Nondestructive detection of pungent and numbing compounds in spicy hotpot seasoning with hyperspectral imaging and machine learning

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Abstract

The levels of capsaicin (CAP) and hydroxy-α-sanshool (α-SOH) are crucial for evaluating the spiciness and numbing sensation in spicy hotpot seasoning. Although liquid chromatography can accurately measure these compounds, the method is invasive. This study aimed to utilize hyperspectral imaging (HSI) combined with machine learning for the nondestructive detection of CAP and α-SOH in hotpot seasoning. Spectral reflectance within the range of 370-1030 nm was used to develop regression models to predict CAP and α-SOH content. The results indicated that the PSO-BPNN model was optimal for predicting CAP (R^2 = 0.9942) and α-SOH (R^2 = 0.9939). Feature selection algorithms and tallow model experiments identified characteristic wavelengths for CAP (740-800 nm and 850-940 nm) and α-SOH (450-550 nm, 650-700 nm, 740-800 nm, and 850-940 nm). These findings demonstrated the potential of HSI for rapid, precise, and nondestructive assessment of CAP and α-SOH levels in hotpot seasoning.

Keywords: HSI; CAP; α-SOH; machine learning; hotpot seasoning; nondestructive detection

1 Introduction

In western China, particularly in regions like Sichuan and Chongqing, diverse spicy cuisines are renowned, especially hotpot, a traditional dish with a long history and famous for its distinctive numbing and pungent flavors (Zheng et al., 2020). Hotpot seasoning typically includes beef tallow, fermented broad bean paste, and a higher concentration of chilies and Szechuan pepper, creating a thicker, oilier, and more aromatic seasoning compared to other variations (Yu et al., 2023). The numbing and pungent flavors are primarily derived from chili peppers and Szechuan pepper (*Zanthoxylum bungeanum*), with capsaicin (CAP) from chili peppers responsible for the pungency and hydroxy-α-sanshool (α-SOH) from Szechuan pepper responsible for the numbing effect (Wang et al., 2023).

The levels of CAP and α-SOH vary across different origins and varieties of chili peppers and Szechuan pepper (Jiang et al., 2018; Wang et al., 2023), leading to varying degrees of pungency and numbness in hotpot seasoning products produced using the same process. Therefore, measuring CAP and α-SOH content in hotpot seasonings is essential to control these pungent and numbing flavors. Traditional methods for evaluating these two compounds are often invasive, time-consuming, and costly. Typically, CAP and α-SOH concentrations are measured using high-performance liquid chromatography (HPLC) (Duelund et al., 2017; Zhang et al., 2019). Alternatively, the total CAP and α-SOH content can be quantified using a spectrophotometric method based on the ultraviolet absorption of sample solutions at different wavelengths (González-Zamora et al., 2015; Zhang et al., 2021),

54 or α-SOH content alone can be screened using differential pulse voltammetry in Szechuan
55 pepper extract (Zhang et al., 2024). Although liquid chromatography offers greater accuracy,
56 the process is complex, impractical for field testing, and requires skilled laboratory personnel
57 (Jing et al., 2023). Moreover, spectrophotometry and differential pulse voltammetry may be
58 affected by other compounds, resulting in inaccurate measurements for target compounds.
59 Consequently, there is an urgent need for a rapid, nondestructive, and precise method to
60 quantitatively determine CAP and α-SOH that can be practically applied to the standardized
61 assessment of hotpot seasoning regarding their pungent and numbing flavors.

62 Hyperspectral imaging (HSI) is a modern method for assessing food quality (Aheto et al.,
63 2019). By combining conventional imaging with spectroscopy, HSI provides insights into the
64 chemical component levels and their spatial distribution within food products (Shi et al.,
65 2018). Unlike point-based fiber optic spectrometers, HSI technology captures spectral data
66 over a significantly larger sample area (Min et al., 2023). enabling the simultaneous analysis
67 of multiple samples. Previous research has demonstrated the effectiveness of HSI techniques
68 in assessing internal compound levels in chili and Szechuan peppers, including CAP and
69 water content in chili peppers (Jiang et al., 2018), as well as total alkylamides and volatile oil
70 content in Szechuan pepper (Tian et al., 2021). However, further research is needed to
71 explore HSI's potential for detecting CAP and α-SOH levels in the complex hotpot seasoning
72 system.

73 This study aims to assess the potential of HSI in conjunction with machine learning for

74 nondestructive detection of pungent and numbing flavor compounds in hotpot seasoning. The
75 primary research contents were as follows: (1) to develop regression prediction models for
76 CAP and α-SOH content based on the full wavelength bands (370-1030 nm); (2) to compare
77 the effectiveness of different feature selection algorithms in processing spectral data for
78 machine learning models; and (3) to obtain distribution maps of CAP and α-SOH within
79 hotpot seasoning.

