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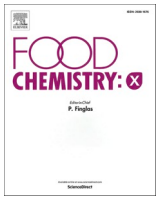

Unraveling the relationship between key aroma components and sensory properties of fragrant peanut oils based on flavoromics and machine learning

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ABSTRACT

Key aroma components of 33 fragrant peanut oils with different aroma types were screened by combined using flavoromics and machine learning. A total of 108 volatile compounds were identified and 100 kinds of them were accurately quantified, and 38 compounds out of them were with odorant activity value ≥1. The 33 peanut oils presented varied intensity of 'fresh peanuts', 'roasted nut', 'burnt', 'over-burnt', 'sweet', 'peanut butter-like', 'puffed food' and 'exotic flavor', and could be classified into four aroma types, namely raw, light, thick and salty. Partial least squares regression analysis, random forest and classification regression tree revealed that 2-acetyl pyrazine had a negative effect on 'fresh peanuts' and could distinguish raw flavor samples well; 2-methylbutanal and 4-vinylguaiacol were key compounds of 'roasted nut' and had significant differences ($P < 0.0001$) in thick and raw flavor samples; furfural contributed to the 'puffed food' as well as key compound of salty flavor.

Introduction

Peanut (*Arachis hypogaea* L.) is an important oilseed for edible purposes with high oil content up to 50%. From 2020 to 2021, the annual production of peanut oil was 6.49 million tons, ranking sixth in the worldwide edible oil consumption. China and India are the two largest consumers of peanut oil, accounting for 71.66 % of the total global production (United States Department of Agriculture, 2021). Peanut oil contains >80% unsaturated fatty acids (linoleic acid and oleic acid), which have a positive effect on reducing cardiovascular risk. It is also rich in other bioactive compounds, such as sterol, phospholipid, vitamin E, choline and so on (Zhang et al., 2022).

In China, peanut oil, especially for fragrant peanut oil, is very popular as cooking oil due to its unique flavor. Flavor is an important aspect of sensory quality of vegetable oils, which largely determines consumer preference and purchase intention. Various peanut oil products are available in the market, which can be simply divided into cold-pressed oil and fragrant oil. Cold-pressed peanut oil is generally processed under the environment of lower than 60 °C, exhibiting a light flavor. In contrast, fragrant peanut oil has a unique strong flavor processed by high-temperature roasting and pressing. During roasting, abundant volatile components could be generated by complex chemical reaction, such as Maillard reactions, Strecker degradation and lipid oxidation. Their formation and abundance are strongly dependent on roasting conditions. Due to the differences in the raw materials and roasting intensity, peanut oil products show different sensory characteristics and can be further divided into different flavor types. However, rare study investigated the sensory characteristics of different type peanut oil. The key aroma compounds of peanut oil significantly affect the sensory property of peanut oil, but they are uncertain from the different flavor types aspects. Flavoromics is an approach to correlate the sensory properties of food to their aroma compounds, which can provide more comprehensive information on the flavor profile of food (Wang et al., 2022). The key is to combine the human perception and evaluation of flavor with instrument analysis and mathematical model analysis, so as to analyze the aromatic regularity of food more deeply. At present, more

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researchers have used this method for flavor research to determine key flavor compounds, characteristic flavor compounds and aroma boundary compounds of citrus fruits (Feng et al., 2021), barley malt (Gu et al., 2022), Baijiu (Wang et al., 2022), wine (Pérez-Jiménez et al., 2021) and mango (Aung et al., 2021), etc. With the help of flavoromics, we could unravel the relationship between aroma compounds of peanut oils and their sensory properties, which can further provide scientific reference for the regulation of oil processing and the production of specific fragrant oil.

At present, some studies have identified the aroma components of peanut oil using headspace solid phase microextraction-gas chromatography-mass spectrometry (HS-SPME-GC–MS) with/without electronic nose. Dun et al. (2019) have identified 101 volatile compounds in hot-pressed peanut oil and 64 volatiles in cold-pressed peanut oil through semi-qualitative analysis by HS-SPME and GC–MS-O. Liu et al. (2011) have characterized 94 volatile compounds by HS-SPME/GC–MS and found 12 pyrazines were considered to be the key contributors to the intense nutty/roasty flavor of aroma roasted peanut oil. Until now, major quantitative results for the volatiles of peanut oil are based on semi-qualitative analysis by the internal standard method. In contrast, external standard method could provide accurate quantitative analysis of volatile components, but it is rarely used in peanut oils.

The multivariate chemometric methods are important tools to reveal the relationship between sensory properties and volatiles. Partial least squares regression (PLSR) is a mathematical model that can analyze and explain the nonlinear relationship of multivariable, which has integrated the advantages of typical correlation analysis, multiple linear regression analysis and principal component analysis (Fan et al., 2006). It is widely used to establish the relationship between sensory properties and volatile compounds in the food field, such as cherry wine (Niu et al., 2011), rose essential oil (Xiao et al., 2017), lavender essential oil (Xiao et al., 2017), burnt scallion oil (Zhang, Wang, et al., 2022). Random forest is a simple and efficient machine learning program to determine outcome predictions using binary segmentation of predicted variables, which can handle data sets with large numbers of predictive variables and provide the highest prediction accuracy compared with other models (Fernández-Delgado et al., 2014). The classification and regression tree (CART) is another common machine learning algorithm based on tree structure, which is suitable for discrete data. When used for classification, CART has the advantages of low computational complexity, easy operation, simple interpretation and implementation. Random forest and CART have been widely used in various fields due to their great flexibility, but little research was related to sensory science. Vigneau et al. (2018) used random forest and CART to predict the important compounds associated with typical sensory attributes in red wine made from Cabernet Franc grape variety. Their results screened out the most important compounds and highlighted few useful compounds closely related to two main olfactory attributes. At the same time, they found that random forest model had better prediction ability than PLSR model. These multivariate data analysis methods could relate and predict the sensory characteristics to their volatile compounds, but they are rarely used in the analysis of peanut oil.

Therefore, this study first identified the aroma compound composition of 33 representative peanut oils by absolute quantification. Then we evaluated the sensory characteristics of peanut oils and classified these oils into different aroma types according to their sensory properties. On this basis, PLSR, random forest and CART were employed to explore the relationship between volatile compounds and sensory properties, and differentiate key compounds of peanut oils with different aroma types. Our results can provide a theoretical basis for the classification of peanut oil based on sensory perspective, and developed a new pathway to screen out the key aroma compounds for the regulation of peanut oil processing.

Material and methods

Oil samples

Thirty-three different brands of peanut oils (numbers were R1-R4, L1-L4, S1-S3, T1-T22) were obtained commercially from the Chinese market. R samples were cold-pressed peanut oil, and the rest samples were processed by roasting and pressing, which were in accordance with national standards and relevant enterprise standards. All samples were stored in a fridge at −20 °C until further analysis. They were sealed and thawed at room temperature for 1 h before the experiment.

Chemicals

All standard chemicals (GC grade, purity ≥ 95 %) were purchased, and their details are shown in Table S1. The *n*-alkanes solution (C6-C24) was obtained from Supelco, Bellefonte, PA, USA.

Analysis of volatile compounds by solid-phase microextraction-gas chromatography-mass spectrometry (SPME-GC–MS)

The extraction of volatile compounds from each sample followed previously published method (Qian et al., 2019) with some modifications. The oil (5 g) was mixed with 10 μL of the internal standard 4-methyl-2-pentanol (1.0018 g/L) in a 20 mL vial capped with a PTFE-silicon septum. An automatic HS-SPME was used to extract volatile compounds on a CTC CombiPAL autosampler (CTC Analytics, Zwingen, Switzerland). Samples were equilibrated at 40 °C for 30 min with a stirring rate of 500 rpm and then extracted at the same temperature for another 30 min by DVB/CAR/PDMS fiber (2 cm, 50/30 μm, Supelco, Bellefonte, PA, USA). After extraction, the SPME fiber were inserted into injector port and desorbed at 250 °C for 8 min, and each sample was tested in triplicate.

