Food Chemistry: X 19 (2023) 100755

Contents lists available at ScienceDirect

Food Chemistry: X

journal homepage: www.sciencedirect.com/journal/food-chemistry-x

Predicting VOCs content and roasting methods of lamb shashliks using deep learning combined with chemometrics and sensory evaluation

Che Shen [a], Yun Cai [a], Meiqi Ding [a], Xinnan Wu [a], Guanhua Cai [a], Bo Wang [a,b,*], Shengmei Gai [a], Dengyong Liu [a,*]

[a] *College of Food Science and Technology, Bohai University, Jinzhou 121013, China*

[b] *Key Laboratory of Meat Processing and Quality Control, MOE, Key Laboratory of Meat Processing, MARA, College of Food Science and Technology, Nanjing Agricultural University, Nanjing 210095, China*

A R T I C L E I N F O

Keywords:
SPME-GC–MS
HS-GC-IMS
Lamb shashliks
Roasting methods
Sensory evaluation
Deep learning

A B S T R A C T

A comparison was made between the traditional charcoal-grilled lamb shashliks (T) and four new methods, namely electric oven heating (D), electric grill heating (L), microwave heating (W), and air fryer treatment (K). Using E-nose, E-tongue, quantitative descriptive analysis (QDA), and HS-GC-IMS and HS-SPME-GC–MS, lamb shashliks prepared using various roasting methods were characterized. Results showed that QDA, E-nose, and E-tongue could differentiate lamb shashliks with different roasting methods. A total of 43 and 79 volatile organic compounds (VOCs) were identified by HS-GC-IMS and HS-SPME-GC–MS, respectively. Unsaturated aldehydes, ketones, and esters were more prevalent in samples treated with the K and L method. As a comparison to the RF, SVM, 5-layer DNN and XGBoost models, the CNN-SVM model performed best in predicting the VOC content of lamb shashliks (accuracy rate all over 0.95) and identifying various roasting methods (accuracy rate all over 0.92).

1. Introduction

Due to their long history, lamb shashliks are considered a traditional Chinese dish. It is due to the unique flavor and sensory experience that these products are loved by consumers and influence their purchase decision (Wang et al., 2023). It should be noted, however, that as a traditional food, lamb shashliks are likely to pollute the environment with the fumes released during the preparation process, particularly those from fuel oil (Wang et al., 2022). As part of traditional food innovation, it is important to process the food in a traditional manner or according to a traditional recipe and ensure the product's sensory characteristics are appropriate to ensure consumer acceptance (Guerrero et al., 2009). The art of cooking meat has evolved into more sophisticated techniques over time (Suman et al., 2016). Myogenic fibers and proteins in sarcoplasmic and connective tissues denature during heating, resulting in structural changes in the meat and altering its mechanical properties (Li et al., 2013). Cooking methods for traditional foods can be improved through innovation. In recent years, technological advances have led to the development of other methods of roasting, such as the use of electric ovens (D), microwaves (W), air fryers (K), and electric grills (L). These methods can be used to avoid the disadvantages associated with traditional lamb shashliks while releasing the flavor of the meat (Wang et al., 2022).

Scientists, chefs, gourmets and consumers in every culture are interested in the effects of different cooking methods on food's sensory and physicochemical properties. Physicochemical indicators and sensory evaluations assess how different cooking methods affect meat quality (Jiang et al., 2023). A sensory evaluation involves assessing food's flavor qualities and sensory properties through human perception. Many industries have used this method, which is irreplaceable in

Abbreviations: HS, headspace; SPME, solid phase micro extraction; GC–MS, gas chromatography-mass spectrometry; GC-IMS, gas chromatography-ion mobility spectrometry; SVM, support vector machine; RF, Random Forest; 5-layer DNN, 5-layer deep neural network; XGBoost, eXtreme Gradient Boosting; CNN-SVM, Convolutional Neural Network-Support Vector Machine; E-nose, electronic nose; E-tongue, electronic tongue. QDA, quantitative descriptive analysis; HCA, hierarchical clustering analysis; PCA, principal component analysis; *t*-SNE, *t*-distributed stochastic neighbor embedding; LSD test, least significant difference test; Tukey's HSD test, Tukey's honestly significant difference test; OPLS-DA, orthogonal partial least squares discrimination analysis; VOC, volatile organic compound.

* Corresponding authors at: College of Food Science and Technology, Bohai University, No. 19, Keji Rd., New Songshan District, Jinzhou 121013, Liaoning Province, China.

E-mail addresses: daqingwb@163.com (B. Wang), jz_dyliu@126.com (D. Liu).

https://doi.org/10.1016/j.fochx.2023.100755
Received 1 May 2023; Received in revised form 1 June 2023; Accepted 12 June 2023
Available online 14 June 2023

food development, quality control, product optimization, and classification (Varela & Ares, 2012). Sensory evaluation is, however, influenced by individual differences among evaluators and is characterized by relatively low reproducibility and subjective nature. For this reason, multivariate intelligent sensory technologies including E-noses and E-tongues are used to obtain relatively complete information on the sensory characteristics of foods.

To analyze volatile organic compounds (VOCs) qualitatively and quantitatively, gas chromatography-mass spectrometry (GC–MS) is an effective and widely used method (Liu, Qian, Dong, Bai, Zhao, Li, & Liu, 2020; Liu et al., 2020; Qian et al., 2023). Due to the complexity of food matrixes, the method usually requires complex sample pretreatment and long simultaneous detection times, which greatly hinders the analytical efficiency of HS-SPME-GC–MS. An important characteristic of gas chromatography with ion mobility spectrometry (GC-IMS) is its ease of operation, high resolution, improved separation, intuitive data visualization, high sensitivity and analytical speed, no sample preparation and atmospheric pressure operation (Yao et al., 2022; Zhu et al., 2022). This method allows samples to be differentiated at a low cost, in real time, and rapidly (Li et al., 2019; Shen et al., 2023).

Data fusion combined with artificial neural network algorithms allows the synthesis and analysis of data from multiple intelligent sensory technologies to simulate human brain activity. In recent years, the rapid development of deep learning technology has proven to be very powerful in a wide range of applications, attributed to its main advantages, including powerful generalization capabilities, and large data training capabilities (Zhu et al., 2023). Convolutional neural networks (CNNs) are one of the most popular deep learning models and have been widely used in many fields from image recognition to speech translation. CNN-SVM models take advantage of their respective models and are applied to process data combining multidimensional techniques with sensory evaluation to explain the differences in sample features from multiple perspectives. Meanwhile, various instruments have been combined to study food flavor profiles as they generate more accurate and comprehensive results.

Thus, this study investigated the effects of four new roasting methods compared to the T method on sensory evaluation, intelligent sensory technologies (E-nose and E-tongues), and VOCs in lamb shashliks. A feature-level data fusion strategy was applied to improve flavor identification accuracy. To predict VOCs and different roasting methods of lamb shashlik, five machine-learning models were applied using data from chemometric, E-nose, E-tongues, and sensory evaluations.

2. Materials and methods

2.1. Sample preparation

A total of 24 six-month-old Sunit sheep (31.5 ± 1.5 kg carcass weight) with similar genetic backgrounds and a similar diet (cereal and silage) were randomly selected from the Xilingol League Yangyang Husbandry Co. and were slaughtered in one day on the commercial slaughter line. As per Chinese standard protocol GB 2707–2016, the longest section of lean backbone and tail fat was removed after slaughter. Using traditional cold chain logistics, meat and tail fat were frozen at −20 °C and transported to Jinzhou, Liaoning, China. In an incubator (MIR-154-PC, Panasonic, Beijing, China) at 4 ± 1 °C, lean meat and fat were thawed until their core temperatures reached a range of −3 °C to −5 °C. The lean and fatty meat was cut into cubes of about 2 cm^3 (2 cm × 1 cm × 1 cm) after removing the surface fat, according to NY/T 3469–2019. Using a 15 cm bamboo skewer, 4 pieces of lean meat were skewered, and 1 piece of fat was skewered. A precision thermometer (Benetech®, Shenzhen, China) was used to measure the internal temperature of the lamb shashliks (80 °C). The effect of roasting methods with different temperatures, times, and powers on the flavor of lamb shashliks was evaluated in a sensory evaluation. The optimal parameters for each of the five methods were determined based on sensory evaluation. Using the T grilling method, a charcoal grill was employed for grilling at 220–230 °C for 12 min, rotating every 1 min. The D method was performed in an electric oven (Panasonic NB-HM3810, Beijing, China) by roasting the lamb shashliks for 10 min at 200 °C and rotating them every minute. For the W roasting method, the lamb shashliks were microwaved (Galanz G70F23CN2P-BM1S0, Foshan, China) at 700 W at 2450 MHz for 8 min, turning every 1 min. For the K method, lamb shashliks were roasted at 1700 W for 5 min, turning every 30 s, in an air fryer (Midea KZ120Q7-400G, Foshan, China). For the L method, the lamb shashliks were roasted on an electric grill (Bear DKL-E20J1, Foshan, China) at 2000 W for 7 min, rotating every 30 s. Lamb shashliks for instrumental analysis were frozen in nylon/polyethylene (9.3 mL $O^2/m^2/24$ h, 0 °C, 0.19 mm thick, Magic Seal®, Guangdong, China) in liquid nitrogen and stored at −80 °C.

The chemicals used in this study, 2-methyl-3-heptanone (99%, internal standard) and *n*-alkanes (C7-C40, 97%, external standard), were obtained from Aladdin (Shanghai, China) and Zhongke Standard Technology Co. All other authentic flavor standards were obtained from Tokyo Chemical Industry (TCI, Shanghai, China): hexanal (98%), heptanal (97%), octanal (99%), nonanal (99.5%), (E)-2-octenal (97%), (E)-2-nonenal (97%), benzaldehyde (99.5%), 1-heptanol (98%), 1-octen-3-ol (98%) and 2-pentylfuran (98%).

