Determination of monosodium glutamate concentration based on Fourier mid-infrared spectroscopy

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ABSTRACT Monosodium glutamate plays an important role in contributing to the umami taste of food. The feasibility of detecting MSG concentration in simple solutions based on mid-infrared spectroscopy was evaluated in this study. Samples (n=144) with different concentration gradients from different batches were prepared and their spectral data were collected. The original and the pre-processed data were analyzed, which both full-wavelength and simplified models for predicting sodium glutamate (MSG) solution were established by employing partial least squares regression (PLSR). The results showed that the root mean squared errors and coefficients of determination of the full-wavelength PLSR model were 1.10mmol/L and 0.98 as well as 1.60mmol/L and 0.95 for cross-validation and prediction, respectively. In addition, a simplified PLSR model based on the uninformative variables elimination method and the competitive adaptive weighting algorithm (UVE-CARS) was developed, where 10 wavelengths were utilized. The root mean squared errors of 0.93 and 1.40mmol/L and coefficients of determination of 0.98 and 0.96 for cross validation and prediction were attained, respectively. The performance of the simplified model was better than that of the full-wavelength PLSR model, and the detection limit of the obtained simplified model was 2.7mmol/L. Therefore, it was shown that it was feasible to use mid-infrared spectroscopy(MIRS) for fast and non-destructive detection of monosodium glutamate concentration and it also testified the ability of mid-infrared spectroscopy in detecting low concentrated analytes.

Keywords: Mid-infrared spectroscopy; Monosodium glutamate; Partial least squares regression; Simplified model; Detection limit.

INTRODUCTION With the development of social economy and the improvement of cooking technology, people's taste has become more and more picky, Therefore, it is important to evaluate the umami taste of food. According to the research, the main umami substances in food includes amino acids, nucleotides and organic acids (Zhang N L et al., 2019). Among them, sodium glutamate has the most obvious umami taste, which can be used as a representative umami amino acid (Yamaguchi S et al., 2000; Kong Y et al., 2018; Phat C et al., 2016). Existing methods for the detection of sodium glutamate includes non-aqueous titration, pH meter, polarimetry, etc (Ferreira C P et al., 2020). Although these methods have high accuracy, some are expensive, some are cumbersome, and these methods require damaged samples. Therefore, it is very important to develop a new efficient, fast and non-destructive detection method. Mid-IR (MIR) spectroscopy is an emerging detection technology, which use the interaction between light and matter to obtain characteristic information. Compared with chemical measurement methods, infrared spectroscopy has the advantages of high efficiency, fastness, non-destructiveness, and online detection. At present, MIR has been widely used in the field of quantitative detection.

Based on previous studies, this paper explored the feasibility of using mid-infrared spectroscopy to detect the concentration of sodium glutamate solution, so as to provide a feasible basis for the detection of complex umami substances in food.

MATERIALS AND METHODS

Experimental materials and equipment The sample used in the experiment was monosodium glutamate (MSG) purchased from Shanghai Yuanye Biotechnology Co., Ltd, with a purity of 99%, and they were stored at 4℃. Thermo Scientific Nicolet IS50 Fourier transform infrared (FT-IR) spectrometer, with scanning range of 400cm^{-1}~4000cm^{-1}, and spectral resolution 4cm^{-1}, were employed for spectral acquisition.

Sample preparation and data collection The experiment was performed in three batches. The first batch was configured with monosodium glutamate solutions with concentrations of 0.8, 1.6, 3.2, 4.8, 6.4, 8, 9.6, 11.2, 14.4, 17.6, 20.8, and 24mmol/L, respectively. , resulting in a total of 48 samples. After repeating twice in different days, a total of 144 samples were obtained, Prepared for spectrum collection.

DATA DIVISION In this paper, 96 samples from the first two batches were used as the training set, 48 samples from the third batch as the prediction set.

MODEL EVALUATION The model built was evaluated with determination coefficients of calibration (R_c^2), cross-validation (R_{cv}^2) and prediction (R_p^2) as well as root mean square errors of calibration ($RMSE_c$), cross-validation ($RMSE_{cv}$) and prediction ($RMSE_p$). Models with larger R_c^2, R_{cv}^2 and R_p^2 values can be considered better models, and models with smaller $RMSE_c$, $RMSE_{cv}$ and $RMSE_p$ values can also be viewed as better models(Yu H D et al., 2021).

RESULTS AND ANALYSIS

Spectral curve analysis The spectrum within $700cm^{-1}$~$4000cm^{-1}$ was taken as the effective spectrum, As shown in *Fig.1* 6846 variables was used in this work. It can be clearly observed that there are absorption peaks near 1650cm^{-1} and 3300cm^{-1}, Where 1650 cm^{-1} is the absorption peak of C=O and C-N bond (Karunakaran C et al., 2019), and 3300 cm^{-1} can be associated with the absorption peak of the N-H bond (Sun D W, 2009).

