMS information on the VOCs in KW fermented by different yeast strains is summarized in Fig. 2.

As shown in Fig. 2 (a), the 3D topographic graph offers a convenient visual representation of how the wines fermented by different strains differ in various sections of the GC-IMS spectrum. Fig. 2 (b) shows the point-by-point differences among samples from the four groups. The main differences regarded features in the range of retention time from 200 to 1200 s. The gallery plot (Fig. 2(c)) shows that VOCs from KW fermented by different yeast strains mainly pertained to the classes of esters and aldehydes. In detail, a total of 52 VOCs were characterized in the samples, including esters (22), aldehydes (9), alcohols (6), ketones (5), acids (4) and others (6), as shown in Table 1.

Among the characterized molecules, 32 VOCs showed significant differences among the four groups. To highlight the overall trend of the above VOCs, an rPCA model was built based on their peak intensities, as shown in Fig. 3.

As shown in Fig. 3 (a), PC 1 accounted for as much as 93.2% of the entire samples' set variability and nicely summarized the differences among the groups. In detail, the highest levels of isoamyl acetate, ethyl hexanoate, (E,E)-2,4-heptadienal, ethyl heptanoate, 4-methyl-2-pentanone, methyl 2-furoate, valeraldehyde, 1-octen-3-one and methyl acetate were quantified in KW fermented by RW. In contrast, the highest amounts of 2-heptanol, 1-pyrazinylethanone, 2-isobutyl-3-methoxypyrazine, diethyl malonate, methyl phenylacetate, butyl propanoate, propyl hexanoate, 2-methylbutyric acid, 2-methyl-2-pentenal, 4-isopropylbenzaldehyde, 1-propanol, 2-butoxyethanol and methyl isovalerate were detected in LA group.

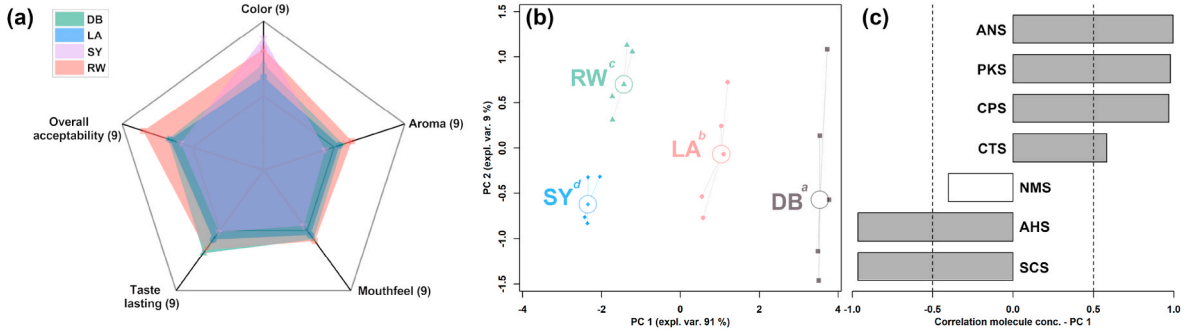

Fig. 1. (a) Radar chart of scores for sensory evaluation of KW fermented by four yeast strains; rPCA model was setup based on E-tongue sensor response values. The scoreplot (b) displays the samples from the four groups as follows: squares (DB), circles (LA), triangles (RW), and diamonds (SY). Each sample group's median is represented by a wide and empty circle and the superscript lowercase letters indicate the significance of the samples along PC 1. The loading plot (c) displays the correlation between the response values and their importance over PC 1. Gray bars indicate significant correlations ($p < 0.05$).

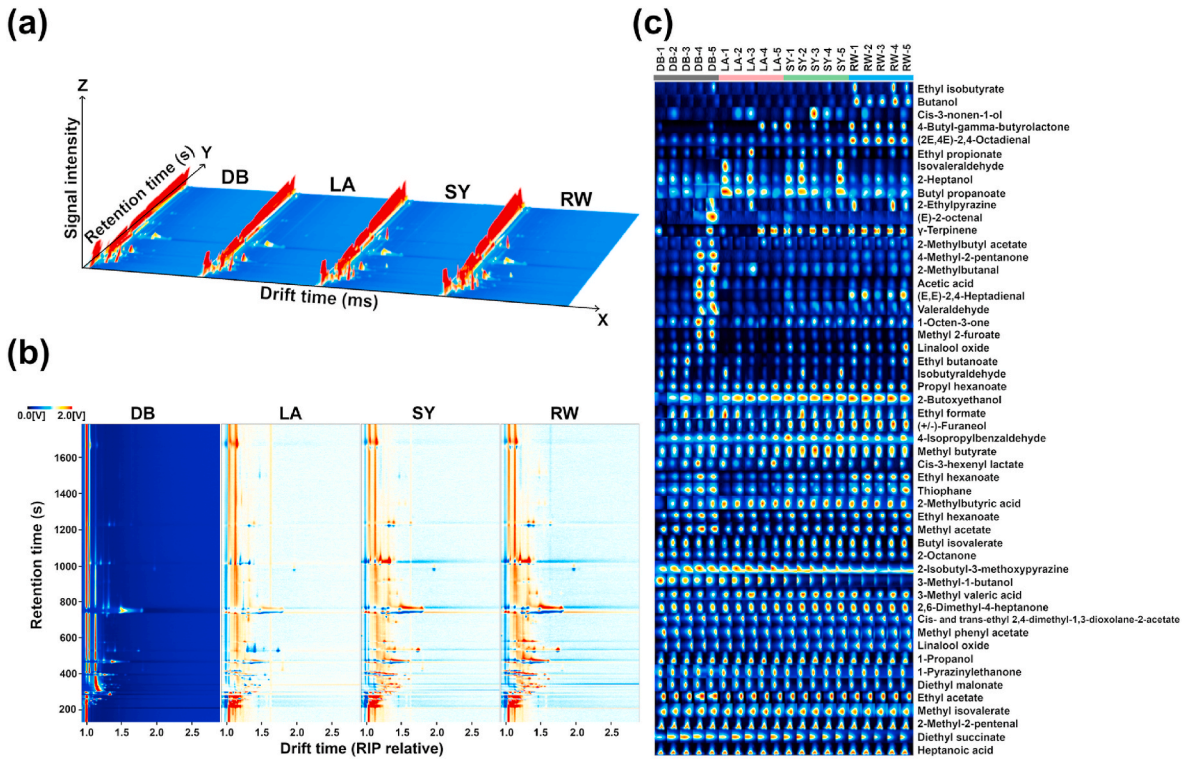

Fig. 2. GC-IMS observation of KW fermented by different yeast strains. (a) 3D topographic plot; (b) 2D difference plot, with spectra from DB group as reference, and the corresponding spectra from LA, SY and RW groups represented as differences from the DB group; (c) Gallery plots indicating the variations of VOCs' concentrations among the four groups. In both (b) and (c), red and blue colors highlight over- and under-expressed components, respectively.

3.3. ^{1}H-NMR analysis

Using ^{1}H-NMR, a total of 77 molecules were identified and quantified in KW, as provided in Table S2. These molecules encompassed various categories, including amino acids, peptides, and analogues (23), carbohydrates and derivatives (4), organic acids and derivatives (26), nucleosides, nucleotides, and analogues (5), as well as alcohols (6). A typical ^{1}H-NMR spectrum of KW is shown in Fig. S2. Taking advantage of ANOVA, the concentrations of thirty-two molecules were found to show significant differences among the four groups, as shown in Table 2.

Similarly to GC-IMS, so as to obtain an overall view of the so observed molecules, an rPCA model was setup based on their concentrations, as shown in Fig. 4.

