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Rapid prediction of Yongchuan Xiuya tea quality by using near infrared spectroscopy coupled with chemometric methods

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Abstract

The current developmental trend is to evaluate the quality of Yongchuan Xiuya tea rapidly. After spectrum pre-processing, near infrared spectroscopy (NIRS) coupled with synergy interval partial least squares (siPLS), principal component analysis (PCA) and back propagation-artificial neural network (BP-ANN) was applied to rapidly and non-destructively predict the quality of Yongchuan Xiuya tea. External Yongchuan Xiuya tea samples were used for the actual application of the proposed model. The best pre-processing method was multiple scattering correction coupled with second derivative, and the characteristic spectral regions selected by siPLS were 4381.5-4755.6 cm^{-1}, 4759.5-5133.6 cm^{-1}, 6266.6-6637.8 cm^{-1} and 7389.9-7760.2 cm^{-1}. The cumulative contribution rate was 99.05% for the first three principal components of the characteristic spectra regions. The transfer function, root mean square error and determinant coefficient of the best BP-ANN prediction model were the tanh function, 0.384 and 0.977, respectively. The root mean square error and determinant coefficient of the external 10 Yongchuan Xiuya tea samples were 0.406 and 0.969, respectively. These results showed that NIRS combined with BP-ANN algorithm can be used to evaluate the quality of Yongchuan Xiuya tea rapidly and accurately.

Keywords: Yongchuan Xiuya tea; quality; near infrared spectroscopy; synergy interval partial least squares; back propagation-artificial neural network.

Practical Application: Rapid detection of Yongchuan Xiuya tea quality.

1 Introduction

Yongchuan Xiuya tea is a famous needle-shaped green tea produced in Chongqing city, China and is one of the most important agricultural products for farmers. Its processing technology mainly includes spreading, fixing, rolling, dewatering, shaping and drying (Xia, 2016). Among them, rolling is a key procedure that promotes the young tea leaves to form the needle-shaped Yongchuan Xiuya tea and destroys the integrity of the mesophyll cells to overflow the inclusions attached to the surface of the tea product. This phenomenon is beneficial to rapidly increase the concentration of tea soup during brewing and form the unique flavour characteristics of freshness and sweet taste for the Yongchuan Xiuya tea. Yongchuan Xiuya tea is popular with tea consumers because it is good for digestion, prevents constipation (Li et al., 2013), has anti-oxidant effects (Zhang et al., 2013) and inhibits gastric injury (Fu et al., 2014). The quality of Yongchuan Xiuya tea should be strictly controlled when sold in the market to maintain its good reputation. Therefore, evaluating the quality of Yongchuan Xiuya tea is very important and urgent.

The national standard method-sensory evaluation method (Gong et al., 2018) is generally used to evaluate the quality of agricultural products (Tikapunya et al., 2018; Kortesniemi et al., 2018). To date, sensory evaluation has been conducted for green tea (Zhu et al., 2017a), black tea (Wang et al., 2017), oolong tea (Zhu et al., 2017b) and Pu'er tea (Chen et al., 2010). Although as a classic standard, this method is highly specialised and easily influenced by many factors, such as differences in reviewers' hobbies, physical conditions and surrounding environments. Hence, the results of sensory evaluation were subjective. Meanwhile, chemical detection method is objective, and the tea quality can be evaluated by analysing its ingredients (Zhang et al., 2015). Although this method is highly accurate, the samples must be crushed prior to the measurement, making this process time-consuming, laborious and not conducive to detecting the tea quality in real time. Therefore, a convenient, scientific and objective method to evaluate the quality of Yongchuan Xiuya tea must be developed.

Near infrared spectroscopy (NIRS) mainly reflects the X–H chemical bond, has the advantages of rapid and non-destructive analysis and has been widely used in agriculture (Khan et al., 2021; Silva et al., 2021; Fagnani et al., 2022), petrochemical industry, textile industry, and pharmaceutical industry (Guillemain et al., 2017; Malegori et al., 2017). NIRS has been broadly used to predict the amounts of polyphenols, caffeine and other components in tea (Wang et al., 2022), assess the quality of fresh tea leaves (Wang et al., 2013) and discriminate the tea varieties (Ren et al., 2013).

