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Evaluation of volatile flavor compounds in rice with different degrees of roasting based on GC-IMS and PCA analysis

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Abstract

The differences of volatile odorants of rice at different roasting levels were analyzed by headspace-gas chromatography-ion mobility spectrometry (HS-GC-IMS) using fingerprints combined with principal component analysis (PCA). GC-IMS and PCA could distinguish the different roasting levels of rice and the results showed that a total of 47 representative flavor compounds were detected in four samples from all roasting stages. The aroma components of roasted rice are mainly aldehydes and ketones, furans and pyrroles, as well as a large number of phenols, esters and alcohols, which make up the special aroma flavor of roasted rice. It can be seen that the flavor characteristics of roasted rice can be reflected more fully when the rice is roasted in medium (18 min), and can have more fruit wood, cream and roasted aromas. The PCA based on the signal intensity of the detected volatile compounds revealed effective differentiation of samples from different stages into comparatively independent spaces. Thus, the differences of volatile compounds from different roasting stages of rice were determined, and the flavor fingerprints of that can be successfully established using HS-GC-IMS and PCA.

Keywords: rice; roasted, flavor fingerprint; principal component analysis; volatile profile; gas chromatography-mass spectrometry.

Practical Application: In this study, GC-IMS was used to analyze and detect the main volatile flavor substances of roasted rice.

1 Introduction

Rice is the main food crop in China, accounting for about a quarter of the food crop acreage in the whole country. Meanwhile, half of population depends on rice for their livelihood in the world (Murtaza et al., 2022). According to archaeological findings, people began to grow and eat rice about 13,000 years ago (Wei et al., 2021). Nowadays, with the development of economy and improvement of living standard, the consumption requirements for rice have long been not limited to cooking (Butardo et al., 2019). Various rice products have also emerged with the needs of the times, such as rice cakes, rice juice drinks, rice wine, rice flour, etc (Jeesan & Seo, 2020). Due to the different processing methods, rice also presents different flavors (Hu et al., 2020). So far, more than 300 volatile compounds have been detected in rice, and these compounds played a vital role in the flavor and quality of rice.

Roast as a traditional pre-gelatinization means of maturing and aromatizing materials can significantly increase the aroma of rice and change the morphological, structural and functional properties of grain starch and protein (Fischer et al., 2016). For example, roasting led to decreased carbohydrates and proteins, increased crude and insoluble dietary fiber (AL Juhaimi et al., 2018), increased non-polar and polar components, and increased antioxidant capacity . More obviously, the color and flavor changed significantly, and some studies suggested that the main reasons were that roasting made the grains undergo a Maillard reaction, and the content of Maillard reaction products (such as pyrazine, pyrrole, furan and their derivatives) increased in the total volatiles (Adelina et al., 2021). Zhou et al. (2010) quantified the flavor substances produced by microwave roasted peanuts and concluded that pyrazines and aldehydes were the main volatile flavor substances of roasted peanuts. Lasekan & Abbas (2010) analyzed volatile flavor compounds in roasted terminalia catappa by supercritical fluid extraction and concluded that Carboxylic acids were the most abundant volatiles in the roasted almond nuts and less significant concentration of acrylamide was generated with mild roasting and shorter roasting period. Roasted rice have many advantages, such as being cooked for direct consumption, enhancing the taste, have an attractive roasted flavor, and being consumed as rice tea. However, little research on rice roasting has been reported.

Flavor substances are generally volatile small molecules containing different chemical types, such as aldehydes, ketones, alcohols, hydrocarbons, esters, phenols, amines, sulfides and mercaptans (Garruti et al., 2021). The process of forming food flavor substances is divided into two types: one is the flavor substances naturally formed during the growth, maturation and storage of raw materials; the other is the flavor substances formed during the processing of food (raw materials). To date, more than 300 volatile compounds have been identified in rice. It was found that the volatile components in rice were alcohols, aldehydes, ketones, esters, hydrocarbons, organic acids, and heterocyclic compounds, among which the most important volatile