As shown in Fig. 4 (a), PC 1 accounted for 63.8% of the variance of the entire samples' set and nicely summarized the differences among the groups. In detail, the highest concentrations of acetoacetate, 2-hydroxyglutarate, 3-hydroxybutyrate, cytosine, leucine, 2-phosphoglycerate, tyrosine, galactonate, galactarate and *myo*-inositol were found in KW fermented by RW, whereas the same samples exhibited the lowest levels of proline, galactose, 2-hydroxybutyrate, asparagine, *sn*-glycero-3-phosphocholine, aspartate, arginine, glycerol, hydroxyacetone and pyroglutamate.

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

E-tongue and ^{1}H-NMR enabled the analysis of KW from distinct perspectives. E-tongue granted the possibility to analyze global taste attributes, and ^{1}H-NMR could provide specific molecules' profiles. Therefore, the correlation of E-tongue and ^{1}H-NMR could highlight which molecules has a direct impact on taste attributes, as shown in Fig. 5.

The NMS, AHS and SCS sensors were positively associated with ornithine, cystine, galactarate and galactonate, but negatively associated with 2-hydroxyisovalerate, isovalerate, isopropanol, betaine, ethanol and proline. The ANS sensor was positively associated with acetoacetate, 2-hydroxyglutarate, *myo*-inositol, 3-hydroxybutyrate, 2-hydroxyisovalerate, isovalerate, 4-aminobutyrate, betaine and tyrosine, but negatively associated with galactose, pyroglutamate, *sn*-glycero-3-phosphocholine and succinate.

3.5. Pathway analysis

To identify the key pathways that distinguish the groups, a pathway enrichment analysis was conducted using the molecules exhibiting significant differences in concentration among the samples characterized by ^{1}H-NMR, as depicted in Fig. 6.

Five pathways were highlighted linked to different yeast strains fermentation, namely butanoate metabolism, glycerolipid metabolism, alanine, aspartate and glutamate metabolism, arginine biosynthesis, arginine and proline metabolism.

4. Discussion

The flavor profile of fruit wines is extremely complex, not only determined by the fruits themselves, but also linked to numerous molecules produced by yeast metabolism (Hoang et al., 2016). Therefore, in order to obtain the comprehensive flavor profile of fruit wine, the combination of different techniques should be considered as necessary. In recent times, the integration of multiple approaches has gained widespread application in the field of wine science. Chen et al. found that the combination of GC-MS and GC-IMS provided a comprehensive flavor analysis of ginkgo rice wine, with 1-pentanol, ethyl heptanoate and isoamyl acetate resulting as the main flavor compounds (Chen et al., 2023). Sherman employed HS-SPME-GC-TOF-MS and UHPLC-MS in an attempt to evaluate the respective contributions of volatile and non-volatile compositions to the expert quality ratings of Pinot noir wine. The results showed that dipeptides and unsaturated fatty acids were positively related to Pinot noir wine quality, while

