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Original Article

Identification of key volatile flavor compounds in cigar filler tobacco leaves via GC-IMS

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Abstract

Cigar filler leaves are the most important component of cigar because they determine its quality. Therefore, the volatile components of eight cigar filler tobacco leaves were studied and compared using gas chromatography–ion mobility spectrometry (GC–IMS). In this study, 84 compounds with high levels of nitrogenous and ketone compounds were identified. Based on the chemometric principal component analysis (PCA) and partial least squares discriminant analysis (PLS-DA), the eight cigar samples were significantly distinguished. Meanwhile, we performed a discriminant analysis of volatile organic compounds in the eight cigar samples based on the variable importance in the projection (VIP) scores of the PLS-DA model, and revealed significant differences in the volatile compounds between the different varieties. 11 volatile compounds (VIP > 1) were screened and compared, among which triamine, acetic acid, acetone, and cyclopentanone were the main differential compounds/flavor substances. This study showed that GC–IMS can rapidly identify and compare the volatile compounds of various cigars, providing a theoretical basis for studying the differences in the volatile aroma of cigars, and laying a foundation for the breeding selection of subsequent varieties.

Keywords: Cigar filler tobacco leaves, Volatile flavor compounds; Gas chromatography–ion mobility spectrometry, Principal component analysis, Partial least squares-discriminant analysis

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Introduction

Cigar tobacco is an important non-food agricultural crop consumed worldwide because of its unique aroma and taste (Allem et al., 2019; Wen and Huang, 2021). Cigar filler tobacco leaves (CFTLs) are an essential component of cigar tobacco, accounting for 70–85% of the weight of the cigar and determining its smoking quality, commodity value, and industrial prospects (Zheng et al., 2022). Generally, CFTLs must undergo additional fermentation before being used in cigars, which can produce several volatile flavor compounds (VFCs) with characteristic flavors (Cornacchione et al., 2022; Yang et al., 2022). Previous research has shown that VFCs in cigar leaves are complex and diverse and include terpenes, aldehydes, alcohols, ketones, esters, and sulfur-containing substances (Kaneko and Harada, 1972). With the development of chromatography–mass spectrometry, more than 100 characteristic flavors have been detected in cigars, including sulfides, terpenes, and aldehydes (Vu et al., 2021; Zhang et al., 2021a). In China, the raw materials of the cigar are mainly imported from Cuba, Dominica, Brazil, and Indonesia (Ying et al., 2018;). The cultivation of CFTLs in China is still in its infancy, therefore the characteristic VFCs of Chinese CFTLs are still unclear (Gao et al., 2015; Ying et al., 2018; Wang et al., 2022). Due to the diversified introduction channels and scattered preservation, various reasons such as repeated naming lead to the unclear genetic relationship between cigar germplasm in China, which brings inconvenience to the quality identification and the promotion and application of superior lines of cigar. Therefore, it is of great significance to study the key VFCs in cigar tobacco leaves that cultivated in China for the understanding and preservation of domestic cigar tobacco germplasm resources. The current research is mainly focused on volatile compounds in cigar, including the extraction, separation, mass spectrometric analysis of characteristic flavor compounds, and exploration of principal flavor components of raw cigar materials that cultured in China. However, there are no systematically reports on the identification and differential analysis of key VFCs in different strains of cigar raw materials in China.

Gas chromatography (GC)–mass spectrometry, GC–olfactometry, and electronic noses are usually employed to identify volatile aroma compounds in tobacco (Rambla-Alegre et al., 2014; Liu et al., 2018; Qi et al., 2022; Zheng et al., 2022). Among these, gas chromatography–ion mobility spectrometry (GC–IMS), which is more sensitive than previous technologies, has emerged. GC–IMS combines the high separation ability of GC with the high sensitivity of IMS and does not require sample pretreatment (Li et al., 2019; Wang et al., 2020; Gu et al., 2021; Li et al., 2022). Studies on drug detection (Li et al., 2022), environmental quality monitoring (Zheng et al., 2022), and food flavor analysis (Wang et al., 2020) demonstrated that trace amounts of VFCs can be rapidly detected through processing.

In our study, GC–IMS was used to detect and identify VFCs in the tobacco leaf raw materials of eight main cigar varieties. Principal component analysis (PCA) was used to analyze the differences in flavor compounds among the different cigar samples. The key VFCs in cigar tobacco raw materials were studied using the variable importance in the projection (VIP) analysis method (Mao et al., 2018). Finally, fingerprints of the volatile flavors of each cigar material were constructed to identify the differences in the volatile compounds among the different materials. The rapid identification of cigar varieties and the efficient differentiation of the flavors of cigar tobacco raw materials will provide a theoretical basis for the qualitative analysis of cigar tobacco raw materials and the research and development of high-quality domestic cigar products.

Material and Methods

Samples and CFTLs preparation

Eight cigar filler tobacco leaves (CFTLs) samples of different varieties were planted and collected from the Chinese Tobacco Hubei Industry Co., Ltd., Wuhan City, Hubei Province (111.34555E, 30.78724N) in 2021. For each sample, 2 kg of the material was collected and dried according to the technical regulations for air-drying high-quality cigars. After drying, the CFTLs were placed in a constant-temperature-and-humidity box at 45 °C and 80% humidity for initial fermentation. After fermentation, the CFTLs were removed and immersed in liquid nitrogen for rapid pre-cooling, stored in a Ziplock bag at −80 °C until further use.

GC–IMS analysis

For the analysis, 1.0 g of each CFTLs was added to a 20 mL headspace bottle sealed and incubated under heating at 80 °C for 20 min at 500 rpm. After cooling to 25°C, the material was injected into a GC injector (Agilent Technologies, Palo Alto, CA, USA) equipped with an MXT-WAX column (30 m × 0.53 mm, film thickness: 1 μm) at a column temperature of 60 °C. High-purity nitrogen (purity > 99.999%) was used as carrier gas. The carrier gas flow rate program was as follows: 2.0 mL/min for 10 min, linear increase to 10.0 mL/min for 10–20 min, and linear increase to 100.0 mL/min for 20–40 min. The flow was then stopped for a total run time of 40 min. The IMS conditions were set as follows: the length of the drift tube was 98 mm, the operating temperature was 60 °C, and the nitrogen concentration was 150 mL/min. The linear voltage inside the tube was 500 V/cm, and the average number of spectral scans was 12. Each GC–IMS analysis was conducted in triplicate.

Qualitative and quantitative analysis of VFCs

By comparing the retention index (RI) and drift time in the GC–IMS library, the VFCs in the CFTL samples were identified. The calculation of the RI for the volatile compounds in the detected material was based on the external standard N-ketone C4–C9. VFCs in CFTLs were identified by comparing the RI to the standard drift time (the time required in milliseconds by ions to reach the collector through the drift tube) in the GC–IMS library using the GC × IMS library search software. Finally, the intensities of the volatile compounds were analyzed according to the peak volumes of the selected signal peaks.

Statistical analysis

Sample analysis was conducted using the VOCal analysis software and three plug-ins (Reporter, Gallery Plot, and Dynamic PCA) built into the device. The 2014 NIST and IMS databases built into the GC × IMS library search software were used for the qualitative analysis of the flavor compounds. Differential maps and fingerprints of VFCs were constructed. SPSS Statistics 21 software was used for variance analysis, and the statistical significance was set at $P < 0.05$. Partial least squares discriminant analysis (PLS-DA) was performed using the website https://www.metaboanalyst.ca/, and Origin 8.6 was used for drawing.

Results

Analysis of VFCs in different CFTLs using GC–IMS

The GC–IMS two-dimensional top view of the volatile compounds in different CFTLs was generated using the Reporter plug-in. As shown in Figure S1, most signals appeared at retention times of 100–1000 s and drift times of 0.3–1.5 s. The compositions of VFCs in the eight CFTLs were the same; however, the VFCs contents were considerably different. In Figure S1, substances exhibiting large differences in their content are mainly concentrated in the red and yellow boxes. Spectrum discrimination showed that the VFC content in the Hainan No. 3, Chuxue No. 14, and Dexue No. 4 samples was relatively high, whereas Yongsheng No. 2, Chuxue No. 80, and Chuxue No. 81 exhibited a relatively low content.

Qualitative and quantitative analysis of VFCs in different varieties of cigar leaves

The ion migration time and RI were used to qualitatively identify VFCs in the detected samples. Totally, 111 peaks were detected in the tobacco leaf samples, and 93 compounds were identified using the NIST 2014 and IMS databases (Figure 1 and Tables S1 and S2), including 12 esters, 4 alkenes, 17 ketones, 4 acids, 20 aldehydes, 13 alcohols, 3 sulfur compounds, 10 nitrogen-containing compounds, and 10 other classes. The monomeric and dimeric forms of nine compounds (acetic acid, sanyamine, cyclopentanone, hexanal, butanol, glutaraldehyde, ethanol, butanal, and propanal) were included. Therefore, 84 compounds were totally identified in the final determination of cigar tobacco samples.

In addition, the quantitative analysis of volatile compounds in these cigars was expressed as the peak volume calculated using the IMS system (Table S1). Among which, nitrogen was the main component in the eight samples, with a content accounting for more than 66%. Chuxue No. 80 exhibited the highest nitrogen content (77.77%) and the main nitrogen-containing compounds were triimine and 2-acetylpyridine. The ketone contents of the different varieties were significantly different: The highest ketone content was observed in Chuxue No. 80 (71.3%) whereas Chuxue No. 81 exhibited the lowest value (14.29%). Additionally, Chuxue No. 81 (7.49%) had the highest aldehyde content, whereas Chuxue No. 80 (5.79%) had the lowest. Dexue No. 4 exhibited the highest alcohol content (6.78%), whereas Chu Xue No. 4 (6.78 %), Chu Xue No. 80, and Chu Xue No. 14 (3.53 %) exhibited lower contents.

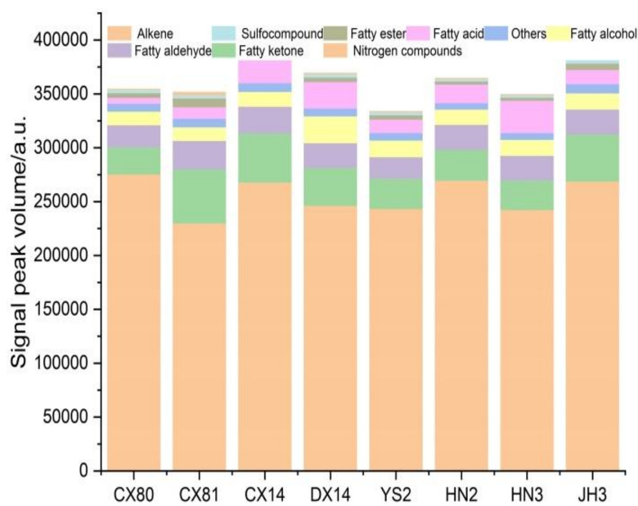

Figure-1. Contents of volatile components in different cigar leaves.