An Agilent 6890 gas chromatography equipped with an Agilent 5975 mass spectrometry (Agilent Technologies, Santa Clara, CA, USA) was used to analyze the volatile compounds based on previous method (Qian et al., 2019) with minor modifications. An HP-INNOWAX capillary column (60 m × 0.25 mm, 0.25 μm thickness, J&W Scientific, Folsom, CA, USA) was used to separate the volatile compounds and the flow rate of the carrier gas (helium) was 1.5 mL/min. The heating procedure was as follows: the oven temperature kept at 50 °C for 1 min, then heated to 220 °C under a 3 °C/min speed, and finally kept at 220 °C for 5 min. The temperature of transfer line heater, ion source and quadrupole in the mass spectrometer were set as 250 °C, 250 °C and 150 °C, respectively. The ionization voltage was set at 70 eV and a full mass scan of 30–350 *m/z* was applied. A series of C6-C24 *n*-alkane standards were analyzed to calculate retention indices (RI). The volatile compounds from various samples were identified by comparing their mass spectrum, RI with the NIST11 MS database and standard reference compounds. The quantification of compounds was based on the calibrated standard curve according to the previous method (Liu et al., 2022). Compounds without standards were relatively quantified using the standard curve of structural analogues. Peak area ratio was used for auxiliary quantification. The standard curve covered 75 standards and was diluted to 15 gradients, with 4-methyl-2-pentanol as the internal standard. The final concentrations (μg/g) were calculated according to the resulting standard curve formulas.

Sensory evaluation

Sensory evaluation of 33 peanut oils was performed using quantitative descriptive analysis (QDA) by a trained and experienced panel (10 females, 40–50 years old) from COFCO Nutrition and Health Research Institute, Beijing (China). Before the experiment, panelist participated six rounds of sensory training in a standard sensory laboratory with a temperature of 25 °C and a humidity of 45% and passed the olfactory

sensitivity test. The first two rounds mainly focused on discussing and merging descriptive words. Peanut oil samples were provided to the evaluator, and they were required to use the tasting cup with 15 mL of peanut oil for pre nasal sniffing and record the felt descriptive words. Sensory analysts collected, deleted duplicates, merged similar words, and then discussed with evaluators to select representative sensory descriptors and improve definitions and corresponding reference samples. The second round of training was based on the preparation and evaluation of the reference samples. Evaluators were required to sniff and determine whether the reference samples were suitable and representative based on different peanut oil samples, and ultimately determine the complete reference sample table. The last two experiments used neutral solution butanol as the intensity training matrix using a 2–10 gradient butanol solution (corresponding to 2–10 odor intensity). The evaluators first sniffed and remembered the corresponding sensory intensity in descending order of intensity; Secondly, butanol solutions with strengths of 3, 5, 7, and 9 were provided and evaluators were required to sort them and provide the correct order after sorting. Evaluators were also required to memorize, repeat intensity scoring exercises, and train their ability to recognize intensity. After training, the panelists were asked to assess the odorant characteristics of 33 peanut oil samples. Oils (10 mL) were presented in 25 mL brown glass bottles to subject according to a William Latin-square arrangement. Sensory attributes were obtained after discussing, screening and merging descriptors, and their intensities were scored on a 10 cm linear scale. The sensory attributes with a citation percentage (percentage of non-null scores, the overall assessors, samples and repetitions) higher than 15% were retained, leading to a list of eight orthonasal sensory attributes including 'fresh peanuts', 'roasted nut', 'burnt', 'over-burnt', 'sweet', 'peanut butter-like', 'puffed food' and 'exotic flavor'. The specific definitions and references to these sensory properties are shown in Table S2. The sensory evaluation experiment of 33 peanut oil was conducted for 7 rounds, with 4–5 groups of samples in each round for 2–3 h. The experiment was repeated 3 times.

Random forest (RF) and classification and regression tree (CART)

Multivariate Random Forest models were developed using the package "Random Forest SRC version 2.12.1" to apply multivariate classification on the dataset of this study. Multivariate trees were constructed for multivariate outcomes. Optimal mtry and nodesize were tuned using out-of-bag error and then were adopted in following modelling. Tree size was set as 1000. Variable importance (VIMP) confidence internals were calculated by subsampling with subratio of 0.2. Variable importances were scaled to 100 and indicated with red color if the value was significantly higher than 0, suggesting positive importance for the classification. Parametric normal confidence regions and Delete-d jackknife variance estimator were used. Level of significance was set at 0.05. Package "mvpart version 1.6–3" was leveraged for generating recursive partitioning trees on multivariates. The size of the trees was 2000. Five multiple cross-validations were applied. Eleven groups of cross validation were built. Trees were selected by cross-validation and best tree was given within one standard error (SE) of the overall best. Root node error was calculated.

Odor activity value (OAV)

The OAV of a volatile compound was calculated through dividing its concentration by its odor threshold in oil. The odor thresholds of acetoin and acetol were determined in refined unscented oil using three-alternative forced-choice (3-AFC) procedure (diluted to ten concentrations for the test) according to ISO 13301:2018. Preliminary experiment was conducted using three olfactory sensitive evaluators to determine the approximate threshold range. The concentration that can be clearly felt by all three evaluators was set as the 7-8th concentration gradient, and was diluted layer by layer to prepared 10 concentration gradient samples. Each concentration gradient had two corresponding blank oil matrices as controls, and all samples were randomly coded with three digits. Ten trained evaluators sniffed the sample pairs according to the given coding order. Three samples were grouped into 10 gradients and sniffed sequentially from low to high. The target solution was required to be selected, and characteristic samples were provided to the evaluators. After sniffing one sample, 5 min break could be taken and the evaluator's sniffing accuracy were recorded. After the evaluation was completed, the results of the sensory evaluation group under each gradient were counted to calculate the experimental detection probability (p) that can correctly select the target compound under that gradient. Then, the probability parameter (chance factor) was used to calculate the corrected detection probability (P), as follows:

$$P = 3 \times p\text{-}12$$

In the formula, p represented the actual detection probability in the experiment, P represented the detection probability corrected by chance probability, and the chance probability in the 3-AFC test is 1/3. The corresponding relationship between sample concentration and detection probability can be fitted using the sigmoid curve, and the fitting formula is as follows:

$$P = \frac{1}{1 + e^{(-(x-x_0)/b)}}$$

In the formula, x represented the logarithmic value of the sample concentration, x_0 represented the logarithmic value of the threshold concentration (when $P = 0.5$, $x_0 = x$), and b represents the slope rate. When the detection probability reaches 50%, the minimum concentration of the corresponding sample is defined as the threshold concentration of the substance, that is, when the vertical axis $P = 0.5$, the corresponding value of horizontal axis is the logarithmic value of the threshold concentration of the target compound. SigmaPlot14.0 software was used to plot the obtained data and calculate the pre nasal threshold of the compound in the oil solution. Thresholds for other substances were obtained from literature and are detailed in Table 1.

Statistical analysis

The heat map and box graphs were processed by Hiplot.com.cn. The standardization method for heat maps was set as row normalization, ward. D2 minimum variance clustering. PLSR and principal components analysis (PCA) was conducted by XLSTAT. The compounds with Variable Importance in the Projection (VIP) > 1 were screened, and the model was considered reliable until $Q^2 > 0.4$ and $R^2Y > 0.6$. One-way ANOVA was performed by IBM SPSS Statistics 26.