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

Compounds	CAS	Formula	RI[a]	RT [s]	DT [ms]	Peak Intensity			
						DB	LA	SY	RW
Esters									
Propyl hexanoate	626-77-7	$C_9H_{18}O_2$	1308.1	1236.921	1.40294	$1.08\times10^3 \pm 1.28\times10^2$ $^{b\#}$	$1.45\times10^3 \pm 1.36\times10^2$ ^{a}	$1.15\times10^3 \pm 1.66\times10^2$ ^{ab}	$1.26\times10^3 \pm 1.23\times10^2$ ^{ab}
Methyl phenylacetate	101-41-7	$C_9H_{10}O_2$	1183.6	780.315	1.24387	$3.08\times10^3 \pm 8.00\times10^2$ ^{ab}	$3.18\times10^3 \pm 2.02\times10^2$ ^{a}	$2.49\times10^3 \pm 2.29\times10^2$ ^{ab}	$2.60\times10^3 \pm 1.58\times10^2$ ^{b}
Diethyl succinate	123-25-1	$C_8H_{14}O_4$	1170.8	729.581	1.29275	$1.40\times10^3 \pm 2.15\times10^2$ ^{a}	$1.55\times10^3 \pm 1.26\times10^2$ ^{a}	$8.38\times10^2 \pm 5.49\times10$ ^{b}	$1.08\times10^3 \pm 1.02\times10^2$ ^{c}
Ethyl heptanoate	106-30-9	$C_9H_{18}O_2$	1101.8	535.435	1.40746	$3.01\times10^3 \pm 4.75\times10^2$ ^{a}	$2.05\times10^3 \pm 6.85\times10^2$ ^{b}	$2.58\times10^3 \pm 2.91\times10^2$ ^{ab}	$2.15\times10^3 \pm 1.71\times10^2$ ^{ab}
Isoamyl acetate	123-92-2	$C_7H_{14}O_2$	1100.7	532.648	1.74685	$2.23\times10^3 \pm 8.82\times10^2$ ^{a}	$8.81\times10^2 \pm 4.79\times10^2$ ^{b}	$1.96\times10^3 \pm 7.00\times10^2$ ^{ab}	$1.14\times10^3 \pm 3.22\times10^2$ ^{a}
cis- and *trans*-ethyl 2,4-dimethyl-1,3-dioxolane-2-acetate	6290-17-1	$C_9H_{16}O_4$	1184.2	782.748	1.31721	$9.01\times10^3 \pm 7.80\times10^2$ ^{a}	$9.74\times10^3 \pm 4.91\times10^2$ ^{a}	$8.31\times10^3 \pm 5.08\times10^2$ ^{a}	$8.68\times10^3 \pm 7.41\times10^2$ ^{a}
Diethyl malonate	105-53-3	$C_7H_{12}O_4$	1074.3	466.694	1.25103	$1.62\times10^3 \pm 2.50\times10^2$ ^{ab}	$1.81\times10^3 \pm 77.40$ ^{a}	$1.18\times10^3 \pm 1.01\times10^2$ ^{bc}	$1.32\times10^3 \pm 88.70$ ^{c}
Methyl isovalerate	556-24-1	$C_6H_{12}O_2$	1031.8	405.941	1.19975	$2.24\times10^3 \pm 1.66\times10^2$ ^{ab}	$2.67\times10^3 \pm 1.63\times10^2$ ^{a}	$2.19\times10^3 \pm 2.34\times10^2$ ^{ab}	$2.27\times10^3 \pm 1.72\times10^2$ ^{b}
Butyl isovalerate	109-19-3	$C_9H_{18}O_2$	1026.3	398.807	1.38394	$1.07\times10^3 \pm 1.76\times10^2$ ^{a}	$9.23\times10^2 \pm 1.44\times10^2$ ^{a}	$9.88\times10^2 \pm 45.50$ ^{a}	$1.07\times10^3 \pm 1.22\times10^2$ ^{a}
Ethyl butanoate	105-54-4	$C_6H_{12}O_2$	1025.6	397.856	1.56275	$3.87\times10^2 \pm 1.67\times10^2$ ^{a}	$2.13\times10^2 \pm 79.50$ ^{b}	$3.07\times10^2 \pm 91.90$ ^{ab}	$2.30\times10^2 \pm 30.00$ ^{ab}
Ethyl hexanoate	123-66-0	$C_8H_{16}O_2$	1006.6	373.125	1.33866	$8.43\times10^2 \pm 2.54\times10^2$ ^{a}	$5.35\times10^2 \pm 1.42\times10^2$ ^{b}	$9.69\times10^2 \pm 72.70$ ^{ab}	$6.84\times10^2 \pm 60.30$ ^{a}
Methyl 2-furoate	611-13-2	$C_6H_6O_3$	977.2	339.834	1.47833	$4.69\times10^2 \pm 4.11\times10^2$ ^{a}	$1.04\times10^2 \pm 44.90$ ^{b}	$2.03\times10^2 \pm 28.10$ ^{ab}	$2.20\times10^2 \pm 25.10$ ^{ab}
Ethyl propionate	105-37-3	$C_5H_{10}O_2$	954.3	326.993	1.45454	$6.54\times10^2 \pm 2.09\times10^2$ ^{a}	$9.46\times10^2 \pm 8.48\times10^2$ ^{a}	$6.28\times10^2 \pm 2.53\times10^2$ ^{a}	$1.09\times10^3 \pm 2.51\times10^2$ ^{a}
Butyl propanoate	590-01-2	$C_7H_{14}O_2$	913.2	303.916	1.27951	$4.25\times10^2 \pm 58.10$ ^{ab}	$6.89\times10^2 \pm 2.05\times10^2$ ^{a}	$2.97\times10^2 \pm 79.10$ ^{a}	$4.88\times10^2 \pm 1.22\times10^2$ ^{b}
Ethyl acetate	141-78-6	$C_4H_8O_2$	890.9	292.506	1.33499	$1.27\times10^4 \pm 1.81\times10^3$ ^{a}	$1.15\times10^4 \pm 1.27\times10^3$ ^{ab}	$9.92\times10^3 \pm 4.34\times10^2$ ^{b}	$9.87\times10^3 \pm 5.50\times10^2$ ^{b}
Methyl acetate	79-20-9	$C_3H_6O_2$	825.1	265.655	1.19287	$3.54\times10^3 \pm 4.61\times10^2$ ^{a}	$2.71\times10^3 \pm 3.30\times10^2$ ^{b}	$2.81\times10^3 \pm 1.16\times10^2$ ^{b}	$2.50\times10^3 \pm 1.47\times10^2$ ^{ab}
Ethyl formate	109-94-4	$C_3H_6O_2$	810.1	259.541	1.22066	$1.93\times10^2 \pm 81.20$ ^{a}	$2.57\times10^2 \pm 74.90$ ^{a}	$2.03\times10^2 \pm 26.10$ ^{a}	$2.43\times10^2 \pm 56.70$ ^{a}
cis-3-Hexenyl lactate	61931-81-5	$C_9H_{16}O_3$	1235.4	985.198	1.97294	$7.26\times10^2 \pm 2.14\times10^2$ ^{a}	$7.82\times10^2 \pm 2.26\times10^2$ ^{a}	$4.57\times10^2 \pm 1.03\times10^2$ ^{ab}	$5.71\times10^2 \pm 54.50$ ^{b}
Methyl butyrate	623-42-7	$C_5H_{10}O_2$	1026.6	399.126	1.43515	$1.99\times10^2 \pm 7.71$ ^{ab}	$2.15\times10^2 \pm 1.46\times10$ ^{ab}	$2.07\times10^2 \pm 1.29\times10$ ^{a}	$2.55\times10^2 \pm 3.36\times10$ ^{b}
2-Methylbutyl acetate	624-41-9	$C_7H_{14}O_2$	900.9	297.037	1.29027	$4.19\times10^2 \pm 1.67\times10^2$ ^{a}	$3.84\times10^2 \pm 1.28\times10^2$ ^{a}	$4.04\times10^2 \pm 28.50$ ^{a}	$3.29\times10^2 \pm 38.20$ ^{a}
Ethyl isobutyrate	97-62-1	$C_6H_{12}O_2$	963.5	332.177	1.56119	56.50 ± 24.80 ^{a}	62.40 ± 18.60 ^{a}	98.10 ± 49.80 ^{a}	55.00 ± 12.80 ^{a}
4-Butyl-gamma-butyrolactone	104-50-7	$C_8H_{14}O_2$	1244.3	1018.717	1.33279	$3.10\times10^2 \pm 60.40$ ^{c}	$3.31\times10^2 \pm 30.90$ ^{bc}	$4.49\times10^2 \pm 33.60$ ^{ab}	$3.94\times10^2 \pm 41.80$ ^{a}
Aldehydes									
2-Methyl-2-pentenal	623-36-9	$C_6H_{10}O$	1177.5	756.238	1.51314	$2.82\times10^4 \pm 3.49\times10^3$ ^{ab}	$3.01\times10^4 \pm 1.97\times10^3$ ^{a}	$2.53\times10^4 \pm 1.89\times10^3$ ^{ab}	$2.64\times10^4 \pm 1.84\times10^3$ ^{b}
(2E,4E)-2,4-Octadienal	30361-28-5	$C_8H_{12}O$	1119.3	579.094	1.26241	$8.25\times10^2 \pm 98.80$ ^{c}	$1.07\times10^3 \pm 1.09\times10^2$ ^{b}	$1.77\times10^3 \pm 1.40\times10^2$ ^{bc}	$9.77\times10^2 \pm 1.36\times10^2$ ^{a}
Valeraldehyde	110-62-3	$C_5H_{10}O$	982	342.518	1.42418	$3.62\times10^2 \pm 2.19\times10^2$ ^{ab}	$1.93\times10^2 \pm 25.20$ ^{b}	$3.03\times10^2 \pm 6.39$ ^{a}	$3.40\times10^2 \pm 40.20$ ^{ab}
(E,E)-2,4-Heptadienal	5910-85-0	$C_7H_{10}O$	1005.3	371.408	1.6159	$2.60\times10^2 \pm 1.91\times10^2$ ^{a}	85.70 ± 26.20 ^{b}	$3.29\times10^2 \pm 67.30$ ^{ab}	$1.52\times10^2 \pm 45.50$ ^{a}
Isovaleraldehyde	590-86-3	$C_5H_{10}O$	913.6	304.159	1.40803	$1.28\times10^2 \pm 74.90$ ^{a}	$2.45\times10^2 \pm 1.92\times10^2$ ^{a}	73.00 ± 25.50 ^{a}	$2.24\times10^2 \pm 1.25\times10^2$ ^{a}
Isobutyraldehyde	78-84-2	C_4H_8O	809.4	259.245	1.28302	$1.91\times10^2 \pm 85.60$ ^{a}	$1.38\times10^2 \pm 1.01\times10^2$ ^{a}	93.00 ± 20.20 ^{a}	$1.62\times10^2 \pm 97.80$ ^{a}
4-Isopropylbenzaldehyde	122-03-2	$C_{10}H_{12}O$	1218.2	917.092	1.32441	$8.60\times10^2 \pm 79.40$ ^{b}	$1.01\times10^3 \pm 76.10$ ^{a}	$8.62\times10^2 \pm 72.20$ ^{ab}	$9.48\times10^2 \pm 84.50$ ^{ab}
2-Methylbutanal	96-17-3	$C_5H_{10}O$	955	327.421	1.39411	$2.32\times10^2 \pm 1.22\times10^2$ ^{a}	$1.88\times10^2 \pm 1.20\times10^2$ ^{a}	$1.63\times10^2 \pm 42.50$ ^{a}	$2.00\times10^2 \pm 24.10$ ^{a}
(E)-2-Octenal	2548-87-0	$C_8H_{14}O$	1058.6	440.708	1.33248	60.90 ± 45.20 ^{a}	51.50 ± 19.10 ^{a}	44.10 ± 7.16 ^{a}	43.20 ± 9.84 ^{a}
Ketones									
(+/-)-Furaneol	3658-77-3	$C_6H_8O_3$	1078	475.771	1.60568	$3.10\times10^2 \pm 60.40$ ^{c}	$3.31\times10^2 \pm 30.90$ ^{bc}	$4.49\times10^2 \pm 33.60$ ^{ab}	$3.94\times10^2 \pm 41.80$ ^{a}
2-Octanone	111-13-7	$C_8H_{16}O$	1305.9	1229.215	1.32942	$1.72\times10^3 \pm 3.96\times10^2$ ^{a}	$1.94\times10^3 \pm 1.94\times10^2$ ^{a}	$1.57\times10^3 \pm 2.28\times10^2$ ^{a}	$1.75\times10^3 \pm 1.33\times10^2$ ^{a}
2,6-Dimethyl-4-heptanone	108-83-8	$C_9H_{18}O$	1177.2	754.976	1.79638	$2.99\times10^3 \pm 3.68\times10^2$ ^{a}	$3.30\times10^3 \pm 2.02\times10^2$ ^{a}	$2.93\times10^3 \pm 2.46\times10^2$ ^{a}	$3.12\times10^3 \pm 2.37\times10^2$ ^{a}
1-Octen-3-one	4312-99-6	$C_8H_{14}O$	977.2	339.834	1.2788	$6.75\times10^2 \pm 1.75\times10^2$ ^{a}	$4.58\times10^2 \pm 1.29\times10^2$ ^{b}	$5.07\times10^2 \pm 21.60$ ^{ab}	$5.55\times10^2 \pm 27.40$ ^{ab}