80 **2 Materials and methods**

81 **2.1 Materials and chemicals**

82 Hotpot seasoning was prepared using beef tallow, garlic, ginger, dried chili peppers,
83 Szechuan pepper, grass fruits, cinnamon, star anise, cumin, corn oil, and broad bean paste. All
84 ingredients were purchased from the local market in Zhenjiang, Jiangsu Province. The
85 chemicals used in this study, including purified α-SOH (≥98 %) and CAP (≥98 %) were
86 purchased from Desite Biotech Co., Ltd. (Chengdu, China). Analytical grade methanol and
87 ethanol were supplied by Sinopharm Chemical Reagent Co., Ltd (China). Capsicum oleoresin
88 (CO), Szechuan pepper oleoresin (SPO) and Capsanthin (CS) were purchased from Chen
89 Guang Glory Biologicals Co., Ltd (Hebei, China), while an alkylamide-rich extract (ALE)
90 was supplied by Xiya Reagent Co., Ltd. (Shandong, China).

91 **2.2 Sample preparation**

92 2.2.1 Hotpot seasoning preparation

93 Spicy hotpot seasoning samples were collected at various processing stages throughout

94 production to analyze changes in CAP and α-SOH levels over time, aiding in the prediction
95 of the product's pungent and numbing flavors.

96 The preparation and conditions for making Szechuan-style spicy hotpot seasoning were
97 as follows: first, 5 kg of dried chili peppers were sliced into 5 cm sections, then boiled in
98 water at a 1:3 ratio for 5 minutes with continuous stirring. After boiling, the peppers were
99 drained to remove surface moisture. Next, 20 kg of beef tallow was added to a cooking pot
100 and heated to 150 ± 5 ℃ over 15 minutes. Then, 5 kg of corn oil was added, and stirred for 5
101 minutes, and 5 kg of broad bean paste was incorporated. The drained chili peppers were then
102 added to the preheated beef tallow and fried at 150 ℃ for 15 minutes, with continuous
103 stirring. Mixed spices were added and heated in the pot for another 10 minutes. To obtain the
104 hotpot seasoning samples with varying spiciness, samples were collected from the pot every
105 10 minutes, three times in total. Following this, 1 kg of Szechuan pepper was added, and
106 additional samples were taken every 10 minutes to analyze numbing levels, again 3 times in
107 total. This sampling process is shown in Fig. 1a. Ultimately, 360 hotpot seasoning samples
108 were collected during 6 processing stages, with all samples stored at 0 ℃ to preserve their
109 original characteristics for further analysis.

110 2.2.2 Tallow model

111 The numbing and pungent extracts (e.g., CO, SPO, and CS) were individually dissolved
112 into melted tallow with various concentrations of 20 g/kg, 60 g/kg, and 100 g/kg. The
113 changes in peak intensity from the hyperspectral curves of tallow with these pungent extracts

indicated specific wavelengths associated with the numbing and pungent substances.

2.3 Hyperspectral imaging system and image acquisition

2.3.1 Hyperspectral Imaging System

In this study, an HSI system was used to acquire hyperspectral images of the samples. The system consisted of a halogen light source (150 W), a hyperspectral imager, and a carrier platform, as shown in Fig. S1a. This line-scanning instrument allowed for dynamic scanning of samples while in motion beneath a stationary camera. Hyperspectral images were captured using the camera (IOC V10E-sCMOS, Isuzu Optics, Taiwan, China). Each pixel contained a complete spectrum within the range of 370–1030 nm with a spectral resolution of 2.8 nm, recording 616 spectral bands with a sampling interval of 1.83 nm. To minimize the influence of natural light, the experiment was conducted in a dark room, using only the HSI system's halogen bulbs.

2.3.2 Hyperspectral Image Acquisition

The petri dish containing the hotpot seasoning was placed on the platform for data collection after setting the relevant parameters, with the platform moving at a speed of 2.58 cm/s. The HSI system was calibrated before data collection to minimize image noise caused by dark current effects on the camera and other environmental factors (ElMasry et al., 2016). To obtain a black calibration image (0% reflectance), the camera lens was covered with a black lid, while a white Teflon board was used to obtain a white calibration image (99% reflectance) (Shi et al., 2022). The hyperspectral images were then calibrated using the

following equation (1):

$$I_c = \frac{I_r - I_b}{I_w - I_b} \quad (1)$$

where I_c represents the calibrated hyperspectral image, I_r is the raw hyperspectral image, I_b is the black reference hyperspectral image, and I_w is the white reference hyperspectral image (Feng et al., 2018; He et al., 2022).

2.4 Determination of CAP and α-SOH using HPLC

Standard solutions of CAP and α-SOH were prepared in ethanol with concentrations of 0.1 mg/L, 1 mg/L, 10 mg/L, 20 mg/L, 40 mg/L, 80 mg/L, and 100 mg/L, based on the purity of CAP and α-SOH standards to plot standard curves.

