

Exploring the aroma profiles and color characteristics of chardonnay wines from the eastern foothills of Ningxia Helan Mountain in China: A Flavoromics approach

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ABSTRACT

This study assessed the chemosensory characteristics of Chardonnay wines from the eastern foothills of the Ningxia Helan Mountain, China. Using Check-All-That-Apply (CATA) and Descriptive Analysis (DA), 29 wines were categorized into lively (QTX and XX sub-regions, marked by citrus and floral aroma) and implicit (YN sub-region, marked by truffle and kerosene aroma) aroma styles. GC-Quadrupole-MS and GC-Orbitrap-MS identified 191 volatile compounds. Subsequent OPLS-DA analysis underscored those volatile compounds, including 1-hexanol, 2-phenylethyl ester, butanedioic acid, diethyl ester, and phenylacetaldehyde, likely form the fundamental volatile framework of the distinct aroma styles. HPLC-QqQ-MS/MS analysis identified 26 non-volatile phenolic compounds. Wines from the YN region exhibited a notable yellowish hue, likely due to their higher flavanol content. This study offers insights into Chardonnay wines' chemistry and sensory traits, guiding vintners to optimize viticulture and oenology practices, and empowering consumers to select wines based on unique aromas and quality.

1. Introduction

Chardonnay is among the oldest and most widely dispersed cultivars of wine grapes, possessing significant commercial value for countries or regions involved in wine production (Kustos et al., 2020). The white wine made from Chardonnay is highly appreciated by wine consumers worldwide due to its unique flavor and rich aroma.

Since the beginning of the twenty-first century, the Eastern Foothills of Helan Mountain in Ningxia has emerged as one of the most significant wine producing regions in China and a hub for tremendous developmental potential. The area is located between the alluvial fan and plain

of the Yellow River, with the Helan Mountains to the west and the Yellow River channel to the east. These natural conditions result in significant differences in the environmental conditions and soil characteristics among the various sub-regions (Qi, Wang, Qin, & Sun, 2019; Tang et al., 2020). In sequential order from North to South, this region can be partitioned into six sub-regions that are adjacent to one another (Fig. 1); namely, Helan (HL), Xixia (XX), Yongning (YN), Qingtongxia (QTX), and Hongsipu (HSP) (Ling et al., 2023).

In recent years, there has been a notable increase in research focused on wines from the eastern side of the Helan Mountains in Ningxia (Song et al., 2022; Tang et al., 2020; Zhang et al., 2022). However, most of the

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research has centered around the sensory quality and volatile composition of the red wines produced in this region. Currently, not enough research has been done on the white wines produced in the region, especially Chardonnay.

Fifty-seven volatile compounds have been shown to make a significant aromatic contribution to Chardonnay wines (Gambetta, Bastian, Cozzolino, & Jeffery, 2014). The principal aroma compounds encompass several types, such as isoprenoids, esters, alcohols, thiols, lactones, monoterpenes, phenols, and acids (Herrero et al., 2016). Gas chromatography-quadrupole-mass spectrometry (GC-QMS) is widely employed method to analyze volatile compounds in wine, and the majority of studies examining diverse wine samples have utilized single quadrupole mass spectrometry to detect these compounds (Khakimov, Bakhtykyzy, Fauhl-Hassek, & Engelsens, 2022; Pinto et al., 2018). Notably, a previous investigation indicated that two-dimensional integrated chromatography-time-of-flight mass spectrometry is superior in detecting trace volatile compounds in Chardonnay wines (Welke, Zanusi, Lazzarotto, & Alcaraz Zini, 2014).

Our recent research has shown that GC-Orbitrap-MS its high accuracy in mass measurements which significantly reduces background signals (Li et al., 2024; Liu et al., 2022; Liu et al., 2022; Wang et al., 2024). This enables enhancement of the signal-to-noise ratio (S/N) of the target analyte while minimizing background ion interference. The GC-Orbitrap-MS method has the capability of achieving high-quality resolution of up to 6000 FWHM (m/z 200) as well as high-precision accuracy of less than 3 ppm (Belarbi et al., 2021). GC-Orbitrap-MS demonstrates the potential for detecting volatile compounds in wine, positioning it as a robust technique for the qualitative analysis of trace aroma compounds (Li et al., 2023; Ma et al., 2023). It is credible to believe that GC-Orbitrap-MS is a powerful method for detecting volatile

compounds in Chardonnay wine, which can provide support and complementary information to the GC-Quadrupole-MS detection results.

The Check-All-That-Apply (CATA) is a rapid sensory descriptive technique that can be conducted by semi-trained or untrained evaluators (Varela & Ares, 2012). This sensory descriptive method has been applied to evaluate a variety of alcoholic beverages, including Chinese-produced wines (Alencar et al., 2019). Descriptive Analysis (DA) is a classic sensory analysis method that is based on a trained panel of sensory experts (Stone, Sidel, Oliver, Woolsey, & Singleton, 2004), and it is also a commonly used method in sensory evaluation of wines. Whether the integration of the two applications will result in a more comprehensive aroma profile of Chardonnay wines is currently unknown.

For Chardonnay wines, the color intensity increases gradually with time, usually from light lemon-green or medium lemon into gold, amber, finally brown color (Zhao et al., 2023). Phenolic compounds in Chardonnay wines are mainly hydroxycinnamic acids, hydroxybenzoic acids, flavanols and flavan-3-ols. The presence of these phenolic compounds and their browning reaction during wine storage together determine the color of Chardonnay wines. HPLC-QQQ-MS/MS has been applied for the detection of phenolic compounds in wines in several studies (Li et al., 2009; Li, Pan, Jin, Mu, & Duan, 2011) and has been applied also to Chardonnay wines (Xing et al., 2016).

This study explores the hypothesis that there is a divergence in the aroma style and color characteristics of Chardonnay wines from Helan Mountain. In this study, the volatile composition and aroma characteristics of Chardonnay wines from this region were investigated using two mass spectrometry methods, GC-Quadrupole-MS and GC-Orbitrap-MS, as well as two sensory evaluation methods, Check-all-that-apply and Descriptive analysis. This study also investigated the phenolic compounds and color of Chardonnay wines from this region using HPLC-

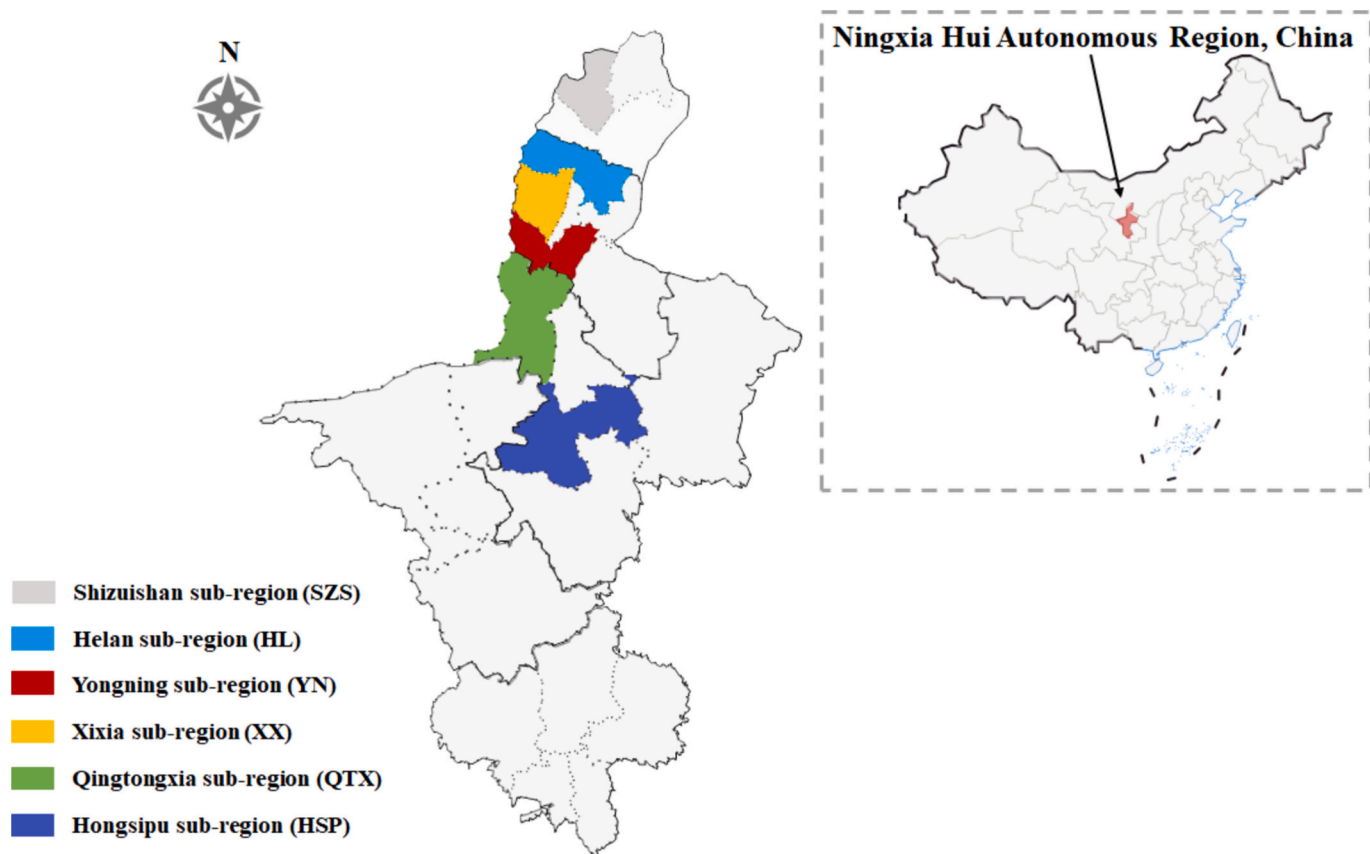


Fig. 1. Distribution of the six sub-regions in the Helan Mountains East Foothills region. Various sub-regions are distinguished by different colors: light grey text for the SZS sub-region, light green text for the HL sub-region, deep red for the YN sub-region, gold for the XX sub-region, green for the QTX sub-region, and indigo for the HSP sub-region. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

QqQ-MS and the CIELAB parameters. To the best of our knowledge, this study represents the first investigation of the volatile and non-volatile compounds, aroma characteristics, and color determination of Chinese Chardonnay wines from the eastern foothills of the Ningxia Helan Mountain.