Results and discussion

Sensory evaluation

Quantitative descriptive sensory analysis (QDA) was applied to evaluate sensory properties of 33 peanut oil samples. Eight sensory attributes were selected for descriptive analysis, which were 'fresh peanuts', 'roasted nut', 'burnt', 'over-burnt', 'sweet', 'peanut butter-like', 'puffed food' and 'exotic flavor'. The intensity values of 8 sensory attributes in all samples have been summarized in Fig. 1a and Fig. S1. Overall, most of the samples showed 'roasted nut', 'burnt', 'over- burnt' flavor, and the 'fresh peanuts' was strong in fractional samples. 'Peanut butter-like', 'puffed food' and 'exotic flavor' were only felt in individual samples. Among these attributes, the intensity values of 'roasted nut' were higher than other properties, with an average value of 5.7 and a maximum value of 8.5 corresponding to T6. The results of 'over-burnt' and 'burnt' were similar, ranging from 0 to 6. The intensities of 'fresh peanuts' were low, and only R1, R2, R3 and R4 exhibited obvious 'fresh peanuts' with the values of 5.0, 6.2, 5.7 and 6.5, respectively; In

Table 1
Volatile compounds with OAV ≥ 1 in 33 peanut oil.

No.	category	odorants	CAS	RI	odor description	odor threshold (ug/kg)	references	OAV (mean)	P value	P value summary
1	aldehyde	2-Methylbutanal	96–17-3	919	malty	2.2	h	203.45	0.0016	**
2	phenol	4-Vinylguaiacol	7786–61-0	2180	smoky, clove-like	20	l	124.28	0.0033	**
3	alcohol	Nonanol	143–08-8	1661	fresh clean fatty floral rose orange dusty wet oily	2	c	71.27	0.0116	*
4	aldehyde	3-Methylbutanal	590–86-3	936	malty	5.4	g	42.83	0.0033	**
5	aldehyde	Hexanal	66–25-1	1081	green, grassy	73	l	36.60	<0.0001	****
6	pyrazine	2-Ethyl-3,5-dimethylpyrazine	13925–07-0	1451	earthy	1.7	e	29.19	0.0024	**
7	acid	Acetic acid	64–19-7	1424	vinegar-like	124	a	24.02	0.0027	**
8	aldehyde	(E)-2-Octenal	2548–87-0	1440	fatty, nutty ; nutty, roasty	4	j	23.65	0.2443	ns
9	aldehyde	2-Methylpropanal	78–84-2	800	malty	15	g	22.37	0.0035	**
10	acid	Butanoic acid	107–92-6	1620	sweaty, cheese-like	7.9	e	17.61	0.1202	ns
11	acid	Hexanoic acid	142–62-1	1855	sweaty, pungent	460	f	13.50	0.3717	ns
12	aldehyde	Benzeneacetaldehyde	122–78-1	1662	Honey-like	22	g	11.83	0.0307	*
13	pyrazine	2,6-Dimethylpyrazine	108–50-9	1333	roasty ; cocoa, roast beef	20	k	10.28	<0.0001	****
14	pyrazine	2,3-Dimethylpyrazine	5910–89-4	1341	nutty nut skin cocoa peanut butter coffee walnut	8	k	6.84	<0.0001	****
15	pyrazine	2,5-Dimethylpyrazine	123–32-0	1328	peanut	2000	l	3.77	0.0005	***
16	pyrazine	Methylpyrazine	109–08-0	1281	roasted	200	l	2.94	<0.0001	****
17	pyrazine	2-Acetylpyrazine	22047–25-2	1617	popcorn-like	10	k	2.76	<0.0001	****
18	aldehyde	(E)-2-Heptenal	18829–55-5	1330	green, fatty	13	j	2.55	<0.0001	****
19	pyrazine	2,3,5-Trimethylpyrazine	14667–55-1	1409	roasted, potato, must	22	l	2.31	0.0001	***
20	pyrazine	3-Ethyl-2,5-dimethylpyrazine	13360–65-1	1439	earthy ; roasted, nut	76	e	1.87	0.0026	**
21	aldehyde	(E,E)-2,4-Nonadienal	5910–87-2	1690	fatty	1.5	g	1.69	0.2853	ns
22	furan	2-Pentylfuran	3777–69-3	1228	fruity green earthy beany vegetable metallic	130	k	1.67	0.3044	ns
23	pyrazine	2-Ethyl-5-methylpyrazine	13360–64-0	1395	nutty ; potato, roasted	320	j	1.65	0.0032	**
24	alcohol	2-Furanmethanol	98–00-0	1670	burnt	680	l	1.62	<0.0001	****
25	aldehyde	Pentanal	110–62-3	978	fermented bready fruity nutty berry	240	i	1.61	0.0431	*
26	furan	2-Methylfuran	534–22-5	874	ethereal acetone chocolate	27	b	1.52	<0.0001	****
27	phenol	p-Cresol	106–44-5	2079	horse stable-like	2.3	g	1.45	0.1961	ns
28	pyrazine	2-Methyl-6-vinylpyrazine	13925–09-2	1486	hazelnut	26	d	0.98	0.0003	***
29	alcohol	Hexanol	111–27-3	1340	grassy	400	i	0.87	<0.0001	****
30	pyrazine	Ethylpyrazine	13925–00-3	1341	roasty, buttery	200	k	0.80	<0.0001	****
31	aldehyde	2-Pyrrolaldehyde	1003–29-8	2000	musty beefy coffee	104		0.79	<0.0001	****
32	aldehyde	(E,E)-2,4-Decadienal	25152–84-5	1790	Deep-fried,fatty	66	f	0.46	0.0149	*
33	ketone	Acetoin	513–86-0	1295	sweet buttery creamy dairy milky fatty	146	m	0.41	0.0002	***
34	aldehyde	Furfural	98–01-1	1455	bread, almond, sweet	700	l	0.39	<0.0001	****
35	lactone	γ-Butyrolactone	96–48-0	1631	caramel, sweet	60	l	0.37	0.0007	***
36	alcohol	Acetol	116–09-6	1300	pungent sweet caramellic ethereal	425	m	0.36	<0.0001	****
37	alcohol	1-Pentanol	71–41-0	1244	fusel oil sweet balsam	470	c	0.34	<0.0001	****
38	aldehyde	5-Methylfurfural	620–02-0	1558	almond, caramel	260	l	0.17	<0.0001	****

a. (Dierkes et al., 2011).
b. (Gemert, 2011).
c. (Jia et al., 2019).
d. (Jia et al., 2020).
e. (Matheis & Granvogl, 2016).
f. (Neugebauer et al., 2020).
g. (Poehlmann & Schieberle, 2013).
h. (Pollner & Schieberle, 2016).
i. (Reboredo-Rodríguez et al., 2013).
j. (Tian et al., 2021).
k. (Yin et al., 2022).
l. (Zhou et al., 2019).
m. Measure according to national standard 《GBT22366-2008》.

contrast, the intensities of other samples ranged from 0 to 2.5. T2 and T13 had higher intensities of 'sweet', with respective intensities of 7.5 and 7, while the intensities of 'sweet' in R2, R3 and R4 were 0. The sensory intensities of 'peanut butter-like', 'puffed food' and 'exotic flavor' were relatively low. There were only 3 'peanut butter-like' flavor samples (T3, T4, T7) and 4 'puffed food' samples (S1, S2, S3 and L2). At the same time, we conducted a correlation analysis on these eight attributes, as shown in the Fig. 1b. Darker color represented a higher

