

Discrimination and quantification of volatile compounds in beer by FTIR combined with machine learning approaches

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ABSTRACT

The composition of volatile compounds in beer is crucial to the quality of beer. Herein, we identified 23 volatile compounds, namely, 12 esters, 4 alcohols, 5 acids, and 2 phenols, in nine different beer types using GC–MS. By performing PCA of the data of the flavor compounds, the different beer types were well discriminated. Ethyl caproate, ethyl caprylate, and phenylethyl alcohol were identified as the crucial volatile compounds to discriminate different beers. PLS regression analysis was performed to model and predict the contents of six crucial volatile compounds in the beer samples based on the characteristic wavelength of the FTIR spectrum. The R^2 value of each sample in the prediction model was 0.9398–0.9994, and RMSEP was 0.0122–0.7011. The method proposed in this paper has been applied to determine flavor compounds in beer samples with good consistency compared with GC–MS.

1. Introduction

Beer is one of the most popular beverages worldwide; its widespread consumption increases its commercial value every year (Alves et al., 2020). In 2020, approximately 1.88 billion liters of beer were consumed globally (Statista, 2022). China is the world's largest beer consumer, accounting for 22.7% of global beer sales (SINDICERV, 2021), which is nearly double the sales of the second largest seller, the United States (Han et al., 2023). People worldwide love beer owing to its various tastes, physicochemical properties, and flavor (Almeida, Aparecida, Lima, Suarez, & Andrade, 2018; Alves et al., 2020; Betancur, Motoki, Spence, & Velasco, 2020). The flavor of beer is characterized by the presence of dozens of volatile organic compounds, including alcohols, esters, fatty acids, carbonyl compounds, sulfur compounds, furanic compounds, monoterpens, and volatile phenols, constituting the unique flavor of each beer at different concentrations (Gagula et al., 2020; Ncube, Dube, & Nindi, 2020). Some of these compounds are pleasant, and their concentrations should be kept stable; however, some have undesirable properties that should be reduced to a minimum (Dong et al., 2014; Liu et al., 2023). Providing consumers with stable-quality beer is extremely essential, and regular beer analysis is warranted to

track, minimize, and correct the concentrations of volatile organic compounds in beer (Betancur et al., 2020; Gagula et al., 2020; Ncube et al., 2020).

At present, beer flavor analysis is achieved via electronic nose (Ghasemi-Varnamkhasti et al., 2011), electronic tongue (Mutz et al., 2021), high-performance liquid chromatography (Scioli et al., 2022), and gas chromatography–mass spectrometry (GC–MS) (Attchelouwa et al., 2020). Furthermore, static headspace technology, solid-phase microextraction (SPME), and headspace solid-phase microextraction (HS-SPME) combined with GC–MS have been effectively used to analyze volatile compounds in beer. For example, these methods have been used to analyze volatile compounds in sorghum beer during storage (Attchelouwa et al., 2020), model and analyze flavor compounds in beer (Giannetti, Mariani, Torrelli, & Marini, 2019), and determine volatile carbonyl compounds in beer (Moreira, Meireles, Brandão, & Pinho, 2013). However, most of these traditional methods have limitations as they are laborious, time-consuming, and destructive; require lengthy sample processing; and lack online tracking and monitoring. Therefore, food researchers are increasing their focus on searching for accurate, rapid, and economical analytical methods to quickly quantify volatile organic compounds in beer.

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Fourier-transform infrared (FTIR) spectroscopy, an advanced chemical analysis technology, has several advantages, including the requirement of a small amount of sample, simple sample pretreatment, good reproducibility, and rapid analysis time at a high spectral resolution. Food researchers have widely used FTIR combined with chemometric models for qualitative and quantitative analyses of volatiles in foods, especially in the application of food classification and adulteration. For example, different brands of Chinese spirits can be discriminated (Dong et al., 2014), the degree of beef spoilage can be analyzed (Zhang, Ye, Xiao, & Dong, 2015), and artificial fragrant rice can be identified from high-quality rice (Liu et al., 2023). In research related to beer, FTIR was employed to monitor sugars in the beer mashing process (Almeida et al., 2018), determine the quality parameters of different beers (Polshin, Aernouts, Saeyns, Lammertyn, et al., 2011), and classify beer samples based on differences in alcohol content and sugars (Gordon et al., 2018). However, the above studies focused on the sugar content, alcohol weight, and degree of surface fermentation in beer to classify and evaluate the quality of the samples. To the best of our knowledge, no studies have classified beer based on volatile compounds or rapidly quantified volatile compounds in beer. As a result, the present study aimed to develop and validate a rapid and simple method for directly quantifying flavor compounds in beer by combining FTIR and chemometric methods. For this purpose, nine beers obtained from Tsingtao Brewery Co. Ltd. (China) were analyzed using SPME-GC-MS and principal component analysis (PCA) to identify and classify the essential odorants dominating the characteristic flavors of different beer samples. Furthermore, a partial least squares (PLS) quantitative analysis model of typical flavor data based on the characteristic wavelength of the FTIR spectrum was successfully established and verified. Our study provides a new and feasible method for evaluating beer flavor and has important and practical significance in the study of beer flavor compounds.

2. Materials and methods

2.1. Sample preparation

Nine beers were obtained from Tsingtao Brewery Co. Ltd. (China) and stored at 4 °C until GC-MS analysis. The beer samples were as follows: No.1 Tsingtao stout black beer, No.2 Tsingtao premium beer, No.3 Tsingtao Craft Beer IPA, No.4 Tsingtao Classical, No.5 Tsingtao pilsner beer, No.6 Tsingtao pure draft beer (batch on May 22), No.7 Tsingtao pure draft beer (batch on May 24), No.8 Tsingtao pure draft beer (batch on May 25), and No.9 Tsingtao pure draft beer (batch on May 27).