2. Materials and methods

2.1. Chemicals and reagents

High-purity analytical-grade sodium hydroxide (NaOH) and sodium chloride (NaCl) were procured from Beijing Chemical Works (Beijing, China). Analytical-grade tartaric acid and glucose were sourced from Shanghai Macklin Biochemical (Shanghai, China). Distilled water was prepared using the Milli-Q® IX 7003 water purification system (Merck KGaA, Darmstadt, Germany). Chromatographic grade ethanol was bought from Fisher (Fairlawn, NJ, USA). All standards were of chromatographic grade and were dissolved in ethanol to prepare concentrated stock solutions. These concentrated solutions were stored at $-20\text{ }^{\circ}\text{C}$ and used within one week after preparation to construct the external standard curves. Information on the standards used in this study is presented in Table S1.

2.2. White wine samples

Fig. S1 presents the experimental design of this study. A total of 29 commercial Chardonnay wines sourced from 15 wineries, representing approximately half of the wineries in this region, were studied across five sub-regions: Helan (HL), Xixia (XX), Yongning (YN), Qingtongxia (QTX), and Hongsipu (HSP) in the Eastern Foothills of Helan Mountain, Ningxia (Table S2).

The vintages of samples ranged from 2012 to 2020 and they were all made from a single variety of Chardonnay grapes. Most of these samples were collected from the XX ($n = 8$), YN ($n = 12$) and QTX ($n = 6$) sub-regions, which are relatively matured sub-regions, while fewer samples were collected from HL ($n = 2$) and HSP ($n = 1$) sub-regions, which are developing wine-producing regions with only three wineries able to offer single varietal Chardonnay wines. All samples were stored unopened and protected from light at $4\text{ }^{\circ}\text{C}$.

2.3. Physical and chemical analyses

Physical and chemical characterization of Chardonnay wines was conducted using Wine Scan FT 120 (FOSS Analytical, Denmark) rapid-scanning infrared Fourier-transform spectrometer. The methodology employed for analysis was in accordance with previously published research (Lan et al., 2022). The indicators measured ethanol, total acidity, volatile acidity, gluconic acid, total sugar, pH, malic acid, citric acid, CO_2 , density, folic acid, glycerol, lactic acid, sorbic acid, tartaric acid, fructose, and glucose. Each sample was repeated three times and the results are shown in Table S3.

2.4. Sensory analysis

Aroma characteristics of Chardonnay wine samples were evaluated using check-all-that-apply (CATA) and descriptive analysis (DA). All sensory experiments were conducted in a lighted, temperature-controlled sensory laboratory, which was kept at a constant temperature of $20\text{ }^{\circ}\text{C}$, with each participant conducting the experiments in a separate compartment. The experimental environment meets the requirements of ISO 8589:2007. To eliminate systematic errors, wine samples were served to participants in a randomized order in International Standards Organization-compliant tasting glasses. All participants were informed that performing these actions was completely voluntary and that their informed consent was obtained in full accordance with the 1975 Declaration of Helsinki. The sample of the informed consent form

signed by the evaluators is presented in Table S4. Ethical approval for participation in this study was granted by the Research Ethics Committee of the Chinese Agricultural University, reference number CAUHR-20220901 (Table S5).

2.4.1. Check-all-that-apply (CATA)

A panel of 16 experts with at least 3 years of experience in wine-making and aroma evaluation (**Panel 1**, 10 men and 6 women, aged 26–58 years) evaluated the aromas of 29 Chardonnay wines. All 29 samples were divided into 5 rounds and presented to the evaluators in **Panel 1**, who were asked to write about the aromatic characteristics of the samples. After each wine sample was smelled, every evaluator in **Panel 1** submitted the aroma characteristics they perceived in that sample. These characteristics were not filtered out, even if mentioned only once, and were compiled into a list of 43 aroma descriptors (Table S6). Subsequently, a panel of six experts (**Panel 2**, 3 men and 3 women, aged 26–40 years) with extensive experience in winemaking and aroma evaluation evaluated all 29 samples again referring to previously constructed list of aroma descriptors. In addition to assessing whether these aroma descriptors were perceived in the samples, **Panel 2** was also tasked with defining these descriptors (Table S6). Forty-three aroma descriptors discussed by **Panel 2** were included in the list of aroma descriptors for the CATA.

A panel of 41 evaluators (**Panel 3**, 21 males and 20 females, aged 18–29 years), who had received at least 3 h of training in wine related knowledge, evaluated the aromas of the samples using the CATA method. All 29 Chardonnay wines were presented to the evaluators in **Panel 3** in 5 rounds, and the evaluators were forced to take a 10-min break between each round to avoid fatigue. During the experiment, the evaluators were asked to sniff the samples carefully and to choose the appropriate word to describe each wine sample from the 43 aroma descriptors list previously formulated.

2.4.2. Descriptive analysis (DA)

A panel of 6 experts with at least 3 years of experience in winemaking and aroma evaluation (**Panel 4**, 3 men and 3 women, aged 26–30 years) generated 12 aroma descriptors based on the 43 aroma descriptors used in the CATA to conduct the DA. Simultaneously, **Panel 3** discussed and identified reference samples for nine of the aroma descriptors. Table S7 shows the aroma descriptors and their interpretations used in the DA, along with a list of reference sample formulations with aroma intensities of 6 on a 0–11-point linear scale.

A panel of 16 fully trained evaluators (**Panel 5**, 5 men and 11 women, aged 23–30 years) from the Center for Viticulture & Enology (CFVE) of China Agricultural University evaluated the aroma characteristics of the samples using the DA method (Lan et al., 2019; Song et al., 2022). Before each formal experiment, the evaluators in **Panel 5** sniffed and discussed the 2 single varietal Chardonnay wines until everyone reached a consensus. During the experiment, all 29 Chardonnay samples were presented to the **Panel 5** evaluators in five rounds, and the evaluators were forced to take a 10-min break between each round to avoid fatigue. Evaluators were asked to evaluate the intensity of 10 aroma attributes in the samples using a linear scale of 0–11 (0 = very low intensity, 10 = strong intensity). Each sample was evaluated 2 times.

2.5. HS-SPME-GC-quadrupole-MS detection of volatile compounds in chardonnay wines

The volatile compounds of Chardonnay wines samples were detected by HS-SPME-GC-Quadrupole-MS, following methods previously reported in the literature (Lan et al., 2019). Briefly, 5 mL of each wine sample was added to a 20 mL vial and spiked with 1.5 g of NaCl and 10 μL of 4-methyl-2-pentanol (solution dissolved in ethanol, 1 g/L). The sample was equilibrated at $40\text{ }^{\circ}\text{C}$ for 30 min. Solid phase micro-extraction fiber (50/30 μm DVB/CAR/PDMS, Supelco, Bellefonte, PA, USA, with a preheat treatment according to the manufacturer's

recommendations before use) was exposed to the vial headspace at 40 °C for 65 min. The compounds were thermally desorbed in the injection port of GC at 250 °C for 8 min with a split ratio of 5:1.

The volatile compounds were analyzed using an Agilent 7890 A GC System (Agilent Technologies, Santa Clara, CA, USA). The separation of compounds was done with a HP-INNOWax capillary column (60 m × 0.25 µm, 0.25 µm, J & W Scientific, Santa Clara, CA). The temperature rise procedure of chromatography was as follows: 50 °C for 1 min, 3 °C per min up to 220 °C and holding for 5 min. The flow rate of carrier gas (nitrogen with 99.99 % purity) was set at 1 mL/min. All mass spectra were acquired in electron ionization mode at 70 eV using full scan with a scan m/z range of 29 to 350. Under the same chromatographic and mass spectrometric conditions, a C₆-C₂₄ n-alkane series (500 µg/L, Supelco, Bellefonte, PA, USA) were analyzed to calculate retention indices (RIs).

The compounds were identified by combining the calculated RI value, the mass spectrum information in NIST13. According to the ten attenuation levels in the synthetic model wine, the aroma standards' calibration curves were obtained. The volatile compounds were quantified through calibration curves built with the ratio of the peak area of the target compound to the peak area of the corresponding internal standard (4-methyl-2-pentanol) against the concentration of each compound. Each sample was repeated three times under the same conditions.

2.6. HS-SPME-GC-Orbitrap-MS detection of volatile compounds in chardonnay wines

The volatile compounds of Chardonnay wines samples were detected by HS-SPME-GC-Orbitrap-MS according to previously published methods by (Liu et al., 2022). Briefly, 5 mL of each wine sample was added to a 20 mL vial and spiked with 1.5 g of NaCl and 10 µL of 4-methyl-2-pentanol (solution dissolved in ethanol, 1 g/L). The sample was equilibrated at 40 °C for 30 min at 450 rpm. Solid phase micro-extraction fiber (50/30 µm DVB/CAR/PDMS, Supelco, Bellefonte, PA, USA, with a preheat treatment according to the manufacturer's recommendations before use) was exposed to the vial headspace at 40 °C for 30 min. The compounds were thermally desorbed in the injection port of GC at 250 °C for 8 min.