Ultrasonic extraction of hotpot seasoning with ethanol was used to effectively capture most of the active flavor components, including pungent and numbing substances (Zhang et al., 2023). Following hyperspectral imaging, the entire 20 g of hotpot seasoning from each petri dish was transferred to a 100 mL centrifuge tube. Subsequently, 30 mL of ethanol was added to the tube, and the mixture was sonicated for 30 minutes before, then centrifuged at 8000 rpm/min for 15 min to collect the supernatant. The remaining residue was re-sonicated in 20 mL of ethanol for 15 minutes, after which the supernatant was collected again. The collected supernatant was transferred to a round-bottomed flask and concentrated in a water bath at 45°C for 1 hour, after which ethanol was added to adjust the final volume to 4 mL, completing the extraction process of hotpot seasoning.

Concentrations of CAP and α-SOH were determined using HPLC (LC-20AT,

SHIMADZU, JP) equipped with an autosampler and UV-vis detector. Both standard solutions and hotpot seasoning extracts were filtered through a 0.22 μm organic filter membrane. The chromatographic separation was achieved using a Sepax HP-C18 (250 × 4.6 mm, 5 μm) with an isocratic mobile phase of deionized water and methanol (35:65, v/v) at a flow rate of 1 mL/min for isocratic elution. The sample auto-injection volume was 20 μL, and chromatographic separation was conducted at a column temperature maintained at 30 ℃.

2.5 Spectral extraction and pre-processing

2.5.1 Spectral data extraction

The HSI system captured data from both the sample and the background, making it necessary to limit the region of interest (ROI) to the entire area of the hotpot seasoning area. Spectral reflectance data of the hotpot seasoning and background were extracted from the calibrated hyperspectral image using ENVI 5.1 software. To eliminate background influence, image segmentation was applied to isolate the ROI from the background. A grayscale image was used to generate a mask image, which was subsequently applied to the hyperspectral image to separate the hotpot seasoning without spices. The final average spectrum for each sample was derived by averaging all pixels within the ROI. Fig. S1b presents a schematic diagram of the workflow. This procedure was applied to all hyperspectral images of the hotpot seasoning, resulting in a spectral matrix with dimensions of 360×616 (360 samples, each containing 616 spectral bands).

2.5.2 Spectral data preprocessing and division

During hyperspectral image acquisition with the HSI system, factors such as spectral response, instrument noise, uneven light source intensity, baseline drift, and grating scattering were unavoidable and could impact modeling accuracy (Zhang et al., 2022). Therefore, preprocessing the spectral data was necessary to enhance relevant spectral information and improve model performance. The Savitzky-Golay (SG) smoothing method was applied to reduce high-frequency noise by averaging several data points (Cheng et al., 2023). Subsequently, multiplicative scatter correction (MSC) and standard normal variate (SNV) were applied to correct spectral scattering (Jia et al., 2017). Additional preprocessing techniques, including min-max scaler (MMS), mean centering (MC), detrending (DT), wavelet transform (WAVE), as well as 1st and 2nd derivative methods, were applied to the spectral data.

After preprocessing, the corresponding concentrations of CAP and α-SOH for each sample were appended to the latter columns of the spectral matrix. The resulting dataset was divided into variables (X) and labels (y), where X included columns 1 to 616 (spectral data) and y included columns 617 and 618 (concentrations). The dataset was randomly shuffled using a uniform distribution before splitting into a calibration set and a prediction set in a 4:1 ratio, resulting in 228 samples for calibration and 74 for prediction. This data processing procedure was conducted using Python 3.10.

2.6 Feature wavelength selection

Although hyperspectral data contains extensive information, much of it is redundant and

exhibits multicollinearity, complicating analysis (Qiao et al., 2022). To address these problems, feature selection algorithms were employed to identify the characteristic wavelengths associated with target chemical compounds. To compare the performance of different feature selection algorithms, the successive projection algorithm (SPA), competitive adaptive reweighted sampling algorithm (CARS), and random frog algorithm (RF) were utilized to select optimal wavelengths.

The SPA method, a feed-forward feature selection algorithm, uses a stepwise iterative process to select the most correlated wavelength in each round, ultimately determining optimal wavelengths with minimal redundancy and collinearity (Xiong et al., 2024). The CARS method, based on the Darwinian concept of "survival of the fittest", is a variable selection algorithm that combines Monte Carlo sampling with regression coefficients from partial least squares regression (PLSR) (Li et al., 2009). Lastly, the RF algorithm iteratively calculates the spectral variable matrix X and target variable matrix y to obtain the average probability value for each variable, which serves as an evaluation index for variable importance (Li et al., 2012).