The six flavor compounds phenylethyl alcohol (C₈H₁₀O), isopentyl alcohol (C₅H₁₂O), ethyl caprylate (C₁₀H₂₀O₂), isopentyl acetate (C₇H₁₄O₂), ethyl caproate (C₈H₁₆O₂), and ethyl acetate (C₄H₈O₂) were purchased from Shanghai McLean Biochemical Technology Co. Ltd. (Shanghai, China). Each flavor compound was dissolved in 5% ethanol and prepared as samples with 20 different concentration gradients at 0.5% intervals. The concentration range of each compound was as follows: phenylethyl alcohol (3–60 mg L⁻¹), isopentyl alcohol (5–100 mg L⁻¹), ethyl caprylate (0.1–2 mg L⁻¹), isopentyl acetate (0.15–3 mg L⁻¹), ethyl caproate (0.1–2 mg L⁻¹), and ethyl acetate (2.5–50 mg L⁻¹). These solutions were prepared for FTIR analysis.

2.2. Determination of the flavor compounds using GC-MS analysis

GC-MS analysis was performed using the Shimadzu Nexis gc2030 GC and Shimadzu QP2020NX MS. The chromatographic column was TR-WaxMS column (30 mL × 0.25 mm × 0.25 μm; Shimadzu Enterprise Management, China). The SPME extraction head divinylbenzene/carboxy/polydimethylsiloxane (DVB/CAR/PDMS) 50/30UM was obtained from Supelco.

Beer samples (5 mL) and 0.6 μL of 2-methyl-3 heptanone solution (0.1632 mg mL⁻¹; internal standard) were added into a 15-mL headspace vial. The headspace vial was placed on an oscillator at a rotation

speed of 500 r min⁻¹ for 15 min under a constant temperature of 30 °C. Then, the DVB/CAR/PDMS 50/30UM extraction head was used for extraction. Before extracting the beer sample, the fiber was aged at 270 °C for 1 h, and then the extraction head was inserted into the headspace of the sample headspace vial. The extraction was performed for 30 min at 60 °C.

GC conditions were as follows: start at 60 °C for 2 min, at 10 °C min⁻¹ to 90 °C, and then at 2 °C min⁻¹ to 130 °C for 5 min. No split injection was applied, and the carrier gas was helium. The flow rate was maintained at 1 mL min⁻¹. The MS conditions were as follows: ionization mode, EI; electron energy, 70 eV, ion source temperature, 230 °C; transfer line temperature, 240 °C; scan mode, full scan mode; and mass scan range, 30–300 *m/z*. Searches were performed using the NISTDEMO database.

The volatile compounds in beers were identified by their mass spectrometry fragment, which was matched with the National Institute of Standards and Technology (NIST 14) and NISTDEMO database, assisted by a mixture of n-alkane series (C₆ - C₄₀) to compare the experimental retention index (RI) with the values available in the NIST MS libraries. In addition, the relative content of volatile compounds was calculated by dividing the peak area of the isolated compound by the peak area of the internal standard. The quantification of phenylethyl alcohol, isopentyl alcohol, ethyl caprylate, isopentyl acetate, ethyl caproate, and ethyl acetate was carried out using an external standard method. The standard curves were prepared by plotting the ratios of the response areas of the standard compounds and internal standard against their concentration ratios. All analyses were carried out in triplicate, and the results are presented as the mean ± standard deviation.

2.3. FTIR spectra acquisition

The PerkinElmer Frontier Optica FTIR spectrometer (PerkinElmer, Norwalk, CT, USA) was used to collect FTIR spectral data of the samples using a previously described method (Wang et al., 2020). The parameter was set to point mode to collect the reflection spectrum, and the spot size was 50 μm × 50 μm. The resolution was 8 cm⁻¹, scanning speed was 1.0 cm s⁻¹, scanning interval was 2 cm⁻¹, scanning range was 5005–1000 cm⁻¹, and number of background scanning times was 100. Each sample was scanned twice, and the spectral data were stored in the form of absorbance. Spectrum IMAGE Software from the “stats” R package (Śliwińska, Wiśniewska, Dymerski, Namieśnik, & Wardencki, 2014) was used for spectrum acquisition and spectral data processing; the drawing and modeling program codes were prepared by us. Before the experiment, corrections were conducted to reduce the experimental error caused by atmospheric interference and instrument noise.

2.4. Characteristic wavelength selection

PCA analysis was performed using the “prcomp” function of the “stats” R package to identify high-dimensional data structures by reducing the dimensions of the data to determine more understandable features and accelerate the processing of valuable sample information.

2.5. Quantification using partial least squares regression models

The PLS regression models were constructed for quantitative analysis of the six flavor compounds based on the spectral information of the samples, which was implemented using the “PLS” function of the R package. The pretreatment methods were smoothing, first-order derivative, and smoothing + first-order derivative, which were applied and compared to select the most appropriate pretreatment method. After the model was established, 10-fold cross-validation was applied to the test set to estimate the predictive ability of the model to reduce the risk of overfitting. The predictive ability of the models was evaluated using correlation coefficients (R²) and root mean square error for prediction (RMSEP). RMSEP was calculated using the following formula:

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (X_{obs,i} - X_{pred,i})^2}{n}}$$

Where X_{obs} is the observed known values of the outcome, X_{pred} is the predicted value obtained using the model, and n is the number of samples in the test set.