The volatile compounds were analyzed using a Thermo Scientific Trace 1300 gas chromatography coupled with a Thermo Scientific Q-Exactive Orbitrap mass spectrometer (GC-Orbitrap-MS, Thermo Scientific, Bremen, Germany). The separation of compounds was done with a HP-INNOWax capillary column (60 m × 0.25 µm, 0.25 µm, J & W Scientific, Santa Clara, CA). The temperature rise procedure of chromatography was as follows: 40 °C for 5 min, 3 °C per min up to 220 °C. The flow rate of carrier gas (helium with 99.99 % purity) was set at 1 mL/min. All mass spectra were acquired in electron ionization mode at 70 eV using full scan with a scan m/z range of 33 to 350. Resolution power was set at 60,000 full widths at half-maximum (FWHM) at m/z 200. Under the same chromatographic and mass spectrometric conditions, a C₆-C₂₄ n-alkane series (500 µg/L, Supelco, Bellefonte, PA, USA) were analyzed to calculate retention indices (RIs).

The compounds were identified by combining the calculated RI value, the mass spectrum information in NIST13. According to the ten attenuation levels in the synthetic model wine, the aroma standards' calibration curves were obtained. The volatile compounds were quantified through calibration curves built with the ratio of the peak area of the target compound to the peak area of the corresponding internal standard (4-methyl-2-pentanol) against the concentration of each compound (Liu et al., 2022). Each sample was repeated three times under the same conditions.

2.7. HPLC-QqQ-MS/MS detection of phenolic compounds in chardonnay wines

An Agilent 1200 series HPLC system coupled with a 6410B triple

quadrupole mass spectrometer (Agilent Technologies, Santa Clara, CA, USA), was employed for phenolic compound detection in the Chardonnay wines, utilizing a Poroshell 120 EC-C18 column (150 × 2.1 mm, 2.7 µm) for compound separation.

The samples were filtered through a 0.22 µm filter before analysis. The mobile phases used for elution were 0.1 % formic acid aqueous solution (A) and 50/50 methanol acetonitrile solution with 0.1 % formic acid (B). The elution procedure of phenolic compounds was 0–10 min, 10 % of B; 10–15 min, 100 % of B. The flow rate of the mobile phase was 0.4 mL/min, the column temperature was maintained at 55 °C, and the injection volume was 5 µL.

The elution program of anthocyanin derivatives was 1 min, 100 % of A; 3 min, 25 % of B; 15 min, 30 % of B; and 20 min, 100 % of B. The posting time was for 5 min. The flow rate of the mobile phase was 0.3 mL/min, the column temperature was controlled at 55 °C, and the injection volume was 10 µL. An electrospray ionization source was used with a spray voltage of 4 kV in negative and positive modes for the non-anthocyanins and anthocyanins, respectively. The temperatures of the ion source and drying gas (N₂) were 150 °C and 350 °C, respectively. The gas flow rate was 12 L/h, and the nebulizer pressure was 35 psi. Multiple reaction monitoring (MRM) was selected as a scanning mode for both identification and quantification.

The qualitative of phenolic compounds was achieved based on their mass information and retention time. The peak areas of the phenolic compounds were used as their relative contents. Three repeated injections were set for each sample.

2.8. Calculation of odor activity value

The odor activity value (OAV) method is an important method currently used to measure the aroma contribution of compounds. It is calculated by dividing the actual concentration of each sample by its threshold value in a wine matrix or hydroalcoholic solution matrix, and compounds with a result greater than or equal to 1 are considered to have a significant contribution to aroma.

2.9. Colorimetric measurements

The chromaticity parameters of the wines using the CIELab method according to OIV (OIV, 2015) were measured with an ultraviolet-visible spectrometer (UV 1101 II, Shanghai Tianmei Scientific, Shanghai, China) and the absorbance spectra of the wines (380–700 nm) were recorded at a wavelength interval of 10 nm (Sáenz Gamasa et al., 2009). Wine samples were filtered through cellulose filters (0.45 µm; Jinteng company, Tianjin, China) and placed in a 2 mm path length glass cuvette with distilled water as a reference. Each wine was analyzed in triplicate. The CIELAB parameters, expressed in terms of the rectangular (L*, a*, b*), were calculated according to a previously published method (Chen et al., 2019).

2.10. Statistical analysis

All data pre-processing was performed by Microsoft Excel (Microsoft, USA). A non-parametric test based on Cochran's Q test was performed on the results of the CATA using XLSTAT 2019 (Addinsoft, New York, NY, USA). One-way ANOVA based on Duncan's test was performed using R 4.1.3 for volatile compound concentrations, CIELAB parameters of the samples, phenolic concentrations and DA results. Statistical significance was deemed at $p = 0.05$. Principal component analysis (PCA) was performed on the results of the CATA and the results of the DA using XLSTAT 2019 (Addinsoft, New York, NY, USA). The species-quantity stacking of volatiles was mapped using Origin 2021 (MicroCal, Massachusetts, USA). Hierarchical cluster analysis and cluster heat maps were performed for key compounds using TBtools 1.112 (Guangdong, China) (Chen et al., 2020). Color swatches of the wine samples were drawn using Adobe Photoshop (Adobe, New York). OPLS-DA analysis for

volatile compounds was conducted by SIMCA (version 14.1 from Umetrics, Malmo, Sweden).

3. Results and discussion

3.1. Aromatic characteristics of chardonnay wines

The aroma characteristics of 29 Chardonnay wines from this region were investigated using the CATA method. Table S8 presents the 38 aroma descriptors with significant differences ($p \leq 0.05$) in their frequency of occurrence as determined by Cochran's Q test, along with the frequency of their selection in each sample.

Among them, the top ten descriptors in terms of total frequency are Honey (502, occurrences), Citrus (486), Pineapple (346), Pear (319), Lemon (306), Candied Fruits (233), Cream (213), Peach (211), Candy (198), and Green Apple (197), indicating that these terms are most used to describe the aroma characteristics of the samples. These fresh fruity, sweet, and creamy aromas are typical aroma characteristics of Chardonnay wines (Gambetta, Cozzolino, Bastian, & Jeffery, 2016; Kustos et al., 2020).

It is worth noting that some aroma descriptors with lower frequency of occurrence may also reveal typical characteristics of certain samples. For instance, although the total frequency of yellow peach was relatively low (102), more than half of the assessors selected this descriptor to describe the YN10–20. Similarly, although withered grass (109) and caramel (105) had lower total frequencies, nearly half of the assessors chose these two descriptors to describe the YN4–17.

In terms of samples, the top ten samples in total frequency of occurrence are YN10–2 (337, occurrences), HL1–19 (303), XX4–20 (288), XX7–20 (273), QTX2–19 (273), HSP1–20 (258), QTX2–18 (250), XX5–20 (248), YN2–17 (243), and QTX12–19 (242), which may exhibit more complex aromatic characteristics and thus lead assessors to select more descriptors to describe them.

Based on the word frequencies of aroma descriptors presented in Table S8, all 29 samples and 38 aroma descriptors were separated using principal component analysis Fig. 2 (a). The first two principal components, F1 (43.45 %) and F2 (14.83 %), cumulatively accounted for 58.28 % of the variance in the data, effectively distinguishing between the aromatic descriptors and the wine samples. Aroma descriptors positioned to the right of F1 exhibited livelier notes, including citrus, lemon, pear, green apple and passion fruit. Conversely, descriptors situated to the left of F1 represented more implicit aromas, including minerals, roasted almonds, licorice, kerosene, animal fur, boiled fruit, clove, withered grass, caramel, and mushrooms. Additionally, aromas like cheese, coconut, butter, cream, and vanilla were distinctly separated and positioned at the top of the plot.

From the distribution of samples in the principal component analysis (Fig. 2 (a)), it is clear that all 29 Chardonnay wines were broadly divided into 2 categories, characterized by their association with sub-regions. The 29 samples exhibited distinct separation into two categories based on their aroma characteristics as determined by F1. Samples positioned on the left side of F1 (represented by YN10–20, XX4–20, XX7–20) were frequently associated by assessors with fresh fruity and floral notes, as well as sweet aromas. Conversely, samples positioned on the right side of F1 (represented by YN4–17, YN3–18, YN3–19) were more commonly described by assessors as possessing implicit and nuanced aromas like withered grass, boiled fruit, and mushrooms. In other words, the 29 wines sourced from five sub-regions can be distinguished by two completely different aroma styles. Samples of QTX and XX were predominantly located on the positive axis of F1, showing livelier aroma characteristics. On the other hand, samples from YN were predominantly located on the negative axis of F1, revealing more implicit aroma characteristics.

A total of 12 attributes were retained, including stone fruit, green fruit, citrus fruit, tropical fruit, floral, flint, leather, truffle, kerosene, boiled fruit, toast and cream and used in the DA. Table S9 shows the

range of intensities for all 12 aroma descriptors, five of which differed significantly ($p < 0.05$) between sub-regions. Among them, tropical fruit had ranging from 5.2 to 3.9, stone fruit (3.4–2.5), green fruit (4.3–3.5), citrus fruit (4.2–3.0), floral (1.4–3.6), flint (1.3–3.3), leather (0.6–4.1), truffle (0.7–3.3), kerosene (1.0–3.8), boiled fruit (1.8–5.2), toast (1.3–3.4), cream (1.2–4.2).