Fingerprint analysis of volatile components in different CFTLs

According to the volatile components in the leaves of different CFTLs, specific volatile components were analyzed in depth. The GalleryPlot plug-in was used to draw the fingerprints of VFCs in the different CFTLs (Figure 2) to visually compare and quantitatively analyze them. As shown in Figure 2, box A shows the characteristic peak area of the 20 VFCs that were detected in all the tested samples. The main compounds identified were aldehydes and ketones, including 2-hexenal, 3-methyl-2-butenal, acrolein, benzaldehyde, hexanal-D/M, methacrolein-D/M, nonanal, valeraldehyde-D/M, 2-butanone, 3-methyl-2-pentanone, 6-methyl-5-hepten-2-one, acetone, cyclopentanone-D, and triimine-D/M. Box B shows that the signal intensity of Chuxue No. 81 was significantly higher than that of the other varieties, mainly including esters and alkenes such as butyl acetate, ethyl 3-methyl butyrate, ethyl butyrate, ethyl isobutyrate ester, hexyl acetate, isobutyl acetate, pentyl methyl 3-methyl butyrate, beta-pinene, limonene, and styrene. Box C indicates that the signal intensity of ketones in Chuxue No. 14 was significantly higher than that of the other varieties, including 1-hexanol, tert-butanol, cyclohexanone, diisobutyl ketone, 1-octen-3-one, 2,3-pentanedione, 4-methyl-2-pentanone, 5-methyl-3-heptanone, (E)-2-heptenal, 2, 6-Dimethylpyridine and benzene. Box D indicates that the signal intensities of alcohols, ketones, and nitrogen-containing substances in Dexue No. 4 were significantly higher than those of the other species, including 1-butanol, 1-penten-3-ol, 2-butanol-D /M, furfuryl alcohol, hydroxyacetone, 1-penten-3-one, 2,5-dimethylpyrazine, and 2-ethyl-5-methylpyrazine. Box E indicates that the signal intensity of acetophenone in Yongsheng No. 2 was significantly higher than that in the other varieties. Box F indicates that the signal intensities of 2-isovaleraldehyde-D, 2-methylpropanal, 2-methylpyrazine, 3-methylbutanal aldehyde-M, and methyl acetate in Hainan No. 2 and Hainan No. 3 was significantly higher than those of the other varieties. Box G indicates that the signal intensity of Jianheng No. 3 was significantly higher than those of the other varieties, including n-propanol, 2-methylpropanol, cyclopentanone-M, 2-pentanone, 3-pentanone, dipropylene glycol monobutylene ether, acetaldehyde, acrylonitrile, diacetyl, ethyl acetate, ethyl lactate, 2-ethylpyrazine, gamma-terpinene, hexyl isobutyrate, and thiophene. The quantitative results demonstrated the differences in the volatile compounds among the eight cultivars.

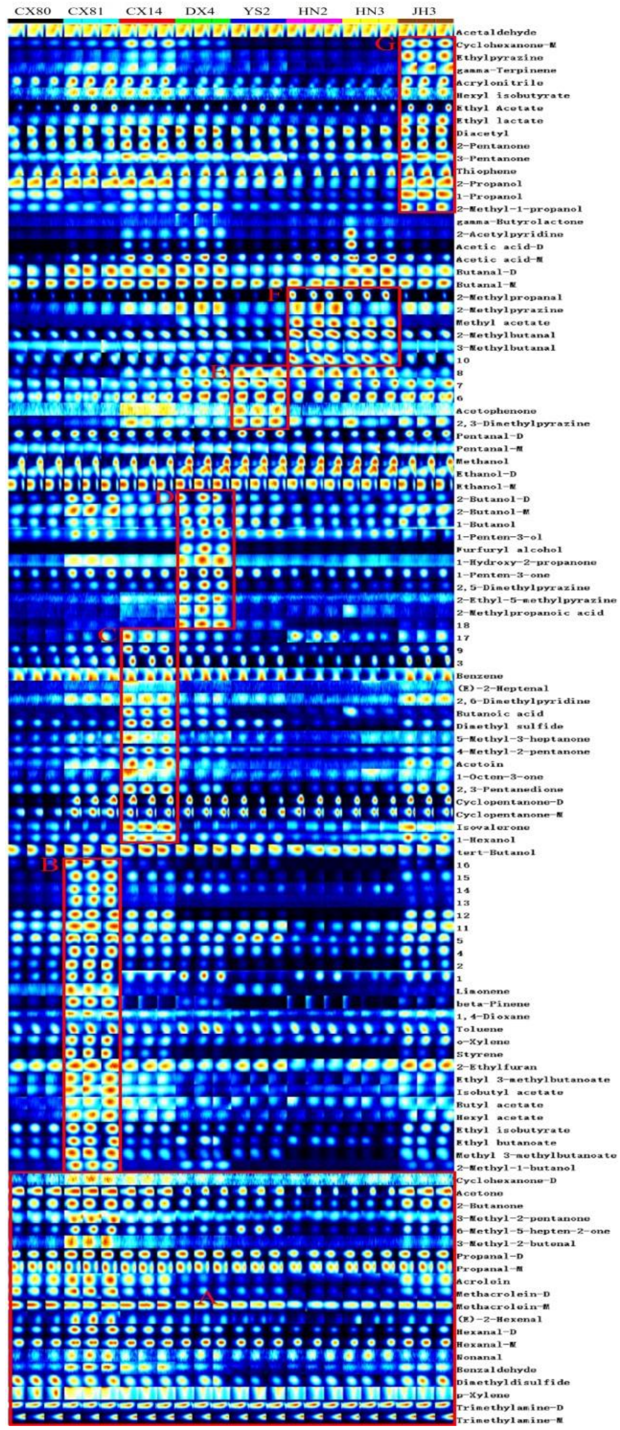

Figure-2. VFCs fingerprint from different cigar leaves;

Each row represents different varieties of cigar samples (3 parallels/sample). Each row is composed of the signal peaks of the volatile compounds contained in the corresponding sample, and each column represents different volatile compounds. The signal peaks represent intensity of the compound. The brightness of the spot represents the concentration of the corresponding volatile compound. Here, monomers and dimers of the same compound were characterized using different columns with the same compound name. Additionally, a small number of volatile compounds were not accurately characterized and are presented in the form of Arabic numerals.

PCA plot for differentiating the volatile compounds in different varieties of cigar leaves

The Dynamic PCA plug-in was used to conduct PCA based on the content (signal peak volume) of volatile compounds in the different varieties of the detected cigar leaves. Distributions of the first and second principal components were obtained through data visualization (Figure 3). The variance contribution rates of the first two principal components were 49% and 17%. The distances between the samples within each variety were similar, showing good parallelism, and the distances between the samples of each variety were significantly separated. By combining PC1 and PC2, the eight cigar samples were divided into six groups: Hainan No. 2 and Hainan No. 3 were classified in the same group, and Chuxue No. 14 and Jianheng No. 3 were categorized in another group, indicating that they had similar volatile compound compositions. However, the other four cigar varieties were clustered into one group, and the distance between them was relatively large, indicating the composition of volatile compounds of these four varieties differed greatly from each other.

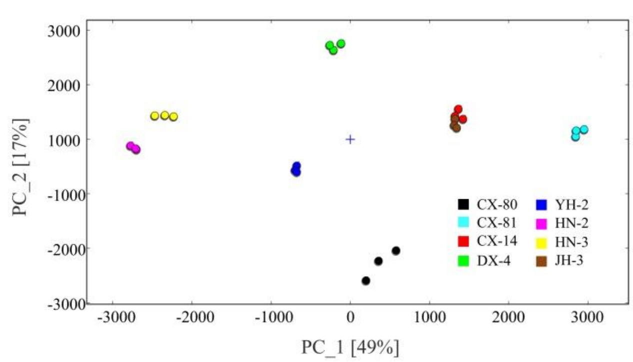

Figure-3. PCA plot for differentiating the volatile compounds of the different cigar samples.

GC–IMS analysis of VFCs in different varieties of cigar leaves

To further explore the key substances causing differences between the tobacco varieties, the VIP scores of all volatile compounds were calculated based on the PLS-DA model, and "VIP> 1" was used as the standard for screening. In this study, 11 (VIP > 1) marker volatile compounds were screened according to the VIP values (Figure 4), among which triimine-M and acetic acid of VIP > 3 were the most important differential compounds, followed by acetone and cyclopentanone-D (2 < VIP < 3), which contributed significantly to the overall difference. Additionally, hexanal, 2-isovaleraldehyde, ethyl isobutyrate, 2-butanone, furfuryl alcohol, methyl 3-methyl butyric acid, amyl, and propionaldehyde (1 < VIP < 2) were important differential compounds. Chuxue No. 80 exhibited the highest triamine-M content, followed by Jianheng No. 3. The highest acetic acid content was found in Hainan No. 3, followed by Dexue No. 4. The highest acetone content was observed in Chuxue No. 81, followed by Jianheng No. 3, and Chuxue No. 80. Furthermore, the cyclopentanone contents in Chuxue No. 81 and Chuxue No. 14 were higher than those in the other varieties. The hexanal contents in Chuxue 81 and Chuxue 14 were the highest among all species. Hainan No. 2 and Hainan No. 3 exhibited a higher content of 2-isovaleraldehyde. Moreover, higher ethyl isobutyrate and furfuryl alcohol contents were observed in Chuxue 81 and Dexue 4. Additionally, the amyl methyl 3-methyl butyrate content was higher in Chuxue No. 81. Chuxue No. 81, Chuxue No. 14, and Dexue No. 4 were rich in propionaldehyde.

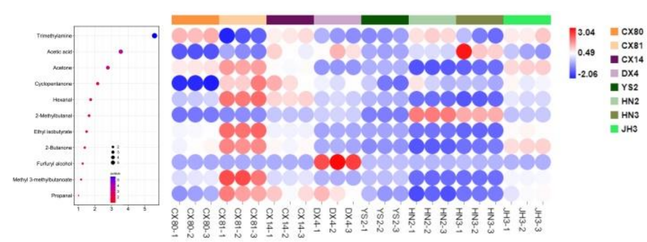

Figure-4. Variable importance in projection scores.

Discussion

Cigar tobacco is an important economic crop that is widely grown worldwide because of its special aroma and taste, which is made from dried and fermented cigar leaves (Allem et al., 2019). At present, most of the cultural cigar species in China are imported, leading to relatively scarce germplasm resources of cigar tobacco in China (Yang et al., 2022; Zheng et al., 2022). Therefore, the cultivation and production of cigar filler tobacco leaves in China are still in their primary stages, and more research should be conducted to explore the germplasm resource presentation, explore the quality differences among different varieties, and identify suitable varieties of cigars in China. As an important flavor substance, the volatile aroma components of cigars are complex and diverse, which determines their smoking quality, commodity value, and industrial prospects. Typically, cigar compounds can be detected using GC–MS (Zheng et al., 2022; Ng et al., 2001). In this study, we used GC–IMS to detect and analyze the key VFCs in eight major CFTLs in China. Totally, 84 volatile compounds were identified: 12 esters, 4 alkenes, 16 ketones, 3 acids, 16 aldehydes, 11 alcohols, 3 sulfur-containing compounds, 10 nitrogen-containing compounds, and 10 other compounds. The quantitative and qualitative results showed that the CFTLs samples mainly contained nitrogen-containing VFCs, followed by ketones, aldehydes, and alcohols. Among these, aldehydes are considered to contribute more to flavor because of their high concentration, low threshold, and high volatility (Zhang et al., 2021a; Wang et al., 2022). In addition, studies have shown that aldehydes were first hydrolyzed by lipids to form free fatty acids; these saturated and unsaturated fatty acids were then thermally decomposed to form hydroperoxides under normal conditions (Kim et al., 2022). Alcohol compounds generally derive from the degradation of secondary hydroperoxides of fatty acids or the reduction of carbonyl compounds (Lawyer et al., 2019). This study revealed significant differences of VFCs between the tested CFTLs, indicating that these differences are the important factors responsible for the different flavor characteristics and sensory qualities of the cigars (Zhang et al., 2021b).

