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Research Article

Characteristic Flavor Substances of Guizhou Black Tea and the Environmental Factors Influencing Their Formation Using Stable Isotopes and Headspace Gas Chromatography-Ion Mobility Spectrometry

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Guizhou is one of the most important black tea producing areas in China. The purpose of this study was to explore the characteristic flavor compounds of Guizhou black tea and investigate the influence of environmental factors on the formation of black tea flavor components. In this study, HS-GC-IMS was used to identify 143 compounds from black tea samples. OPLS-DA was employed to analyze the data, effectively distinguishing black tea from different origins. A total of 83 significant flavor compounds were selected as potential markers using the VIP variable selection method and OAV screening. Cluster analysis was used to identify the characteristic flavor compounds in black tea samples from different origins. In addition, by investigating the climate environment of various production regions and analyzing the volatile components along with stable C and N isotope ratios of samples, it was discovered that the development of volatile components in black tea could be significantly influenced by ambient temperature and light. In regions with higher temperatures, the concentration of volatile components with floral, fruity, and sweet aromas is higher, resulting in a more intense aroma in black tea. In regions with low ambient temperatures but strong sunlight, black tea contains higher levels of components that give it a fresh and nutty aroma. As a result, the aroma of black tea is relatively elegant and fresh. At the same time, it was found that the stable isotope ratios of C and N in black tea were also significantly affected by ambient temperature and were positively correlated. This study introduces a fresh perspective for the comprehensive examination of Guizhou black tea, offering theoretical guidance for optimizing planting conditions and enhancing product quality. Its positive influence on promoting the development of the Guizhou black tea industry is noteworthy.

1. Introduction

Tea is among the most consumed beverages worldwide [1]. Tea contains many healthy active ingredients, such as polyphenols, caffeine, theanine, and theaflavins [2, 3]. According to the Food and Agriculture Organization of the United Nations statistics (FAOSTAT) database (https://www.fao.org/faostat/), China is one of the world's largest tea producers and consumers, with a large production and market share of black tea. Guizhou Province is also among the major black tea-producing areas in China. In 2022, tea plantations in Guizhou covered an area of more than 4,666 square kilometers, with an output value of 57.09 billion Chinese yuan.

Tea's flavor is the most important determinant of its quality. Flavor refers to tea taste and aroma, with volatile organic compounds (VOCs) being significant contributors to its characteristic flavor. The aroma of tea is predominantly made up of volatile flavor compounds [4]. Plant volatiles are mainly divided into terpenoids (with floral, fruity aroma), fatty acid metabolic compounds (alcohols, ketones, aldehydes, etc., with sweet aroma), and phenylalanine/aromatic

cyclic metabolic compounds (including volatile phenylpropanoids and aromatic compounds with floral, nutty aroma) [1, 5]. The terpenoids are synthesized primarily through the methylerythritol-4-phosphate (MEP) or mevalonate (MVA) pathways. Fatty acid metabolic compounds are primarily synthesized through the degradation of the unsaturated C18 fatty acids linolenic and linoleic acid in the lipoxygenase (LOX) pathway [6]. Phenylalanine/aromatic cyclic metabolites are primarily synthesized through the shikimic acid pathway [7]. At present, it has been found that the synthesis pathways of the above volatile components will be affected by external environmental factors.

Ion mobility spectroscopy (IMS) is a highly effective and sensitive analytical technique based on ion mobility differences in the gas phase under a constant electric field. In addition, headspace-gas chromatography ion mobility spectrometry (HS-GC-IMS) combines the advantages of high resolution provided by gas chromatography and high sensitivity provided by ion transfer spectrometry [8–11] to rapidly detect trace VOCs in samples without requiring a sample pretreatment. Currently, HS-GC-IMS has been widely used in the detection of volatile components such as fruit juices [9], peppers [4], huajiao [12], green tea [13], and other foods.

In recent years, stable isotope technology has emerged as an excellent novel method for origin identification and has been widely utilized in various fields such as soil science, medicine, agriculture, biology, ecology, and environmental studies. The isotopic fractionation effect is influenced by various factors, including altitude, soil composition, water sources, topography, and atmospheric composition. These factors lead to variations in isotope ratios among organisms in different regions, contributing to distinct regional profiles in isotope ratios. Therefore, the detection of the isotope composition of organisms can reflect their growth environment and their characteristics as a result of adaptation to environmental changes. Moreover, since the stable isotope composition in living organisms is an intrinsic property that is not affected during processing or storage [14], stable isotope technology has also been used to identify tea-producing areas [15–18].

Numerous studies have been conducted on the identification and characterization of volatile compounds in tea to explore the mechanism of pleasurable aroma formation and reveal the relationship between tea metabolite composition and aroma production [10, 19–21]. However, there are few studies on the relationship between the volatile components of tea and environmental factors. In this study, HS-GC-IMS was used to analyze the characteristic flavor components of black tea and to investigate the key flavor components of black tea from various regions. According to the characteristics that the synthesis of volatile components and isotopic composition of plants are affected by natural factors in the plant environment, the influence of environmental factors on the unique flavor components of Guizhou black tea and the relationship between the isotopic composition and environmental factors were innovatively determined by the ratio of C and N stable isotopes in black tea samples. It is hoped that a correlation model can be established between the formation of Guizhou black tea flavor and environmental factors. This would provide a new research direction for the comprehensive study of Guizhou black tea and offer theoretical guidance for the future development of the black tea industry.

2. Materials and Methods

2.1. Samples. All black tea samples used in this experiment were collected in the spring of 2022 from four main black tea-producing areas in Guizhou and two main black tea-producing areas outside of Guizhou in China. The samples were collected by picking one bud, one leaf, one bud, and two leaves, and they were processed aseptically to make black tea using Chen's methods [19]. The information on sampling locations is shown in Table 1 and Figure 1.

2.2. Headspace Gas Chromatography-Ion Mobility Spectrometry (HS-GC-IMS)

2.2.1. Instruments and Equipment. The FA2204 Electronic analytical balance was purchased from China, and the Flavor Spec® HS-GC-IMS was purchased from G.A.S. Germany.

2.2.2. HS-GC-IMS Determination Method. Prior to the experiment, the tea samples were processed as described previously with minor modifications [13, 22]. Accordingly, an HS-GC-IMS FlavourSpec® (GAS mbH, Dortmund, Germany) instrument was utilized for the study. About 1 g of samples was injected into a 20 mL headspace vial and incubated for 20 min at 85°C. Subsequently, 500 μL of headspace gas was automatically collected with a heated syringe (85°C) and was injected into the HS-GC-IMS for analysis. The samples were then carried into the capillary column (FS-SE-54-CB-1, 15 m × 0.53 mm, 60°C) by nitrogen (purity ≥99.999%) using the following flow procedure: initial flow rate was maintained at 2 mL/min for 2 min, increased to 10 mL/min at 10 min, then 100 mL/min at 20 min, and finally 150 mL/min at 30 min. After preseparation, analytes were ionized in positive ion mode using a 3H ionization source located in the ion mobility spectrometer ionization chamber and then transferred to the drift tube at 45°C under the drift gas (nitrogen, purity ≥99.999%) at 150 mL/min. The drift tube length was 98 mm, and its linear voltage was 500 V/cm. Volatile compounds were identified by comparing retention indices (RIs) and were then compared with the data obtained from the NIST17 mass spectral library and the IMS database (GAS mbH, Dortmund, Germany).

2.2.3. HS-GC-IMS Result Analysis. The VOC analysis software was used to inspect the analytical spectrogram to determine the retention and migration time for qualitative analysis. The internal standard method was used to calculate the substance content, and the content calculation formula is as follows:

$$C_s = \frac{(A_i \times C_i)}{A_s}, \quad (1)$$

Table 1: Sample information.

Samples	Place of collection
WY	Wuyishan City, Fujian Province
BS	Baoshan City, Yunnan Province
GZZY	Zunyi City, Guizhou Province
GZAS	Anshun City, Guizhou Province
GZPA	Puan County, Guizhou Province
GZDY	Duyun City, Guizhou Province

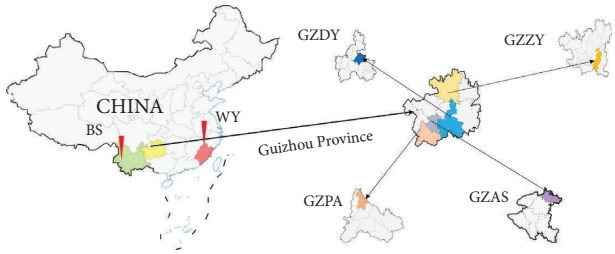


Figure 1: Sample collection locations.

where C_s is the concentration of volatile substances, C_i is the concentration of standard substances, A_s is the peak area of volatile substances, and A_i is the peak area of standard substances.

In addition, the HS-GC-IMS Library Search software was compared with the NIST and IMS databases for qualitative analysis of characteristic flavor compounds. The 3D difference map, 2D overhead difference map, and fingerprint map of VOCs were constructed using Reporter and Gallery Plot. Orthogonal Partial Least Squares Discriminant Analysis (OPLS-DA) and Partial Least Squares Discriminant Analysis (PLS-DA) were used to analyze the differences between the sample groups. The key flavor substances were selected by calculating the volatile component VIP value and odor activity value (OAV) value.

2.3. Stable Isotope Analysis

2.3.1. Instruments and Equipment. The XP6 electronic balance was purchased from Mettler-Toledo International Inc in Switzerland; the DI/CF-MAT253 gas isotope ratio mass spectrometer was purchased from Thermo Fisher Scientific; and the YXQM-0.4L planetary ball mill was purchased from MITR in China.

2.3.2. Measurements of C and N Element Content and Their Stable Isotope Ratios. Tea samples were crushed with a ball mill and sieved through a 100-mesh screen prior to the experiment. Approximately 1 mg from each tea sample was weighed and transferred to a 3.5 × 5 mm pressed tin capsule. The samples were placed sequentially into the automatic solid sample tray of the element analyzer. After reduction resulting from combustion, the carbon and nitrogen elements in the samples were converted into pure CO_2 and N_2 gas. Then, the isotope ratio mass spectrometer was used for the detection of isotope composition.

The δ-value (‰) was determined by comparing the isotope value of the examined sample to internationally accepted standard materials. The isotopic values were expressed according to the following formula:

$$\delta‰ = \left[\left(R_{sample}/R_{standard}\right)\text{-}1\right] \times 1000, \quad (2)$$

where R_{sample} and $R_{standard}$ are the isotopic ratios of the sample and the standard materials, respectively. Isotope standards IAEA-CH-3 and IAEA-N1 were used for the $\delta^{13}C$ and $\delta^{15}N$ calibration.

2.3.3. Meteorological Information Collection. GPS was used to locate and record the sampling locations' longitude, latitude, and altitude. Moreover, the China Meteorological Science Data Center was queried for the average annual precipitation, average high temperature, average low temperature, and number of sunny days.

2.3.4. Data Analysis. The correlation model between the carbon and nitrogen isotope ratios and environmental factors was established by the partial least squares (PLS) method. The least squares method is a commonly implemented method in unitary linear regression analysis. It minimizes the sum of the squared errors between the observed and predicted values, generating a best-fitting line to obtain the functional relationship between the independent variable and the dependent variable. A quantitative prediction model was established to assess the relationship between carbon and nitrogen isotope ratios and environmental factors, using 8 environmental factors as independent variables and each stable isotope ratio as dependent variables. The model included 18 samples, of which 16 were randomly selected and used as the training set and 2 as the prediction sets. The model results were expressed in terms of coefficient of determination (R), root mean square error (RMSE), and relative prediction deviation (RPD) for all samples (where RPD = DS/RMSE).

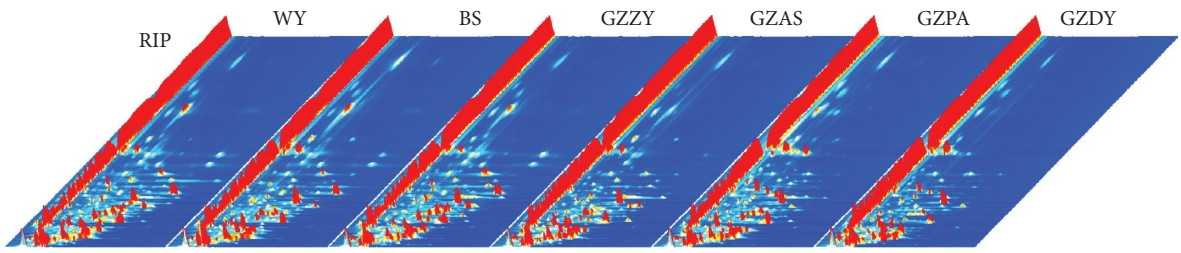
The box diagrams and bar diagrams were created using the Origin 2021 software. OPLS-DA was conducted on the SIMCA 14.1 program, and VIP value, partial least squares, and PLS analysis were performed on XLSTAT.

3. Results and Discussion

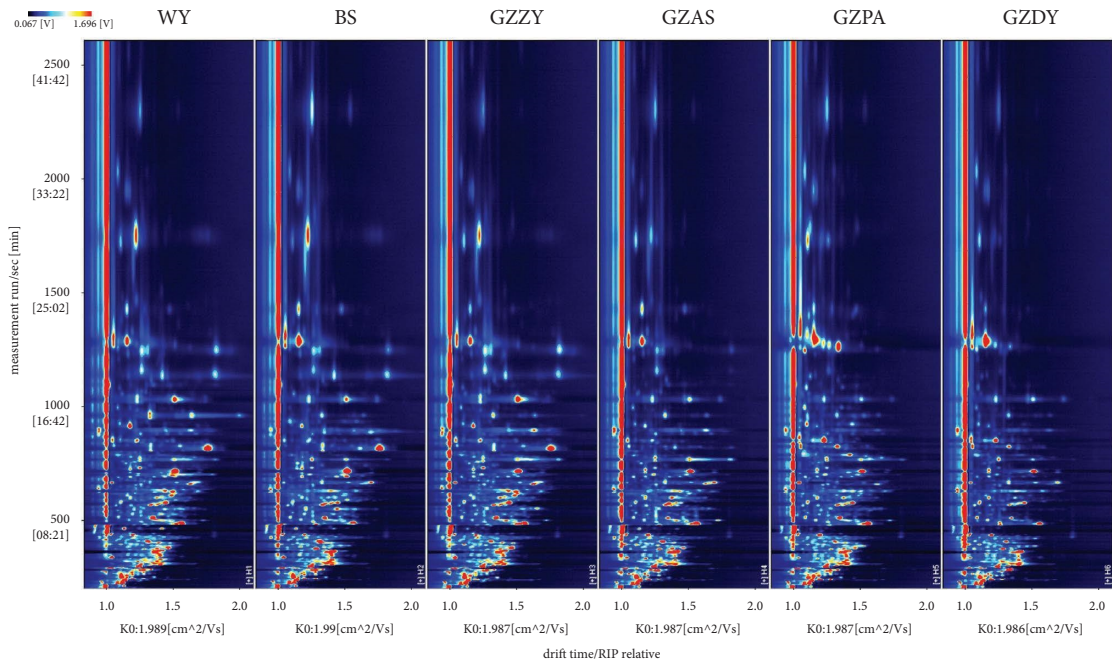
3.1. Black Tea Volatile Flavor Compounds

3.1.1. Analysis of Volatile Compounds of Black Tea Samples from Different Regions by HS-GC-IMS. The volatile flavor compounds in 4 black tea samples from different regions in Guizhou and 2 black tea samples from regions outside of Guizhou were determined by GC-IMS. Using the Reporter plug-in of the included VOC analysis software, the volatile compounds of black tea from different regions were compared, and the results are shown in Figure 2.