All 29 samples and 12 aroma descriptors were separated using principal component analysis (Fig. 2 (b)). The first two principal components, F1 (69.52 %) and F2 (15.51 %), contributed to 85.04 % of the data variance, resulting in good separation between aroma attributes and samples. Aroma descriptors positioned to the left of F1 exhibited livelier notes, including stone fruit, green fruit, citrus fruit, tropical fruit, and floral. Conversely, aroma descriptors situated to the right of F1 represented more implicit aromas, including flint, leather, truffle, kerosene, and boiled fruit. In addition, aroma descriptors like toast and cream were distinctly separated and positioned at the top of the plot. The distribution pattern of these aroma descriptors is consistent with the results obtained by CATA.

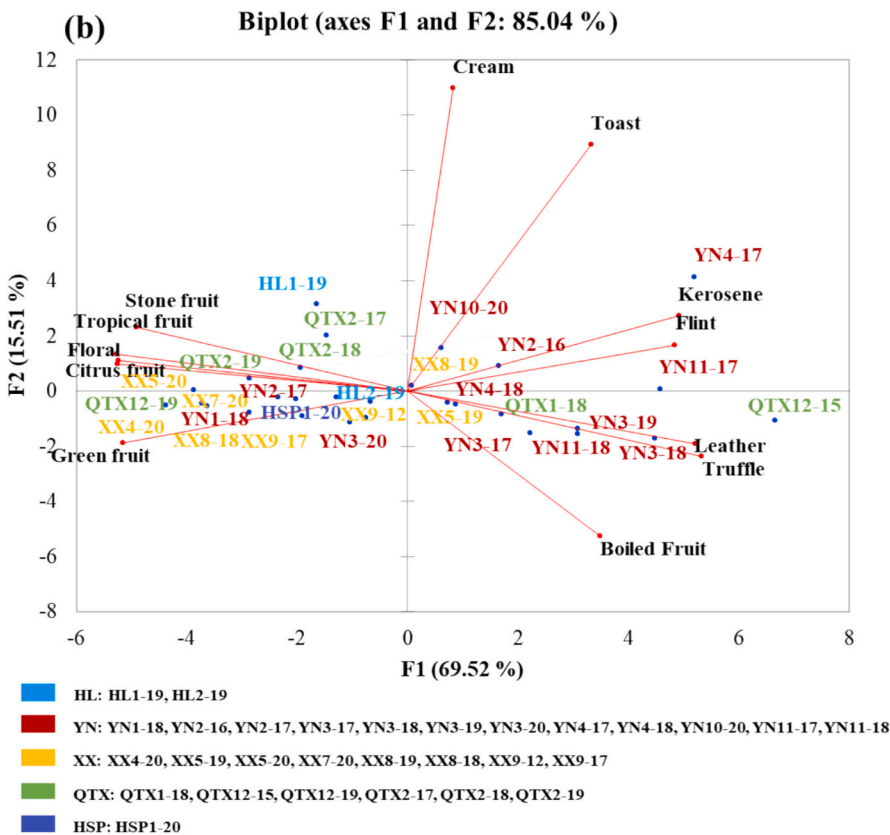
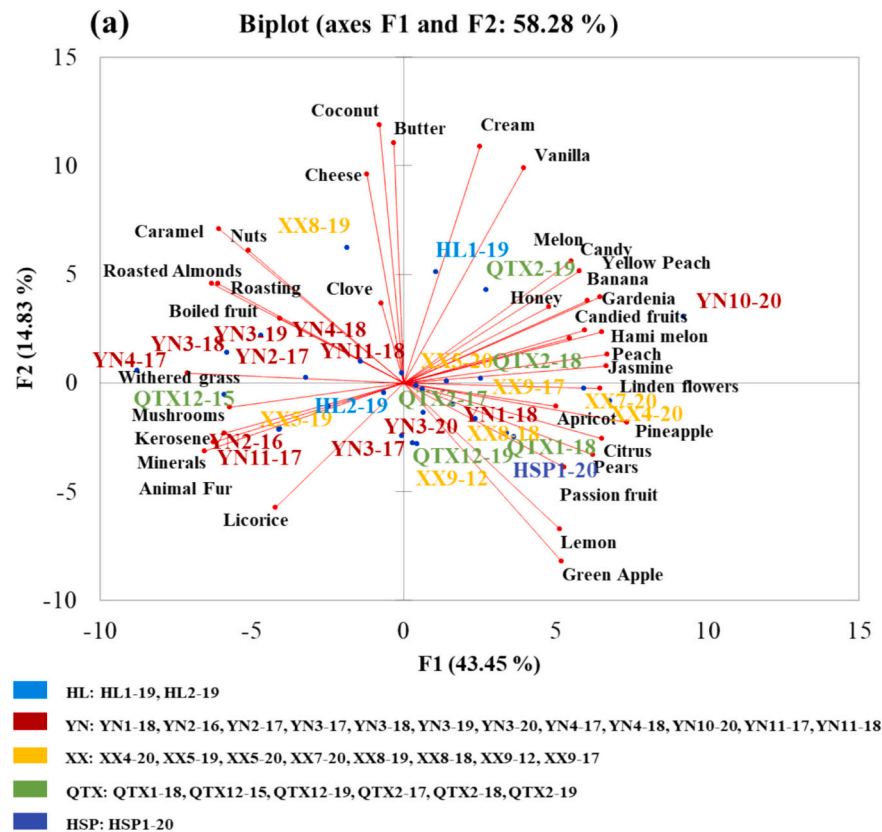
From the distribution of samples in the principal component analysis (Fig. 2 (b)), it is clear that all 29 Chardonnay wines were broadly divided into 2 categories, characterized by their association with sub-regions. Samples characterized by kerosene, flint, leather, and truffle, represented by QTX12–15, YN3–19, YN3–18, YN11–17, and YN4–17, were primarily distributed in the positive half of F1 axis. Samples characterized by stone fruit, green fruit, citrus fruit, tropical fruit, and floral, represented by XX4–20, XX5–20, XX7–20, and QTX12–19, were primarily distributed in the negative half of F1 axis. The distribution pattern of these samples is consistent with the results obtained by CATA. The wines from the QTX and XX sub-regions show a lively aroma characteristic, while the samples from the YN sub-region show an implicit aroma characteristic; these two aroma characteristics are gradually developing into two aroma styles. However, there are also exceptions to this pattern. For example, QTX12–15 exhibits pronounced characteristics of kerosene, flint, leather, and truffle. YN1–18 and YN2–17 also show some characteristics of stone fruit, green fruit, citrus fruit, tropical fruit, and floral. QTX12–15 may have undergone aroma changes during storage due to its earlier production year. The aroma characteristics of YN1–18 and YN2–17, on the other hand, may have been influenced by the winemaking process.

3.2. Composition of volatile compounds

The volatile compounds of Chardonnay wines from the eastern foothills of the Ningxia Helan Mountain were studied using HS-SPME-GC-Quadrupole-MS (LRMS, low-resolution mass spectrometry) and HS-SPME-GC-Orbitrap-MS (HRMS, high-resolution mass spectrometry). Fig. 3 displays the qualitative results of volatile compounds in the samples, with a total of 191 volatile compounds identified, including 30 alcohols, 13 aldehydes, 10 acids, 73 esters, 1 alkane, 18 aromatics, 8 furans, 12 ketones, 2 lactones, 5 volatile phenols, 1 pyridine, 2 pyrroles, 7 pyrazines, 2 sulfurous compounds, and 7 terpenes.

HRMS effectively complements the qualitative results of LRMS, especially in the detection of volatile compounds with relatively lower levels. A total of 154 volatile compounds, including 21 alcohols, 12 aldehydes, 5 acids, 54 esters, 1 alkane, 17 aromatic compounds, 8 furans, 12 ketones, 1 lactone, 5 volatile phenols, 1 pyridine, 2 pyrroles, 7 pyrazines, 2 sulfurous compounds, and 6 terpenes were qualitatively detected by HRMS. In addition, the LRMS has an irreplaceable role in the characterization of compounds, and a total of 37 volatiles including 9 alcohols, 1 aldehyde, 5 acids, 19 esters, 1 aromatic compound, 1 lactone, and 1 terpene were qualitatively detected.