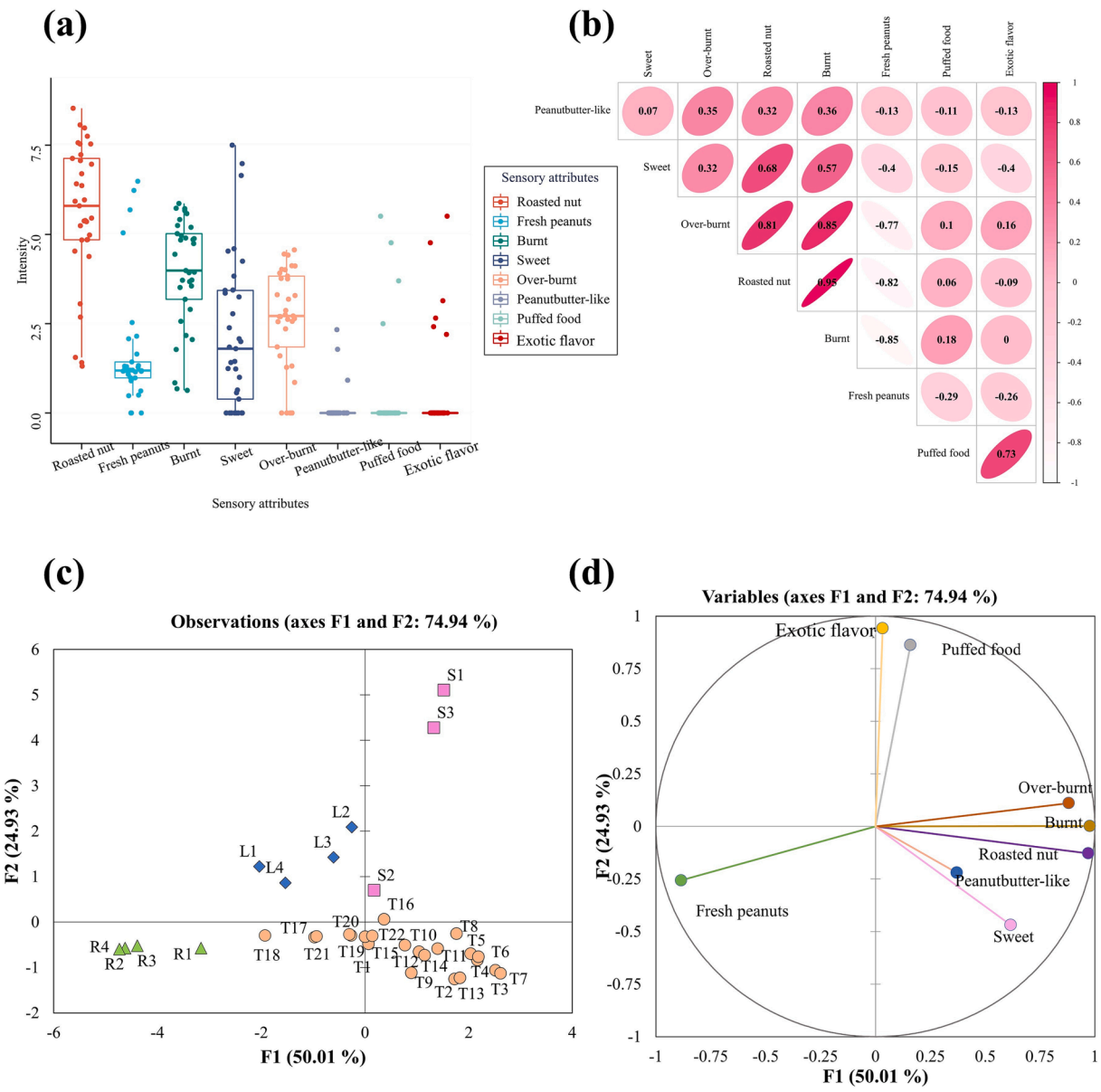

Fig. 1. Sensory evaluation and principal component analysis of 33 peanut oil samples. (a) QDA score of sensory attributes; (b) Sensory attribute correlation matrix; (c) Sample distribution scatter plot; (d) Loading plot of sensory attributes.

correlation between two attributes, that is, the closest correlation coefficient was 1. The positive correlation between 'burnt' and 'roasted nut' was high, followed by 'burnt' and 'over-burnt', 'roasted nut' and 'over-burnt', 'puffed food' and 'exotic flavor', 'roasted nut' and 'sweet', 'burnt' and 'sweet'. In addition, some attributes existed significantly negative correlation, such as 'fresh peanuts' and 'roasted nut', 'burnt', 'over-burnt'. This provided a good reference for the follow-up machine learning.

The principal component analysis (PCA) was performed to demonstrate the relationship between peanut oils and their sensory attributes (as shown in Fig. 1c), and the two principal components F1 and F2 explained 74.94 % of the variance. The samples R1-4 were located in the third quadrant and closely related to the 'fresh peanuts' attribute. S1 and S3 samples with 'puffed food' were clearly separated from other samples. S2 was classified as S sample because its process was similar to S1 and S3, and its 'puffed food' flavor was second after S1 and S3, which was placed in the first quadrant together with S1 and S3. l and T samples could be distinguished on F2. The characteristics of 'roasted nut', 'burnt' and 'over-burnt' in T samples were stronger than those in L samples.

In the Fig. 1d, 'roasted nut', 'over-burnt' and 'burnt' attributes were obviously similar and located closely, and 'peanut butter-like' and 'sweet' aroma were closed to each other. Most samples were associated with these five attributes. The four L samples in the second quadrant had low levels of 'roasted nut', 'burnt', 'over-burnt' and 'exotic flavor', so they were distributed near the middle. According to the results of PCA, we divided all 33 peanut oil samples into four types, namely, raw (R1-R4), light (L1-L4), salty (S1-S3) and thick (T1-T22) flavor. The differences in the aroma of peanut oils were closely related to their processing methods. Previous studies have reported that the peanut oil extracted from roasted peanuts had a 'baking smell' similar to 'roasted nut', while the cold pressed peanut oil was often 'green' and 'fatty' (Dun et al., 2019).

Characterization of volatile compounds in peanut oils

A total of 108 compounds were identified in the 33 samples by GC–MS, including 21 aldehydes, 16 pyrazines, 13 alcohols, 11 acids, 6 phenols, 7 esters, 7 alkanes, 5 lactones, 4 terpenes, 4 pyrroles, 4 ketones,

4 furans, 3 compounds containing benzene ring, 1 thiazole, 1 amide, and 1 pyridine (Table S3). Most of the 33 peanut oil samples contained all the 108 compounds, except for T1 and T10 (detected 107 compounds), T8 (106 compounds), *R*3 (95 compounds), R4 (94 compounds) and R2 (92 compounds). In peanut oils, the compound with higher concentration was hexanoic acid (3.92–13.41 μg/g), followed by acetic acid (1.68–2.22 μg/g), 2-ethylhexanoic acid (2.86–2.97 μg/g), hexanal (0.71–8.25 μg/g) and 4-vinylguaiacol (0.86–7.14 μg/g). The compound with lower concentration was 2-ethyl-6-methylpyrazine, followed by 2-acetylfuran, ethyl acetate, 6-methyl-5-heptene-2-one and benzothiazole. Based on the distribution of volatile compounds, a cluster heat map was used to reveal the differences among various peanut oil samples (Fig. 2).