2.7 Model construction and evaluation

2.7.1 Partial least squares regression

Partial least squares regression (PLSR), a commonly used method in chemometrics analysis, combines principal component analysis to facilitate data analysis (Zhang et al., 2023). Following principal component analysis on the raw spectral data, PLSR constructs a

prediction model using the dimensionality-reduced data as variables and the concentrations as response values. To determine the optimal number of principal components, cross-validation was performed on the calibration set. The number of potential factors that yielded the minimum root mean square error of cross-validation was selected as the optimal number of principal components.

2.7.2 Support vector regression

Support vector regression (SVR), a branch of support vector machine (SVM), is widely used for quantitative concentration prediction (Leng et al., 2021). Selecting an appropriate kernel function is crucial for SVR, with common options including the linear kernel, polynomial kernel, and radial basis function. The model's optimization objective is to minimize total loss while maximizing the margin for optimal performance. Given that the spectral reflectance of hotpot seasoning is not linearly related to the concentrations of CAP and α-SOH, a nonlinear analytical method is more suitable for this study. Therefore, a polynomial kernel was selected as the kernel function. Additionally, setting the optimal penalty factor C and kernel function parameter γ is necessary for effective SVR. To achieve this, grid search combined with cross-validation was used

2.7.3 Back propagation neural network

Back propagation neural network (BPNN) is a highly effective feed-forward network based on error backpropagation. During BPNN training, the first layer of neurons serves as the input layer to receive spectral data, and each layer's output is used as input for the next

234 layer. The final layer, or output layer, provides the network's predictions. In this study, the
235 input layer contained the same number of neurons as the spectral feature dimensions, the
236 hidden layer included 10 neurons, and the output layer contained 2 neurons.

237 Although BPNN has proven to be a valuable deep-learning algorithm in chemometrics,
238 it requires further optimization. Random initialization of connection weights can lead to
239 variability in BPNN predictions, and gradient descent training may converge slowly or get
240 trapped in local minima with multidimensional spectral data. Particle swarm optimization
241 (PSO) addresses these issues by simulating individual particles within a "swarm" (analogous
242 to a flock of birds) with attributes of velocity and position (Jin et al., 2012). In this study,
243 PSO was used to optimize the initial algorithm for BPNN, producing the optimal PSO-BPNN
244 model.

245 2.7.4 Evaluation of model performance

246 To evaluate the performance of the regression models, various evaluation indexes were
247 employed to assess the three models (PLSR, SVM, PSO-BPNN). A well-performing
248 regression model is indicated by a lower root mean square error (RMSE), ideally approaching
249 0, and a higher coefficient of determination (R^2) close to 1 (Sun et al., 2024). Moreover, the
250 relative percent deviation (RPD) served as an indicator of predictive performance. An RPD
251 below 1.5 signifies an unreliable model, while an RPD between 1.5 and 2.0 indicates
252 moderate reliability, and an RPD above 2.0 denotes high reliability (Bai et al., 2024). The
253 prediction model with the highest stability and accuracy was selected based on these

evaluation indexes. In addition, the above indicators were calculated using equations (2), (3), and (4) respectively.

$$RMSE = \sqrt{\frac{1}{n}\Sigma_{i=1}^{n}(y_i - \hat{y}_i)^2} \quad (2)$$

$$R^2 = 1 - \frac{\Sigma_{i=1}^{n}(y_i - \hat{y}_i)^2}{\Sigma_{i=1}^{n}(y_i - \bar{y})^2} \quad (3)$$

$$RPD = \frac{\sqrt{\frac{1}{n-1}\Sigma_{i=1}^{n}(y_i - \bar{y})^2}}{RMSE} \quad (4)$$

Where n is the total number of samples, y_i represents the measured value of sample i, and $\hat{y}_i$ is the predicted target value, $\bar{y}$ is the mean value of all samples.

2.8 Chemical information visualization

Each pixel in the hyperspectral image contains spectral information that can be used to predict the target compounds through the established regression model. With the focus on the target areas, the hyperspectral image of hotpot seasoning was masked to isolate the ROI. The spectral data of all pixels were preprocessed, and effective wavelengths were used to predict CAP and α-SOH concentrations. Grayscale images were then generated to represent the distribution of these compounds based on the predicted values. Finally, pseudo-color images were synthesized to visualize the spatial distributions of CAP and α-SOH within hotpot seasoning.

2.9 Software

Data analysis and model construction were conducted using four software tools: ENVI 5.6, Origin 2018, Visual Studio Code 2022, and Python 3.10. ENVI 5.6 was used to extract spectral data from regions of interest within the hotpot seasoning. Origin 2018 was utilized

for processing HPLC data and plotting chromatograms. Visual Studio Code 2022 facilitated data preprocessing, feature wavelength selection, regression model construction, and visualization of chemical information. All programming tasks were conducted using Python 3.10.