Table S10 presents the results of one-way ANOVA based on Duncan's test for all compounds quantitatively detected in this study, with the samples grouped by geographical origin of production. Out of all the 191 volatile compounds detected in this study, 141 compounds had significant differences ($p < 0.05$) in their content across 5 sub-regions. These



(caption on next page)

Fig. 2. Analysis of the aroma characteristics of Chardonnay dry white wine from the eastern foot of the Helan Mountains in Ningxia. (a) Results of principal component analysis of word frequency of aroma descriptors in CATA. (b) Results of principal component analysis of word frequency of aroma descriptors in QDA. The explanation of the sample abbreviations depicted in the figure can be found in Table S2. Samples from various sub-regions are distinguished by different colors: light green text for the HL sub-region, deep red for the YN sub-region, gold for the XX sub-region, green for the QTX sub-region, and indigo for the HSP sub-region. The black text in these figures represents aroma descriptors. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

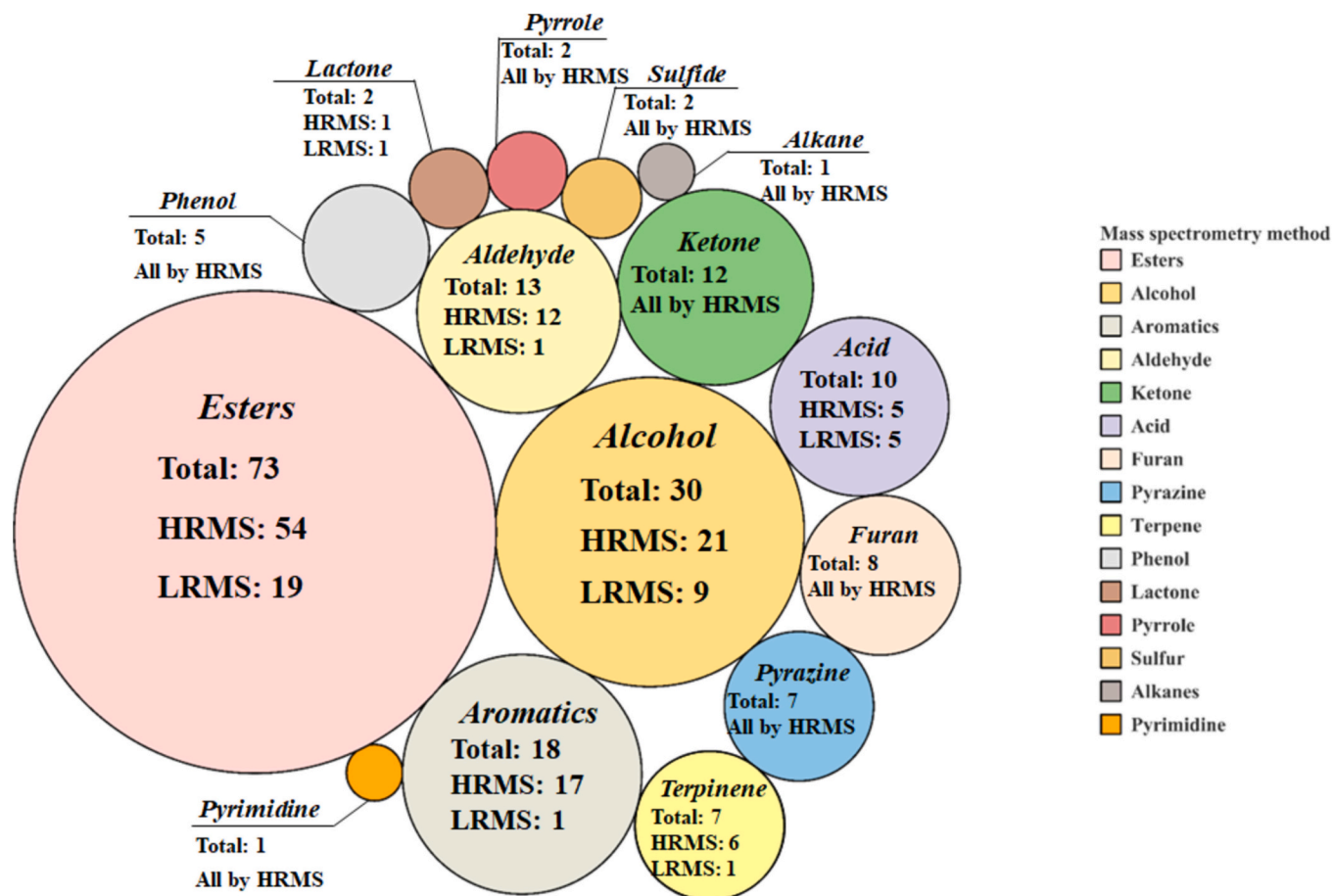


Fig. 3. Qualitative detection results of volatile compounds in Chardonnay dry white wine from the eastern foot of the Helan Mountains in Ningxia. In the figure, HRMS stands for HS-SPME-GC-Orbitrap-MS method, and LRMS stands for HS-SPME-GC-Quadrupole-MS method.

include, 30 alcohols, 9 aldehydes, 5 acids, 53 esters, 1 alkane, 17 aromatic compounds, 7 furans, 7 ketones, 2 lactone, 5 volatile phenols, 1 pyridine, 2 pyrroles, 7 pyrazines, 1 sulfurous compound, and 6 terpenes.

3.3. Volatile base of two aroma styles in chardonnay wines

The wines from the QTX and XX sub-regions show a lively aroma characteristic, while the samples from the YN sub-region show an implicit aroma characteristic; these two aroma characteristics are gradually developing into two aroma styles (Fig. 2). To further analyze the volatile basis of two aroma styles in Chardonnay wines from the eastern foothills of the Ningxia Helan Mountain, four samples (XX4–20, XX5–20, XX7–20, and QTX12–19) with a typical lively style and five samples (QTX12–15, YN3–19, YN3–18, YN11–17, and YN4–17) with a typical implicit style were selected. O-PLSDA analysis was performed using the concentration of compounds with significant differences in content among these samples. The results demonstrate good discrimination between the two groups of samples (Fig. 4 (a)). Fig. S2 shows the results of 200 fitting calculations, from which it can be seen that the model has an R^2 of 0.979 and a Q^2 of 0.898, indicating that the model is reliable, and the fitting results are good. Fig. 4 (b) shows the contribution of all

compounds to the discriminant analysis of groups DA(1) and DA(2), where compounds closer to DA(1) or DA(2) indicate a greater contribution to their discrimination. Table S11 lists the detailed information of 84 volatile compounds with VIP values greater than 1, including aroma description, aroma threshold, and odor activity value.

Regarding the volatile compounds that may contribute to the lively style, 1-hexanol (AL5, grassy), acetic acid, 2-phenylethyl ester (E64, rose-like), linalool (T3, citrus-like and flowery), pyrazine, trimethyl-(PY6, earthy and roasty), pyrazine, 2-ethyl-3-methyl-(PY4, roasty), and pyrazine, (2-methylpropyl)-(PY1) generally have higher odor activity values (OAVs) in samples with more lively aroma characteristics than in samples with more implicit aroma characteristics. In addition, six ester compounds with high VIP values ($VIP > 1.5$), including isobutyl acetate (E7, fruity), isoamyl acetate (E14, banana-like), dodecanoic acid, methyl ester (E63), 2-pentanol, acetate (E11), dodecanoic acid, ethyl ester (E65), and hexyl acetate (E19, green and fruity), may also be potential volatile compounds that contribute to the lively aroma style of Chardonnay wine. Except for T3, the aforementioned volatile compounds are all derived from the fermentation process of wine (Gambetta et al., 2014).

Regarding the volatile compounds that may contribute to the

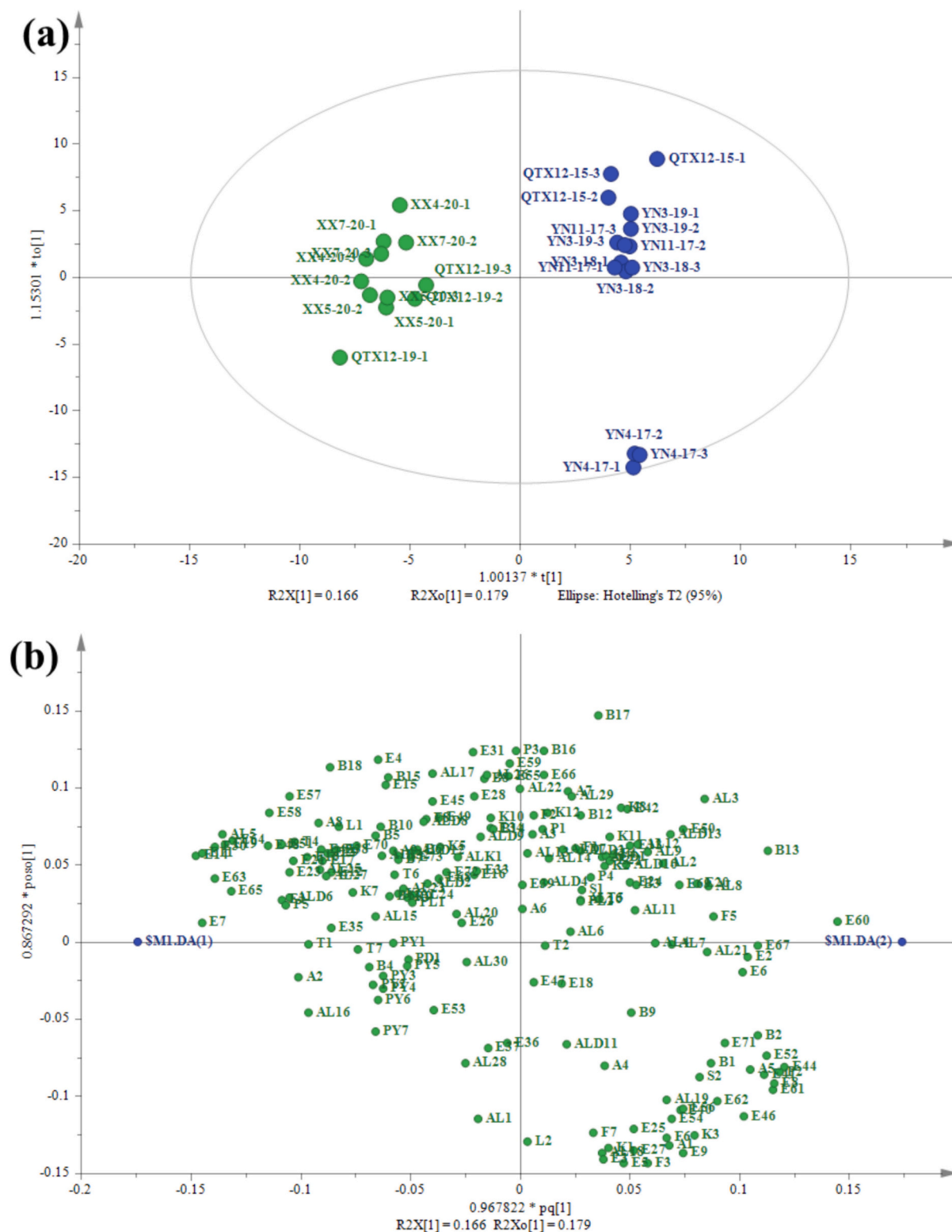


Fig. 4. Signature compounds and potential volatiles of two aromatic styles in the Chardonnay dry white wine from the eastern foothills of Ningxia Helan Mountains. (a) OPLS-DA analysis of typical samples of two aroma styles based on volatile compound contents. In Fig. 4(a), typical samples with the lively style are labeled in green, while typical samples with the implicit style are labeled in indigo. (b) Loading plot for the volatile compounds of typical samples of two aroma styles. The sample abbreviation explanations shown in Fig. 4(b) are detailed in Table S2, while the abbreviations of volatile compounds highlighted in green text are listed in Table S11. The text highlighted in indigo indicates the group of samples, where DA(1) denotes samples with the lively style and DA(2) denotes samples with the implicit style.