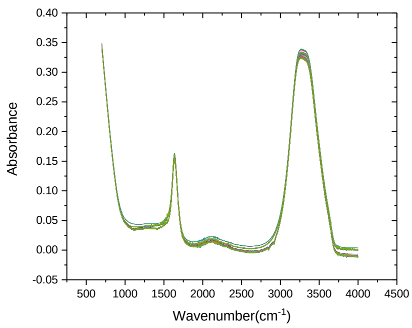

Figure 1. Absorption spectrum curve of monosodium glutamate solution

Full wavelength model analysis The original and the pre-processed data were analyzed, which full-wavelength models for predicting sodium glutamate (MSG) solution were established by employing partial least squares regression (PLSR). Among them, the model established based on the mean centralization preprocessing is the optimal model. As shown in *Fig.2*, The results showed that the root mean squared errors and coefficients of determination of the full-wavelength PLSR model were 1.10mmol/L and 0.98 as well as 1.60mmol/L and 0.95 for cross-validation and prediction, respectively.

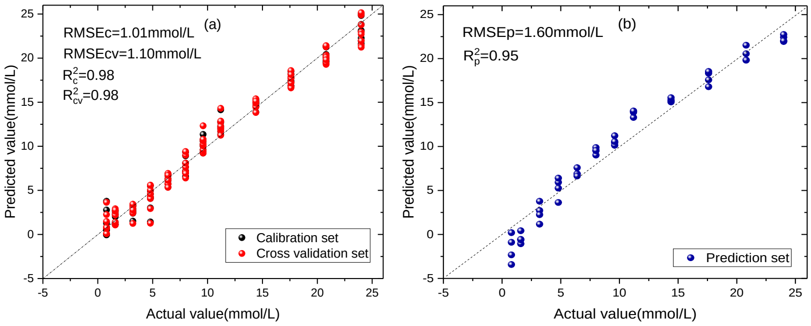

Figure 2. PLSR detection model based on Mean Center preprocessing

Feature wavelength model analysis The simplified PLSR model based on the uninformative variables elimination method and the competitive adaptive weighting algorithm (UVE-CARS) was developed, where 10 wavelengths were utilized, the 10 feature wavelength distributions are shown in *Fig.3*. The model results are shown in *Table 1*. The root mean squared errors of 0.93 and 1.40mmol/L and coefficients of determination of 0.98 and 0.96 for cross validation and prediction were attained, respectively. The SE_c of this simplified model is 0.9mmol/L, Therefore, its detection limit is 2.7mmol/L (Li D et al., 2010).

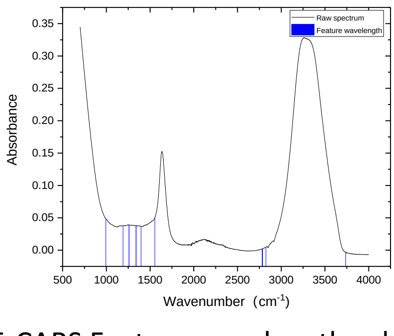

Figure 3.UVE-CARS Feature wavelength selection results

Table 1. Feature wavelength model results

Wavelength selection	Number of variables	RMSE(mmol/L)			R^2			SE(mmol/L)	
		c	cv	p	c	cv	p	c	p
UVE-CARS	10	0.89	0.93	1.40	0.98	0.98	0.96	0.90	1.40

CONCLUSION In this paper, the full-wavelength and feature wavelength model quantitative detection models for MSG concentration prediction were established by mid-infrared spectroscopy, respectively. For the Full-spectrum model, better results were obtained using mean centralization preprocessing data, with $R_{cv}^2 = 0.98, R_p^2 = 0.95, RMSE_{cv} = 1.10$ mmol/L and $RMSE_p = 1.60$ mmol/L. To select informative wavelengths and eliminate redundant and noisy wavelengths, UVE-CARS was applied to MIR data to improve the predicted performance of the model. The performance of the simplified model was better than that of the full-wavelength, and the values of R_{cv}^2, R_p^2, $RMSE_{cv}$ and $RMSE_p$ were 0.98, 0.98, 0.93mmol/L and 1.40mmol/L. In addition, the detection limit of the obtained simplified model was 2.7mmol/L. Therefore, it was shown that it was feasible to use mid-infrared spectroscopy (MIRS) for fast and non-destructive detection of monosodium glutamate concentration and it also testified the ability of mid-infrared spectroscopy in detecting low concentrated analytes.

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