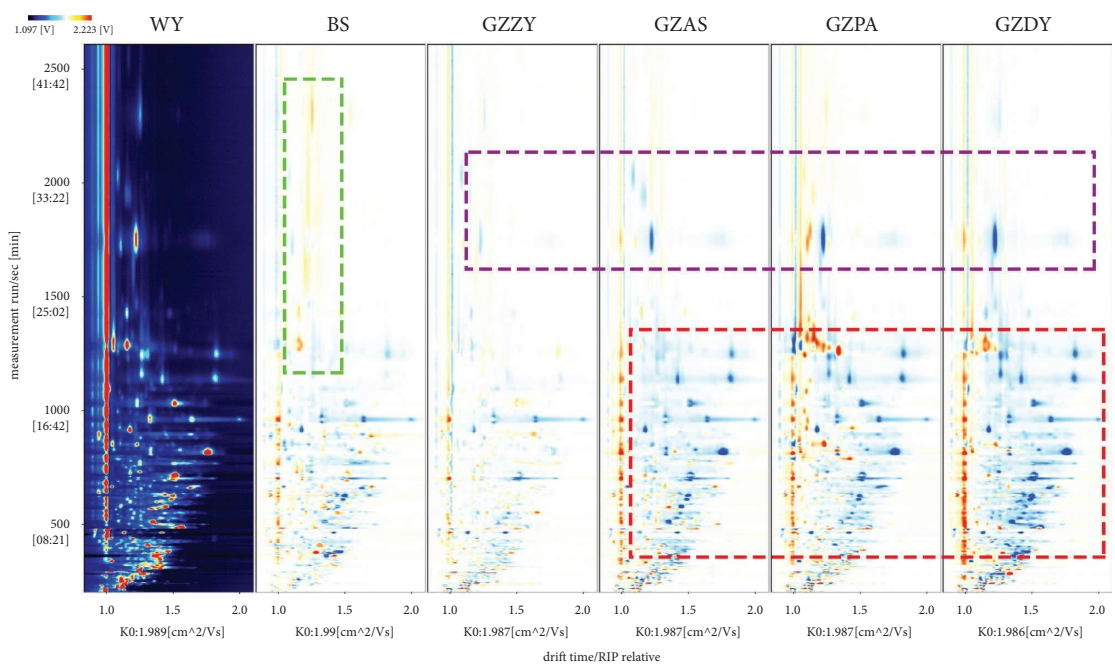
The GC-IMS 3D spectra of black tea samples from 6 regions are shown in Figure 2(a). The variation in volatile compounds across different samples is clearly visible in the figure. The top view of the 2D GC-IMS diagram of black tea samples from 6 regions is shown in Figure 2(b). The background of the image is blue, with the vertical axis representing the retention time (s) of gas chromatography, and the horizontal axis representing the ion migration time.



(a)



(b)



(c)

Figure 2: GC-IMS results of black tea from different regions.

The red vertical line at 1.0 on the horizontal axis indicates the reaction ion peak (RIP). Both the migration time and RIP were normalized. Each peak on the left and right sides of the RIP corresponds to a volatile organic compound, and the color indicates the compound concentration: white indicates a lower concentration, red is a higher concentration, and a darker color corresponds to a greater concentration. As shown in Figure 2(b), most volatile compound signals of the black tea samples from 6 different Guizhou regions were in a retention time range of 0~1750 s and drift time range of 1.0~1.7 s, indicating that the volatile compounds of the black tea samples from different regions were highly similar. However, their content in the different regions was different. For example, the two GZZY samples were similar to WY and BS, while the GZAS, GZPA, and GZDY samples shared a higher similarity. The WY sample was taken as a reference to accentuate the differences, and the signal peak in the reference spectrum was deducted to obtain the differential spectral map between different samples (Figure 2(c)). The background was white after deduction, and red indicated that the corresponding compound content was higher than WY, while a darker color indicated greater differences and a blue color indicated that the corresponding compound content was lower than WY. As shown in Figure 2(c), the volatile compound contents of GZAS, GZPA, and GZDY were significantly different from those of WY and BS (red box in the figure). In contrast, the volatile compound contents of BS, GZZY, and WY were relatively low, with BS and WY still exhibiting some differences (green box in the figure). Finally, the volatile compounds of GZZY and WY samples were very similar. Therefore, overall, the differences between Guizhou tea samples and non-Guizhou tea samples are small (purple box in figure) and cannot be clearly distinguished.

3.1.2. Qualitative and Quantitative Analysis of Volatile Flavor Compounds. To more intuitively assess the changes in the content of volatile compounds in different samples, the retention time and migration time of volatile flavor compounds from samples from different regions were compared, and the HS-GC-IMS migration time data were compared with the NIST database to perform qualitative analysis of volatile compounds. Quantitative analysis was performed using the content calculation formula, and the results are shown in Table 2. A total of 184 volatile compounds were detected in the black tea samples, and 143 volatile compounds (including dimers and monomers) were identification through the database. As shown in Figure 3, there were 30 aldehydes (accounting for 21%~27% of the total volatile compounds), 30 alcohols (16%~24% of the total volatile compounds), 26 ketones (21%~28% of the total volatile compounds), and 21 heterocyclic classes (7%~14% of the total volatile compounds). There were 18 esters (4%–7% of the total volatile compounds), 9 terpenes (1% of the total volatile compounds), 5 acids (11%–21% of the total volatile compounds), and 4 sulfides (2%-3% of the total volatile compounds). The total volatile compound content in the GZZY, BS, and WY samples was higher than that in the other three samples, and the volatile compounds of the WY and GZZY samples were highly similar.

The Gallery Plot plug-in was used to plot the fingerprint spectrum of volatile compounds (Figure 4). Each row in the figure represents all the signal peaks identified in a sample, and each column represents the signal peaks of the same volatile organic compound in different samples, followed by *M* and *D*, which correspond to the monomers and dimers of the same compounds, and the number indicates the unidentified peaks.

The detailed volatile organic compound information for each sample and the differences in volatile content between samples are shown in Figure 4. Volatile compounds that were present in high amounts (in mg/kg) across all samples were as follows: Acetic acid (15.37~30.05 mg/kg), Linalool (2.44~15.53 mg/kg), 2-Octanone (0.59~12.60 mg/kg), (E)-2-Hexenal (6.57~10.57 mg/kg), Furfural (0.79~9.83 mg/kg), (Z)-3-Hexenol (2.90~7.46 mg/kg), 1-Hydroxy-2-propanone (2.19~7.28 mg/kg), Acetone (3.97~6.97 mg/kg), Hexanal (5.29~6.61 mg/kg), 4-Methyl-3-penten-2-one (2.37~6.42 mg/kg), Linalool oxide (0.64~6.13 mg/kg), 1-Penten-3-ol (4.91~5.93 mg/kg), 2-Butanone (4.10~5.71 mg/kg), Dimethyl sulfide (3.57~5.11 mg/kg), 1-Pentanol (2.44 to 4.60 mg/kg), and Propanal (3.48~3.93 mg/kg). Among these compounds, Linalool, (E)-2-Hexenal, (Z)-3-Hexenol, Hexanal, Linalool oxide, and 1-Pentanol have been shown to be the main aroma compounds in black tea [19, 20, 25–30].

The types of volatile flavor compounds identified in the black tea from different regions or varieties were similar. However, they differed in relative abundance in the different samples (i.e., compounds that were only present in high amounts in a specific sample but very low or no amounts in other samples). For example, the characteristic compounds in the WY sample are 22, Dimethyl disulfide, Myrcene, 5-Methyl-3-heptanone, 6-Methyl-5-hepten-2-one, 2-Propanol, and 1-Hexano1-D. The distinct compounds in the BS samples were 33, 34, 35, and 36 and included Pyrrolidine, beta-Pinene, Diacetyl, 1-Penten-3-one-D, cis-4-Heptenal, Benzaldehyde, and Phenylacetaldehyde. The compounds characteristic of the GZZY sample are 12, Linalool oxide, 4-Methyl-2-pentanone, 3-Methyl-2-pentanone, 4-Methyl-3-penten-2-one, 2-Hexanone, Ethyl pentanoate-D, 1-Propanethiol, and 4-Methy1-1 pentanol. The characteristic compounds in the GZAS sample were Ethyl isobutyrate, 1-Octen-3-one, Camphene, Heptanal-D, and Octanal. The characteristic compounds in the GZPA samples are 1, 4, 26, 27, Styrene, o-Xylene, 2-acetylfuran, 2-Methylpyrazine, 2-acety1-1 pyrroline, 2, 3-dimethylpyrazine, Pyridine, 3-Ethylpyridine, 5-Methyl-2-furfural, Propanoic acid, 2-Methylpropanoic acid, 2-Cyclohexen-1-one, 5-Methyl-2 (3H)-furanone, Methyl acetate, (Z)-3-Hexenyl propionate, and 3-Methyl-3-buten-1-ol. The distinct compounds in the GZDY sample were 10, 39, 40, and Ethyl acetate.

3.1.3. Analysis of Volatile Aroma Compounds in Black Tea with OPLS-DA. OPLS-DA is a supervised discriminant analysis statistical method that can establish a relationship model between the samples and their volatile compound abundance to categorize them. The model evaluation parameters were the independent variable fit index (*R2X*),

Table 2: Sample volatile composition.

Category	Number	Compound	CAS#	Formula	MW	RI	Rt (sec)	Dt (RIPrel)	Odor description	WY	BS	GZZY	GZAS	GZPA	GZDY
Acid	1	2-Methylpropanoic acid	79-31-2	$C_4H_8O_2$	88.1	1697.5	1951.345	1.15266	Burnt, butter, cheese, sweat	1.19 ± 0.14^{bc}	1.32 ± 0.08^{b}	0.91 ± 0.08^{d}	0.56 ± 0.04^{e}	1.73 ± 0.08^{a}	1.11 ± 0.1^{c}
Acid	2	Acetic acid-D	64-19-7	$C_2H_4O_2$	60.1	1504.7	1284.11	1.15619	Acid, fruit, pungent, sour, vinegar	7.65 ± 0.27^{d}	11.85 ± 1.01^{c}	7.55 ± 0.75^{d}	7.58 ± 0.21^{d}	15.14 ± 0.49^{b}	17.32 ± 0.63^{a}
Acid	3	Acetic acid-M	64-19-7	$C_2H_4O_2$	60.1	1505.3	1285.78	1.05804	Acid, fruit, pungent, sour, vinegar	8.33 ± 0.07^{d}	10.01 ± 0.44^{b}	8.79 ± 0.31^{d}	9.51 ± 0.14^{c}	9.43 ± 0.3^{c}	12 ± 0.05^{a}
Acid	4	Propanoic acid-D	79-09-4	$C_3H_6O_2$	74.1	1642	1729.802	1.26584	Fat, fruit, pungent, silage, soy	0.47 ± 0.01^{b}	0.33 ± 0.03^{cd}	0.52 ± 0.02^{b}	0.37 ± 0.02^{c}	0.98 ± 0.03^{a}	0.29 ± 0.04^{d}
Acid	5	Propanoic acid-M	79-09-4	$C_3H_6O_2$	74.1	1641.6	1728.11	1.11074	Fat, fruit, pungent, silage, soy	2.28 ± 0.06^{d}	1.46 ± 0.09^{e}	2.66 ± 0.16^{c}	2.8 ± 0.19^{ab}	5.28 ± 0.14^{a}	2.98 ± 0.28^{b}
Alcohols	6	(Z)-3-Hexenol-D	928-96-1	$C_6H_{12}O$	100.2	1404.8	1033.73	1.51285	Grass, green fruit, green leaf, herb, unripe banana	3.71 ± 0.12^{b}	2.77 ± 0.01^{c}	5.08 ± 0.04^{a}	1.84 ± 0.05^{d}	1.29 ± 0.02^{f}	1.56 ± 0.04^{e}
Alcohols	7	(Z)-3-Hexenol-M	928-96-1	$C_6H_{12}O$	100.2	1404.2	1032.52	1.23471	Grass, green fruit, green leaf, herb, unripe banana	2.09 ± 0.11^{b}	2.04 ± 0.03^{b}	2.29 ± 0.05^{a}	1.89 ± 0.01^{c}	1.64 ± 0.03^{d}	1.89 ± 0.02^{c}
Alcohols	8	1-Butanol-D	71-36-3	$C_4H_{10}O$	74.1	1166.3	604.308	1.37934	Fruity	1.02 ± 0.02^{d}	0.47 ± 0.02^{f}	1.39 ± 0.03^{b}	1.52 ± 0.01^{a}	1.09 ± 0.02^{c}	0.53 ± 0.02^{e}
Alcohols	9	1-Butanol-M	71-36-3	$C_4H_{10}O$	74.1	1166	603.685	1.18554	Fruity	0.77 ± 0.02^{e}	0.59 ± 0.02^{f}	0.86 ± 0.01^{d}	1.14 ± 0.02^{a}	1.02 ± 0.02^{b}	0.99 ± 0.02^{c}
Alcohols	10	1-Hexanol-D	111-27-3	$C_6H_{14}O$	102.2	1372	962.71	1.64035	Green, grassy	1.61 ± 0.04^{a}	0.35 ± 0.1^{c}	0.56 ± 0.01^{b}	0.37 ± 0.01^{c}	0.21 ± 0.01^{d}	0.17 ± 0.01^{d}
Alcohols	11	1-Hexanol-M	111-27-3	$C_6H_{14}O$	102.2	1372	962.71	1.33404	Green, grassy	2.38 ± 0.06^{a}	1.34 ± 0.14^{d}	1.85 ± 0^{b}	1.6 ± 0.01^{c}	1.09 ± 0.05^{e}	1.08 ± 0.02^{e}
Alcohols	12	1-Octen-3-ol	3391-86-4	$C_8H_{16}O$	128.2	1487.7	1237.46	1.1669	Cucumber, earth, fat, floral, mushroom	0.51 ± 0.02^{a}	0.53 ± 0.02^{a}	0.39 ± 0.02^{b}	0.32 ± 0.02^{c}	0.26 ± 0^{d}	0.14 ± 0.01^{e}
Alcohols	13	1-Pentanol-D	71-41-0	$C_5H_{12}O$	88.1	1267.6	769.74	1.50845	Balsamic, fruit, green, pungent, yeast	1.85 ± 0.04^{c}	1.35 ± 0.03^{e}	2.46 ± 0.03^{b}	2.59 ± 0.02^{a}	1.75 ± 0.02^{d}	0.85 ± 0.09^{f}
Alcohols	14	1-Pentanol-M	71-41-0	$C_5H_{12}O$	88.1	1268.1	770.47	1.25621	Balsamic, fruit, green, pungent, yeast	1.62 ± 0.03^{e}	1.46 ± 0.01^{f}	1.82 ± 0.04^{c}	1.99 ± 0.02^{a}	1.89 ± 0.04^{b}	1.68 ± 0.03^{d}
Alcohols	15	1-Penten-3-ol-D	616-25-1	$C_5H_{10}O$	86.1	1179.4	631.085	1.35481	Butter-like, pungent	3.51 ± 0.09^{c}	3.32 ± 0.05^{d}	4.07 ± 0.05^{a}	3.73 ± 0.02^{b}	3 ± 0.06^{e}	2.68 ± 0.1^{f}
Alcohols	16	1-Penten-3-ol-M	616-25-1	$C_5H_{10}O$	86.1	1179.9	632.33	0.94636	Butter-like, pungent	1.51 ± 0.04^{e}	2.06 ± 0.02^{c}	1.75 ± 0^{d}	2.18 ± 0.01^{b}	2.11 ± 0.13^{cb}	2.71 ± 0.09^{a}
Alcohols	17	1-Propanethiol	107-03-9	C_3H_8S	76.2	841.4	251.238	1.36193	Cabbage, onion	0.29 ± 0.01^{b}	0.22 ± 0.03^{c}	0.5 ± 0.01^{a}	0.2 ± 0^{c}	0.27 ± 0.01^{b}	0.12 ± 0^{d}
Alcohols	18	1-Propanol-D	71-23-8	C_3H_8O	60.1	1056.8	426.27	1.25264	Alcohol, candy, pungent	0.02 ± 0^{c}	0.03 ± 0^{ab}	0.03 ± 0^{a}	0.02 ± 0^{c}	0.03 ± 0^{a}	0.03 ± 0^{bc}
Alcohols	19	1-Propanol-M	71-23-8	C_3H_8O	60.1	1055.4	424.398	1.11251	Alcohol, candy, pungent	0.3 ± 0^{e}	0.34 ± 0.01^{c}	0.32 ± 0.02^{d}	0.36 ± 0.01^{b}	0.4 ± 0^{a}	0.25 ± 0^{f}
Alcohols	20	2-Butanol	78-92-2	$C_4H_{10}O$	74.1	1041.7	407.55	1.14851	N	0.17 ± 0.01^{e}	0.2 ± 0.01^{d}	0.16 ± 0^{e}	0.23 ± 0.01^{c}	0.26 ± 0^{b}	0.27 ± 0.01^{a}
Alcohols	21	2-Methyl-1-propanol	78-83-1	$C_4H_{10}O$	74.1	1113.4	507.056	1.17464	Apple, bitter, cocoa, wine	0.34 ± 0.01^{f}	0.52 ± 0.03^{d}	0.38 ± 0.01^{e}	0.55 ± 0.02^{c}	0.6 ± 0.01^{b}	0.67 ± 0.01^{e}
Alcohols	22	2-Methylisoborneol	2371-42-8	$C_{11}H_{20}O$	168.3	1671.8	1845.11	1.27805	N	0.46 ± 0.06^{a}	0.51 ± 0.03^{a}	0.46 ± 0.02^{a}	0.26 ± 0.04^{b}	0.17 ± 0.01^{c}	0.32 ± 0.03^{b}
Alcohols	23	2-Propanol	67-63-0	C_3H_8O	60.1	951.4	321.906	1.23079	Floral	0.58 ± 0.02^{a}	0.21 ± 0.01^{e}	0.38 ± 0.01^{b}	0.29 ± 0^{c}	0.27 ± 0^{d}	0.18 ± 0^{f}
Alcohols	24	3-(Methylthio)-1-propanol	505-10-2	$C_4H_{10}OS$	106.2	1803.8	2457.37	1.09841	Earth, garlic, potato, soy	0.83 ± 0.01^{d}	0.94 ± 0.1^{cd}	0.99 ± 0.06^{c}	1 ± 0.09^{c}	1.2 ± 0.02^{b}	1.37 ± 0.07^{a}
Alcohols	25	3-Methyl-1-butanol-D	123-51-3	$C_5H_{12}O$	88.1	1224.4	703.789	1.48669	Burnt, cocoa-like, winey	0.61 ± 0.02^{a}	0.47 ± 0.05^{b}	0.23 ± 0.02^{e}	0.39 ± 0.01^{c}	0.35 ± 0.01^{d}	0.07 ± 0.01^{f}
Alcohols	26	3-Methyl-1-butanol-M	123-51-3	$C_5H_{12}O$	88.1	1224.5	703.94	1.24564	Burnt, cocoa-like, winey	0.43 ± 0.01^{e}	0.59 ± 0.03^{d}	0.63 ± 0.01^{c}	0.83 ± 0.01^{a}	0.75 ± 0.03^{b}	0.38 ± 0.01^{f}
Alcohols	27	3-Methyl-3-buten-1-ol-D	763-32-6	$C_5H_{10}O$	86.1	1284.8	797.543	1.43554	N	0.25 ± 0.01^{b}	0.11 ± 0^{c}	0.23 ± 0^{b}	0.11 ± 0.01^{c}	1.86 ± 0.11^{a}	0.29 ± 0.02^{b}
Alcohols	28	3-Methyl-3-buten-1-ol-M	763-32-6	$C_5H_{10}O$	86.1	1284.8	797.543	1.18599	N	0.19 ± 0.01^{b}	0.2 ± 0.01^{b}	0.2 ± 0.01^{b}	0.05 ± 0.01^{d}	0.23 ± 0.03^{a}	0.13 ± 0.01^{c}
Alcohols	29	4-Methyl-1-pentanol	626-89-1	$C_6H_{14}O$	102.2	1339.3	896.812	1.63176	N	1.24 ± 0.01^{c}	0.62 ± 0.02^{d}	2.42 ± 0.03^{a}	1.41 ± 0.03^{b}	0.47 ± 0.02^{f}	0.53 ± 0.01^{e}
Alcohols	30	cis-2-Penten-1-ol	1576-95-0	$C_5H_{10}O$	86.1	1339.3	896.77	0.94842	Mushroom-like, green, grassy	2.01 ± 0.02^{c}	1.32 ± 0.03^{d}	2.49 ± 0.02^{a}	2.47 ± 0.04^{a}	2.05 ± 0.02^{c}	2.37 ± 0.02^{b}
Alcohols	31	Ethanol	64-17-5	C_2H_6O	46.1	951.4	321.906	1.12793	N	0.83 ± 0.06^{a}	0.48 ± 0.01^{f}	0.63 ± 0.01^{c}	0.77 ± 0.01^{b}	0.54 ± 0.02^{e}	0.75 ± 0.01^{b}
Alcohols	32	Linalool oxide-D	60047-17-8	$C_{10}H_{18}O_2$	170.3	1488.8	1240.573	1.82461	Floral	2.68 ± 0.16^{b}	1.72 ± 0.23^{c}	3.65 ± 0.04^{a}	0.7 ± 0.09^{d}	0.28 ± 0.01^{e}	0.27 ± 0.03^{e}
Alcohols	33	Linalool oxide-M	60047-17-8	$C_{10}H_{18}O_2$	170.3	1487.7	1237.636	1.27169	Floral	2.08 ± 0.04^{b}	1.81 ± 0.09^{c}	2.42 ± 0.07^{a}	1.32 ± 0.07^{d}	0.66 ± 0.02^{e}	0.41 ± 0.03^{f}
Alcohols	34	Linalool-D	78-70-6	$C_{10}H_{18}O$	154.3	1646.1	1745.37	1.69315	Coriander, floral, lavender, lemon, rose	1.69 ± 0.08^{a}	1.59 ± 0.06^{a}	1.33 ± 0^{b}	0.66 ± 0.19^{c}	0.74 ± 0.04^{c}	0.84 ± 0.14^{c}
Alcohols	35	Linalool-M	78-70-6	$C_{10}H_{18}O$	154.3	1645.1	1741.53	1.22912	Coriander, floral, lavender, lemon, rose	12.65 ± 0.63^{a}	13.12 ± 0.71^{a}	12.23 ± 0.96^{a}	5.87 ± 0.72^{b}	2.83 ± 0.54^{c}	1.77 ± 0.11^{c}
Aldehydes	36	(E)-2-Heptenal	18829-55-5	$C_7H_{12}O$	112.2	1338.6	895.50	1.23452	Green, fatty	0.22 ± 0.04^{a}	0.11 ± 0.01^{d}	0.18 ± 0.01^{b}	0.16 ± 0^{cb}	0.14 ± 0.02^{cd}	0.15 ± 0.02^{bc}
Aldehydes	37	(E)-2-Hexenal-D	6728-26-3	$C_6H_{10}O$	98.1	1235.7	720.456	1.51231	N	7.92 ± 0.17^{b}	8.82 ± 0.15^{a}	7.39 ± 0.18^{c}	5.41 ± 0.03^{d}	5.1 ± 0.14^{e}	4.85 ± 0.23^{e}
Aldehydes	38	(E)-2-Hexenal-M	6728-26-3	$C_6H_{10}O$	98.1	1234.5	718.73	1.18153	N	1.19 ± 0.02^{e}	1.58 ± 0.03^{c}	1.53 ± 0.01^{d}	1.68 ± 0.03^{b}	1.57 ± 0.02^{dc}	1.86 ± 0.02^{a}
Aldehydes	39	(E)-2-Nonenal	18829-56-6	$C_9H_{16}O$	140.2	1540.4	1387.41	1.41852	Paper	0.14 ± 0.01^{dc}	0.17 ± 0.02^{b}	0.14 ± 0.02^{d}	0.16 ± 0.01^{dcb}	0.21 ± 0^{a}	0.16 ± 0.01^{cb}
Aldehydes	40	(E)-2-Octenal	2548-87-0	$C_8H_{14}O$	126.2	1440.2	1116.217	1.33973	Dandelion, fat, fruit, grass, green, spice	0.38 ± 0^{b}	0.41 ± 0.01^{b}	0.47 ± 0.03^{a}	0.3 ± 0.02^{c}	0.15 ± 0.01^{d}	0.08 ± 0.01^{e}
Aldehydes	41	(E)-2-Pentenal	1576-87-0	C_5H_8O	84.1	1130.3	536.192	1.11327	Grassy, green	0.09 ± 0^{e}	0.13 ± 0.01^{d}	0.14 ± 0^{c}	0.21 ± 0.01^{a}	0.16 ± 0.01^{b}	0.14 ± 0^{c}