3. Results and discussion

3.1. Analysis of the volatile compounds in the nine beer samples via GC–MS analysis

Beer flavor is affected by various volatile organic compounds, including alcohols, esters, aldehydes, ketones, and phenols (Giannetti et al., 2019). In the present study, the volatile organic compounds in the nine beer samples were identified via SPME–GC–MS. The volatile organic compounds and their relative concentrations in different beer samples are shown in Table 1. In total, 23 volatile flavor compounds were identified: 12 esters, 5 acids, 4 alcohols, and 2 phenols. Significant differences were observed in volatile organic compound types and content among the different beers. Among them, ethyl caproate, phenylethyl alcohol, and ethyl caprylate, as ideal alcohols and esters in beer (Riu-Aumatell, Miró, Serra-Cayuela, Buxaderas, & López-Tamames, 2014), accounted for an essential proportion in each sample, with significant differences in content (Table 1). Almost every type of beer contains a distinctive volatile compound, giving each kind of beer its characteristic flavor. Beer sample No. 1 contains n-caprylic acid with

fresh cheese flavor (Ferreira et al., 2022), No. 2 contains ethyl myristate with an oil fragrance, No. 3 contains neopentyl butyrate with a strong banana flavor (Han et al., 2023), No. 4 contains 1-octanol with a lemon flavor, and No. 5 contains chavicol, contributing to its distinctive odor, which can be considered as characteristic fingerprints to identify different beers. Interestingly, samples 6–9 were different batches of the same kind of beer, and their relative contents of the volatile flavor compounds ethyl caproate, phenylethyl alcohol, ethyl caprylate, dimethyl salicylic acid, and ethyl laurate were comparatively stable. Some amount of malonic acid and pentadecanoic acid was detected in the samples, whereas it was not detected in some. The difference in flavor compounds in beer may be caused by the raw materials used, technological parameters, and yeast (Ferreira et al., 2022; Li et al., 2022). Although the proportion of these organic acids was <1%, thereby not seriously affecting beer flavor, it is important for brewers to identify these unstable flavor compounds and determine solutions to maintain their stability in products.

In order to screen for volatile compounds that can help distinguish different beer samples, PCA, a technique used to explore high-dimensional data structures by reducing the dimension of the data to identify more understandable features and accelerating the processing of valuable sample information, could be used to screen feature components effectively to distinguish different samples (Wang & Huang, 2022) and was used to analyze the differences in major flavor compounds in different beer samples. As shown in Fig. 1A, PC1 and PC2 explained 63% and 16.4%, respectively, of the variance in the total variables of the sample; the cumulative contribution rate of the two principal components was 79.4%, indicating that the two components

Table 1
Relative contents (mg L⁻¹) of flavor components for 9 beer samples by GC–MS.

Flavor compounds	Relative content (mean ± standard deviation)								
	NO.1	NO.2	NO.3	NO.4	NO.5	NO.6	NO.7	NO.8	NO.9
Phenylethyl alcohol	15.80 ± 0.87	11.01 ± 0.96	8.35 ± 0.45	5.91 ± 0.29	7.76 ± 0.33	11.41 ± 0.51	7.13 ± 0.31	10.77 ± 0.52	5.47 ± 0.27
Ethyl caproate	22.64 ± 1.68	8.83 ± 0.57	13.69 ± 0.89	12.92 ± 0.67	23.98 ± 1.89	17.75 ± 0.71	20.20 ± 2.12	16.32 ± 0.89	16.94 ± 0.85
Ethyl caprylate	21.36 ± 1.98	26.75 ± 1.06	22.79 ± 1.32	11.01 ± 0.51	10.73 ± 0.08	21.66 ± 1.05	27.66 ± 2.15	27.73 ± 1.12	25.72 ± 1.08
Octoic acid	5.36 ± 0.22	ND	ND	ND	ND	ND	ND	ND	ND
Ethyl acetate	4.64 ± 0.31	12.80 ± 0.54	ND	1.21 ± 0.03	1.54 ± 0.09	3.03 ± 0.12	ND	2.49 ± 0.11	ND
Malonic acid	1.93 ± 0.02	ND	3.61 ± 0.29	3.38 ± 0.11	2.88 ± 0.02	2.88 ± 0.09	ND	ND	3.44 ± 0.18
Ethyl decanoate	4.93 ± 0.38	9.77 ± 0.31	2.70 ± 0.25	2.32 ± 0.09	0.54 ± 0.04	ND	ND	ND	ND
Ethyl dodecanoate	1.84 ± 0.13	ND	ND	0.48 ± 0.02	ND	3.36 ± 0.13	5.14 ± 0.39	6.53 ± 0.34	5.24 ± 0.31
3-Methylsalicylic acid	0.49 ± 0.02	1.47 ± 0.23	1.70 ± 0.13	1.84 ± 0.07	0.63 ± 0.04	0.560 ± 0.03	0.55 ± 0.04	0.46 ± 0.02	ND
Salicylic acid - 2-ethyl ethyl ester	0.14 ± 0.018	ND	0.073 ± 0.001	ND	0.14 ± 0.01	ND	ND	ND	ND
Ethyl laurate	0.37 ± 0.089	ND	0.095 ± 0.065	0.74 ± 0.03	ND	0.41 ± 0.02	ND	0.33 ± 0.01	ND
Caproic acid	ND	0.21 ± 0.021	ND	ND	ND	ND	ND	ND	ND
n-decanol	ND	0.46 ± 0.078	ND	ND	ND	ND	ND	ND	ND
Ethyl myristate	ND	0.038 ± 0.001	ND	ND	ND	ND	ND	ND	ND
Homosalate	ND	0.20 ± 0.02	0.21 ± 0.09	ND	ND	ND	ND	ND	ND
Butyl phthalate	ND	0.21 ± 0.08	ND	ND	ND	ND	ND	ND	ND
Neoamyl Butyrate	ND	ND	2.10 ± 0.21	ND	ND	ND	ND	ND	ND
Linalool	ND	ND	0.95 ± 0.08	ND	ND	ND	ND	ND	ND
P-allylphenol derivative	ND	ND	ND	0.17 ± 0.01	ND	ND	ND	ND	ND
P-allylphenol	ND	ND	ND	0.42 ± 0.009	ND	ND	ND	ND	ND
Ethyl palmitate	ND	ND	ND	0.15 ± 0.01	ND	ND	ND	ND	ND
N-Octanol	ND	ND	ND	ND	0.77 ± 0.06	ND	ND	ND	ND
Ethyl 9-Hexadecenoate	ND	ND	ND	ND	0.54 ± 0.05	ND	ND	ND	ND