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component was aldehydes, and the highest content was hexanal (Zhou et al., 2019). At the same time, some studies have found that glutaraldehyde and hexanal were important indicators for evaluating the quality of rice (Cho & Kays, 2013). The current research mainly focused on the effect of heat treatment on flavor substances of rice (Maleki et al., 2020). Mainly starch, fat and protein-like substances in rice were changed during heat treatment. After heat treatment, starch in rice degraded to form reducing sugars, which react with amino acids in a Maillard reaction to form important flavor substances, such as glucose, a starch degradation product, reacts with 1-pyrroline (a Strecker degradation product of proline) to form 2-acetyl-1-pyrroline, which is an important volatile component of aromatic rice with a popcorn flavor (Wei et al., 2017). In addition, rice is also degraded by heat to produce volatile flavor substances. Heating separates the starch-fat complex and promotes the degradation of fat to form oleic and linoleic acids, which were free fatty acids, resulting in volatile flavor substances. Volatile flavor substances from fats are mainly produced by fat hydrolysis and oxidation, in addition, enzymatic reactions as well as heating can also induce the breakdown of esters in rice to produce breakdown products such as aldehydes, ketones, alcohols, acids, furans, lactones, and hydrocarbons. Flavor is an important sensory attribute of food products used to assess their nutrition-related properties and freshness. However, although rice has been extensively studied in recent years, little research has been conducted to evaluate flavor substances of rice after roasting. Therefore, the aim of this study was to develop a simple method to characterize the flavor profile of roasted rice and to establish its flavor fingerprinting. Fingerprinting refers to detecting the unique profile of flavor compounds, or the flavor fingerprint, and quantifying the similarities within the same group (Zhou et al., 2019). Flavor fingerprinting can provide a more comprehensive picture of food quality information and reveal the complexity and relevance of food components. Therefore, it is reasonable and feasible to use flavor fingerprinting to evaluate the flavor characteristics of roasted rice.

Gas chromatography-ion mobility spectrometry (GC-IMS) is a recent technique that combines two aspects of gas chromatography and ion mobility spectrometry into one (Rahman et al., 2022), and simultaneously obtains information on the composition of flavor compounds and sample quality discrimination. GC-IMS combines the advantages of high separation in gas chromatography and high sensitivity in ion mobility spectrometry without any special sample pre-treatment and can rapidly detect trace volatile organic compounds (VOCs) in the sample. Compared with GC-MS, GC-IMS combines the advantages of high separation of gas chromatography and high resolution and sensitivity of ion mobility spectrometry, which is especially suitable for trace detection of VOCs (Zhang et al., 2022). Moreover, GC-IMS technology requires lower temperature for sample processing and analysis, which was more favorable for the detection of volatile compounds with poor thermal stability. In addition, after the initial separation of gas phase ions by GC, further separation is achieved in ion mobility spectrometry, which has stronger separation capability than ordinary chromatography (Yin et al., 2021). Therefore, gas phase ion mobility spectrometry has good application prospects in the fields of food volatiles detection.

In this study, the volatile organic compounds of rice at different roasting stages were firstly analyzed and detected using GC-IMS, and then subjected to principal component analysis and fingerprinting of the volatile components. This study analyzed the flavor substance changes of rice after roasting treatment and revealed the formation mechanism of aroma substances during the roasting process of rice. It aimed to provide a theoretical basis for the further development and utilization of rice resources, and also broadened the idea of rapid and efficient analysis of rice volatile compounds for the modern production and consumption of rice products.

2 Materials and methods

2.1 Materials

The rice in this study was obtained from Wuchang City, Heilongjiang Province, China, and roasted in a constant temperature oil bath in the laboratory. All of the chemical reagents used in this study were of analytical grade and purchased from LongShengJingKe reagent Distribution Department (Harbin, China).

2.2 Rice roasting process

The rice was removed from impurities and roasted in a constant temperature oil bath at 200 ± 20 °C. The rice was roasted with lightly, medium and heavy degrees for 9, 18, 27 min, respectively.

2.3 GC-IMS analysis

An Agilent 490 gas chromatograph (Agilent Technologies, Palo Alto, CA, USA) and IMS instrument (FlavourSpec®, Gesellschaft für Analytische SensorSysteme 156 8 MBh) equipped with an automatic sampling device were used to detect the flavor substances in samples collected from different production stages. The sample (2 g) from each stage was weighed and added to the 20 mL headspace glass sampling vial, labeled, and inserted into the sampling tank of the automatic sampler. After setting the relevant parameters of the instrument according to yang's method (Yang et al., 2021), the test starts.

Headspace injection conditions

The incubation temperature of the autosampler was 100 °C, and the incubation time was 15 min. The heating mode of the automatic headspace injection was oscillation heating, with an oscillation rate of 500 rpm, an injection needle temperature of 85 °C, and an injection volume of 500 μL; cleaning time is 0.5 min.

