





## Research Article

# Exploring Relationships between Aroma, Tasty Components Properties, and Marketing Price of Chinese Cabernet Sauvignon Using Gas Chromatography Mass Spectrum and High-Performance Liquid Chromatography

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The purpose of this paper was to find the relationship between aroma and tasty component properties and marketing price of Chinese Cabernet Sauvignon red wines. One-way ANOVA was used to compare differences ( $p < 0.05$ ) between concentrations of phenolic compounds, organic acids, monosaccharides and total acidity, total polyphenols, total sugars, and total reducing sugars in various Chinese Cabernet Sauvignon red wines with different marketing prices. Principal component analysis revealed that the presence of higher amount of alcohol appears to be the characteristic feature for the wine samples, which have a lower marketing price, and the higher level of esters and acids were the features of the wine samples with a higher marketing price. Moreover, samples in marketing price area 39 to 79 RMB and samples in marketing price area 188 to 258 RMB can be totally clustered into their own marketing price area by volatile compounds with OAV > 1. Acetic acid, succinic acid, and glucose made a great contribution to most of the wine samples in the marketing price area ranging from 39 to 79 RMB, and glycerol, fructose, and malic acid were the features of most wine samples in the marketing price area ranging from 188 to 258 RMB. Concentrations of total acidity, total polyphenols, total sugars, total reducing sugars, and alcohol content seemed to have no significant distinguishing ( $p < 0.05$ ) ability on different samples belonging to different marketing price areas.

## 1. Introduction

Researchers have demonstrated that taste, type, alcohol content, age, color, marketing price, brand label, usability of purpose, and region of origin were influential attributes when consumers purchase wine [1]. Especially, marketing price seems to play one of the most important roles in choosing a wine [2].

Moreover, the producers pursue objective quality related to wine aroma taste characteristics, and the purchasers usually care about quality of the extrinsic factors like those mentioned earlier except for experienced drinkers.

In recent decades, the motivation of wine consumption has turned into the pleasure of drinking. There is no doubt that wine aroma and taste characteristics will be paid more attention as key drivers of wine choice. Therefore, as consumers, understanding the relationship between the marketing price and wine aroma taste characteristics has become necessary.

Aroma taste characteristics are typically studied by evaluating the aroma and tasting profile. Gas chromatography mass spectrum (GC-MS) is a common way to analyze aroma compounds, and it has become a mature technology to study all kinds of volatile compounds, although there are

TABLE 1: Code list of 12 wine samples with different marketing prices analyzes here.

Wine sample code	Grape variety	Areas of wine sources	Vintage	Price (RMB)
W1	Cabernet sauvignon	Yantai, Shandong	2011	39
W2	Cabernet sauvignon	Changli, Hebei	2011	49
W3	Cabernet sauvignon	Yantai, Shandong	2011	59
W4	Cabernet sauvignon	Yantai, Shandong	2011	65
W5	Cabernet sauvignon	East of Helan Mountain, Ningxia	2011	68
W6	Cabernet sauvignon	Jichang, Xinjiang	2011	79
W7	Cabernet sauvignon	Changli, Hebei	2011	239
W8	Cabernet sauvignon	Yantai, Shandong	2011	188
W9	Cabernet sauvignon	Lulong, Hebei	2011	198
W10	Cabernet sauvignon	Hangu, Tanjin	2011	228
W11	Cabernet sauvignon	Changli, Hebei	2011	258
W12	Cabernet sauvignon	Yibin, Sichuan	2011	208

some deficiencies in accurate quantification of these compounds [3]. More than 800 different volatile compounds have been found in different wines, and their concentrations range from hundreds of mg/L to several ng/L [4]. However, the formation mechanism of aroma compounds is very complex; no single compound can contribute to the whole aroma of a wine. Therefore, we should take many comprehensive factors into account. In recent years, the threshold and odor active value (OAV) were brought in to express the contribution of a single compound in wine [5], only those odorants with OAV > 1 can contribute to the entire aroma of the wine.

The classical way to analyze compounds related to tasting which mainly include phenolic compounds, organic acids, and monosaccharides is high-performance liquid chromatography (HPLC). Increasing knowledge on wine analytical chemistry makes contributions to the development of the wine industry and scientific research. Moreover, as a wine grape, Cabernet Sauvignon was thought to be a classic type to study. Hundreds of aroma compounds of Cabernet Sauvignon wines were identified and quantified.

The purpose of this paper is to find the relationship between aroma and tasty component characteristics and marketing price of Chinese red wines. Marketing price is representative of the extrinsic cues, and it has a significant influence on wine consumption. The findings provide insights into the relative impact of marketing price on Chinese consumer's preferences and furthermore provide some references for developing targeted wines.

## 2. Materials and Methods

**2.1. Chemicals and Materials.** All the standards for the HPLC analysis and Folin-Ciocalteu reagent were obtained from Sigma-Aldrich (St. Louis, MO, USA). HPLC-grade acetonitrile, methanol, and ethanol were obtained from the Sinopharm Chemical Reagent Co., Ltd (Shanghai, China). A C7-C30 n-alkane mixture used for calculating linear retention indices was obtained from Supelco (Bellefonte, PA, USA). 2-octanol was purchased from Sigma-Aldrich (Saint Luis, EUA). Double-distilled water was purchased from Watsons Company. Other reagents were purchased from the Sinopharm Chemical Reagent Co., Ltd (Shanghai, China).

Twelve different commercial Cabernet sauvignon red wines were purchased from the Jiuxian net. These wines were all made in China and aged 3 years with marketing price ranging 39 to 79 RMB and 188 to 258 RMB, respectively, per bottle. They were made by different companies in 2012 and had very high popularity to the red wine consumers in China. All the samples were stored at 10°C before the analysis. The details of these wines are listed in Table 1.

**2.2. Extraction, Identification, and Quantification of the Volatile Compounds.** A 75  $\mu\text{m}$  DVD/CAR/PDMS fiber length 1 cm (Supelco, Bellefonte, PA, USA) was used to perform the headspace solid-phase microextraction (HS-SPME) of the wine samples. Before the extraction, 10  $\mu\text{L}$  of 2-octanol solution (700 mg/L in hydroalcoholic solution) was spiked as an internal standard and mixed with 10 mL of wine. About 5 g of sodium chloride was added into the sample wine. Then the SPME fiber was exposed to the headspace for 30 min at 60°C. It was loaded into the injector of a GC-MS (7890 series gas chromatograph and 5973C mass spectrometer selective detector, Agilent Technologies, USA). The temperature of the injector port and desorption time were 250°C with splitless mode and 5 min, respectively. The GC-MS was equipped with an HP-INNOWAX fused-silica capillary column (60 m  $\times$  0.25 mm I.D., 0.25  $\mu\text{m}$  film thickness, Agilent Technologies, USA). The carrier gas was helium at a flow rate of 1.0 mL/min. The program of oven temperature was set as follows: the initial temperature at 40°C for 2 min; to 180°C at 5°C/min; then to 230°C at 15°C/min and at 230°C for 15 min. The MS ionization source was set at 70 eV of ionization energy and in a range of 30 to 450 amu at 3.2 scans/s with 3 min of a solvent delayed time.