implicit style, butanedioic acid, diethyl ester (E52), furfural (F5, sweet and cereal-like), phenylacetaldehyde (B13, honey-like), 1-octanol (AL21, intense citrus, roses), and methionol (S2, cooked potato-like) generally have higher odor activity values (OAVs) in samples with more implicit aroma characteristics than in samples with more lively aroma characteristics. In addition, two ester compounds with high VIP values ($VIP > 1.5$), including pentanedioic acid, diethyl ester (E60) and benzeneacetic acid, ethyl ester (E61, honey-like), may also be potential volatile compounds that contribute to the implicit aroma style of Chardonnay wine. Phenylacetaldehyde has been reported in previous research as a Strecker degradation product of phenylalanine during wine bottle storage. At low concentrations, it presents a honey-like aroma, while at high concentrations, it presents a mossy aroma (Bueno et al., 2018; Echave, Barral, Fraga-Corral, Prieto, & Simal-Gandara, 2021). It is noteworthy that this group of compounds includes four diethyl esters (E60, E52, E71, and E69), which are typically formed by the esterification and condensation reaction of the corresponding organic acid molecule with two ethanol molecules during wine aging (Mato, Huidobro, Simal-Lozano, & Sancho, 2006; Schreiner & Morlock, 2023). It can be inferred that the wine samples from the YN sub-region have a more implicit aroma style possibly because they contain more aldehydes and diethyl esters produced during wine aging or bottle storage. These compounds may occur in samples from recent vintages and could be attributed to certain factors, such as oxidation reactions, related to grape growing practices or winemaking techniques in the YN sub-region that have yet to be elucidated, leading to premature aging of the wine.

3.4. Color characteristics and detection of non-volatile phenols

The CIELAB parameters were determined for 29 samples, expressed in terms of the rectangular (L , a^* , b^*) system, to represent wine color. The absorption spectra of the samples were shown in Fig. 5(a), the color palette was shown in Fig. 5(b), and the principal component analysis was shown in Fig. 5(c). Fig. 5(a) indicates that the samples have the highest absorbance at 380 nm wavelength of visible light, indicating that the samples have a blue-green hue. Table S12 presents the one-way ANOVA of variance results for the CIELAB parameters, and the wines from the five sub-regions showed significant differences only in the b^* value. Combining Fig. 5(b) and Fig. 5(c), wines produced in the YN sub-region have higher b^* values, which means that these samples tend to

have a yellow tone, while wines from other sub-regions do not show a consistent color pattern.

Using HPLC-QqQ-MS, 26 non-volatile phenolic compounds were detected in 29 samples, including 11 flavanols, 2 flavanones, 4 dihydrochalcones, 5 hydroxycinnamic acids, and 4 hydroxybenzoic acids. The peak areas of the compounds were subjected to one-way ANOVA of variance, and the results are shown in Table S13. Among them, the relative contents of 10 compounds were significantly different. Principal component analysis (PCA) was performed on peak areas of all 26 non-volatile phenolic compounds, and the results are shown in Fig. S3. Through this graph, it can be observed that the total variation of the analysis is 43.71 %. Moreover, the wine products from different sub-regions cannot be well distinguished, and most samples are concentrated in the negative half axis of F1. Thus, OPLS-DA was employed to analyze the peak areas of all 26 non-volatile phenolic compounds, as shown in Fig. 6 (a-b), and a good discrimination was achieved among the samples. Fig. 6 (b) shows the results of fitting calculation 200 times, from which the model has an R^2 value of 0.667 and Q^2 value of 0.435, indicating a good fitting result. There are 10 compounds with $VIP > 1$, which are marked in Table S13. Among them, 4 flavonol compounds have a close correlation with the yellow color of white wine. According to previous studies, quercetin, kaempferol, and isorhamnetin are the most important flavonol compounds in the winemaking grapes of white varieties (Castillo-Muñoz, Gómez-Alonso, García-Romero, & Hermosín-Gutiérrez, 2010; Mattivi, Guzzon, Vrhovsek, Stefanini, & Velasco, 2006). The quercetin-rhamnoside, dihydrokaempferol, myricetin, and dihydroquercetin detected in this study are derivatives of the above-mentioned compounds. The accumulation of flavonols in white grape varieties is mainly related to sunlight, especially to ultraviolet radiation. The stronger the ultraviolet radiation, the higher the accumulation of flavonols in grapes (Figueiredo-González et al., 2013). The yellow color of wines from the YN sub-region may be because of ultraviolet radiation and oxidation reactions.

4. Conclusion

The commercial Chardonnay wines from the Eastern Foothills of the Helan Mountain have been effectively characterized through a comprehensive analysis of their volatile compounds, aroma styles, and color characteristics. The wines from the region demonstrated

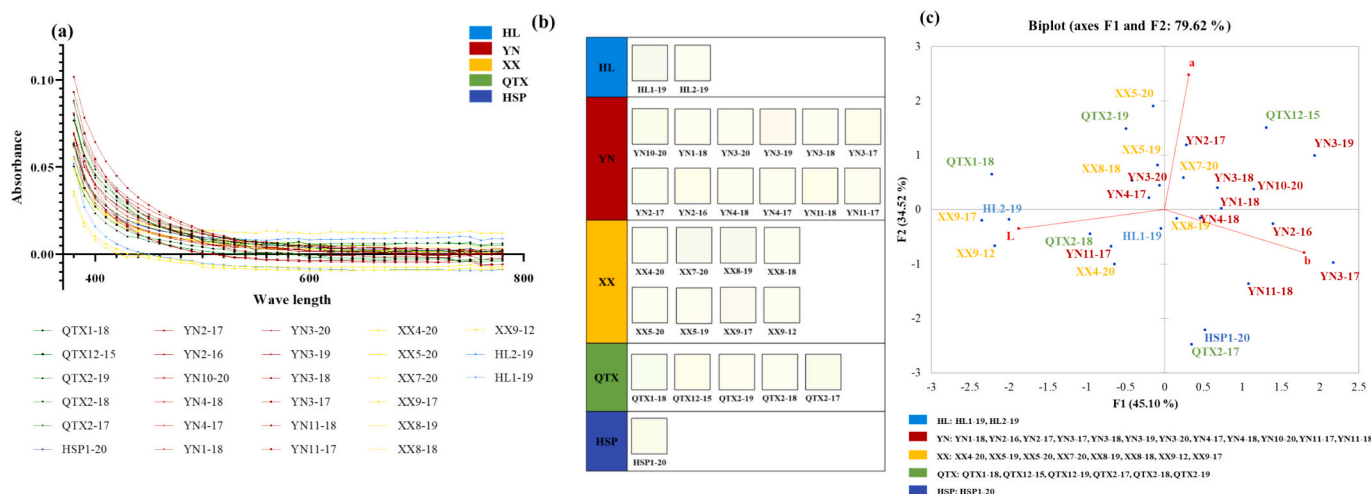


Fig. 5. Color Characteristics in the Chardonnay dry white wine from the eastern foothills of Ningxia Helan Mountains. (a) Absorption curve of wine samples. (b) Wine sample color chart. (c) Results of principal component analysis of the CIELAB parameters, expressed in terms of the rectangular (L , a^* , b^*) system for wine samples. The sample abbreviations explanation depicted in Fig. 5(a) and Fig. 5(c) is detailed in Table S2. Samples from the HL sub-region are denoted by light green text, samples from the YN sub-region are indicated in deep red, samples from the XX sub-region are highlighted in gold, samples from the QTX sub-region are shown in green, and samples from the HSP sub-region are represented in indigo. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