GC conditions

The sample entered the FS-SE-54-CB-1 quartz capillary column (15 m × 0.53 mm, 0.5 m) as a gas. The chromatographic column temperature was set at 60 °C, the carrier gas was N_2 (purity ≥ 99.999%), and the carrier gas flow rate was programmed as follows: the initial flow rate reached 2.0 mL/min within 2 min; the internal linearity was increased to 10.0 mL/min within 8 min, followed by 100.0 mL/min within 10 min and then to 150.0 mL/min within 10 min; the total running time was 30 min.

IMS conditions

The length of the drift tube was 98 mm, the linear voltage in the tube was 500 V/cm, the drift tube temperature was 45 °C, the drift gas was N_2 (purity ≥ 99.999%), the drift gas flow rate was 150 mL/min, the radioactive source was tritium (^3H) in carbon dioxide as the carrier gas, and the ionization mode was positive ion.

2.4 Statistical analysis

The following analytical software packages were used: (i) the Laboratory Analytical Viewer (LAV) for viewing the analytical spectra, in which each point refers to a VOC that can be quantitatively analyzed by establishing a standard curve; (ii) the Reporter plug-in for directly comparing the spectral differences between samples (two-dimensional top view and three-dimensional spectrum); (iii) the Gallery plot plug-in for fingerprint comparison, i.e., visual and quantitative comparisons of VOC differences between different samples; (iv) the Dynamic PCA plug-in for sample cluster analysis; (v) GC-IMS Library search software using NIST and IMS databases for qualitative analysis of the VOCs.

3 Results and discussion

3.1 Analysis of volatile odor components of rice at different roasting times by GC-IMS spectroscopy

The flavor compounds in the samples were determined by GC-IMS. The FlavourSpec® flavour analyzer was used to analyse the volatile flavour compounds of rice during roasting. Figure 1 shows the 3D spectra of the volatile components of rice at different roasting times obtained by the Reporter plug-in program in the LAV analysis software that comes with the instrument. The vertical coordinate represents the retention time (s) of the GC, the horizontal coordinate represents the ion migration time (normalized treatment), the red vertical line at the horizontal coordinate 1.0 is the reactive ion peak (RIP) peak, and each point on either side of the RIP peak represents a volatile organic compound. The color represents the response of the substance, with white, red, darker colors indicating a low, high and larger response, respectively. A compound may produce 1, 2 or more spots (representing monomers, dimers or trimers), depending on the concentration and nature of the volatile component. The four sections of the graph from left to right are: unroasted rice, lightly roasted rice, moderately roasted rice and heavily roasted rice. The three-dimensional spectra shown that the types and concentrations of VOCs increased significantly with the increase of roasting time, and there were significant differences in the types and concentrations of VOCs between the untreated rice and the heavily roasted rice.

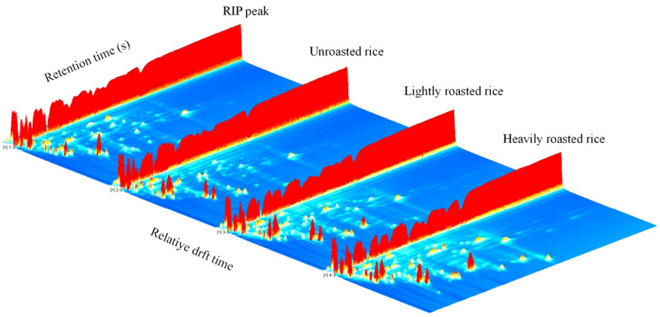


Figure 1. GC-IMS three-dimensional profiles of rice with different roasting degrees. From left to right, the picture shows unroasted rice, lightly roasted rice, moderately roasted rice and heavily roasted rice.

The differences in volatile flavor compounds between the four samples from different roasting stages were mainly reflected in the position, number, intensity and timing of ion peaks (Figure 1). The top view of HS-GC-IMS was obtained by normalizing the ion migration time and the position of the RIP (Figure 2A). The entire spectrum represents the total flavor compounds, and the points to the right of the RIP indicate the volatile organic compounds detected from the sample. The colors indicate the signal intensity of individual compounds. Red indicates high intensity and blue indicates low intensity. Darker colors indicate higher intensities. The results showed that most of the signals appear at hold times of 100-800 seconds and drift times of 1.0-1.9. In order to compare the differences between samples more obviously, a difference comparison model was used: the spectrum of unroasted rice was selected as a reference, and the spectra of other samples were deducted from the reference. If the VOCs of the two were the same, the background after deduction was white, while red color represented the concentration of the substance higher than the reference, and blue color represented the concentration of the substance lower than the reference. It can be seen from Figure 2B that the volatiles of the four rice