(*continued on next page*)

Table 1 (*continued*)

Compounds	CAS	Formula	RI[a]	RT [s]	DT [ms]	Peak Intensity			
						DB	LA	SY	RW
4-Methyl-2-pentanone	108-10-1	$C_6H_{12}O$	1006.1	372.516	1.47887	$1.62\times10^2 \pm 1.23\times10^2$ ^{ab}	67.50 ± 5.94 ^{b}	$1.25\times10^2 \pm 8.12$ ^{ab}	84.80 ± 7.46 ^{a}
Alcohols									
3-Methyl-1-butanol	123-51-3	$C_5H_{12}O$	1173.5	740.521	1.24303	$7.48\times10^2 \pm 1.85\times10^2$ ^{a}	$6.52\times10^2 \pm 1.12\times10^2$ ^{a}	$2.02\times10^2 \pm 31.70$ ^{b}	$3.19\times10^2 \pm 15.30$ ^{c}
1-Propanol	71-23-8	C_3H_8O	1026.3	398.807	1.26805	$5.60\times10^3 \pm 4.87\times10^2$ ^{ab}	$6.25\times10^3 \pm 2.98\times10^2$ ^{a}	$5.02\times10^3 \pm 4.19\times10^2$ ^{a}	$5.90\times10^3 \pm 5.53\times10^2$ ^{b}
2-Heptanol	543-49-7	$C_7H_{16}O$	912.3	303.431	1.37572	$4.08\times10^2 \pm 70.60$ ^{ab}	$4.98\times10^2 \pm 1.89\times10^2$ ^{a}	$2.66\times10^2 \pm 66.10$ ^{ab}	$4.79\times10^2 \pm 1.69\times10^2$ ^{b}
(Z)-3-Nonen-1-ol	10340-23-5	$C_9H_{18}O$	1159.2	684.044	1.43516	99.10 ± 74.80 ^{a}	$1.98\times10^2 \pm 1.61\times10^2$ ^{a}	$1.32\times10^2 \pm 90.30$ ^{a}	$2.87\times10^2 \pm 1.98\times10^2$ ^{a}
Butanol	71-36-3	$C_4H_{10}O$	1120.8	582.779	1.38099	$1.37\times10^2 \pm 16.30$ ^{b}	$1.47\times10^2 \pm 19.20$ ^{b}	$5.24\times10^2 \pm 75.00$ ^{b}	$1.43\times10^2 \pm 33.00$ ^{a}
Linalool oxide	60047-17-8	$C_{10}H_{18}O_2$	1082.5	487.13	1.25198	$3.49\times10^3 \pm 4.50\times10^2$ ^{a}	$4.01\times10^3 \pm 2.22\times10^2$ ^{a}	$3.89\times10^3 \pm 2.49\times10^2$ ^{a}	$3.75\times10^3 \pm 3.13\times10^2$ ^{a}
Acids									
Heptanoic acid	111-14-8	$C_7H_{14}O_2$	1078.4	476.912	1.37522	$1.08\times10^4 \pm 1.32\times10^3$ ^{a}	$1.21\times10^4 \pm 5.45\times10^2$ ^{a}	$1.20\times10^4 \pm 9.23\times10^2$ ^{a}	$1.16\times10^4 \pm 1.12\times10^3$ ^{a}
3-Methylvaleric acid	105-43-1	$C_6H_{12}O_2$	956.8	328.42	1.26805	$1.24\times10^3 \pm 2.84\times10^2$ ^{a}	$1.60\times10^3 \pm 2.87\times10^2$ ^{a}	$1.26\times10^3 \pm 1.18\times10^2$ ^{a}	$1.43\times10^3 \pm 1.57\times10^2$ ^{a}
2-Methylbutyric acid	116-53-0	$C_5H_{10}O_2$	869.7	283.848	1.2045	$1.35\times10^2 \pm 17.70$ ^{b}	$1.91\times10^2 \pm 19.80$ ^{a}	$1.56\times10^2 \pm 17.20$ ^{a}	$1.63\times10^2 \pm 9.63$ ^{ab}
Acetic acid	64-19-7	$C_2H_4O_2$	1433.9	1666.756	1.15833	$4.17\times10^3 \pm 4.14\times10^3$ ^{a}	$3.43\times10^3 \pm 9.92\times10^2$ ^{a}	$2.35\times10^3 \pm 2.50\times10^2$ ^{a}	$2.00\times10^3 \pm 5.97\times10^2$ ^{a}
Others									
Thiophane	110-01-0	C_4H_8S	1101.1	533.577	1.31076	$1.30\times10^3 \pm 1.08\times10^2$ ^{a}	$9.39\times10^2 \pm 2.85\times10^2$ ^{a}	$1.27\times10^3 \pm 1.30\times10^2$ ^{a}	$1.03\times10^3 \pm 1.04\times10^2$ ^{a}
1-Pyrazinylethanone	22047-25-2	$C_6H_6N_2O$	1023.4	395.002	1.20128	$1.38\times10^3 \pm 1.54\times10^2$ ^{a}	$1.52\times10^3 \pm 1.09\times10^2$ ^{a}	$1.02\times10^3 \pm 97.40$ ^{b}	$1.10\times10^3 \pm 75.20$ ^{b}
2-Isobutyl-3-methoxypyrazine	24683-00-9	$C_9H_{14}N_2O$	1173.6	740.728	1.31076	$1.37\times10^3 \pm 87.50$ ^{b}	$1.62\times10^3 \pm 55.70$ ^{a}	$9.17\times10^2 \pm 55.30$ ^{c}	$1.17\times10^3 \pm 70.00$ ^{d}
2-Ethylpyrazine	13925-00-3	$C_6H_8N_2$	962.5	331.583	1.51022	67.00 ± 49.20 ^{a}	59.30 ± 40.10 ^{a}	79.10 ± 41.00 ^{a}	72.70 ± 24.20 ^{a}
2-Butoxyethanol	111-76-2	$C_6H_{14}O_2$	905.6	299.654	1.20644	$4.95\times10^2 \pm 1.33\times10^2$ ^{b}	$8.43\times10^2 \pm 39.90$ ^{a}	$6.72\times10^2 \pm 71.40$ ^{a}	$7.25\times10^2 \pm 55.10$ ^{a}
γ-Terpinene	99-85-4	$C_{10}H_{16}$	1243.9	1017.288	1.20778	$1.35\times10^3 \pm 1.09\times10^3$ ^{a}	$2.04\times10^3 \pm 1.72\times10^3$ ^{a}	$2.57\times10^3 \pm 2.39\times10^2$ ^{a}	$2.31\times10^3 \pm 6.23\times10^2$ ^{a}

[#] For each molecule, sd values followed by a common superscript identify no significant differences.
[a] RI, RT, and Dt stand for retention index, retention time, and drift time, respectively.