2.2. Evaluation of the sensory characteristics of lamb shashliks

According to Ramirez et al. (2020), thirty sensory assessors underwent an initial screening process (including matching and ranking tests) and nine training sessions on descriptors and methods applicable to meat products, from which final panel of 18 (nine males and nine females, aged 20 to 26 years) were selected. Sensory attributes (odor, flavor, appearance, and texture) of lamb shashliks using various roasting methods were analyzed using quantitative descriptive analysis (QDA). A total of 19 descriptors were identified characterize the lamb shashliks after discussion with panelists. A total of three sessions over a two-week period were conducted after a high level of agreement among the panelists. Samples were held at 50 °C on white trays coded with random three-digit numbers and randomly handed to panelists, with three replicates of each sample assessed by panelists. Each assessor received an assessment form and were invited to rate the intensity of each attribute on a linear scale with 10 cm (unstructured) anchored on the left end by "none" and on the right end by "strong". During the QDA procedure, panelists were able to use filtered portable water or/and unsalted crackers provided between sample evaluations as materials for palate cleansing. The average sensory scores obtained by panelists for 19 descriptors of the five roasting methods lamb shashlik samples were collected and used for further analysis.

2.3. E-nose measurement

PEN3 E-nose (Airsense Analytics GmbH, Schwerin, Germany) was used for the analysis by referring to the method of Shi et al. (2020). Ten metal oxide monolayer thick film sensors exist in the PEN3 system: W1C, W5S, W3C, W6S, W5C, W1S, W1W, W2S, W2W, and W3S, which can generate signals about different VOCs. Table S1 describes the performance of the E-nose gas sensor array. Various roasting methods were used for cooking lamb shashliks in a 20 mL headspace sample bottle. The sample vial was heated for 40 min in a water bath at 50 °C. The parameters for the system were determined using an E-nose system with a chamber flow rate of 200 mL/min, an injection flow rate of 200 mL/min, and a measurement time of 120 s. Following the return of the sensor signal to baseline, the chamber was cleaned with fresh air, and the next sample was then measured.

2.4. E-tongue measurement

Among the five chemical sensors contained in the E-tongue (SA402b, Insent Inc., Japan) are CA0 (sourness sensor), AE1 (astringency sensor), AAE (umami sensor), CT0 (saltiness sensor), and C00 (bitterness sensor). According to Shen et al. (2023), the lamb shashliks samples of variety roasting methods were homogenized (10000 rpm) with 200 mL distilled water (40 °C) for 60 s and then centrifuged at 5000 rpm for 40 min at 4 °C. Supernatants were removed, and membrane passes (0.22 μm) were taken for analysis. Each sample was subjected to the E-tongue test to determine its water solubility. Four cycles of each sample were performed, and the average of the three cycles was calculated after the first cycle. Before measurement, each sensor was checked to ensure it was operating within the specified mV range according to the manufacturer's instructions. As a result of electrostatic or hydrophobic interactions between taste-presenting substances and artificial lipid membranes, an E-tongue was used to detect changes in membrane potential, leading to the evaluation of eight basic taste indicators, including umami, astringency, saltiness, bitterness, richness, sourness, aftertaste astringency (aftertaste-A), and aftertaste bitterness (aftertaste-B).

2.5. Analysis of headspace solid-phase microextraction/gas chromatography-mass spectrometry (HS-SPME/GC–MS)

Various roasting methods were used to process lamb shashliks, and VOCs were detected, as described by Liu et al. (2021), with some modifications. Headspace solid-phase microextraction (HS-SPME) was used to extract VOCs. As an internal standard, 2 g of chopped sample and 1.5 μL of 2-methyl-3-heptanone (1.7 μg/mL in methanol) were quickly transferred to a 20 mL headspace vial, and the vial sealed with a PTFE spacer. In the following steps, the vial was placed in a water bath and kept at 55 °C for 15 min. For 45 min following incubation, carboxene-polydimethylsiloxane (CAR/PDMS, 75 μm) coated fibers (Supelco, Inc., Bellefonte, PA, USA) were exposed to the headspace vial to absorb VOCs from the sample. Immediately after coating, the fibers were injected into the gas chromatography (GC) unit port to desorb for 2 min. The VOCs were separated and identified using a gas chromatography-mass spectrometer (GC–MS) (TQ8040NX, Shimadzu Corporation) equipped with an Rtx-5MS (30 mm × 0.25 mm × 0.25 μm). At a 1 mL/min rate, helium was used as the carrier gas in a constant flow mode. Inlet and ion source temperatures were 200 ℃. The oven temperature was ramped-up as follows: hold the temperature at 40 °C for 3 min, ramp up to 120 °C at 5 °C/min, ramp up to 200 °C at 10 °C/min, and hold at 200 °C for 13 min. A full electron collision scan mode was utilized to obtain mass spectra at 70 eV and 400 *m/z*. Using 2-methyl-3-heptanone as an internal standard, the contents of each component were quantified.

2.6. Analysis of Headspace-gas chromatography-ion mobility spectrometry (HS-GC-IMS)

HS-GC-IMS (FlavorSpec®, Gesellschaft für Analytische Sensorsysteme mbH, Dortmund, Germany, Department of Shandong HaiNeng Science Instrument Co., Ltd., Shandong, China) was used for the analysis of VOCs. The analytical method proposed by Yao et al. (2021) was slightly modified. 3.00 g of chopped lamb shashliks was accurately weighed, transferred to a 20 mL headspace vial, and incubated at 60 °C for 15 min at 500 rpm. After this, 500 μL of volatile gas was collected from the headspace vial and automatically injected into the injector at 85 °C without splitting. A metal capillary column (MXT-5, 15 m × 0. 53 mm, 1 μm) was used to separate the VOCs bound to IMS at 45 °C. As a carrier/drift gas, high-purity nitrogen was used. The initial carrier gas flow rate was set at 2 mL/min, which was maintained at 2 mL/min for 0–2 min, and then increased linearly from 2 mL/min to 100 mL/min for 2–20 min. The total run time was 20 min, and the drift gas flow rate was 150 mL/min. Ionization was carried out in an IMS ionization chamber at 45 °C at a column temperature of 60 °C. GC-IMS analysis was conducted in triplicate. Retention indices (RI) were calculated using *n*-ketones (C4-C9).

2.7. Machine learning prediction

Each dataset was divided into 70% for model training and 30% for data prediction. A root mean square error (RMSE) and correlation coefficient (R^2) were used to evaluate the performance of each model. R^2 represents the correlation between the predicted and measured values in a training or test set. RMSE represents the deviation between predicted and measured values in training or test sets. The closer the R^2 is to 1, the smaller the RMSE and the higher the accuracy and stability.

The use of data fusion strategies is widespread. A data fusion method combines data from different sources to allow for more extensive use of sample features and more accurate identification of samples. Data fusion includes three strategies: data-level fusion, feature-level fusion, and decision-level fusion (Xu et al., 2019). The feature-level fusion strategy was chosen to integrate data obtained from GC–MS, GC-IMS, E-nose, E-tongue, and sensory evaluations.

To identify lamb shashliks processed in various roasting methods according to their flavor characteristics, five models were developed: SVM (Cortes and Vapnik, 1995), RF (Leo & Breiman, 2001), XGBoost (Chen & Guestrin, 2016), 5-Layer DNN (Hinton, 2006), and CNN-SVM (Islam et al., 2021).

2.8. Statistical analysis

To determine differences between means, one-way analysis of variance (ANOVA) and LSD tests were conducted using SPSS 26.0 software (SPSS Inc., USA). ANOVA was also performed to assess the variation in mean attribute scores between samples prepared using various roasting methods. To identify groups with significant differences, Tukey's HSD test was used. WPS Office (Kingsoft Corporation, Beijing, China) and Origin 2022 (OriginLab Inc., Northampton, MA, USA) were used to determine radar plots and PCA. The OPLS-DA analysis was conducted using SIMCA-P 14.1 software (Umetrics, Umea, Sweden), and the clustering heat maps were generated using TBtools version 1.098. Python 3.7.3 was used to run SVM, RF, XGBoost, DNN 5-layer, CNN-SVM, and *t*-SNE.

3. Results

3.1. Effect of the roasting methods on sensory evaluation

In Fig. 1A and Table S2, 19 sensory descriptors were used to rate the average strength of all lamb shashliks. Umami flavor exhibited the highest (from 6.7 to 9.1), followed by roasting-lamb odor (from 6.8 to 8.9), intensity odor (from 6.5 to 8.9), buttery odor (from 3.8 to 8.9), fatty flavor (from 6.5 to 8.8), dryness (from 6.4 to 8.7), gravy flavor (from 5.6 to 8.7), greasy appearance (from 5.2 to 8.7), bloody flavor (from 7.1 to 8.6), hardness (from 6.5 to 8.5), juicy appearance (from 6.2 to 8.5), fatty odor (from 6.6 to 8.4), gamy flavor (from 6.4 to 8.3), liver odor (from 4.5 to 8.3), chewy texture (from 5.9 to 8.2), rubbery texture (from 5.4 to 8.2), wet appearance (from 5.0 to 8.1), sour flavor (from 5.3 to 7.7), and dark appearance (from 5.3 to 7.7). A significant difference was found in the above descriptors ratings of the samples differed significantly, indicating that these attributes were capable of revealing differences between lamb shashliks treated with various roasting methods.

