Current Research in Food Science 6 (2023) 100418

Contents lists available at ScienceDirect

Current Research in Food Science

journal homepage: www.sciencedirect.com/journal/current-research-in-food-science

Characterization of wine volatile compounds from different regions and varieties by HS-SPME/GC-MS coupled with chemometrics

Lin Zhang [a], Qianqian Liu [a], Yuanyuan Li [a], Shuzhen Liu [a], Qian Tu [a], Chunlong Yuan [a,b,*]

[a] College of Enology, Northwest A&F University, Yangling, 712100, China
[b] Ningxia Helan Mountain's East Foothill Wine Experiment and Demonstration Station of Northwest A&F University, Yongning, Ningxia, 750104, China

ARTICLE INFO

Keywords:
Wine
Volatile
Sensory analysis
Marker
Chemometric
GC-MS

ABSTRACT

HS-SPME/GC-MS and aroma descriptive analysis were used to gain insights into the volatile and sensory details of 99 red wine samples collected from four varieties in five regions. The general volatile fingerprints of Cabernet Sauvignon and Merlot wine samples in Xinjiang and Ningxia regions were similar, even though chemometric models could not discriminate between them. The main drivers of the diversity were secondary metabolites of grape such as terpenes, benzene-derivatives, and ketones. Fermentation-derivatives (esters and alcohols) were also responsible for region and variety-related differences in wines. Analysis of volatile compounds also showed that the primary factor accounting for diversity in wines in this study was region rather than variety. These results highlight the sensory attributes and volatiles of different regions and varieties, and provide a quantitative basis for screening for differential metabolites and potential markers in wines.

1. Introduction

Volatile compounds are the main determinants of wine aroma performance, which relate to particular attributes that characterize the overall sensory profile (Chen and Darriet, 2021). Hundreds of volatile compounds have been identified in wine, including terpenes, phenols, alcohols, esters, aldehydes, ketones, and lactones, with concentrations ranging from a few ng/L to hundreds of mg/L (Tang et al., 2019). Some of the volatile compounds are formed during the process of fermentation and aging while others emit directly from the grape berries (González-Barreiro et al., 2015). As for a young wine, the composition and content of aroma compound largely depend on the variety and vineyard (Luzzini et al., 2021; Wei et al., 2019; Zhang et al., 2020).

The different combinations of volatiles provide us with aromatically diverse and distinctive wines (Chen and Darriet, 2021; Liu et al., 2017; Sherman et al., 2020), which could become chemical markers to differentiate between wine samples. In recent years, large amounts of evidence implicating geographic or varietal effects on wine quality have been reported (Alem et al., 2019; Dourtoglou et al., 2014; Slaghenaufi et al., 2019). For instance, Cabernet Sauvignon wines show common sensory attributes related to the geographic origin that have been confirmed by many authors (Zhang et al., 2021; Kustos et al., 2020). Sauvignon Blanc wines are well known for their characteristic aromas related to varietal thiols, which can exhibit variations in their concentration due to the yeast used during the winemaking process (Pavez et al., 2016; Dubourdieu et al., 2006). Surveyed consumers have reported a willingness to pay more for wines exhibiting typical qualities (Goode, 2021). Therefore, the recognition of a compound or group of compounds that are associated with a certain region or variety is a goal for researchers trying to develop a better understanding of geographical and varietal typicality. However, many studies focus on origin traceability and pursue the perfect identification model, though it may not adapt to other samples. Large amounts of samples and characteristic flavors attributable should be studied in depth.

The wine grape cultivation region in China has a very scattered distribution, with a distance of over 2000 km on an east-west orientation, containing entirely different environments and eco-climate conditions (Pan et al., 2022; Wei et al., 2019; Li et al., 2011). This wide geographic and ecological distribution raises the question of which is more significant in wine diversity and typicality: region or variety. Common practice is making wines in the laboratory, which are not reflective of the retail wine market. This method produces typically young, mostly unoaked wines under the same standardized winemaking protocols, which will limit some of the authenticity and characteristic of the local areas (Costello et al., 2018; Kustos et al., 2020). Moreover, previous studies have had a limited number of samples fermented in the

* Corresponding author. College of Enology, Northwest A&F University, Yangling, 712100, China.
E-mail address: yuanchl69@nwsuaf.edu.cn (C. Yuan).

https://doi.org/10.1016/j.crfs.2022.100418
Received 12 August 2022; Received in revised form 14 December 2022; Accepted 15 December 2022
Available online 16 December 2022

same laboratory and were not extensive enough to draw conclusions about wine grapes grown and fermented across China.

The present study investigated commercial wines collected from different regions and varieties to identify volatile compounds by GC-MS and evaluate the diversity driver of red wines in China. In addition, the sensory attributes were assessed to investigate the wine aroma features. Chemometric approach models were established to distinguish volatile compounds, contributing to finding evidence of potential volatile markers associated with regions and varieties.

2. Materials and methods

2.1. Wine samples

In this study, a total of 99 commercial wine samples in three groups were collected. The first group was Cabernet Sauvignon wines from five different regions, including Hebei (HB), Xinjiang (XJ), Shanxi (SX), Nei Mongol (NMG), and Ningxia (NX), where HB was located in the east and XJ, SX, NMG, NX were in the west; the second group was three different varieties of wines from the Xinjiang region, including Merlot (ML), Syrah (SR), and Cabernet Sauvignon; the third group was three different varieties of wines from the Ningxia region, including Cabernet Gernischt (CG), Merlot, and Cabernet Sauvignon. The sample size was marked in Fig. 1. The physical and chemical parameters of the sample wines can be found in Table S1. Wines were collected evenly in all vintages to select important compounds with persistence and representativeness (Table S1). Original and monovarietal wines were collected to guarantee the varietal and geographical typicality. All samples were stored in the underground cellar of the College of Enology of Northwest A & F University for low-temperature storage until analysis.

2.2. Chemicals and reagents

Chromatographically pure standards included ethyl acetate, ethyl isobutyrate, isobutyl acetate, butyl acetate, ethyl 2-methylbutyrate, 2-methyl-1-propanol, isoamyl acetate, 1-butanol, 3-methyl-1-butanol, ethyl hexanoate, hexyl acetate, propanoic acid, ethyl L(-)-lactate, 1-hexanol, cis-3-hexenol, ethyl octanoate, 1-heptanol, 2,3-butanediol, 1-octanol, isobutyric acid, diethyl succinate, L-α-terpineol, phenethyl acetate, hexanoic acid, benzyl alcohol, phenylethyl alcohol, octanoic acid, decanoic acid, ethyl lactate, ethyl decanoate (Sigma-Aldrich, Shanghai, China). Ultrapure 18.2 MΩ cm water used for these experiments was produced from the Milli-Q Ultrapure water system (Human Corp., Seoul, Korea). Absolute ethanol (analytically pure) was purchased from Sichuan Xilong Chemical Industry Co. Ltd. (Chengdu, Sichuan, CHN).

2.3. Volatile compounds analysis

The method for qualitative and quantitative analysis of volatile compounds in wine samples used head space solid-phase microextraction GC-MS (HS-SPME–GC–MS) and was based on the method by Kong et al. (2019), with some modifications. Eight mL of the supernatant were held in a 20 mL headspace vial containing 40 μg/L internal standard (2-octanol) and 2 g NaCl. The vial was tightly capped and heated at 40 °C for 15 min on a heating platform. Then, the activated solid-phase fiber was exposed to the headspace vial at 40 °C for 30 min until the distribution was balanced. Subsequently, the fiber was desorbed in the GC injector for 5 min at 230°C. The solid-phase fiber of divinylbenzene/carboxen/polydimethylsiloxane (DVB/CAR/PDMS) was purchased from Supelco Corporation (Bellefonte, PA, USA).

The QP2020 GC-MS system (Shimadzu Corporation, Kyoto, JPN) coupled with a DB-Wax column (60 m × 0.25 mm × 0.25 μm, St. Louis, MO, USA) was used to analyze volatile compounds. Gas chromatography conditions: The carrier gas was ultrapure helium (purity >99.999%) in the splitless mode at 1 mL/min flow rate. The temperature program was 40 °C for 5 min, ramping to 130 °C at 2 °C/min, increasing to 220 °C at 5 °C/min, and maintaining for 10 min. Mass spectrometer conditions: Electron ionization (EI) mass spectrometric data from m/z 35 to 350 were scanned at 0.2 s intervals. The ion source and the injector temperature were 200 °C and 230 °C, respectively.