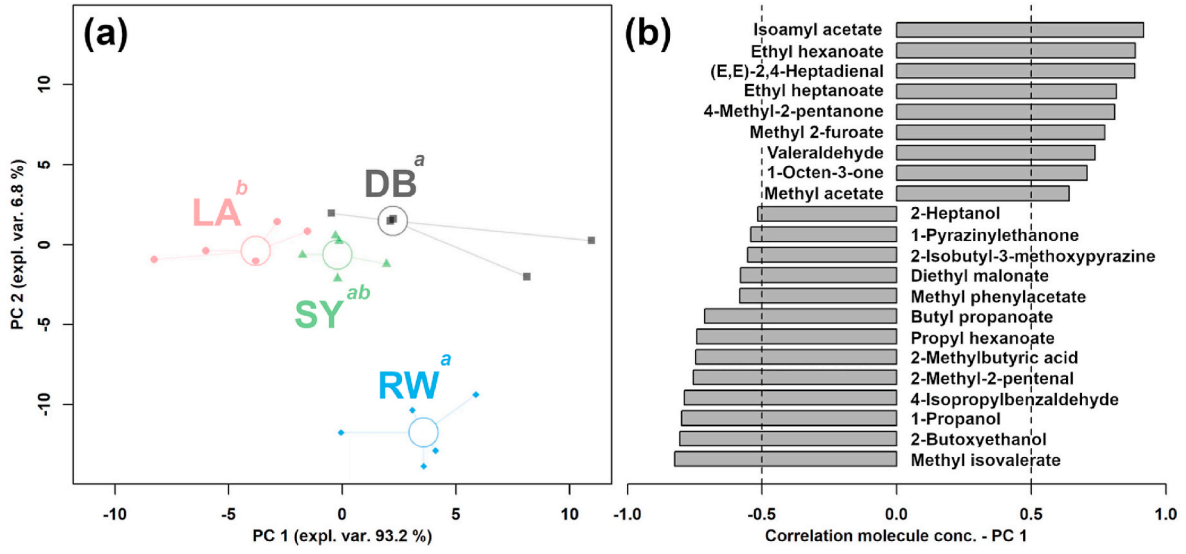

Fig. 3. rPCA model calculated on the basis of VOCs showing significant differences in peak intensities among KW fermented by DB, LA, SY and RW strains respectively. The scoreplot (a) displays the samples from the four groups as follows: squares (DB), circles (LA), triangles (SY), and diamonds (RW). Each sample group's median was represented by a wide and empty circle, while the superscript lowercase letters indicate significant differences among the samples along PC 1. The loading plot (b) evidences significant correlations ($p < 0.05$) between the peak intensity of each VOC and its importance over PC 1.