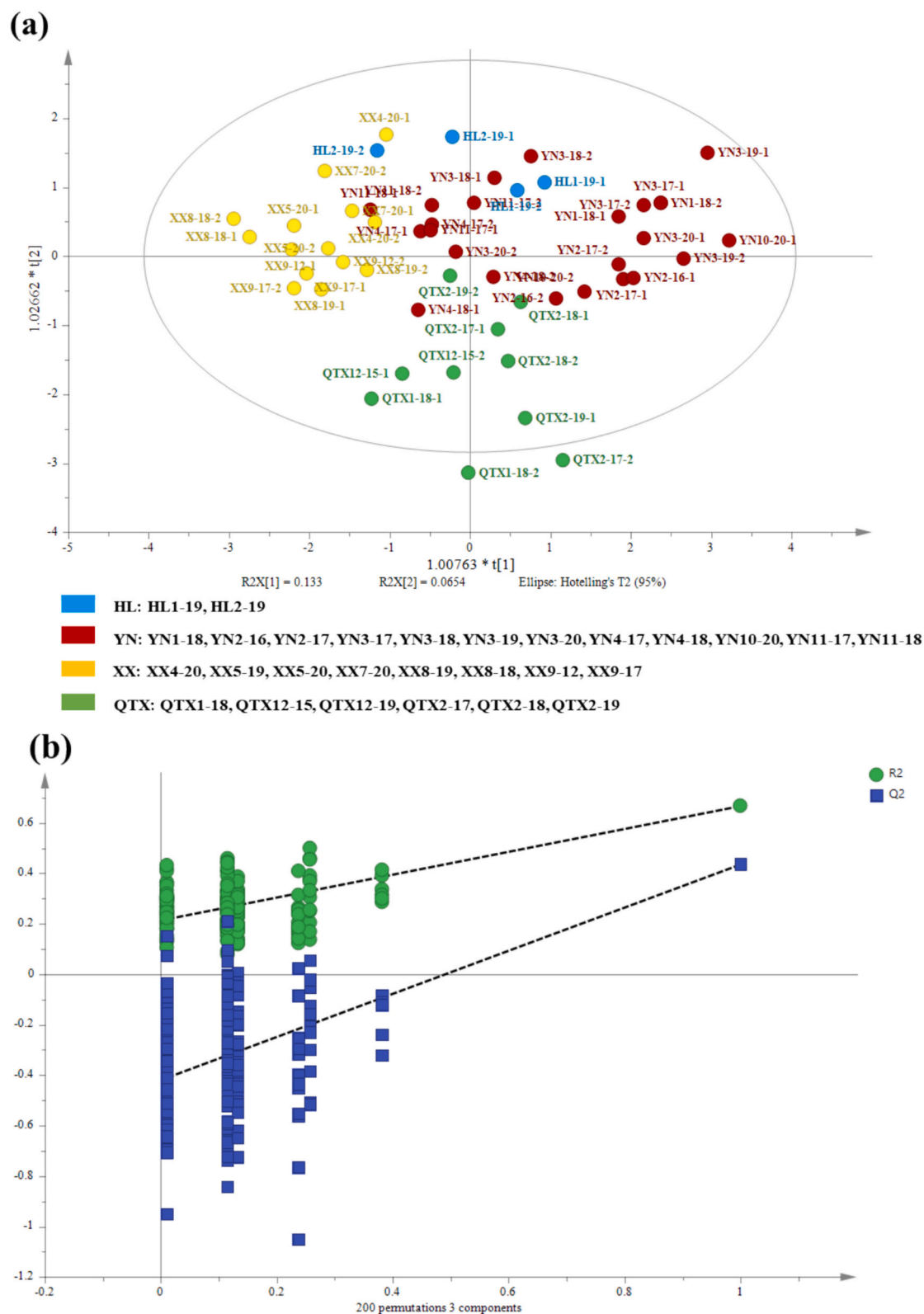


Fig. 6. Screening model construction for signature non-volatile phenolic compounds in the Chardonnay dry white wine from the eastern foothills of Ningxia Helan Mountains. (a) OPLS-DA analysis of wine samples based on the relative content of non-volatile phenolic compounds. The sample abbreviations explanation depicted in Fig. 6(a) is detailed in Table S2. Samples from the HL sub-region are denoted by light green text, samples from the YN sub-region are indicated in deep red, samples from the XX sub-region are highlighted in gold, samples from the QTX sub-region are shown in green. (b) Results of 200 rounds of fitting and calculation of the OPLS-DA model in Fig. 6(a). In the figure, R^2 is represented by green and Q^2 is represented by indigo. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

pronounced differences in their aroma styles. Specifically, the QTX and XX sub-regions were characterized by a lively aroma style, marked by distinct fresh fruit and floral notes. In contrast, the YN sub-region's wines exhibited a more implicit aroma style, marked by distinct truffle, kerosene, and flint. A total of 191 volatile compounds were identified, with 141 compounds demonstrating significant differences in content across the five sub-regions, highlighting the influence of regional terroir on wine chemistry. The OPLS-DA and odor activity value (OAV) analysis revealed that compounds like 1-hexanol, 2-phenylethyl ester, and linalool contribute to the lively style, while butanedioic acid, diethyl ester, and phenylacetaldehyde are associated with the implicit style. In terms of color, YN sub-region wines had higher b^* values, indicating a yellowish hue, possibly due to ultraviolet radiation and oxidation reactions. HPLC-QqQ-MS/MS detection of non-volatile phenolic compounds revealed significant differences in the content of 10 compounds, with flavonol compounds closely related to wine color. Although the study faced limitations in sample size and detection conditions, the findings suggest the potential for geographical traceability of Chinese Chardonnay wines and provide insights into the development of region-specific wine quality. This study holds significance for the Ningxia region by enhancing its viticultural reputation. It provides a scientific foundation for the region's Chardonnay wines, emphasizing the unique chemosensory attributes that can be associated with local terroir. This understanding can lead to the development of wines with distinct regional identities, potentially increasing the market value and consumer appeal of Ningxia wines, and contributing to the growth of the local wine industry.

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CRediT authorship contribution statement

Jiani Liu: Writing – original draft, Data curation. **Xinyue Zhang:** Formal analysis. **Yuxuan Zhu:** Formal analysis. **Shuying Wang:** Data curation. **Xiaoyue Hu:** Visualization. **Mengqi Ling:** Writing – review & editing. **Demei Li:** Resources. **Changqing Duan:** Conceptualization. **Haibin Mu:** Conceptualization. **Baoqing Zhu:** Resources, Methodology, Conceptualization. **Yibin Lan:** Conceptualization.

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.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.fochx.2024.102038>.

Data availability

Data will be made available on request.