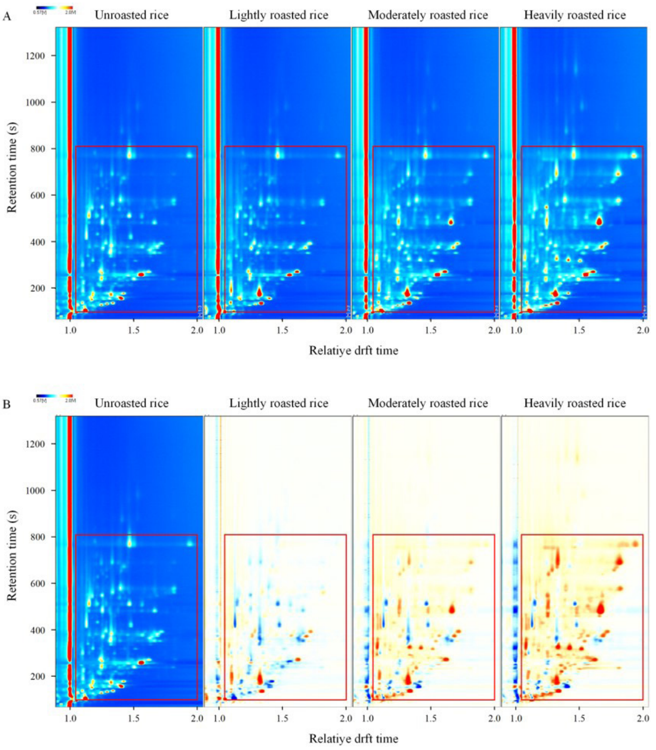


Figure 2. Two-dimensional GC-IMS profiles of rice with different roasting degrees (A: original spectrum; B: difference comparison spectrum). From left to right, the picture shows unroasted rice, lightly roasted rice, moderately roasted rice and heavily roasted rice.

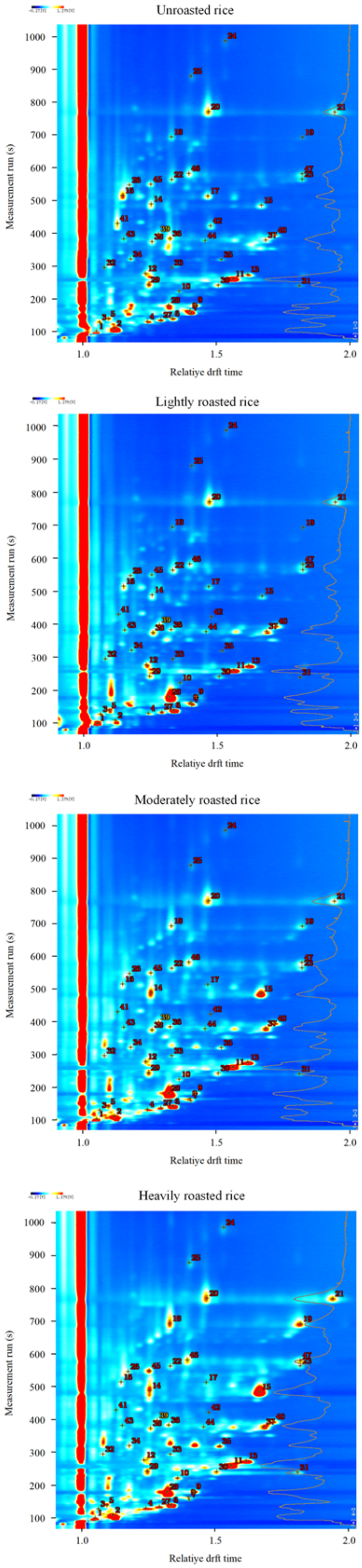
samples with different frying stages can be better separated by GC-IMS technique, and the GC-IMS characteristic spectrum information presented by the rice samples with different frying times has some differences, and some volatile components in the rice with different frying times appear to be higher or lower, showing more obvious differences (shown in the red box in Figure 2B). Among the four rice samples, the signal intensity of VOCs in the heavily roasted rice samples was significantly higher than that in the unroasted rice and lightly roasted rice. The retention times of most of the flavor ions ranged from 100-800 s, and the drift times were mainly between 1.0 and 1.9. Some ions had retention times between 800 and 1000 s, mainly due to the low polarity of these compounds, and non-polar compounds were retained on non-polar columns longer than polar compounds (Fan et al., 2021).