The relative content of volatile compound was calculated by dividing the peak area of the isolated compound by the peak area of internal standard. No.1–No.9 were Tsingtao stout black beer, Tsingtao premium beer, Tsingtao Craft Beer IPA, Tsingtao Classical, Tsingtao pilsner beer, Tsingtao pure draft beer batch on May 22, Tsingtao pure draft beer batch on May 22, Tsingtao pure draft beer batch on May 24, Tsingtao pure draft beer batch on May 25, Tsingtao pure draft beer batch on May 27.

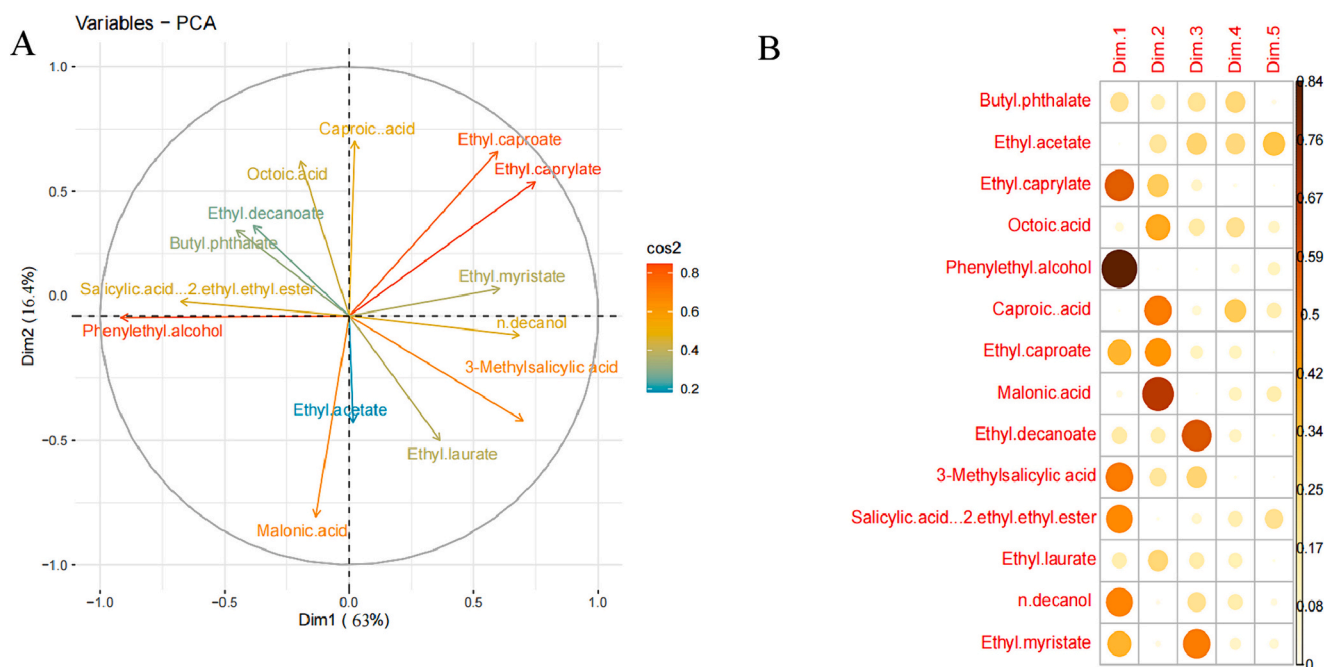


Fig. 1. PCA analysis of GC-MS data of 9 beer samples. A: Variable correlation plots of various flavor compounds; B: Contribution plots of various flavor compounds.

explained 79.4% of the variance; thus, the prepared principal components represented most of the sample information. PC1 explained 63% of the total samples, indicating that it was the most significant principal component. Fig. 1B shows the significant contributions of the differences. The larger the circle area in the figure is, the greater the contribution of that variable. Additionally, the closer the color was to red, the lower the contribution, and the closer the color was to blue, the greater the contribution. Fig. S1 shows the contributions of different volatile compounds to the differences in the beer samples. Finally, ethyl caproate, ethyl caprylate, and phenylethyl alcohols with contributions >10% were selected as the volatile compounds to distinguish among the different beers.