Table 2: Continued.

Category	Number	Compound	CAS#	Formula	MW	RI	Rt (sec)	Dt (RIPrel)	Odor description	WY	BS	GZZY	GZAS	GZPA	GZDY
Aldehydes	42	(E,E)-2,4-Hexadienal	142-83-6	C_6H_8O	96.1	1414.8	1056.549	1.12376	Green	0.22 ± 0.01^{b}	0.37 ± 0.03^{a}	0.24 ± 0.01^{b}	0.21 ± 0.01^{b}	0.22 ± 0.01^{b}	0.14 ± 0.01^{c}
Aldehydes	43	2-Hexenal	505-57-7	$C_6H_{10}O$	98.1	1274.1	780.10	1.17889	N	0.16 ± 0^{b}	0.1 ± 0.01^{c}	0.21 ± 0^{a}	0.04 ± 0^{e}	0.05 ± 0^{e}	0.07 ± 0.01^{d}
Aldehydes	44	2-Methyl-2-pentenal-D	623-36-9	$C_6H_{10}O$	98.1	1170.2	612.292	1.49183	Fruit	1.52 ± 0.13^{a}	0.32 ± 0.02^{b}	1.59 ± 0.05^{a}	0.26 ± 0.01^{b}	0.26 ± 0.02^{b}	0.1 ± 0.02^{c}
Aldehydes	45	2-Methyl-2-pentenal-M	623-36-9	$C_6H_{10}O$	98.1	1170.6	613.026	1.15978	Fruit	0.24 ± 0.01^{b}	0.09 ± 0.01^{f}	0.28 ± 0^{a}	0.15 ± 0^{e}	0.16 ± 0.01^{d}	0.17 ± 0.01^{c}
Aldehydes	46	2-Methylpropanal	78-84-2	C_4H_8O	72.1	833.1	246.558	1.2835	Burnt, caramel, cocoa, green, malt	0.56 ± 0.01^{c}	0.75 ± 0.01^{b}	0.48 ± 0.01^{d}	0.58 ± 0.02^{c}	0.76 ± 0^{b}	0.79 ± 0^{a}
Aldehydes	47	3-Methyl-2-butenal-D	107-86-8	C_5H_8O	84.1	1217.3	693.527	1.36324	Burnt, cocoa-like	0.23 ± 0.02^{a}	0.14 ± 0.01^{b}	0.21 ± 0.01^{a}	0.22 ± 0^{a}	0.22 ± 0^{a}	0.06 ± 0.01^{c}
Aldehydes	48	3-Methyl-2-butenal-M	107-86-8	C_5H_8O	84.1	1217.8	694.266	1.09612	Burnt, cocoa-like	0.19 ± 0^{e}	0.11 ± 0^{f}	0.28 ± 0.01^{c}	0.43 ± 0.01^{a}	0.4 ± 0.01^{b}	0.23 ± 0.01^{d}
Aldehydes	49	3-Methylbutanal	590-86-3	$C_5H_{10}O$	86.1	931.6	307.866	1.40821	N	1.53 ± 0.02^{b}	1.62 ± 0.09^{b}	1.34 ± 0.17^{f}	1.37 ± 0.04^{f}	1.45 ± 0.04^{ef}	1.79 ± 0.01^{a}
Aldehydes	50	Acetaldehyde	75-07-0	C_2H_4O	44.1	767.8	212.862	0.98394	Floral, green apple	1.02 ± 0.02^{c}	1.03 ± 0.05^{c}	1.08 ± 0.09^{c}	1.06 ± 0.02^{c}	1.16 ± 0.02^{b}	1.31 ± 0.01^{a}
Aldehydes	51	Acrolein	107-02-8	C_3H_4O	56.1	886.9	278.382	0.98137	N	0.38 ± 0.01^{d}	0.28 ± 0.01^{e}	0.63 ± 0.01^{a}	0.47 ± 0^{c}	0.53 ± 0.02^{b}	0.46 ± 0^{c}
Aldehydes	52	Benzaldehyde-D	100-52-7	C_7H_6O	106.1	1552.6	1424.845	1.47264	Bitter almond-like, marzipan-like	0.33 ± 0.03^{d}	0.75 ± 0.04^{a}	0.23 ± 0.02^{e}	0.58 ± 0.02^{b}	0.46 ± 0.02^{c}	0.12 ± 0.01^{f}
Aldehydes	53	Benzaldehyde-M	100-52-7	C_7H_6O	106.1	1552.9	1425.73	1.15798	Bitter almond-like, marzipan-like	2.32 ± 0.09^{c}	3.44 ± 0.1^{a}	1.92 ± 0.1^{d}	3.29 ± 0.04^{b}	2.37 ± 0.02^{c}	1.38 ± 0.05^{e}
Aldehydes	54	Butanal	123-72-8	C_4H_8O	72.1	896.5	284.466	1.28093	Malty, sweaty	1.21 ± 0^{d}	1.5 ± 0.08^{b}	1.62 ± 0.02^{a}	1.36 ± 0.01^{c}	1.38 ± 0.02^{c}	0.69 ± 0.01^{e}
Aldehydes	55	cis-4-Heptenal	6728-31-0	$C_7H_{12}O$	112.2	1257.5	753.80	1.15253	Dairy	0.24 ± 0.02^{c}	0.41 ± 0.03^{a}	0.28 ± 0.01^{b}	0.29 ± 0.01^{b}	0.09 ± 0^{d}	0.1 ± 0.01^{d}
Aldehydes	56	Diethyl acetal	105-57-7	$C_6H_{14}O_2$	118.2	911.6	294.294	1.03922	Creamy, fruit, pleasant, tropical fruit	1.86 ± 0.05^{b}	1.66 ± 0.05^{c}	2.44 ± 0.05^{a}	1.57 ± 0.07^{e}	1.7 ± 0.02^{c}	1.19 ± 0.03^{f}
Aldehydes	57	Heptanal-D	111-71-7	$C_7H_{14}O$	114.2	1204.1	674.758	1.69562	Citrus-like, fatty	0.7 ± 0.02^{d}	1.42 ± 0.08^{b}	0.74 ± 0.02^{d}	1.54 ± 0.03^{a}	0.16 ± 0.01^{e}	1.16 ± 0.01^{c}
Aldehydes	58	Heptanal-M	111-71-7	$C_7H_{14}O$	114.2	1204.9	675.988	1.33193	Citrus-like, fatty	0.32 ± 0.02^{c}	0.61 ± 0.01^{b}	0.32 ± 0^{c}	0.7 ± 0^{a}	0.24 ± 0.01^{d}	0.69 ± 0.01^{a}
Aldehydes	59	Hexanal-D	66-25-1	$C_6H_{12}O$	100.2	1102.8	489.574	1.56546	Apple, fat, fresh, green, oil	4.34 ± 0.05^{b}	3.96 ± 0.08^{c}	4.29 ± 0.19^{b}	4.77 ± 0.01^{a}	4.8 ± 0.11^{a}	3.21 ± 0.23^{d}
Aldehydes	60	Hexanal-M	66-25-1	$C_6H_{12}O$	100.2	1102	488.157	1.26797	Apple, fat, fresh, green, oil	1.05 ± 0.05^{f}	1.54 ± 0.04^{c}	1.16 ± 0.02^{e}	1.43 ± 0^{d}	1.69 ± 0.02^{b}	2.27 ± 0.04^{a}
Aldehydes	61	Nonanal	124-19-6	$C_9H_{18}O$	142.2	1403.5	1030.971	1.47774	Citrus-like, soapy	0.46 ± 0.01^{c}	0.52 ± 0.01^{ab}	0.55 ± 0.01^{a}	0.5 ± 0.02^{b}	0.38 ± 0.01^{d}	0.54 ± 0.03^{a}
Aldehydes	62	Octanal	124-13-0	$C_8H_{16}O$	128.2	1297.1	818.26	1.40049	Citrus-like, soapy	0.09 ± 0^{d}	0.12 ± 0.01^{d}	0.14 ± 0.01^{d}	0.64 ± 0.01^{a}	0.27 ± 0.04^{c}	0.34 ± 0.05^{b}
Aldehydes	63	Pentanal	110-62-3	$C_5H_{10}O$	86.1	1006.6	367.302	1.43007	Almond-like, malty	1.41 ± 0.04^{f}	2.46 ± 0.05^{c}	1.65 ± 0.02^{d}	2.53 ± 0.03^{b}	1.55 ± 0.02^{e}	2.73 ± 0.02^{a}
Aldehydes	64	Phenylacetaldehyde	122-78-1	C_8H_8O	120.2	1766.9	2268.35	1.25576	Honey-like, beeswax-like	4.34 ± 0.18^{d}	7.97 ± 0.14^{a}	4.47 ± 0.28^{d}	5.14 ± 0.1^{c}	5.77 ± 0.22^{b}	3.73 ± 0.37^{e}
Aldehydes	65	Propanal	123-38-6	C_3H_6O	58.1	822	240.474	1.14208	Fruity, malty	3.8 ± 0.04^{b}	3.48 ± 0.11^{d}	3.79 ± 0.07^{b}	3.93 ± 0.04^{a}	3.61 ± 0.06^{c}	3.74 ± 0.06^{b}
Esters	66	(Z)-3-Hexenyl propionate	33467-74-2	$C_9H_{16}O_2$	156.2	1387.9	996.517	1.36251	Fruit	0.19 ± 0.01^{b}	0.08 ± 0^{c}	0.15 ± 0.02^{b}	0.09 ± 0.01^{c}	0.28 ± 0.04^{a}	0.08 ± 0.03^{c}
Esters	67	Butyl acetate-D	123-86-4	$C_6H_{12}O_2$	116.2	1090.7	471.238	1.625	Apple, banana	0.02 ± 0^{a}	0.01 ± 0^{ab}	0.01 ± 0^{ab}	0.01 ± 0^{c}	0.01 ± 0^{bc}	0.01 ± 0^{ab}
Esters	68	Butyl acetate-M	123-86-4	$C_6H_{12}O_2$	116.2	1089.2	469.258	1.24931	Apple, banana	0.13 ± 0.01^{a}	0.12 ± 0^{b}	0.08 ± 0^{c}	0.07 ± 0^{d}	0.04 ± 0^{f}	0.06 ± 0^{e}
Esters	69	Ethyl acetate	141-78-6	$C_4H_8O_2$	88.1	902.3	288.21	1.33878	Aromatic, brandy, contact glue, grape	0.93 ± 0.03^{b}	0.93 ± 0.03^{b}	0.74 ± 0.03^{c}	0.33 ± 0.03^{d}	0.9 ± 0.02^{b}	4.77 ± 0.11^{a}
Esters	70	Ethyl butanoate	105-54-4	$C_6H_{12}O_2$	116.2	1055.4	424.398	1.2025	Apple, butter, cheese, pineapple, strawberry	0.5 ± 0.04^{b}	0.32 ± 0.02^{c}	0.68 ± 0.02^{a}	0.48 ± 0.01^{b}	0.31 ± 0.02^{c}	0.11 ± 0.01^{d}
Esters	71	Ethyl crotonate	623-70-1	$C_6H_{10}O_2$	114.1	1147.9	568.477	1.56079	Tropical fruit	0.06 ± 0^{b}	0.03 ± 0^{e}	0.09 ± 0^{a}	0.05 ± 0^{c}	0.04 ± 0^{d}	0.02 ± 0^{f}
Esters	72	Ethyl isobutyrate	97-62-1	$C_6H_{12}O_2$	116.2	967.3	333.609	1.18242	N	0.19 ± 0.01^{d}	0.21 ± 0.01^{c}	0.21 ± 0^{c}	0.62 ± 0.01^{a}	0.32 ± 0.01^{b}	0.13 ± 0.01^{e}
Esters	73	Ethyl pentanoate-D	539-82-2	$C_7H_{14}O_2$	130.2	1140.8	555.248	1.65995	Apple, dry fish, herb, nut, Yeast	0.17 ± 0.02^{c}	0.07 ± 0.01^{d}	1 ± 0.06^{a}	0.28 ± 0.01^{b}	0.22 ± 0^{c}	0.04 ± 0^{d}
Esters	74	Ethyl pentanoate-M	539-82-2	$C_7H_{14}O_2$	130.2	1140.8	555.248	1.28197	Apple, dry fish, herb, nut, Yeast	0.32 ± 0.02^{d}	0.11 ± 0.01^{f}	0.72 ± 0^{a}	0.63 ± 0.01^{b}	0.44 ± 0.01^{c}	0.23 ± 0^{e}
Esters	75	gamma-Butyrolactone	96-48-0	$C_4H_6O_2$	86.1	1714.7	2025.33	1.08916	Caramel, cheese, roasted nut	2.28 ± 0.13^{c}	1.83 ± 0.07^{d}	1.35 ± 0.07^{e}	0.75 ± 0.04^{f}	3.21 ± 0.15^{a}	2.9 ± 0.09^{d}
Esters	76	Hexyl propionate	2445-76-3	$C_9H_{18}O_2$	158.2	1339.9	898.04	1.44599	Fruit	0.62 ± 0.03^{b}	0.25 ± 0.01^{d}	0.79 ± 0.01^{a}	0.48 ± 0^{c}	0.25 ± 0^{d}	0.23 ± 0.01^{d}
Esters	77	Isoamyl acetate	123-92-2	$C_7H_{14}O_2$	130.2	1137.8	549.718	1.73675	Apple, banana, glue, pear	0.05 ± 0^{b}	0.07 ± 0.01^{a}	0.04 ± 0^{c}	0.03 ± 0^{d}	0.02 ± 0^{e}	0.03 ± 0^{cd}
Esters	78	Linalyl acetate	115-95-7	$C_{12}H_{20}O_2$	196.3	1567.2	1470.72	1.23114	Fruit	0.93 ± 0.04^{b}	0.72 ± 0.06^{c}	1.17 ± 0.1^{a}	0.67 ± 0.04^{c}	0.46 ± 0.03^{d}	0.3 ± 0.04^{e}
Esters	79	Methyl 3-methylbutanoate	556-24-1	$C_6H_{12}O_2$	116.2	1027.5	390.702	1.52778	Apple, fruit, pineapple	0.2 ± 0.01^{d}	0.3 ± 0.02^{c}	0.11 ± 0.01^{e}	0.05 ± 0^{f}	0.74 ± 0.02^{a}	0.52 ± 0.02^{b}
Esters	80	Methyl acetate	79-20-9	$C_3H_6O_2$	74.1	860.2	262.121	1.20045	Ester, green	0.69 ± 0.02^{b}	0.69 ± 0.01^{b}	0.65 ± 0.02^{c}	0.63 ± 0.01^{cd}	1.09 ± 0.01^{a}	0.62 ± 0.01^{d}
Esters	81	Methyl hexanoate-D	106-70-7	$C_7H_{14}O_2$	130.2	1190.4	654.748	1.68967	Ester, fresh, fruit, pineapple	0.05 ± 0^{a}	0.04 ± 0^{b}	0.03 ± 0^{c}	0.02 ± 0^{d}	0.01 ± 0^{e}	0.02 ± 0^{d}
Esters	82	Methyl hexanoate-M	106-70-7	$C_7H_{14}O_2$	130.2	1190.4	654.748	1.26282	Ester, fresh, fruit, pineapple	0.12 ± 0.01^{b}	0.14 ± 0^{a}	0.08 ± 0^{c}	0.12 ± 0^{b}	0.05 ± 0^{d}	0.12 ± 0^{b}
Esters	83	Methyl salicylate	119-36-8	$C_8H_8O_3$	152.1	1820.7	2549.173	1.17556	Almond, caramel, peppermint, sharp	0.86 ± 0.08^{bc}	0.67 ± 0.01^{d}	0.92 ± 0.03^{b}	0.72 ± 0.07^{cd}	1.14 ± 0.13^{a}	0.85 ± 0.06^{bc}
Heterocyclic	84	2,3-Diethyl-6-methylpyrazine	18138-04-0	$C_9H_{14}N_2$	150.2	1455.8	1154.776	1.26764	Earth, meat, potato, roast	2.11 ± 0.03^{b}	1.7 ± 0.09^{c}	2.33 ± 0.06^{a}	1.67 ± 0.06^{c}	0.66 ± 0.04^{d}	0.27 ± 0.04^{e}