3.2 Qualitative analysis of volatile flavor substances in rice roasting process

The changes in flavor substances during rice roasting were detected by HS-GC-IMS spectroscopy, comparing their drift times and retention indices, using instrumental analysis methods. The figures shown in Figure 3, with the marked points representing a specific volatile substance for qualitative analysis. According to the NIST 2014 gas phase retention index database built into the flavor meter software and the IMS migration time database of G.A.S, a total of 47 volatile components (monomers and dimers of some substances) could be clearly characterized, mainly including 24 aldehydes, 8 esters, 8 ketones, 4 alcohols, 2 pyrrolylins, and 1 furan. As some individual compounds were present in different concentrations, they produced some signals or spots which represented the formation of the corresponding dimers. The results are shown in Table 1 and Figure 3.

3.3 Fingerprint analysis of volatile flavor substances in rice roasting process

The volatile organic compound contents of rice samples at different roasting stages were determined and their characteristic flavor fingerprints were established. The brighter the signal of each compound represents the stronger signal intensity, while the darker the signal represents the weaker signal intensity. Each row in Figure 4 represents a sample (from top to bottom, unroasted rice, lightly roasted rice, moderately roasted rice and heavily roasted rice, respectively), and each column represents the same volatile component in different samples (the darker the red signal, the higher the relative content of the substance), and the two with the same name on the fingerprint profile are compound monomer and dimer, respectively. It can be observed from the fingerprint spectrum above that: 3-methylbutyraldehyde, 2-methylbutyraldehyde, benzaldehyde, 2-acetyl-1-pyrroline, acetone, hexanal and methylheptenone have the highest concentrations when the rice is first fried and are higher than the other stages, and the concentrations decrease sharply when the frying is continued. The main reason is that aldehydes and ketones have carbonyl structures and are more active in nature, which can easily react with other substances under high temperature conditions, so continued heat will decrease the content of aldehydes and ketones. Moon & Shibamoto (2009) roasted coffee


Unroasted rice

Lightly roasted rice

Moderately roasted rice

Heavily roasted rice

Figure 3. Qualitative analysis of ion mobility spectra of volatile components of rice with different roasting degrees. (A: unroasted rice; B: lightly roasted rice; C: moderately roasted rice; D: heavily roasted rice).

Table 1. List of qualitative compounds of volatile components of rice with different roasting degrees.