To explore the key VFCs in different CFTLs, all volatile compounds were analyzed using fingerprints, PCA, and PLS-DA. The similarities and differences in the volatile compounds among the different varieties were clarified, and the eight varieties were divided into six groups. Significant differences were observed in the structures of flavor substances. Chuxue No. 14, Jianheng No. 3, Hainan No. 2, and Hainan No. 3 exhibited similar flavor substance structures, which can provide a reference for the blending of tobacco leaves in industrial production. The contribution of all identified volatile compounds to the structural differences in flavor compounds was studied using VIP analysis, and 11 marker compounds with important contributions to the structural differences in flavor compounds were selected. Among these, triamine-M and acetic acid were identified as the most important differential markers, followed by acetone and cyclopentanone D. Acetic acid and acetone are important and common aromatic substances in cigars and are known to impart pungent odors (Li et al., 2023). Other compounds such as hexanal, 2-isovaleraldehyde, ethyl isobutyrate, and 2-butanone, which endow CFTLs with typical fruity and ethereal properties, are also important differential flavor compounds (Baker et al., 2004). Our study revealed that each cigar variety exhibits characteristic marker compounds in different contents. For example, signal intensity of esters and alkene in Chuxue No. 81 are significantly higher than that in the other varieties., and so as to the ketones in Chuxue No. 14, the alcohols in Dexue No. 4, and the acetophenone in Yongsheng No. 2, which may be the main reason for the flavor differences between the different varieties. Yu et al. (2021) used GC–MS analysis and revealed that the biomarkers of two volatile compounds screened on cigar raw materials were α-curcumene and cedrol, which differs from our results. The differences in volatile compounds among the different varieties can affect the results, whereas the detection ability of GC–IMS and GC–MS may lead to such differences. The volatile components detected by GC–IMS were mostly small molecules with high volatility and low contents, and the detection time was short. Thus, GC–IMS can rapidly identify volatile compounds in different varieties of cigar leaves, as well as the flavors of different samples (Zeki et al., 2020). However, the correlation between the flavor substances in cigar leaves, style characteristics of cigars, and the mechanism of their influence on the sensory quality of cigars among the different varieties requires further research.

Conclusion

In this study, we used GC–IMS to detect, analyze, and build the fingerprints of volatile compounds contained in eight major Chinese CFTLs. We identified and classified 84 volatile compounds, mainly composed of nitrogen, ketones, aldehydes, alcohols, and esters. The GC–IMS fingerprint of the flavor substances contained in cigar tobacco is an efficient tool for the effective identification of the different varieties of cigar tobacco. Additionally, the exploration of key differential volatile compounds can help in revealing the mechanism of flavor differences in the different cigar varieties. This study provides data support for the application of GC–IMS analysis in the rapid grading of cigar tobacco leaves as well as a theoretical basis for studying the flavor-formation mechanism of cigar tobacco leaves. The correlation between these findings via GC-IMS and via GC-MS should be further studied.

Supporting information: Figure S1. Two-dimensional GC–IMS spectra of the different cigar tobacco leaves. The ordinate represents the retention time of the volatile compounds during GC separation. The background of the entire graph is blue, the abscissa represents the ion migration time and the red vertical line at 1.0 of the abscissa is the RIP peak (reactive ion peak, normalized). Each point on the right side of the RIP peak represents a volatile compound and the color indicates the signal intensity of a single compound. Red represents high intensity and blue represents low intensity. **Table S1.** Analysis of volatile organic compounds in different varieties of cigar leaves. **Table S2.** Peak position and volume of each compound.

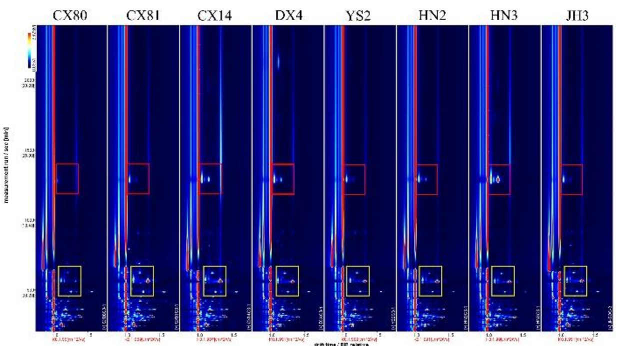

Figure S1. Two dimensional GC–IMS spectra of the different cigar tobacco leaves

Table-1: Analysis of volatile organic compounds in different varieties of cigar leaves

Name	Molecular formula	Retention index	Retention index/s	Drift time/ms	Signal peak volume /a.u.							
					CX80	CX81	CX14	DX4	YS2	HN2	HN3	JH3
gamma-Butyrolactone	C4H6O2	1711.1	2009.558	1.0904	436.58±23.47	471.33±44.34	484.31±11.88	609.92±15.34	449.69±12.55	542.97±29.11	600±77.18	487.74±43.61
2-Acetylpyridine	C7H7NO	1638.8	1717.593	1.11686	430.39±51.7	505.63±40.74	811.02±50.2	1005.78±115.39	514.77±46.93	553.42±26.89	964.93±429.92	487.98±59.23
Benzaldehyde	C7H6O	1551.3	1420.55	1.15887	315.74±19.37	605.52±36.74	464.51±17.54	342.37±44.55	244.35±27.52	277.2±23.82	281.05±28.99	473.12±8.71
Acetic acid-M	C2H4O2	1504.5	1283.453	1.05773	4352.2±275.34	8781.97±1645.09	15011.85±1247.79	16462.86±1691.04	10141.39±268.41	13187.88±447.8	18354.16±2526.2	10360.84±1560.49
Acetic acid-D	C2H4O2	1503.6	1280.914	1.15576	350.39±47.51	1102.5±413.71	5218.92±1385.23	5977.37±1281.7	1573.73±165.91	3072.38±142.67	10094.41±5849.88	1773.57±592.49
6-Methyl-5-hepten-2-one	C8H14O	1347.1	912.089	1.18021	554.81±92.05	1207.46±36.02	803.81±29.29	671.43±6.89	1023.82±21.98	316.74±22.57	311.8±12.98	801.16±26.14
1-Hexanol	C6H14O	1345.6	909.114	1.32839	671.87±101.6	859.86±37.49	1281.45±44.45	745.38±112.35	873.81±28.35	540.51±9.63	791.65±119.66	1148.63±87.18
Trimethylamine-M	C6H15N	1198.2	666.695	0.84871	171895.56±1547.69	127912.33±5008.94	167734.93±1415.76	139864.06±3145.22	137434.58±1920.76	164163.94±2465.54	136605.22±6333.01	168589.63±4299.14
Trimethylamine-D	C6H15N	1197.2	665.207	0.90521	102190.77±1444.66	100406.72±1193.46	98181.48±686.01	103938.36±661.62	104605.31±362.61	104096.21±978.44	104170.04±1890.12	98347.85±753.53
2,5-Dimethylpyrazine	C6H8N2	1313.6	848.138	1.10613	222.72±16.22	325.02±26.71	251.45±2.72	641.42±40	149.79±8.76	176.01±2.83	198.58±39.5	215.39±3.23
Styrene	C8H8	1281.2	791.623	1.04836	181.02±21.25	1276.62±76.84	503.19±26.83	121.94±16.52	148.49±39.39	108.01±30.8	75.22±7.45	332.91±19.53
(E)-2-Hexenal	C6H10O	1227.1	707.701	1.18042	125.63±9.83	264.95±15.21	167.62±0.84	165.12±7.89	149.52±7.16	89.11±8.12	147.95±22.58	145.19±18.97
Isovalerone	C9H18O	1195.1	662.33	1.33415	637.99±76.97	502.11±43.52	1601.18±47.9	511.54±136.4	509.43±7.59	733.99±63.34	856.96±35.84	1325.3±207.89
1-Butanol	C4H10O	1160.5	592.761	1.18498	401.55±17.81	525.76±15.95	431.19±29.49	576.62±39.8	481.95±10.26	382.95±37.16	365.32±17.3	506.53±30.09
Cyclopentanone-M	C5H8O	1143.5	560.245	1.1104	4477.49±409.65	7992.82±172.91	6815.21±448.88	6344.29±262.64	5624.33±651.62	6153.03±837.33	5584.59±104.34	6372.22±294.64
Cyclopentanone-D	C5H8O	1144.3	561.758	1.32349	2060.83±200.73	18534.6±3014.13	17290.16±2214.05	14126.89±908.44	8231.66±2963.77	13221.45±2666.83	10979.78±833.63	14708.64±756.49
p-Xylene	C8H10	1145.4	563.753	1.07393	553.92±17.09	273.65±50.07	282.72±36.79	377.72±58.5	492.63±90.83	333.47±72.81	405.25±22.3	427.33±156.91
2-Methyl-1-propanol	C4H10O	1107.7	497.493	1.16921	255.07±19.3	290.68±13.29	339.18±7.07	338.79±71.58	221.86±21.19	256.16±11.85	243.26±12.52	358.25±42.9
Hexanal-M	C6H12O	1101.4	487.217	1.25937	2668.27±61.23	3500.59±45.46	3064.12±15.27	2702.02±65.6	2557.82±32.67	2071.76±31.04	1945.42±75.88	2735.32±57.09
Hexanal-D	C6H12O	1101.7	487.795	1.56113	1717.59±58.04	3619.51±60.75	2672.74±48.74	1768.1±49.13	1426.18±40.65	896.82±26.31	784.5±50.34	1913.77±94.45
2,3-Pentanedione	C5H8O2	1077.9	453.718	1.22483	760.31±14.55	952.57±24.11	1320.94±5.77	659.48±25.19	306.39±3.3	326.49±3.49	367.32±27.84	1133.25±42.51