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

	DB	LA	SY	RW
Amino Acids, Peptides And Analogues				
4-Aminobutyrate	$2.01\times10^{-3}\pm1.15\times10^{-4}$ ^{a*}	$1.84\times10^{-3}\pm3.28\times10^{-4}$ ^{ab}	$1.60\times10^{-3}\pm1.19\times10^{-4}$ ^{b}	$1.60\times10^{-3}\pm7.86\times10^{-5}$ ^{b}
Alanine	$9.64\times10^{-4}\pm2.04\times10^{-4}$ ^{b}	$1.56\times10^{-3}\pm2.97\times10^{-4}$ ^{a}	$1.43\times10^{-3}\pm2.32\times10^{-4}$ ^{a}	$1.25\times10^{-3}\pm1.23\times10^{-4}$ ^{ab}
Arginine	$2.18\times10^{-3}\pm4.48\times10^{-4}$ ^{b}	$1.56\times10^{-3}\pm1.16\times10^{-3}$ ^{b}	$4.08\times10^{-3}\pm7.01\times10^{-4}$ ^{a}	$1.46\times10^{-3}\pm4.98\times10^{-4}$ ^{b}
Asparagine	$3.43\times10^{-4}\pm1.53\times10^{-4}$ ^{b}	$1.10\times10^{-3}\pm2.93\times10^{-4}$ ^{a}	$9.48\times10^{-4}\pm2.64\times10^{-4}$ ^{a}	$3.20\times10^{-4}\pm4.96\times10^{-5}$ ^{b}
Aspartate	$3.93\times10^{-4}\pm2.50\times10^{-4}$ ^{b}	$5.10\times10^{-4}\pm2.17\times10^{-4}$ ^{ab}	$8.98\times10^{-4}\pm2.85\times10^{-4}$ ^{a}	$2.11\times10^{-4}\pm1.36\times10^{-4}$ ^{b}
Betaine	$2.53\times10^{-4}\pm1.43\times10^{-5}$ ^{a}	$2.40\times10^{-4}\pm3.17\times10^{-5}$ ^{a}	$2.01\times10^{-4}\pm2.12\times10^{-5}$ ^{b}	$1.96\times10^{-4}\pm1.10\times10^{-5}$ ^{b}
Cystine	$3.10\times10^{-3}\pm3.40\times10^{-4}$ ^{bc}	$2.37\times10^{-3}\pm3.89\times10^{-4}$ ^{c}	$3.94\times10^{-3}\pm6.05\times10^{-4}$ ^{ab}	$4.87\times10^{-3}\pm8.27\times10^{-4}$ ^{a}
Leucine	$4.30\times10^{-4}\pm2.77\times10^{-4}$ ^{ab}	$4.54\times10^{-4}\pm1.04\times10^{-4}$ ^{a}	$2.15\times10^{-4}\pm7.84\times10^{-5}$ ^{b}	$4.14\times10^{-4}\pm4.27\times10^{-5}$ ^{ab}
Ornithine	$5.79\times10^{-5}\pm1.36\times10^{-5}$ ^{b}	$1.49\times10^{-4}\pm3.49\times10^{-5}$ ^{a}	$1.24\times10^{-4}\pm2.86\times10^{-5}$ ^{a}	$1.39\times10^{-4}\pm2.39\times10^{-5}$ ^{a}
Proline	$3.01\times10^{-3}\pm9.40\times10^{-4}$ ^{ab}	$4.27\times10^{-3}\pm5.37\times10^{-4}$ ^{a}	$3.79\times10^{-3}\pm8.88\times10^{-4}$ ^{a}	$1.83\times10^{-3}\pm3.15\times10^{-4}$ ^{b}
Pyroglutamate	$4.48\times10^{-3}\pm9.21\times10^{-4}$ ^{b}	$7.43\times10^{-3}\pm3.16\times10^{-3}$ ^{b}	$1.38\times10^{-2}\pm2.72\times10^{-3}$ ^{a}	$4.47\times10^{-3}\pm1.18\times10^{-3}$ ^{b}
Tyrosine	$1.87\times10^{-4}\pm7.45\times10^{-5}$ ^{a}	$1.82\times10^{-4}\pm3.55\times10^{-5}$ ^{a}	$1.10\times10^{-4}\pm2.02\times10^{-5}$ ^{b}	$1.52\times10^{-4}\pm2.12\times10^{-5}$ ^{ab}
Carbohydrates				
Galactose	$1.13\times10^{-3}\pm5.77\times10^{-4}$ ^{ab}	$7.71\times10^{-4}\pm1.72\times10^{-4}$ ^{b}	$1.50\times10^{-3}\pm2.97\times10^{-4}$ ^{a}	$1.01\times10^{-3}\pm1.20\times10^{-4}$ ^{ab}
Organic Acids and Derivates				
2-Hydroxybutyrate	$1.38\times10^{-3}\pm6.23\times10^{-5}$ ^{ab}	$1.06\times10^{-3}\pm1.79\times10^{-5}$ ^{c}	$1.67\times10^{-3}\pm2.25\times10^{-4}$ ^{a}	$1.22\times10^{-3}\pm1.10\times10^{-4}$ ^{b}
2-Hydroxyglutarate	$3.13\times10^{-3}\pm2.69\times10^{-4}$ ^{a}	$2.74\times10^{-3}\pm3.72\times10^{-4}$ ^{a}	$9.48\times10^{-4}\pm3.03\times10^{-4}$ ^{b}	$2.98\times10^{-3}\pm3.02\times10^{-4}$ ^{a}
2-Hydroxyisovalerate	$3.38\times10^{-4}\pm3.40\times10^{-5}$ ^{a}	$2.23\times10^{-4}\pm3.51\times10^{-5}$ ^{b}	$1.07\times10^{-4}\pm3.16\times10^{-5}$ ^{c}	$1.06\times10^{-4}\pm1.71\times10^{-5}$ ^{c}
2-Phosphoglycerate	$1.02\times10^{-2}\pm4.00\times10^{-4}$ ^{ab}	$1.01\times10^{-2}\pm5.14\times10^{-4}$ ^{ab}	$9.61\times10^{-3}\pm4.45\times10^{-4}$ ^{b}	$1.03\times10^{-2}\pm3.89\times10^{-4}$ ^{a}
3-Hydroxybutyrate	$9.68\times10^{-4}\pm1.86\times10^{-4}$ ^{a}	$8.93\times10^{-4}\pm7.99\times10^{-5}$ ^{a}	$6.01\times10^{-4}\pm1.95\times10^{-4}$ ^{b}	$9.48\times10^{-4}\pm3.33\times10^{-5}$ ^{a}
Acetoacetate	$2.46\times10^{-4}\pm2.32\times10^{-5}$ ^{a}	$2.16\times10^{-4}\pm2.91\times10^{-5}$ ^{a}	$8.18\times10^{-5}\pm2.84\times10^{-5}$ ^{b}	$2.35\times10^{-4}\pm2.16\times10^{-5}$ ^{a}
Butyrate	$4.86\times10^{-3}\pm1.99\times10^{-4}$ ^{a}	$3.49\times10^{-3}\pm2.98\times10^{-4}$ ^{b}	$5.26\times10^{-3}\pm6.07\times10^{-4}$ ^{a}	$5.53\times10^{-3}\pm5.31\times10^{-4}$ ^{a}
Galactarate	$2.73\times10^{-4}\pm1.33\times10^{-4}$ ^{b}	$4.33\times10^{-4}\pm9.25\times10^{-5}$ ^{b}	$3.51\times10^{-4}\pm1.27\times10^{-4}$ ^{b}	$6.55\times10^{-4}\pm4.50\times10^{-5}$ ^{a}
Galactonate	$2.13\times10^{-3}\pm5.87\times10^{-4}$ ^{b}	$2.21\times10^{-3}\pm3.28\times10^{-4}$ ^{b}	$2.07\times10^{-3}\pm5.67\times10^{-4}$ ^{b}	$3.60\times10^{-3}\pm4.99\times10^{-4}$ ^{a}
Isovalerate	$1.87\times10^{-4}\pm2.60\times10^{-5}$ ^{a}	$1.07\times10^{-4}\pm2.91\times10^{-5}$ ^{b}	$6.29\times10^{-5}\pm2.24\times10^{-5}$ ^{c}	$5.54\times10^{-5}\pm8.48\times10^{-6}$ ^{c}
Succinate	$1.34\times10^{-2}\pm2.72\times10^{-3}$ ^{ab}	$1.08\times10^{-2}\pm2.59\times10^{-3}$ ^{b}	$1.56\times10^{-2}\pm1.52\times10^{-3}$ ^{a}	$1.66\times10^{-2}\pm2.51\times10^{-3}$ ^{a}
Nucleotides				
Cytosine	$1.19\times10^{-4}\pm5.49\times10^{-5}$ ^{ab}	$1.13\times10^{-4}\pm4.60\times10^{-5}$ ^{b}	$8.55\times10^{-5}\pm1.04\times10^{-5}$ ^{b}	$1.94\times10^{-4}\pm2.58\times10^{-5}$ ^{a}
Alcohols				
Glycerol	$9.46\times10^{-2}\pm1.11\times10^{-2}$ ^{b}	$9.15\times10^{-2}\pm9.41\times10^{-3}$ ^{b}	$1.40\times10^{-1}\pm1.83\times10^{-2}$ ^{a}	$7.92\times10^{-2}\pm1.07\times10^{-2}$ ^{b}
Ethanol	$1.66\pm6.99\times10^{-2}$ ^{a}	$1.60\pm6.63\times10^{-2}$ ^{ab}	$1.65\pm1.68\times10^{-1}$ ^{a}	$1.48\pm7.19\times10^{-2}$ ^{b}
Isopropanol	$3.49\times10^{-2}\pm2.07\times10^{-2}$ ^{a}	$1.81\times10^{-2}\pm2.18\times10^{-3}$ ^{ab}	$1.69\times10^{-2}\pm1.23\times10^{-3}$ ^{b}	$1.77\times10^{-2}\pm1.00\times10^{-3}$ ^{ab}
myo-Inositol	$8.64\times10^{-3}\pm2.45\times10^{-4}$ ^{a}	$7.22\times10^{-3}\pm5.24\times10^{-4}$ ^{b}	$7.09\times10^{-3}\pm4.22\times10^{-4}$ ^{b}	$7.60\times10^{-3}\pm5.22\times10^{-4}$ ^{b}
Propylene glycol	$2.33\times10^{-2}\pm2.40\times10^{-2}$ ^{a}	$9.87\times10^{-3}\pm2.52\times10^{-3}$ ^{ab}	$1.67\times10^{-2}\pm1.60\times10^{-3}$ ^{a}	$5.06\times10^{-3}\pm1.42\times10^{-3}$ ^{b}
Miscellaneous				
sn-Glycero-3-phosphocholine	1.73×10-5 $\pm3.71\times10^{-6}$ ^{b}	4.33×10-5 $\pm2.50\times10^{-5}$ ^{a}	5.59×10-5 $\pm1.74\times10^{-5}$ ^{a}	2.92×10-5 $\pm4.55\times10^{-6}$ ^{ab}
Hydroxyacetone	$4.77\times10^{-5}\pm1.21\times10^{-5}$ ^{b}	$8.95\times10^{-5}\pm4.32\times10^{-5}$ ^{ab}	$1.61\times10^{-4}\pm5.73\times10^{-5}$ ^{a}	$5.19\times10^{-5}\pm1.31\times10^{-5}$ ^{b}

* For each molecule, sd values followed by a common superscript identify no significant differences.

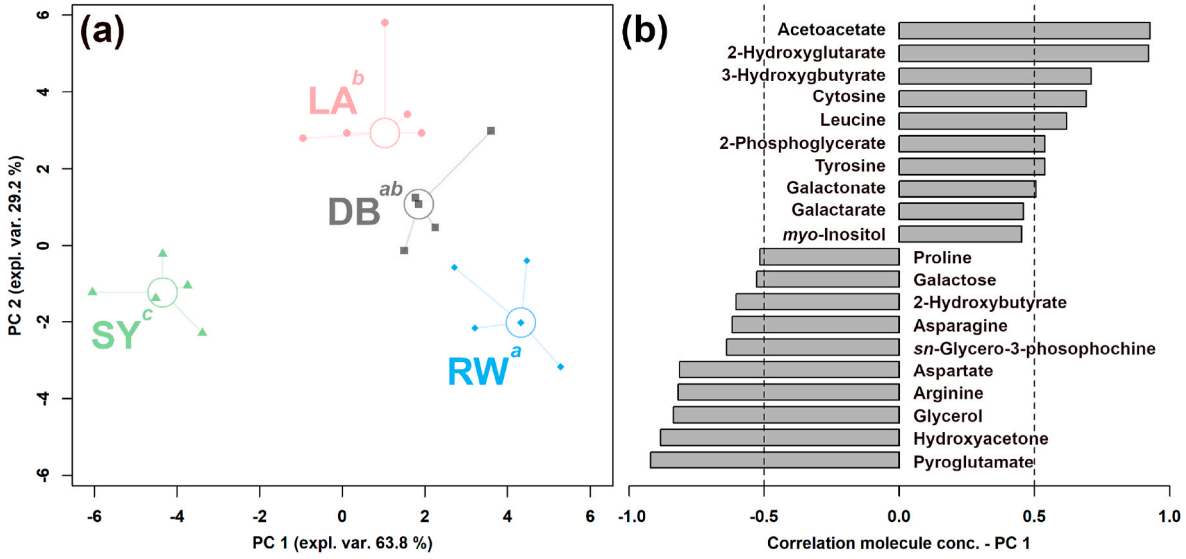

Fig. 4. rPCA model performed on the basis of molecules showing significantly different concentration in KW fermented by DB, LA, SY and RW strains. The scoreplot (a) displays the samples from the four groups as follows: squares (DB), circles (LA), triangles (SY), and diamonds (RW). Each sample group's median is represented by a wide and empty circle and the superscript lowercase letters indicate the significance of the samples along PC 1. The loading plot (b) evidences a significant correlation ($p < 0.05$) between the concentration of each molecule and its importance over PC 1.