In addition, these data suggest that odor, flavor, appearance, and texture all play important roles in defining the sensory characteristics of lamb shashliks roasted in different methods. As shown in Table S2, the attribute intensity ratings showed trends in different methods of perceiving lamb shashliks. Sample T exhibited the highest umami flavor (9.1), roasting-lamb odor (8.9), intense odor (8.9), fatty flavor (8.8), dark appearance (8.7), greasy appearance (8.7), and juicy appearance (8.5) and the lowest buttery odor (3.8). Umami is the dominant flavor characteristic of roasted lamb (Liu et al., 2020). Besides sample T, the highest-rated samples were sample K (8.5), sample L (8.0), D (7.4), and

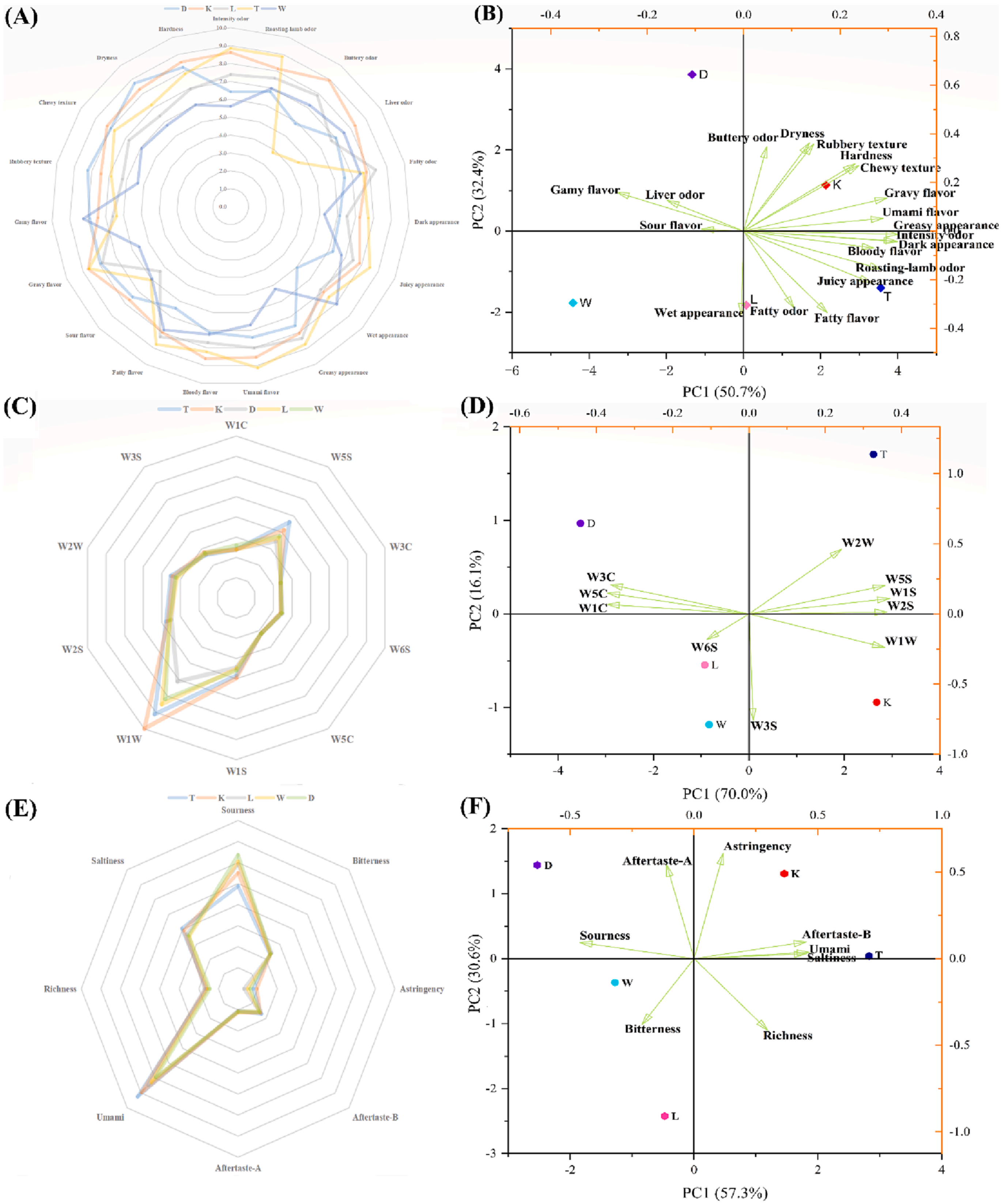

Fig. 1. Radar chart (A) and principal component analysis (B) of QDA for lamb shashliks with different roasting methods; Radar chart (C) and principal component analysis (D) of E-nose data for lamb shashliks with different roasting methods; Radar chart (E) and principal component analysis (F) of E-tongue data for lamb shashliks with different roasting methods.

W (6.7). Sample K was rated highest in terms of buttery odor (8.9), gravy flavor (8.7), bloody flavor (8.6), hardness (8.5), liver odor (8.3), chewy texture (8.2), and sour flavor (7.7).

Compared to the control sample T, sample K ranked second in the attribute ratings of umami flavor, intensity odor, dark appearance, roasting-lamb odor, and juicy appearance. Based on the findings of Wang et al. (2022), consumers were attracted to lamb shashliks treated by the K method due to their buttery odor, making them unique and popular. Among the samples, sample L presented the highest fatty odor (8.4), the second greasy appearance (8.4), the second fatty flavor (8.3), and the second buttery odor (7.9). Sample D exhibited the highest dryness (8.7), highest rubbery texture (8.2), second hardness (8.2), and second gamy flavor (8.1). The highest rating was given to sample W for gamy flavor (8.8), wet appearance (8.1), and liver odor (7.6). From these ratings, it is apparent that the flavor and odor attributes are more indicative of the samples processed in different roasting methods.

The sensory data from the evaluated lamb shashlik samples were subjected to PCA to differentiate between different roasting methods. For the analysis, the first two principal components (PC1 and PC2) explained 83.1% of the total variance (Fig. 1B). With PC1 accounting for 50.7% of the variance, the positive end of the axis is formed by buttery odor, dryness, rubbery texture, hardness, chewy texture, gravy flavor, umami flavor, greasy appearance, intense odor, dark appearance, bloody flavor, roasting-lamb odor, juicy appearance, fatty flavor, and fatty odor. In contrast, the negative axis is formed by liver odor, gamy flavor, sour flavor, and wet appearance.

The samples K, T, and L were grouped on the positive side of PC1. They were identified by characteristics that described buttery, intense, roasting-lamb, and fatty odors, gravy, umami, fatty, bloody flavor, rubbery, chewy, dry, hardness texture, as well as greasy, dark, and juicy appearance. Samples D and W were associated with a gamy flavor, liver odor, sour flavor, and wet appearance. Furthermore, these were the negative effects of PC1.

3.2. Effect of roasting methods on the development of intelligent sensory technologies

Fig. 1C illustrates the responses of the E-nose to lamb shashliks treated with various roasting methods. As indicated by the strong responses of the sensors W1W, W2W, W5S, W2S, and W1S, lamb shashliks that have been roasted by various methods contain high levels of alcohols, aldehydes, ketones and sulfides.

Nevertheless, the intensity of the signal in lamb shashliks varied based on the roasting method. Compared to the control sample T, sample K showed the strongest response at W1W and W1S (K > T > L > W > D), suggesting that the shashlik with K used contained more sulfur-containing compounds. However, the responses of W3S, W6S, W1C, W3C, and W5C were less variable. The E-nose system was effective in identifying the characteristic aromas of a variety of samples. According to the radar plot, the lamb shashliks treated with the five roasting methods showed similar odor profiles. Nevertheless, there was a considerable variation in the intensity and proportion of the various volatile gases.

An analysis of the spatial distribution and distances of lamb shashlik odors was conducted using PCA (Fig. 1D). In all samples, and the first two main components contributed 88.1% to the cumulative variance, which indicates that they covered the bulk of the information (PC1 70.3%, PC2 17.8%). A significant difference between the shashliks treated by various roasting methods can be found primarily on PC1, where the E-nose completely distinguishes the five roasting methods. In each roasting method, shashliks occupied a different aroma region. It was found that samples T and K clustered on the positive PC1 axis and were associated with sensors W1S, W2S, W3S, W5S, W1W, and W2W. On the other hand, samples D, L, and W clustered on the negative PC1 axis and were associated with sensors W1C, W3C, W5C, and W6S. This indicates that the E-nose sensor can distinguish between different roasting methods for lamb shashliks.

Using the E-tongue, differences in taste characteristics were evaluated. Fig. 1E illustrates responses to bitterness, saltiness, astringency, sourness, aftertaste-B, aftertaste-A, richness, and umami. The lamb shashliks with various roasting methods responded strongly to the umami, sourness, and saltiness sensors. Umami and saltiness were the strongest responses for lamb shashliks treated by the T method, followed by those treated by the K method. Additionally, lamb shashliks treated with the D method showed the strongest response regarding sourness. There was less variation in richness than aftertaste-A, aftertaste-B, and astringency responses. As indicated by the shape of the radar plot, the taste profiles of lamb shashliks treated by the five roasting methods were similar. The intensity and proportion of each taste, however, varied significantly.

For the electronic tongue, PCA plots of taste differences are shown in Fig. 1F. PC1 (60.1%) and PC2 (27.1%) contributed 87.2% of the cumulative contribution and can reflect the overall characteristics of the samples as a whole. As determined by the T and K methods, lamb shashliks clustered on the positive PC1 axis associated with umami, saltiness, richness, astringency, aftertaste-A, and aftertaste-B are highly correlated with these attributes. On the other hand, lamb shashlik treated with the L, D, and W methods clustered on the negative PC1 axis associated with sourness and bitterness. The results of this study suggest that E-tongue may prove to be an effective method of separating the taste of lamb shashliks prepared using different roasting methods.

3.3. Identification and quantification of VOCs

Using SPME-GC–MS to analyze lamb shashliks treated with five roasting methods revealed significant differences in the volume and composition of VOCs. In total, 79 VOCs were identified and quantified, of which 57, 57, 34, 52, and 36 VOCs were found in T, K, D, L, and W, respectively (Table S3). Among these, 17, 18, 13, 18, and 15 were aldehydes; 14, 13, 5, 12, and 7 were alcohols; 0, 4, 6, 3, and 2 were ketones; 21, 15, 9, 10, and 9 were hydrocarbons; 4, 6, 0, 8, and 2 were esters; and 1, 1, 1, 1, 1, and 1 were furans. Using a clustered heat map hierarchical clustering analysis (HCA) based on the contents of VOCs, lamb shashliks treated with each roasting method were compared. As shown in Fig. 2., the heat map displays the overall profile of each VOC in the form of colored boxes. A normalized color intensity scale ranges from a maximum value of 3.00 (red) to a minimum value of 3.00 (blue), which indicates a high or low concentration of VOCs (Florentino-Ramos et al., 2019). Based on the HCA results, the lamb shashliks were categorized into three groups: K method and L method, D method and W method, and T method alone. Moreover, the tree diagram could be used to categorize the VOCs into four groups. Using the K and L methods, a total of 15 VOCs with a high concentration in Group A were detected. T, K and L methods revealed 22 VOCs with high contents in Group B. The five roasting methods detected hexanal, heptanal, octanal, nonanal, 2-pentylfuran, 1-pentanol, 1-octen-3-ol, pentadecanal, toluene and heptadecane in the samples, amongst others. In group C, 35 VOCs were found to be more abundant in T samples, predominantly hydrocarbons, long-chain aldehydes, and long-chain alcohols. The VOCs with higher content in group D were pentadecane, formic acid heptyl ester, 2-heptanone, eicosane, 5-pentyldihydro-2(3H)-Furanone, 2-decanone, and 5-butyldihydrofuranone-2(3H)-Furanone.