The identification of the volatiles was carried out by comparing the retention indices (RIs) in NIST Chemistry database [6] and mass spectrum Wiley7n.1 database (Hewlett-Packard, Palo Alto, CA). The RI of the volatile compounds was calculated using an n-alkane series under the same conditions according to Van Den Dool and Kratz equation [7]. The equation was proved to be in good correlation with experience and adequate for practice [8]. Quantification analysis was performed based on the method reported in Tufariello et al.'s study [9].

**2.3. Physicochemical Analysis and Analysis of Phenolic Compounds, Organic Acids, and Monosaccharides.** The total sugars and reducing sugars were determined based on the reaction with 3,5-dinitrosalicylic acid (DNS), and the total phenols were measured by Folin–Ciocalteu reagent. Alcohol content and total acidity analyses were performed for the wine according to standard methods [10].

The phenolic compounds, organic acid, and monosaccharides in the wine samples were extracted using a 150 mg solid-phase extraction (SPE) cartridge filled with ProElut™ PLS resin (Dikma Technologies, Beijing, China) and concentrated by using a VAC ELT 20 station (Varian, city, nation). First, the cartridge was balanced by rinsing with 6 mL methanol, 6 mL acetonitrile, and 10 mL water followed by passing a 4 mL wine sample through the SPE cartridge at a rate of 4 to 6 drops/min. Then the cartridge was flushed with 10 mL water, 10 mL of water-methanol mixture (5%, v/v), and 10 mL methanol. The first two elution phases were combined and dried under nitrogen flow. Then the dried extract was dissolved in 2 mL of water and stored at  $-20^{\circ}\text{C}$  for HPLC analysis of organic acid and monosaccharides. The last methanol elution phase was collected and dried under nitrogen flow as well. The dried extract was dissolved in 2 mL acetonitrile and stored at  $-20^{\circ}\text{C}$  for HPLC analysis of phenolic compounds.

The analysis of phenolic compounds [11–13] and organic acids was performed by an Agilent 1200 infinity series (Agilent Technologies, USA) HPLC system with a Spursil C18 column ( $5\ \mu\text{m}$ ,  $250 \times 4.6\ \text{mm}$ , Dikam Technologies Inc, Beijing, China) and a UV detector. The mobile phase for the analysis of phenolic compounds consisted of 0.1% orthophosphate in water (A) and acetonitrile (B) by gradient elution. The mobile-phase elution was programmed as 0 to 2 min, A 95%; 2 to 6 min, A 95% to 90%; 6 to 20 min, A 90% to 85%; 20 to 30 min, A 58% to 70%; 30 to 32 min, A 70% to 90%; and 32 to 35 min, A 90% to 95%. The flow rate and column temperature were 0.7 mL/min and  $35^{\circ}\text{C}$ , respectively. The wavelength of the UV detector was set at 280 nm.

For the analysis of organic acids, the mobile phases consisted of 0.08 mol/L potassium dihydrogen phosphate (adjusted pH to 2.9 using orthophosphoric acid) in water (A) and acetonitrile (B). The elution program was 90% of A with 10% of B at a flow rate of 0.7 mL/min. The column temperature was  $30^{\circ}\text{C}$ . The wavelength of the UV detector was 210 nm.

The analysis of monosaccharides was performed using an Agilent 1200 infinity series (Agilent Technologies, USA) HPLC system with a PlatwasilHN2 column ( $5\ \mu\text{m}$ ,  $250 \times 4.6\ \text{mm}$ , Dikam Technologies Inc, Beijing, China) and reflective index detector. The mobile phase was 0.001 mL/L acetic acid in water at a flow rate of 0.3 mL/min with a column temperature of  $55^{\circ}\text{C}$ .

The standard curves set up through the standards of phenolic compounds, organic acids, and monosaccharides were used in the quantification of those compounds in the wine samples.

**2.4. Statistics and Data Processing.** Principal component analysis (PCA) was used to examine the following items: first, to reveal the relationship among wine samples with different marketing price on all detected aroma compounds, aroma compounds with  $\text{OAV} > 1$ , and the total content related to tasting and tasty compounds. Second, to identify the constituents that act as the chemotypical factors. Statistical data processing was performed using unscramble 9.7 (CAMO Software AS, Norway).

One-way ANOVA was performed to find the significant differences for phenolic compounds, organic acids, monosaccharides, and the total content related to tasting using SAS 9.3 (North Carolina state university, Raleigh, USA). Duncan's multiple comparison tests were performed to determine the significance among different samples.

### 3. Results

**3.1. Aroma Compounds of Cabernet Sauvignon Wines.** A total of 59 different volatile compounds of 12 different Cabernet Sauvignon wines were identified and quantified by HS-SPME/GC-MS, which are shown in Table 2, and their identified information and odor description were also given. Fifty-nine compounds included alcohols (16), phenols (6), aldehydes (4), acids (7), ketones (3), esters (17), terpenes (3), sulfur-contained compound (1), and furans (2). Thirteen compounds included isoamyl acetate, ethyl hexanoate, ethyl octoate, diethyl succinate, *cis*-3-hexene-1-ol, 2,3-butanediol, nonanal, 5-methyl-2-furfural, 2-amylfuran, DL-limonene, octanoic acid, decanoic acid, and guaiacol made a greater contribution to these wine aromas with  $\text{OAV} > 1$ . Their  $\text{OAV}$  values are listed in Table 3.

As shown in Table 2, esters and alcohols are the largest groups. Among the identified major esters, most of them have floral and fruity odors. For the esters with  $\text{OAV} < 1$ , it was found that nine esters including ethyl acetate which associated with fruity aroma, ethyl caprate which associated with grape aroma, ethyl 2-hexenoate which associated with fruity and green aroma, ethyl lactate which associated with fruity and anise aroma, ethyl hydrogen succinate which associated with chocolate aroma, methyl salicylate, ethyl 3-hydroxybutyrate, and ethyl 3-methylbutyl butanedioate whose odor was not found, did not differ in concentration between the lower marketing price group and the higher marketing price group. Indeed, the concentrations of compounds in the six lower marketing price samples were almost the same as that in the six higher samples. Moreover, for another four esters, isopentyl formates are associated with apple-like aroma [11] and have a significant difference on the two categories. Some researchers have proved that isopentyl formate is produced during the alcoholic fermentation, and this ester content depends on the yeast [12]. As it can be observed, lower marketing price samples are mainly characterized by a higher concentration of isopentyl formate which only exists in the sample W9 for the higher marketing price samples. Isoamyl lactate with fatty aroma and ethyl methyl were in low concentration and only existed in samples W5, W6, and W10. Phenethyl acetate which associated with fruity aroma was common to all

TABLE 2. Volatile compounds identified in 12 Cabernet sauvignon red wines with different marketing prices, including concentration (mg/L), the Kovats Index of aroma compounds on HP-INNOWAX (KI) and sensory descriptor for each compound detected by SPME/GC-MS. Each sample was analysed in triplicate. The obtained coefficients of regression ( $R^2$ ) were >0.998, and the relative standard deviations (RSD) were <5%.