Studies on Yongchuan Xiuya tea are currently focused on processing technology (Jing et al., 2009), aroma component analysis (Zhang et al., 2012) and amino acid composition (Yuan et al.,

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2011) analysis. Some research works have also been performed on quality evaluation (Yuan et al., 2010); however, estimating the quality of Yongchuan Xiuya tea by NIRS has not been reported. In the present study, NIRS combined with synergy interval partial least squares (siPLS), principal component analysis (PCA) and back propagation-artificial neural network (BP-ANN) (Xu et al., 2022; Pranoto et al., 2022) was used to establish the quality prediction model of Yongchuan Xiuya tea that can be used for rapid and accurate quality evaluation.

2 Materials and methods

2.1 Yongchuan Xiuya tea samples and its classification

A total of 130 Yongchuan Xiuya tea samples processed between 27 March 2020 and 1 May 2020 were obtained from Chongqing Junshan Tea Co., Ltd., Chongqing Stalagmite Mountain Ecological Agriculture Co., Ltd. and Chongqing Yunling Tea Technology Co., Ltd. Among which, the 120 samples used to build the model were divided into two sets of calibration (90 samples) and prediction (30 samples) according to the quality scores. The prediction set was used to test the robustness of the calibration model. The remaining external 10 Yongchuan Xiuya tea samples were used to test the actual prediction effect of the calibration model.

2.2 Sensory evaluation

According to the reference (Gong et al., 2018), 3.0 g of Yongchuan Xiuya tea samples were obtained through quartering, placed in a 150 mL evaluation cup filling with boiling water and soaked for 3 minutes. The tea soup was then poured into the tea bowl at a constant speed according to the brewing order. Five sensory evaluation experts evaluated the quality (including appearance, soup colour, aroma, taste and leaf bottom) of Yongchuan Xiuya tea. The full score was 100 points, and a higher score indicated the better quality.

2.3 Spectrum collection

NIR spectra were obtained in the reflectance mode using a Thermo Antaris II Fourier transform (FT) NIR spectrometer (Thermo Fisher, USA) with an integrating sphere. The spectral scanning range was from 4000 cm^{-1} to 10000 cm^{-1} with InGaAs as the detector. Prior to scanning, the instrument must be warmed up for 1 hour. During scanning, the Yongchuan Xiuya tea sample (15 g) was loaded into the sample cup specifically designed for this application. This sample cup was rotated 360° during the scanning to ensure that the NIRS information of each sample was collected. Each sample was scanned for 64 times, and the three selected spectra were averaged as the final spectrum of the sample (Figure 1).

2.4 Spectral data analysis

Pretreatment of optical data

Each spectrum was transformed into 1557 pairs of data points with 3.86 cm^{-1} interval between two adjacent data points saved in an excel sheet. The pre-processed data were analysed by using TQ Analyst 9.4.45 software package (Thermo Fisher Scientific Inc., USA) and Matlab V. 7.0 software package (MathWorks, Natick, USA) in Win 10 software system. The effects of spectrum pre-processing methods of standard normal variation (SNV), multiple scatter correction (MSC), first derivative (FD) and second derivative (SD) and some combination pre-treatment methods were compared. The best pre-treatment method that improves the signal-to-noise ratio of the spectra was selected.

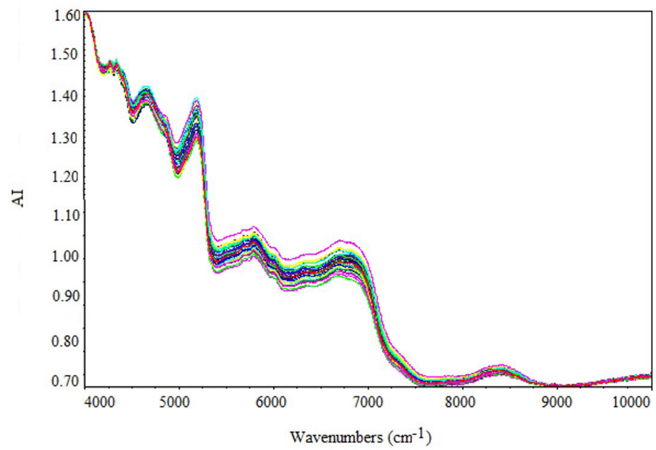

Figure 1. Near infrared spectroscopy of Yongchuan Xiuya tea samples.