Count	Compound	CAS#	Formula	MW	RI	Rt [sec]	Dt[RIPrel]	Comment
1	Ethanol	C64175	C_2H_6O	46.1	513.8	100.389	1.05471	
2	Acetone	C67641	C_3H_6O	58.1	532.3	108.472	1.12106	
3	Butanone monomer	C78933	C_4H_8O	72.1	576.8	127.873	1.06576	monomer
4	Butanone dimer	C78933	C_4H_8O	72.1	581.4	129.893	1.24429	dimer
5	Ethyl acetate monomer	C141786	$C_4H_8O_2$	88.1	601.8	138.785	1.09736	monomer
6	ethyl acetate dimer	C141786	$C_4H_8O_2$	88.1	602.7	139.189	1.33909	dimer
7	Methylbutanal	C590863	$C_5H_{10}O$	86.1	640.4	155.638	1.40735	
8	Methylbutanal	C96173	$C_5H_{10}O$	86.1	657.8	163.274	1.40371	
9	Pentanal	C110623	$C_5H_{10}O$	86.1	693.9	180.946	1.4237	
10	(E)-2-Pentenal	C1576870	C_5H_8O	84.1	745.6	222.214	1.36405	
11	Hexanal	C66251	$C_6H_{12}O$	100.2	790.3	259.759	1.5652	
12	Butyl acetate monomer	C123864	$C_6H_{12}O_2$	116.2	805.3	276.204	1.23781	monomer
13	Butyl acetate dimer	C123864	$C_6H_{12}O_2$	116.2	803.6	274.342	1.62069	dimer
14	(F)-2-heptenal monomer	C18829555	$C_7H_{12}O$	112.2	958.1	488.956	1.25922	monomer
15	(E)-2-heptenal dimer	C18829555	$C_7H_{12}O$	112.2	955.7	484.648	1.67043	dimer
16	Benzaldehyde monomer	C100527	C_7H_6O	106.1	972.6	514.805	1.15156	monomer
17	Benzaldehyde dimer	C100527	C_7H_6O	106.1	971.7	513.082	1.471	dimer
18	(F)-2-octenal monomer	C2548870	$C_8H_{14}O$	126.2	1066.6	693.839	1.33409	monomer
19	(E)-2-octenal dimer	C2548870	$C_8H_{14}O$	126.2	1065.7	692.033	1.82517	dimer
20	Nonanal monomer	C124196	$C_9H_{18}O$	142.2	1105.9	770.327	1.47392	monomer
21	Nonanal dimer	C124196	$C_9H_{18}O$	142.2	1105.3	769.123	1.94503	dimer
22	Butyl butanoate monomer	C109217	$C_8H_{16}O_2$	144.2	999.3	562.657	1.33617	monomer
23	Butyl butanoate dimer	C109217	$C_8H_{16}O_2$	144.2	1000.3	564.573	1.82341	dimer
24	Decanal	C112312	$C_{10}H_{20}O$	156.3	1216.7	986.151	1.53555	
25	(E) -2-nonenal	C18829566	$C_9H_{16}O$	140.2	1161.6	878.825	1.40672	
26	6-methyl-5-hepten-2-one	C110930	$C_8H_{14}O$	126.2	990.3	546.115	1.17827	
27	Butanal	C123728	C_4H_8O	72.1	592.4	134.71	1.2945	
28	Acetoin	C513860	$C_4H_8O_2$	88.1	692.5	179.799	1.32485	
29	pentanol monomer	C71410	$C_5H_{12}O$	88.1	770.9	242.423	1.24817	monomer
30	pentanol dimer	C71410	$C_5H_{12}O$	88.1	768.9	240.753	1.51019	dimer
31	pentanol polymer	C71410	$C_5H_{12}O$	88.1	766.2	238.665	1.81375	polymorph
32	Furfurol monomer	C98011	$C_5H_4O_2$	96.1	822.4	295.026	1.0836	monomer
33	Furfurol dimer	C98011	$C_5H_4O_2$	96.1	822.4	295.026	1.33604	dimer
34	(F)-2-hexenal monomer	C6728263	$C_6H_{10}O$	98.1	845.9	321.015	1.18181	monomer
35	(E)-2-hexenal dimer	C6728263	$C_6H_{10}O$	98.1	844.4	319.361	1.52155	dimer
36	Heptanal monomer	C111717	$C_7H_{14}O$	114.2	898.3	382.763	1.32946	monomer
37	Heptanal dimer	C111717	$C_7H_{14}O$	114.2	896.1	378.904	1.6864	dimer
38	Heptanone	C110430	$C_7H_{14}O$	114.2	893.3	373.942	1.26209	
39	Butyl propanoate monomer	C590012	$C_7H_{14}O_2$	130.2	906.7	397.649	1.28646	monomer
40	Butyl propanoate dimer	C590012	$C_7H_{14}O_2$	130.2	904.5	393.79	1.72367	dimer
41	acetyl-1-pyrroline monomer	C85213225	C_6H_9NO	111.1	924.4	429.075	1.13308	monomer
42	acetyl-1-pyrroline dimer	C85213225	C_6H_9NO	111.1	920.3	421.908	1.48141	
43	Cyclohexanone monomer	C108941	$C_6H_{10}O$	98.1	897.7	381.661	1.15601	monomer
44	Cyclohexanone dimer	C108941	$C_6H_{10}O$	98.1	895.5	377.801	1.45991	dimer
45	Pentylfuran	C3777693	$C_9H_{14}O$	138.2	992	549.171	1.25814	
46	Octanal monomer	C124130	$C_8H_{16}O$	128.2	1009	581.615	1.39931	monomer
47	Octanal dimer	C124130	$C_8H_{16}O$	128.2	1008.4	580.367	1.82284	dimer

MW represents molecular mass, RT represents relative retention index, Rt represents retention time, Dt represents relative migration time.

beans from Ethiopia, Yegashephine, Nicaragua and Sumatra. It was found that furfural, 2-acetylfuran, 5-methylfurfural and furanylmethanol reached their highest levels at 240 °C for 14 min. Furfural acetate reached its highest level at 250 °C for 17 min and then decreased with increasing roasting. However, the content of 5-hydroxymethylfurfural decreases continuously with the deepening of baking, and further 5-methylfurfural is produced.