Code	Compous	CKI <sup>m</sup>	KI <sup>n</sup>	IM <sup>o</sup>	ODE <sup>p</sup>	OTS <sup>q</sup> (mg/L)	Concentration (mg/L)											
							W1	W2	W3	W4	W5	W6	W7	W8	W9	W10	W11	W12
Esters																		
ES1	Ethyl acetate	897	888	A	Fruity, pineapple2	12.000a	1.92	1.33	1.20	1.97	1.54	1.52	1.89	1.73	2.36	2.97	1.60	4.08
ES2	Isoamyl acetate	1128	1131	A	Banana, sweet2	0.066d	0.06	0.07	0.11	0.09	0.09	0.24	0.07	0.15	0.10	0.15	0.05	0.20
ES3	Isopentyl formate	1233		B	Apple-like	NF	6.30	10.55	9.85	7.78	8.59	8.77	ND	ND	5.89	ND	ND	ND
ES4	Ethyl hexanoate	1239	1241	A	Apple peel, fruit2	0.008a	ND	0.16	0.21	0.20	ND	0.65	0.18	0.55	0.22	ND	ND	0.58
ES5	Ethyl 2-hexenoate	1350	1343	A	Fruity, green apple1	0.014c	ND	ND	0.01	ND	0.01	0.01	ND	0.01	ND	0.01	0.01	ND
ES6	Ethyl lactate	1357	1352	A	Fruity, anise2	154.000c	ND	2.13	1.40	ND	ND	2.13	1.40	1.95	ND	1.82	2.01	
ES7	Ethyl octanoate	1443	1436	A	Fruity, fatty1	0.240a	0.36	0.37	0.45	0.61	0.36	0.69	0.68	0.65	0.52	1.28	0.49	1.88
ES8	Ethyl 3-hydroxybutyrate	1534	1524	A	NF	20.000c	ND	ND	0.01	ND	0.01	0.02	ND	0.01	0.01	0.02	0.02	ND
ES9	Isoamyl lactate	1581	1523	A	Fatty, rancid1	NF	ND	ND	ND	ND	0.06	0.06	ND	ND	ND	0.09	ND	ND
ES10	Ethyl caprate	1648	1636	A	Grape4	0.500a	0.05	0.04	0.08	0.12	0.12	0.05	0.18	0.05	0.08	0.19	0.13	0.22
ES11	Ethyl methyl succinate	1650		C	NF	NF	ND	ND	ND	0.04	0.04	0.04	ND	ND	ND	0.04	ND	ND
ES12	Diethyl succinate	1689	1688	A	Fruity, sweet1	1.200a	0.94	1.37	1.68	1.55	1.07	1.26	2.96	2.20	2.75	3.21	2.24	3.12
ES13	Methyl salicylate	1809	1788	A	NF	NF	ND	ND	0.03	0.02	0.03	0.02	0.11	0.12	0.04	0.07	0.08	0.06
ES14	Phenethyl acetate	1843		B	Floral1	1.800a	ND	0.02	ND	0.03	ND	ND	0.06	0.05	0.04	0.07	0.03	0.10
ES15	Ethyl 3-methylbutyl succinate	1920		C	Fruity1	NF	ND	ND	0.04	ND	0.03	0.03	0.05	ND	0.04	0.06	0.03	ND
ES16	Diethyl malate	2066	2041	A	NF	10.000c	ND	ND	ND	ND	ND	ND	ND	ND	ND	0.03	ND	ND
ES17	Ethyl hydrogen succinate	2400		C	Chocolate1	NF	0.10	0.10	ND	0.11	ND	ND	0.15	ND	0.10	0.20	ND	0.21
Total esters																		
AL1	1-propanol	1054	1037	A	Alcohol, ripe fruit1	306.000a	0.23	0.45	0.40	0.50	0.50	0.25	0.23	0.24	0.41	0.45	0.42	0.28
AL2	2-methyl-1-propanol	1106	1099	A	Alcohol, solvent1	75.000a	0.66	1.44	0.70	0.95	0.83	0.47	0.62	0.53	0.51	0.67	0.61	0.68
AL3	1-butanol	1162	1163	A	Medicine, fruit1	150.000a	0.04	0.04	0.04	0.04	0.06	0.04	ND	0.04	0.04	0.07	0.08	0.08
AL4	3-methyl-1-butanol	1221	1220	A	Cheese1	30.000b	ND	ND	ND	ND	ND	ND	6.02	6.43	5.89	8.39	5.14	9.06
AL5	1-pentanol	1263	1254	A	Almond, synthetic, balsamic6	64.000a	0.03	0.01	0.01	0.02	0.02	0.02	ND	ND	0.01	ND	ND	ND
AL6	3-ethyl-1-butanol	1334	1343	A	Vinous, herbaceous, cacao6	50.000a	ND	ND	0.02	ND	ND	0.02	2.10	ND	ND	0.01	ND	0.02
AL7	3-methyl-2-pentanol	1362		C	Fruity, Cocoa2	NF	ND	ND	ND	ND	ND	ND	ND	ND	ND	2.48	ND	ND
AL8	3-Ethoxypropanol	1387		C	Fruity6	NF	ND	0.02	0.01	0.01	ND	0.02	ND	ND	0.02	ND	ND	0.02
AL9	cis-3-hexene-1-ol	1392	1391	A	Fruity, plant1	0.040c	0.02	0.02	0.02	0.02	0.02	0.03	0.04	0.05	0.02	0.03	0.02	0.04
AL10	1-heptanol	1461	1467	A	NF	0.425d	0.01	ND	0.01	ND	0.01	ND	ND	ND	ND	ND	ND	ND
AL11	2-ethyl-1-hexanol	1493	1503	A	Fruity, green cucumber2	8.000a	ND	ND	0.01	ND	ND	0.02	ND	ND	ND	ND	0.01	0.03
AL12	2,3-butanediol	1551	1583	A	Fruity, onion2	0.030d	0.26	ND	0.13	0.26	0.22	0.39	0.24	0.31	0.29	0.57	0.48	0.35
AL13	1-octanol	1564	1553	A	Chemical, metal, burnt1	0.200d	0.02	0.04	0.02	0.02	0.02	0.02	ND	0.04	0.06	0.03	0.04	0.06
AL14	1,3-butanediol	1587		C	Fruity1	NF	ND	ND	ND	0.12	ND	ND	0.10	0.10	ND	0.13	0.19	ND
AL15	Benzyl alcohol	1902	1903	A	Floral, sweet1	200.000a	0.02	0.04	0.02	ND	0.02	0.08	0.08	0.09	0.04	0.06	0.16	0.05
AL16	Phenethyl alcohol	1941	1938	A	Rose, sweet2, honey6	200.000a	1.71	2.71	1.29	2.19	1.35	3.13	3.43	3.55	3.38	4.43	4.15	5.39
Total alcohols																		
AD1							3.30	4.77	2.68	4.13	3.05	4.45	12.90	11.40	10.64	17.34	11.30	16.06



TABLE 2: Continued.