According to the clustering heat map, S- and R- samples were obviously clustered into two categories. The contents of 2-methylfuran (0.064–0.080 μg/g), 2-acetyl pyrazine (0.037–0.046 μg/g), 2-furanmethanol (3.55–4.56 μg/g), 5-methyl-2-furanmethanol (0.08–0.13 μg/g), and pyrrole (0.029–0.350 μg/g) were higher in S-samples. 5-Methylfurfural (0.28 μg/g) and 2-pyrrolaldehyde (0.36 μg/g) were especially

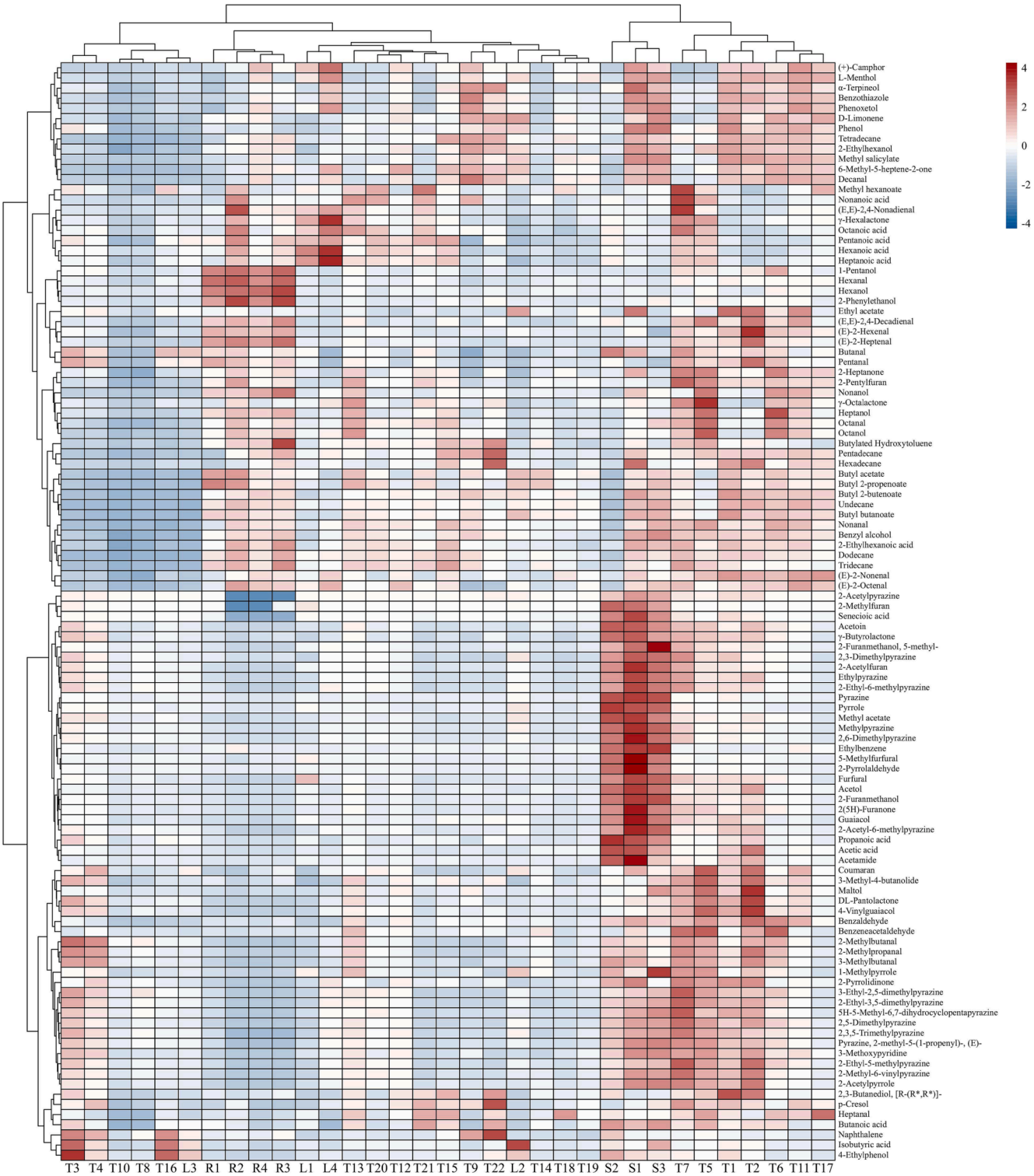

Fig. 2. Heat map of volatile compounds distributed in the 33 peanut oil samples.

higher in S1. 2-Methylfuran, 2-acetyl pyrazine, 5-methylfurfural and 2-pyrrolaldehyde reached their thresholds in oil, which had 'chocolate', 'popcorn', 'caramel', 'burnt' and 'nutty' flavors, respectively. Other compounds with higher contents belonged to pyrazines. Studies have found that *N*-heterocyclic compounds accounted for the highest proportion (61.68 %) in roasted peanut oils and pyrazines were the most abundant volatile compounds. Pyrazines were formed by the Maillard reaction between sugars and amino acids during seed roasting, usually accompanied by the generation of other *N*-heterocyclic compounds such as pyrrole and pyridine. Most of them exhibited 'baked', 'nutty', 'butter', 'baked potato' aroma attributes, and played a dominant role in the flavor of roasted seed oil because of their low thresholds and high dilution factors (Liu et al., 2011). In addition, roasting produced other volatile compounds, including furans, furanones, pyranones and cycloketones, and they together contributed to the 'nutty', 'roasted', and 'over-burnt' flavors, which were typical sensory characteristics of vegetable oils extracted from roasted seeds (Zhang et al., 2019).

R samples had distinct aroma of 'fresh peanuts' and slight aroma of 'roasted nut'. The compounds with higher contents in R samples were (E, E)-2,4-nonadienal (0.086 μg/g, R2) ('fatty'), hexanol (2.32 μg/g, *R*3) ('grassy'), hexanal (8.25 μg/g, R2) ('green'), (E) −2-hexenal (0.049 μg/g, *R*3) ('almon-like'), (E)-2-heptenal (0.094 μg/g, *R*3) ('green'). Butyl 2-propenoate (0.088 μg/g) and butylacetate (0.0027 μg/g) ('fruity') were higher in R1 and R2, while nonanol (0.30 μg/g) was higher in *R*3. Previous studies found that aldehydes mostly with 'green', 'fatty' and 'earthy' flavor were the main aroma odorants in cold pressed peanut oil, followed by alcohols and terpenes (Dun et al., 2019). Aldehydes and alcohols were formed by lipid oxidation and played an important role in the overall aroma of cold pressed peanut oil (Yin et al., 2022). Lipid oxidation mainly involved two pathways. One was lipoxygenase pathway that occurred during the division of oilseed cells, and the other was auto-oxidation during processing and storage. Hexanal and nonanal were the oxidation products of linoleic acid and oleic acid, respectively (Dun et al., 2019). Some alcohols were also formed by the reduction of their corresponding aldehydes, such as 1-hexanol, 1-octanol, 1-nonanol, 1-decanol, etc. (Wang et al., 2020). 4-Vinylguaiacol was a key phenolic compound in roasted peanut oil, which had a 'smoky' flavor and commonly produced by the thermal degradation of 4-hydroxycinnamic acid and ferric acid (Tańska et al., 2018), but this phenolic substance has not been detected in cold pressed peanut oil (Yin et al., 2022). However, in our study, 4-vinylguaiacol was detected in all four R samples, and the contents of R1-R4 were 1.28 μg/g, 0.86 μg/g, 0.96 μg/g and 0.91 μg/g, respectively.