Toluene	C7H8	1063.9	435.235	1.04093	846.83±30.91	1326.31±37.3	1003.02±14.95	1121.58±145.92	854.72±17.54	984.86±27.77	909.01±24.77	1048.93±33.78
Ethyl butanoate	C6H12O2	1063.4	434.658	1.20044	173.49±9.69	445.63±18.7	182.48±8.47	266.67±64.65	104.21±14.85	204.58±15.08	146.61±13.66	239.08±39.29
Dimethyl disulfide	C2H6S2	1063.4	434.658	1.13948	316.76±7.13	299.45±15.98	209.75±10.28	243.03±13.41	134.22±1.09	214±12.03	197.14±13.62	269.33±15.36
1-Propanol	C3H8O	1053.4	421.951	1.11205	769.03±24.23	217.49±30.02	649.18±15.4	450.91±21.54	251.56±8.08	262.24±12.24	274.34±6.87	1061.62±59.07
Methyl 3-methylbutanoate	C9H18O2	1052.9	421.373	1.21263	840.74±44.88	1910.97±138.82	813.12±35.3	536.58±25.02	633.64±34.12	120.89±10.92	141.27±6.1	950.97±10.83
1-Penten-3-one	C5H8O	1042.1	408.089	1.07852	481.96±26.31	864.48±19.23	736.09±5.74	934.01±3.85	761.99±9.63	528.52±2.5	604.19±2.75	637.01±4.18
3-Methyl-2-pentanone	C6H12O	1035.4	400.003	1.18215	215.49±13.49	300.16±13.36	216.46±5.45	188.27±19.91	170.61±16.14	184.57±10.98	168.41±20.63	194.3±2.25
2-Butanol-M	C4H10O	1038.8	404.046	1.14456	137.15±7.97	218.15±20.05	142.07±6.32	176.99±15.78	148.21±4.44	122.23±4.81	116.97±8.98	179.41±2.89
2-Butanol-D	C4H10O	1040.2	405.779	1.30814	116.39±8.23	355.28±23.47	285.3±15.17	368.05±33.24	209.84±6.19	127.84±3.67	181.33±23.46	199.86±17.59
Thiophene	C4H4S	1030	393.65	1.03178	2060.48±78.59	2247.45±464.61	1952.72±23.86	2271.85±52.67	2076.02±58	1618.4±73.87	1891.38±97.75	2673.4±35.69
3-Pentanone	C5H10O	1029.5	393.072	1.11306	259.96±9.24	286.13±18.13	370.94±7.94	332.05±20.88	380.83±8.98	245.76±26.92	306.21±11.43	396.92±26.91
Acrylonitrile	C3H3N	1013.8	375.167	1.08258	427.37±12.31	551.18±24.72	456.39±1.48	343.41±3.36	307.88±5.52	206.69±5.81	221.97±3.31	562.94±16.68
4-Methyl-2-pentanone	C6H12O	1019.4	381.521	1.17402	920.34±40.17	1024.58±25.66	1424.16±15.06	1066.12±15.03	804.3±7.78	562.71±13.5	764.28±12.81	1141.24±26.6
Pentanal-M	C5H10O	1003.8	364.193	1.18114	1331.19±30.8	1139.19±21.62	1453.57±27.08	1551.75±145.29	1393.06±39.8	1394.6±143.73	1425.24±103.78	1487.36±8.98
Pentanal-D	C5H10O	1003.2	363.616	1.42397	2275.4±70.46	2665.19±32.16	2241.33±67.25	1921.64±7.13	2606.24±39.45	1600.37±43.51	1647.52±64.19	2416.09±98.48
2-Pentanone	C5H10O	1000	360.15	1.3498	1120.31±22.61	1273.86±30.11	1495.49±14.5	1196.85±35.4	1023.21±2.35	984.55±12.14	1019.78±34.5	1520.54±20.09
Benzene	C6H6	969.5	335.314	1.0267	755.35±9.46	739.37±94.53	816±13.2	854.78±9.4	762.91±8.81	634.55±13.4	600.2±4.64	770.6±7.2
Ethyl isobutyrate	C6H12O2	967.2	333.582	1.18622	1874.43±41.24	3285.64±68.72	1795.42±2.91	1065.78±27.68	1043.15±8.48	551.13±1.53	404.33±5.6	1975.94±40.31
Ethanol-M	C2H6O	946.7	318.473	1.04224	1679.66±25.47	1734±126.12	1859.46±87.78	2052.11±15.63	1988.03±27.86	1976.8±48.69	2007.66±51.8	1811.83±17.29
Ethanol-D	C2H6O	947.2	318.821	1.12682	2916.54±28.68	2581.71±50.35	2771±116.31	3788.38±70.24	3443.8±52.73	3153.32±85.08	3351.71±21.02	2983.22±6.11
3-Methylbutanal	C5H10O	938.3	312.55	1.16815	269.17±5.26	311.42±57.07	367.84±10.25	331.08±8.14	270.8±10.79	392.34±16.02	356.32±39.32	272.85±7.4
2-Propanol	C3H8O	947.2	318.821	1.22966	1664.43±51.22	1732.93±113.54	1822.71±99.25	1279.18±42.84	1337.89±13.85	795.57±35.37	836.58±30.21	1891.22±28.12
2-Methylbutanal	C5H10O	929.8	306.628	1.39497	2543.39±65.59	2919.29±35	3920.64±64.93	4187.87±63.77	2675.83±23.08	7269.34±10.54	6424.1±15.34	3984.73±78.15
Diacetyl	C4H6O2	998.2	358.188	1.16815	1836.27±45.46	1754.78±174.16	2238.38±152.17	1982.57±223.38	1630.07±99.63	1894.4±188.04	1879.52±232.35	2374.63±64.81
Methanol	CH4O	909.2	292.693	1.02687	3755.92±81.69	3411.51±126.1	3824.49±15.77	4841.21±110.67	4925.19±97.67	4699.51±185.85	4816.11±184.28	4445.14±38.8
2-Butanone	C4H8O	916.5	297.57	1.24792	2289.73±97.68	3277.88±51.04	2298.19±85.57	1527.32±46.16	1288±43.47	798.96±38.71	1043.15±47.98	2634.64±58.71
Ethyl Acetate	C4H8O2	899	286.073	1.3373	438.07±49.69	1128.87±37.09	806.51±41.13	708.11±40.71	1002.13±74.63	514.79±20.04	811.73±47.09	1276.16±9
Methacrolein-M	C4H6O	898	285.377	1.04609	672.55±20.86	646.01±76.99	692.93±30.87	639.54±22.11	635.61±13.09	511.47±25.03	533.57±17.62	628.47±22.67
Butanal-M	C4H8O	892.5	281.893	1.11144	600.51±15.27	675.51±10.66	715.93±30.19	746.26±13.64	659.48±18.74	757.88±4.59	833.22±12.99	686.3±14.38
Butanal-D	C4H8O	893.1	282.241	1.2854	291.25±8.99	410.83±10.63	406.51±7.79	400.53±14.34	273.55±4.57	260.15±46.17	397.57±60.71	358.77±3.39
Methacrolein-D	C4H6O	898	285.377	1.22101	1027.09±106.82	1387.54±36.76	847.31±44.41	615.43±16.35	597.52±21.53	350.1±9.96	439.81±5.53	728.73±29.58
tert-Butanol	C4H10O	928.3	305.583	1.15662	517.71±14.73	591.08±66.58	655.49±63.5	612.93±33.46	575.71±23.73	596.38±40.85	591.3±15.24	559.48±8.97
2-Methylpropanal	C4H8O	835.2	247.752	1.28444	272.72±3.63	305.06±8.22	405.5±15.34	566.38±6.31	204.26±9.99	1470.11±16.36	1520.62±19.67	368.24±15.64
Acrolein	C3H4O	867.1	266.216	1.08934	379.3±7.6	456.81±18.61	359.63±7.29	187.89±8.43	132.07±1.58	158.96±10.51	182.53±6.26	376.91±19.05
Methyl acetate	C3H6O2	851.1	256.809	1.03456	122.41±3.25	80.57±3.71	126.19±7.1	306.11±11.81	224.21±11.98	383.97±48.82	330.33±12.18	100.08±7.39
Acetone	C3H6O	842.6	251.932	1.11337	10958.04±143.57	13199.66±215.25	10197.57±180.56	6614.58±15.13	7514.64±53.11	4433.88±87.22	5112.33±243.89	11606.94±216.94
Propanal-M	C3H6O	821.9	240.436	1.04801	1534.03±24.61	1518.65±43.6	1504.8±17	1569.66±69.07	1447.25±43.74	1320.5±6.86	1498.75±49.26	1539.78±40.71
Propanal-D	C3H6O	822.5	240.784	1.14604	3875.6±75.17	5165.31±127.62	4716.1±175.89	4676.14±150.95	3985.45±76.05	3585.9±95.53	3631.14±37.4	4443.3±69.52
Dimethyl sulfide	C2H6S	796.8	227.197	0.95575	451.15±23.06	450.58±13.15	976.95±7	711.08±7.4	593.9±2.33	262.69±9.75	164.59±4.25	608.12±2.29
Acetaldehyde	C2H4O	774.4	216.049	0.96536	386.28±6.61	331.37±3.59	365.93±6.48	361.8±9.03	374.43±7.43	353.02±6.93	354.5±3.72	373.64±7.05
2-Ethylfuran	C6H8O	936.4	311.157	1.32289	948.06±32.59	1164.38±45.74	1010.06±25.54	820.11±13.89	936.57±14.47	587.7±38.85	869.98±9.65	1097.72±4.47
Nonanal	C9H18O	1399.3	1021.501	1.48151	161.93±19.9	264.46±23.9	209.32±15.1	237.94±17.83	211.34±19.8	231.53±13.31	263.89±33.05	186.44±6.96