3 Results and discussion

3.1 Reference concentrations of CAP and α-SOH

This study collected a total of 360 hotpot seasoning samples at intervals of 10, 20, 30, 40, 50, and 60 min. during processing. Fig. 1b and Fig. 1c demonstrate the HPLC graphs and average concentrations of CAP and α-SOH in samples from each time point. Based on the HPLC profiles of purified CAP and α-SOH the retention times were 25.7 minutes for CAP and 28.0 minutes FOR α-SOH. As the simmering time increased, CAP was continuously released from the chili peppers, leading to a gradual increase in CAP concentration. Samples collected at 10, 20, 30, 40, 50, and 60 minutes were labeled as S10, S20, S30, S40, S50, and S60, respectively, as presented in Fig. 1c. The CAP concentrations ranked as follows: S60 (0.62 ± 0.00 mg/g) > S50 (0.37 ± 0.01 mg/g) > S40 (0.33 ± 0.00 mg/g) > S30 (0.28 ± 0.01 mg/g) > S20 (0.26 ± 0.00 mg/g) > S10 (0.23 ± 0.00 mg/g). When evaluating the numbness of the hotpot seasoning samples, they were ranked as follows: S60 (0.25 ± 0.00 mg/g) > S50 (0.11 ± 0.01 mg/g) > S40 (0.07 ± 0.01 mg/g) > S30 (0.00 ± 0.00 mg/g) = S20 (0.00 ± 0.00 mg/g) = S10 (0.00 ± 0.00 mg/g). The hotpot seasoning samples S10, S20, and S30 did not contain α-SOH because Szechuan pepper was not yet added. According to the average

concentrations of hotpot seasoning samples S40, S50, and S60, α-SOH was gradually released from the Szechuan pepper as heating time increased.

3.2 Dataset construction and description

The dataset was randomly selected based on a uniform distribution and divided into 288 calibration samples and 72 prediction samples at a 4:1 radio. Table S1 presents the ranges, means, and standard deviation of CAP and α-SOH in both the calibration and prediction sets. According to Table S1, the hotpot seasoning samples exhibited considerable variability in CAP content, with a difference of 0.4125 mg/g between the maximum and minimum values. The mean CAP values for the calibration and prediction sets were 0.3501 mg/g and 0.3359 mg/g, respectively, showing no significant difference. The standard deviation was 0.1319 mg/g in the calibration set and 0.1163 mg/g in the prediction set. The α-SOH was not detected in the hotpot seasoning samples collected at 10, 20, and 30 min as shown in Fig. 1b and Fig. 1c resulting in a minimum α-SOH content of 0 mg/g in the total set, with a maximum difference of 0.2501 mg/g. The average α-SOH value in the calibration set was 0.7320 mg/g, slightly higher than the prediction set at 0.6310 mg/g. The standard deviations for α-SOH were 0.9050 mg/g in the calibration set and 0.8270 mg/g in the prediction set.

Both CAP and α-SOH exhibited wider data distributions of data in the calibration set compared to the prediction set, ensuring a reasonable data distribution for modeling after random shuffling and uniform sample division.

3.3 Regression models based on the overall spectral for CAP and α-SOH

The raw spectral curves extracted from hyperspectral images of hotpot seasoning samples, shown in Fig. 1d, displayed a consistent trend within the effective range of 370-1030 nm. Three distinct absorption peaks were observed at 665 nm, 757 nm, and 927 nm, with an additional relatively flat peak at 839 nm. The wavelengths around 665 nm fall within the red range of the visible spectrum, where certain pigment molecules absorb light energy (Li et al., 2023).

Preprocessing the original spectral data was essential to eliminate interference from factors such as background noise and light scattering. In this study, the methods described in Section 2.4.1 were applied to optimize original data. PLSR, SVR, and PSO-BPNN models were then constructed to predict CAP and α-SOH, each showing varying performance when combined with different pretreatment methods. Model performance was evaluated using R^2, RMSE, and RPD. The spectral curves following various pretreatments are shown in Fig. S2, while the average raw spectral curves of hotpot seasoning sampled at 6 different times are shown in Fig. S2a. Notably, most pretreatments preserved the differences in the original spectral curves of different samples at the absorption peaks, except for the SG+2nd derivative method.

3.3.1 Prediction based on PLSR

The original spectral data were used to construct the PLSR model, and its performance was compared with datasets preprocessed using 9 different methods. In all datasets, the 616 columns of spectral data were assigned to matrix X, while matrices comprising CAP and α-

SOH concentrations were assigned to variable y. The PLSR model was employed to capture the intricate relationship between spectral data X and concentration data y for quantitative prediction.