3.2. Establishment of a rapid quantitative prediction model for the six flavor compounds

The above results demonstrated that ethyl caproate, phenylethyl alcohol, and ethyl caprylate significantly contributed to the flavor differences among different beer samples. Studies have reported that ethyl acetate, isopentyl alcohol, and isopentyl acetate have a strong effect on beer flavor (Alves et al., 2020; Giannetti et al., 2019). Therefore, these six flavor compounds were selected to establish a rapid infrared spectrum quantitative analysis method.

3.2.1. Selection of the characteristic infrared spectra for the different flavor compounds

Fig. 2 illustrates the original spectra of the 20 concentration gradients of the six flavor compounds. The information range and shape of the characteristic peaks of the infrared spectrum of each flavor compound were different. To establish an efficient and accurate calibration model using infrared spectral data, the characteristic wavelengths in the infrared spectra of each flavor compound were screened using PCA, as shown in the PCA load diagram in Fig. 3. It reflected the score coefficients of each observation wave number in the principal components PC1 and PC2. The sum of the product of each observation object and the PC1 score coefficient was the score of the principal component PC1, and the sum of the product with the PC2 score coefficient was the score of the principal component PC2. The wave number range was included when the value of at least one of the two principal components was >0 and

was depicted as the characteristic wavelength range. The characteristic wavelengths of each flavor compound were finally selected as follows: phenylethyl alcohol, 5000–4876 and 2369–2353 cm^{-1} ; isopentyl alcohol, 4970–4876 and 1566–1474 cm^{-1} ; ethyl caprylate, 2898–2608, 1455–1381, 1335–1300, 1285–1273, and 1103–1022 cm^{-1} ; isopentyl acetate, 2372–2311 cm^{-1} ; ethyl caproate, 2921–2650, 1431–1377, 1331–1304, and 1103–1022 cm^{-1} ; and ethyl acetate, 2372–2315 and 1802–1709 cm^{-1} .

Analysis of the selected characteristic wavelengths combined with the published data revealed that the bands at 2925 and approximately 1465 cm^{-1} were attributed to the (C–H) tensile vibration and variable angle vibration in alcohols and esters, respectively (Majstorović, Živković, Mitrović, Munćan, & Kijevčanin, 2016). The bands at approximately 1080 and 1430 cm^{-1} were characteristics of the (C–O) stretching vibration and (C–OH) in-plane bending vibration in esters, respectively (Majstorović, Živković, Matija, & Kijevčanin, 2017). The band at the range 1750–1800 cm^{-1} was the characteristic of the (C=O) stretching vibration in ester carbonyls (Shigley, Bonhorst, Liang, Althouse, & Triebold, 1955). Thus, selection of this region for the analysis of the six volatile compounds is fully addressable.

3.2.2. Quantification model for single flavor compounds

PLS, a mathematical optimization technique (Yamashita, Anzanello, Soares, Rocha, & Fogliatto, 2022), is widely used to analyze infrared spectral data (Costa, Morgano, Ferreira, & Milani, 2019; Kahmann et al., 2018). It can support regression modeling when the number of variables is greater than the number of samples. The independent variables have multiple correlations (Yao et al., 2022). Furthermore, the final model contains all the original independent variables. Recently, infrared spectroscopy combined with the PLS method has been applied for the quantitative analysis of food ingredients (Bassbasi, Platikanov, Tauler, & Oussama, 2014; Wang et al., 2020). In the present study, we established quantitative prediction models for the six flavor compounds by combining infrared spectral data with PLS.

Smoothing and derivative processing can reduce interference from noise and baseline drift and efficiently highlight the differences between samples in the spectrogram. The derivative-processed spectrogram can reveal the absorption peak position of the original spectrogram and the absorption intensity of the peak position, facilitating further analysis. In