Code	Compous	CKI <sup>m</sup>	KI <sup>n</sup>	IM <sup>o</sup>	ODE <sup>p</sup>	OTS <sup>q</sup> (mg/L)	Concentration (mg/L)												
							W1	W2	W3	W4	W5	W6	W7	W8	W9	W10	W11	W12	
KE2	Butyrolactone	1664	1635	A	Sweet, buttery <sup>5</sup>	20.000c	0.04	0.04	0.03	0.03	0.04	0.09	0.07	0.07	0.07	0.04	0.08	0.11	0.11
	Total lactones						0.04	0.04	0.03	0.03	0.04	0.09	0.07	0.07	0.07	0.04	0.08	0.11	0.11
ME1	Methionol	1735	1727	A	Cooked potato1		0.03	0.04	0.02	0.03	0.03	0.06	0.04	0.07	0.03	0.10	0.05	0.03	0.03
	Total Sulfur compounds						0.03	0.04	0.02	0.03	0.03	0.06	0.04	0.07	0.03	0.10	0.05	0.03	0.03

Sulfur compounds

NF: not found ND: not detected mCKI: calculated Kovats Index of aroma compounds on HP-INNOWAX. nKI: theoretical retention index obtained from the database (<http://webbook.nwast.gov/chemwastry/>). oIM: identification methods: A, mass spectrum and KI agreed with authentic compounds tested in the same GC-MS condition; B, mass spectrum agreed with mass spectral data base; C, mass spectrum and KI agreed with mass spectral literature data base. pODE: odor description shown in literatures: 1 (Tuñariello, Capone, & Siciliano, 2012); 2 (Niu et al., 2011); 3 (Li, Tao, Wang, & Zhang, 2008); 4 (Acree & Arn, 2004); 5 (Capone et al., 2013); 6 (Welke, Zanus, Lazzarotto, & Zini, 2014); 7 (Zheng et al., 2012); 8 (Loscos, Hernandez-Orte, Cacho, & Ferreira, 2007). qOTS: odor threshold of the volatile compounds shown in literatures: a (Welke et al., 2014); b (Alvarez, González-Barreiro, Cancho-Grande, & Simal-Gándara, 2011); c (Tuñariello et al., 2012); d (Pino & Queris, 2011). wClass 1: including samples W1 to W6 belonging to marketing price area 39 to 79 RMB. zClass 2: including samples W7 to W12 belonging to marketing price area 188 to 258 RMB.

TABLE 3: The compounds whose OAV &gt; 1 in all samples or partial samples.

	Compounds	OAV <sub>W1</sub>	OAV <sub>W2</sub>	OAV <sub>W3</sub>	OAV <sub>W4</sub>	OAV <sub>W5</sub>	OAV <sub>W6</sub>	OAV <sub>W7</sub>	OAV <sub>W8</sub>	OAV <sub>W9</sub>	OAV <sub>W10</sub>	OAV <sub>W11</sub>	OAV <sub>W12</sub>
ES2	Isoamyl acetate	0.91	1.06	1.67	1.36	1.36	3.64	1.06	2.27	1.52	2.27	0.76	3.03
ES4	Ethyl hexanoate	ND	20.00	26.25	25.00	ND	81.25	22.50	68.75	27.50	ND	ND	72.50
ES7	Ethyl octanoate	1.50	1.54	1.88	2.54	1.50	2.88	2.83	2.71	2.17	5.33	2.04	7.83
ES12	Diethyl succinate	0.78	1.14	1.40	1.29	0.89	1.05	2.47	1.83	2.29	2.68	1.87	2.60
AL9	cis-3-Hexene-1-ol	0.50	0.50	0.50	0.50	0.50	0.75	1.00	1.25	0.50	0.75	0.50	1.00
AL12	2,3-Butanediol	8.67	ND	4.33	8.67	7.33	13.00	8.00	10.33	9.67	19.00	16.00	11.67
AD2	Nonanal	ND	1.33	0.67	0.67	0.67	0.67	1.33	2.67	0.00	1.33	ND	4.00
AD4	5-Methyl-2-furfural	3.33	13.33	3.33	3.33	3.33	16.67	10.00	16.67	6.67	6.67	ND	86.67
FU1	2-Amylfuran	ND	ND	ND	ND	ND	1.67	ND	ND	ND	3.33	ND	5.00
TE1	DL-Limonene	0.44	0.66	0.60	0.80	0.70	1.18	1.68	1.40	1.02	1.34	0.78	3.04
AC6	Octanoic acid	11.67	13.33	8.33	15.00	11.67	16.67	23.33	0.00	15.00	21.67	10.00	48.33
AC7	Decanoic acid	ND	ND	1.00	1.00	3.00	ND	3.00	4.00	ND	4.00	ND	3.00
PH1	Guaiacol	ND	ND	ND	ND	ND	1.00	1.00	1.00	1.00	1.00	ND	2.00

higher marketing price samples and typically found in all samples of higher marketing price category. However, it only existed in two samples belonging to the lower marketing price group and lower than the higher marketing price group.

For the four esters with OAV > 1, the compound that made the greatest contribution to wine aroma is ethyl hexanoate due to its high OAV which is mainly from enzymatic reaction between free alcohols and acetyl CoA derivatives of fatty acids [13]. The highest concentration of ethyl hexanoate is 0.65 mg/L in sample W6 and its OAV reached 81.25. The higher concentration next to sample W6 is 0.58 mg/L in sample W12 (OAV = 72.5) and 0.55 mg/L in sample W8 (OAV = 68.75) and then 0.22 mg/L (OAV = 27.50) in sample W9, 0.21 mg/L (OAV = 26.25) in sample W3, 0.20 mg/L (OAV = 25.00) in sample W4, 0.18 mg/L (OAV = 22.50) in sample W7 and 0.16 mg/L (OAV = 20.00) in sample W2, and it was not detected in other four samples. For ethyl hexanoate, there were no significant differences on two categories. Ethyl octoate which was described as fruity and fatty aroma was the second contributor. The OAV of it ranged 1.50 to 2.88 in the lower marketing price group but ranged 2.04 to 7.83 in the higher marketing price group. The same phenomenon happened for diethyl succinate whose OAV ranged 0.78 to 1.40 in the lower marketing price group but ranged 1.83 to 2.63 in the higher marketing price group as shown in Table 3. So, we can conclude that ethyl octoate and diethyl succinate had more influence on the higher marketing price group. Isoamyl acetate has banana and sweet aroma, which is a common volatile compound in wine, and almost reported in any literature about wine aroma compounds, it shows that there

is no significant function to separate these two groups as shown in Tables 2 and 3. However, for the concentration of total esters, the most samples in the lower marketing price team are relatively higher than these samples in the higher marketing price team.