References

- Alencar, N. M. M., Ribeiro, T. G., Barone, B., Barros, A. P. A., Marques, A. T. B., & Behrens, J. H. (2019). Sensory profile and check-all-that-apply (cata) as tools for evaluating and characterizing syrah wines aged with oak chips. *Food Research International*, 124, 156–164. <https://doi.org/10.1016/j.foodres.2018.07.052>
- Belarbi, S., Vivier, M., Zaghouani, W., Sloovere, A., Agasse-Peulon, V., & Cardinael, P. (2021). Comparison of new approach of GC-HRMS (Q-Orbitrap) to GC-MS/MS (triple-quadrupole) in analyzing the pesticide residues and contaminants in complex food matrices. *Food Chemistry*, 359, Article 129932. <https://doi.org/10.1016/j.foodchem.2021.129932>
- Bueno, M., Marrufo-Curtido, A., Carrascón, V., Fernández-Zurbano, P., Escudero, A., & Ferreira, V. (2018). Formation and accumulation of acetaldehyde and Strecker aldehydes during red wine oxidation. *Frontiers in Chemistry*, 6, 20. <https://doi.org/10.3389/fchem.2018.00020>
- Castillo-Muñoz, N., Gómez-Alonso, S., García-Romero, E., & Hermosín-Gutiérrez, I. (2010). Flavonol profiles of *Vitis vinifera* white grape cultivars. *Journal of Food Composition and Analysis*, 23(7), 699–705. <https://doi.org/10.1016/j.jfca.2010.03.017>
- Chen, C., Chen, H., Zhang, Y., Thomas, H. R., Frank, M. H., He, Y., & Xia, R. (2020). TBtools: An integrative toolkit developed for interactive analyses of big biological data. *Molecular Plant*, 13(8), 1194–1202. <https://doi.org/10.1016/j.molp.2020.06.009>
- Chen, Y., Ouyang, X., Laaksonen, O., Liu, X., Shao, Y., Zhao, H., ... Zhu, B. (2019). Effect of *Lactobacillus acidophilus*, *Oenococcus oeni*, and *Lactobacillus brevis* on composition of bog bilberry juice. *Foods*, 8(10), 430. <https://doi.org/10.3390/foods8100430>
- Echave, J., Barral, M., Fraga-Corral, M., Prieto, M. A., & Simal-Gandara, J. (2021). Bottle aging and storage of wines: A review. *Molecules*, 26(3), 713. <https://doi.org/10.3390/molecules26030713>
- Figueiredo-González, M., Cancho-Grande, B., Boso, S., Santiago, J. L., Martínez, M. C., & Simal-Gándara, J. (2013). Evolution of flavonoids in Mouratón berries taken from both bunch halves. *Food Chemistry*, 138(2), 1868–1877. <https://doi.org/10.1016/j.foodchem.2012.11.083>
- Gambetta, J. M., Bastian, S. E. P., Cozzolino, D., & Jeffery, D. W. (2014). Factors influencing the aroma composition of chardonnay wines. *Journal of Agricultural and Food Chemistry*, 62(28), 6512–6534. <https://doi.org/10.1021/jf501945s>
- Gambetta, J. M., Cozzolino, D., Bastian, S. E. P., & Jeffery, D. W. (2016). Towards the creation of a wine quality prediction index: Correlation of chardonnay juice and wine compositions from different regions and quality levels. *Food Analytical Methods*, 9(10), 2842–2855. <https://doi.org/10.1007/s12161-016-0467-9>
- Herrero, P., Sáenz-Navajas, P., Culleré, L., Ferreira, V., Chatin, A., Chaperon, V., ... Escudero, A. (2016). Chemosensory characterization of chardonnay and pinot noir base wines of champagne. Two very different varieties for a common product. *Food Chemistry*, 207, 239–250. <https://doi.org/10.1016/j.foodchem.2016.03.068>
- Khakimov, B., Bakhytkyzy, I., Faul-Hassek, C., & Engelsens, S. B. (2022). Non-volatile molecular composition and discrimination of single grape white wines of chardonnay, Riesling, sauvignon blanc and Silvaner using untargeted GC-MS analysis. *Food Chemistry*, 369, Article 130878. <https://doi.org/10.1016/j.foodchem.2021.130878>
- Kustos, M., Gambetta, J. M., Jeffery, D. W., Heymann, H., Goodman, S., & Bastian, S. E. P. (2020). A matter of place: Sensory and chemical characterisation of fine Australian chardonnay and shiraz wines of provenance. *Food Research International*, 130, Article 108903. <https://doi.org/10.1016/j.foodres.2019.108903>
- Lan, Y., Liu, M., Zhang, X., Li, S., Shi, Y., & Duan, C. (2022). Regional variation of chemical characteristics in young Marselan (*Vitis vinifera* L.) red wines from five regions of China. *Foods*, 11(6), 787. <https://doi.org/10.3390/foods11060787>
- Lan, Y.-B., Xiang, X.-F., Qian, X., Wang, J.-M., Ling, M.-Q., Zhu, B.-Q., ... Duan, C.-Q. (2019). Characterization and differentiation of key odor-active compounds of 'Beibinghong' icewine and dry wine by gas chromatography-olfactometry and aroma reconstitution. *Food Chemistry*, 287, 186–196. <https://doi.org/10.1016/j.foodchem.2019.02.074>
- Li, J., Zou, S., Yang, W., Peng, M., Chen, B., Deng, J., ... Zheng, G. (2023). Identification of volatile and nonvolatile compounds in Citri Reticulatae Pericarpium Viride using GC-MS, UPLC-Q-Exactive Orbitrap-MS, and HPLC-PDA. *Food Science & Nutrition*, 11 (3), 1415–1425. <https://doi.org/10.1002/fsn3.3181>
- Li, Y., Li, R., Hu, X., Liu, J., Liu, G., Gao, L., ... Zhu, B. (2024). Changes of the volatile compounds and odors in one-stage and three-stage infant formulas during their secondary shelf-life. *Current Research in Food Science*, 8. <https://doi.org/10.1016/j.crf.2024.100693>
- Li, Z., Pan, Q., Jin, Z., Mu, L., & Duan, C. (2011). Comparison on phenolic compounds in *Vitis vinifera* cv. Cabernet sauvignon wines from five wine-growing regions in China. *Food Chemistry*, 125(1), 77–83. <https://doi.org/10.1016/j.foodchem.2010.08.039>
- Li, Z., Pan, Q., Jin, Z.-M., He, J.-J., Liang, N., & Duan, C.-Q. (2009). Evolution of 49 phenolic compounds in shortly-aged red wines made from cabernet Gernischt (*Vitis vinifera* L. cv.). *Food Science and Biotechnology*, 18, 1001–1012.
- Ling, M., Chai, R., Xiang, X., Li, J., Zhou, P., Shi, Y., ... Lan, Y. (2023). Characterization of key odor-active compounds in Chinese Dornfelder wine and its regional variations by application of molecular sensory science approaches. *Food Chemistry: X*, 17, Article 100598. <https://doi.org/10.1016/j.fochx.2023.100598>
- Liu, Y., Li, N., Li, X., Qian, W., Liu, J., Su, Q., ... Cheng, J. (2022). A high-resolution Orbitrap mass spectral library for trace volatile compounds in fruit wines. *Scientific Data*, 9(1), 496. <https://doi.org/10.1038/s41597-022-01594-x>
- Liu, Y., Qian, X., Xing, J., Li, N., Li, J., Su, Q., ... Zhu, B. (2022). Accurate determination of 12 lactones and 11 volatile phenols in nongrape wines through headspace-solid-phase microextraction (HS-SPME) combined with high-resolution gas chromatography-Orbitrap mass spectrometry (GC-Orbitrap-MS). *Journal of*

- Agricultural and Food Chemistry*, 70(6), 1971–1983. <https://doi.org/10.1021/acs.jafc.1c06981>
- Ma, Y., Yao, J., Zhou, L., Zhao, M., Liu, J., & Marchioni, E. (2023). Characterization and discrimination of volatile organic compounds and lipid profiles of truffles under different treatments by UHPLC-QE Orbitrap/MS/MS and P&T-GC-MS. *Food Chemistry*, 410. <https://doi.org/10.1016/j.foodchem.2023.135432>
- Mato, I., Huidobro, J. F., Simal-Lozano, J., & Sancho, M. T. (2006). Simultaneous determination of organic acids in beverages by capillary zone electrophoresis. *Analytica Chimica Acta*, 565(2), 190–197. <https://doi.org/10.1016/j.aca.2006.02.043>
- Mattivi, F., Guzzon, R., Vrhovsek, U., Stefanini, M., & Velasco, R. (2006). Metabolite profiling of grape: Flavonols and anthocyanins. *Journal of Agricultural and Food Chemistry*, 54(20), 7692–7702. <https://doi.org/10.1021/jf061538c>
- Oiv, Organisation Internationale de la Vigne et du Vin. (2015). *Résumé de Méthodes Internationales d'Analyse des Vins et des Moûts*. <http://www.oiv.org/fr/normes-et-documents-techniques/methodes-danalyse>
- Pinto, J., Oliveira, A. S., Azevedo, J., De Freitas, V., Lopes, P., Roseira, I., ... Guedes de Pinho, P. (2018). Assessment of oxidation compounds in oaked chardonnay wines: A GC-MS and ¹H NMR metabolomics approach. *Food Chemistry*, 257, 120–127. <https://doi.org/10.1016/j.foodchem.2018.02.156>
- Qi, Y., Wang, R., Qin, Q., & Sun, Q. (2019). Soil affected the variations in grape and wine properties along the eastern foot of Helan Mountain, China. *Acta Agriculturae Scandinavica, section B — Soil & Plant. Science*, 69(6), 494–502. <https://doi.org/10.1080/09064710.2019.1611914>
- Sáenz Gamasa, C., Hernández, B., de Santiago, J. V., Alberdi, C., Alfonso, S., & Diñeiro, J. M. (2009). Measurement of the colour of white and rosé wines in visual tasting conditions. *European Food Research and Technology*, 229(2), 263–276. <https://doi.org/10.1007/s00217-009-1050-z>
- Schreiner, T., & Morlock, G. E. (2023). Investigation of the estrogenic potential of 15 rosé, white and red wines via effect-directed ten-dimensional hyphenation. *Journal of Chromatography A*, 1690, Article 463775. <https://doi.org/10.1016/j.chroma.2023.463775>
- Song, X., Ling, M., Li, D., Zhu, B., Shi, Y., Duan, C., & Lan, Y. (2022). Volatile profiles and sensory characteristics of cabernet sauvignon dry red wines in the sub-regions of the eastern foothills of Ningxia Helan Mountain in China. *Molecules*, 27(24), 8817. <https://doi.org/10.3390/molecules27248817>
- Stone, H., Sidel, J., Oliver, S., Woolsey, A., & Singleton, R. C. (2004). Sensory evaluation by quantitative descriptive analysis. In M. C. G. Jr. (Ed.). *In Descriptive sensory analysis in practice*: Wiley.
- Tang, K., Tian, X., Ma, Y., Sun, Y., Qi, X., Miu, C., & Xu, Y. (2020). Aroma characteristics of cabernet sauvignon wines from loess plateau in China by QDA®, napping® and GC-O analysis. *European Food Research and Technology*, 246(4), 821–832. <https://doi.org/10.1007/s00217-020-03448-5>
- Varela, P., & Ares, G. (2012). Sensory profiling, the blurred line between sensory and consumer science. A review of novel methods for product characterization. *Food Research International*, 48(2), 893–908. <https://doi.org/10.1016/j.foodres.2012.06.037>
- Wang, S., Su, Q., Zhu, Y., Liu, J., Zhang, X., Zhang, Y., & Zhu, B. (2024). Sensory-guided establishment of sensory lexicon and investigation of key flavor components for goji berry pulp. *Plants-Basel*, 13(2). <https://doi.org/10.3390/plants13020173>
- Welke, J. E., Zanus, M., Lazzarotto, M., & Alcaraz Zini, C. (2014). Quantitative analysis of headspace volatile compounds using comprehensive two-dimensional gas chromatography and their contribution to the aroma of chardonnay wine. *Food Research International*, 59, 85–99. <https://doi.org/10.1016/j.foodres.2014.02.002>
- Xing, R.-R., Liu, D., Li, Z., Tian, Y., Zhang, X.-X., Li, J.-M., & Pan, Q.-H. (2016). Impact of different types of stoppers on sensorial and phenolic characteristics evolution during a bottle storage time of a white wine from chardonnay grape variety. *Journal of Food Science and Technology*, 53(11), 4043–4055. <https://doi.org/10.1007/s13197-016-2411-9>
- Zhang, X., Wang, K., Gu, X., Sun, X., Jin, G., Zhang, J., & Ma, W. (2022). Flavor chemical profiles of cabernet sauvignon wines: Six vintages from 2013 to 2018 from the eastern foothills of the Ningxia Helan Mountains in China. *Foods*, 11(1), 22. <https://doi.org/10.3390/foods11010022>
- Zhao, X., Duan, C.-Q., Li, S.-Y., Zhang, X.-K., Zhai, H.-Y., He, F., & Zhao, Y.-P. (2023). Non-enzymatic browning of wine induced by monomeric flavan-3-ols: A review. *Food Chemistry*, 425, Article 136420. <https://doi.org/10.1016/j.foodchem.2023.136420>