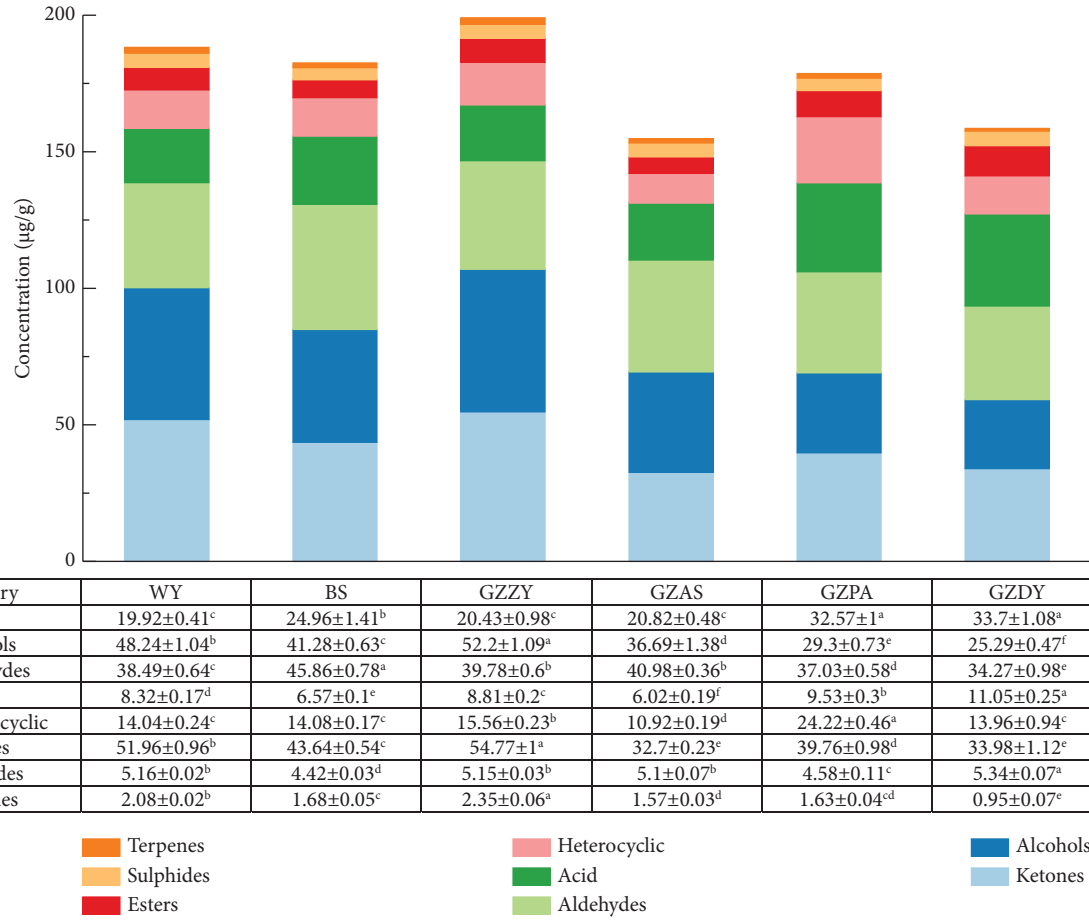
Table 2: Continued.