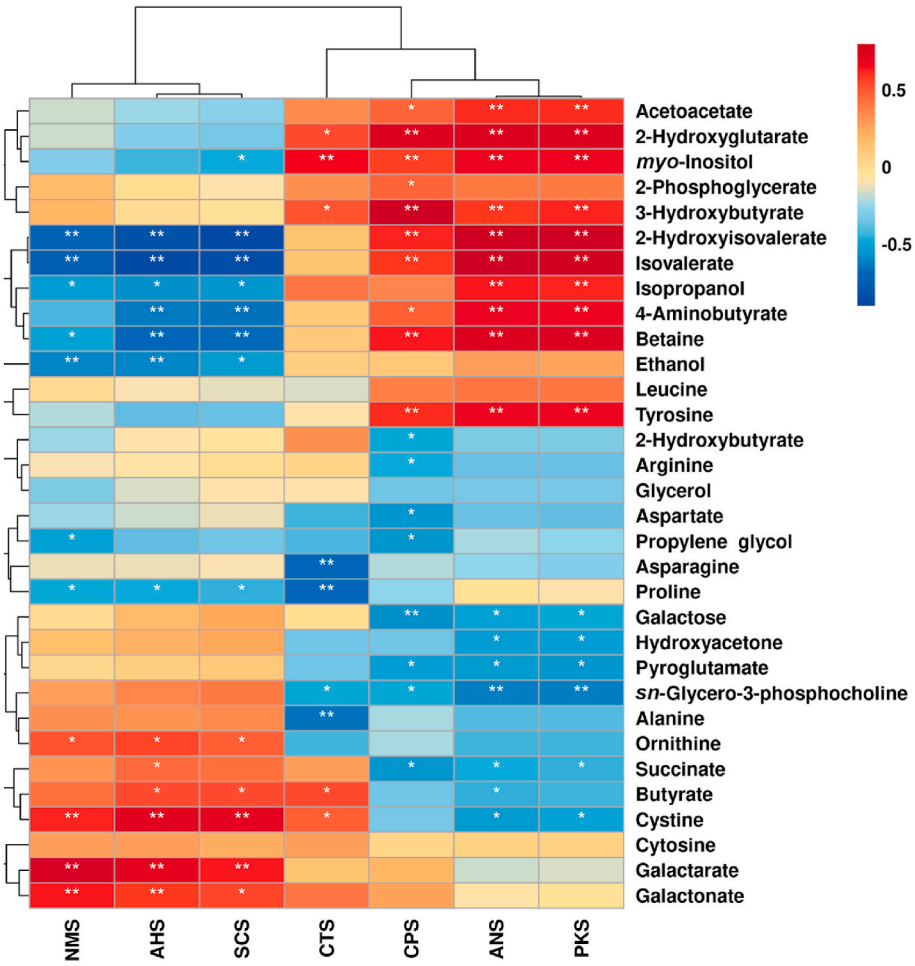

Fig. 5. Spearman's correlation heatmap showing the correlation between molecules' levels and E-tongue sensor responses. The colors represent the correlation coefficient, with red and blue indicating positive and negative correlations, respectively. The symbols "*" and "**" represent significances at $p < 0.05$ and $p < 0.01$, respectively.

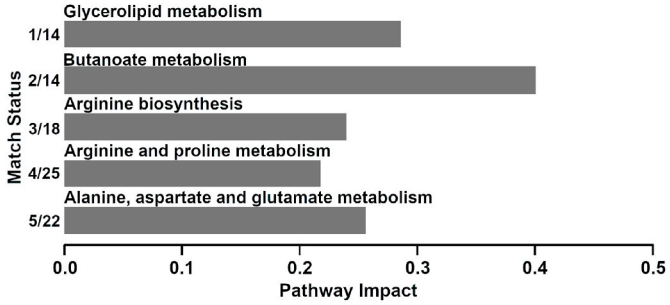

Fig. 6. Metabolic pathways evaluated through enrichment analysis based on statistically significant molecules quantified from KW samples among the four groups (impact value > 0.2).

N-(3-methylbutyl)acetamide and xanthine were negatively associated to it (Sherman et al., 2020). To the best of our knowledge, this study represents the first attempt to comprehensively characterize the flavor profile of KW fermented by four commercial *S. cerevisiae* strains by sensory evaluation, E-tongue, GC-IMS and ^{1}H-NMR.

In this study, E-tongue could effectively distinguish KW fermented by different yeast strains. Sensory evaluation indicated that KW fermented by RW obtained the highest total score, mainly due to color and overall acceptability. The total score of sensory evaluation of KW fermented by SY was the lowest, mainly in connection to sourness and bitterness. Both of the taste characteristics are known to be negatively correlated to wine quality (Bi et al., 2019; Cosme et al., 2021). Such finding agreed with E-tongue analysis, with KW fermented by SY showing the highest response values of AHS and SCS, indeed mainly linked to sourness and bitterness respectively.

Esters are important for the flavor of the wine, mainly contributing to a strong fruity and floral aroma. In our study, esters were detected as the most abundant compounds in all KW samples by means of GC-IMS, which is in line with Qi et al. (Qi et al., 2019). In particular, ethyl acetate, ethyl butanoate, ethyl heptanoate, isoamyl acetate and ethyl hexanoate were also identified in KW by GC-MS (Chen et al., 2022). Several esters could come from kiwifruit itself, such as ethyl hexanoate (Zhao et al., 2021) and methyl acetate (Lan et al., 2021). However, most of esters were formed by esterification of alcohols and acids, as a result of yeast metabolism (Vararu et al., 2020).

In comparison to the other three groups, KW fermented by RW exhibited elevated levels of esters, resulting in enhanced sensory characteristics characterized by a desirable and fruity full-bodied ester aroma (Muñoz-Redondo et al., 2021; Wang et al., 2015). Such findings could partially explain its sensory score higher than the others. In particular, KW fermented by RW contained the highest level of ethyl hexanoate, which has been considered as one of the key odor-active compounds in KW (Lan et al., 2022). Apart from ethyl hexanoate, it is worth to note that several esters, such as isoamyl acetate, ethyl heptanoate, methyl acetate and methyl 2-furoate, play important roles in distinguishing KW fermented by different yeast. Isoamyl acetate is an

important flavor component of yeast fermented alcoholic beverages. The variation of isoamyl acetate content in KW could be linked to isoamyl alcohol production and ATF genes transcription abilities of different yeast strains (Yoshimoto et al., 2002). Ethyl heptanoate was formed from propionyl-CoA during fermentation by the metabolism of yeast, which has an odour note (tropical fruit). Wang et al. found that ethyl heptanoate, together with ethyl hexanoate, ethyl pentanoate, nonanal and ethyl butyrate, were the major contributors to the gingko wine aroma (Wang et al., 2015).

As one of the most intensively studied compounds in fruit wines, sugars are not only able to affect the metabolism of yeast, but they are also directly related to the sensory of fruit wines. In the study, among the sugars quantified by ^{1}H-NMR, the concentration of galactose was found to be significantly different among the KW fermented by distinct yeast strains. As the widely characterized sugars in fruit wine, such differences could be linked to the sugar metabolic ability of different yeast (Apolinar-Valiente et al., 2014).