The identification of volatile compounds was based on comparing the mass spectra and retention time with those of pure standards in the NIST 17 library. Moreover, the quantification was performed according to the internal standard-standard curve method. The internal standard substance was 2-Octanol, and the standard curve was plotted using the 5-point method. For the volatile compounds without pure standards, the standard curve of substance with similar chemical structure was used for calculation.

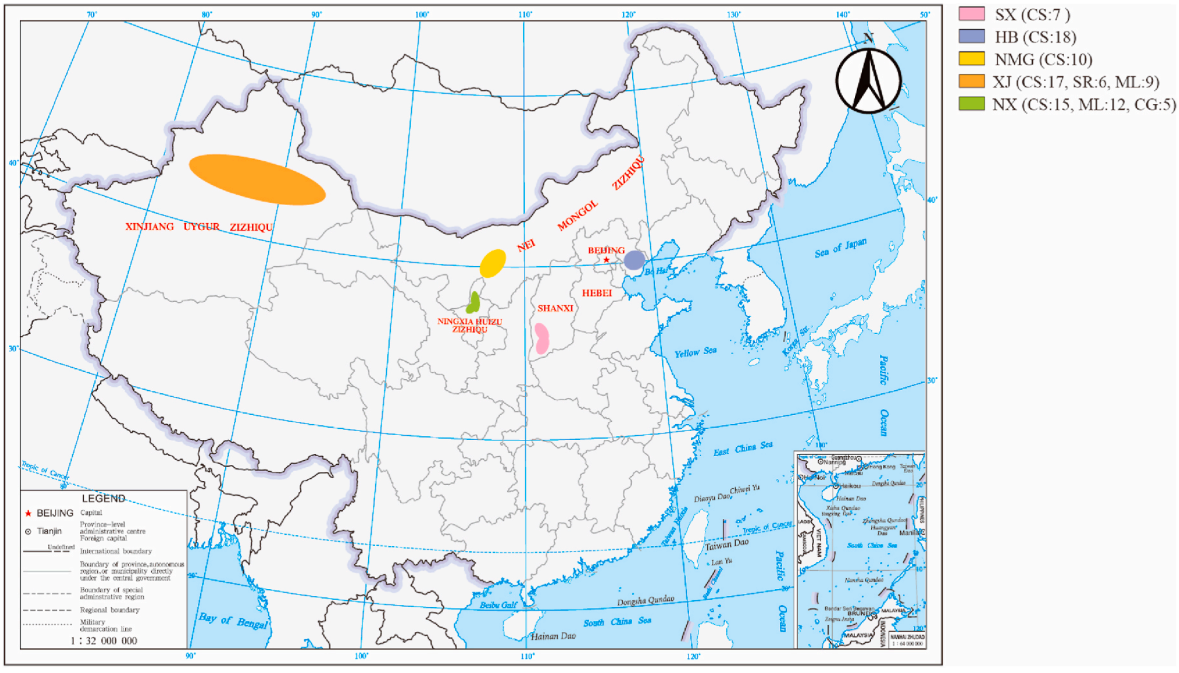

Fig. 1. The distribution of wine regions. The numbers in parentheses indicated the sample sizes.

2.4. Sensory analysis

The sensory panel was composed of ten experts, including five males and five females aged 20 to 30. All of them came from the College of Enology and have related education backgrounds. They were trained to identify typical wine aromas with a 54-aroma kit (Le Nez du Vin®, France) and evaluate aromatic descriptors by tasting real wines (Sun et al., 2018; Lan et al., 2021). Wine samples were numbered with three-digit random codes in black wine-tasting glasses. Recognition training sessions were performed repeatedly for two months (two or three times a week) until the accuracy exceeded 90%. Every participant was asked to describe the aroma by at least five trained descriptors, and assign a value (0–5) according to the intensity of the aroma.

To simplify the analysis of the aroma characteristics of wines, the 54 aroma descriptors were divided into seven groups referring to reported literature and participants' opinion (Panceri et al., 2015): tropical fruity, berry, floral, vegetal, roasted, spicy, and fatty.

2.5. Statistical analysis

International Business Machines Statistical Package for Social Sciences (IBM SPSS) 26 was used for Duncan test of ANOVA and linear discriminant analysis (LDA). The online platform MetaboAnalyst 5.0 performed principal component analysis (PCA) with sample normalization by sum. PCA and LDA models were established to observe the differentiation of volatiles on regions and varieties and to screen for important characteristic compounds. Sensory analysis was performed by SPSS to calculate the mean and standard deviation. And the radar charts were plotted by Origin 2022b.

3. Results and discussion

3.1. Volatile compounds profile

In the present study, a total of 54 volatile compounds were identified qualitatively and quantitatively (Table 1), including esters, alcohols, fatty aldehydes, monoterpenoids, benzene-derivatives, C_6 compounds, and volatile fatty acids, as well as volatile sulfides with very low odor thresholds. Fermentation-derived esters and alcohols were the main volatile components in the wine studied as expected. Most compounds showed significant differences in five regions, and some could be found only in specific regions. For example, nonanal could be identified only in HB and NMG, and trans-linalool oxide could be found in part samples of HB, indicating that the region factor strongly influenced the synthesis, accumulation, and release of volatiles (Avellone et al., 2018; Petretto et al., 2021; Tang et al., 2019). Moreover, compared to HB and SX, XJ has longer sunshine hours and greater temperature differences which were important factors affecting the chemical composition of wine and grapes, too (Pan et al., 2022; Xu et al., 2015). As many previous studies suggested that the component contributes to wine aroma when its concentration is at least 20% of the threshold, the volatiles with odor activity values (OAV)>0.2 were listed respectively (Tables S2–S4) (Lan et al., 2019; Peng et al., 2013; Wang et al., 2016; Zhu et al., 2021).

Fermentation-derived esters have long been associated with wine fruitiness (Cameleyre et al., 2021; Previtali et al., 2022), including acetate esters, such as ethyl acetate, isobutyl acetate, isoamyl acetate, and ethyl fatty acid esters butyl acetate, ethyl hexanoate, and ethyl octanoate. Most of the esters were higher than the odor threshold in concentration. Ethyl acetate ranged from 40.8 to 264.3 mg/L concentration in CS samples and was the most abundant ester analyzed. A noteworthy phenomenon was that the OAV of ethyl octanoate far exceeded other compounds and contained higher concentrations in the four western regions (XJ, NX, NMG, and SX) than in the eastern region (HB) (Table S2). These results indicate that, to some extent, ethyl octanoate played a vital role in the aroma composition and presentation of the samples. In previous studies, the OAV of ethyl octanoate reached a concentration of more than 4000 (Jiang et al., 2013).

Branched-chain esters ethyl 2-methylbutyrate (threshold 18 μg/L) and ethyl 3-methylbutyrate (threshold 3 μg/L) were significantly higher in HB than other four regions (Table 1), which might be related to the low altitude of HB area. As reported, branched-chain esters may be the source of the aroma of red fruit in some wines (Lan et al., 2019), which was easy to present at lower elevations (Falcão et al., 2007).

Compared with other varieties in XJ (Table 2), CS wines contained the highest concentrations of branched-chain ester, and the same situation also occurred in NX (Table 3). As branched-chain esters tend to show higher levels in older wines, we checked the vintages table and found that the difference in each treatment was not significant (Table S1). This high concentration of branched-chain esters is presumably due to the basic situation of grape varieties, such as juice turbidity, sugar, and other nutrient conditions (Binati et al., 2020; Chen et al., 2021; Tufariello et al., 2021).

The majority of the higher alcohols in this study have significant differences between different regions (Table 1), which may have resulted from the vineyard and winemaking environment (Ciani et al., 2016; Clemente-Jimenez et al., 2004). Branched alcohols such as 2-methyl-1--propanol, 3-methyl-1-butanol, and aromatic alcohol phenylethyl alcohol were identified in this study, with concentrations ranging from 35.0–108.0 mg/L, 216.0–476.5 mg/L, and 21.7–76.0 mg/L in CS samples, respectively (Table 1). Despite the observed concentration of 1-hexanol being below the threshold, this volatile compound still provided contributed partly to wine aroma together with other volatiles (Zhu et al., 2021).

Volatile fatty acids in wine include both straight and branched chains. In this study, three straight-chain fatty acids and one branched-chain fatty acid, namely hexanoic acid, octanoic acid, decanoic acid, and isobutyric acid, showed significant differences among regions. As a whole, the concentrations in the west four regions were significantly higher than HB, because they were in arid and semi-arid areas. Less rainfall is more conducive to the formation of fatty acids (Ju et al., 2018).