The alcohols, detected in appreciative concentration in wine samples, were 3-methyl-1-butanol, 1-pentanol, 1-heptanol, 1,3-butanediol, benzyl alcohol, and phenethyl alcohol. 3-methyl-1-butanol associated with cheese aroma was only detected in the higher marketing price group, and its concentration ranged from 5.14 mg/L to 9.06 mg/L, and it can be a typical compound for higher marketing price group although its OAV < 1. 1,3-butanediol associated with fruity aroma is detected in four samples belonging to the higher marketing price group but just in one sample belonging to the lower marketing price. As opposed to 3-methyl-1-butanol, 1-pentanol only detected in the lower marketing price groups except 0.01 mg/L in sample W9. But the concentration of 1-pentanol (ranged 0.01–0.03 mg/L) was far lower than its threshold (64 mg/L) as shown in Table 2. 1-heptanol is also only detected in three of samples in the lower marketing price groups. Benzyl alcohol and phenethyl alcohol are the ones that found in all samples except W4, but the concentration of it in samples belonging to the higher marketing price group was commonly higher than that in samples belonging to the lower marketing price group. For the alcohols with OAV > 1, as it shown in Tables 2 and 3, the OAV of 2,3-butanediol ranged from 0 to 8.67 in samples in higher marketing price team except 13 in W6 and ranged 9.67 to 19.00 in samples in higher marketing price team except 8.00 in W7. 2,3-butanediol in two groups has a greater difference, and 2,3-butanediol made a greater contribution

to wine aroma of samples in the higher marketing price team. The concentration of total alcohols of the lower marketing price team is far lower than the higher marketing price team.

Four aldehydes and two ketones and two furans were found not largely differ in concentration and OAV for two marketing price groups. Moreover, both total aldehydes and total ketones were not found big changes in two marketing price groups. However, the concentration of total furans in higher marketing price groups was slightly higher than those in the lower marketing price groups.

For seven acids, there were no special changes, and change rule because of marketing price except heptanoic acid was only found in higher marketing price group. However, the concentration of total acids in higher marketing price groups was also slightly higher than those in lower one, which was similar to the concentration of total furans. Especially, for octanoic acid and Decanoic acid whose  $OA V > 1$ , octanoic acid ( $OA V = 48.33$ ) in sample W12 have the greatest contribution in acids to the wine aroma.

Terpenes have been proved to form for sensory expression of the wine bouquet and belong to the secondary plant constituents and are synthesized by microorganisms [14]. There were no much changes in samples because of marketing price for dl-limonene and Styrene shown in Table 2. Moreover, vitispirane existed in lower marketing price samples W1 (0.03 mg/L) and W6 (0.04 mg/L).

Volatile phenols were determined, but all concentrations of these compounds were lower than their threshold except guaiacol. Volatile phenols have been proved to play a negative effect on wine quality, and most of the phenols are responsible for phenolic and animal smoky [9]. Guaiacol were detected in sample W7 with  $OA V = 1$ . Phenol commonly existed in two groups, but it is not detected in W8 and W11 belonging to the higher marketing price group. Moreover, 2,4-bis(1,1-dimethylethyl)-phenol was commonly found in the lower marketing price samples and had a higher concentration ranging from 0.008 to 1.95 mg/L compared to other volatile phenols, but its threshold had not been determined, and it has the potential negative effect on the wine aroma. It was not detected in higher marketing price samples. p-ethylguaiacol and 4-ethylphenol which have unpleasant odor and were only detected in sample W1 and their concentrations were 0.02 mg/L and 0.13 mg/L, respectively. Different from former five volatile phenols, 3-methyl-phenol were detected in three samples belonging to the higher marketing price group, and their concentrations were 0.02 mg/L in sample W7, 0.02 mg/L in sample W8, 0.01 mg/L in sample W11, but only 0.01 mg/L in sample W4 belonging to the lower marketing price group.

Moreover, one lactone (butyrolactone, 0.03–0.11 mg/L, sweet and buttery smell) and one sulfur compound (methionol, 0.02–0.10 mg/L, cooked potato smell) were found in all wine samples, but their concentration was lower than their threshold. Intuitively, there were no significant differences in different samples with different marketing price level. So, these two kinds of compounds cannot be divided by marketing price.

**3.2. Statistical Analysis of Aroma Volatiles.** In order to reveal the variations of aroma compounds in different samples in two different marketing price areas, the composition data were analysed by PCA. The results are shown in Figure 1.

As shown in Figure 1(a) and 1(b), the 2D graphical representation of PCA contains 94% of the total variance in the data set. Wine samples were classified into two categories, the samples on the left side of the PCA score plot which belonged to Class 2, while the samples on the right belonged to Class 1 according to PC1 shown as Figure 1(a). The class 2 samples variability derived mostly from 3-methyl-1-butanol (AL4) and while isopentyl formate (ES3), ethyl lactate (ES6), diethyl succinate (ES12), 3-ethyl-1-butanol (AL6), and phenethyl alcohol (AL16) most influenced the Class 1.

As shown in Figures 1(c) and 1(d), the 2D graphical representation of PCA contains 94% of the 13 variances in the data set. Wine samples were also classified into two categories. Interesting, the two categories which include samples same as the aforementioned results shown in Figure 1(a), samples in two groups belonging to the different marketing price areas were totally separated. Figure 1(d) shows that Class 2 sample variability derived mostly from ethyl octoate (ES7, abscissa value: 0.1312; ordinate value: 0.8711), diethyl succinate (ES12, abscissa value: 0.2558; ordinate value: 0.4114), DL-limonene (TE1, abscissa value: 0.2558; ordinate value: 0.4114), and ethyl hexanoate (ES4, abscissa value: 0.1764; ordinate value: -0.0456), but no compound most influenced Class 1.

Hence, samples in discussed different marketing prices area can be significantly separated by volatile compounds and aroma compounds with  $OA V > 1$ , namely, the wine samples with different marketing price have significant different on their concentration of volatile compounds and aroma compounds. Moreover, the presence of the high amount of alcohol appears to be the characteristic for the Class 1 which has a lower marketing price and the high level of esters and acids were the feature of the Class 2 which has a higher marketing price. Moreover, volatile compounds who  $OA V > 1$  appears to have the same function, which divides different sample as all the volatile compounds.