1-Penten-3-ol	C5H10O	1176.6	625.367	0.94082	930.93±32	1226.38±63.54	1069.1±22.84	1550.6±4.31	1341.13±25.35	1141.18±53.95	1213.33±86.48	1189.39±269.3
Cyclohexanone-M	C6H10O	1298.6	820.984	1.16128	276.6±21.92	386.3±37.22	690.69±21.6	365.85±82.44	99.39±11.24	133.66±10.94	122.79±12.44	810.96±18.47
beta-Pinene	C10H16	1138.1	550.363	1.21943	131.74±9.2	734.94±18.01	206.15±39.98	296.96±46.13	40.89±5.5	204.98±56.05	116.38±89.7	210.75±16.79
Ethyl lactate	C5H10O3	1354.8	927.408	1.53592	145.55±4.88	190.09±9.92	197.96±11.18	194.65±7.79	152.73±9.92	138.03±17.67	106.76±5.81	250.79±9.4
o-Xylene	C8H10	1226.2	706.452	1.05037	184.84±13.13	291±20.56	188.23±8.86	155.52±1.64	149.99±8.28	174.2±9.3	120.74±9.23	247.16±2.29
Acetoin	C4H8O2	1298	819.971	1.06119	95.42±0.8	169.63±10.56	212.3±9.06	137.37±5.99	102.62±5.79	94.45±2.56	91.84±3.62	181.51±8.74
2-Methylpyrazine	C5H6N2	1275.6	782.469	1.09365	38.54±5.52	57.04±1.3	73.33±8.6	108.68±1.53	55.95±0.27	111.34±11.08	74.79±13.08	88.21±8.27
5-Methyl-3-heptanone	C8H16O	1262.9	762.198	1.28435	90.64±9.1	128.49±9.22	103.04±18.52	100.01±6.62	89.46±4.59	58.59±2.48	70.68±15.3	77.7±5.52
3-Methyl-2-butenal	C5H8O	1215	690.235	1.09365	37.41±2.15	69.95±4.33	32.97±7.6	35.23±2.89	25.65±5.5	23.67±5.57	25.04±3.8	36.47±0.57
Hexyl isobutyrate	C10H20O2	1354.7	927.23	1.45844	124.14±15.3	202.69±21.27	187.32±8.54	180.83±6.3	153.66±19.33	143.09±17.77	121.21±9.79	187.86±12.57
2,3-Dimethylpyrazine	C6H8N2	1334.8	888.139	1.09352	52.84±1.71	76.22±7.36	186.23±14.99	124.8±10.45	225.69±7.55	153.11±33.97	144.19±49.83	167.64±11.25
gamma-Terpinene	C10H16	1259.8	757.317	1.22082	37.21±6.39	76.41±6.96	67.76±2.7	45.11±2.73	38.22±1.46	27.29±3.24	29.74±4.7	94.04±9.64
Hexyl acetate	C8H16O2	1249.8	741.8	1.41846	41.48±3.53	122.25±11.82	93.75±6.88	53.57±1.79	47.4±4.86	34.3±2.36	42.94±5.78	84.9±6.68
2-Methyl-1-butanol	C5H12O	1227.6	708.423	1.23333	41.2±7.17	201.73±7.73	35.47±5.62	113.31±2.02	30.57±10.03	29.85±6.06	26.07±4.2	61.23±6.35
Butyl acetate	C6H12O2	1089.4	469.448	1.23501	35.86±1.9	92.58±24.76	64.86±12.28	67.04±4.82	55.6±10.53	67.19±6.31	62.18±2.67	53.62±4.73
Ethyl 3-methylbutanoate	C7H14O2	1084.6	462.894	1.26078	64.39±3.85	132.28±15.2	69.05±3.16	46.15±6	36.93±4.56	31.71±7.34	42.4±6.13	72.59±7.79
1,4-Dioxane	C4H8O2	1085.3	463.768	1.12256	67.18±7.07	126.89±2.24	95.1±5.05	85.75±7.09	67.09±2.6	48.7±4.09	79.35±6.68	107.95±3.29
Isobutyl acetate	C6H12O2	1033.5	397.782	1.23267	57.01±7.37	111.09±1.7	61.3±1.32	37.85±9.46	37.12±2.59	39.27±7.19	38.4±0.57	64.08±9.36
Limonene	C10H16	1204.7	675.712	1.22187	49.97±11.59	125.23±18.9	30.24±2.21	41.25±3.28	84.76±2.84	19.96±1.69	22.23±5.02	35.15±2.21
Butanoic acid	C9H18O2	1694.1	1936.957	1.15526	677.87±135.78	606.31±53.85	1914.53±66.53	1419.97±199.81	537.14±67.73	769.78±61.43	1299.5±486.21	848.71±149.73
Furfuryl alcohol	C5H6O2	1740.2	2140.588	1.12118	332.02±34.15	405.09±51.89	468.78±50.41	9409.67±1085.14	1020.18±76.36	804.45±26.99	805.77±164.23	558.54±62.69
2-Methylpropanoic acid	C4H8O2	1629.2	1682.418	1.14796	236.41±26.13	255.49±47.28	305.71±16.02	756.59±115.33	289.43±22.15	382±46.76	402.56±139.17	237.75±11.23
Acetophenone	C8H8O	1675.4	1859.578	1.19663	323.27±56.19	373.22±52.67	374.93±84.7	461.79±43.9	612.41±6.93	396.94±23.21	389.71±85.24	360.36±5.77
(E)-2-Heptenal	C7H12O	1314.9	850.539	1.25885	32.83±2.77	52.79±5.37	78.72±19.42	47.35±5.88	45.59±5.68	43.38±7.46	48.2±6.39	62.66±17.21
Cyclohexanone-D	C6H10O	1296.7	817.531	1.4629	49.7±1.37	70.33±5.49	69.69±6.93	59.57±7.51	56.38±5.08	55.4±1.58	55.49±4.17	53.56±5.83
1-Octen-3-one	C8H14O	1292.2	809.95	1.27148	51.25±6.1	63.92±9.43	104.83±25.46	75.61±6.06	54.42±8.87	55.86±9.97	73.67±16.78	83.89±10.03
2,6-Dimethylpyridine	C7H9N	1256.3	751.829	1.09281	45.09±9.88	55.9±3.03	63.6±7.85	54.03±6.01	47.45±1.13	42.28±4.23	40.69±4.47	67.02±1.8
Ethylpyrazine	C6H8N2	1346.6	911.031	1.12401	72.94±10.29	122.05±18.73	178.91±2.24	138.65±4.66	106.01±10.94	71.63±2.2	61.44±0.7	295.28±16.49
1-Hydroxy-2-propanone	C3H6O2	1312.5	846.171	1.05028	57.48±15.54	144.52±6.82	102.22±5.65	184.01±9.09	98.98±39.05	99.54±30.17	82.22±12.43	71.66±20.04
2-Ethyl-5-methylpyrazine	C7H10N2	1408.6	1042.435	1.17364	164.78±20.93	156.44±4.17	199.42±30.55	299.49±9.58	205.15±23.54	161.01±2.9	174.25±8.09	192.05±17.64

Table-2: Peak position and peak volume of compound

	[+] CX80 C3-1	**[+] CX80 C3-2**	**[+] CX80 C3-3**	**[+] CX81 C3-1**	**[+] CX81 C3-2**	**[+] CX81 C3-3**	**[+] CX14C3-1**	**[+] CX14C3-2**	**[+] CX14C3-3**	**[+] DX4 C3-1**	**[+] DX4 C3-2**	**[+] DX4 C3-3**	**[+] YS2B 2-1**	**[+] YS2B 2-2**	**[+] YS2B 2-3**	**[+] YS2 C3-1**	**[+] YS2 C3-2**	**[+] YS2 C3-3**	**[+] HN2 C3-1**	**[+] HN2 C3-2**	**[+] HN2 C3-3**	**[+] HN3 C3-1**	**[+] HN3 C3-2**	**[+] HN3 C3-3**	**[+] JH3 OC-1**	**[+] JH3 OC-2**	**[+] JH3 OC-3**
gamma-Butyrolactone	428.41486	463.04407	418.2856	455.15884	521.4956	437.3488	484.76233	472.20462	495.95584	627.6117	600.3656	601.7698	409.9716	434.18048	518.38727	462.33755	437.2488	449.48657	548.41064	511.53076	568.978	682.05066	528.8387	589.101	455.47214	470.40497	537.3527
2-Acetylpyridine	373.065	444.62302	473.49106	465.89468	503.69662	547.3064	868.9586	783.4432	780.6526	950.3015	1138.4315	928.5988	458.97815	482.78934	474.2598	537.5149	460.80228	545.98224	547.6064	582.74884	529.9118	1460.497	742.3885	691.89996	549.1394	483.9225	430.88553
Benzaldehyde	293.50403	324.7694	328.942	584.2352	647.94135	584.3752	472.64676	444.38748	476.50385	393.61456	320.5813	312.90936	289.38257	294.03503	317.02417	237.44095	274.66748	220.9551	304.1132	258.8526	268.62192	249.08994	288.4005	305.64847	482.44052	471.7225	465.1837
Acetic acid-M	4653.621	4113.8975	4289.094	10526.714	8560.159	7259.0483	16384.705	14704.151	13946.708	15000.321	18314.557	16073.689	8256.386	9758.102	9736.947	10395.691	9860.799	10167.683	13568.177	13301.128	12694.33	21268.69	17001.05	16792.752	12039.399	10088.966	8954.145
Acetic acid-D	404.26596	332.40802	314.4824	1560.021	992.73816	754.73065	6772.535	4771.626	4112.609	4769.5596	7321.992	5840.5635	960.11523	1131.4484	1287.3508	1738.9415	1407.1378	1575.1093	2952.6748	3230.244	3034.2087	16843.426	6963.098	6476.707	2424.4248	1630.728	1265.5637