Category	Number	Compound	CAS#	Formula	MW	RI	Rt (sec)	Dt (RIPrel)	Odor description	WY	BS	GZZY	GZAS	GZPA	GZDY
Heterocyclic	85	2,3-Dimethylpyrazine	5910-89-4	$C_6H_8N_2$	108.1	1354	925.93	1.10702	Caramel, cocoa, hazelnut, peanut butter, roasted	0.4 ± 0.01^{c}	0.41 ± 0.02^{c}	0.46 ± 0.03^{c}	0.42 ± 0.01^{c}	1.25 ± 0.02^{a}	0.62 ± 0.09^{b}
Heterocyclic	86	2,5-Dimethylfuran	625-86-5	C_6H_8O	96.1	939	313.014	1.33493	Savory	0.95 ± 0.03^{b}	1.1 ± 0.05^{a}	0.97 ± 0.01^{b}	0.93 ± 0.02^{bc}	0.88 ± 0^{c}	0.76 ± 0.06^{d}
Heterocyclic	87	2,5-Dimethylpyrazine	123-32-0	$C_6H_8N_2$	108.1	1317	854.52	1.10803	Earthy, roasty, nutty	0.57 ± 0.09^{a}	0.2 ± 0.07^{d}	0.35 ± 0.02^{c}	0.25 ± 0.01^{d}	0.51 ± 0.04^{ba}	0.47 ± 0.03^{b}
Heterocyclic	88	2-Acetyl-1-pyrroline	85213-22-5	C_6H_9NO	111.1	1329.8	878.509	1.11716	Savory	0.13 ± 0.01^{b}	0.08 ± 0^{d}	0.1 ± 0^{c}	0.05 ± 0.01^{e}	0.17 ± 0.01^{a}	0.13 ± 0.01^{b}
Heterocyclic	89	2-Acetylfuran	1192-62-7	$C_6H_6O_2$	110.1	1544.7	1400.553	1.11988	Balsamic, cocoa, coffee	0.17 ± 0.01^{c}	0.17 ± 0.01^{c}	0.21 ± 0.01^{b}	0.18 ± 0.02^{c}	0.7 ± 0.01^{a}	0.19 ± 0.02^{bc}
Heterocyclic	90	2-Butylfuran	4466-24-4	$C_8H_{12}O$	124.2	1147.6	568.005	1.18981	Wet hay	0.4 ± 0.01^{c}	0.18 ± 0.01^{f}	0.44 ± 0.01^{b}	0.51 ± 0.01^{a}	0.36 ± 0.01^{d}	0.28 ± 0.01^{e}
Heterocyclic	91	2-Ethylfuran	3208-16-0	C_6H_8O	96.1	974.7	339.222	1.04565	Butter, caramel	2.69 ± 0.09^{b}	2.46 ± 0.22^{c}	3.23 ± 0.07^{a}	1.44 ± 0.03^{d}	0.73 ± 0.04^{f}	0.99 ± 0.06^{e}
Heterocyclic	92	2-Methylpyrazine	109-08-0	$C_5H_6N_2$	94.1	1280.6	790.72	1.08187	Cocoa, green, hazelnut, popcorn, roasted	0.66 ± 0.01^{b}	0.28 ± 0.01^{e}	0.59 ± 0.02^{c}	0.39 ± 0.01^{d}	0.92 ± 0.02^{a}	0.9 ± 0.01^{a}
Heterocyclic	93	2-Pentylfuran	3777-69-3	$C_9H_{14}O$	138.2	1244.6	733.88	1.25403	Butter, floral, fruit, green bean	1.1 ± 0.1^{b}	0.45 ± 0.03^{c}	1.31 ± 0.03^{a}	0.48 ± 0.01^{c}	0.42 ± 0.03^{c}	0.22 ± 0.03^{d}
Heterocyclic	94	3-Ethylpyridine	536-78-7	C_7H_9N	107.2	1368.3	955.10	1.11324	Nuts	0.14 ± 0.01^{d}	0.21 ± 0.01^{c}	0.19 ± 0.01^{dc}	0.15 ± 0.01^{d}	0.89 ± 0.05^{a}	0.33 ± 0.06^{b}
Heterocyclic	95	5-Methyl-2(3H)-furanone	591-12-8	$C_5H_6O_2$	98.1	1427.4	1085.84	1.10444	Floral	0.22 ± 0.01^{d}	0.18 ± 0^{ed}	0.35 ± 0.01^{c}	0.15 ± 0.01^{e}	1.09 ± 0.06^{a}	0.53 ± 0.03^{b}
Heterocyclic	96	5-Methyl-2-furfural	620-02-0	$C_6H_6O_2$	110.1	1657.9	1790.404	1.13094	N	0.35 ± 0.01^{b}	0.27 ± 0.01^{c}	0.35 ± 0.02^{b}	0.24 ± 0.02^{c}	1.83 ± 0.06^{a}	0.34 ± 0.08^{b}
Heterocyclic	97	Furfural-D	98-01-1	$C_5H_4O_2$	96.1	1496.2	1260.518	1.33413	Almond, baked potatoes, bread, burnt, spice	0.95 ± 0.02^{b}	0.89 ± 0.04^{b}	1.04 ± 0.1^{b}	0.47 ± 0.02^{c}	7.19 ± 0.2^{a}	1.11 ± 0.24^{b}
Heterocyclic	98	Furfural-M	98-01-1	$C_5H_4O_2$	96.1	1496.2	1260.518	1.09033	Almond, baked potatoes, bread, burnt, spice	0.57 ± 0.01^{c}	0.43 ± 0.01^{d}	0.45 ± 0.01^{d}	0.35 ± 0.01^{d}	2.39 ± 0.01^{a}	1.56 ± 0.15^{b}
Heterocyclic	99	Pyridine	110-86-1	C_5H_5N	79.1	1199.1	667.825	1.04448	N	1.14 ± 0^{d}	0.61 ± 0.01^{e}	1.65 ± 0.04^{b}	0.36 ± 0.06^{f}	2.32 ± 0.18^{a}	1.31 ± 0.08^{c}
Heterocyclic	100	Pyrrolidine	123-75-1	C_4H_9N	71.1	1016	377.598	1.28864	N	0.62 ± 0.02^{d}	3.54 ± 0.12^{a}	0.48 ± 0.01^{e}	1.5 ± 0.04^{c}	0.67 ± 0.02^{d}	2.4 ± 0.09^{b}
Heterocyclic	101	Thiophene	110-02-1	C_4H_4S	84.1	1034.3	398.658	1.0328	N	0.49 ± 0.02^{d}	0.42 ± 0.02^{e}	0.64 ± 0.01^{c}	1.03 ± 0.03^{a}	0.51 ± 0.01^{d}	0.84 ± 0.02^{b}
Heterocyclic	102	o-Xylene	95-47-6	C_8H_{10}	106.2	1173.4	618.824	1.07315	N	0.1 ± 0^{c}	0.09 ± 0^{c}	0.12 ± 0^{b}	0.12 ± 0.01^{b}	0.25 ± 0.01^{a}	0.08 ± 0.01^{d}
Heterocyclic	103	p-Xylene	106-42-3	C_8H_{10}	106.2	1147.1	567.06	1.07315	N	0.26 ± 0.01^{d}	0.39 ± 0.01^{b}	0.24 ± 0.01^{d}	0.2 ± 0.01^{e}	0.36 ± 0.01^{c}	0.55 ± 0.01^{a}
Heterocyclic	104	Styrene	100-42-5	C_8H_8	104.2	1229	710.553	1.05222	N	0.03 ± 0^{d}	0.03 ± 0^{d}	0.05 ± 0^{c}	0.03 ± 0^{d}	0.12 ± 0.01^{a}	0.09 ± 0.01^{b}
Ketones	105	1-Hydroxy-2-propanone-D	116-09-6	$C_3H_6O_2$	74.1	1317	854.52	1.23587	Butter, herb, malt, pungent	1.64 ± 0.04^{c}	1.17 ± 0.05^{d}	1.52 ± 0.12^{dc}	0.73 ± 0.02^{e}	5.07 ± 0.31^{a}	3.99 ± 0.41^{b}
Ketones	106	1-Hydroxy-2-propanone-M	116-09-6	$C_3H_6O_2$	74.1	1316.5	853.51	1.05427	Butter, herb, malt, pungent	2.09 ± 0.03^{b}	1.27 ± 0.31^{c}	1.93 ± 0.11^{b}	1.9 ± 0.08^{b}	2.11 ± 0.16^{b}	2.76 ± 0.06^{a}
Ketones	107	1-Octen-3-one	4312-99-6	$C_8H_{14}O$	126.2	1332.6	883.886	1.25903	Mushroom-like	0.49 ± 0.04^{b}	0.35 ± 0.03^{c}	0.22 ± 0.01^{e}	0.56 ± 0.02^{a}	0.27 ± 0.02^{d}	0.13 ± 0^{f}
Ketones	108	1-Penten-3-one-D	1629-58-9	C_5H_8O	84.1	1045.2	411.762	1.31179	Fish, green, mustard, pungent	2.31 ± 0.06^{c}	3.93 ± 0.05^{a}	2.24 ± 0^{c}	2.91 ± 0.02^{b}	1.25 ± 0.02^{e}	1.66 ± 0.08^{d}
Ketones	109	1-Penten-3-one-M	1629-58-9	C_5H_8O	84.1	1044.8	411.294	1.08165	Fish, green, mustard, pungent	0.14 ± 0.01^{e}	0.22 ± 0.01^{d}	0.24 ± 0.01^{c}	0.3 ± 0.01^{b}	0.13 ± 0.01^{f}	0.34 ± 0.01^{a}
Ketones	110	2,3-Pentanedione	600-14-6	$C_5H_8O_2$	100.1	1065.1	436.83	1.20157	N	1.43 ± 0.09^{d}	1.19 ± 0.04^{e}	1.18 ± 0.02^{e}	2.19 ± 0.01^{b}	2.39 ± 0.03^{a}	2 ± 0.06^{c}
Ketones	111	2-Butanone	78-93-3	C_4H_8O	72.1	920	299.91	1.24879	Fragrant, fruit, pleasant	5.15 ± 0.11^{c}	4.99 ± 0.1^{c}	5.4 ± 0.13^{b}	5.19 ± 0.03^{c}	5.61 ± 0.15^{a}	4.16 ± 0.11^{d}
Ketones	112	2-Cyclohexen-1-one	930-68-7	C_6H_8O	96.1	1447.7	1134.771	1.13097	Solvent	0.1 ± 0^{c}	0.09 ± 0^{c}	0.09 ± 0.01^{c}	0.05 ± 0.01^{d}	0.57 ± 0.02^{a}	0.21 ± 0^{b}
Ketones	113	2-Heptanone-D	110-43-0	$C_7H_{14}O$	114.2	1194.5	661.598	1.63447	Blue cheese, fruit, green, nut, spice	1.31 ± 0.1^{b}	0.42 ± 0^{e}	1.66 ± 0.07^{a}	0.93 ± 0.01^{c}	0.58 ± 0.01^{d}	0.21 ± 0.02^{f}
Ketones	114	2-Heptanone-M	110-43-0	$C_7H_{14}O$	114.2	1194.5	661.598	1.26404	Blue cheese, fruit, green, nut, spice	0.23 ± 0.01^{d}	0.16 ± 0^{e}	0.3 ± 0^{a}	0.24 ± 0^{c}	0.26 ± 0^{b}	0.1 ± 0^{f}
Ketones	115	2-Hexanone	591-78-6	$C_6H_{12}O$	100.2	1100.5	485.841	1.49596	N	0.76 ± 0.02^{b}	0.31 ± 0.01^{d}	1.26 ± 0.06^{a}	0.69 ± 0.01^{c}	0.74 ± 0.01^{b}	0.36 ± 0.02^{c}
Ketones	116	2-Octanone-D	111-13-7	$C_8H_{16}O$	128.2	1297.5	819.08	1.7618	Fat, fragrant, mold	9.92 ± 0.11^{a}	9.41 ± 0.11^{b}	9.44 ± 0.1^{b}	0.2 ± 0.06^{c}	0.23 ± 0.03^{c}	0.22 ± 0.02^{c}
Ketones	117	2-Octanone-M	111-13-7	$C_8H_{16}O$	128.2	1296.4	817.05	1.33321	Fat, fragrant, mold	2.39 ± 0.05^{c}	3.02 ± 0.09^{a}	2.76 ± 0.02^{b}	0.51 ± 0.07^{e}	2.77 ± 0.15^{b}	2.08 ± 0.1^{d}
Ketones	118	2-Pentanone	107-87-9	$C_5H_{10}O$	86.1	1001.9	362.154	1.36964	Fruit, pungent	3.88 ± 0.06^{a}	1.64 ± 0.08^{d}	3.97 ± 0.1^{a}	2.3 ± 0.01^{c}	2.53 ± 0.07^{b}	1.35 ± 0.06^{f}
Ketones	119	3-Hydroxy-2-butanone	513-86-0	$C_4H_8O_2$	88.1	1304.3	831.23	1.06299	Butter, creamy, green pepper	0.52 ± 0.01^{d}	0.19 ± 0.02^{f}	0.48 ± 0.01^{e}	0.75 ± 0.01^{c}	1.53 ± 0.04^{b}	1.76 ± 0.01^{a}
Ketones	120	3-Methyl-2-pentanone	565-61-7	$C_6H_{12}O$	100.2	1038.6	403.778	1.48107	N	0.52 ± 0.06^{b}	0.18 ± 0.01^{d}	0.72 ± 0.07^{a}	0.18 ± 0.01^{d}	0.34 ± 0^{c}	0.07 ± 0.01^{e}
Ketones	121	4-Methyl-2-pentanone	108-10-1	$C_6H_{12}O$	100.2	1020.5	382.746	1.46735	N	2.48 ± 0.27^{b}	0.24 ± 0.01^{d}	3.54 ± 0.26^{a}	1.42 ± 0.04^{c}	1.49 ± 0.03^{c}	0.29 ± 0.02^{d}
Ketones	122	4-Methyl-3-penten-2-one-D	141-79-7	$C_6H_{10}O$	98.1	1153.9	580.021	1.44681	Plastic, earthy	4.29 ± 0.11^{b}	2.7 ± 0.11^{d}	5.21 ± 0.07^{a}	1.39 ± 0.01^{f}	3.24 ± 0.06^{c}	2.4 ± 0.12^{e}
Ketones	123	4-Methyl-3-penten-2-one-M	141-79-7	$C_6H_{10}O$	98.1	1153.6	579.399	1.1144	Plastic, earthy	1.07 ± 0.01^{e}	1.2 ± 0.03^{c}	1.16 ± 0^{d}	1 ± 0.01^{f}	1.25 ± 0.02^{b}	1.49 ± 0.01^{a}
Ketones	124	5-Methyl-3-heptanone	541-85-5	$C_8H_{16}O$	128.2	1232.9	716.34	1.69299	N	0.2 ± 0.01^{a}	0.14 ± 0.01^{d}	0.2 ± 0.01^{a}	0.16 ± 0^{c}	0.09 ± 0^{e}	0.19 ± 0.01^{b}
Ketones	125	6-Methyl-5-hepten-2-one	110-93-0	$C_8H_{14}O$	126.2	1348.3	914.52	1.18166	Citrus, mushroom, pepper, rubber, strawberry	2.64 ± 0.01^{a}	1.03 ± 0.02^{c}	1.84 ± 0.05^{b}	0.74 ± 0.02^{d}	0.33 ± 0.02^{e}	0.36 ± 0.01^{e}
Ketones	126	Acetone	67-64-1	C_3H_6O	58.1	842.2	251.706	1.11765	Pungent	5.59 ± 0.14^{c}	6.47 ± 0.45^{a}	6.34 ± 0.22^{ab}	5.97 ± 0.06^{bc}	4.15 ± 0.16^{e}	5.16 ± 0.05^{d}
Ketones	127	Acetophenone	98-86-2	C_8H_8O	120.2	1693.3	1933.34	1.17861	Floral	0.91 ± 0.03^{c}	0.67 ± 0.05^{d}	1.1 ± 0.04^{b}	0.16 ± 0.04^{e}	0.96 ± 0.13^{c}	1.25 ± 0.04^{a}

Table 2: Continued.

Category	Number	Compound	CAS#	Formula	MW	RI	Rt (sec)	Dt (RIPrel)	Odor description	WY	BS	GZZY	GZAS	GZPA	GZDY
Ketones	128	Cyclohexanone	108-94-1	$C_6H_{10}O$	98.1	1305.1	832.623	1.16556	Mint, cool	0.07 ± 0.02^{b}	0.03 ± 0^{c}	0.04 ± 0^{c}	0.06 ± 0^{b}	0.1 ± 0.01^{a}	0.09 ± 0^{a}
Ketones	129	Cyclopentanone	120-92-3	C_5H_8O	84.1	1148.4	569.422	1.33214	Mint, cool	1.64 ± 0.08^{dc}	2.24 ± 0.09^{a}	1.75 ± 0.02^{c}	2.01 ± 0.03^{b}	1.63 ± 0.06^{d}	1.18 ± 0.04^{e}
Ketones	130	Diacetyl	431-03-8	$C_4H_6O_2$	86.1	988.6	349.986	1.1665	Butter, pastry, yeast	0.18 ± 0.01^{cb}	0.35 ± 0.01^{a}	0.19 ± 0.02^{b}	0.17 ± 0.01^{cd}	0.16 ± 0.01^{d}	0.17 ± 0.01^{cd}
Sulphides	131	Dimethyl disulfide	624-92-0	$C_2H_6S_2$	94.2	1087.2	466.423	1.13615	Cabbage-like, sulfury	1.12 ± 0.01^{a}	0.71 ± 0.03^{b}	0.26 ± 0.02^{d}	0.58 ± 0.02^{c}	0.1 ± 0.01^{e}	0.12 ± 0.01^{e}
Sulphides	132	Dimethyl sulfide-D	75-18-3	C_2H_6S	62.1	796.2	226.902	1.12279	Asparagus-like, putrid, cooked corn-like	2.9 ± 0.01^{c}	2.48 ± 0.18^{d}	3.66 ± 0.05^{a}	3.31 ± 0.05^{b}	3.03 ± 0.12^{c}	3.54 ± 0.09^{a}
Sulphides	133	Dimethyl sulfide-M	75-18-3	C_2H_6S	62.1	795.3	226.434	0.96723	Asparagus-like, putrid, cooked corn-like	1.02 ± 0.02^{e}	1.16 ± 0.11^{c}	1.11 ± 0.01^{cd}	1.03 ± 0.02^{ed}	1.33 ± 0.02^{b}	1.5 ± 0.02^{a}
Sulphides	134	Methional	3268-49-3	C_4H_8OS	104.2	1475.1	1204.093	1.09824	Cooked potato-like	0.12 ± 0.01^{b}	0.07 ± 0.02^{c}	0.12 ± 0.01^{b}	0.18 ± 0.01^{a}	0.12 ± 0.01^{b}	0.18 ± 0.01^{a}
Terpenes	135	3-Carene	13466-78-9	$C_{10}H_{16}$	136.2	1160	591.853	1.28612	Lemon	0.12 ± 0^{c}	0.08 ± 0.01^{e}	0.13 ± 0^{b}	0.08 ± 0^{e}	0.1 ± 0^{d}	0.15 ± 0^{a}
Terpenes	136	alpha-Phellandrene	99-83-2	$C_{10}H_{16}$	136.2	1178.8	629.839	1.68231	Citrus, fresh, mint, pepper, spice, wood	0.49 ± 0.01^{a}	0.06 ± 0.01^{f}	0.47 ± 0.01^{b}	0.25 ± 0.01^{d}	0.4 ± 0.02^{c}	0.13 ± 0.01^{e}
Terpenes	137	alpha-Terpinene	99-86-5	$C_{10}H_{16}$	136.2	1187.5	648.433	1.22012	Citrus, woody, spicy, lemon-like	0.13 ± 0.01^{a}	0.08 ± 0.01^{c}	0.11 ± 0.01^{b}	0.1 ± 0^{b}	0.08 ± 0^{c}	0.06 ± 0.01^{d}
Terpenes	138	beta-Pinene	127-91-3	$C_{10}H_{16}$	136.2	1139.1	552.162	1.21279	Pine, polish, wood	0.42 ± 0.02^{b}	0.87 ± 0.02^{a}	0.21 ± 0.01^{d}	0.16 ± 0.01^{e}	0.34 ± 0.01^{c}	0.14 ± 0^{f}
Terpenes	139	Camphene	79-92-5	$C_{10}H_{16}$	136.2	1110.9	502.761	1.72608	Camphor, mothball, oil, warm	0.19 ± 0.03^{c}	0.04 ± 0.01^{d}	0.26 ± 0^{b}	0.62 ± 0.02^{a}	0.25 ± 0.01^{b}	0.03 ± 0^{d}
Terpenes	140	gamma-Terpinene	99-85-4	$C_{10}H_{16}$	136.2	1261.6	760.18	1.21317	Citrus, lemon-like, woody, spicy, juicy	0.3 ± 0.01^{b}	0.18 ± 0.01^{c}	0.64 ± 0.01^{a}	0.18 ± 0^{c}	0.19 ± 0.01^{c}	0.18 ± 0.01^{c}
Terpenes	141	Limonene	138-86-3	$C_{10}H_{16}$	136.2	1206.1	677.599	1.2187	Citrus-like, carrot-like	0.16 ± 0^{c}	0.19 ± 0.01^{b}	0.26 ± 0.02^{a}	0.1 ± 0^{e}	0.14 ± 0.02^{cd}	0.14 ± 0.01^{d}
Terpenes	142	Myrcene	123-35-3	$C_{10}H_{16}$	136.2	1175.9	623.836	1.22062	Balsamic, fruit, geranium, herb, must	0.1 ± 0^{a}	0.05 ± 0^{c}	0.09 ± 0.01^{b}	0.05 ± 0^{cd}	0.04 ± 0^{d}	0.04 ± 0^{e}
Terpenes	143	Terpinolene	586-62-9	$C_{10}H_{16}$	136.2	1287.5	802.002	1.22298	Pine	0.17 ± 0.02^{ab}	0.14 ± 0.01^{b}	0.18 ± 0.04^{a}	0.03 ± 0.01^{d}	0.08 ± 0.02^{c}	0.08 ± 0.02^{c}

N, no aroma description of the substance was found. a, b, c, and d indicate significant difference. Odor descriptions were from the literature [4, 12, 23, 24] or from FEMA database.



Category	WY	BS	GZZY	GZAS	GZPA	GZDY
Acid	19.92±0.41^{c}	24.96±1.41^{b}	20.43±0.98^{c}	20.82±0.48^{c}	32.57±1^{a}	33.7±1.08^{a}
Alcohols	48.24±1.04^{b}	41.28±0.63^{c}	52.2±1.09^{a}	36.69±1.38^{d}	29.3±0.73^{e}	25.29±0.47^{f}
Aldehydes	38.49±0.64^{c}	45.86±0.78^{a}	39.78±0.6^{b}	40.98±0.36^{b}	37.03±0.58^{d}	34.27±0.98^{e}
Esters	8.32±0.17^{d}	6.57±0.1^{e}	8.81±0.2^{c}	6.02±0.19^{f}	9.53±0.3^{b}	11.05±0.25^{a}
Heterocyclic	14.04±0.24^{c}	14.08±0.17^{c}	15.56±0.23^{b}	10.92±0.19^{d}	24.22±0.46^{a}	13.96±0.94^{c}
Ketones	51.96±0.96^{b}	43.64±0.54^{c}	54.77±1^{a}	32.7±0.23^{e}	39.76±0.98^{d}	33.98±1.12^{e}
Sulphides	5.16±0.02^{b}	4.42±0.03^{d}	5.15±0.03^{b}	5.1±0.07^{b}	4.58±0.11^{c}	5.34±0.07^{a}
Terpenes	2.08±0.02^{b}	1.68±0.05^{c}	2.35±0.06^{a}	1.57±0.03^{d}	1.63±0.04^{cd}	0.95±0.07^{e}

Figure 3: Volatile compound content and their proportion in samples from different tea-producing regions.