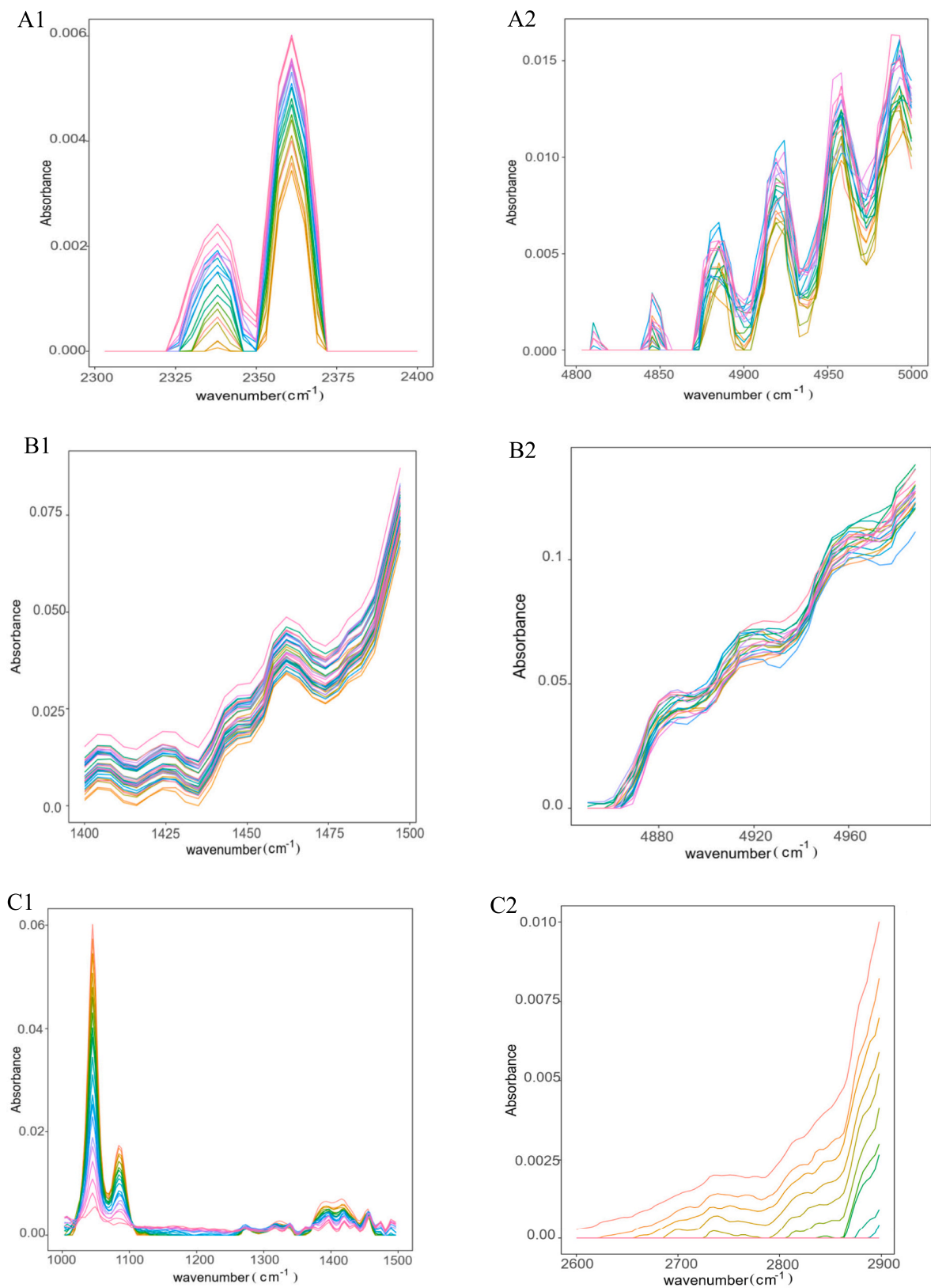


Fig. 2. Stacked FTIR spectra of 20 concentration gradients of six flavor compounds in 5% ethanol. A: Phenylethyl alcohol; B: Isopentyl alcohol; C: Ethyl caprylate; D: Isopentyl acetate; E: Ethyl caproate; F: Ethyl acetate. The numbers 1 and 2 represented FIRT maps of flavor compounds in different wavelength ranges.

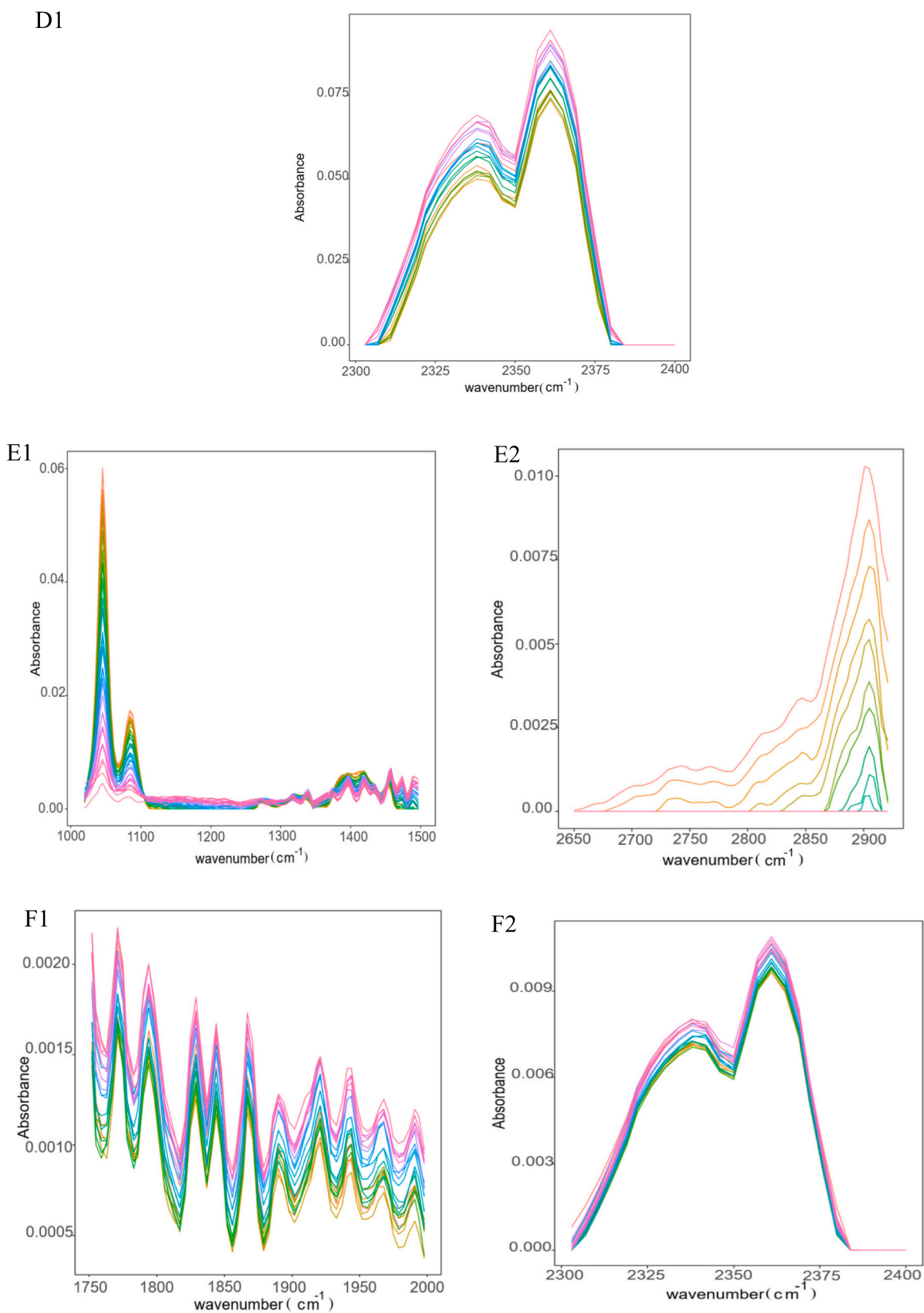


Fig. 2. (continued).