### 3.3. Concentrations of Phenolic Compounds, Organic Acids, and Monosaccharides.

The common polyphenolic compounds, monosaccharides, and the organic acids were quantified by HPLC, and the results were showed in Table 4. Concentrations of total acidity, total polyphenols concentration, the total sugar, and other index related to sensory were also detected and are shown in Table 5. As shown in Tables 4 and 5, for concentrations of each phenolic compound, organic acid, and monosaccharide, there were significant difference among different samples, and there were also no significant rules in each of the two groups by marketing price.

According to Table 4, four monosaccharides and alcohol including, fructose, glucose, sucrose, maltose, and glycerol were quantified, and they are responsible for the sweetness of wine, especially, glycerol also contributes positively to the



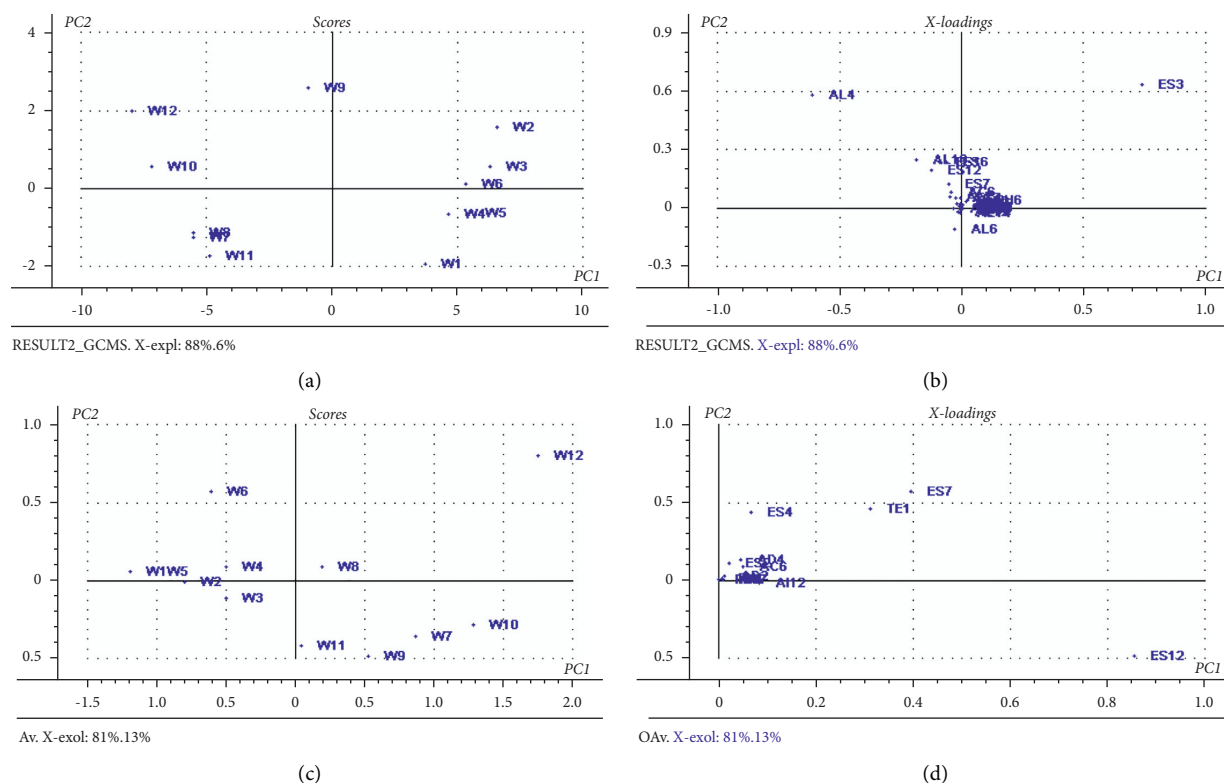


FIGURE 1: (a) Score plot (PCA) for all aroma variation among wine samples which were W1 to W6 belonging to lower marketing price group and W7 to W12 belonging to higher marketing price group. (b) The loading plot (PCA) for all aroma compounds which explains 88% of on the horizontal axis (PC1) and 6% on the vertical axis (PC2). (c) Score plot (PCA) for 14 aroma variation with OAV > 1 among the wine samples (W1–W12). (d) The loading plot (PCA) for all aroma compounds with OAV > 1 which explains 81% of on the horizontal axis (PC1) and 13% on the vertical axis (PC2).

quality of wine by providing wine mellow and sweetness [15]. The content of glycerol showed a higher level ranging from 374.29 to 8255.88 mg/L and concentration of fructose ranged from 750.26 to 1420.43 mg/L, while the concentration of glucose ranged from 116.47 to 898.13 mg/L. Sucrose and maltose were not detected in wine samples.

Polyphenolic compounds are responsible for bitterness, astringency, and the color of red wines and will change as wine ages [16]. Eight polyphenolic compounds were quantified. Among them, the concentration of gallic acid kept a highest level in all the wine samples, which was from 27.11 to 94.37 mg/L. After gallic acid, (+)-catechin ranked the second one, whose concentration ranged from 9.49 to 31.60 mg/L. Then (–)-epicatechin concentration was from 1.57 to 14.59 mg/L, and concentrations varied greatly in different samples. Trans-ferulic acid ranged from 2.12 to 6.08 mg/L. As most researchers have reported previously, trans-ferulic acid has not been found [17]. Moreover, other compounds with a lower level in wine samples are listed in Table 3.

Both the phenols and organic acid compounds have been proved to link to health benefits. Organic acids were another kind of compounds which should be paid attention to. Tartaric acid (144.16–369.12 mg/L) and lactic acid (224.95–561.67 mg/L) almost kept the same level. The concentration ranged from 6.10 to 721.23 mg/L for malic acid, 23.54 to 87.60 mg/L for L(+)-Ascorbic acid,

7.43–878.29 mg/L for acetic acid, 16.99–29.33 mg/L for citric acid but it was not detected in four samples, 18.38 to 403.56 mg/L for succinic acid.

Table 5 shows the total acidity concentration ranged from 4547.55 to 6299.48 mg/L, the total polyphenol concentration ranged from 1297.95 to 2972.82 mg/L, and polyphenols are not only main contributors to the antioxidant properties of red and white wines but also the main reasons for the wine having astringency and bitterness [18, 19]. The total sugars concentration ranged from 3009.21 to 4865.12 mg/L and the total reducing sugars concentration was from 1458.21 to 3075.73 mg/L.

Moreover alcohol content was one of the most important index given also in Table 5 due to its great influence on wine color and the stability of tartaric acid and polyphenolic compounds, and it greatly affects mouth-feel [20]. Alcohol content in samples was from 11.00 to 13.00% (v/v), and there were no special significant difference from each other.