As we all know, the secondary metabolites of grapes are recognized as the basis of varietal typicality in wine. Terpenes α-terpinol, linalool, and citronellol, benzene-derivatives benzyl alcohol, phenylethyl alcohol and phenethyl acetate, C13-norisoprenoids damascone and epoxy-α-ionone, volatile phenols Guaiacol, 4-Ethyl-2-methoxyphenol and 2,4-Di-tert-butylphenol, C_6 compound 1-hexanol and thiols 3-methylthio-propanol were important secondary metabolites identified in this study, contributing to the unique aroma in wines. Terpenes are regarded as key odorants in aromatic grape varieties of *Vitis vinifera*, such as Muscat of Alexandria, Riesling, and Gewürztraminer, to which they impart their characteristic floral aromas. Citronellol and L-α-terpinol contribute floral, fruity, and citrus attributes, presenting concentrations ranging from 0 to 5.4 μg/L and from 0 to 40.3 μg/L. Several authors studied the effect of light on terpene concentrations in grapes (Rienth et al., 2021; Yang et al., 2019), proposing a general conclusion that monoterpenes increased with sunshine levels. Reports from the literature were consistent with this study, where the concentration of L-α-terpinol in HB was significantly higher than in SX, as the HB area is stronger in both effective accumulated temperature and solar radiation intensity (Table 1). However, NMG with high sunlight radiation did not show a high L-α-terpinol concentration. A possible explanation for this phenomenon was the heat stress on grapes (Alem et al., 2019; Scafidi et al., 2013).

In XJ (Table 2), L-α-terpinol in CS wines was significantly higher than in ML and SR samples. Of the three wine varieties in the NX, the concentration of phenethyl alcohol, characterized by rose aroma, exceeded its odor threshold and showed significantly more aromatic in CS and ML wines than in CG (Table 3). Several C13-norisoprenoids, such as damascenone with stewed apple, rose, and honey aroma (Francis and Newton, 2005), are powerful odorants in wine, which can be present in

Table 1
Volatile compounds of CS wine samples from five regions.

volatile compounds (μg/L)	HB			XJ			SX			NMG			NX		
	Max	Min	Mean	Max	Min	Mean	Max	Min	Mean	Max	Min	Mean	Max	Min	Mean
Ethyl acetate	264260.04	52031.27	103269.44a	115508.24	59124.5	77482.76 ab	102485.79	64448.87	80825.20 ab	122303.85	55965.28	71224.14b	104552.9	40761.98	72901.28b
Ethyl isobutyrate	621.81	nd	34.54ns	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
Isobutyl acetate	1148.39	41.48	330.32a	467.84	nd	51.03c	470.51	nd	225.45 ab	480.32	30.3	127.60bc	210.87	nd	70.31c
Butyl acetate	1382.11	368.35	633.81ns	1011.15	nd	645.63ns	1067.31	630.16	852.03ns	944.37	nd	696.25ns	944.19	415.96	634.21ns
Ethyl 2-methylbutyrate	147.23	6.46	41.32a	51.75	5.77	14.96b	60.07	6.87	28.41 ab	34.95	nd	15.15b	39.91	13.19	26.41 ab
Ethyl 3-methylbutyrate[a]	208.27	11.19	63.20a	59.61	8.6	27.59b	96.96	11.71	46.36 ab	53.51	10.27	26.89b	81.29	30.24	53.09 ab
isoamyl acetate	819.5	281.21	456.71ns	1712.81	334.94	637.62ns	762.53	254.6	483.46ns	1017.61	312.1	554.06ns	1137.57	294.77	579.27ns
Ethyl hexanoate	2968.35	1369.41	2187.58b	3468.96	2178.71	2866.19a	3260.17	2132.72	2607.26a	3027.25	2169.1	2569.32a	3793.44	2323.51	2906.90a
Hexyl acetate	30.16	26.7	28.10a	50.08	nd	24.16 ab	27.77	nd	3.97c	29.84	nd	13.88bc	47.21	nd	21.79 ab
Ethyl heptanoate[a]	293.29	nd	141.14a	160.7	nd	74.65b	nd	nd	nd	nd	nd	nd	256.51	nd	27.62b
Ethyl L(-)-lactate	801138.67	nd	189050.02a	nd	nd	nd	nd	nd	nd	29486.09	nd	2948.61b	nd	nd	nd
Ethyl octanoate	2807.15	855.64	1628.26ns	2668.4	1438.02	1986.80ns	1924.84	1371.64	1689.43ns	2223.54	1138.36	1739.93ns	3096.02	1239.51	1840.25ns
Ethyl 2-hydroxy-4-methylvalerate[a]	738.73	nd	281.11ns	458.54	nd	299.56ns	473.42	367.86	412.92ns	391.35	nd	291.52ns	515.04	391.74	438.23ns
Isoamyl lactate[a]	864.67	322.47	529.57a	501.05	318.87	412.69bc	546.68	355.53	430.92b	449.85	nd	324.29c	727.13	464.28	537.70a
Diethyl succinate	33276.14	4678.57	10989.39 ab	26813.72	7769.14	16557.26a	17015.62	40.16	7195.70b	22178.55	757.46	12290.17 ab	25235.56	1734.22	15860.56a
Ethyl isopentyl succinate[a]	1593.58	354.12	795.14a	1607.29	345.36	929.88a	899.37	287.39	434.85b	1529.71	271.84	802.62a	2105.19	nd	991.62a
Ethyl lactate	369204.25	nd	165039.49c	402383.04	147702.6	257700.56 ab	478816.31	137907.27	252793.42 ab	348086.25	nd	190098.31bc	409498.13	201514.37	282042.98a
Ethyl decanoate	833.8	nd	291.59bc	1516.85	322.76	604.05a	329.94	180.43	276.06c	616.15	239.37	413.36bc	823.45	nd	476.95 ab
Diethyl glutarate[a]	194.26	nd	130.22a	165.64	nd	76.07 ab	172.02	nd	47.55 ab	170.48	nd	65.62 ab	172.49	nd	45.20 ab
2-Methyl-1-propanol	107984.9	46916.21	66331.25b	58967.37	34981.56	46107.49c	104980.5	58142.81	76757.08a	77789.95	49285.56	63724.47b	89483.62	46726.95	65096.16b
1-Butanol	5498.26	1452.48	2852.84b	5369.22	430.25	3661.32b	4881.18	2773.25	3660.97b	7471.64	3281.59	4308.00 ab	15692.58	nd	5862.13a
3-Methyl-1-butanol	476549.62	215937.65	299251.87b	439389.26	245020.77	323482.93b	420265.67	299086	371731.34a	437919.4	285071.34	376871.73a	429674.46	342889.42	382937.42a
4-Methyl-1-pentanol[a]	253.3	112.84	144.32b	255.52	138.2	163.76b	160.25	107.35	133.68b	184.1	145.27	163.67b	961.72	nd	265.64a
2-Heptanol[a]	5.98	0.39	2.84a	8.37	0.65	2.58 ab	2.19	nd	0.56c	4.32	nd	1.08bc	10.21	nd	0.94c
3-Methyl-1-pentanol[a]	245.07	123.35	161.92c	362.12	139.04	228.32b	236.37	131.07	183.84bc	308.54	155.35	228.48b	545.26	156.07	346.72a
1-Heptanol	40.32	nd	22.46ns	54.59	12.39	27.70ns	28.96	12.74	18.62ns	26.34	9.82	14.93ns	44.12	nd	24.10ns
3-Ethyl-4-methylpentan-1-ol[a]	13784.29	nd	7055.85a	9549.47	nd	3111.73b	2870.29	nd	410.04b	5437.51	nd	1628.16b	11418.5	nd	2905.09b
2,3-Butanediol	34806.98	nd	16207.70a	21212.55	9838.02	15468.80a	15571.6	nd	9235.44b	11968.39	5750.42	9078.42b	23833.98	nd	12303.10 ab
trans-2-Octen-1-ol[a]	1177.01	nd	339.10a	334.92	nd	52.76b	nd	nd	nd	nd	nd	nd	nd	nd	nd
Isobutyric acid	451.8	61.15	141.29a	166.12	nd	44.17b	200.03	nd	93.54a	70.16	nd	19.79b	nd	nd	nd
Hexanoic acid	3603.03	1471.75	2484.81b	3974.35	1512.32	2893.31b	3117.68	1706.09	2402.77b	3213.08	1586.53	2513.07b	4742.35	2647.88	3445.73a
Octanoic acid	1160.65	410.93	626.54b	1147.17	477.02	800.68a	763.14	449.01	634.15b	888.25	480.24	687.09 ab	1083.16	607.14	799.66a
Decanoic acid	173.03	nd	99.30 ab	231.69	92.14	130.77a	109.72	nd	70.27b	151.87	nd	108.64 ab	214.71	nd	116.12a
Linalool	nd	nd	ndns	20.45	nd	1.20ns	nd	nd	ndns	4.43	nd	0.44ns	nd	nd	ndns
trans-Linalool oxide[a]	4.43	nd	0.54ns	1.61	nd	0.39ns	nd	nd	ndns	nd	nd	ndns	nd	nd	ndns
Citronellol	2.70	nd	0.44b	3.54	nd	1.69a	1.33	nd	0.64 ab	2.29	nd	1.19 ab	5.45	nd	1.10 ab
Nerolidol	56.80	nd	9.51a	26.16	nd	1.54 ab	nd	nd	ndb	12.16	nd	1.36 ab	nd	nd	ndb
epoxy-α-ionone[a]	3.37	nd	0.19ns	nd	nd	ndns	nd	nd	ndns	nd	nd	ndns	nd	nd	ndns
2-Undecanone[a]	3.42	nd	1.53a	1.43	nd	0.21b	2.50	nd	0.36b	nd	nd	ndb	nd	nd	ndb
Damascone	nd	nd	ndns	nd	nd	ndns	nd	nd	ndns	nd	nd	ndns	5.61	nd	0.37ns
Guaiacol	127.76	nd	7.10ns	nd	nd	ndns	nd	nd	ndns	nd	nd	ndns	nd	nd	ndns
4-Ethyl-2-methoxyphenol	14.23	nd	1.58ns	93.74	nd	5.51ns	nd	nd	ndns	nd	nd	ndns	nd	nd	ndns
2-Nonanone	2.71	nd	0.27ns	nd	nd	ndns	nd	nd	ndns	nd	nd	ndns	nd	nd	ndns
Methyl salicylate	43.29	nd	4.59ns	27.03	nd	7.27ns	13.67	nd	1.95ns	26.51	nd	7.24ns	nd	nd	ndns
1-Hexanol	4680.61	1662.32	3276.09 ab	4663.19	2318.92	3072.88bc	3234.74	1955.61	2474.00c	4022.68	1732.2	2905.67bc	5701.27	2416.37	3868.96a
cis-3-Hexen-1-ol	254.26	120.36	196.59a	306.68	126.69	200.08a	242.42	130.59	186.31a	241.48	nd	154.98a	307.86	nd	80.89b
Nonanal[a]	4.27	nd	0.93ns	3.29	nd	0.30ns	1.09	nd	0.16ns	3.23	nd	1.17ns	6.71	nd	0.45ns
trans-2-Hexen-1-ol[a]	733.19	nd	166.13ns	511.5	nd	145.61ns	nd	nd	nd	396.39	nd	105.84ns	nd	nd	nd
L-α-Terpineol	26.58	nd	10.06a	9.52	nd	4.56 ab	4.5	nd	0.64b	5.67	nd	1.91b	40.29	nd	6.32 ab
2,4-Di-tert-butylphenol[a]	379.5	125.41	180.25c	1446.55	108.68	805.77b	1140.42	586.86	845.42b	1617.11	478.07	1113.77b	2265.84	794.83	1572.35a
Benzyl alcohol	2164.95	170.04	1013.23a	840.34	241.05	538.52b	582.5	nd	224.33c	979.08	214.92	524.73b	1097.3	nd	610.95b
Phenylethyl alcohol	75339.61	35382.12	50041.99ns	75640.64	21658.13	49735.32ns	68816.23	26019.14	45822.93ns	76013.13	34305.56	56325.12ns	68367.05	41337	55862.88ns
Phenethyl acetate	86.48	37	50.25ns	109.47	21.89	45.15ns	52.61	25.27	33.11ns	60.83	26.2	39.03ns	130.17	28.79	53.96ns
3-Methylthiopropanol[a]	4214.33	1149.35	1955.87 ab	1489.1	nd	694.96b	1237.22	nd	631.46b	1962.42	nd	840.45b	12989.72	nd	3141.51a