Table 1 demonstrates the prediction results using different preprocessed spectral datasets, showing that different pretreatment methods impacted PLSR prediction results. As smoothing the raw spectral curves using the SG method improved the PLSR predictions for CAP and α-SOH, further preprocessing was based on SG-smoothed spectral data. All preprocessing methods yielded satisfactory predictions, except for the 2nd derivative method.

For CAP predicting, the DT, WAVE, SNV, MMS, and MC methods improved the model performance. However, for α-SOH concentration prediction, the SNV method did not yield enhancements compared to the raw spectral data. The DT, WAVE, MMS, and MC methods improved the R^2 of PLSR on both the validation and prediction sets. Considering the overall prediction performance, DT was ultimately selected as the most suitable data preprocessing method for PLSR, achieving R^2 values above 0.98 for both CAP and α-SOH.

3.3.2 Prediction based on SVR

The SVR model was constructed to assess its performance across various preprocessing methods. To determine the most suitable kernel function, different functions were tested on the original spectral data, with the polynomial kernel ultimately selected for SVR. Cross-validation and grid search were employed to identify optimal values for C and γ, enhancing model performance.

According to Table 1, data processing with the 2nd derivative yielded the poorest prediction in the SVR model, likely due to reduced variation across samples, as shown in Fig. S2c. The WAVE and MC methods enhanced the predictive capability of the SVR model, as reflected by higher RPD values for CAP and α-SOH compared to the original spectral data. In contrast, the 1st derivative reduced the SVR predictive capability in both CAP and α-SOH, while the MSC and SNV methods did not contribute to the optimization. The DT method enhanced the prediction only for α-SOH, while MMS exclusively improved CAP predictions. Although the SVR model with the WAVE method predicted CAP slightly less effectively than MC, it performed better for α-SOH prediction. Considering overall results for both CAP and α-SOH, the WAVE method was identified as the most suitable preprocessing approach for SVR.

3.3.3 Prediction based on PSO-BPNN

The PSO-BPNN model consists of one or more hidden layers, enabling it to effectively model complex data and efficiently search for optimal solutions (Lei et al., 2022). In this study, a BPNN with ten hidden-layer networks was established to analyze the relationship between spectral data and the measured values of CAP and α-SOH, with the initial weights and thresholds optimized using the PSO algorithm.

Table 2 shows the PSO-BPNN prediction results for CAP and α-SOH using various spectral preprocessing methods. Due to its superior modeling capabilities, PSO-BPNN outperformed both PLSR and SVR overall. The PSO-BPNN constructed in this study

achieved its best performance in predicting CAP when combined with the SNV method, yielding an R^2 value of 0.9953, an RMSE value of 0.0080, and the highest RPD of 10.3345 on the prediction set. However, for α-SOH, the best preprocessing method was MSC, resulting in an R^2 value of 0.9944, an RMSE value of 0.0065, and an RPD of 9.4933 on the prediction set. Thus, while SNV was ideal for predicting CAP, MSC was more suitable for predicting α-SOH. To select a method for simultaneous prediction of CAP and α-SOH, both sets of model results were considered, with MMS emerging as the most suitable method, as it achieved RPD values above nine for both CAP and α-SOH.

Fig. S3 presents scatter plots for the MMS-PSO-BPNN model, comparing the true CAP and α-SOH content measured by HPLC with the predicted values for the calibration and prediction sets. In Fig. S3a, the scatter plot of CAP shows blue dots for the calibration and prediction results, with points evenly distributed around the y=x line, indicating minimal deviation in the prediction results. Meanwhile, the points in the plot were divided into six regions corresponding to CAP levels in the hotpot seasoning samples collected at six separate times. The scatter plot of α-SOH in Fig. S3b indicates a strong correlation between predicted and measured values. The 180 samples from the first three collection times lack α-SOH, resulting in true values of 0. The model accuracy predicted samples from the first three time points with very low values below 0.02 mg/g, clearly distinguishing them from samples containing α-SOH.

3.4 Feature wavelengths screened by selection algorithms

Three different feature selection algorithms (CARS, RF, and SPA) were used for spectral data of hotpot seasoning.

3.4.1 CARS

In the CARS method for selecting feature wavelengths, Monte Carlo sampling was set to 100 iterations and 10-fold cross-validation was employed to determine the minimum number of latent variables based on the root mean square error of cross-validation (RMSECV). Fig. S4a(1) illustrates the number of sampled variables in each sampling. Fig. S4a(2) depicts the trend in RMSECV values across iterations, and Fig. S4a(3) shows the regression coefficients of each variable. The blue vertical dashed line in Fig. S4a(3) indicates the sampling iteration with the minimum RMSECV.

The final set of 48 selected feature wavelengths is shown in Fig. 2a and detailed in Table S2. The characteristic wavelengths screened by CARS were distributed in the ranges of 450-550 nm, 650-700 nm, 740-800 nm, and 850-940 nm.