As the degree of rice roasting increased, the concentrations of E-2-heptanal, cyclohexanone and butyl propionate increased and then decreased. The main reason may be that during the roasting process of rice, α-amino acids react with α-dicarbonyl compounds to lose one molecule of CO2 and become aldehydes and amino ketones with one less carbon atom, a process called Strecker degradation reaction. The ketones and aldehydes

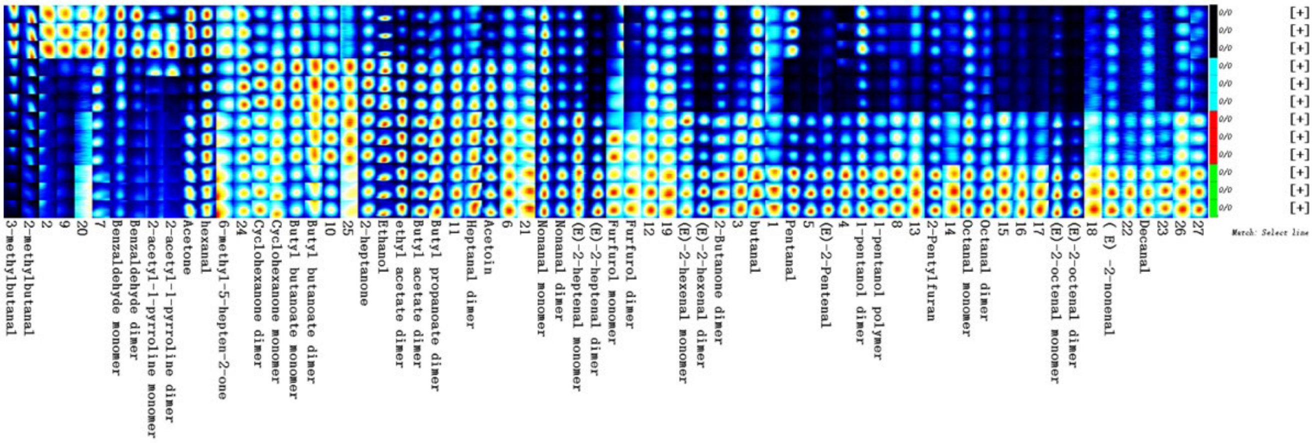


Figure 4. Fingerprint of volatile components of rice with different roasting degrees. (Right side down is unroasted rice, lightly roasted rice, medium roasted rice, and heavily roasted rice, respectively).

produced by this reaction, such as 2-methylbutyraldehyde, 3-methylbutyraldehyde, methylthiopropionaldehyde, and acetylacetone, are important factors in the production of aroma. showed experimentally that the content of Strecker aldehydes and ketones increased rapidly at the beginning of roasting, and then decreased as the temperature increased. Therefore, under moderate roasting conditions, rice was more fruity, floral and creamy aromas, and these aromas gradually decrease as the roasting degree increases.

The concentration of volatile substances such as nonanal, furfural, E-2-hexanal, 2-butanone, butanal, pentanal, E-2-pentanal, pentanol, 2-pentylfuran, octanal, E-2-octanal, E-2-nonanal and decanal gradually increased and reached the highest in the heavily roasted rice. It indicated that the main flavor substances added to rice during roasting were aldehydes. The increase in the relative content of aldehydes is mainly due to fat oxidation (Zhu et al., 2021), and they are one of the characteristic flavor compounds of rice when subjected to heat, which can impart a certain fatty flavor to fried rice. Studies have shown that functional fatty acids in rice are mainly linoleic acid, palmitic acid and oleic acid, and these functional fatty acids may be easily converted to aldehydes by oxidation reactions during frying, thus making lipid oxidation an important pathway for the characteristic aroma of fried rice.