Note: nd: not detected. ns: not significant. Different letters in the row mean significant differences by ANOVA among the areas ($p < 0.05$). Data are the mean of three replicates.
[a] Quantified with a calibration curve of a compound of the same chemical class.

Table 2
Volatile compounds of wine samples from three varieties of XJ.

volatile compounds(μg/L)	CS			ML			CG		
	Max.	Min.	Mean	Max.	Max.	Min.	Mean	Min.	Max.
Ethyl acetate	115508.24	59124.5	77482.76ns	103101.14	41748.79	70791.97ns	135703.12	72474.29	91559.76ns
Isobutyl acetate	467.84	nd	51.03ns	233.15	nd	47.86ns	182.36	30.15	76.67ns
Butyl acetate	1011.15	nd	645.63ns	1185.44	577.21	785.02ns	1047.56	584.6	782.14ns
Ethyl 2-methylbutyrate	51.75	5.77	14.96ns	27.31	4.74	11.37ns	20.77	nd	8.03ns
Ethyl 3-methylbutyrate[a]	59.61	8.6	27.59ns	46.52	10.61	22.3ns	46.11	4.82	18.34ns
isoamyl acetate	1712.81	334.94	637.62ns	1353.64	279.63	621.24ns	2435.58	417.79	1124.18ns
Ethyl hexanoate	3468.96	2178.71	2866.19ns	4001.83	2301.8	2741.09ns	3187.48	2317.27	2639.23ns
Hexyl acetate	50.08	nd	24.16ns	32.62	nd	22.28ns	48.51	nd	31.72ns
Ethyl heptanoate[a]	160.7	nd	74.65ns	157.7	nd	34.82ns	160.38	nd	80.07ns
Ethyl octanoate	2668.4	1438.02	1986.8ns	2375.38	1477.74	1786.87ns	2387.37	1395.5	1780.13ns
Ethyl 2-hydroxy-4-methylvalerate[a]	458.54	nd	299.56ns	400.2	nd	240.58ns	439.22	nd	139.86ns
Isoamyl lactate[a]	501.05	318.87	412.69ns	492.25	316.05	388.66ns	445.78	311.15	366.49ns
Diethyl succinate	26813.72	7769.14	16557.26ns	19950.61	8658.21	14332.41ns	20237.85	8573.99	13218.02ns
Ethyl isopentyl succinate[a]	1607.29	345.36	929.88a	1193.48	335.38	635.09b	1022.98	456.36	682.1 ab
Ethyl lactate	402383.04	147702.6	257700.56ns	392610.57	196812.61	279798.25ns	404329.71	175101.77	238208.42ns
Ethyl decanoate	1516.85	322.76	604.05ns	1071.68	319.89	581.89ns	579.73	246.97	449.77ns
Diethyl glutarate[a]	165.64	nd	76.07ns	162.52	nd	71.7ns	169.34	nd	28.22ns
2-Methyl-1-propanol	58967.37	34981.56	46107.49ns	52860.69	36069.87	45727.47ns	66339.81	46866.74	52635.92ns
1-Butanol	5369.22	430.25	3661.32ns	10668.48	2441.81	4618.75ns	9248.44	nd	4957.19ns
3-Methyl-1-butanol	439389.26	245020.77	323482.93ns	388222.37	242221.29	313743.05ns	398244.19	241807.5	301043.08ns
4-Methyl-1-pentanol[a]	255.52	138.2	163.76a	161.9	131.11	145.73a	158.41	nd	112.8b
2-Heptanol[a]	8.37	0.65	2.58ns	3.35	nd	1.79ns	3.59	1.28	2.62ns
3-Methyl-1-pentanol[a]	362.12	139.04	228.32ns	427.17	143.48	224ns	244.74	138.42	173.87ns
1-Heptanol	54.59	12.39	27.7ns	33.82	10.26	17.78ns	37.53	19.35	26.9ns
3-Ethyl-4-methylpentan-1-ol[a]	9549.47	nd	3111.73ns	6418.46	nd	2159.32ns	nd	nd	ndns
2,3-Butanediol	21212.55	9838.02	15468.8b	22443.5	7439.78	14079.67b	28068.24	10801.36	21211.48a
trans-2-Octen-1-ol[a]	334.92	nd	52.76ns	267.68	nd	29.74ns	nd	nd	ndns
Isobutyric acid	166.12	nd	44.17ns	126.06	nd	22.41ns	120.44	nd	55.38ns
Hexanoic acid	3974.35	1512.32	2893.31ns	4988.97	1741	3048.08ns	3361.13	475.07	2063.97ns
Octanoic acid	1147.17	477.02	800.68a	1270.1	580.54	770a	715.56	382.21	550.06b
Decanoic acid	231.69	92.14	130.77a	167.72	89.96	118.23 ab	146.39	nd	88.07b
Linalool	20.45	nd	1.20ns	5.77	nd	0.64ns	21.87	nd	6.25ns
trans-Linalool oxide[a]	1.61	nd	0.39ns	nd	nd	ndns	1.4	nd	0.4ns
Citronellol	3.54	nd	1.69ns	3.41	nd	1.68ns	3.52	nd	2.14ns
Nerolidol	26.16	nd	1.54ns	22.03	nd	4.19ns	19.78	nd	5.84ns
2-Undecanone[a]	1.43	nd	0.21	nd	nd	nd	nd	nd	nd
Benzyl alcohol	840.34	241.05	538.52b	1665.82	378.05	1002.08a	455.71	116.8	218.23c
Phenylethyl alcohol	75640.64	21658.13	49735.32ns	67802.59	24044.05	41944.28ns	55450.72	24691.79	34195.14ns
Phenethyl acetate	109.47	21.89	45.15ns	74.29	24.79	38.66ns	72.92	30.63	48.31ns