3.4.2 RF

The RF algorithm was used to extract feature wavelengths, calculating the average selection probability for each wavelength, as displayed in Fig. S4b. Based on the RF results, the top 30 wavelengths with the highest average selection probabilities were chosen as feature wavelengths, marked by red dots in Fig. S4b. Unlike the CARS and RF algorithms, the SPA algorithm did not rely on the measured values of CAP and α-SOH for feature selection. Its primary objective is to identify wavelength combinations containing minimal

redundancy and reduced covariance, based solely on raw spectral data (Wang et al., 2022).

As shown in Fig. 2b and detailed in Table S2, the distribution of the 30 feature wavelengths selected by the RF algorithm were mainly distributed in the ranges of 450-560 nm, 650-695 nm, 740-800 nm, and 850-930 nm, which closely align with the feature wavelengths revealed by the CARS method.

3.4.3 SPA

The feature variables selected by SPA showed a more concentrated distribution overall, identifying variables near the prominent absorption peaks at 665 nm and 927 nm. However, no feature variables were selected in the range of 700-850 nm, despite the presence of two inconspicuous absorption peaks within this range. Moreover, a significant number of feature variables were concentrated in the visible range of 550-600 nm, whereas the CARS and RF methods exhibited few variables in this range.

The feature wavelengths selected by SPA were distributed around absorption peaks in the ranges of 570-600 nm, 660-670 nm, 920-930 nm, and 1020-1030 nm, as shown in Fig. 2c and detailed in Table S2. This differs from the characteristic wavelengths selected by CARS and RF, possibly SPA is an unsupervised variable selection method, resulting in more clustered feature wavelengths.

3.5 Feature wavelengths validation through tallow model experiments

A tallow model simulating hotpot seasoning was constructed by dissolving the numbing and pungent substances in the tallow. By measuring the characteristic absorption peaks of

these substances in the model, it was verified whether the characteristic wavelengths selected by the algorithms corresponded to the numbing and pungent substance. Fig. 2d depicts the reflectance curves of tallow before and after adding different CO concentrations. Notable increases in absorption peak intensity were observed at 400–550 nm, 635–700 nm and 850–950 nm as CO concentration increased, with a moderate increase seen at 735–800 nm. The spectral curve of pure CAP, shown in the inset, displays prominent absorption peaks at 735-800 nm, 850-950 nm, and 970-1000 nm. Accordingly, the variation in absorption peak intensity in the tallow model at 735–800 nm and 850–950 nm can be attributed to the presence of CAP, suggesting that CAP's characteristic absorption peaks in hotpot seasoning are within these ranges of 735–800 nm and 850–950 nm, which is consistent with feature wavelength selected by the CARS and RF algorithms.

The differences in the absorption peak intensity within the visible range of 400–550 nm and 635–700 nm may be attributed to capsanthin in CO. Previous studies reported that capsanthin, a type of carotenoid, exhibits strong light absorption range in the 400-500 nm range, and the visible range near 680 nm is useful for the quantification of total carotenoids (Ignat et al., 2013; J. Li et al., 2024). The spectra of tallow with different concentration gradients of capsanthin (CS) are shown in Fig. 2e, demonstrating increased peak intensity at 400-550 nm and 635-700 nm as CS concentration in the tallow increased. Therefore, the variability in peak intensity within ranges at 400-550 nm and 635-700 nm is primarily due to the CS. During hotpot seasoning processing, CS content may increase as CAP was

continuously released from chili peppers, making CS-related wavelengths beneficial for machine learning models in predicting CAP content.

On the other hand, Fig. 2f demonstrated the average spectrum of tallow with added SPO, revealing that tallow with increasing SPO concentrations exhibits higher peak intensities at 380–470 nm, 520–555 nm, 590–625 nm, and 630–690 nm. The inset shows the spectrum of ALE, with strong absorption peaks at 410 nm and 670 nm, and moderate absorption peaks at 530nm, 605nm, and 955nm. This increase in absorption peak intensification in the tallow spectrum with added SPO is attributed to the presence of alkylamides, indicating that α-SOH characteristic peak in hotpot seasoning falls within the four feature wavelength segments identified by the CARS and RF algorithms.

3.6 Regression model performance

Table 3 presents the modeling results of the three different feature wavelength selection methods. Although SPA's prediction performance for CAP and α-SOH was inferior to CARS and RF in both PLSR and SVR models, it showed improved prediction accuracy compared to the PLSR model built with all wavelengths. In the PLSR model, CARS provided superior results for CAP prediction, while RF was more effective for α-SOH prediction. Nonetheless, prediction accuracy slightly decreased after screening feature wavelengths using these three feature selection methods compared to the SVR model built with a full wavelength set. Scatter plots of the CAP and α-SOH predictions in the PLSR model are depicted in Fig. 3, demonstrating a high linear correlation in predicting CAP and α-SOH content.