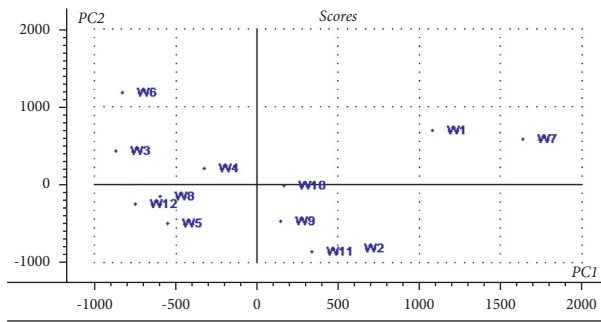
**3.4. Statistical Analysis of Monosaccharides, Phenolic Compounds, and Organic Acids in Wine Samples.** In order to know whether or not the compounds related to tasting follow the same separated principle and to reveal the relationship between those and samples with different marketing price, these composition data and total content data

TABLE 4: Concentration (mg/L) of the monosaccharide compounds, the phenolic compounds, and organic acids in wines determined by HPLC analysis, as well as, their retention time (RT) and correlation coefficient ( $R^2$ ) were also given. The recovery ratio of all the standards dealt with as the same conditions reached over 96%, and the recovery ratio of wine with adding standards on the same conditions range from 95.5% to 103.4%.

Compounds	RT (min)	$R^2$	Concentration											
			W1	W2	W3	W4	W5	W6	W7	W8	W9	W10	W11	W12
Monosaccharides (mg/L)														
Fructose	8.39	0.996	1072.08e	1261.90cd	968.36f	1420.43a	750.26h	1081.43e	1311.45bc	1223.53d	1220.52d	1221.90d	1333.35b	893.90g
Glucose	9.61	0.994	611.33d	898.13a	631.11d	706.38c	752.62b	340.37e	710.63c	116.47f	640.75d	120.65f	687.75c	714.88c
Sucrose	13.17	0.992	0.00a	0.00a	0.00a	0.00a	0.00a	0.00a	0.00a	0.00a	0.00a	0.00a	0.00a	0.00a
Maltose	15.52	0.997	0.00a	0.00a	0.00a	0.00a	0.00a	0.00a	0.00a	0.00a	0.00a	0.00a	0.00a	0.00a
Phenolic compounds (mg/L)														
Gallic acid	7.36	0.999	72.78e	27.11j	56.51gh	76.55d	57.73g	91.22b	82.27c	62.26f	94.37a	53.76h	33.17j	43.01i
(+)-catechin	12.02	0.999	18.89d	4.84h	3.90i	31.60a	3.20i	26.37b	24.05c	11.39f	17.23e	17.22e	16.99e	9.49g
(-)-Epicatechin	13.67	0.999	9.87c	1.57i	5.56f	14.23a	5.33f	14.59a	13.23b	4.62g	9.08d	9.13d	8.16e	2.62h
p-Coumaric acid	18.26	0.999	9.43a	3.62f	5.37e	3.62f	3.00f	8.06b	7.18c	9.44a	6.90c	7.28c	2.44g	6.02
Trans-ferulic acid	19.58	0.999	5.14b	2.12h	1.78i	3.83e	3.00j	3.39f	3.14g	3.95e	4.45c	6.08a	5.05b	4.12d
Rrans-resveratrol	26.32	0.999	0.54a	0.00h	0.22f	0.16g	0.24ef	0.55a	0.48bc	0.47c	0.36d	0.50b	0.25e	0.14g
Quercetin	30.12	0.998	0.53f	0.00h	0.52f	0.77d	0.00h	1.17c	1.39b	0.28g	0.00h	1.14c	0.71e	2.31a
Organic acids (g/L)														
Tartaric acid	3.89	0.999	224.66g	191.53h	279.00de	276.15e	144.16i	327.80b	315.30c	282.32d	143.04i	237.85f	220.30g	369.12a
Malic acid	5.21	1.000	12.18e	679.62b	10.13e	69.93d	6.10e	15.04e	303.44c	753.45a	18.61e	721.23ab	759.70a	9.48e
(+)-ascorbic acid	5.86	0.998	23.54e	0.00f	23.66e	23.47e	23.59e	23.85e	57.18d	87.60b	23.52e	92.22a	80.07c	23.63e
Lactic acid	6.78	1.000	486.05bc	0.00f	374.10d	341.34d	224.95e	453.76c	344.55d	484.93bc	468.53c	561.67a	369.09d	245.45e
Acetic acid	7.62	0.999	749.64b	0.00h	727.40bc	698.76d	448.57f	878.29a	20.00gh	0.00h	712.54cd	7.43h	0.00h	629.89e
Citric acid	9.02	1.000	0.00h	19.53d	0.00h	28.01b	13.99f	0.00h	25.52c	29.33a	0.00h	0.00h	16.99e	0.00h
Succinic acid	12.63	0.997	279.17cd	0.00g	341.86b	72.86e	269.08d	403.56a	0.00g	20.39f	0.00g	18.38f	22.71f	282.31c
Alcohol (mg/L)														
Glycerol	5.51	0.988	1937.84ef	2959.08b	2906.19b	1281.41gh	507.76i	2059.93e	2523.9d	374.29i	8255.88a	1356.29g	2698.46c	1148.06h

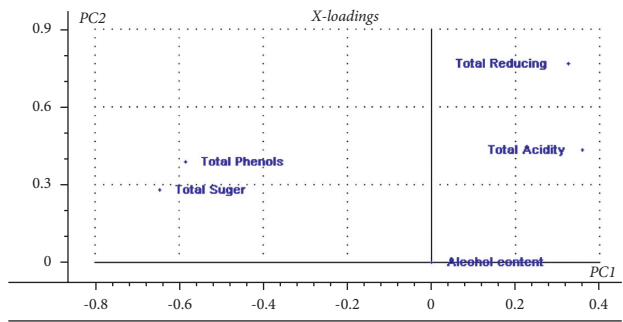
TABLE 5: Concentrations of the total acidity, the total phenols, and some other index related to sensory. Each analysis was performed in triplicate.

Parameter	Concentration (g/L)±ΔS											
	W1	W2	W3	W4	W5	W6	W7	W8	W9	W10	W11	W12
Total acidity	5.59cd	5.14efg	5.553.98cd	5.66c	4.65h	5.33defg	6.29a	5.06g	5.29defg	5.96b	5.03g	4.54h
Total phenols	2.06cd	1.56e	2.97a	2.50b	2.14c	2.92a	1.29f	2.61b	1.99d	2.14c	1.50e	2.62b
Total sugars	3.00f	3.20f	4.50b	4.16c	4.17c	4.86a	3.12f	4.06c	3.56e	3.81d	3.52e	4.08c
Total reducing sugars	3.07a	1.52ef	1.74c	1.76c	1.57de	2.74b	2.87b	1.60de	1.55def	1.61de	1.45fg	1.76c
Alcohol strength (% vol)	12.00ab	12.00ab	12.50a	12.50a	12.50a	12.50a	12.00ab	12.00ab	12.00ab	13.00a	12.00ab	11.00b