SiPLS algorithm

After pre-treatment, the pre-processed spectral data points were equally divided into 10-24 spectral intervals by siPLS (Nørgaard et al., 2000), and the partial least squares (PLS) model was established by combining two, three or four spectral intervals. When the root mean square error of cross validation (RMSECV) was the lowest, the selected spectral intervals built for the best model at this time were closely related to the quality of Yongchuan Xiuya tea.

RMSECV was calculated as follows (Equation 1):

$$RMSECV = \sqrt{\frac{\sum_{i=1}^{n}\left(y_i^{'} - y_i\right)^2}{n}} \quad (1)$$

Where n is the number of samples in the calibration set, y_i is the true value of sample i and $y_i^{'}$ is the predicted value of sample i in the calibration set.

PCA and BP-ANN algorithms

PCA (Ghaziri & Qannari, 2015) was performed on the best spectral intervals obtained by siPLS. BP-ANN algorithm (Liu et al., 2010) was used to establish the NIRS models with the number of principal components (PCs) as the input value and the quality score of Yongchuan Xiuya tea sample as the output value. The results were expressed as the determination coefficient of cross validation (R_c^2), determination coefficient of prediction (R_p^2), root mean square error of cross validation (RMSECV) and root mean square error of prediction (RMSEP).

A higher R^2 and a lower RMSEP indicated the better prediction effect of the calibration model.

RMSEP was calculated as follows (Equation 2):

$$RMSEP = \sqrt{\frac{\sum_{i=1}^{n}\left(y_i - y_i^{'}\right)^2}{n}} \quad (2)$$

Where n is the number of samples in the prediction set, y_i is the true value of sample i and $y_i^{'}$ is the predicted value of sample i in the prediction set.

R^2 was calculated as follows (Equation 3):

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

Where yi and yi' are the true value and predicted value of sample i, respectively, and $\bar{y}$ is the average true value of all samples.

3 Results and discussion

3.1 Quality scores of Yongchuan Xiuya tea using sensory evaluation

Table 1 showed that the sensory quality scores ranged from 75.00 to 93.00 for all Yongchuan Xiuya tea samples, from 75.00 to 93.00 for the calibration set samples and from 83.00 to 90.00 for the prediction set samples. The quality score range of the prediction set samples was within that of the calibration set samples, indicating that sample division was reasonable and provided a pre-condition for establishing the robust quality prediction model of Yongchuan Xiuya tea.

3.2 Comparison of pre-processing methods for spectral data

The NIR spectral data of Yongchuan Xiuya tea samples were pre-treated by various spectrum pre-processing methods. The models of quality score were established by PLS method, and the results were shown in Table 2.

Table 2 showed the comparison of PLS model results of quality scores. The different pre-treatment methods had varying effects on the original spectra of Yongchuan Xiuya tea. Without pre-processing, the result of PLS model was the worst ($R_c^2 = 0.597$, RMSECV = 1.774). When different pre-processing methods were used to de-noise the original spectra, the results of PLS models were improved to varying degrees. Compared with the model without pre-processing, the model established by the combined pre-treatment method of (MSC + SD) produced the best values ($R_c^2 = 0.728$, RMSECV = 1.205) with RMSECV reduced by 32.1%. Therefore, spectral pre-treatment can effectively improve the signal-to-noise ratio, and this finding was consistent with previous conclusions (Li & Altaner, 2019). However, the results of NIRS models for the quality score of Yongchuan Xiuya tea (Table 2) were still poor. Accurately predicting the quality score of the external Yongchuan Xiuya tea samples was still difficult. Therefore, further screening the characteristic spectra intervals that reflecting Yongchuan Xiuya tea quality was necessary to improve the prediction effect of the model.