Note: nd: not detected. ns: not significant. Different letters in the row mean significant differences by ANOVA among the areas ($p < 0.05$). Data are the mean of three replicates.

[a] Quantified with a calibration curve of a compound of the same chemical class.

wine at up to 5.6 μg/L far higher than its odor threshold of 0.05 μg/L. (Geffroy et al., 2020).

3.2. Sensory description analysis

According to data obtained from ANOVA and post-hoc test (Duncan) (Fig. 2), the berry group scored the highest, vegetal, roasted, spicy floral, and tropical fruity groups scored the second-highest, and the fatty groups scored the lowest. CS wine samples from five regions showed significant differences in the odor characteristics of the berry aroma (Fig. 2A). HB showed the highest intensity, which may be due to the elevation. In Fig. 2A, the sum scores of the vegetal group, including bell pepper, green grass, and herbal, were significantly higher in four western regions than in HB, which may be due to the elevation (Falcão et al., 2007). The vegetal odor was presumably related to 1-hexanol and 3-methylthiopropanol (Lan et al., 2019). The C_6 compound 1-hexanol produces a typical herbal aroma. Volatile sulfides 3-methylthiopropanol, with a concentration range in wine from 0 to 4.5 mg/L, elicits unpleasant flavors of potatoes, cauliflower, and cooked cabbage (Lan et al., 2019). The fatty group included oil, fat meat, cream, and butter, which had a significant difference in the five regions. As same as the study of Pearson et al. (2020), three wines originating from the Heathcote region can be distinguished from other wines based on beef stock odor. As for three different varieties in XJ (Fig. 2B), SR wine samples showed the highest fatty odor value, which may relate to some long-chain fatty acids

3.3. Chemometric approach

To assess more detailed information about the volatile compounds, the relevant quantitative data were subject to principal component analysis (PCA) (Petretto et al., 2021). The overlapping ellipses seemed inevitable as all the volatile data was entered into the model, which did not suggest the failure in the modeling even if the separation was less fine. Because our aim was to find the important compounds that can separate the model, rather than strictly classify or traceability research.

According to Fig. 3, the differences between varieties were relatively small in the same region, whereas for the same variety (CS) larger differences among regions were highlighted. Due to the scattered and far away regions, geographic diversity has remained dominant in China, although some studies have reported that variety rather than region showed a more obvious difference in wine (Ziółkowska et al., 2016). Another interesting phenomenon was the volatile fingerprints of Cabernet Sauvignon and Merlot samples overall were similar in quantification in the same region. However, a previous study reported that in the north-eastern part (Ebro Valley) of Spain, only quantitative differences in volatiles were observed in young Cabernet Sauvignon and Merlot wines, and no odorants were characteristic of a single variety (Ferreira et al., 2000).

Table 3
Volatile compounds of wine samples from three varieties of NX.

volatile compounds(μg/L)	CS			ML			CG		
	Max.	Min.	Mean	Max.	Min.	Mean	Max.	Min.	Mean
Ethyl acetate	104552.9	40761.98	72901.28b	114631.68	43668.28	62640.41b	155706.96	68151.44	117762.87a
Isobutyl acetate	210.87	nd	70.31b	170.17	nd	24.8b	541.28	20.47	204.9a
Butyl acetate	944.19	415.96	634.21b	721.47	337.66	594.37b	953.62	835.46	884.01a
Ethyl 2-methylbutyrate	39.91	13.19	26.41ns	37.64	nd	23.14ns	38.25	5.71	18.7ns
Ethyl 3-methylbutyrate[a]	81.29	30.24	53.09ns	77.23	19.1	45.83ns	64.73	7.81	29.64ns
isoamyl acetate	1137.57	294.77	579.27ns	809.77	305.04	489.13ns	748.81	339.45	472.74ns
Ethyl hexanoate	3793.44	2323.51	2906.9ns	3384.57	1956.5	2606.46ns	3317.69	2049.88	2758.37ns
Hexyl acetate	47.21	nd	21.79a	29.25	nd	2.44a	29.52	nd	22.67b
Ethyl heptanoate[a]	256.51	nd	27.62ns	207.47	nd	17.29ns	nd	nd	ndns
Ethyl octanoate	3096.02	1239.51	1840.25ns	2368.84	1164.71	1755.07ns	1691.08	1075.67	1415.39ns
Ethyl 2-hydroxy-4-methylvalerate[a]	515.04	391.74	438.23ns	617.82	nd	404.91ns	587.9	nd	406.75ns
Isoamyl lactate[a]	727.13	464.28	537.7ns	823.72	340.18	491.24ns	575.89	497.6	525.68ns
Diethyl succinate	25235.56	1734.22	15860.56ns	23565.4	1192.3	14595.56ns	19755.52	14090.21	16279.09ns
Ethyl isopentyl succinate[a]	2105.19	nd	991.62a	1619.52	371.43	912.19a	678.39	213.42	409.77b
Ethyl lactate	409498.13	201514.37	282042.98b	450198.35	123261.12	253182.64b	501518.48	397586.3	472161.41a
Ethyl decanoate	823.45	nd	476.95ns	873.74	236.54	502.51ns	975.77	263.05	584.49ns
Diethyl glutarate[a]	172.49	nd	45.2ns	200.9	nd	45.87ns	163.94	nd	65.2ns
2-Methyl-1-propanol	89483.62	46726.95	65096.16a	98028.85	51699.83	67661.39a	58155.69	34118.77	47990.42b
1-Butanol	15692.58	nd	5862.13ns	9386.87	nd	5100.47ns	4457.09	2501.44	3158.75ns
3-Methyl-1-butanol	429674.46	342889.42	382937.42a	471071.17	316557.45	383475.34a	305825.67	244292.24	281690.66b
4-Methyl-1-pentanol[a]	961.72	nd	265.64ns	476.66	nd	258.27ns	144.8	101.67	130.29ns
2-Heptanol[a]	10.21	nd	0.94ns	11.47	nd	1.04ns	5.49	0.23	1.99ns
3-Methyl-1-pentanol[a]	545.26	156.07	346.72a	495.67	171.24	330.64a	185.16	125.65	148.77b
1-Heptanol	44.12	nd	24.1ns	51.29	nd	20.09ns	22.39	12.4	16.88ns
3-Ethyl-4-methylpentan-1-ol[a]	11418.5	nd	2905.09a	nd	nd	ndb	5942.77	2732.52	3938.74a
2,3-Butanediol	23833.98	nd	12303.1ns	34914.83	nd	11126.08ns	12604.02	nd	8758.04ns
Isobutyric acid	nd	nd	ndns	69.13	nd	11.21ns	nd	nd	ndns
Hexanoic acid	4742.35	2647.88	3445.73ns	4492.47	nd	2931.71ns	6032.7	2554	3845.63ns
Octanoic acid	1083.16	607.14	799.66ns	1027.71	659.6	807.82ns	1305.4	638.32	921.8ns
Decanoic acid	214.71	nd	116.12ns	159.71	nd	110.31ns	196.5	92.62	135.44ns
trans-Linalool oxide (furanoid)[a]	nd	nd	ndb	nd	nd	ndb	1.84	nd	0.37a
Citronellol	5.45	nd	1.10ns	5.10	nd	1.47ns	3.35	nd	0.67ns
Nerolidol	nd	nd	ndns	19.64	nd	1.64ns	19.16	nd	3.83ns
Damascone	5.61	nd	0.37ns	nd	nd	ndns	nd	nd	ndns
Methyl salicylate	nd	nd	ndb	46.74	nd	12.10a	18.05	nd	15.74a
1-Hexanol	5701.27	2416.37	3868.96b	5540.18	2375.62	3503.62b	6874.48	3523.15	4899.88a
cis-3-Hexen-1-ol	307.86	nd	80.89ns	1063.12	nd	153.83ns	248.87	161.18	187.47ns
Nonanal[a]	6.71	nd	0.45ns	27.74	nd	2.69ns	0.78	nd	0.16ns
trans-2-Hexen-1-ol[a]	nd	nd	ndb	309.35	nd	25.78b	266.07	nd	150.15a
L-α-Terpineol	40.29	nd	6.32ns	16.14	nd	2.72ns	13.7	6.36	8.73ns
2,4-Di-tert-butylphenol[a]	2265.84	794.83	1572.35a	2131.53	817.88	1692.59a	1223.88	949.97	1095.81b
Benzyl alcohol	1097.3	nd	610.95ns	1334.68	nd	830.61ns	752.94	423.49	588.77ns
Phenylethyl alcohol	68367.05	41337	55862.88a	84359.26	48379.84	57647.85a	34489.19	20788.5	28495.83b
Phenethyl acetate	130.17	28.79	53.96a	67.14	34.68	48.22a	30.79	24.65	27.69b
3-Methylthiopropanol[a]	12989.72	nd	3141.51ns	13027.07	nd	2930.01ns	695.78	nd	283.81ns