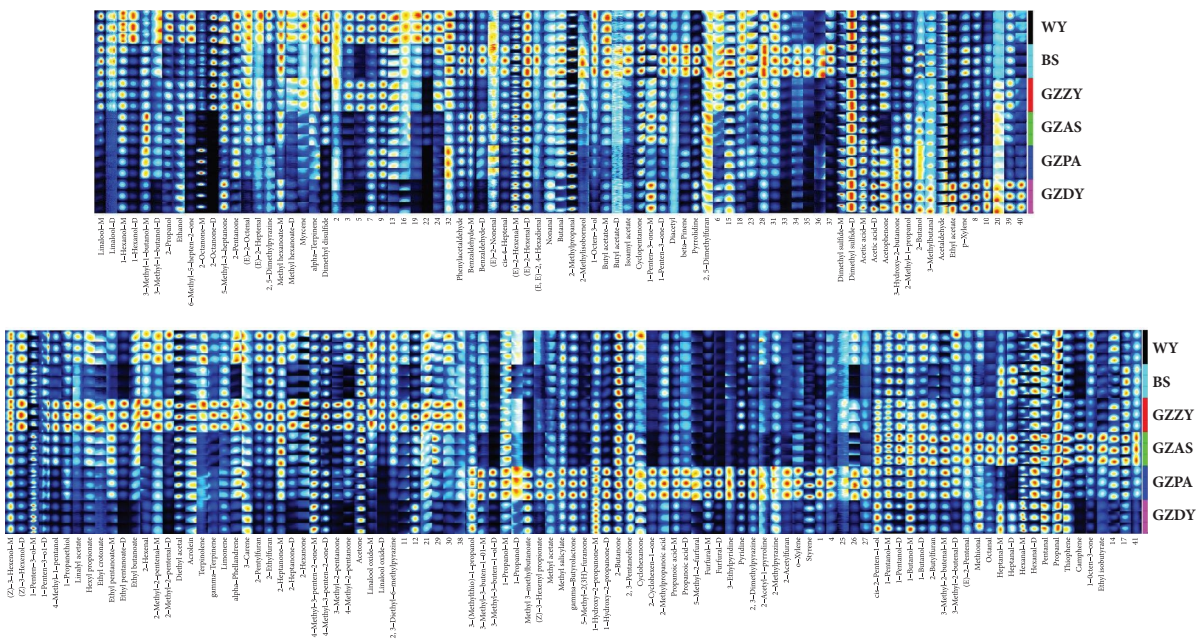


Figure 4: Volatile compound fingerprint spectrum from each tea sample.

dependent variable fit index ($R2Y$), and model prediction index ($Q2$). $R2X$ and $R2Y$ represent the interpretation rate of the built model for X and Y matrices, respectively, and $Q2$ represents the prediction ability of the model. The model is considered highly reliable when all three indices approach 1. $Q2 > 0.5$ indicates a reliable model, and $Q2 > 0.9$ indicates a highly reliable predictive model.

The OPLS-DA model was established according to the volatile compounds identified in black tea samples from 6 different regions. The results are shown in Figure 5(a). The six samples could be distinguished effectively, and the model indices $R2X = 0.983$, $R2Y = 0.997$, and $Q2 = 0.993$ indicate a very high and reliable prediction ability. Thus, the model can be used to distinguish black tea samples from different regions. In addition, to prevent the model from overfitting the data, a replacement test ($n = 200$) was also carried out on the model. The results are shown in Figure 5(b). All the green $R2$ values and blue $Q2$ values on the left are lower than the original point on the right, and the intercept between the regression line and the vertical axis (on the left) of the $Q2$ point is negative, indicating that the model does not overfit and has good prediction ability. Thus, it can be used for discriminant analysis of aroma compounds from black tea samples of different origins.

3.1.4. Analysis of Volatile Aroma Compounds of Black Tea with PLS-DA. The 143 compounds identified in Table 2 were assessed with PLS-DA. PLS-DA is a supervised discriminant analysis method, a multivariate statistical analysis method, which can determine the classification of research objects according to the observed or measured values of several variables. PLS-DA maximizes the difference between groups according to a predefined classification (Y variable), achieving better separation results than principal component analysis.

According to the PLS-DA score plots (Figure 6), WY and GZZY were in close proximity, indicating that the two samples have similar aroma types. In comparison, the other four samples were relatively dispersed and independent, indicating that the model can distinguish different black tea origins.

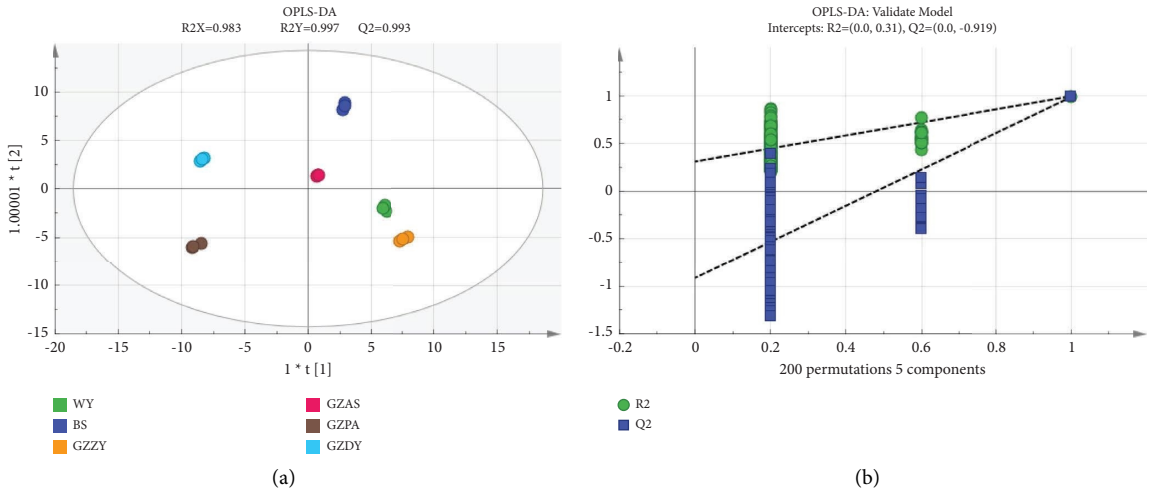
WY black tea is known for its floral, fruity, and dried longan aroma, while GZZY black tea is known for its fruity and sweet aroma. As is shown in Figure 6, Terpinolene, Limonene141, Butanal, 2-Hexenal, 3-Methyl-1-butanol, 4-Methyl-1-pentanol, 2-Propanol, Diethyl acetate, gamma-Terpinene, 1-Pentanol-D, 2-Methyl-2-pentenal, Hexyl propionate, Ethyl crotonate, 2-Heptanone, and Butyl acetate were significantly correlated with the aromas of WY and GZZY samples, which exhibited strong fruity and floral aroma, in line with the common aroma characteristics of WY and GZZY samples. The BS sample was highly correlated with Diacetyl, Methyl hexanoate, Heptanal, beta-Pinene, Nonanal, etc., which are associated with sweetness and woody fragrance. The PA sample was correlated 2-cyclohexen-1-one, 5-Methyl-2 (3H)-furanone, 2, 3-dimethylpyrazine, 3-Ethylpyridine, 2-Methylpyrazine, and Propanoic acid, which give a floral and sweet aroma. The GZDY sample was highly correlated with 1-Penten-3-ol, 2-Methyl-1-propanol, 2-Methylpropanal, Acetic acid, Dimethyl sulfide, and Ethyl acetate. These compounds potentially give GZDY black tea a subtle floral and fruity aroma.

3.1.5. Analysis of Key Flavor Compounds of Black Tea from Different Guizhou Regions. In order to further analyze the contribution rates of key flavor compounds of black tea products from 4 Guizhou regions and 2 regions outside of Guizhou, a variable importance (VIP) >1 and a predicted P value <0.05 were used to identify the key volatile compounds. A total of 50 flavor compounds were screened and are listed in Figure 7. They include 13 aldehydes, 10 alcohols, 7 ketones, 6 terpenes, 5 esters, 5 heterocycles, 3 sulfur-containing compounds, and 1 acid.

The OAV is the ratio of the concentration of each compound to its detection threshold. The odor activity value can determine the contribution of each volatile compound in the sample to the overall aroma. When OAV ≥1, the aroma compound can theoretically be considered to contribute to the overall aroma. Moreover, the higher the OAV, the larger the contribution to aroma. Using the threshold values of related compounds provided by references [31, 32], the OAV of all volatile compounds was calculated. Finally, 83 compounds with OAV ≥1 in at least one sample were obtained, including 1 acid, 13 alcohols, 22 aldehydes, 11 esters, 11 heterocyclic compounds, 16 ketones, 3 sulfides, and 6 terpenes. When a volatile compound has an OAV ≥100 in the sample, it can be considered to have a greater contribution to the overall aroma. Therefore, all the volatile compounds with VIP greater than 1 or OAV ≥100 in the sample were considered as the main aroma compounds of black tea (68 in total), and cluster analysis was conducted accordingly (Figure 3). A stronger correlation between the compound and the overall aroma of the sample is indicated by a lighter color, while weaker correlations are indicated with darker colors.

As shown in Figure 8, the cluster analysis showed that GZZY and WY samples had a high similarity. The GZDY and GZPA samples were also similar, while GZAS samples exhibited some overlap with the GZZY, WY, GZDY, and GZPA samples, while the BS samples were distinct.

At the same time, although no significant difference in volatile compounds was found between Guizhou black tea samples and non-Guizhou black tea samples, it can be seen from Figure 8 that although there was a certain overlap between samples from the same production area, each sample had distinct volatile compounds that were highly correlated with that particular sample, and these patterns had a high similarity with the PLS-DA results. In accordance with these criteria, the distinct compounds present in each sample could be the ones that give the characteristic aroma of each sample. For example, the compounds with high correlation with the WY sample were Dimethyl disulfide, 1-Octen-3-one, 2-Octanone, 2-Methylisoborneol, Butyl



(a) (b)

Figure 5: OPLS-DA analysis of volatile aroma compounds in black tea samples from different regions.

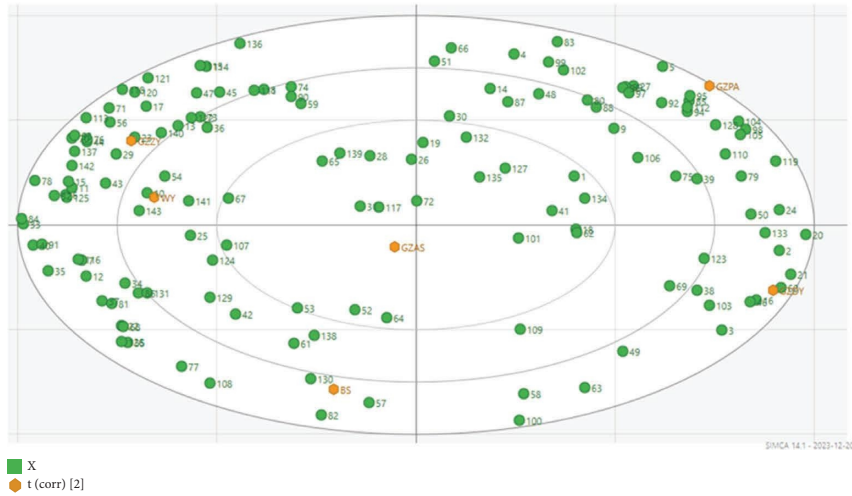


Figure 6: PLS-DA analysis of volatile aroma compounds in black tea samples from different regions.

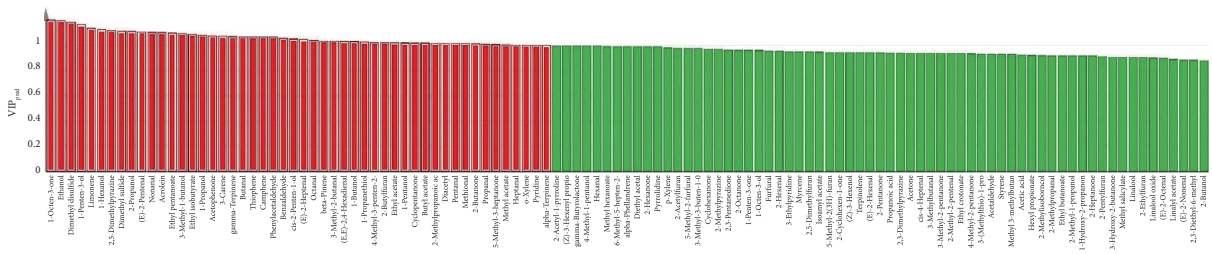
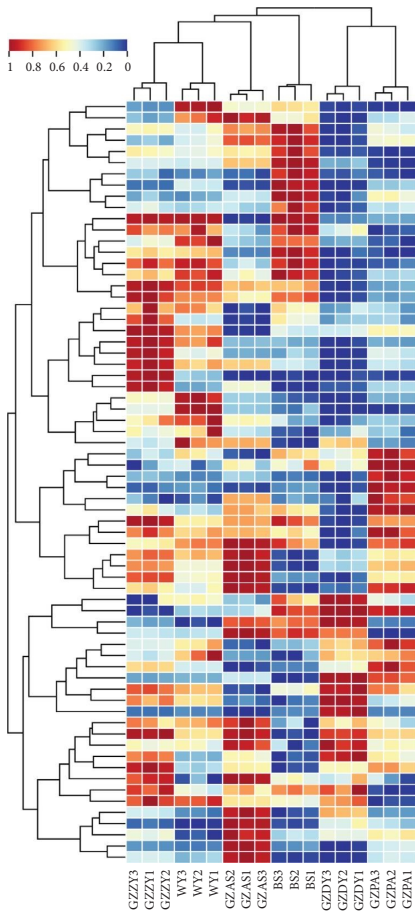


Figure 7: VIP analysis of volatile compounds in black tea samples.

acetate and Linalool, 1-Octen-3-ol, 2, 3-diethyl-6-methylpyrazine, 2-propanol, 1-Hexanol, alpha-Terpinene, 2, 5-dimethylpyrazine, and 5-Methyl-3-heptanone. Most of these compounds have a floral and fruity aroma, while some have a nutty aroma and sour taste and may be the source of the dry longan aroma in WY black tea. Among them, Dimethyl disulfide, 2-Propanol, 1-Hexanol, alpha-Terpinene, 2, 5-dimethylpyrazine, and 5-Methyl-3-heptanone had the strongest correlation with the WY sample. These compounds may be the distinct flavor compounds in WY samples. Compounds with high correlation with the BS sample included Cyclopentanone, Benzaldehyde, cis-4-Heptenal, 1-Penten-3-one, Diacetyl, beta-Pinene, Phenylacetaldehyde, (E, E)-2, 4-Hexadienal, 2-Octanone (2-Methylisoborneol, Butyl) acetate, (E)-2-Hexenal, 1-Octen-3-ol, (E)-2-Octenal, Butanal, 3-Methyl-1-butanol,