Ketone flavors were less in type and content in both unroasted and roasted rice, and overall roasting increased the type and content of ketones. Ketone formation may be a product of oxidation of alcohols or a product of ester decomposition (Moon & Shibamoto, 2009). Alcoholic flavor substances were higher in unroasted rice, but their content gradually decreased with increasing roasting. It is possible that the alcohols were oxidized to the corresponding aldehydes during the roasting process (Zhang et al., 2022). The content of esters in unroasted rice was lower but more diverse, while the content and diversity of roasted rice were relatively lower. The high aroma threshold of esters had little effect on the roasted flavor (Guo et al., 2019). Compared to unroasted rice, the content and variety of furan-like flavor substances increased after roasting. Furan is a five-membered aromatic ring heterocyclic organic compound consisting of four carbon atoms and one oxygen atom. Compounds containing this five-membered aromatic ring are usually furan congeners. The mechanism of formation of furans in roasted rice involves the melad reaction, caramelization reaction, oxidation of polyunsaturated fatty acids, such as linoleic and linolenic acids, and the decomposition of ascorbic acid and its derivatives.

3.4 Analysis of volatile flavor substances PCA in rice roasting process

PCA is a multivariate statistics-based assay that uses the signal intensity of flavor substances to highlight their differences between samples (Fu et al., 2022). Figure 5 shows the results of PCA of flavor compounds in rice samples from different roasting stages. The GC-IMS chromatographic data of rice with different roasting levels were selected for PCA analysis of all volatile compounds in different roasting stages of rice to detect whether there were significant differences in volatiles between samples. The results were shown in Figure 5, where the contribution of PC1 is 66% and PC2 is 28%, and the cumulative contribution of both is up to 94%, which indicated that most of the information in the volatile components of the characterized samples can be obtained by PCA. The differences in characteristics between the samples can be visualized in Figure 5, where all four samples are far away from each other, while the parallel results of each sample are close together and almost overlap. This is due to the relatively obvious differences in the characteristics of the four samples at different roasting stages and the good reproducibility of the individual samples. It can be seen that the four different roasting stages of rice samples can be accurately distinguished by PCA analysis, which is consistent with the results of fingerprinting, which indirectly indicated the potential of GC-IMS mobility spectrometry for the identification of flavor substances in rice roasting.

A total of 47 volatile organic compounds, including dimers of some substances, were analyzed and identified by GC-IMS technique for the analysis of volatile odor substances in rice with different roasting degrees. The main compounds included 24 aldehydes, 8 esters, 8 ketones, 4 alcohols, 2 pyrroline, and

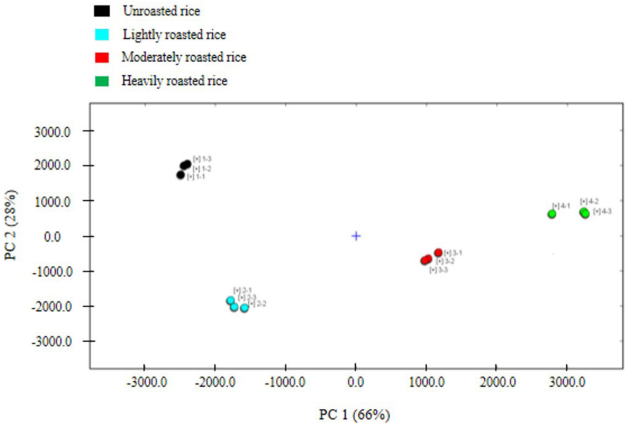


Figure 5. PCA analysis of volatile components of rice with different roasting degree.

1 furan. The aldehyde volatiles were the main flavor components in both unroasted and roasted rice, but there were large differences in the types and contents of aldehydes in rice with different roasting levels, and their relative contents decreased with increasing roasting levels.

4 Conclusion

Forty-seven flavor substances were identified from the volatile odor substances of rice at different roasting levels. The analysis showed that aldehydes, ketones and aromatic compounds such as E-2-hexanal, 2-butanone and butyraldehyde had a greater influence on the characteristic flavor of roasted rice. Alcohols and furans also contributed to the characteristic aroma composition of roasted rice. These analytically identified volatile flavor compounds may be contributors to the volatile components of rice at different roasting stages.In addition, the results of PCA showed that the distribution of volatile compounds from samples at different roasting stages occupied relatively independent spaces and could be easily distinguished. Therefore, a specific and feasible method was developed to establish the flavor fingerprint of a given sample using GC-IMS and PCA to successfully characterize the volatile organic compounds in samples from different roasting stages. The combination of GC-IMS and PCA allowed the rapid detection and analysis of unique flavor fingerprints across roasting stages, thus allowing a scientific approach to determine the processing endpoints, avoiding the involvement of human senses. This method has great potential for industrial application to detect flavor differences in rice at different roasting levels and provides a basis for future research on rice roasting processes and the development of their products.

Conflict of interest

The authors declare that they have no conflict of interest.

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