Note: nd: not detected. ns: not significant. Different letters in the row mean significant differences by ANOVA among the areas ($p < 0.05$). Data are the mean of three replicates.

[a] Quantified with a calibration curve of a compound of the same chemical class.

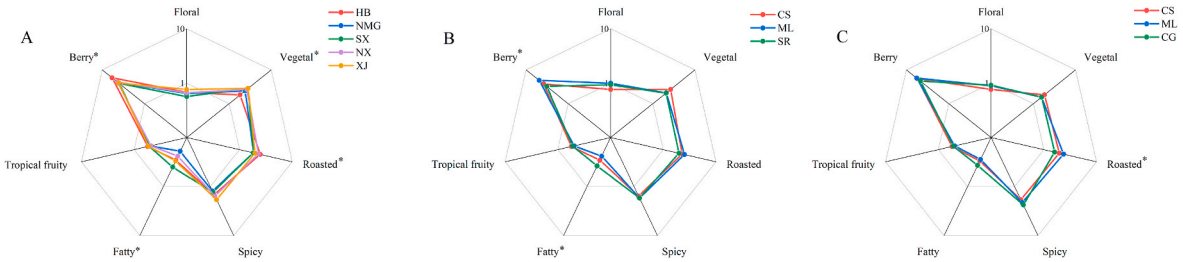

Fig. 2. Graphical representation of the sensory profiles of CS wine samples in five regions(A), three varieties in Xinjiang (B) and three varieties in Ningxia (C). The values were converted as a nonlinear normalized logarithmic function for each attribute. The individual attributes marked with the asterisk * represent significant differences between the samples ($p < 0.05$).

In the score plot (Fig. 3A), it was clear that the sample could be divided into two groups, the first group was represented by samples in HB, and the second was represented by NMG, XJ, SX, and XJ. Geography was undoubtedly the most significant driver of variation in wines since the two PCA groups isolated the location in eastern China and from the four locations in western China (Jiang et al., 2013; Xu et al., 2015). The two components explained about 95% of the total variance.

For the PCA of three varieties in XJ, two components explained more than 90% of the total variance, including PC1 explained 60.7% of the overall variance (Fig. 3B). It can be noticed this dataset was not

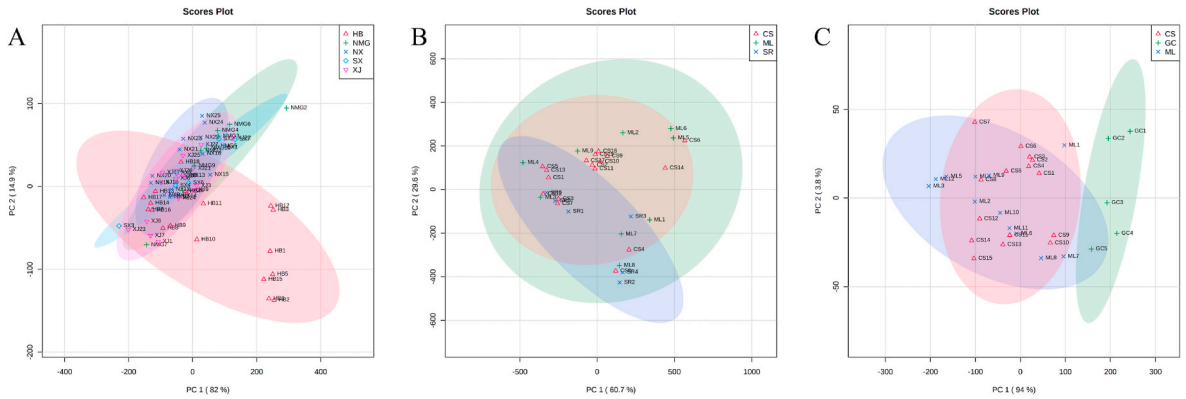

Fig. 3. PCA performed with CS wine from five regions (A), three varieties in Xinjiang (B) and three varieties in Ningxia (C). Ellipses display 95% confidence regions.

separated among the CS, ML and SR samples. Moreover, regarding different varieties in NX, the first two PCs explained 94% and 3.8% of the variance. In Fig. 3B and C, CS and ML wine samples showed great similarities in XJ and NX, while CG showed a big separation from them.

Unavoidably, the PCA models built for different varieties had some problems, whether in XJ or NX (Fig. 3B and C). As mentioned earlier, the volatile compounds of CS and ML wines in the same region showed great similarities. However, when contrasting the two regions carefully, the individual volatile compounds that demonstrated similarity in CS and ML samples were not the same. For example, ethyl acetate showed no significant difference in CS and ML samples from the XJ region but differed greatly in NX, suggesting that regions were of vital importance to wine quality within the same variety (Yue et al., 2014).

To observe the differences of wines in regions and varieties more intuitively and screen differential metabolites for the markers of different regions and varieties, the scores of PCA components were used in the LDA (Garde-Cerdán et al., 2021; Cosme et al., 2020).

The application of forwarding stepwise LDA on a volatile compounds data matrix allowed an 88.1% correct discrimination rate among CS samples from the five regions studied (Table S5). The key volatile compounds associated with the discriminant classification were 2,4-Di-tert-butylphenol, 2-methyl-1-propanol, 3-ethyl-4-methylpentan-1-ol, 2-undecanone, isoamyl lactate, and trans-2-hexen-1-ol. In Fig. 4A, the data were concentrated essentially around the group means based on the first two discriminant functions. The coordinate points from the NMG and NX regions appeared in the same area, which may have resulted from their close geographic locations and similar climate.

In XJ, the LDA analysis allowed us to distinguish among three varieties with a 93.8% certainty rate (Table S6). Benzyl alcohol, 2,3-butanediol, L-α-terpineol, 3-ethyl-4-methylpentan-1-ol, ethyl decanoate, and methyl salicylate were the key volatile compounds associated with the discriminant classification. Despite the relatively dispersed data, each group of variety could be clearly distinguished (Fig. 4B). In the LDA analysis concerning the three varieties in NX, the validation rate was 90.6% (Table S7), involving the diversity drivers phenylethyl alcohol, hexyl acetate, ethyl decanoate, nerolidol, trans-2-hexen-1-ol, ethyl octanoate, isobutyl acetate, diethyl succinate, and ethyl hexanoate. As shown in Fig. 4C, the data of the same variety were concentrated together, and different varieties of wine have been distinguished clearly.

Cross-validations were established to validate the region identification and prediction ability of LDA models. The principle is to randomly select n-1 samples from n samples as the training sample. The remaining 1 sample is used as the test sample so that each sample will be predicted by the established model once (Hao et al., 2021). The rates of the CS wines in the five regions, the three different varieties in XJ, and the three different varieties in NX were 82.1%, 78.1%, and 75.0%, respectively.