6-Methyl-5-hepten-2-one	471.43143	539.399	653.5958	1167.5773	1217.1859	1237.6178	770.31	824.59784	816.5371	665.88916	669.24854	679.1378	1003.79614	989.2588	1056.5687	1028.9448	999.728	1042.7845	330.45724	329.07306	290.689	303.18448	305.48184	326.72238	801.39764	774.907	827.1818
1-Hexanol	565.16095	683.01715	767.4372	818.40125	869.8118	891.3745	1235.476	1324.1908	1284.6958	629.3936	753.0576	853.6925	905.15643	874.9864	840.27277	847.2315	903.6434	870.5561	542.2629	530.1296	549.1505	667.37335	801.47986	906.08514	1248.3158	1086.6654	1110.901
Trimethylamine-M	170412.19	171774.08	173500.42	122132.69	130611.44	130992.85	166941.42	166893.89	169369.47	143162.27	139531.67	136898.23	127744.58	128656.164	127053	135977.94	136714.45	139611.34	161952.86	166822.62	163716.34	143908.5	133275.44	132631.72	166932.84	165365.39	173470.67
Trimethylamine-D	103752.445	100902.06	101917.805	99472.95	99995.89	101751.33	97456.945	98821.06	98266.42	104472.13	103198.125	104144.83	105815.164	105369.78	104453.766	104192.55	104750.79	104872.6	104889.125	103002.75	104396.74	105770.586	104654.766	102084.766	98174.83	99172.84	97695.88
2,5-Dimethylpyrazine	204.11372	230.20673	233.84161	294.48163	344.07697	336.48947	250.02531	249.74315	254.58893	599.6191	679.3289	645.3018	125.88361	130.63385	129.71846	140.58092	158.01328	150.79016	178.68504	176.30327	173.05052	243.92865	171.68411	180.11368	217.86232	216.56256	211.739
Styrene	162.9746	175.63449	204.44478	1346.149	1289.6016	1194.1235	482.93378	493.01193	533.6245	109.54883	140.7009	115.56995	254.63559	239.7161	295.2126	177.22087	103.59658	164.66539	119.4559	131.4426	73.12216	77.98572	80.882965	66.77666	354.77945	326.7446	317.21747
(E)-2-Hexenal	127.25891	115.08115	134.53758	255.14215	282.47272	257.23288	166.7539	168.42471	167.67151	166.57393	172.17735	156.6002	159.27306	177.5697	175.8078	157.72444	146.23988	144.58463	98.470856	83.86464	85.00665	172.44176	127.969894	143.43373	144.19359	126.743454	164.63873
Isovalerone	554.4362	653.5114	706.01514	551.7478	484.08466	470.50937	1553.0667	1648.8602	1601.6178	362.47137	542.01184	630.1224	527.89886	465.14813	418.5389	515.35004	500.87048	512.0684	663.3474	752.9265	785.7094	824.7045	895.53595	850.6353	1555.9395	1267.6101	1152.3401
1-Butanol	382.6366	403.99045	418.0101	536.6462	533.1846	507.45816	464.42383	420.9851	408.1608	596.3241	602.7207	530.8028	480.59644	453.70135	478.77896	493.41406	478.8101	473.62213	419.23877	384.63843	344.97015	358.64542	352.3577	384.96506	503.96103	477.80804	537.8326
Cyclopentanone-M	4794.693	4622.7646	4014.998	8051.0254	7798.3228	8129.1245	7276.672	6788.8877	6380.0693	6316.5986	6096.5923	6619.683	5921.5977	6834.348	6244.5986	6373.97	5305.495	5193.5244	7103.128	5833.1963	5522.753	5495.236	5699.2515	5559.284	6712.2505	6192.295	6212.1177
Cyclopentanone-D	2194.0938	2158.4402	1829.9603	16651.959	16940.826	22011.023	19620.201	17036.27	15213.998	14338.576	13131.3	14910.8	9219.496	14415.944	10896.893	11625.595	6915.276	6154.1216	16102.16	12723.492	10838.688	11661.615	11227.293	10050.417	15482.645	13970.981	14672.3
p-Xylene	534.8887	558.9043	567.9582	239.59612	331.13712	250.21861	242.48003	291.0467	314.63348	328.7198	361.94705	442.49228	550.03705	352.81537	449.0622	390.9395	565.7142	521.2401	257.15735	341.0731	402.1908	391.17056	393.61237	430.9655	498.9575	535.65076	247.38802
2-Methyl-1-propanol	235.96346	254.68446	274.56528	293.73508	276.13165	302.1869	344.66797	331.19934	341.65964	371.89633	387.83118	256.64856	196.2485	211.24576	209.48607	233.08397	197.42162	235.07916	249.43431	269.84836	249.21213	234.05046	238.20749	257.5084	388.52438	309.15225	377.06204
Hexanal-M	2608.2668	2665.8918	2730.6643	3485.7192	3464.43	3551.6272	3065.954	3048.0173	3078.4006	2668.3025	2777.6157	2660.1372	2512.9575	2514.8372	2496.7073	2595.4958	2537.3865	2540.579	2105.8167	2064.3975	2045.0565	1885.4169	1920.135	2030.7214	2801.1758	2700.0032	2704.769
Hexanal-D	1668.2922	1702.9059	1781.5626	3616.9287	3560.09	3681.5146	2681.1711	2620.3445	2716.718	1735.2178	1824.5814	1744.5116	1331.9761	1340.63	1282.0519	1473.0857	1401.1456	1404.3094	898.78204	922.08887	869.58075	736.0852	780.8592	836.55786	2022.6829	1864.3252	1854.3092
2,3-Pentanedione	744.7147	762.6781	773.5317	957.9401	973.53503	926.22815	1316.3545	1319.0583	1327.4147	664.325	681.89954	632.22644	289.6225	278.61563	286.0676	302.6068	308.64124	307.93692	330.2462	323.3541	325.8692	336.37393	390.35294	375.22015	1084.6436	1151.6512	1163.4536
Toluene	813.51544	852.41724	874.5687	1366.3142	1320.1316	1292.4766	1019.7688	998.2616	991.02515	1194.699	1216.4883	953.56537	764.83105	764.64215	751.5468	873.2556	838.3887	852.5083	1012.8434	984.4264	957.31134	890.88794	898.8954	937.23724	1085.7922	1019.43774	1041.5714
Ethyl butanoate	164.49654	172.21068	183.75746	467.16333	433.47394	436.25565	190.75618	173.81927	182.85762	269.23737	330.004	200.781	63.823864	62.908478	61.615383	111.670654	87.11516	113.85026	196.80618	221.96379	194.9643	152.3832	131.00711	156.44246	281.22406	203.46495	232.5574
Dimethyldisulfide	324.86716	313.91583	311.48294	307.20596	281.07074	310.07877	221.52165	205.12465	202.59178	247.2747	253.80019	228.00046	104.41199	94.007225	92.99408	134.92195	132.96231	134.77754	206.39554	207.72195	227.8716	211.45238	195.63083	184.33734	262.93628	258.2016	286.8519
1-Propanol	741.0621	782.4611	783.58093	205.26018	251.69612	195.52197	631.70654	660.7923	655.0356	471.42255	428.47485	452.82596	205.50014	216.72253	197.6038	260.83667	247.81017	246.03494	276.11832	252.98256	257.62616	279.8932	276.4627	266.65784	995.13104	1108.0237	1081.7063
Methyl 3-methylbutanoate	790.30634	855.6566	876.2595	1987.2893	1994.8925	1750.7327	781.608	806.4745	851.2663	562.8369	533.9022	513.0127	874.6709	863.57513	926.03485	620.3397	608.17084	672.40576	124.67716	108.57567	129.40297	140.33429	147.78181	135.69958	947.6509	942.1808	963.0636
1-Penten-3-one	455.41214	482.4272	508.0314	857.5807	849.6555	886.2066	729.74414	737.6338	740.9021	937.1617	929.723	935.1332	516.7787	519.5537	517.5941	768.1193	750.88916	766.9506	530.4162	525.6859	529.44525	606.4134	601.1232	605.04694	641.74023	635.45026	633.82837
3-Methyl-2-pentanone	201.19426	217.28687	228.00269	289.92245	295.27704	315.2667	210.33258	218.30669	220.74402	185.49936	209.41054	169.88889	160.8061	175.71893	160.46394	180.3403	151.97884	179.50046	172.5395	194.04224	187.13461	168.2092	147.87514	189.14314	194.82654	191.82709	196.23517
2-Butanol-M	137.2082	129.14967	145.08453	220.10635	197.19499	237.15878	138.97455	137.89474	149.34154	178.7806	191.80264	160.38618	132.2069	133.08896	125.996925	143.12268	150.21693	151.28784	116.71196	125.55478	124.42832	109.01781	115.18113	126.70346	181.90002	176.23883	180.08035
2-Butanol-D	109.76878	113.803604	125.60588	357.09683	330.95715	377.79303	267.7954	293.44403	294.65048	361.08942	404.22375	338.84238	120.56903	111.972824	101.67693	215.57607	203.28276	210.65475	125.42592	126.01914	132.06693	157.35118	182.41548	204.22482	220.15968	190.1985	189.2209
Thiophene	1981.8148	2060.6426	2138.997	2469.0366	2559.7822	1713.5328	1927.647	1975.1538	1955.3574	2306.0798	2298.2703	2211.1995	2328.0137	2227.6387	2454.295	2009.2386	2113.7974	2105.0188	1533.1437	1658.8562	1663.2109	1784.3999	1913.694	1976.0381	2645.8286	2660.6482	2713.7097
3-Pentanone	261.93204	249.89423	268.05978	295.457	297.69882	265.2381	379.53937	369.38568	363.8978	336.93384	350.05588	309.15448	286.80524	283.1326	283.56363	375.6712	375.62454	391.19724	217.75568	248.09679	271.43918	306.4239	294.66382	317.5285	425.85535	372.6473	392.2526
Acrylonitrile	427.81274	414.85068	439.45062	534.23773	539.7567	579.5427	455.95425	455.16995	458.03833	346.94757	343.0216	340.26212	305.92618	328.57092	320.96344	313.45593	302.4224	307.74808	200.30331	211.64568	208.1241	219.4487	220.73956	225.72533	564.4788	545.53564	578.79846
4-Methyl-2-	877.23047	927.048	956.727	1013.4677	1053.927	1006.34235	1435.3971	1407.0468	1430.0403	1061.9521	1053.616	1082.7994	779.9838	780.3793	774.7648	797.2384	812.6401	803.0085	549.44824	562.23926	576.43884	753.1087	778.25745	761.4805	1112.1096	1164.2423	1147.381