T samples mainly presented the flavor of 'roasted nut', 'burnt' and 'over-burnt', and some samples also had obvious 'sweet' aroma, such as T2, T3 and T9 or 'peanut butter' such as T13 and T7. Samples with 'roasted nut' flavor tended to contain higher concentrations of pyrazines, as well as individual aldehydes such as 2-methylbutanal (1.18 μg/g, T3), 3-methylbutanal (0.50 μg/g, T2), and 2-methylpropanal (0.81 μg/g, T2), exhibiting 'malty' aroma. Some acids were also detected in T samples. Most acids were 'sweet' and 'cheese' flavor, and a few had 'vinegar' flavor, such as acetic acid. The contents of some acids in T samples were higher, for example nonanoic acid (0.10 μg/g, T7) ('moldy'), isobutyric acid (0.075 μg/g, T3) ('cheese-like'). However, their threshold values were relatively high, so their contributions to the overall flavor of peanut oil were not outstanding. In addition, there were esters, lactones, alkanes in peanut oils, but these odorants were not generally considered to have an important contribution to the flavor of oil due to their high odor thresholds. Among terpenes, D-limonene was widely concerned as a monoterpene and existed in many plants, which had 'citrus' and 'mint' flavor (Zhou et al., 2019). It generally disappeared in the later stage of peanut roasting, which may be related to its low volatility (Liu et al., 2011). In this study, D-limonene was detected in all samples ranging from 0.046 μg/g to 0.079 μg/g. Dimethyl sulfoxide and dimethyl trisulfide have been identified in peanut oil, which were less identified in previous studies (Yin et al., 2022). These sulfides were produced by sulfur-containing amino acids such as methionine, cysteine and cystine in peanuts through Maillard reaction or Strecker degradation (Jia et al., 2019). As for L samples, only the contents of acid compounds in L1 and L4 samples were high.

Comparison of odorant activity value (OAV) in various peanut oil samples

The concentrations of volatiles were not enough to reflect their importance to the flavor of peanut oil, and the contributions of key aroma compounds were also closely related to their aroma thresholds. The lower the threshold, the easier it could be perceived. OAV was the ratio of the concentration of compound to its threshold value in the same matrix. Generally, odorants with OAV greater than or equal to 1 were regarded as aroma-activate compounds, which had greater contribution to the flavor (Xu et al., 2022).

The OAVs of odorants in 33 peanut oil samples have been shown in the Fig. S2. The 38 compounds with OAV ≥ 1 were ranked according to the mean values of OAV in 33 samples, and their retention index, aroma description, detectable threshold and significance between different samples are listed in Table 1. Among these compounds, 10 pyrazines and 10 aldehydes accounted for the highest proportion. Pyrazines such as 2,3-dimethylpyrazine, 2-ethyl-3,5-dimethylpyrazine, 2-ethyl-5-methylpyrazine, 2,5-dimethylpyrazine, methylpyrazine, 2,6-dimethylpyrazine, 3-ethyl-2,5-dimethylpyrazine and 2-methylbutanal had high OAV values, which had 'roasted nut' and 'roasted potato' flavor and provided 'roasted nut' aroma to roasted peanut oil (Yin et al., 2022). Through one-way analysis of variance, 2,3-dimethylpyrazine, methylpyrazine, 2,6-dimethylpyrazine, 2-acetyl pyrazine and methylpyrazine had high significance in different flavor samples and were important odorants in peanut oil.

Aldehydes were another aroma-active volatile compounds in peanut oils and were important to the overall aroma profile of peanut oil. 2- and 3-Methylbutanal with average OAVs of 203 and 43 contributed to the aroma of 'roasted nut'. Benzeneacetaldehyde, hexanal and pentanal contributed to 'sweet', 'green' and 'fruit' aroma, and 2-pyrolaldehyde, furfural and 5-methylfural exhibited 'coffee', 'bread' and 'caramel' flavor. In addition, the average OAV values of 2-methylbutanal and 4-vinylguaiacol were the highest, which were 203 and 124, respectively. 4-Vinylguaiacol generally appeared in roasted peanut oil and was less detected in cold pressed peanut oil. At the same time, through the comparison between different types of samples, 2-furanmethanol, furfural, 2,6-dimethylpyrazine and methylpyrazine had significant differences between S and other samples, which proved that these compounds could well distinguish S samples; hexanal and hexanol had significant differences between R and other samples. The results of OAV played an important role in revealing the aroma-active odorants of peanut oil, and it also made a certain comparison and reference for the subsequent modeling analysis.

Partial least squares regression (PLSR) analysis

PLSR could reveal the relationship between volatile compounds and sensory attributes (Zhang, Wang, et al., 2022). The compounds with Variable Importance in the Projection (VIP) > 1 were screened, and the model was considered reliable until $Q^2 > 0.4$ and $R^2Y > 0.6$ (Liu, Gu, Laaksonen et al., 2022). Based on the modeling results, six ideal attributes were selected as the representative flavor of peanut oils including 'fresh peanuts', 'roasted nut', 'over-burnt', 'burnt', 'puffed food' and 'exotic flavor'. Twenty-nine compounds were strongly related to these sensory attributes, and 18 of them had a OAV great than 1. The modeling of 'peanut butter-like' and 'sweet' were not ideal due to the data structure of the sample so it was not discussed here (Table S4 for specific model parameters). Through PLSR analysis, the correlation coefficients between volatile compounds and each sensory attribute are summarized in the Table 2.

Some of these compounds had one-way positive or negative effects

Table 2
Correlation between sensory properties and compounds by PLSR.

Compounds	Fresh peanuts	Roasted nut	Burnt	Over-burnt	Puffed food	Exotic flavor
2-Methylpropanal		0.058	0.057			
3-Methylbutanal		0.071	0.073	0.107		
Hexanal	0.148	−0.181	−0.154			
(E)-2-Heptenal	0.109					
Benzeneacetaldehyde		0.084				
2-Pyrrolaldehyde					0.208	0.22
1-Pentanol	0.108					
Acetol					−0.006	−0.207
Hexanol	0.137	−0.142	−0.128			
2-Furanmethanol					0.055	
Guaiacol					−0.016	
2-Phenylethanol	0.128	−0.158	−0.137			
2-Furanmethanol, 5-methyl-	−0.072		0.055	0.209	0.029	
2(5H)-Furanone					−0.07	−0.202
2-Methylfuran	−0.074					
Furfural					−0.088	
2-Acetylfuran					−0.094	
5-Methylfurfural					0.208	0.309
Pyrazine					0.211	0.175
Methylpyrazine					0.06	
2,5-Dimethylpyrazine				−0.037		
2,6-Dimethylpyrazine					0.038	
2-Acetylpyrazine	−0.095	0.094	0.091	0.374		
2-Acetyl-6-methylpyrazine					−0.04	
Propanoic acid					0.011	−0.132
Methyl acetate					−0.023	
Ethylbenzene					0.381	0.308
Pyrrole					0.154	0.379
Acetamide					−0.031	

The bold indicate that OAV > 1 in at least one sample.

on the sensory attributes, such as (E)-2-heptenal ('green, fat'), 1-pentanol ('sweet, fat'), which only had a positive effect on the odour of 'fresh peanuts'. 2-Methylpropanal ('malt') had a positive effect on the odour of 'roasted nut' and 'burnt'; 3-methylbutanal ('malt') had a positive effect on 'roasted nut', 'burnt' and 'over-burnt'; nonanol ('fat, fresh') had a negative effect on 'roasted nut', 'burnt' and 'over-burnt'. Zhang et al. (2022) analyzed the relationship between compounds and sensory properties of fried *Allium tenuissimum L.* flower oil by PLSR. Their results suggested that *N*-heterocyclic compounds such as methylpyrazine, 2,5-dimethylpyrazine, were positively correlated with the sensory properties of 'roasty', and 2-pentylfuran, furfural and 2-furanmethanol had significant positive effects on 'caramel' properties. Furthermore, some compounds had positive correlations to some sensory attributes but negative correlations to other attributes, such as 2-acetyl pyrazine with 'popcorn' flavor had positive effects on 'roasted nut', 'burnt' and 'over-burnt', but a negative effect on the 'fresh peanuts'. On the other hand, hexanol ('grassy') had a positive effect on 'fresh peanuts' but a negative effect on 'roasted nut', 'burnt' and 'over-burnt', as did hexanal ('green', 'fresh', 'leaf') and 2-phenylethanol ('floral'). The PLSR results were well consistent with the aroma description of volatiles.