3.4. Identification of VOCs using HS-GC-IMS

HS-GC-IMS was used to analyze the VOC content of lamb shashliks roasted with five different methods. GC-IMS analysis detected 43 signals, as shown in Table S4. Based on retention and migration times for each VOC, retention indices were calculated using *n*-ketone C4-C9 as an external reference standard and compared with the GC-IMS library. We identified 43 VOCs (including monomers and dimers) containing 22 aldehydes, 7 alcohols, 6 ketones, and 2 acids. Seven peaks, however,

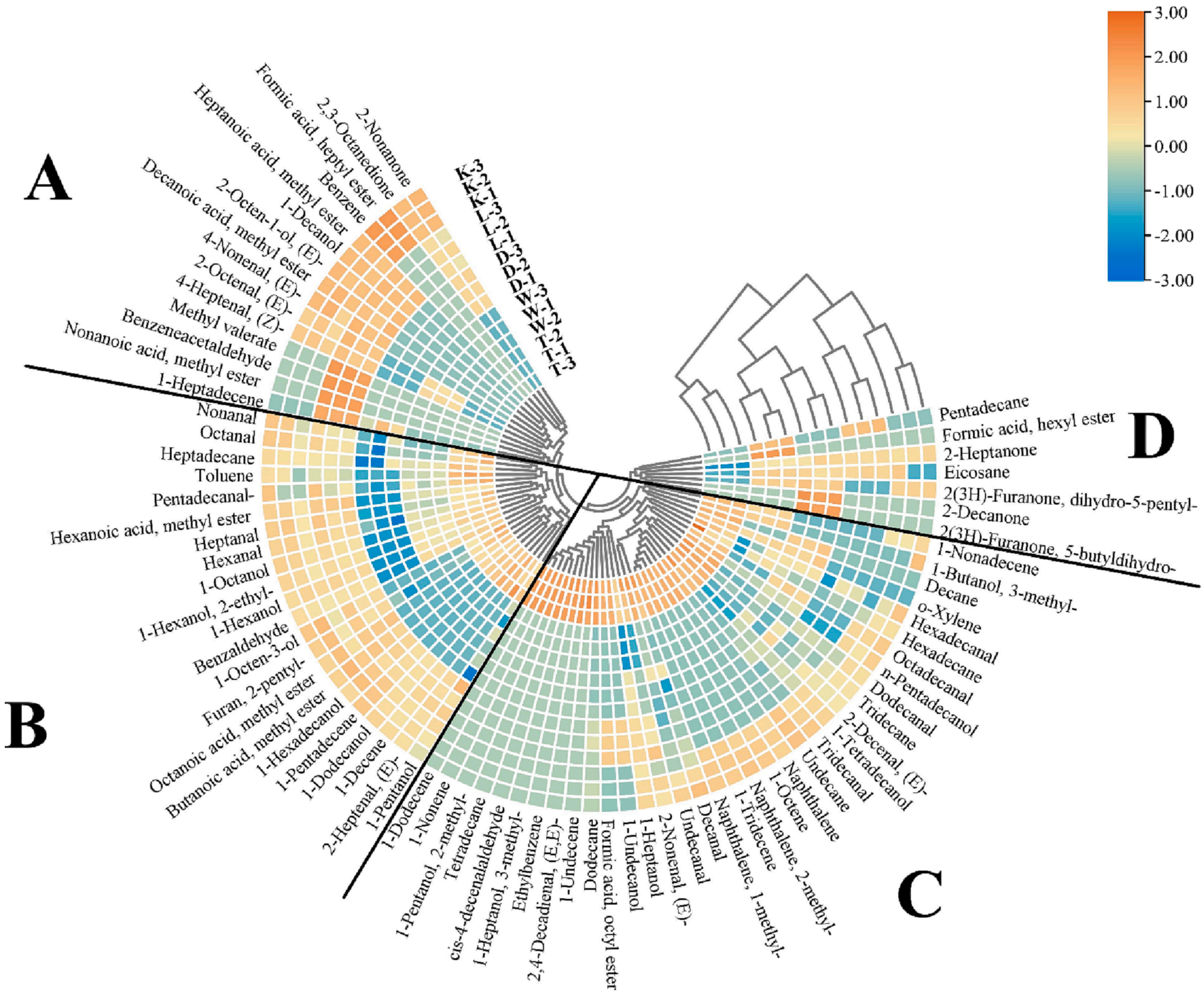

Fig. 2. Hierarchical clustering and heatmap visualization of volatile organic compounds of lamb shashliks with five roasting methods.

remain unidentified. A significant proportion of the compounds detected by GC-IMS were aldehydes, accounting for 51.2% of all compounds detected. Due to the incorporation of ions and neutral molecules in some compounds, multiple signals are observed (monomer and dimer) (Li et al., 2019). For example, the monomer and dimer of pentanal exhibited similar retention times ($Rt_{\text{pentanal monomer}} = 163.045$, $Rt_{\text{pentanal dimer}} = 164.811$) but different drift times ($Dt_{\text{pentanal monomer}} = 1.18537$, $Dt_{\text{pentanal dimer}} = 1.42954$).

Fig. S1 illustrates the three-dimensional spectra of VOCs from lamb shashliks roasted using five different methods. The X-, Y-, and Z-axes display the ion drift time, GC retention time, and ion peak intensity, respectively. The ion drift time and ion peak intensity were used to quantify each aroma component. As shown in Fig. S2, the vertical coordinates indicate the retention time and the horizontal coordinates indicate the drift time for lamb shashliks treated by five roasting methods. The spectrum has a blue background, and a red vertical line is visible on the left side, representing the reactive ion peak (RIP, normalized drift time of 2.043–2.045 ms). Each dot on either side of the RIP represents a VOC. A substance's color corresponds to its concentration, with white indicating a lower concentration and red indicating a higher concentration. Furthermore, the darker the red, the darker the color. GC-IMS successfully separated the VOCs in lamb shashliks using five roasting methods. In addition, all the spectra contained several signal peaks, which indicate that the lamb shashliks roasted according to different methods contained a high level of VOCs.

Using the difference comparison model, various roasting methods were used to compare the differences between lamb shashlik samples (Fig. S3). Using the D-method lamb shashlik spectra as a reference, white indicates the same concentration of VOCs in both samples after deductions. Contrary to the reference compound, the red color indicates a higher concentration of compounds, and the blue color indicates a lower concentration. Most signals appeared in the range of retention time 100 to 550 s and drift time 1.0 to 1.75 s. Compared to lamb shashliks prepared by different roasting methods, some volatile components were significantly increased, and others markedly decreased. It appears that roasting methods have varying degrees of influence on lamb shashliks' VOCs.

For a comprehensive visual comparison of VOCs from lamb shashliks roasted in five different ways, Gallery Plot was used (Fig. 3). Each row represents a peak signal from one sample. In addition, each column indicates the presence of the same VOC in different samples. A brighter color indicates a higher concentration of VOCs. In regions A and B of Fig. 3, the K-method lamb shashliks were found to contain higher concentrations of pentanal, heptanal, hexanal, 2-butanone, 2-pentenal, (E)-2-octenal, (E)-2-heptenal, (E)-2-hexenal octanal, and (Z)-4-heptenal, as well as unidentified peaks at 2, 3, and 7 than the samples of other roasting methods.

Compared to other roasting methods, the W-method lamb shashliks

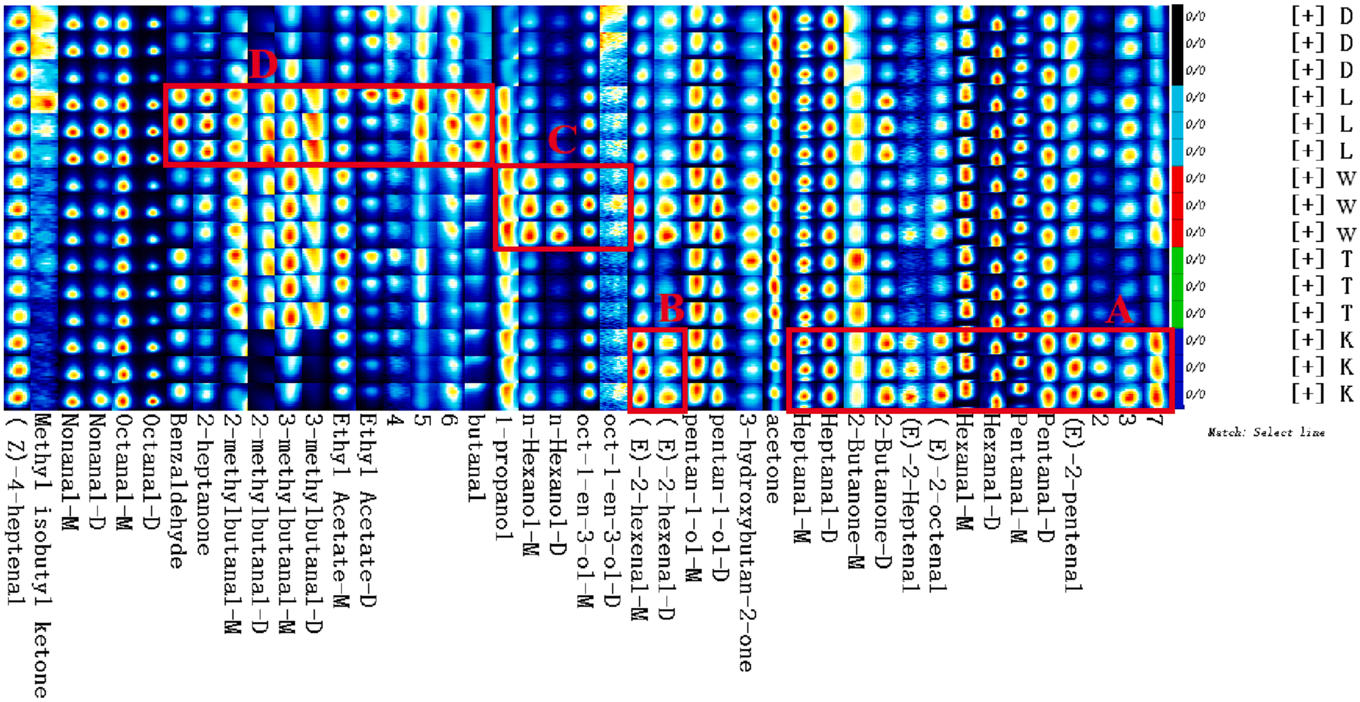

Fig. 3. Dynamic fingerprints of lamb shashliks with five roasting methods, generated by Gallery Plot (Please refer to supplementary materials for topographic map, three-dimensional topographic map, and difference comparison plots). Each row represents the signal peak of one sample while each column represents the same volatile organic compound in different samples. Colors represent the content of a volatile organic compound, and the brighter the color is, the higher the content.