this study, the infrared spectral data corresponding to the filtered characteristic wave numbers were preprocessed in three different ways: smoothing, first-order derivative, and smoothing + first-order

derivative. The PLS model was established using the processed data. The determined coefficient (R^2) and RMSEP of the model are shown in Table S1. Higher R^2 values and lower RMSEPs were considered signs of



Fig. 3. PCA loading plot of six flavor compounds. A: Phenylethyl alcohol; B: Isopentyl alcohol; C: Ethyl caprylate; D: Isopentyl acetate; E: Ethyl caproate; F: Ethyl acetate.

the successful model prediction. Therefore, this experiment adopted the smoothing and the first-order derivative pretreatment methods.

The spectral data corresponding to the selected characteristic

wavelength of each flavor compound (40 samples: 20 concentrations, two in parallel) were randomly divided into an 80% training set and 20% test set after smoothing + first-order derivative pretreatment to

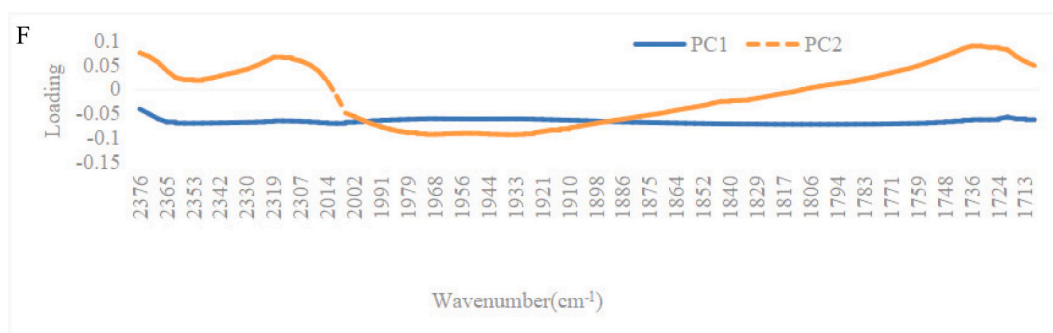


Fig. 3. (continued).