Aldehydes play an important role on the flavor of KW. They could be generated through oxidation during sample preparation and fermentation (Vavoura et al., 2015; Zhu et al., 2021). In general, the flavor threshold is low for aldehydes and most of aldehydes have unique fatty aromas (Wang et al., 2021). Two of the aldehydes we identified in the present investigation, isovaleraldehyde and isobutyraldehyde, have been also found in KW by Li et al. (Li et al., 2022, 2023). (E,E)-2,4-Heptadienal could be generated from the degradation of fat during food processing (Zhu et al., 2015). High levels of (E,E)-2,4-heptadienal in KW fermented by RW could contribute to a superior fatty flavor and green aroma compared to the other groups (Wang et al., 2020; Wei et al., 2013). In addition, a higher amount of valeraldehyde in KW fermented by RW could provide a stronger fruity and nutty note.

Ketones are mainly produced by the degradation of unsaturated fatty acids and amino acids, giving a strong flavor even at low concentrations (Sun et al., 2018). In our study, higher levels of two ketones were found in KW fermented by RW compared to the other groups, namely 1-octen-3-one and 4-methyl-2-pentanone. 1-Octen-3-one, associated to herbal and mushroom notes (Wang et al., 2021), has been previously detected in KW by means of GC-MS (Huang et al., 2022). In addition, Chen et al. found that 1-octen-3-one was the main contributor to the characteristic aroma of Chinese rice wine (Chen et al., 2019). Similarly to 1-octen-3-one, 4-methyl-2-pentanone, a typical volatile aroma compound for dry red wines, could give KW fruity and green herbs aromas (Jin et al., 2021).

In the process of wine fermentation, alcohols can be considered the main compounds formed as a result of the catabolism and anabolism of yeast (Lan et al., 2022; Wang et al., 2014). In agreement with our study, 3-methyl-1-butanol and butanol were identified in KW by Huang et al. through GC-MS (Huang et al., 2022). However, it is worthy to note that some alcohols were negatively correlated with wine flavor, such as 1-propanol and 2-heptanol. The flavor of 1-propanol has been described as musty and usually associated with low quality wines (Gambetta et al., 2017). 2-Heptanol was described as earthy and unripe fruit flavored. Focusing on ^{1}H-NMR analysis, concentration of glycerol was less abundant in KW fermented by RW than other groups. Such molecule is one of the main by-products of yeast during alcohol fermentation, with slightly sweet taste and viscous properties (Liu et al., 2018). In our study, distinct glycerol levels were mainly determined by different yeast strains, which was consistent with Nieuwoudt et al. (Nieuwoudt et al., 2017).

Organic acids are mainly produced by yeasts through fatty acid metabolism and tricarboxylic acid cycle (TCA cycle) (Swiegers & Pretorius, 2005), representing essential VOCs for complexity and fruity balance in fruit wines (Milovanovic et al., 2019; Mu et al., 2019; Qin et al., 2018). An exception is represented by 2-methylbutyric acid, with a flavor described as pungent and acidic, which was less abundant in KW fermented by RW compared to the others. In combination with the variations of ketones and alcohols, higher amounts of 1-octen-3-one and 4-methyl-2-pentanone, and lower levels of 1-propanol and 2-heptanol might have positive consequences on flavor features. In terms of ^{1}H-NMR analysis, six organic acids exhibited significant differences among the four groups, with the highest levels of acetoacetate, 2-hydroxyglutarate, 3-hydroxybutyrate, 2-phosphoglycerate, galactonate and galactarate and lower levels of 2-hydroxybutyrate in RW samples. Acetoacetate is a ketone body that produces reactive oxygen species, beneficial for human health (Rathee et al., 2016). Shimizu et al. found that acetoacetate could be formed by two acetyl-CoA molecules condensing to one acetoacetyl-CoA, then decarboxylated to acetone. Finally, in yeast cells, acetone could be converted to isopropanol by ethanol dehydrogenase (Shimizu et al., 1974). As a substrate of glycolysis, 2-phosphoglycerate plays a key role on pyruvate synthesis, and the reduction of 2-phosphoglycerate regulated the synthesis of acetyl-CoA in the TCA cycle (He et al., 2020).

Amino acids are widely found in different types of fruit wines, such as pear wine (Yang et al., 2021), grape wine (Malagoli et al., 2022) and KW (Liu, D., Xu, et al., 2020). Aromatic amino acids, in particular, not only play fundamental roles on the aroma of wine, but they are also precursors of most VOCs during wine fermentation (El Hadi et al., 2013). Besides, they are nitrogen sources for yeast growth and reproduction (Zhang et al., 2018). In line with the present study, some amino acids have been characterized in KW by means of reversed-phase high-performance liquid chromatography, namely alanine, aspartate, arginine, valine, proline, tyrosine, isoleucine and leucine (Chen et al., 2022). Univariate and multivariate analyses showed that the higher concentrations of leucine and tyrosine and the lower concentrations of proline, asparagine, aspartate, and arginine made KW fermented by RW stand out from the others. During wine fermentation, leucine could be converted to isoamyl alcohol via the Ehrlich pathway, providing whiskey, alcoholic, pungent, cheese or herbal scents in wines (Genovese et al., 2009). Tyrosine is produced by the oxidation of phenylalanine by phenylalanine hydroxylase. A previous study indicated that red wines produced by organic management could lead to higher levels of tyrosine than biodynamic management (Laghi et al., 2014). Moreover, Kamal et al. found that tyrosine could be converted to tyramine with wine aging, with adverse effects on wine quality (Kamal et al., 2016). Proline could be converted to glutamate via proline oxidase and pyrroline-5-carboxylate reductase in the mitochondria of *S. cerevisiae* in aerobic environment (Salmon & Barre, 1998). As proline could not be consumed by yeast during alcoholic fermentation (Tzachristas et al., 2021), we suggest that the variation of proline concentration in KW could be linked to distinct proline metabolism related enzyme activities in different yeast strains during aerobic respiration. Arginine can provide two opposite flavors, namely sweetness and bitterness, when present in low or high concentrations in wine (Yu et al., 2022). Arginine is a precursor of putrescine, commonly detected in wine, but harmful to human health in connection with an excessive intake (Torres et al., 2017). Therefore, higher levels of arginine may have a negative impact on the quality of KW, both from flavor and safety points of view.

5. Conclusion

To the best of our knowledge, this is the first work that comprehensively characterizes the sensory feature and flavor profile of KW through the combination of sensory evaluation, E-tongue, GC-IMS and ^{1}H-NMR. The combination of several techniques has been confirmed to provide a more comprehensive flavor fingerprint than single techniques. As suggested by sensory evaluation and E-tongue analyses, KW fermented by different yeast strains exhibited varied flavor features, and KW fermented by RW obtained the highest sensory score, thus being one of the potential candidates for KW production. The present study will facilitate screening suitable S. cerevisiae strains for KW production and provide a theoretical basis for large-scale production of KW.

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CRediT authorship contribution statement

Qian Zhang: Formal analysis, Writing – original draft, Writing – review & editing. **Jian Ma:** Formal analysis, Writing – review & editing. **Yupei Yang:** Formal analysis, Writing – review & editing. **Jing Deng:** Writing – review & editing. **Kaixian Zhu:** Methodology, Writing – review & editing. **Yuwen Yi:** Methodology, Writing – review & editing. **Junni Tang:** Writing – review & editing. **Xiaole Jiang:** Writing – review & editing. **Chenglin Zhu:** Conceptualization, Data curation, Formal analysis, Funding acquisition, Methodology, Writing – original draft, Writing – review & editing. **Luca Laghi:** Methodology, Writing – original draft, Writing – review & editing.

Declaration of competing interest

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

Data availability

Data will be made available on request.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.lwt.2023.115193.

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