contained higher levels of 1-octen-3-ol, *n*-hexanol, 1-propanol, and pentan-1-ol, 3-hydroxybutan-2-one in the C region. The D region of the lamb shashliks treated with the L-method contained higher levels of benzaldehyde, 2-methylbutanal, 3-methylbutanal, butanal, 2-heptanone, as well as unidentified peaks of 4, 5 and 6 as well as ethyl acetate than those treated with other roasting methods. A relatively small difference in aroma composition was observed between lamb shashliks prepared by different roasting methods, among which samples L and K contained high amounts of aldehydes and ketones, including nonanal, octanal, benzaldehyde, 2-methylbutanal, 3-methylbutanal, 2-heptanone, 2-butanone, heptanal, hexanal, pentanal, (E)-2-pentenal, (E)-2-pentenal, (E)-2-heptenal. Samples W contained relatively high levels of alcohols.

3.5. Multivariate statistical analysis

To achieve the greatest possible separation and differentiation between lamb shashliks treated with five roasting methods, OPLS-DA was applied to data derived from VOCs (SPME-GC–MS and GC-IMS), an E-nose, an E-tongue, as well as a sensory evaluation (QDA). The quality parameters in the generated OPLS-DA model showed a good fit ($R^2Y = 0.961$) and high predictive power ($Q^2 = 0.875$). According to Fig. 4A, the lamb shashliks were well separated based on the grilling methods. OPLS-DA results indicate that GC-based methods, intelligent sensory technologies, and sensory evaluation can be combined to characterize the profiles of lamb shashliks prepared in five different ways. Notably, the flavors of samples K and L were relatively similar, suggesting that the two roasting methods may be similar in characterizing the flavors. Cross-validation of the substitution test was conducted 200 times to test the robustness of the model, and no overfitting was detected ($R^2 = 0.512$, $Q^2 = -1.01$; Fig. 4B).

For an in-depth analysis of the characteristics of lamb shashliks with five roasting methods, *t*-SNE was used to visualize the data space of the fused data (SPME-GC–MS and GC-IMS, E-nose, E-tongues, and sensory evaluation). Placing similar data points close to each other makes it possible to represent high-dimensional data in a low-dimensional nonlinear manifold (Van & Hinton, 2008). The eigenvalues of lamb shashliks with five roasting methods were collected for the raw data processing, and the eigenvalues were separated explicitly. Fig. S4 shows clear boundaries between the visualized data that distinguish five roasting methods for lamb shashliks. As a result, the method significantly impacts the classification of fused data of features from GC-based methods, intelligent sensory technologies, and sensory evaluation methods.

3.6. Prediction modeling of lamb shashliks roasted in different methods

3.6.1. Prediction results of the content of VOCs

With five roasting methods, five models were developed for detecting VOCs in lamb shashliks. Based on the fusion of data, including intelligent sensory technologies (E-nose and E-tongue), sensory evaluation, and GC-based methods, five models are developed to predict the content of six VOCs (aldehydes, alcohols, ketones, hydrocarbons, esters, and furans) in lamb shashliks. Table 1 presents the results. A CNN-SVM system best predicted aldehydes, achieving recognition accuracy of 0.9522 and 0.984, respectively, with RMSEs of 0.07049 and 0.06857. In addition, CNN-SVM performed the best for predicting ketones, hydrocarbons, and esters in the training and test sets compared to the other four models. Based on the training set, RF performed well in predicting furan compounds (RMSE = 0.06822, R2 = 0.9926) but did not perform as well in the test set as CNN-SVM (RF: RMSE = 0.0982, $R^2 = 0.9427$; CNN-SVM: RMSE = 0.08796, $R^2 = 0.9627$). As for alcohols, CNN-SVM obtained the highest accuracy on the training set ($R^2 = 0.9849$), whereas DNN 5-Layer achieved the highest accuracy on the test set ($R^2 = 0.9554$), while CNN-SVM came in second ($R^2 = 0.9503$). As a result, the CNN-SVM model provides more accurate predictions than the other four models. For each compound type, the accuracy in both the training set and test set is higher than 0.95, and the RMSE is lower than 0.10, indicating good performance and greater stability.

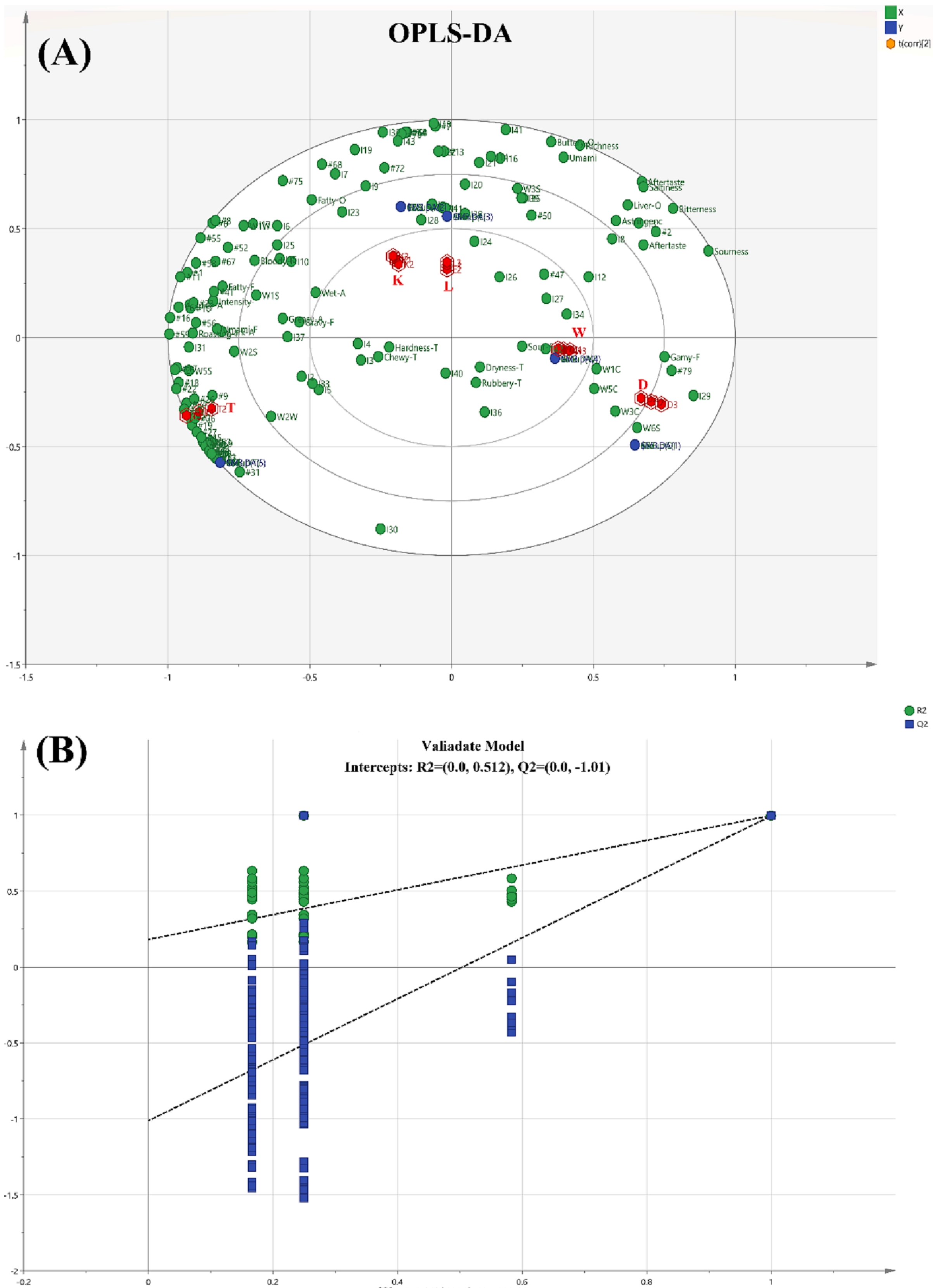

Fig. 4. OPLS-DA analysis of lamb shashliks of different roasting methods obtained using GC–MS, GC-IMS, E-nose, E-tongue and QDA. (A) Double-labeled plot of OPLS-DA of lamb shashliks with different roasting methods (R2Y = 0.961, Q2 = 0.875). Red hexagons represent lamb shashlik samples and green circles represent individual factors; (B) cross-validation by 200 substitution tests (R2 = 0.512, Q2 = − 1.01). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table 1
Quantitative prediction results of volatile compounds content of lamb shashlik based on different modeling methods.