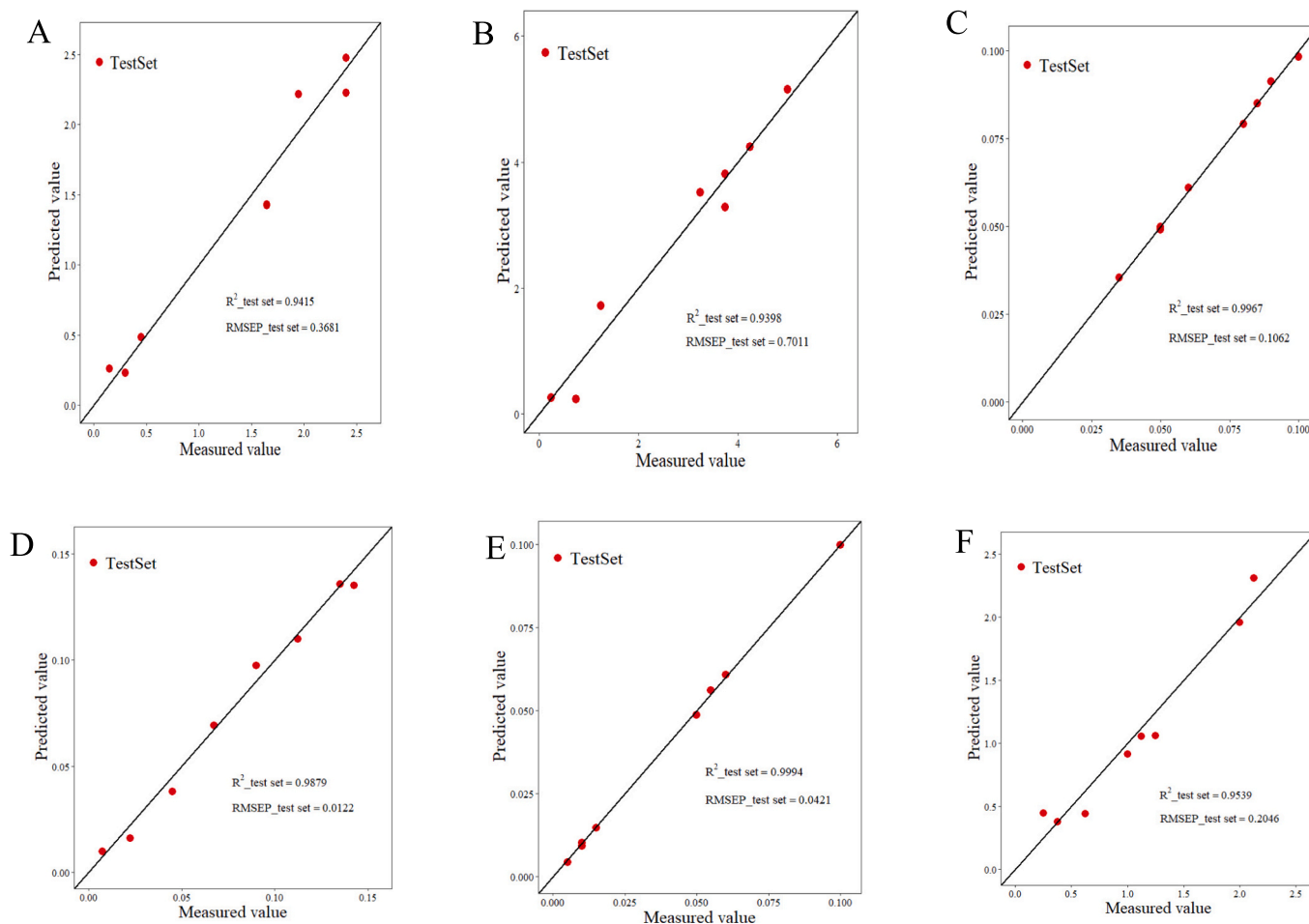


Fig. 4. Quantification models for the six flavor compounds using PLS. A: Phenylethyl alcohol; B: Isopentyl alcohol; C: Ethyl caprylate; D: Isopentyl acetate; E: Ethyl caproate; F: Ethyl acetate.

establish the final PLS model. A linear relationship was observed between the spectral data established using the PLS model of each flavor compound and the content of flavor compounds (Fig. 4). The R^2 value of each sample was 0.9398–0.9994, and the RMSEP was 0.012–0.0013. These results indicate that the prediction performance of the model is perfect.

3.3. Determination of six flavor compounds in three beer samples

The concentrations of six flavor compounds in three beer samples were detected using the PLS calibration model and GC–MS. The results are presented in Table 2. The relative standard error of the

concentrations of the six flavor compounds measured by the two detection methods was 1.38%–25.61%, suggesting the feasibility of the proposed method. Wang et al. (2020) used FTIR spectroscopy combined with machine learning methods to rapidly quantify the content of artificial sweeteners in beverages. The relative standard error between the results of their proposed method and the reference HPLC method was within the range of 2.52–11.01%. Further, Martins, Nascimento, Barbosa, and Barauna (2022) analyzed wheat protein content in wheat flour via FTIR spectroscopy. The predicted error range was 6–29%. These studies suggest that FTIR is a reliable method to rapidly detect the content of flavor compounds in beer.

Table 2

PLS calibration model and GC–MS were used to analyze and compare the contents of six flavor compounds in three beer samples.

Flavor compounds	PLS (mg L ⁻¹)		GC–MS (mg L ⁻¹)		RSE (%)
	Mean value	RSD	Mean value	RSD	
Sample 1					
Phenylethyl Alcohol	33.88	0.48	30.26	0.41	2.98
Isopentyl alcohol	56.12	0.47	48.42	0.55	1.38
Ethyl caprylate	1.25	0.06	1.01	0.05	24.67
Isopentyl acetate	13.62	0.09	11.34	0.08	20.18
Ethyl Caproate	3.71	0.07	3.12	0.05	19.27
Ethyl Acetate	12.54	0.14	14.06	0.12	-15.81
Sample 2					
Phenylethyl Alcohol	35.9	1.79	32.80	1.64	5.68
Isopentyl alcohol	58.34	2.92	50.60	2.53	5.55
Ethyl caprylate	2.59	0.01	2.18	0.0095	19.25
Isopentyl acetate	1.69	0.12	2.42	0.12	-22.54
Ethyl Caproate	3.83	0.0069	3.25	0.0075	17.89
Ethyl Acetate	17.48	0.87	15.20	0.76	15
Sample 3					
Phenylethyl Alcohol	32.66	1.63	28.70	1.44	-13.79
Isopentyl alcohol	55.02	2.75	43.80	2.19	25.61
Ethyl caprylate	6.24	0.026	5.2	0.024	20.17
Isopentyl acetate	1.12	0.045	0.91	0.036	23.32
Ethyl Caproate	5.67	0.019	4.52	0.018	25.61
Ethyl Acetate	14.46	0.50	13.12	0.66	10.25

4. Conclusions

In this study, we identified volatile compounds in 9 types of beer using GC–MS, and employed PCA analysis, ethyl caproate, phenylethyl alcohol, and ethyl caprylate with a contribution of >10% to beer differentiation were selected as key compounds to distinguish different beers. Our results highlight the feasibility of establishing a PLS quantification model for beer volatile compounds based on infrared spectrum data for the rapid and nondestructive detection of beer flavor compounds. The quantitative method proposed in this study was validated within a certain concentration of six volatile compounds in beer. The RSD value between the rapid quantitative method and the GC–MS for measuring the concentrations of six flavor compounds is 1.38–25.61%. In short, FTIR spectroscopy combined with machine learning is a promising tool to quantification of some volatile compounds in beer.

Ethical approval

This article does not contain any studies with human participants or animals performed by any of the authors.

Informed consent

Not applicable.

CRedit authorship contribution statement

Yi-Fang Gao: Writing – review & editing, Writing – original draft, Software. **Xiao-Yan Li:** Software, Data curation. **Qin-Ling Wang:** Investigation. **Zhong-Han Li:** Software. **Shi-Xin Chi:** Data curation. **Yan Dong:** Software. **Ling Guo:** Writing – review & editing, Supervision. **Ying-Hua Zhang:** Writing – review & editing, Supervision, Funding acquisition, Conceptualization.

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.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.fochx.2024.101300>.

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