Among these important variables, it was obvious that most alcohol compounds had a positive correlation with 'fresh peanuts', and some had a negative correlation with 'roasted nut' and 'burnt' at the same time. The odorants positively related to 'roasted nut', 'burnt' and 'over-burnt' aroma attributes were often negatively related to 'fresh peanuts', such as pyrazines and individual aldehydes. In addition, five compounds, 2-pyrrolaldehyde ('coffee'), 5-methylfural ('caramel'), pyrazine ('hazelnut'), ethylbenzene and pyrrole ('nutty'), were also positively correlated with two highly correlated attributes (correlation coefficient = 0.73) of 'puffed food' and 'exotic flavor' (Fig. 2b). Such results could guide us to study the interaction of interrelated odorants in the further and to clarify the effect of these compounds on the overall flavor in oil matrix.

Random forest

Random forest could establish a prediction model through variable selection. On the basis of reducing the burden of data analysis, key variables related to sensory attributes or aroma characteristics were accurately screened. Through the analysis and comparison of parameters, the R^2 of 'fresh peanuts', 'roasted nut', 'burnt' and 'over-burnt' were all above 0.7, indicating that the prediction results of these sensory attributes were better in this model. The random forest screened out 5 important compounds (red compounds in the Fig. 3) that affect these four attributes.

The important volatile for 'roasted nut' was 2-methylbutanal; for 'fresh peanuts' were furfural, 2-furanmethanol, 5-methylfurfural, 2-acetyl pyrazine; for 'burnt' was 2-methylbutanal, and 2-acetyl pyrazine; for 'over-burnt' was 2-methylbutanal. The correlation matrix of sensory attribute (Fig. 2b) had confirmed that 'roasted nut', 'burnt' and 'over-burnt' attribute were highly correlated. 2-Methylbutanal ('cocoa', 'nut' and 'wheat') was served as the important compound for all these 3 attributes by random forest, which was also an important aromatic compound in roasted almonds and made an important contribution to roasted almond flavor (Erten & Cadwallader, 2017). It was produced by Strecker degradation of isoleucine (Whitfield & Mottram, 1992). The selected five important variables could be used as indicators of different sensory characteristics, providing basis for processing control of peanut oil. In this study, fewer important variables were screened out by random forest (5 variables) than PLSR (29 variables), and there were four compounds overlapped by the two methods, except 2-methylbutanal. Random forest and PLSR were always better than null model. Moreover, random forest retained fewer variables, which provided higher prediction accuracy and lowest prediction error (Vigneau et al., 2018).

Classification and regression tree (CART)

Each CART was constructed by means of the recursive binary partitioning of the dataset (Breiman, 2001). It is grown from a root at which

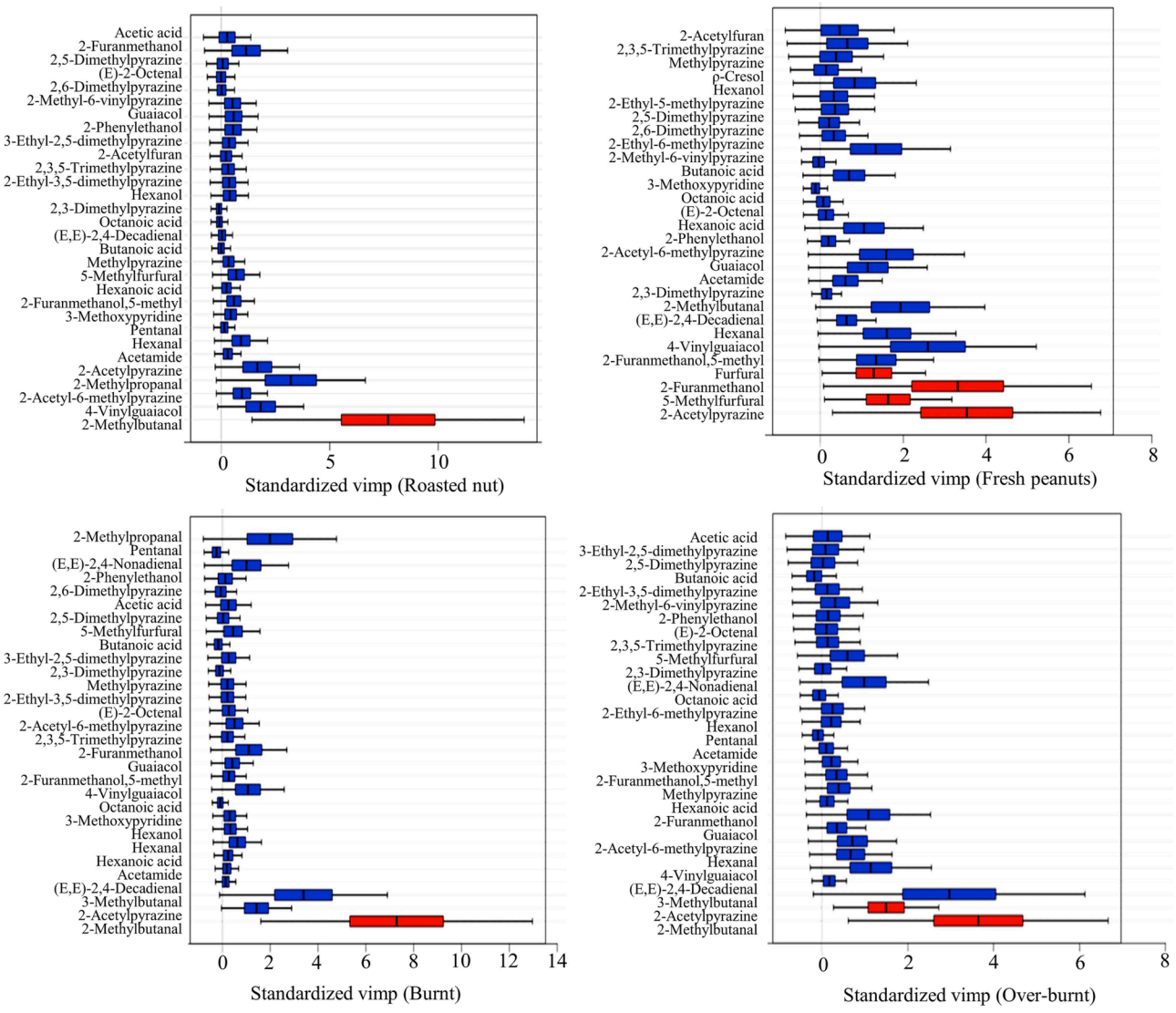

Fig. 3. The key variables related to corresponding sensory properties selected by random forest (red module on the right side of the ordinate). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

all the observations are merged, and then is split into two subsets through successive nodes. The terminal nodes are usually called leaves and may contain a single observation if the tree is completely built. As shown in the Fig. 4, there are 9 nodes in the regression tree and 6 compounds retained for prediction, including 4-vinylguaiacol ('smoky'), hexanol ('grass'), 2-acetyl pyrazine ('popcorn'), 2-methylbutanal ('nutty', 'cocoa', 'malt'), benzeneacetaldehyde ('green', 'floral') and furfural ('toasted', 'almond', 'sweet'). The number of variables screened by CART was significantly lower than that by PLSR, and there were four replicates (hexanol, 2-acetyl pyrazine, benzeneacetaldehyde, furfural). Three compounds (2-acetyl pyrazine, 2-methylbutanal, furfural) were the same with the results of random forest. Two subsets were distinguished after nodes according to the concentrations of the compounds, and 'n' represented the number of samples. In the first step, 4-vinylguaiacol with a concentration of 1.34 μg/g was selected, and the compounds in node one were divided into two subsets. The left subset (No. 1–2) was further distinguished by hexanol at a concentration of 1.758 μg/g. Hexanol was described as 'grassy', and the samples in this subset were screened for R1, R2, *R*3, R4 and L1. Meanwhile, the bar chart also showed that the first subset had a distinct odour of 'fresh peanuts'. The rightmost subset (No. 11) was separated by 2-acetyl pyrazine at a concentration of 0.03583 μg/g. It showed only three samples S1, S2 and S3, which exhibited higher 'puffed food' and 'exotic flavor' than other groups. In the middle of eight group samples (No. 3–10), the No. 3–5 groups all had clear flavor of 'roasted nut', 'burnt', 'over-burnt' compared with the No. 6–10 groups. The 'sweet' was relatively weak when benzeneacetaldehyde < 0.2161 μg/g and furfural < 0.1839 μg/g. However, when the concentration of furfural > 0.1839 μg/g, the 'sweet' could not be perceived but 'puffed food' and 'exotic flavor' could be perceived. When the concentration of benzeneacetaldehyde > 0.2161 μg/g, 'sweet' was obviously perceived. The No. 6–10 groups had obvious flavor of 'roasted nut', 'burnt' and 'over-burnt', but almost no 'fresh peanuts', 'puffed food' and 'exotic flavor'.