pentanone																											
Pentanal-M	1295.876	1345.258	1352.4457	1117.2931	1160.5297	1139.7579	1424.1747	1459.015	1477.516	1554.1086	1405.2915	1695.8405	1416.5272	1407.8777	1330.2875	1397.5262	1430.438	1351.2236	1513.7072	1234.9515	1435.1372	1378.221	1544.2128	1353.2899	1477.0516	1493.471	1491.5691
Pentanal-D	2355.522	2223.095	2247.5793	2628.414	2679.1738	2687.9944	2190.0388	2216.4985	2317.4644	1913.6918	1923.7566	1927.4758	2420.9387	2492.4058	2496.3828	2651.7942	2582.9048	2584.0356	1562.3872	1590.882	1647.8381	1581.2637	1651.8574	1709.4269	2331.2263	2524.0798	2392.9683
2-Pentanone	1099.7075	1116.7333	1144.5015	1279.0857	1241.477	1301.0172	1498.15	1508.477	1479.8423	1167.4995	1236.1669	1186.8738	929.7364	920.2337	976.5367	1024.2213	1020.5153	1024.8812	975.2747	998.2927	980.07385	989.1855	1012.9745	1057.1686	1528.2401	1535.6343	1497.7323
Benzene	745.8656	755.42163	764.7755	669.02637	846.8227	702.25806	826.1354	820.803	801.0755	844.04095	861.50885	858.7938	839.6151	845.2896	879.0745	760.2785	755.7149	772.74066	649.79877	629.23145	624.62335	604.8203	595.5487	600.21674	764.1423	778.3619	769.2902
Ethyl isobutyrate	1839.1587	1864.3474	1919.775	3292.3215	3213.829	3350.7817	1792.1962	1796.2133	1797.8574	1037.5411	1092.8688	1066.9357	1323.8575	1339.7257	1339.9724	1042.1335	1035.2148	1052.0918	550.63916	549.9126	552.84766	409.5161	398.3848	405.0836	1966.222	2020.2211	1941.3866
Ethanol-M	1663.7664	1666.1859	1709.0337	1710.3268	1621.3853	1870.2797	1870.9862	1940.9111	1766.4921	2039.2621	2047.5583	2069.512	2070.3386	2108.505	2056.9255	1991.2886	1958.6879	2014.1222	1945.9747	2032.9387	1951.4915	2065.506	1965.5422	1991.9307	1796.4598	1808.491	1830.5425
Ethanol-D	2894.4944	2906.1565	2948.96	2524.38	2601.9702	2618.765	2790.009	2876.633	2646.3486	3829.6274	3707.2832	3828.23	3631.237	3722.758	3547.1814	3494.0889	3448.3862	3388.9304	3077.0454	3137.843	3245.0745	3345.4717	3334.5203	3375.1396	2981.7717	2989.928	2977.9612
3-Methylbutanal	263.95166	274.4786	269.08627	302.72232	259.19254	372.3407	357.46786	368.10147	377.96188	323.47632	330.0862	339.66446	282.3727	301.66696	316.171	269.324	260.8322	282.25052	373.94263	403.2106	399.87122	385.20502	372.20517	311.5363	266.58673	270.93704	281.01297
2-Propanol	1616.6594	1658.103	1718.5142	1715.7546	1628.9683	1854.0804	1850.1389	1905.3533	1712.6307	1288.0641	1316.8766	1232.5964	1535.2366	1548.9496	1553.6066	1326.9948	1333.2025	1353.481	835.4181	783.3699	767.91266	825.36884	813.5821	870.7872	1882.162	1868.7422	1922.7434
2-Methylbutanal	2469.2388	2567.1008	2593.825	2878.977	2941.9324	2936.9487	3987.6384	3916.2783	3858.0068	4150.331	4261.5015	4151.775	2000.6224	1980.826	2024.9092	2701.8562	2667.7869	2657.8489	7260.3726	7266.7026	7280.942	6440.234	6422.384	6409.6904	3896.1597	4014.0293	4043.9949
Diacetyl	1791.954	1834.0574	1882.7974	1753.0945	1581.4703	1929.7754	2258.7664	2379.3308	2077.0374	1890.2871	2237.3013	1820.1089	1493.3464	1508.8636	1539.7869	1626.4999	1532.2727	1731.4451	1783.4467	2111.5178	1788.2502	2041.9905	1613.3756	1983.1924	2442.3306	2313.1562	2368.3997
Methanol	3661.936	3809.8467	3795.9849	3311.4956	3553.1604	3369.8828	3807.1382	3828.3567	3837.9683	4937.262	4866.1733	4720.182	4137.751	4139.744	4238.9883	4931.221	5019.705	4824.643	4884.161	4512.4756	4701.901	4680.4873	4741.909	5025.924	4406.8394	4444.166	4484.412
2-Butanone	2185.713	2303.9736	2379.5176	3317.668	3220.337	3295.643	2358.788	2200.306	2335.4812	1529.1244	1572.5453	1480.2822	1376.6545	1228.786	1371.7355	1238.5309	1305.361	1320.1049	756.07263	809.50507	831.3033	1001.02997	1033.0486	1095.3749	2568.1584	2656.398	2679.3647
Ethyl Acetate	407.82086	410.97806	495.4226	1091.2534	1129.9419	1165.4176	846.43164	808.8274	764.26447	661.30554	727.7467	735.2787	1157.6302	1153.8909	1191.655	925.6349	1074.7388	1006.00244	521.87994	530.31396	492.16318	758.39	829.2703	847.5336	1279.0857	1266.0614	1283.3405
Methacrolein-M	693.38855	651.66284	672.5857	652.9671	565.7786	719.27936	690.2269	725.0539	663.5007	615.9005	643.0245	659.7058	689.4626	685.9966	689.46704	641.35583	620.633	644.8486	484.89563	534.591	514.93677	553.80304	525.32825	521.57556	603.09174	635.6258	646.6971
Butanal-M	585.7972	599.45245	616.2871	687.303	666.56683	672.6568	725.78705	739.9578	682.0351	758.961	731.8482	747.95636	607.7176	606.76666	621.56836	679.7288	642.75336	655.9487	756.11707	763.0914	754.4218	847.10486	821.35846	831.20996	670.7727	688.94714	699.1675
Butanal-D	282.25275	291.26886	300.2361	422.29376	401.29538	408.894	413.1932	397.95377	408.38297	416.47705	396.3963	388.7088	250.08531	249.30989	245.32617	277.95352	273.8654	268.83298	252.84036	218.06673	309.5433	327.88217	425.85977	438.97293	355.97037	362.54025	357.80557
Methacrolein-D	1149.4761	952.61444	979.1784	1363.7725	1429.8848	1368.9738	809.6317	836.0091	896.2758	597.9194	630.30676	618.0601	660.74786	618.4712	663.93616	586.28815	583.9264	622.3438	339.4845	351.5667	359.2431	445.66504	439.09293	434.67816	695.7015	737.6915	752.7932
tert-Butanol	505.5385	513.4971	534.09106	586.98584	526.64575	659.61475	649.39215	721.82556	595.2576	578.6362	614.6696	645.49286	648.14575	665.1493	656.6975	572.113	553.9852	601.0433	630.02686	550.9235	608.19525	585.9638	608.493	579.45166	549.4172	562.3903	566.6407
2-Methylpropanal	269.31735	276.5449	272.29013	295.6814	310.99637	308.5035	421.93607	403.02618	391.5505	568.04706	571.6886	559.4086	187.64119	178.44954	183.45306	214.85399	202.91617	195.00429	1463.1654	1488.7917	1458.3729	1499.7053	1523.381	1538.7626	353.5708	366.4551	384.70288
Acrolein	372.98724	377.19092	387.7312	449.411	443.0322	477.9769	359.59415	352.36212	366.9328	193.43568	192.03816	178.18736	141.32967	142.52501	148.45059	132.20912	130.42722	133.57997	156.50911	149.90366	170.47989	175.30345	186.39697	185.87929	356.03033	381.36792	393.3324
Methyl acetate	125.01488	118.769356	123.43961	80.580795	76.85925	84.28012	131.8803	128.46758	118.2339	319.40594	296.8523	302.07578	179.86261	193.21573	185.07054	236.35005	212.39221	223.89899	396.15634	425.5354	330.21286	341.88184	317.61072	331.5104	94.47159	97.31773	108.45569
Acetone	10814.588	10957.786	11101.737	13414.072	12983.584	13201.322	10272.128	9991.668	10328.91	6625.5776	6620.8384	6597.3203	8732.636	8371.24	8576.0625	7454.508	7534.2666	7555.1494	4352.996	4422.359	4526.2954	4835.892	5203.9937	5297.103	11361.799	11684.904	11774.128
Propanal-M	1510.8899	1531.3107	1559.8921	1533.7947	1552.669	1469.4976	1518.5441	1485.7878	1510.0546	1635.8159	1575.1582	1498.0012	1579.6351	1545.8013	1613.9711	1497.0813	1429.4026	1415.252	1326.9325	1313.2839	1321.2914	1441.9581	1529.8375	1524.4586	1494.7062	1550.776	1573.8628
Propanal-D	3800.6372	3875.197	3950.9807	5309.9854	5068.7026	5117.227	4868.106	4523.449	4756.7397	4843.922	4633.118	4551.366	3475.6035	3404.2566	3469.1936	4062.6382	3910.5881	3983.135	3512.8254	3694.0012	3550.883	3669.4302	3594.6882	3629.302	4366.9204	4460.0854	4502.8955
Dimethyl sulfide	425.59982	457.44955	470.40717	435.41803	457.5673	458.76263	969.9179	983.922	977.00995	711.4919	703.4734	718.264	681.3108	638.80743	680.3243	592.6403	592.46924	596.5885	261.74094	253.44691	272.88113	159.77518	167.84482	166.13846	610.72815	607.1888	606.45337
Acetaldehyde	382.25665	382.67212	393.90787	328.60648	330.08398	335.42746	371.7208	358.92316	367.14163	371.65637	359.82965	353.92184	360.95834	358.8365	355.51266	381.25018	366.5173	375.52676	345.18567	358.3566	355.53043	355.20828	350.4758	357.8189	365.56638	378.57956	376.7821
2-Ethylfuran	910.6243	963.4124	970.1334	1207.1522	1169.8391	1116.1533	1017.4159	981.6513	1031.1089	831.19	824.6268	804.52374	896.8557	878.2925	889.2949	936.27075	951.19025	922.2533	547.21313	624.67224	591.22284	859.0649	873.46	877.40594	1102.4092	1097.2457	1093.5175
Nonanal	149.83478	151.05011	184.89948	243.71759	290.5979	259.07922	225.23874	195.20425	207.52422	239.4317	254.97774	219.41759	172.59727	194.0489	191.95818	211.48793	231.05547	191.46494	216.37148	241.32246	236.88106	256.86185	234.91031	299.88507	179.27383	186.86356	193.18018
1-Penten-3-ol	894.16736	952.51	946.1045	1267.7656	1258.1562	1153.2177	1049.0367	1093.9552	1064.3007	1545.7703	1554.0509	1551.9669	790.2197	778.904	814.88855	1324.1152	1329.0099	1370.2623	1104.1422	1116.3245	1203.0796	1129.7552	1207.7832	1302.4414	1438.2766	1226.3754	903.5101
Cyclohexanone-M	252.90479	280.71747	296.16797	347.78296	389.03986	422.0716	702.59357	665.75586	703.7267	444.1631	373.57602	279.81763	104.12315	117.3074	122.33537	98.048706	111.237404	88.88594	141.56296	138.23691	121.166695	136.87938	118.17835	113.317024	809.44507	793.2858	830.13904
beta-Pinene	121.23335	138.368	135.61295	714.16254	746.1589	744.48364	230.57999	227.86937	160.00847	326.969	320.0636	243.84422	37.08654	50.30412	44.638493	46.811428	35.926754	39.941574	186.6236	267.8998	160.40173	218.87547	78.12347	52.154892	212.09894	193.31793	226.8229
Ethyl lactate	140.37651	150.07474	146.18878	196.32404	195.29756	178.65839	191.06056	191.9515	210.85472	200.16779	198.03262	185.73932	150.20583	164.05217	162.82573	142.44946	162.23473	153.50745	135.40187	121.824356	156.87793	111.17424	108.99559	100.17054	240.52928	252.85591	258.99478