Category	Compound	CAS#	Formula	MW	VIP	Odor description	OT (ppb/L)	OAV					
								WY	BS	GZZY	GZAS	GZPA	GZDY
Sulfur-containing	Dimethyl disulfide	624-92-0	$C_2H_6S_2$	94.2	1.19	Cabbage-like, sulfury	0.0011	1018	645	236	527	91	109
Ketones	1-hexen-3-one	4312-99-6	$C_6H_{10}O$	126.2	1.20	Mushroom-like	0.000016	30625	21875	13750	35000	16875	9125
Ketones	Cyclopentanone	120-92-3	C_5H_8O	84.1	1.02	Mint, Cool	9.3	< 1	< 1	< 1	< 1	< 1	< 1
Aldehydes	Benzaldehyde	100-52-7	C_7H_6O	106.1	1.06	Bitter almond-like, marzipan-like	0.35	8	12	6	11	8	4
Aldehydes	cis-4-Heptenal	6728-31-0	$C_7H_{12}O$	112.2	< 1	Dairy	0.000087	2759	4713	3218	3218	1034	1149
Ketones	1-Penten-3-one	1629-58-9	C_5H_8O	84.1	< 1	Fish, Green, Mustard, Pungent	0.023	107	181	108	140	60	87
Ketones	Diacetyl	431-03-8	$C_4H_6O_2$	86.1	1.02	Butter, Pastry, Yeast	0.015	12	23	13	11	11	11
Terpenes	beta-Pinene	127-91-3	$C_{10}H_{16}$	136.2	1.04	Pine, Pelish, Wood	0.14	3	6	2	1	2	1
Aldehydes	Phenylacetaldehyde	122-78-1	C_8H_8O	120.2	1.07	Honey-like, hennwax-like	0.0052	835	1533	860	988	1110	717
Aldehydes	(E,E)-2,4-hexadienal	142-83-6	C_6H_8O	96.1	1.03	Green	0.01	22	37	24	21	22	14
Ketones	2-Octanone	111-13-7	$C_8H_{16}O$	128.2	< 1	Fat, Fragrant, Mold	0.0502	245	248	243	14	60	46
Alcohols	3-Methylisoborneol	2371-42-8	$C_{11}H_{20}O$	168.3	< 1	-	0.0000018	255556	283333	255556	144444	94444	177778
Esters	Butyl acetate	123-86-4	$C_6H_{12}O_2$	116.2	1.02	Apple, Banana	0.038	3	2	2	1	< 1	1
Aldehydes	(E)-2-Hexenal	6728-26-3	$C_6H_{10}O$	99.1	< 1	-	0.03	304	347	297	237	222	224
Alcohols	Linalool	78-70-6	$C_{10}H_{18}O$	154.3	< 1	Coriander, Floral, Lavender, Lemon, Rose	0.00022	65227	68909	61636	29682	16227	11864
Alcohols	1-Octen-3-ol	3391-86-4	$C_8H_{16}O$	128.2	< 1	Cucumber, Earth, Fat, Floral, Mushroom	0.0015	340	353	260	213	173	93
Heterocyclic	2,3-Diethyl-5-methylpyrazine	18138-04-0	$C_9H_{14}N_2$	150.2	< 1	Earth, Meat, Potato, Roast	0.005	422	340	466	334	132	54
Aldehydes	(E)-2-Octenal	2548-87-0	$C_8H_{14}O$	126.2	< 1	Dandelion, Fat, Fruit, Grass, Green, Spice	0.003	127	137	157	100	50	27
Terpenes	Terpinolene	586-62-9	$C_{10}H_{16}$	136.2	< 1	Pine	0.0002	850	700	900	150	400	400
Terpenes	Limonene	138-86-3	$C_{10}H_{16}$	136.2	1.14	Citrus-like, carro-like	2	< 1	< 1	< 1	< 1	< 1	< 1
Ketones	4-Methyl-3-penten-2-one	141-79-7	$C_6H_{10}O$	98.1	1.03	Plastic, earthy	1.2	4	3	5	2	4	3
Heterocyclic	2-Pentylfuran	3777-69-3	$C_9H_{14}O$	138.2	< 1	Butter, Floral, Fruit, Green Bean	0.0059	186	76	222	81	71	37
Alcohols	1-Propanethiol	107-03-9	C_3H_8S	76.2	1.03	Cabbage, Onion	0.0003	94	71	161	65	87	39
Esters	Ethyl butanoate	105-54-4	$C_6H_{12}O_2$	116.2	< 1	Apple, Butter, Cheese, Pineapple, Strawberry	0.0009	556	356	756	533	344	122
Terpenes	gamma-Terpinene	99-85-4	$C_{10}H_{16}$	136.2	1.07	Citrus, lemon-like, woody, spicy, juicy	0.055	5	3	12	3	3	3
Esters	Ethyl pentanoate	539-82-2	$C_7H_{14}O_2$	130.2	1.10	Apple, Dry Fish, Herb, Nut, Yeast	0.0058	86	31	295	155	114	47
Alcohols	2-Propanol	67-63-0	C_3H_8O	60.1	1.13	Floral	9.7479	< 1	< 1	< 1	< 1	< 1	< 1
Alcohols	1-Butanol	111-27-3	$C_4H_{10}O$	102.2	1.13	Green, grassy	0.056	71	36	43	35	27	22
Terpenes	alpha-Terpinene	99-86-5	$C_{10}H_{16}$	136.2	1.09	Citrus, woody, spicy, lemon-like	0.085	2	< 1	1	1	< 1	< 1
Aldehydes	(E)-2-Heptenal	18829-55-5	$C_7H_{12}O$	112.2	1.05	Green, fatty	0.0018	122	61	100	89	78	83
Alcohols	Ethanol	64-17-5	C_2H_6O	46.1	1.20	-	3	< 1	< 1	< 1	< 1	< 1	< 1
Acid	2-Methylpropanoic acid	79-31-2	$C_4H_8O_2$	88.1	1.02	Burnt, Butter, Cheese, Sweat	6.5505	< 1	< 1	< 1	< 1	< 1	< 1
Aldehydes	(E)-2-Nonenal	18829-56-6	$C_9H_{16}O$	140.2	< 1	Paper	0.0004	350	425	350	400	525	400
Heterocyclic	o-Xylene	95-47-6	C_8H_{10}	106.2	1.09	-	0.45023	< 1	< 1	< 1	< 1	< 1	< 1
Esters	Methyl acetate	79-20-9	$C_3H_6O_2$	74.1	1.01	Ester, Green	1.5	< 1	< 1	< 1	< 1	< 1	< 1
Aldehydes	Hexanal	66-25-1	$C_6H_{12}O$	100.2	< 1	Apple, Fat, Fresh, Green, Oil	0.0045	1198	1222	1211	1378	1442	1218
Alcohols	1-Propanol	71-23-8	C_3H_8O	60.1	1.08	Alcohol, Candy, Pungent	8.5056	< 1	< 1	< 1	< 1	< 1	< 1
Aldehydes	Butanal	123-72-8	C_4H_8O	72.1	1.07	Malty, sweaty	0.0082	148	183	198	166	168	84
Ketones	2-Butanone	78-93-3	C_4H_8O	72.1	1.01	Fragrant, Fruit, Pleasant	35.4002	< 1	< 1	< 1	< 1	< 1	< 1
Alcohols	3-Methyl-1-butanol	123-51-3	$C_5H_{12}O$	88.1	1.10	Burnt, cocoa-like, winey	0.004	263	265	215	305	273	113
Heterocyclic	2-Butylfuran	4466-24-4	$C_8H_{12}O$	124.2	1.03	Wet Hay	0.005	80	56	88	102	72	56
Alcohols	1-Butanol	71-36-3	$C_4H_{10}O$	74.1	1.03	Fruity	0.4392	4	2	5	6	5	3
Alcohols	1-Pentanol	71-41-0	$C_5H_{12}O$	88.1	1.02	Balsamic, Fruit, Green, Pungent, Yeast	5	< 1	< 1	< 1	< 1	< 1	< 1
Aldehydes	3-Methylbutanal	107-86-8	$C_5H_{10}O$	84.1	1.04	Burnt, cocoa-like	0.0005	860	500	980	1300	1240	580
Aldehydes	2-Methylbutanal	590-86-3	$C_5H_{10}O$	86.1	< 1	-	0.0011	1391	1473	1218	1245	1318	1627
Aldehydes	2-Methylpropanal	78-84-2	C_4H_8O	72.1	< 1	Burnt, Caramel, Cocoa, Green, Malt	0.0015	373	500	320	387	507	527
Aldehydes	Pentanal	110-62-3	$C_5H_{10}O$	86.1	1.01	Almond-like, malty	0.0012	1175	2050	1375	2108	1292	2275
Aldehydes	Heptanal	111-71-7	$C_7H_{14}O$	114.2	1.01	Citrus-like, fatty	0.0028	364	721	379	3905	143	661
Heterocyclic	2-Acetyl-1-pyrroline	85213-22-5	C_6H_9NO	111.1	< 1	Savory	0.0001	1300	800	1000	500	1700	1300
Heterocyclic	2,5-Dimethylpyrazine	123-32-0	$C_6H_8N_2$	108.1	1.12	Earthy, roasty, nutty	0.02	29	10	18	13	26	24
Heterocyclic	Pyridine	110-86-1	C_5H_5N	79.1	1.00	-	0.00079	1443	772	2089	456	2057	1658
Ketones	3-Hydroxy-2-butanone	513-86-0	$C_4H_8O_2$	88.1	< 1	Butter, Creamy, Green Pepper	0.0014	571	136	343	536	1093	1257
Ketones	Acetophenone	98-86-2	C_8H_8O	120.2	1.08	Floral	0.065	14	10	17	2	15	19
Terpenes	3-Carene	13466-78-9	$C_{10}H_{16}$	136.2	1.07	Lemon	0.77	< 1	< 1	< 1	< 1	< 1	< 1
Esters	Ethyl acetate	141-78-6	$C_4H_8O_2$	88.1	1.02	Aromatic, Brandy, Contact Glue, Grape	6.2	< 1	< 1	< 1	< 1	< 1	< 1
Aldehydes	Propanal	123-38-6	C_3H_6O	58.1	1.01	Fruity, malty	0.0093	409	374	408	423	388	402
Alcohols	cis-2-Penten-1-ol	1576-95-0	$C_5H_{10}O$	86.1	1.03	Mushroom-like, grass, grassy	0.72	3	2	3	3	3	3
Sulfur-containing	Methional	3268-49-3	C_4H_8OS	104.2	1.02	Cooked potato-like	0.00043	279	163	279	419	279	419
Sulfur-containing	Dimethyl sulfide	75-18-3	C_2H_6S	62.1	1.13	Asparagus-like, putrid, cooked corn-like	0.0005	13067	12133	15933	14467	14533	16800
Aldehydes	Acrolein	107-02-8	C_3H_4O	56.1	1.10	almond cherry, burnt, sweet, pungent	0.11	3	3	6	4	5	4
Alcohols	1-Penten-3-ol	616-25-1	$C_5H_{10}O$	86.1	1.17	Butter-like, pungent	0.3581	14	15	16	17	14	15
Aldehydes	Nonanal	124-19-6	$C_9H_{18}O$	142.2	1.13	Citrus-like, soapy	0.0011	418	473	500	455	345	491
Ketones	5-Methyl-3-heptanone	541-85-5	$C_8H_{16}O$	128.2	1.01	-	0.041	5	3	3	4	2	5
Heterocyclic	Thiophene	110-02-1	C_4H_4S	84.1	1.07	-	0.084	6	5	8	12	6	10
Aldehydes	Octanal	124-13-0	$C_8H_{16}O$	128.2	1.04	Citrus-like, soapy	0.0034	26	35	41	188	79	100
Aldehydes	(E)-2-Pentenal	1576-87-0	C_5H_8O	84.1	1.11	Grassy, green	0.31	< 1	< 1	< 1	< 1	< 1	< 1
Esters	Ethyl isobutyrate	97-62-1	$C_6H_{12}O_2$	116.2	< 1	-	0.0001	1900	2100	2100	6200	3200	1300
Terpenes	Camphene	79-92-5	$C_{10}H_{16}$	136.2	1.07	Camphor, Menthall, Oil, Warm	26	< 1	< 1	< 1	< 1	< 1	< 1

Figure 8: Cluster analysis of key flavor compounds in black tea samples.

2-Methylpropanal, Pentanal, and Heptanal. The aroma of these compounds may serve as the source of BS black tea's rich, sweet, fruity, and fragrant aroma. cis-4-Heptenal, 1-Penten-3-one-D, Diacetyl, beta-Pinene, Phenylacetaldehyde, and (E, E)-2, 4-Hexadienal had the highest correlation with the BS samples. Therefore, these compounds may be the distinct flavor compounds in BS samples. The compounds with high correlation with the GZZY samples were 2-octanone, 2-methylisoborneol, Linalool, 2, 3-diethyl-6-methylpyrazine, (E)-2-Octenal, Limonene, 4-Methyl-3-penten-2-one, 2-Pentylfuran, 1-Propanethiol, Ethyl butanoate, gamma-Terpinene, Ethyl pentanoate, Butanal1-Pentanol, Acetophenone, cis-2-Penten-1-ol, Dimethyl sulfide, Acrolein, 1-Penten-3-ol, Nonanal, and 5-Methyl-3-heptanone. Most exhibit floral and fruit aromas and may be the source of the intensely floral and fruitarian aromas of GZZY samples. The correlation between Limonene, 4-Methyl-3-penten-2-one, 2-Pentylfuran, 1-Propanethiol, Ethyl butanoate, gamma-Terpinene, Ethyl pentanoate, and GZZY samples was the strongest, which suggested that these compounds might be the compounds giving the characteristic aroma in GZZY tea samples. The compounds with high correlation with GZAS samples were 1-Octen-3-one, Cyclopentanone, Benzaldehyde, Cism-4-Heptenal, 3-Methyl-1-butanol, 2-Butylfuran, 1-Butanol, 1-Pentanol, 3-Methyl-2-butenal, Pentanal, Heptanal, Propanal, cis-2-Penten-1-ol, Methional, 1-Penten-3-ol, Thiophene, Octanal, (E)-2-Pentenal, Ethyl isobutyrate, and Camphene, most of which confer a grassy aroma alongside with floral and fruity notes and potentially contribute to the fresh smell of the GZAS samples. Among them, Limonene, 4-Methyl-3-penten-2-one, 1-Propanethiol, Ethyl butanoate, gamma-Terpinene, and Ethyl pentanoate had the strongest correlation with the GZAS samples. Thus, they might be the key contributing volatiles to the characteristic aroma of the GZAS samples. The compounds with high correlation with the GZPA samples were 2-Methylpropanoic acid, (E)-2-Nonenal, o-Xylene, Methyl acetate, Hexanal, 1-Propanol, 2-Butanone, 3-Methyl-1-butanol, 3-Methyl-2-butenal, 2-Methylpropanal, 2-Acetyl-1-pyrroline, Pyridine, and 3-Hydroxy-2-butanone, which contribute to the sweet smell of the PA black tea. 2-Methylpropanoic acid, (E)-2-Nonenal, o-Xylene, Methyl acetate, Hexanal, 1-Propanol, and 2-Acetyl-1-pyrroline exhibited the strongest correlation with the GZPA samples. Thus, they might be the key contributing volatile compounds to the aroma of the GZPA tea samples. The compounds with high correlation with the GZDY sample were 3-Methylbutanal, 2-Methylpropanal, Pentanal, 3-Hydroxy-2-butanone, Acetophenone, 3-Carene, Ethyl acetate, CS-2-penten-1-OL, Methional, Dimethyl sulfide, and Nonanal which can bring various flavors to GZDY black tea, including floral, fruity, nutty, and sweet flavors. Among

them, 3-Methylbutanal, 3-Carene, and Ethyl acetate strongly correlated with the characteristics of the GZDY sample, suggesting that these compounds might be the distinct aroma compounds in the GZDY sample.

3.1.6. Summary of the Volatile Compound Profiles in Different Black Tea Samples. In summary, GC-IMS technology was implemented to determine volatile compounds from 4 black tea samples from Guizhou and 2 black tea samples from regions outside of Guizhou. A total of 184 volatile compounds were detected, and 143 compounds were annotated through database comparisons. Among them, 30 aldehydes (accounting for 21%~27% of total volatile compounds), 30 alcohols (16%~24% of total volatile compounds), 26 ketones (21%~28% of total volatile compounds), 21 heterocyclic compounds (7%~14% of total volatile compounds), and 18 esters (4%~7% of total volatile compounds), 9 terpenes (1% of total volatile compounds), 5 acids (11%~21% of total volatile compounds), and 4 sulfides (2%~3% of total volatile compounds) were analyzed by OPLS-DA. The results showed that OPLS-DA could effectively distinguish the black tea samples from different regions. By calculating the VIP and OAV values of the volatile compounds in the samples, a total of 83 important volatile aroma compounds were selected. After analysis by PLS-DA and cluster analysis, the distinctive aroma compounds of black tea samples from different regions in Guizhou were identified. The analysis of the main aroma compounds in the black tea samples from different regions revealed that three samples, GZAS, GZPA, and GZDY, had high similarity. Similarly, the GZZY and WY samples had a high similarity, consistent with the OPLS-DA and PLS-DA results. At the same time, although no significant difference in volatile compounds between Guizhou black tea samples and non-Guizhou black tea samples was found, distinct flavor compounds were identified in black tea samples from different regions. The distinctive aroma compounds in the WY sample were Dimethyl disulfide, 2-Propanol, 1-Hexanol, alpha-Terpinene, 2, 5-dimethylpyrazine, and 5-Methyl-3-heptanone. The distinctive aroma compounds in BS samples were cis-4-Heptenal, 1-Penten-3-one-D, Diacetyl, beta-Pinene, Phenylacetaldehyde, and (E, E)-2, 4-Hexadienal. The distinctive aroma compounds in the GZZY sample were Limonene, 4-Methyl-3-penten-2-one, 2-Pentylfuran, 1-Propanethiol, Ethyl butanoate, gamma-Terpinene, and Ethyl pentanoate. The characteristic aroma compounds in the GZAS sample were Limonene, 4-Methyl-3-penten-2-one, 2-Pentylfuran, 1-Propanethiol, Ethyl butanoate, gamma-Terpinene, and Ethyl pentanoate. In GZPA samples, the distinctive aroma compounds were 2-Methylpropanoic acid, (E)-2-Nonenal, o-Xylene, Methyl acetate, Hexanal, 1-Propanol, and 2-Acetyl-1-pyrroline, while in the GZDY sample, the characteristic aroma compounds were 3-Methylbutanal, 3-Carene, and Ethyl acetate.

3.2. Effects of Environmental and Meteorological Factors on the Formation of the Characteristic Flavor of Black Tea. Through HS-GC-IMS analysis, the distinctive flavor components of black tea samples from various origins were identified. However, it was also observed that the similarity in volatile components between the GZZY sample, a black tea produced in Guizhou Province, and the WY sample, a black tea produced in Fujian Province, was higher than that of other black teas from Guizhou Province. To investigate this phenomenon further, the researchers conducted the following study.

3.2.1. Effects of Environmental Factors in Different Black Tea Regions on Volatile Components of Black Tea. Through the weather website, we checked the annual climate conditions of each producing area. It was found that the sample producing areas with similar volatile components had similar climate conditions. Therefore, it was speculated that environmental factors may be one of the reasons for the difference in volatile components of black tea.