Available studies have shown that norisoprenoids, terpenes, and fermentation-derivatives like esters and alcohols play important roles in geographic difference and typicality (Slaghenaufi et al., 2019). A previous study using only seven volatiles achieved the discrimination of varietal wines. The volatiles used were 3-methyl-1-butanol, 2,3-butanediol, ethyl lactate, 3-methyl-1-butylacetate, 2-phenylethanol, phenyl ethyl acetate, and p-hydroxy phenylethanol (Dourtoglou et al., 2014), suggesting that alcohols, esters, and benzene-derivatives were likely to play a role in the expression of varietal features of wines. Our data agreed that the diversity of region and variety relied mainly on secondary metabolites of grapes compounds such as benzene-derivatives, terpenes, ketones, and some esters and alcohols.

4. Conclusion

The results obtained showed great variability among the volatile compound profiles of wines from different regions and varieties except for CS and ML. One further point to make was that the main primary

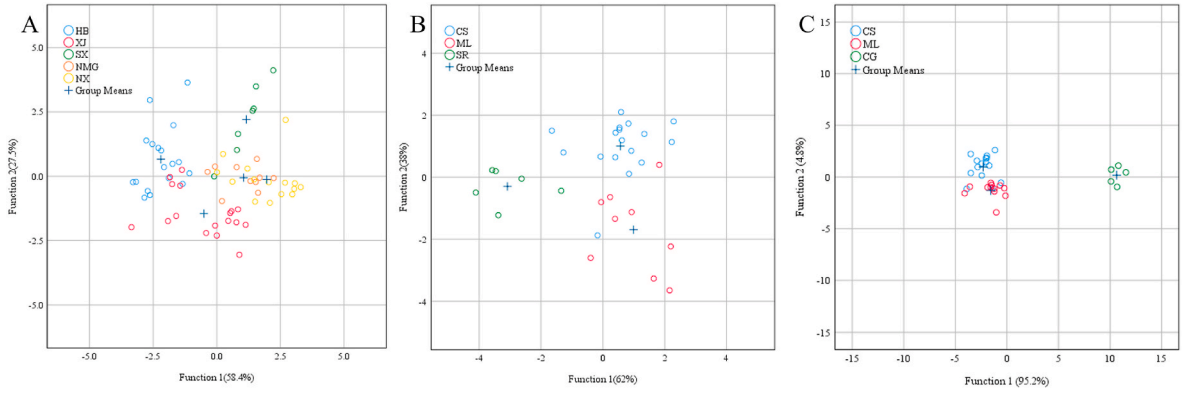

Fig. 4. LDA classification of CS wines from five regions (A), three varieties of wines in Xinjiang (B), and three varieties of wines in Ningxia (C).

factor of wine diversity in China seemed to be region rather than variety. Terpenes L-α-terpineol, nerolidol, benzene-derivatives benzyl alcohol, phenylethyl alcohol, ketones 2-undecanone, and methyl salicylate played obvious roles among the groups. Fermentation-derivatives such as esters and alcohols were also important secondary metabolites partly responsible for the region- and variety-related differences in wines. It is not enough to screen for differential metabolites through volatiles alone, and these characteristic compounds could only be considered as potential markers for wine volatiles. Further research and verification are needed to confirm the representative markers of each region and variety.

CRediT authorship contribution statement

Lin Zhang: Conceptualization, Methodology, Software. **Qianqian Liu:** Data curation, Writing – original draft, preparation. **Yuanyuan Li:** Visualization, Investigation. **Shuzhen Liu:** Supervision. **Qian Tu:** Software, Validation. **Chunlong Yuan:** 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.

Acknowledgments

This work was supported by The Key Industry Innovation Chain (Group), Agriculture of Shaanxi Province, China (no. 2020ZDLNY05-05); National key research and development program of Ningxia (2021BEF02016).

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.crfs.2022.100418.

References

Alem, H., Rigou, P., Schneider, R., Ojeda, H., Torregrosa, L., 2019. Impact of agronomic practices on grape aroma composition: a review. J. Sci. Food Agric. 99 (3), 975–985.
Avellone, G., Salvo, A., Costa, R., Saija, E., Bongiorno, D., Di Stefano, V., Calabrese, G., Dugo, G., 2018. Investigation on the influence of spray-drying technology on the quality of Sicilian Nero d'Avola wines. Food Chem. 240, 222–230.
Binati, R.L., Lemos Junior, W.J.F., Luzzini, G., Slaghenaufi, D., Ugliano, M., Torriani, S., 2020. Contribution of non-Saccharomyces yeasts to wine volatile and sensory diversity: a study on Lachancea thermotolerans, Metschnikowia spp. and Starmerella bacillaris strains isolated in Italy. Int. J. Food Microbiol. 318, 108470.
Cameleyre, M., Monsant, C., Tempere, S., Lytra, G., Barbe, J.C., 2021. Toward a better understanding of perceptive interactions between volatile and nonvolatile compounds: the case of proanthocyanidic tannins and red wine fruity esters-methodological, sensory, and physicochemical approaches. J. Agric. Food Chem. 69 (34), 9895–9904.
Chen, K., Liu, C., Wang, Y., Wang, Z., Li, F., Ma, L., Li, J., 2021. Predominance of indigenous non-Saccharomyces yeasts in the traditional fermentation of greengage wine and their significant contribution to the evolution of terpenes and ethyl esters. Food Res. Int. 143, 110253.
Chen, L., Darriet, P., 2021. Strategies for the identification and sensory evaluation of volatile constituents in wine. Compr. Rev. Food Sci. Food Saf. 20 (5), 4549–4583.
Ciani, M., Capece, A., Comitini, F., Canonico, L., Siesto, G., Romano, P., 2016. Yeast interactions in inoculated wine fermentation. Front. Microbiol. 7, 555.
Clemente-Jimenez, J.M., Mingorance-Cazorla, L., Martinez-Rodriguez, S., Heras-Vazquez, F.J.L., Rodriguez-Vico, F., 2004. Molecular characterization and oenological properties of wine yeasts isolated during spontaneous fermentation of six varieties of grape must. Food microbiology 21 (2), 149–155.
Cosme, F., Vilela, A., Moreira, L., Moura, C., Enríquez, J., Filipe-Ribeiro, L., Nunes, F.M., 2020. Terroir effect on the phenolic composition and chromatic characteristics of Mencía/Jaen monovarietal wines: Bierzo D.O. (Spain) and Dão D.O. (Portugal). Molecules 25, 6008.
Costello, M., Smith, R., Lane, L., 2018. Australian wine labels: terroir without terror. Gastronomica 18 (3), 54–65.
Dourtoglou, V., Antonopoulos, A., Dourtoglou, T., Lalas, S., 2014. Discrimination of varietal wines according to their volatiles. Food Chem. 159, 181–187.
Dubourdieu, D., Tominaga, T., Masneuf, I., Peyrot des Gachons, C., Murat, M.L., 2006. The role of yeasts in grape flavor development during fermentation: the example of Sauvignon blanc. Am. J. Enol. Vitic. 57, 81–88.
Falcão, L.D., de Revel, G., Perello, M.C., Moutsiou, A., Zanus, M.C., Bordignon-Luiz, M.T., 2007. A survey of seasonal temperatures and vineyard altitude influences on 2-Methoxy-3-isobutylpyrazine, C13-norisoprenoids, and the sensory profile of Brazilian Cabernet Sauvignon wines. J. Agric. Food Chem. 55 (9), 3605–3612.
Ferreira, V., Lopez, R., Cacho, J.F., 2000. Quantitative determination of the odorants of young red wines from different grape varieties. J. Sci. Food Agric. 80 (11), 1659–1667.
Francis, I.L., Newton, J.L., 2005. Determining wine aroma from compositional data. Aust. J. Grape Wine Res. 11, 114–126.
Garde-Cerdán, T., Rubio-Bretón, P., Marín-San Román, S., Sáenz de Urturi, I., Pérez-Álvarez, E.P., 2021. Pre-fermentative maceration with SO2 enhanced the must aromatic composition. Food Chem. 345, 128870.
Geffroy, O., Morère, M., Lopez, R., Pasquier, G., Condoret, J.-S., 2020. Investigating the aroma of Syrah wines from the northern rhone valley using supercritical CO2-dearomatized wine as a matrix for reconstitution studies. J. Agric. Food Chem. 68 (41), 11512–11523.
González-Barreiro, C., Rial-Otero, R., Cancho-Grande, B., Simal-Gándara, J., 2015. Wine aroma compounds in grapes: a critical review. Crit. Rev. Food Sci. Nutr. 55 (2), 202–218.
Goode, J., 2021. The Science of Wine: from Vine to Glass, third ed. University of California Press, Oakland, California.
Hao, X., Gao, F., Wu, H., Song, Y., Zhang, L., Li, H., Wang, H., 2021. From soil to grape and wine: geographical variations in elemental profiles in different Chinese regions. Foods 10 (12), 3108.
Jiang, B., Xi, Z., Luo, M., Zhang, Z., 2013. Comparison on aroma compounds in Cabernet Sauvignon and Merlot wines from four wine grape-growing regions in China. Food Res. Int. 51 (2), 482–489.
Ju, Y.-l., Liu, M., Tu, T.-y., Zhao, X.-f., Yue, X.-f., Zhang, J.-x., Fang, Y.-l., Meng, J.-f., 2018. Effect of regulated deficit irrigation on fatty acids and their derived volatiles in 'Cabernet Sauvignon' grapes and wines of Ningxia, China. Food Chem. 245, 667–675.
Kong, C.-l., Li, A.-h., Jin, G.-J., Zhu, X.-l., Tao, Y.-s., 2019. Evolution of volatile compounds treated with selected non-Saccharomyces extracellular extract during Pinot noir winemaking in monsoon climate. Food Res. Int. 119, 177–186.
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 Res. Int. 130, 108903.
Lan, H., Li, S., Yang, J., Li, J., Yuan, C., Guo, A., 2021. Effects of light exposure on chemical and sensory properties of storing Meili Rosé wine in colored bottles. Food Chem. 345, 128854.
Lan, Y.B., Xiang, X.F., Qian, X., Wang, J.M., Ling, M.Q., Zhu, B.Q., Liu, T., Sun, L.B., Shi, Y., Reynolds, A.G., 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 Chem. 287, 186–196.
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 Chem. 125 (1), 77–83.
Liu, J., Zhu, X.L., Ullah, N., Tao, Y.S., 2017. Aroma glycosides in grapes and wine. J. Food Sci. 82 (2), 248–259.
Luzzini, G., Slaghenaufi, D., Ugliano, M., 2021. Volatile compounds in monovarietal wines of two amarone Della Valpolicella terroirs: chemical and sensory impact of grape variety and origin, yeast strain and spontaneous fermentation. Foods 10 (10).
Pan, Y., Gu, H.W., Lv, Y., Yin, X.L., Chen, Y., Long, W., Fu, H., She, Y., 2022. Untargeted metabolomic analysis of Chinese red wines for geographical origin traceability by UPLC-QTOF-MS coupled with chemometrics. Food Chem. 394, 133473.
Panceri, C.P., De Gois, J.S., Borges, D.L.G., Bordignon-Luiz, M.T., 2015. Effect of grape dehydration under controlled conditions on chemical composition and sensory characteristics of Cabernet Sauvignon and Merlot wines. LWT - Food Sci. Technol. (Lebensmittel-Wissenschaft -Technol.) 63 (1), 228–235.
Pavez, C., Agosin, E., Steinhaus, M., 2016. Odorant screening and quantitation of thiols in carmenere red wine by gas chromatography–olfactometry and stable isotope dilution assays. J. Agric. Food Chem. 64 (17), 3417–3421.
Pearson, W., Schmidtke, L.M., Francis, I.L., Carr, B.T., Blackman, J.W., 2020. Characterising inter- and intra-regional variation in sensory profiles of Australian Shiraz wines from six regions. Aust. J. Grape Wine Res. 26 (4), 372–384.
Peng, C.T., Wen, Y., Tao, Y.S., Lan, Y.Y., 2013. Modulating the formation of Meili wine aroma by prefermentative freezing process. J. Agric. Food Chem. 61 (7), 1542–1553.
Petretto, G.L., Mercenaro, L., Urgeghe, P.P., Fadda, C., Valentoni, A., Del Caro, A., 2021. Grape and wine composition in Vitis vinifera L. Cv. Cannonau explored by GC-MS and sensory analysis. Foods 10 (1), 101.
Previtali, P., Dokoozlian, N.K., Pan, B.S., Wilkinson, K.L., Ford, C.M., 2022. The effect of ripening rates on the composition of Cabernet Sauvignon and Riesling wines: further insights into the sugar/flavor nexus. Food Chem. 373, 131406.
Rienth, M., Vigneron, N., Darriet, P., Sweetman, C., Burbidge, C., Bonghi, C., Walker, R. P., Famiani, F., Castellarin, S.D., 2021. Grape berry secondary metabolites and their modulation by abiotic factors in a climate change scenario-A review. Front. Plant Sci. 12, 643258.