Class	Model	Training set		Test set	
		RMSE	R^2	RMSE	R^2
Aldehydes	SVM	0.07584	0.9361	0.06966	0.8936
	RF	0.11202	0.9181	0.09665	0.8905
	XGBoost	0.08315	0.9376	0.06915	0.9604
	DNN 5-Layer	0.08116	0.9337	0.10294	0.9356
	CNN-SVM	**0.07049**	**0.9522**	**0.06857**	**0.984**
Alcohols	SVM	0.0634	0.9762	**0.07642**	0.9022
	RF	0.08385	0.9384	0.08114	0.9103
	XGBoost	**0.05456**	0.9506	0.13059	0.9212
	DNN 5-Layer	0.11323	0.9019	0.08088	**0.9554**
	CNN-SVM	0.05458	**0.9849**	0.0918	0.9503
Ketones	SVM	0.09741	0.9628	0.09785	0.9382
	RF	0.05337	0.9721	0.07449	0.8943
	XGBoost	0.08979	0.9059	0.13755	0.9077
	DNN 5-Layer	0.11009	0.921	0.07414	0.9177
	CNN-SVM	**0.04976**	**0.983**	**0.0537**	**0.9636**
	SVM	0.12646	0.9055	0.08313	0.9113
	RF	0.10655	0.9595	0.12261	0.9182
	XGBoost	0.09614	0.9545	0.1448	0.9162
	DNN 5-Layer	0.11648	0.9692	0.11076	0.9655
	CNN-SVM	**0.07263**	**0.9621**	**0.08066**	**0.9682**
Esters	SVM	0.0918	0.9384	0.14169	0.9439
	RF	0.10604	0.9751	0.11424	0.9099
	XGBoost	0.12146	0.9455	0.12998	0.9213
	DNN 5-Layer	0.05193	0.9893	0.14528	0.9342
	CNN-SVM	**0.04269**	**0.9921**	**0.09563**	**0.9556**
Furan	SVM	0.09153	0.9272	0.08849	0.9002
	RF	**0.06822**	**0.9926**	0.0982	0.9427
	XGBoost	0.1265	0.9921	0.14535	0.8952
	DNN 5-Layer	0.11573	0.9141	0.14199	0.9013
	CNN-SVM	0.09321	0.9686	**0.08796**	**0.9627**

3.6.2. *Prediction of the results of the various roasting methods for lamb shashliks*

Five different models were developed using intelligent sensory technologies, sensory evaluation, and GC-based methods to identify lamb shashliks in various roasting methods. Five models were developed using the fusion data. The CNN-SVM provided the best results in predicting various types of roasting methods. It achieved recognition accuracy higher than 0.95 for both the training and 0.92 for the test set, which was higher than the recognition accuracy for the other four models. In addition, the RMSEs for this model's training and test sets are lower than 0.05, which is also significantly lower than the RMSEs for the other models. The results demonstrate that CNN-SVM can predict the five roasting methods for lamb shashliks well.

4. Discussion

4.1. *Effect of roasting methods on the types and concentrations of VOCs*

VOCs have a significant impact on the aroma of meat products. Also, lamb shashliks treated by five roasting methods differed in the types and contents of VOCs. SPME-GC–MS detected 57, 57, 34, 52, and 36 VOCs in samples treated by T, K, D, L, and W, respectively. HS-GC-IMS detected 43 VOCs at the same time. As part of the T method, coals were burned under the oven to generate heat, and the sample was heated on top of the oven to produce VOCs. Alternatively, the L method treats samples like the T method but uses electricity as the heat source. In addition, the K, W, and D methods generate significant amounts of heat in a confined space to produce VOCs from the sample.

HS-SPME-GC–MS detected 21 aldehydes in lamb shashliks from the five roasting methods, while HS-GC-IMS detected 22 (containing monomers and dimers). Aldehydes are important intermediates in the oxidation of sweeteners and lipids and can interact with amino acids and carbonyl groups (Watanabe et al., 2015; Vidal et al., 2020). Because of their low threshold and high concentration in cooked meat, aldehydes containing six to ten carbons are the main compounds with odor properties (Mottram, 1998). Nonanal and octanal levels were highest in lamb shashliks prepared by the *T*-method, followed by K and L. By oxidizing oleic acid, octanal and nonanal are generated, which are responsible for imparting fruity, green, fatty, and grassy flavors to lamb shashliks (Huang et al., 2022) which are considered to be important flavor components (Domínguez et al., 2014a; Xi et al., 2018). Using the new method, hexanal and heptanal were found in the highest amounts in K samples. In cooked lamb samples, hexanal is the predominant compound (Meinert et al., 2007). As oxidation products of linoleic and arachidonic acids, hexanal and heptanal provide the fatty, fruity, herbaceous, and pungent aroma of grilled lamb shashlik (Domínguez et al., 2014b; Bassam et al., 2022). By Strecker degradation, phenylacetaldehyde and benzaldehyde are generated from phenylalanine and contribute to the fatty aroma of cooked lamb (Xi et al., 2018). In both K and L samples, abundant unsaturated aldehydes were detected (Tables S3 and S4), including (E)-2-pentenal, (E)-2-hexenal, (E)-2-octanal, (E)-2-nonenal, and (E)-2-decanal, which have significant effects on the fatty aroma of roasted lamb (Liu et al., 2021). Additionally, 2-methylbutyraldehyde and 3-methylbutyraldehyde were detected by GC-IMS in L samples at higher levels than in T samples, and these compounds may contribute to the pleasant aroma (Bassam et al., 2022).

In the muscle, linoleic acid is degraded by lipoxygenase and peroxidase, which lead to the production of alcohols. In most cases, they are characterized by pleasant aromas such as sweetness, freshness, fruit and vegetable aromas, as well as floral aromas that enhance the volatile flavor of meat products. As a result of various roasting methods, the primary alcohols detected in lamb shashliks were propanol, pentanol, hexanol, 1-heptanol, and 1-octen-3-ol. Pentanol may be generated through the auto-oxidation of polyunsaturated fatty acids. In samples from the grilling and roasting treatments, 1-hexanol was predominant. In contrast, 2-ethyl-1-hexanol has an aroma described as resinous, floral, and green (Calkins & Hodgen, 2007). A high alcohol threshold ensures that alcohol has little effect on the volatile flavor of roasted lamb shashliks and plays a synergistic role in the overall volatile flavor. The aroma of roasted meat is characterized by 1-octen-3-ol, formed by the degradation of secondary hydroperoxides of fatty acids and has a pleasant mushroomy, grassy flavor with a low threshold and a significant contribution to lamb flavor (Wang et al., 2021). The lamb shashliks treated by the W method contained more alcohols than those treated by other methods, including propanol, hexanol, 1-octen-3-ol, pentanol, heptanol, and 2-ethyl-1-hexanol. The presence of long-chain alcohols in cooked meat is rare and is considered a potential biomarker for meat from grazing animals (Gkarane et al., 2019). Various grilling methods have generated long-chain alcohols and aldehydes, including 1-pentadecanol and pentadecanal. As a result of lipid oxidation, these aldehydes and alcohols may be generated (Kerth, 2016).

As amino acids are degraded, unsaturated fatty acids are oxidized or degraded, and oxidation of β-keto acids generates ketones. In particular, 2-ketones significantly affect the aroma of meat and meat products since they are present in large quantities and have a distinct aroma. In samples treated with the K method, 2-heptanone, 2,3-octanedione and 2-butanone were present in higher concentrations than in samples treated in other ways. In the case of lamb shashliks, 2-heptanone imparted a fruity aroma and a blue cheese aroma. As a result of the thermal oxidation of linoleic acid during meat cooking, 2,3-octanedione is formed, which is described as having a herbal aroma, whereas 2-butanone is formed as a result of the reaction between sulfur atoms and amino acids (Moran et al., 2022). Ketones have a higher threshold than other aldehydes and, therefore, positively affect the volatile flavor of lamb shashliks. In the overall volatile flavor of meat products, ketones usually play a coordinating role.

Hydrocarbons, both aliphatic and aromatic, are formed by the thermal homogenization of long-chain fatty acids or the thermal degradation of lipids. As a result of the incomplete combustion of meat and fat during grilling, alkanes are generated (Bassam et al., 2022). As a result, roasting over a fire generates more aromatic hydrocarbons. Because of this, the T method yielded a higher percentage of alkanes and a different type of alkane than the other roasting methods. Table S3 shows that the T sample contained more toluene, ethylbenzene, o-xylene, naphthalene, 2-methylnaphthalene, and 1-methylnaphthalene than the other samples. Particularly, toluene, which can contribute to the aroma of lamb shashliks, was described as having a fruity and sweet aroma (Madruga et al., 2010). As an oxidation product of linoleic acid, furans, such as 2-pentylfuran, are found in various meat products and provide a sweet or caramel-like aroma in foods containing fats (Liu et al., 2021; Yao et al., 2022).

As a result of the degradation of alcohols, esters are usually synthesized through esterification reactions between fats or proteins and acids or through ester exchange reactions between triglycerides and fatty acids in ethanol (alcoholysis). Esters are highly aromatic compounds that have a low detection threshold for odors. K and L samples contained more esters of different types and concentrations than T samples. The T method samples were likely roasted on a charcoal fire, resulting in incomplete fat combustion to generate alkanes and aromatic hydrocarbons, leading to the degradation of esters. The K-treated samples had the highest concentration of esters, including butanoic acid methyl ester, heptanoic acid methyl ester, and decanoic acid methyl ester. The L-treated samples contained higher concentrations of methyl valerate, hexanoic acid methyl ester, octanoic acid methyl ester, nonanoic acid methyl ester, and ethyl acetate. As a result of these methyl and ethyl esters, the lamb shashliks acquired creamy, fruity, floral, and sweet flavors (Li et al., 2021; Wang et al., 2021).

Meat volatility is influenced by the cooking method (Lorenzo & Domínguez, 2014), and the abundance of most VOCs in lamb shashliks varied significantly between roasting methods ($p < 0.05$). Several VOCs may influence sensory evaluation, including aldehydes, alcohols, ketones, furans, and esters.

4.2. Influence of new roasting methods on sensory evaluation

Despite similar sensory profiles between the lamb shashliks treated by the four new roasting methods and those treated by the traditional T roasting method (Fig. 1A), odor, flavor, appearance, and texture were the four sensory dimensions that differentiated the different roasting methods. There is a significant difference in the intensity of each sensory attribute between the various roasting methods of lamb shashliks (Table S2). For the odor dimension, the intensity of buttery odor, liver odor, and fatty odor sensory attributes was higher in lamb shashliks treated with the new roasting method than in lamb shashliks treated with the *T*-method.