3.3 Establishment of quality score prediction model

Characteristic spectral intervals screened by siPLS

siPLS was used to establish the prediction models with two, three or four spectral intervals. When the RMSECV was the lowest, the modelled spectral intervals were those that exactly reflecting the quality of Yongchuan Xiuya tea. The results were shown in Table 3.

Table 1. Quality scores of Yongchuan Xiuya tea.

Index	Statistics	All samples	Calibration set	Prediction set
Quality scores	Max	93.00	93.00	90.00
	Min	75.00	75.00	83.00
	Average	80.75	82.35	82.72
	Standard deviation	3.25	3.46	2.66

Table 2. Comparison of PLS model results of quality scores using different preprocessing methods.

Pretreatment methods	R_c^2	RMSECV
None	0.597	1.774
SNV	0.601	1.651
FD	0.623	1.532
SD	0.625	1.537
MSC	0.658	1.445
SNV + FD	0.671	1.412
SNV + SD	0.683	1.389
MSC + FD	0.692	1.316
MSC + SD	0.728	1.205

SNV: standard normal variation; FD: first derivative; SD: second derivative; MSC: multiple scatter correction.

Table 3. Results of siPLS calibration models for Yongchuan Xiuya tea quality scores.

Number of intervals	Factors	Modeling intervals	Proportion (%)	RMSECV
10	11	[5 8 9 10]	40.00	1.421
11	11	[5 8 9 10]	36.36	1.254
12	12	[6 9 11 12]	33.33	1.335
13	11	[7 10 11 13]	30.77	1.241
14	12	[7 9 12 14]	28.57	1.114
15	12	[7 10 14 15]	26.67	1.002
16	**13**	**[2 3 7 10]**	**25.00**	**0.854**
17	13	[6 7 10 16]	23.53	0.884
18	12	[5 8 11 17]	22.22	0.907
19	11	[11 12 15 19]	21.05	0.921
20	13	[11 12 17 20]	20.00	0.952
21	12	[7 12 17 20]	19.05	0.987
22	12	[7 8 9 20]	18.18	1.029
23	14	[4 13 15 18]	17.39	1.135
24	11	[6 13 22 24]	16.67	1.203

SiPLS: synergy interval partial least squares; RMSECV: root mean square error of cross validation.

Table 3 showed that when the numbers of spectral intervals gradually increased from 10 to 24, the best siPLS models were all established by applying four spectral intervals. This finding indicated that the four spectral intervals contained more useful information than the two or three spectral intervals. Therefore, when the full spectra were divided into a certain number of spectral intervals, the best prediction effect was observed from the siPLS models established by four intervals. With gradual increase in the numbers of spectral intervals, the RMSECV of siPLS models showed a trend of first decreasing and then gradually increasing. The lowest RMSECV (0.854) was observed when the whole spectra were divided into 16 intervals and four spectral intervals of [2 3 7 10] were selected to build the model (Figure 2). Hence, the four spectral intervals of [2 3 7 10] were the best characteristic spectral intervals reflecting the quality of Yongchuan Xiuya tea. The corresponding spectral wavenumbers were 4381.5-4755.6 cm^{-1}, 4759.5-5133.6 cm^{-1}, 6266.6-6637.8 cm^{-1} and 7389.9-7760.2 cm^{-1}, which only accounted for 25.00% of the whole spectra data. Therefore, the prediction effect of the model has been further improved. RMSECV was reduced by 29.1% compared with the best results of the PLS model built with (MSC + SD) combined pre-treatment. The region of 4381.5-5133.6 cm^{-1} is the first-order frequency-doubling absorption region of C-H bond and the second-order frequency-doubling absorption region of C=O bond, that of 6266.6-6637.8 cm^{-1} is the second-order frequency-doubling absorption region of N-H bond, and that of 7389.9-7760.2 cm^{-1} is the secondary absorption zone of C-H bond (Jill & Lois, 2009). During rolling, Yongchuan Xiuya tea released a large amount of polyphenols, free amino acids, coffee and other beneficial ingredients which were positively correlated with the quality of Yongchuan Xiuya tea. Polyphenols and free amino acids contained many C-H and N-H chemical bonds, whose information was screened out by the siPLS method in the NIR spectral regions. Hence, the characteristic spectral regions can effectively reflect the quality of Yongchuan Xiuya tea.