o-Xylene	173.74596	181.43344	199.32794	300.97153	304.67087	267.35992	187.37013	179.82928	197.48827	154.29619	157.38673	154.89163	192.66693	191.09166	213.44536	141.7607	158.31767	149.90143	182.28883	176.28549	164.03662	111.86395	120.07801	130.29169	247.7324	249.09882	244.6352
Acetoin	94.7582	96.30458	95.19812	170.98201	179.4538	158.46208	217.38463	201.84747	217.67569	137.70811	143.18933	131.21597	93.580635	96.91114	102.69453	108.78896	101.77247	97.29774	92.92298	97.40883	93.01408	95.74468	91.19885	88.59044	191.53159	177.5608	175.45009
2-Methylpyrazine	33.007286	38.55294	44.051933	55.54316	57.87829	57.689434	70.63373	66.414505	82.95592	109.997635	109.03336	107.004845	45.160618	51.215065	49.65757	56.23859	55.707573	55.916424	98.70415	119.43368	115.87434	63.575024	71.63799	89.159225	97.750984	83.06256	83.831314
5-Methyl-3-heptanone	80.22308	94.64266	97.05778	137.30374	129.25188	118.91377	124.41943	92.600815	92.105354	107.39811	94.62267	98.00205	77.71687	75.61726	73.93757	94.71154	86.18866	87.47509	57.64722	61.399864	56.709614	53.92568	83.92685	74.17753	82.23827	79.296585	71.55134
3-Methyl-2-butenal	39.208374	35.022476	37.988598	73.53542	71.18474	65.136955	30.098932	41.579052	27.223902	37.286503	31.918598	36.47332	21.029482	26.092999	23.906733	22.269255	22.682512	31.99414	25.446451	17.423475	28.12596	23.67344	29.330183	22.11595	37.002113	35.8601	36.53553
Hexyl isobutyrate	124.88602	108.475685	139.0523	227.24283	190.6762	190.1474	197.18166	182.23773	182.55324	179.86928	175.06349	187.55676	158.93977	199.56345	178.49176	149.42819	174.76355	136.79716	163.41896	135.293	130.5472	127.903244	125.752525	109.96875	192.02039	173.73262	197.82155
2,3-Dimethylpyrazine	54.338936	50.970665	53.20803	71.30916	72.673355	84.686714	203.53383	177.52304	177.63412	119.991356	136.79272	117.62957	175.74115	183.63303	162.59244	232.74182	226.61404	217.72456	190.97835	143.02713	125.31483	196.34627	139.1523	97.07333	158.83313	163.76334	180.31364
gamma-Terpinene	34.838062	32.340744	44.438526	69.733894	75.868324	83.62469	67.78536	70.45154	65.05253	43.75865	48.251163	43.320953	49.984177	49.824207	40.592564	38.939533	39.17727	36.542194	23.653446	28.379246	29.850088	34.715862	29.13022	25.366465	83.12922	101.39699	97.60657
Hexyl acetate	37.755306	41.90788	44.78513	114.541245	116.35647	135.86179	101.49252	88.34827	91.39659	55.61648	52.74367	52.337082	52.305977	46.171543	45.451675	46.160435	52.757004	43.28763	36.971004	32.498493	33.422768	42.3478	37.48647	48.993248	77.203636	89.12145	88.37937
2-Methyl-1-butanol	48.611095	40.674774	34.309273	203.42274	193.28682	208.4707	39.834927	37.444252	29.134665	113.5081	111.19297	115.22334	25.668633	23.722322	22.486992	34.964706	37.66421	19.092058	36.642178	27.910444	24.995422	30.621058	22.327023	25.270927	67.01217	62.230824	54.44114
Butyl acetate	34.493683	35.046913	38.02859	88.730415	69.967186	119.03375	78.71669	60.52447	55.325424	62.695183	72.23122	66.20121	57.87607	70.038284	63.892742	67.31656	52.519268	46.9514	74.18197	65.49023	61.90644	60.828857	65.26138	60.45115	51.599438	59.0203	50.24191
Ethyl 3-methylbutanoate	63.530586	61.03549	68.59188	126.58126	120.75122	149.50151	65.66353	69.58726	71.9135	51.435024	47.375767	39.626076	47.653496	45.365025	46.63146	38.952866	31.716413	40.13265	26.36184	40.081547	28.696966	41.34354	36.857693	48.98436	80.760765	65.24361	71.757965
1,4-Dioxane	65.23028	61.284332	75.02404	126.736786	124.73937	129.20523	89.37919	96.98668	98.93743	83.222534	80.276405	93.75394	83.75577	84.95777	79.3899	67.40543	69.51616	64.337105	44.365208	52.4815	49.25098	75.121796	75.868324	87.05072	108.597885	110.86858	104.39199
Isobutyl acetate	48.817726	59.095844	63.10622	112.819336	109.41107	111.03078	62.264153	61.842007	59.797935	34.693645	48.486675	30.369993	28.55477	31.154293	35.577927	34.729195	36.76882	39.87492	31.16096	41.78346	44.85845	38.53072	37.777527	38.88843	73.959785	55.345417	62.946247
Limonene	44.334103	63.29285	42.27226	146.53316	110.47532	118.69604	28.254826	29.845644	32.61847	40.42593	38.45962	44.865116	90.9189	99.91281	101.92355	81.58506	87.077385	85.604324	19.891912	21.673807	18.301092	18.683245	20.02522	27.974876	35.964523	36.83992	32.64513
Butanoic acid	562.3215	827.4218	643.8532	614.5608	548.81726	655.5644	1955.8595	1837.7811	1949.9362	1285.2379	1649.54	1325.1462	523.09753	542.4384	559.5553	487.81955	614.3586	509.23117	698.9253	808.18756	802.222	1855.2958	952.9099	1090.2825	996.75964	852.0128	697.34784
Furfuryl alcohol	317.45297	307.577	371.0387	373.98483	376.29776	464.9904	454.05682	524.9172	427.3706	8582.55	10638.36	9008.107	1157.6146	1080.4465	910.3999	1025.2589	941.3965	1093.8707	831.7721	803.775	777.81085	992.8137	739.29346	685.18787	619.71985	494.44278	561.44385
2-Methylpropanoic acid	206.29332	253.03143	249.89423	226.20079	230.22227	310.03656	312.30725	287.44513	317.3752	689.19824	889.7615	690.81793	305.69067	336.56058	346.2077	264.02054	304.6664	299.59402	417.37466	399.64236	328.99307	562.788	333.04788	311.8318	242.21341	246.05716	224.96991
Acetophenone	277.798	305.92175	386.09152	326.09805	430.08124	363.46677	352.42657	468.60974	303.74658	504.1321	416.4904	464.75266	478.86563	525.34375	520.76904	612.76556	605.3025	619.15546	422.7648	390.22632	377.8219	340.842	340.1488	488.13727	364.4688	353.75964	362.84467
(E)-2-Heptenal	31.463127	31.009876	36.02007	51.830505	47.96899	58.582603	101.07482	69.07624	66.02346	41.412415	47.47797	53.17026	44.34521	47.149143	44.694035	47.006947	39.330574	50.428543	38.33742	51.94604	39.86381	45.02953	55.563156	44.020824	82.416016	50.921783	54.652214
Cyclohexanone-D	49.295414	51.22173	48.57999	71.97793	64.2038	74.80186	70.82703	75.979416	62.266373	67.22102	52.203773	59.293583	41.079144	50.466312	43.176537	51.537228	61.666485	55.929756	54.3456	54.6411	57.209522	56.971786	58.704803	50.779587	50.019726	60.29118	50.37966
1-Octen-3-one	44.45408	53.019176	56.263027	74.57967	60.544468	56.64518	133.77994	94.802635	85.910934	70.269356	74.3486	82.2005	47.555733	57.213966	47.57351	64.65482	49.306526	49.28875	46.42705	54.86106	66.298965	58.818115	91.87873	70.32712	87.80392	91.37882	72.49561
2,6-Dimethylpyridine	42.55443	36.722164	55.99419	52.62814	58.622597	56.45188	62.110847	56.596302	72.09124	54.6611	47.73126	59.7024	57.64944	53.410217	52.701458	47.6846	48.446682	46.22931	46.818092	41.570164	38.450737	35.59348	42.529987	43.956394	69.0118	66.56558	65.49023
Ethylpyrazine	61.988647	74.42637	82.413795	103.49438	121.702156	140.94753	180.21144	180.1981	176.33215	136.6683	135.30634	143.97807	94.1472	97.23108	93.09406	106.29609	94.924835	116.805275	69.76278	71.078094	74.05088	62.233047	60.91551	61.164352	302.12912	276.4649	307.23483
1-Hydroxy-2-propanone	46.42705	75.246216	50.764034	143.49594	138.268	151.79442	98.75525	99.161835	108.74453	174.59024	184.71283	192.73804	76.32158	74.875175	176.31659	75.81722	77.06144	144.0714	91.847626	132.80013	73.957565	96.56009	75.559494	74.53968	94.678215	62.146397	58.14935
2-Ethyl-5-methylpyrazine	169.6556	182.83762	141.8318	154.47838	153.61409	161.23714	177.48972	186.45251	234.3193	304.51312	305.5107	288.44717	162.66576	186.20367	209.31055	230.9577	199.63899	184.86613	158.84203	164.2988	159.88849	167.18938	183.08202	172.49286	186.16812	178.09406	211.87453

1	201.39645	210.00375	231.46205	419.74313	398.79364	425.9153	381.09244	396.05856	396.3674	399.77344	408.52518	414.37744	141.974	136.40613	107.95356	156.8957	147.09084	132.64015	292.79083	292.86414	309.43887	252.42265	205.1402	239.30951	381.59012	365.39975	382.80545
2	478.4346	489.16153	522.71313	1300.4707	1298.2045	1211.878	330.1373	351.04236	360.7095	285.0478	293.7751	295.75027	145.08676	148.40837	155.52484	122.37314	123.28853	132.98898	88.40603	85.366585	105.7473	62.22416	64.66815	69.77833	522.5843	510.9664	508.53354
3	1377.8876	1600.8379	1768.3939	2840.582	2908.0295	2917.9966	2834.7075	2734.988	2766.0867	2179.5208	2107.963	1984.1033	4118.8945	4068.017	4073.205	1953.9622	1931.8173	1993.0571	1112.5051	1133.2324	1223.8403	1636.387	1641.2594	1667.4746	2015.1465	2011.6183	1886.3812
4	303.5644	318.64163	327.67776	549.0794	538.19257	550.7969	350.34695	348.40063	334.06326	368.07037	378.9728	375.70895	315.41333	317.48407	312.70718	307.22818	308.17245	318.46167	222.68144	220.173	222.67033	231.56203	259.59467	282.37494	467.0389	439.52173	428.53708
5	1779.7251	1853.696	1907.053	2706.4	2526.2373	2817.6128	1995.4656	1855.7179	1940.8778	1424.128	1711.7198	1414.3499	2115.3704	2100.1797	2242.2427	1903.6869	2022.4341	1987.6937	899.9463	1007.88654	820.7519	902.94574	808.74963	989.08105	1945.7458	1811.986	1802.7432
6	575.539	591.5072	594.5089	597.1417	626.2564	577.8808	668.2065	647.75024	667.30664	714.1536	734.9409	716.17773	674.392	652.99817	668.4709	729.3442	743.13055	731.27716	582.44	553.3831	581.18243	620.55524	618.99554	640.4871	731.7304	735.3986	738.7958
7	293.80396	308.0658	322.4165	256.20642	257.11514	273.6943	370.38104	346.76315	348.59616	538.44806	522.07104	519.93365	500.72162	511.8396	514.5791	603.82495	618.10455	590.39185	289.07593	143.40929	287.46735	218.33334	400.41556	353.3553	437.86426	437.60873	423.4469
8	252.16493	270.8926	287.10965	227.37392	248.90775	253.92682	804.4793	766.99066	758.6077	1040.9049	1107.7771	1045.2664	842.3702	866.04803	890.2903	1284.207	1308.1426	1329.8431	1201.962	1102.6825	1168.1327	1061.0479	1085.4368	1100.3807	733.1168	643.3977	611.89014
9	538.55023	554.7673	578.734	855.4611	854.1058	853.6814	1053.096	994.8689	1028.265	784.1653	774.2382	725.5582	547.76855	522.44434	545.4201	564.7899	559.2176	572.8706	349.5982	357.7767	373.27606	245.86607	252.29156	259.8435	809.85834	805.72797	805.8813
10	342.9261	356.3525	351.94443	381.61234	458.51602	402.57516	448.97775	459.36032	461.7932	573.6505	560.51514	558.99316	304.61533	267.9176	301.58255	342.25952	331.12158	326.90012	678.31573	721.3768	637.23663	703.96216	679.3467	696.919	403.3239	375.8467	357.78558
11	548.444	512.9794	567.6694	886.0155	804.72595	893.56964	615.034	577.14984	628.98035	553.4097	580.34924	552.17	704.8287	675.7207	708.5991	590.54736	624.57007	603.6117	323.60297	244.69518	327.32227	405.91455	468.1165	458.6338	696.7991	710.301	706.3284
12	1694.9252	1788.7057	1822.053	3144.133	3226.86	2877.5664	2280.631	2198.9817	2370.85	239.29395	241.2136	230.76662	508.26025	489.9147	494.5361	263.6406	270.98593	267.3688	102.69675	97.28885	114.15909	107.24036	111.86395	119.76917	1969.1682	2053.0818	2048.7693
13	30.792137	39.05729	36.322235	140.78755	139.4989	144.74016	36.942123	41.53906	42.101177	31.638649	29.758993	31.796398	34.009327	25.135397	26.195202	27.628273	28.345919	30.154476	23.960056	26.088554	37.621998	28.079302	24.57772	29.796764	49.259865	47.238014	47.078045
14	40.25263	41.29688	53.814587	137.8192	169.76224	182.63544	67.05438	51.21284	63.539474	96.36457	127.03007	101.13036	56.891804	55.196556	54.89661	61.11103	74.83296	81.57839	43.980835	45.14062	41.25689	38.388523	60.726654	92.07203	53.383556	49.059902	51.697197
15	183.62859	191.26497	187.91669	1033.8862	997.49066	1066.1381	630.0468	539.1368	545.2535	319.71255	324.86493	379.63492	285.42328	409.29614	330.09067	311.39407	232.72626	202.49402	170.85538	117.294075	111.901726	108.900055	125.35926	129.23856	592.2315	532.8779	548.1574
16	117.94951	121.651054	125.705864	502.47018	457.6984	488.38834	128.32538	127.92546	138.77458	67.19881	66.483376	50.835133	154.48059	157.2712	161.89923	96.69118	93.85392	104.436424	35.753452	27.12392	28.752512	27.095037	41.219116	31.56755	142.78273	119.58476	122.09319
17	46.88919	55.223217	52.91031	56.21415	69.69168	103.40106	147.97511	134.94196	117.00079	100.54381	92.30754	93.147385	46.382614	65.074745	45.418346	65.35248	44.51407	46.7781	157.40895	139.95659	141.62517	86.344185	71.55801	64.38821	74.7152	73.24436	99.17517
18	39.748276	40.041553	36.459988	50.408546	51.95715	47.149143	49.695343	40.492584	50.48631	180.88908	199.70343	175.35455	84.75781	85.6843	87.79503	81.10292	85.4399	89.32364	38.550716	30.414429	27.877117	36.86436	34.862503	38.535164	48.802174	47.637943	43.572018

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Contribution of Authors

Wang J: Performed the experiments & collected data

Pan Y, Liu L & Wu C: Analyzed and interpreted data and wrote the manuscript

Shi Y & Yuan X: Conceived idea, designed and performed the experiments & collected data