In a previous study, the buttery odor was identified as an important sensory attribute of lamb shashliks treated by the K method (Wang et al., 2022). As a result of this attribute, consumers prefer lamb shashliks that have been treated with the K method. According to the results of HS-SPME-GC–MS and HS-GC-IMS, the attributed buttery odor may result from a combination of processing methods with multiple VOCs. Upon sensory evaluation, the buttery odor of K lamb shashliks is not quite the same as the sweet odor in the actual cream, but rather a slightly sweet and intermingled fat odor that can fill the nasal cavity briefly. In Fig. 3, unsaturated aldehydes in lamb shashliks prepared using the K-method, including (E)-2-pentenal, (E)-2-octenal, (E)-2-heptenal, and (E)-2-hexenal, were significantly higher than in lamb shashliks prepared using other methods. Unsaturated aldehydes were responsible for the fatty odor. Also, the K-method samples contained a higher concentration of methyl esters, which generated similar aromas, such as creamy and fruity. It was also possible to bring sweet aromas with 2-heptenal. The lamb shashliks prepared with the K method also contained higher short-chain aldehydes. As mentioned, the lamb shashliks had a mixture of sweet, fatty, and buttery odors. On the other hand, the air fryer activates a high-powered fan while processing the sample, causing the VOCs generated during the process to be released faster as well. As a result, the ability to perceive buttery odor is not simply determined by a consumer's ability to associate (Wang et al., 2022). Lamb shashliks prepared by the K-method contain a variety of short-chain aldehydes with unsaturated aldehydes, esters, as well as a high concentration of 2-heptanone. In addition to the intensely sweet aroma caused by a variety of VOCs generated during the air fryer processing, the buttery odor is also a result of the synergistic effect of these VOCs. Short-chain aldehydes with unsaturated aldehydes, methyl esters, and ketones may be the chemical basis of the buttery odor in lamb shashliks prepared using the K-method, which complemented the research on butter odor by Wang et al. (2022). Similar to the buttery odor of the L-method samples, the strength of the buttery odor was lower than that of the K-method samples due to the differences in processing methods.

Furthermore, the L-method samples had a higher level of fatty odor than the *T*-method samples. In contrast to the T samples, the L-method samples exhibited a fatty odor. In T samples, aldehydes may contribute to the fatty odor. The synergistic effect of aldehydes and esters may explain the fatty odor of lamb shashliks prepared with the L method (Tables S3 and S4).

Umami is the most important sensory attribute in the taste dimension. The taste characteristics of lamb are primarily influenced by free amino acids and 5′ -nucleotides, where a synergistic effect of monosodium glutamate-like amino acids and 5′-nucleotides provides the taste profile. The direct heating of lamb by thermal radiation and thermal convection may significantly increase glutamate and 5′-inosine monophosphate concentrations (Liu et al., 2021). Thus, the umami intensity of roasted lamb shashliks treated with the T, K, and L methods was greater. The texture in the samples treated by the K, D, and W methods changed significantly, making them drier and harder than those treated by the T method. Possibly, this is because the samples were processed in the three ways mentioned above, which resulted in more moisture loss in the samples as they were enclosed. In addition, the textures of the samples treated by the K and D methods were rubberier and chewier than those treated by the T method. Contrary to this, the texture of the samples treated with the W method was rougher, which may be due to the microwave heating process. The L method, however, generated more tender samples than the T method. A possible explanation is that the L method uses a milder electric heat and is not processed in a closed environment. Because of their outstanding sensory attributes, as well as their health benefits and quickness, K and L methods may replace traditional charcoal grilling as a new roasting method.

4.3. Model for the prediction of lamb shashliks

CNN-SVM combines the strengths of both SVM and CNN models by using CNN to extract the feature vector, which is not easy to fit and more scientific, and the power of SVM to perform classification and generalization. Tables 1 and 2 show that CNN-SVM performs more efficiently and is more stable than the other models. This is because deep learning models typically involve deep architectures, which can extract more abstract and invariant data features and perform better than shallow classifiers. In addition, CNN-SVM can establish a good correlation between appropriate chemometrics obtained from GC–MS, GC-IMS, E-nose, and E-tongues, as well as sensory evaluation results, which predict various types of VOCs in lamb shashliks and provide a new method for quantitatively predicting specific VOCs in other food matrixes. Moreover, the model performs well in identifying the flavor characteristics of lamb shashliks with different roasting methods and can distinguish the various roasting methods of lamb shashliks with greater clarity.

5. Conclusion

The results showed that HS-GC-IMS and HS-SPME-GC–MS techniques, as well as sensory evaluation, E-nose, and E-tongue, were effective at identifying the characteristic flavors in lamb shashliks to differentiate between the five roasting methods. K and L treated samples

Table 2
Prediction results of the roasting method of lamb shashliks using different models.

Class	Model	Training set		Test set	
		RMSE	R^2	RMSE	R^2
T	SVM	0.1003323	0.924288	0.0929575	0.947582
	RF	0.0555048	0.961542	0.0782145	0.840642
	XGBoost	0.0879942	0.896841	0.1306725	0.898623
	DNN 5-Layer	0.1122918	0.91179	0.077847	0.936054
	CNN-SVM	**0.0507552**	**0.98402**	**0.054774**	**0.96178**
K	SVM	0.1003323	0.922056	0.0949145	0.89129
	RF	0.0544374	0.95821	0.0774696	0.840642
	XGBoost	0.0879942	0.949	0.13755	0.853238
	DNN 5-Layer	0.1056864	0.921	0.0771056	0.925056
	CNN-SVM	**0.0507552**	**0.95951**	**0.054774**	**0.926877**
D	SVM	0.0944877	0.912428	0.0929575	0.947582
	RF	0.0517689	0.952658	0.0715104	0.840642
	XGBoost	0.0888921	0.851546	0.1361745	0.953085
	DNN 5-Layer	0.1133927	0.88416	0.0756228	0.908523
	CNN-SVM	**0.047272**	**0.97402**	**0.054237**	**0.962144**
L	SVM	0.0915654	0.943544	0.09785	0.947582
	RF	0.0512352	0.981821	0.0722553	0.930072
	XGBoost	0.0888921	0.933077	0.1389255	0.944008
	DNN 5-Layer	0.1056864	0.94863	0.077847	0.890169
	CNN-SVM	**0.0487648**	**0.983215**	**0.052089**	**0.953964**
W	SVM	0.0983841	0.933916	0.0988285	0.881908
	RF	0.0539037	0.991542	0.0722553	0.867471
	XGBoost	0.0844026	0.887782	0.129297	0.953085
	DNN 5-Layer	0.1078882	0.96705	0.0719158	0.954408
	CNN-SVM	**0.032248**	**0.99283**	**0.051015**	**0.982872**

contained higher concentrations of unsaturated aldehydes, ketones and esters among the new roasting methods. These VOCs may greatly influence the sensory evaluation of buttery odor. Alcohol concentrations were higher in samples treated by the W method. Using a data fusion strategy, sensory evaluation, intelligent sensory technologies, and GC-based methods were combined. The CNN-SVM performed better than other models in quantifying the compounds of six types in lamb shashliks and in identifying the roasting method of lamb shashliks. The results of this study indicate that combining sensory evaluation, intelligent sensory technologies, and chemometric analysis can be a valuable tool for identifying and characterizing food products in the food industry. This study provide insight into the changes in lamb shashliks following different roasting methods, thus offering new ideas and theoretical guidance for developing traditional grilled lamb shashliks.

CRediT authorship contribution statement

Che Shen: Methodology, Conceptualization, Investigation, Visualization, Formal analysis, Data curation, Writing – original draft, Writing – review & editing. **Yun Cai:** Data curation, Formal analysis. **Meiqi Ding:** Data curation. **Xinnan Wu:** Data curation. **Guanhua Cai:** Writing – review & editing. **Bo Wang:** Methodology, Formal analysis, Visualization, Funding acquisition, Writing – review & editing. **Shengmei Gai:** Supervision. **Dengyong Liu:** Project administration, Funding acquisition.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The data that has been used is confidential.

Acknowledgement

The authors would like to express their gratitude to EditSprings (https://www.editsprings.cn) for the expert linguistic services provided.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.fochx.2023.100755.