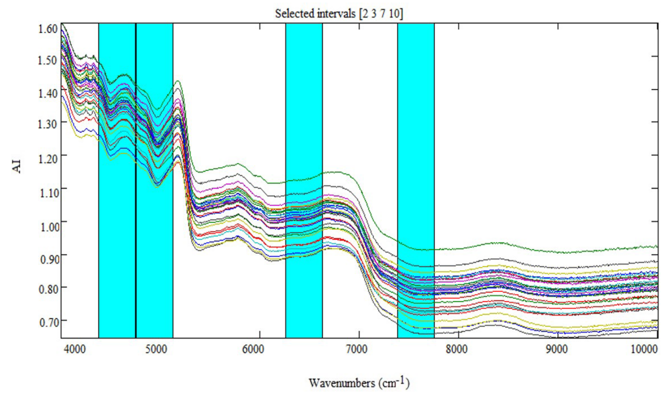

Figure 2. Optimal spectral regions ([2 3 7 10]) selected by siPLS method.

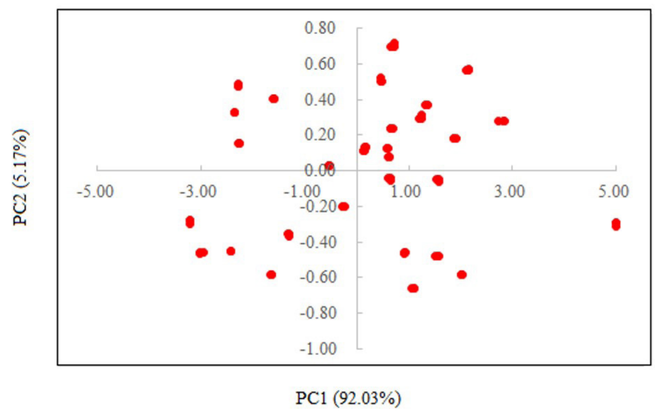

Figure 3. PC1 and PC2 contribution rate of the optimal spectral regions.

Results of PCA analysis

PCA was applied to the characteristic spectral intervals. The contribution rate of the first seven principal components decreased rapidly. Particularly, the contribution rate of PC1 was 92.03%, that of PC2 was 5.17%, that of PC3 was 1.85% and those of PC4-PC7 were all less than 1.00% (Figure 3). The cumulative contribution rate of the first three principal components was 99.05%. Therefore, the first three principal components can represent the characteristic spectral intervals (Wolfgang & Leopold, 2011) and can be used to establish the BP-ANN prediction model in the next step.

Establishment of quality score prediction model with BP-ANN algorithm

The quality score prediction model was established by using BP-ANN algorithm and optimised by regulating the number of hidden neurons in the neural network. After multiple tests, the optimal quality score prediction model was calibrated using three PCs input neurons, four hidden neurons, and one output neuron (quality score value). During model establishment, varying transfer functions were applied between the transfer layers, and the prediction effect of the model was greatly altered. Three kinds of information transfer functions, namely, linear [-1,1] function, logistic function and tanh function were used in building the BP-ANN models. The model results of these three kinds of transfer functions were compared and were shown in Table 4.