Selecting an optimal model to predict CAP and α-SOH content is essential after comparing the performance of different feature selection algorithms for regression analysis. Therefore, the effectiveness of PLSR, SVR, and PSO-BPNN in analyzing spectral data of hotpot seasoning was evaluated. Unlike traditional models, the deep learning model PSO-BPNN model can automatically learn the most useful feature variables without manual feature extraction, using full-band spectral data as input (Xiong et al., 2024). Therefore, feature extraction methods were not applied in the PSO-BPNN model.

A comparison of the data in Table 1 and Table 3 reveals that the PLSR model outperforms in predicting CAP and α-SOH. When combined with DT and CARS, the PLSR model achieved an optimal R^2 value of 0.9868, an RMSE value of 0.0338, and an RPD value of 8.8351 for the CAP prediction set. For α-SOH prediction, the PLSR model attained an optimal R^2 value of 0.9856 with the RF feature selection algorithm, corresponding with RMSE and RPD values of 0.0399 and 8.3275, respectively. In contrast, Table 2 reveals that PSO-BPNN achieved R^2 values exceeding 0.99 on the prediction set for CAP when combined with different preprocessing methods to predict CAP, except the 1st and 2nd derivative methods. The combination of the MSC method yielded the best results in predicting α-SOH in the prediction set, with the highest R^2 value of 0.9944, RMSE value of 0.0065, and RPD value of 9.400. Overall, PSO-BPNN outperformed traditional machine learning methods for predicting CAP and α-SOH in hotpot seasoning. Traditional machine learning models often require extensive manual preprocessing and feature selection steps, which might limit the

model from achieving optimal predictive results (Singh et al., 2021). In contrast, PSO-BPNN benefits from powerful nonlinear capabilities, with the PSO algorithm optimizing the initial weights of the neural network to better analyze the relationship between spectral data and the measured CAP and α-SOH values.

3.7 Visualization map for CAP and α-SOH

Based on previous analysis, the PSO-BPNN model combined with the MMS method was identified as the optimal approach for detecting the CAP and α-SOH content in hotpot seasoning. First, spectral information from all pixel points was extracted from the hyperspectral image of the hotpot seasoning, generating a grayscale map, as depicted in Fig. 4a. Subsequently, a mask file was then created, as illustrated in Fig. 4b and compared with the original hyperspectral image to identify the ROI. The raw spectral data within the ROI was subsequently processed using MMS and fed into the trained model to calculate the CAP and α-SOH values for each pixel. To visualize the distribution of CAP and α-SOH in the hotpot seasoning, the model-generated concentrations for CAP and α-SOH were calculated to create grayscale distribution maps, as shown in Fig. 4c and Fig. 4d. Pseudo-colored images in Fig. 4e and Fig. 4f further illustrate the spatial distribution of CAP and α-SOH. The overall distribution of both CAP and α-SOH was uniform, reflecting the homogeneity of the hotpot seasoning, though α-SOH was more concentrated in the central region and higher near the Szechuan pepper. In summary, compared to traditional detection methods, HSI technology provides an intuitive means of detecting CAP and α-SOH distribution in hotpot seasoning,

offering a new technical reference for quality evaluation and product quality control.

4 Conclusions

This study utilized hyperspectral imaging (HIS) technology to analyze CAP and α-SOH content in hotpot seasoning, leveraging the abundant spectral information provided. The predictive performance of two conventional machine learning models (PLSR and SVR), along with different feature selection algorithms, was assessed for CAP and α-SOH content. Although both models demonstrated high reliability, PLSR outperformed SVR. Additionally, the study also investigated the feasibility of applying deep learning to analyze the spectral data of hotpot seasoning. The results indicated that the PSO-BPNN method was optimal for predicting CAP and α-SOH. Different preprocessing methods were tested in the PSO-BPNN model to optimize prediction outcomes, with the MMS method ultimately selected for its ability to improve regression model performance for both CAP and α-SOH. The model demonstrated high reliability, achieving an R^2 value of 0.9942, an RMSE value of 0.0092, and an RPD value of 9.3741 for CAP, and an R^2 value of 0.9939, RMSE value of 0.0068, and RPD value of 9.0678 in the α-SOH prediction set.

Additionally, feature selection algorithms and the tallow model were used to identify the characteristic wavelengths of CAP and α-SOH. CAP's feature wavelengths were identified in the ranges of 740-800 nm and 850-940 nm, while α-SOH feature wavelengths were within 450-550 nm, 650-700 nm, 740-800 nm, and 850-940 nm. The pseudo-color distribution images of CAP and α-SOH effectively depict the distribution of these two compounds in

hotpot seasoning. The results of this study provide a theoretical foundation for the online monitoring of CAP and α-SOH content in hotpot seasoning.

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