References

Bassam, S. M., Clarice, N.-D., & Farag, M. A. (2022). Dissecting grilled red and white meat flavor: Its characteristics, production mechanisms, influencing factors and chemical hazards. *Food Chemistry, 371*, Article 131139. https://doi.org/10.1016/j.foodchem.2021.131139
Calkins, C. R., & Hodgen, J. M. (2007). A fresh look at meat flavor. *Meat Science, 77*, 63–80.
Chen, T., & Guestrin, C. (2016). *Xgboost: A scalable tree boosting system.* ACM.
Cortes, C., & Vapnik, V. (1995). Support-vector networks. *Machine Learning, 20*(3), 273–297. https://doi.org/10.1007/BF00994018
Domínguez, R., Gomez, M., Fonseca, S., & Lorenzo, J. M. (2014a). Effect of different cooking methods on lipid oxidation and formation of volatile compounds in foal meat. *Meat Science, 97*(2), 223–230. https://doi.org/10.1016/j.meatsci.2014.01.023
Domínguez, R., Gomez, M., Fonseca, S., & Lorenzo, J. M. (2014b). Influence of thermal treatment on formation of volatile compounds, cooking loss and lipid oxidation in foal meat. *LWT, 58*(2), 439–445.
Florentino-Ramos, E., Villa-Ruano, N., Hidalgo-Martínez, D., Ramírez-Meraz, M., Mendez-Aguilar, R., Velasquez-Valle, R., & Becerra-Martínez, E. (2019). 1H NMR−based fingerprinting of eleven Mexican Capsicum annuum cultivars. *Food Research International, 121*, 12–19. https://doi.org/10.1016/j.foodres.2019.03.025
Gkarane, V., Brunton, N. P., Harrison, S. M., Gravador, R. S., Allen, P., Claffey, N. A., … Monahan, F. J. (2018). Volatile profile of grilled lamb as affected by castration and age at slaughter in two breeds. *Journal of food science, 83*(10), 2466–2477.
Guerrero, L., Guardia, M. D., Xicola, J., Verbeke, W., Vanhonacker, F., Zakowska-Biemans, S., Sajdakowska, M., Sulmont-Rosse, C., Issanchou, S., Contel, M., Scalvedi, M. L., Granli, B. S., & Hersleth, M. (2009). Consumer-driven definition of traditional food products and innovation in traditional foods. A qualitative cross-cultural study. *Appetite, 52*(2), 345–354. https://doi.org/10.1016/j.appet.2008.11.008
Huang, Q., Dong, K., Wang, Q., Huang, X., Wang, G., An, F., Luo, Z., & Luo, P. (2022). Changes in volatile flavor of yak meat during oxidation based on multi-omics. *Food Chemistry, 371*, Article 131103. https://doi.org/10.1016/j.foodchem.2021.131103
Hinton, G. E. (2007). To recognize shapes, first learn to generate images. Editor(s): Paul Cisek, Trevor Drew, John F. Kalaska, Progress in Brain Research, Elsevier, 165, 535-547. https://doi.org/10.1016/S0079-6123(06)65034-6.
Islam J., Bhuiyan S., Hossain A., Surja A. S. and Iqbal M. S. (2021). Classification of Gastric Precancerous Diseases using Hybrid CNN-SVM. *2021 3rd International Conference on Electrical & Electronic Engineering (ICEEE)*, Rajshahi, Bangladesh, pp. 137-140, https://doi.org/10.1109/ICEEE54059.2021.9718790.
Jiang, S., Zhu, Y., Peng, J., Zhang, Y., Zhang, W., & Liu, Y. (2023). Characterization of stewed beef by sensory evaluation and multiple intelligent sensory technologies combined with chemometrics methods. *Food Chemistry, 408*, Article 135193. https://doi.org/10.1016/j.foodchem.2022.135193
Kerth, C. (2016). Determination of volatile aroma compounds in beef using differences in steak thickness and cook surface temperature. *Meat Science, 117*, 27–35. https://doi.org/10.1016/j.meatsci.2016.02.026
Leo, & Breiman. (2001). Random forests. *Machine Learning*. Springer Science and Business Media LLC. 45(1), 5-32. https://doi.org/10.1023/a:1010933404324.
Li, C., Wang, D., Xu, W., Gao, F., & Zhou, G. (2013). Effect of final cooked temperature ontenderness, protein solubility and microstructure of duck breast muscle. *LWT, 51*(1), 266–274. https://doi.org/10.1016/j.lwt.2012.10.003
Li, M., Yang, R., Zhang, H., Wang, S., Chen, D., & Lin, S. (2019). Development of a flavor fingerprint by HS-GC-IMS with PCA for volatile compounds of Tricholoma matsutake Singer. *Food Chemistry, 290*, 32–39. https://doi.org/10.1016/j.foodchem.2019.03.124
Li, W., Chen, Y. P., Blank, I., Li, F., Li, C., & Liu, Y. (2021). GC × GC-ToF-MS and GC-IMS based volatile profile characterization of the Chinese dry-cured hams from different regions. *Food Research International, 142*, Article 110222. https://doi.org/10.1016/j.foodres.2021.110222
Liu, D., Bai, L., Feng, X., Chen, Y. P., Zhang, D., Yao, W., Zhang, H., Chen, G., & Liu, Y. (2020). Characterization of Jinhua ham aroma profiles in specific to aging time by gas chromatography-ion mobility spectrometry (GC-IMS). *Meat Science, 168*, Article 108178. https://doi.org/10.1016/j.meatsci.2020.108178
Liu, X., Qian, M., Dong, H., Bai, W., Zhao, W., Li, X., & Liu, G. (2020). Effect of ageing process on carcinogen ethyl carbamate (EC), its main precursors and aroma compound variation in Hakka Huangjiu produced in southern China. *International Journal of Food Science & Technology, 2020*(55), 509–516.
Liu, H., Ma, J., Pan, T., Suleman, R., Wang, Z., & Zhang, D. (2021). Effects of roasting by charcoal, electric, microwave and superheated steam methods on (non)volatile

compounds in oyster cuts of roasted lamb. *Meat Science, 172*, Article 108324. https://doi.org/10.1016/j.meatsci.2020.108324
Lorenzo, J. M., & Domínguez, R. (2014). Cooking losses, lipid oxidation and formation of volatile compounds in foal meat as affected by cooking procedure. *Flavour and Fragrance Journal, 29*(4), 240–248.
Madruga, M. S., Elmore, J. S., Oruna-Concha, M. J., Balagiannis, D., & Motrram, D. S. (2010). Determination of some water-soluble aroma precursors in goat meat and their enrolment on flavour profile of goat meat. *Food Chemistry, 123*(51), 3–520.
Meinert, L., Andersen, L. T., Bredie, W. L. P., Bjergegaard, C., & Aaslyng, M. D. (2007). Chemical and sensory characterisation of pan-fried pork flavour: Interactions between raw meat quality, ageing and frying temperature. *Meat Science, 75*(2), 229–242. https://doi.org/10.1016/j.meatsci.2006.07.004
Moran, L., Vivanco, C., Lorenzo, J. M., Barron Luis Javier, R., & Aldai, N. (2022). Characterization of volatile compounds of cooked wild Iberian red deer meat extracted with solid phase microextraction and analysed by capillary gas chromatography - mass spectrometry. *LWT, 163*, Article 113472. https://doi.org/10.1016/j.lwt.2022.113472
Mottram, D. S. (1998). Flavour formation in meat and meat products: A review. *Food Chemistry, 62*, 415–424.
Qian, M., Ruan, F., Zhao, W., Dong, H., Bai, W., Li, X., Huang, X., & Li, Y. (2023). The dynamics of physicochemical properties, microbial community, and flavor metabolites during the fermentation of semi-dry Hakka rice wine and traditional sweet rice wine. *Food Chemistry, 416*, Article 135844. https://doi.org/10.1016/j.foodchem.2023.135844
Ramirez, J. L., Du, X., & Wallace, R. W. (2020). Investigating sensory properties of seven watermelon varieties and factors impacting refreshing perception using quantitative descriptive analysis. *Food Research International, 138*(Part A), Article 109681. https://doi.org/10.1016/j.foodres.2020.109681
Shen, C., Cai, Y., Wu, X., Gai, S., Wang, B., & Liu, D. (2023). Characterization of selected commercially available grilled lamb shashliks based on flavor profiles using GC-MS, GC × GC-TOF-MS, GC-IMS, E-nose and E-tongue combined with chemometrics. *Food Chemistry, 423*, Article 136257.
Shi, J., Nian, Y., Da, D., Xu, X., Zhou, G., Zhao, D., & Li, C. (2020). Characterization of flavour volatile compounds in sauce spareribs by gas chromatography-mass spectrometry and electronic nose. *LWT-Food Science and Technology, 124*, Article 109182. https://doi.org/10.1016/j.lwt.2020.109182
Suman, S. P., Nair, M. N., Joseph, P., & Hunt, M. C. (2016). Factors influencing internalcolor of cooked meats. *Meat Science, 120*, 133–144. https://doi.org/10.1016/j.meatsci.2016.04.006
Varela, P., & Ares, G. (2012). Sensory profiling, the blurred line between sensory and consumer science. A review of novel methods for product characterization. *Food Research International*, 48(2), 893–908. https://doi.org/10.1016/j.foodres.2012.06.037.
Van der Maaten, L., & Hinton, G. (2008). Viualizing data using t-SNE. *Journal of Machine Learning Research, 1*, 1–48.
Vidal, N. P., Manful, C., Pham, T. H., Wheeler, E., Stewart, P., Keough, D., & Thomas, R. (2020). Novel unfiltered beer-based marinades to improve the nutritional quality, safety, and sensory perception of grilled ruminant meats. *Food Chemistry, 302*, Article 125326. https://doi.org/10.1016/j.foodchem.2019.125326
Wang, B., Shen, C., Cai, Y., Dai, L., Gai, S., & Liu, D. (2023). Consumer culture in traditional food market: The influence of Chinese consumers to the cultural construction of Chinese barbecue. *Food Control, 143*, Article 109311. https://doi.org/10.1016/j.foodcont.2022.109311
Wang, B., Shen, C., Zhao, T., Zhai, X., Ding, M., Dai, L., Gai, S., & Liu, D. (2022). Development of a Check-All-That-Apply (CATA) Ballot and Machine Learning for Generation Z Consumers for Innovative Traditional Food. *Foods, 11*, 2409. https://doi.org/10.3390/foods11162409
Wang, L., Zhang, H., De, C., Deng, W., Yang, Z., & Wu, X. (2021). Volatile flavor compounds in muscles from different carcass cuts of Qianbei Ma goat. *Meat Research, 35*(1), 47–52.
Wang, Y. Q., Shen, Y. Y., Wu, Y. Y., Li, C. S., Li, L. H., Zhao, Y. Q., Hu, X., Wei, Y., & Huang, H. (2021). Comparison of the microbial community and flavor compounds in fermented Mandarin fish (Siniperca chuatsi): Three typical types of Chinese fermented Mandarin fish products. *Food Research International, 144*(2), Article 110365. https://doi.org/10.1016/j.foodres.2021.110365
Watanabe, A., Kamada, G., Imanari, M., Shiba, N., Yonai, M., & Muramoto, T. (2015). Effect of aging on volatile compounds in cooked beef. *Meat Science, 107*, 12–19. https://doi.org/10.1016/j.meatsci.2015.04.004
Xi, J., Zhan, P., Tian, H., Wang, P., Geng, Q., Wang, Y., Zhang, F., & Ji, Y. (2018). Comparison of different extraction fibers for analysis of characteristic aroma compounds in Xinjiang roasted lamb by SPME-GC-MS and PCA. *Food Science, 39*(10), 234–241.
Xu, M., Wang, J., & Gu, S. (2019). Rapid identification of tea quality by E-nose and computer vision combining with a synergetic data fusion strategy. *Journal of Food Engineering, 241*, 10–17. https://doi.org/10.1016/j.jfoodeng.2018.07.020
Yao, W., Cai, Y., Liu, D., Chen, Y., Li, J., Zhang, M., Chen, N., & Zhang, H. (2022). Analysis of flavor formation during production of Dezhou braised chicken using headspace-gas chromatography-ion mobility spec-trometry (HS-GC-IMS). *Food Chemistry, 370*, Article 130989. https://doi.org/10.1016/j.foodchem.2021.130989
Zhu, J., Jiang, X., Rong, Y., Wei, W., Wu, S., Jiao, T., & Chen, Q. (2023). Label-free detection of trace level zearalenone in corn oil by surface-enhanced Raman spectroscopy (SERS) coupled with deep learning models. *Food Chemistry, 414*, Article 135705. https://doi.org/10.1016/j.foodchem.2023.135705
Zhu, Z., Bassey, A. P., Cao, Y., Du, X., Huang, T., Cheng, Y., & Huang, M. (2022). Meat quality and flavor evaluation of Nanjing water boiled salted duck (NWSD) produced by different Muscovy duck (Cairina moschata) ingredients. *Food Chemistry, 397*, Article 133833.