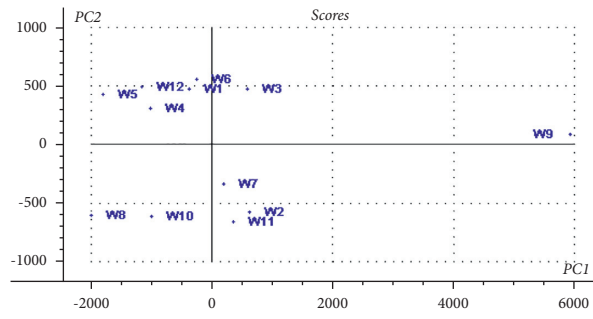
RESULT3. X-expl: 53%.33%

(a)



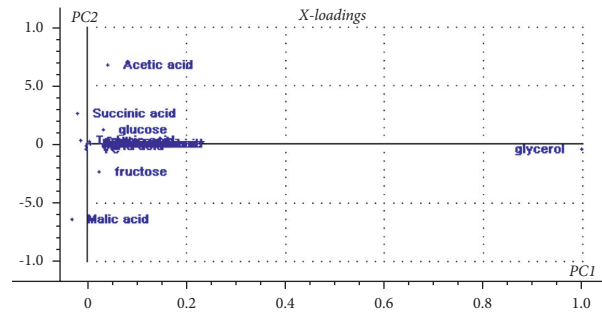
RESULT3. X-expl: 53%.33%

(b)



compounds-19. X-expl: 92%.6%

(c)



compounds-19. X-expl: 92%.6%

(d)

FIGURE 2: (a) Score plot (PCA) for monosaccharides, phenolic compounds, and organic acids variation among wine samples which were W1 to W6 belonging to lower marketing price group and W7 to W12 belonging to higher marketing price group. (b) The loading plot (PCA) for monosaccharides, phenolic compounds, and organic acids which explains 92% of on the horizontal axis (PC1) and 6% on the vertical axis (PC2). (c) Score plot (PCA) for total content of polyphenol, sugar, reduce sugar, acids, alcohol variation among the wine samples (W1–W12). (d) The loading plot (PCA) for total content of polyphenol, sugar, acids, alcohol variation which explains 53% of on the horizontal axis (PC1) and 33% on the vertical axis (PC2).

in Tables 4 and 5 were also analysed by PCA. Results are shown in Figure 2.

As shown in Figures 2(a) and 2(b), the 2D graphical representation of PCA contains 88% of total contents of polyphenol, sugar, sugar, acids, and alcohol variance in the data set. Wine samples were also classified into two categories according to PC1, the samples on the left side of the PCA score plot were Samples 3, 4, 5, 6, sample 8, and sample 12 which most of them belonged to Class 1 except Samples 8 and sample 12, while the samples on the right belonged to Class 2 except sample 1, sample 2. The samples could not be totally separated by marketing price areas. However, samples W1, W3, W4, and W6 were held together according to PC2, the sample 2, sample 5, sample 8, sample 9, sample 10, sample 11 and sample 12 were gathered. The loading plot

showed total reducing sugar and total acidity played a positive role to divide the samples on the right side of its score plot and total phenols and total sugar made positive contributions on the samples on the left side of its score plot shown as Figures 2(a) and 2(b).

In Figures 2(c) and 2(d), the scores scatter plot of PCA accounted 98% of the total variance in the data set. The corresponding loading showed the relative importance of each compounds to each sample. Figure 2(c) shows samples W2, W3, W7, W9, and W11 were on the right held together, and the rest samples were held together according to PC1. However, samples W1, W3, W4, W5, W6, W9, and W12 were cluster to one group according to PC2. Corresponding to the scores scatter plot, Figure 2(d) shows the variability of new group including samples W1, W3, W4, W5, W6, W9,

and W12 derived mostly from acetic acid (abscissa value: 0.0398; ordinate value: 0.6707), and to a lesser extent, succinic acid (abscissa value:  $-0.0203$ ; ordinate value: 0.2592) and the second lesser extent, glucose (abscissa value: 0.0315; ordinate value: 0.1207). while glycerol (abscissa value: 0.9976; ordinate value:  $-0.0416$ ), fructose (abscissa value: 0.0223; ordinate value:  $-0.2395$ ), malic acid (abscissa value:  $-0.0317$ ; ordinate value:  $-0.6376$ ) most influenced successively another group combining with W2, W7, W8, W10 and W11.

Hence, it can be concluded that there are intercommunity and difference for tasting index belonging to the same marketing price area. The samples belonging to the same marketing price area cannot totally cluster to one group by monosaccharides, phenolic compounds, and organic acids or concentrations of total acidity, total polyphenols, the total sugar, total reducing sugar, and the alcohol content. However, it found that the present of acetic acid, succinic acid, and glucose appears to be the characteristic for most of samples in the lower marketing price area and glycerol, fructose, malic acid were the feature of most of samples in the higher marketing price area. Total acid and the total polyphenol have the mostly influence on different samples with different marketing price on tasting.

#### 4. Conclusions

The purpose of this paper is to find the relationship between aroma, tasty component properties, and marketing price. In this paper, 59 compounds were detected and quantified in 12 samples with different marketing prices by GC-MS. Five monosaccharides and 7 phenolic compounds and 7 organic acids were detected and quantified by HPLC. Principal component analysis (PCA) was used to reveal the relationship among wine samples with different marketing prices on all detected aroma compounds, aroma compounds with  $OAV > 1$ , and the total content related to tasting monosaccharides, phenolic compounds, and organic acids. One-way ANOVA was carried out to find the significant differences for phenolic compounds, organic acids, monosaccharides, and concentrations of total acidity, total polyphenols, total sugars, total reducing sugars, and alcohol content.

Principal component analysis for aroma compounds showed the main difference between the Class 1 and Class 2 is the fermentation and ripening aromas, which are represented by higher alcohols, ethyl, and acetic esters. For instance, 3-methyl-1-butanol, 3-ethyl-1-butanol, isopentyl formate, and ethyl lactate. According to Cabernet sauvignon varietal wines, as well as representatives of grape varietal aromas, for example, terpenes and DL-limonene, the high level of esters and acids were the feature of the wine samples with a higher marketing price. Moreover, samples in Class 1 including W1–W6 belonging to marketing price area 39–79RMB and samples in Class 2 including W7–W12 belonging to marketing price area 188 to 258 RMB can be totally clustered into their own marketing price area by volatile compounds or aroma compounds with  $OAV > 1$ .

PCA for concentrations of phenolic compounds, organic acids, and monosaccharides revealed acetic acid, succinic acid, and glucose made a great contribution to most of the wine samples in Class 1 and glycerol, fructose, malic acid, was the feature of most of the wine samples in Class 2. Concentrations of total acidity, total polyphenols, total sugars, total reducing sugars, and alcohol content seemed to have no significant distinguishing ability on different samples belonging to different marketing price areas.

#### Data Availability

The data used to support the findings of this study are available from the corresponding author and co-corresponding author upon request.

#### Conflicts of Interest

The authors declare that there are no conflicts of interest.

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