Table 4 showed that the linear function BP-ANN model had the worst results (R_p^2 = 0.908, RMSEP = 0.525), and the hyperbolic tanh function BP-ANN model had the best results (R_p^2 = 0.977, RMSEP = 0.384). This phenomenon occurred because Yongchuan Xiuya tea contained many kinds of internal components, and its NIR spectral information was highly complicated. Therefore, the prediction effect of the linear transfer function BP-ANN model was relatively poor. The logistic function was an S-shaped function, indicating the existence of a certain non-linear factor in the spectral information. Hence, the model prediction result was better than that of the linear function model. The tanh function was a hyperbolic tangent function which had faster convergence speed and reduced the numbers of iterations. Hence, the model with this function had the best prediction result and was the most robust among the three kinds of transfer function BP-ANN models (Lv, 2006).

Actual application of the best BP-ANN model

The quality scores of the external 10 Yongchuan Xiuya tea samples were predicted to test the actual application of the best BP-ANN model. The results were shown in Figure 4.

Table 4. Results of three kinds of transfer functions BP-ANN model.

Transfer functions	Calibration set		Prediction set	
	R_c^2	RMSECV	R_p^2	RMSEP
Linear [-1,1]	0.914	0.514	0.908	0.525
logistic	0.956	0.475	0.942	0.489
tanh	0.982	0.377	0.977	0.384

R_c^2: the coefficient of determination for calibration; R_p^2: the coefficient of determination for prediction; RMSEP: root mean square error of prediction; RMSECV: root mean square error of cross validation.

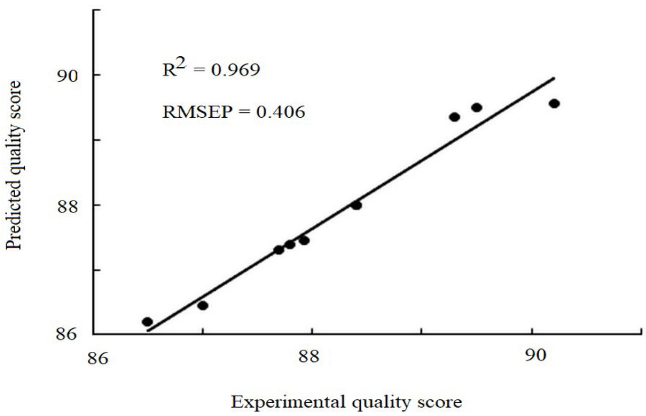

Figure 4. Predicted quality scores of external 10 Yongchuan Xiuya tea samples by the best BP-ANN model. R^2 was the determination coefficient of external 10 Yongchuan Xiuya tea samples; RMSEP was root mean square error of external 10 Yongchuan Xiuya tea samples; BP-ANN was back propagation-artificial neural network.

Figure 4 showed that the actual application of the best BP-ANN model can accurately predict the quality score of the external 10 Yongchuan Xiuya tea samples ($R^2 = 0.969$, RMSEP = 0.406). The results were close to the prediction set model ($R_p^2 = 0.977$, RMSEP = 0.384), indicating that the BP-ANN model established by using the tanh transfer function can accurately predict the quality of Yongchuan Xiuya tea.

4 Conclusion

The current developmental trend is to evaluate the quality of Yongchuan Xiuya tea non-destructively. In this paper, a robust prediction model ($R_p^2 = 0.977$, RMSEP = 0.384) for Yongchuan Xiuya tea quality was established by combining NIR spectroscopy, siPLS, PCA and BP-ANN with the tanh transfer function. Without destroying the sample, the quality of Yongchuan Xiuya tea can be predicted ($R^2 = 0.969$, RMSEP = 0.406) quickly and accurately, and the cost of product sales was therefore reduced. The selected characteristic spectral intervals (4381.5-4755.6 cm^{-1}, 4759.5-5133.6 cm^{-1}, 6266.6-6637.8 cm^{-1} and 7389.9-7760.2 cm^{-1}) have eliminated a large amount of irrelevant spectral information. In future applications, these intervals can be used to develop a targeted near-infrared spectral instrument that detects the quality of Yongchuan Xiu tea without using the full wavelength near-infrared spectral detector. This method can greatly reduce the research cost and advance the commercialisation of the instrument. Additionally, Yongchuan Xiuya tea samples produced in different years should be collected to enhance the prediction accuracy of the model. Existing databases should be appropriately expanded to improve the model's adaptability.

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