Scafidi, P., Pisciotta, A., Patti, D., Tamborra, P., Di Lorenzo, R., Barbagallo, M.G., 2013. Effect of artificial shading on the tannin accumulation and aromatic composition of the Grillo cultivar (Vitis vinifera L.). BMC Plant Biol. 13, 175.
Sherman, E., Coe, M., Grose, C., Martin, D., Greenwood, D.R., 2020. Metabolomics approach to assess the relative contributions of the volatile and non-volatile composition to expert quality ratings of pinot noir wine quality. J. Agric. Food Chem. 68 (47), 13380–13396.
Slaghenaufi, D., Guardini, S., Tedeschi, R., Ugliano, M., 2019. Volatile terpenoids, norisoprenoids and benzenoids as markers of fine scale vineyard segmentation for Corvina grapes and wines. Food Res. Int. 125, 108507.
Sun, W.X., Hu, K., Zhang, J.X., Zhu, X.L., Tao, Y.S., 2018. Aroma modulation of Cabernet Gernischt dry red wine by optimal enzyme treatment strategy in winemaking. Food Chem. 245, 1248–1256.
Tang, K., Xi, Y.-R., Ma, Y., Zhang, H.-N., Xu, Y., 2019. Chemical and sensory characterization of Cabernet Sauvignon wines from the Chinese loess plateau region. Molecules 24 (6), 1122.
Tufariello, M., Fragasso, M., Pico, J., Panighel, A., Castellarin, S.D., Flamini, R., Grieco, F., 2021. Influence of non-Saccharomyces on wine chemistry: a focus on aroma-related compounds. Molecules 26 (3), 644.
Wang, J., Capone, D.L., Wilkinson, K.L., Jeffery, D.W., 2016. Chemical and sensory profiles of rosé wines from Australia. Food Chem. 196, 682–693.
Wei, Z., Liu, X., Huang, Y., Lu, J., Zhang, Y., 2019. Volatile aroma compounds in wines from Chinese wild/hybrid species. J. Food Biochem. 43 (10), e12684.
Xu, X.Q., Liu, B., Zhu, B.Q., Lan, Y.B., Gao, Y., Wang, D., Reeves, M.J., Duan, C.Q., 2015. Differences in volatile profiles of Cabernet Sauvignon grapes grown in two distinct regions of China and their responses to weather conditions. Plant Physiol. Biochem. 89, 123–133.
Yang, Y., Jin, G.J., Wang, X.J., Kong, C.L., Liu, J., Tao, Y.S., 2019. Chemical profiles and aroma contribution of terpene compounds in Meili (Vitis vinifera L.) grape and wine. Food Chem. 284, 155–161.
Yue, T.-X., Chi, M., Song, C.-Z., Liu, M.-Y., Meng, J.-F., Zhang, Z.-W., Li, M.-H., 2014. Aroma characterization of Cabernet Sauvignon wine from the plateau of Yunnan (China) with different altitudes using SPME-GC/MS. Int. J. Food Prop. 18 (7), 1584–1596.
Zhang, X., Kontoudakis, N., Šuklje, K., Antalick, G., Blackman, J.W., Rutledge, D.N., Schmidtke, L.M., Clark, A.C., 2020. Changes in red wine composition during bottle aging: impacts of grape variety, vineyard location, maturity, and oxygen availability during aging. J. Agric. Food Chem. 68 (47), 13331–13343.
Zhang, X., Wang, K., Gu, X., Sun, X., Jin, G., Zhang, J., Ma, W., 2021. 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).
Zhu, J., Niu, Y., Xiao, Z., 2021. Characterization of the key aroma compounds in Laoshan green teas by application of odour activity value (OAV), gas chromatography-mass spectrometry-olfactometry (GC-MS-O) and comprehensive two-dimensional gas chromatography mass spectrometry (GC × GC-qMS). Food Chem. 339, 12813.
Ziółkowska, A., Wąsowicz, E., Jeleń, H.H., 2016. Differentiation of wines according to grape variety and geographical origin based on volatiles profiling using SPME-MS and SPME-GC/MS methods. Food Chem. 213, 714–720.