At present, studies have shown that the synthesis of volatile components in plants is affected by environmental factors. For example, high temperature can promote the synthesis and subsequent release of floral and fruity terpene compounds by inducing and increasing the activity of enzymes related to MEP and MVA pathways. It can also significantly express LOX in plants, promoting the accumulation of related metabolites (alcohols, ketones, aldehydes, etc.), most of which can bring a sweet odor [33]. The average temperature of the WY region and GZZY region is higher than that of the other four regions. Therefore, the content of related volatile components in the WY sample and GZZY sample is significantly higher than that of the other four samples, making their floral, fruity, and sweet fragrance stronger. The shikimic acid pathway in plants is inhibited under long-term high-temperature conditions but can be activated under intense light and low-temperature conditions, thus promoting the synthesis of phenylpropane and aromatic compounds with sweet, floral, and nutty aromas in plants [34]. GZAS, GZPA, and GZDY, thanks to their high altitude, low average temperatures, and abundant sunlight, produce black teas that are fresh and light, with some nutty notes. This provides theoretical guidance for the study of the flavor of black tea produced in Guizhou. However, as GC-IMS technology is an emerging technology, its database is not complete and refined, and there are still many compounds that cannot be annotated, so it is

impossible to know whether these compounds are the key flavor compounds in black tea. We anticipate that GC-IMS results will become more precise as technology advances and GC-IMS data become more and more refined.

3.2.2. Relationship between C and N Stable Isotope Composition and Environmental Factors in Black Tea. Environmental and meteorological factors not only affect the synthesis of volatile aroma compounds but also have a great influence on the fractionation of stable isotopes in plants. Different environmental meteorological factors can alter the ratio of stable isotopes in plants. For example, the carbon isotope fractionation of carbon assimilated in organisms is affected by multiple environmental factors such as temperature, precipitation, light, and atmospheric pressure [35]. Specifically, in arid areas with low air humidity and strong evaporation, plants reduce stomatal conductance, decreasing intercellular CO_2 concentration and increasing the $\delta^{13}C$ value of carbon assimilated by photosynthates. During respiration, temperature also affects the CO_2 produced by the leaves and the $\delta^{13}C$ values of the main organic compounds of the leaves [35]. Nitrogen is an important biological element and one of the key components of amino acids, significantly impacting organisms' growth and development [36]. Nitrogen isotope fractionation in plant tissues is mainly affected by soil properties, fertilization, altitude, temperature, and other factors [37, 38]. For example, when the ambient temperature increases, the biological activity of nitrifying bacteria and ammoniating bacteria in the soil is enhanced. This accelerates the rate of soil mineralization and nitrification, leading to an increase in the content of soil ^{15}N, consequently raising $\delta^{15}N$ of plants [39–41].

Based on the aforementioned as a preliminary reference, it is hypothesized that there might exist a potential correlation between the volatile components of black tea and its internal isotopic compositions. By measuring the $\delta^{13}C$ and $\delta^{15}N$ values of black tea samples from six distinct regions, in conjunction with local environmental factors, we assessed the relationship between environmental factors and isotope fractionation across different regions, with the aim of establishing a relational model capable of reflecting both the isotope ratios and volatile composition of black tea.

The stable isotope ratios of black tea samples from 4 Guizhou regions and 2 non-Guizhou regions were obtained, as shown in Table 3. In addition, the $\delta^{13}C$ values of the samples from Guizhou province ranged from −28.71‰ to −25.37‰, while the $\delta^{15}N$ values ranged from 0.75‰ to 3.31‰. The $\delta^{13}C$ values of the WY samples ranged from −26.11‰ to −25.52‰, while the $\delta^{15}N$ values ranged from 2.77‰ to 2.99‰. Furthermore, the $\delta^{13}C$ and $\delta^{15}N$ values of BS samples ranged between −27.53‰ and −26.44‰ and between 0.02‰ and 0.22‰, respectively.

In order to investigate the impact of environmental and meteorological factors on the ratio of stable isotopes of carbon and nitrogen in plants, a quantitative prediction model was developed using PLS analysis of the environmental meteorological factors and the $\delta^{13}C$ values in each sample region (Figure 9). The quantitative prediction model results are shown in Table 4. As R^2 and RPD increase, the RMSE decreases, and the model accuracy improves. The R^2 values of the $\delta^{13}C$ and $\delta^{15}N$ models were 0.09 and 0.63, respectively. The RMSE values were 0.94 and 0.64, respectively, and the RPD values were 0.94 and 1.06, respectively. This indicates that the $\delta^{15}N$ prediction model based on eight environmental and meteorological factors is more accurate than the $\delta^{13}C$ prediction model.

Further analysis of the importance of the model variables shows that if the VIP value of the environmental factor is all greater than 1, it indicates that the environmental factor has a significant impact on the ratio of carbon and nitrogen isotopes. The results are depicted in Figure 9. Variables with VIP values of carbon isotope ratios greater than 1 include annual rainfall, mean low temperature, mean high temperature, and altitude, indicating that temperature, rainfall, and altitude have significant effects on $\delta^{13}C$ values. In addition, the positive correlation coefficients of the four factors showed that the $\delta^{13}C$ value of black tea was positively correlated with the temperature and rainfall of the producing area and negatively correlated with the altitude of the producing area. Regarding the $\delta^{15}N$ values, four environmental factors, total rainfall, number of sunny days, number of cloudy days, and mean low temperature, had VIP values greater than 1. Among the four factors, only the normalized correlation coefficients of number of sunny days were negative, while those of the other three factors were positive. This result shows that the $\delta^{15}N$ value is affected by several factors, such as precipitation temperature and sunshine.

At present, a large number of studies show that when the environmental precipitation decreases or the soil moisture decreases, the water stress increases. In order to reduce water transpiration loss in the body, plants often close part of their stomata, reducing stomatal conductance and intercellular CO_2 concentration, resulting in an increase in plant $\delta^{13}C$ [42]. However, when the precipitation is too high or the soil moisture is too high, the soil microbial activity decreases, the respiration rate decreases sharply, the soil nitrification is inhibited, and the availability of soil inorganic nitrogen decreases, thus making the soil ^{15}N poor and resulting in the decrease of plant $\delta^{15}N$ [43]. According to Wang et al. [44], as the altitude increases, the temperature decreases, the atmospheric CO_2 partial pressure decreases, and the amount of CO_2 available to plants decreases. Plants, due to insufficient CO2 supply, cause carboxylase enzymes to be unable to fractionate 13C, leading to a direct synthesis of organic compounds, thereby resulting in an increase in plant $\delta^{13}C$.

In this study, the $\delta^{13}C$ and $\delta^{15}N$ values of black tea are positively correlated with the temperature of the producing area, which is consistent with the results of Julien et al. [35]. However, the correlation results of $\delta^{13}C$ and $\delta^{15}N$ values of black tea with environmental elevation and rainfall are different from the current mainstream research results. Water et al. [45] believe that the positive ratio of $\delta^{13}C$ value to environmental elevation may be due to the influence of regional water use efficiency and drought stress elimination.

Table 3: Stable isotope data of black tea samples from 4 Guizhou regions and 2 non-Guizhou regions.

Origins	δ^{13}C value			δ^{15}N value		
	Min value	Max value	Average ± standard deviation	Min value	Max value	Average ± standard deviation
WY	−26.11	−25.52	−25.79 ± 0.24	2.77	2.99	2.89 ± 0.09
BS	−27.53	−26.44	−26.97 ± 0.44	0.02	0.22	0.12 ± 0.08
GZZY	−26.97	−26.34	−26.67 ± 0.26	0.75	2.82	1.58 ± 0.89
GZAS	−26.43	−25.37	−26.08 ± 0.50	1.34	1.68	1.57 ± 0.16
GZPA	−28.50	−25.86	−26.83 ± 1.19	2.59	3.31	2.86 ± 0.33
GZDY	−28.71	−26.12	−27.77 ± 1.18	0.80	2.38	1.51 ± 0.65

Table 4: Partial least squares regression models of δ^{13}C and δ^{15}N.

Model	Model establishment			Model results		
	Variable number	Sample number for training dataset	Sample number for test dataset	R^2	RMSE	RPD
δ^{13}C	8	16	2	0.16	0.90	1.06
δ^{15}N	8	16	2	0.62	0.65	1.06

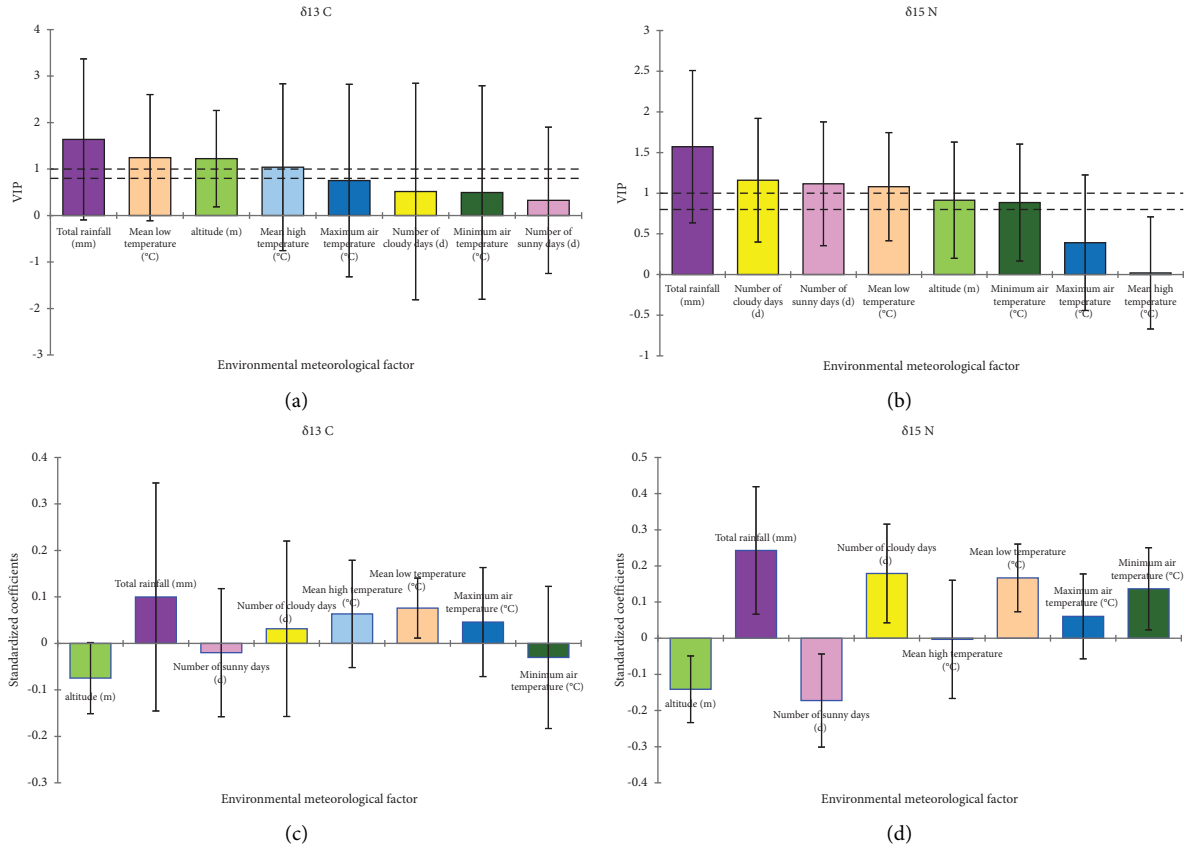


Figure 9: PLS analysis results of black tea samples from 6 regions.

In addition, Schulze [46], Heaton [47], and Codron [48] also found that the δ^{13}C and δ^{15}N values in plants were positively correlated with regional rainfall under some special circumstances. To sum up, the effects of other factors on the stable isotope ratio of black tea may be superimposed, making the situation more complicated. Therefore, the

mechanism of how various environmental factors affect the stable isotope ratio of black tea still needs to be further studied.

3.3. Summary of the Effects of Environmental Factors on the Formation of Volatile Components in Black Tea. According to the environmental and meteorological conditions of six black tea samples and the variation in volatile components in each sample, it was observed that the volatile components of black tea were significantly influenced by temperature, sunlight, and other factors. The levels of terpenoids, alcohols, ketones, and aldehydes in black tea samples were found to be higher in regions with elevated temperatures. These compounds contribute to the stronger floral, fruity, and sweet flavors characteristic of teas produced in these regions. In regions with slightly lower average temperatures and abundant sunshine, the plants contain higher levels of substances with fragrant, floral, and nutty aromas. This results in tea produced in these areas having a lighter, sweeter smell, a fresher aroma, and a hint of nuttiness.

In addition to the volatile components, external environmental factors also influence the internal isotopic composition of tea. The $\delta^{13}C$ and $\delta^{15}N$ values of black tea samples from six regions were detected, and a PLS-VIP regression model was used for analysis. The results showed that the $\delta^{13}C$ value of black tea samples was mainly affected by the temperature of origin, altitude, and rainfall. It was positively correlated with temperature and rainfall but negatively correlated with altitude. The $\delta^{15}N$ value is mainly affected by precipitation, temperature, and sunshine. It is positively correlated with precipitation and temperature but negatively correlated with sunshine.

Combined with the analysis of the relationship between the two and the environmental factors in the producing area, it was found that the content of volatile components in black tea samples was positively correlated with $\delta^{13}C$ and $\delta^{15}N$ due to the environmental temperature in the producing area, indicating that the stable isotope ratio in black tea samples may reflect the content of volatile components. However, due to the small sample size, this conclusion needs to be further studied after expanding the sample size.

4. Conclusion and Discussion

In this study, GC-IMS technology was implemented to determine volatile compounds from 4 black tea samples from Guizhou and 2 black tea samples from regions outside of Guizhou. A total of 184 volatile compounds were detected, and 143 compounds were annotated through database comparisons. The data were analyzed by OPLS-DA, and the results showed that the HS-GC-IMS could effectively distinguish black tea samples from different regions. By calculating the VIP and OAV values of the volatile compounds in the samples, a total of 83 important volatile aroma compounds were selected. After analysis by PLS-DA and cluster analysis, the distinctive aroma compounds of black tea samples from different regions in Guizhou were identified. The distinctive aroma compounds in the GZZY sample were Limonene, 4-Methyl-3-penten-2-one, 2-Pentylfuran, 1-Propanethiol, Ethyl butanoate, gamma-Terpinene, and Ethyl pentanoate. These substances give GZZY samples strong floral and fruity aromas. The distinctive aroma compounds in the GZAS sample were Limonene, 4-Methyl-3-penten-2-one, 2-Pentylfuran, 1-Propanethiol, Ethyl butanoate, gamma-Terpinene, and Ethyl pentanoate. These substances give the GZAS sample a fresh grassy, floral, and fruity aroma. The characteristic aroma compounds in GZPA samples were 2-Methylpropanoic acid, (E)-2-Nonenal, o-Xylene, Methyl acetate, Hexanal, 1-Propanol, and 2-Acetyl-1-pyrroline. These substances have a strong sweet fragrance, which makes the GZPA sample smell with some honey odor; and in the GZDY sample 3-Methylbutanal, 3-Carene and Ethyl acetate. In addition, among the black tea samples from the other two regions, the characteristic flavor substances in WY black tea are Dimethyl disulfide, 2-Propanol, 1-Hexanol, alpha-Terpinene, 2, 5-Dimethylpyrazine, and 5-Methyl-3-heptanone. These ingredients give WY sample a special dry longan aroma. The characteristic flavor substances in BS black tea samples were cis-4-Heptenal, 1-Penten-3-one-D, Diacetyl, beta-Pinene, Phenylacetaldehyde, and (E, E)-2, 4-Hexadienal which gave BS black tea samples a strong fruity flavor.

In addition, through the investigation of the climate environment of different producing areas, combined with the analysis of the volatile component content and stable C and N isotope ratios in each sample, it was found that the formation of volatile components in black tea was greatly affected by ambient temperature and light. In the regions with higher temperature, the volatile components with floral, fruity, and sweet aroma were higher, and the black tea had a stronger aroma. In the regions where the temperature is low but the light is strong, the fragrant and nutty components in black tea are higher, and the aroma of black tea is relatively elegant and fresh. At the same time, it was found that the stable C and N isotope ratios in black tea were also significantly affected by ambient temperature and were positively correlated.

This study examined how characteristic flavor compounds and environmental factors affect the flavor of Guizhou black tea. It offers a theoretical framework for optimizing planting conditions and enhancing product quality. Additionally, it sets a new direction for in-depth research on Guizhou black tea and contributes positively to the industry's development.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Authors' Contributions

Yonghui Ge was responsible for project administration, supervision, and review and editing. Yongji Huang was responsible for investigation, review and editing, visualization, software, and manuscript revision. Ling Wang was responsible for conceptualization, methodology, software, validation, formal analysis, original draft preparation, and visualization. Luyu Jia was responsible for investigation, resources, and validation. All authors have read and approved the manuscript.

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