The concentration distribution of six variables in the four flavor types of peanut oils have been shown in the Fig. 4. 2-Acetyl pyrazine could distinguish the raw flavor (R samples) well ($P < 0.05$). This result was consistent with the PLSR result, and 2-acetyl pyrazine had a significant negative correlation with 'fresh peanuts'. Similarly, hexanol could well distinguish raw flavor from the other three flavor types ($P < 0.001$), so it might make a significant contribution to the raw flavor type samples. The content of furfural in S samples was significantly higher than that in the other three flavor types and it was considered as a candidate compound of salty flavor type; 4-vinylguaiacol and 2-methylbutanal had significant differences in thick (T samples) and raw flavor

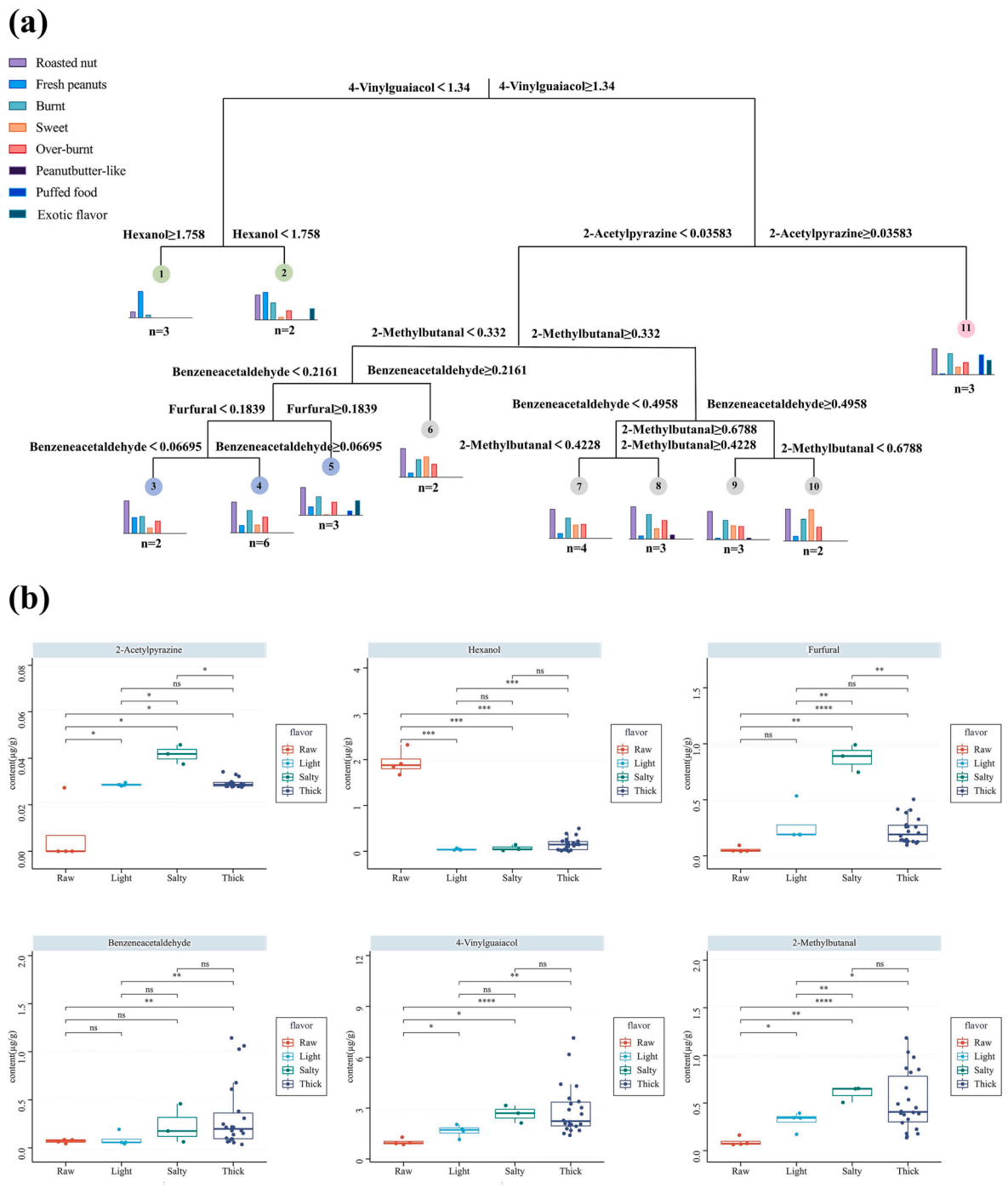

Fig. 4. CATR (a) and the distribution of key variables in four type flavor samples (b). (Numbers next to the compounds in (a) represented the compound concentration μg/g; 'n' represented the number of samples; (b) performed one way ANOVA, * is $P < 0.05$, * * is $P < 0.01$, * * * is $P < 0.001$, * * * * is $P < 0.0001$, NS is $P > 0.05$).

($P < 0.0001$).

Conclusion

In this study, flavoromics was carried out to evaluate the characteristic of 33 fragrant peanut oils in China market from the aroma composition and sensory perspective. Among all identified compounds, 100 were accurately quantified, which mainly included aldehydes, pyrazines, alcohols, acids, phenols, esters, terpenes and other heterocyclic compounds. And 38 volatile compounds were detected with OAV ≥ 1. From the perspective of sensory properties, most commercial peanut oils presented 'fresh peanuts', 'roasted nut', 'burnt', 'over-burnt' and 'sweet' flavor, and a few samples had 'puffed food' and 'exotic flavor'. They can be classified into four aroma types, namely raw, light, thick and salty. The relationship between the volatiles and sensory characteristics has been established using multi-analytical approach. Partial least squares regression analysis identified 29 compounds with potential contributions to the specific aroma of peanut oil, while random forest and regression tree screened out 5 and 6 key aroma compounds. The concentration of 2-acetyl pyrazine was lower in the raw aroma type oil, while hexanol was higher. 2-Methylbutanal and 4-vinylguaiacol contributed significantly to the 'roasted nut' of peanut oil, which

could be used as the signature compound of thick flavor. Furfural was the characteristic compounds in the salty type peanut oil. Compared with PLSR, random forest and regression tree could greatly reduce the number of variables while finding the key compounds that affect the aroma types of peanut oil. Furthermore, CART provided complementary information about the effects of volatile concentrations on sensory attributes and flavor type, which was more conducive to the process control of specific flavor. In the future research, these important variables can be applied to study the formation mechanism of characteristic aroma and evaluate the quality and grade of peanut oil. The important variables selected in this study need to be verified by aroma omission and recombination test, so as to provide scientific basis for processing specific fragrant oils.

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

Data will be made available on request.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.fochx.2023.100880.

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