



Article The Analysis and Rapid Non-Destructive Evaluation of Yongchuan Xiuya Quality Based on NIRS Combined with Machine Learning Methods

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Abstract: This paper attempts to analyze and assess Yongchuan Xiuya tea quality quickly, accurately, and digitally. The sensory evaluation method was first used to assess Yongchuan Xiuya tea quality, and then near infrared spectroscopy (NIRS) was obtained, and standard methods were applied to the testing of the chemical components. Next, principal component analysis (PCA) and the correlation coefficient method were used to comprehensively screen out the representative components. Finally, NIRS combined with partial least squares regression (PLSR) and back propagation artificial neural network (BP-ANN) methods were applied to build quality evaluation models for Yongchuan Xiuya tea, respectively, and external samples were employed to examine the practical application results of the best model. The cumulative variance contribution rate of the first three principal components of the ingredients in tea was 97.73%. Seven components closely related to tea quality were screened out, namely, amino acids, total catechin, epigallocatechin gallate (EGCG), tea polyphenols, water extracts, epicatechin gallate (ECG), and epigallocatechin (EGC) (p < 0.01). Between the two models established to predict the tea quality, the model built by the PLS method had the better results, whose coefficient of determination of prediction (Rp2) and root mean square error of prediction (RMSEP) were 0.7955 and 1.2263, respectively, and the best results were obtained by the nonlinear BP-ANN model, whose R_p^2 and RMSEP were 0.9315 and 0.6787, respectively. The 10 external Yongchuan Xiuya samples were employed to test the best BP-ANN model, and the results of R² and RMSEP were 0.9579 and 0.6086, respectively, meaning that the model has good robustness. Therefore, the model established by NIRS combined with the BP-ANN method can be used to assess Yongchuan Xiuya tea quality rapidly, accurately, and digitally, and it can also provide new ideas and methods for evaluating the quality of other teas.

Keywords: Yongchuan Xiuya; quality evaluation; near infrared spectroscopy; principal component analysis; artificial neural network

1. Introduction

Tea, one of the world's three major non-alcoholic beverages [1], is known as the health liquid in Britain [2], while in China, tea is known as the national drink [3]. Yongchuan Xiuya, as one of the representatives of China's famous green tea [4], is a tea product of geographical indication in China [5]. It is processed by fresh tea leaves of Zaobaojian No.1, Nanjiang No.1, and Nanjiang No.2 tea varieties from Yongchuan district, Chongqing City [6]. It is produced according to the processes of de-enzyme, rolling, shaping, and drying. Yongchuan Xiuya Nature Reserve is located within an altitude range of 500–800 m. The climate in the reserve is warm and humid all year round, with clouds and mist shrouding the day and night, producing a lot of diffuse light and shortwave ultraviolet light. This makes the tea buds and leaves grow very young and tender, and the contents



Citation: Zang, Y.; Wang, J.; Wu, X.; Chang, R.; Wang, Y.; Luo, H.; Zhong, Y.; Wu, Q.; Chen, Z.; Deng, M. The Analysis and Rapid Non-Destructive Evaluation of Yongchuan Xiuya Quality Based on NIRS Combined with Machine Learning Methods. *Processes* **2023**, *11*, 2809. https:// doi.org/10.3390/pr11092809

Academic Editors: Xiong Luo and Jie Zhang

Received: 7 August 2023 Revised: 18 September 2023 Accepted: 19 September 2023 Published: 21 September 2023



Copyright: © 2023 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). of proteins, amino acids, and alkaloids are abundant, laying a solid foundation for the formation of excellent-quality Yongchuan Xiuya.

Yongchuan Xiuya has the quality characteristics of a tight, round, thin, and straight appearance, a fresh and lush green appearance color, a clear and bright soup color, a fresh and tender aroma, a long and mellow taste, and a tender, even, and bright leaf bottom [7]. It has won honors such as the China International Tea Expo Gold Award and the China Excellent Tea Regional Public Product Brand [8]. After research, it has been confirmed that Yongchuan Xiuya not only has the functions of protecting the heart [9], anticancer [10], antioxidant [11], and antiviral [12], but also has good gastric injury prevention effects [13], DPPH free radical scavenging ability [14], and constipation prevention effects [15]. Therefore, Yongchuan Xiuya is deeply loved by consumers and has become a daily drink that people cannot put down; therefore, it is urgent to evaluate Yongchuan Xiuya tea quality.

Usually, the sensory evaluation method is used to evaluate the quality [16]. It is a practical technology for professionals to comprehensively evaluate the quality by using their own human sensory organs, such as vision, taste, smell, and touch. It has been realized to evaluate the quality of wheat [17], rice [18], honey [19], Chinese medicine [20], green tea [21], black tea [22], Oolong [23], and Pu'er tea [24]. Although the sensory evaluation method is classic, it is highly specialized during evaluation, and reviewers need to undergo strict professional training, making it difficult to master and popularize the sensory evaluation method. To effectively reduce the shortcomings of sensory evaluation methods, instrumental methods are currently used to detect tea quality. The wet chemical detection method is used to apply a variety of chemical detection instruments, for example, high-performance liquid chromatography (HPLC) [25], gas chromatography [26], high-performance liquid chromatography/mass spectrometry (HPLC-MS) [27], and gas chromatography/mass spectrometry (GC-MS) [28], to accurately determine the contents of Yongchuan Xiuya tea [29,30], so as to evaluate the quality [31]. Although this method is objective, fair, and accurate, it requires complex sample pretreatment before determination. The determination is time-consuming and laborious, and a large number of chemical detection reagents are required, which will put great pressure on external environmental protection. So, there is an urgent need to develop an objective new approach to assess Yongchuan Xiuya tea quality quickly and digitally.

Near infrared spectroscopy (NIRS), an electromagnetic wave with a wavelength in the range of 780–2526 nm, mainly reflecting the chemical information of the X–H bond and having the characteristics of fast and non-destructive analysis, has now been popularly applied in agriculture [32], the petrochemical industry, the textile industry, and the pharmaceutical industry [33]. NIRS, combined with si-PLS methods, has been extensively utilized to check the contents of polyphenols and caffeine [34], assess the quality of fresh tea leaves [35], and discriminate between varieties of tea [36]. However, there are few reports on the application of NIRS technology to assess Yongchuan Xiuya tea quality.

The current research on Yongchuan Xiuya mainly focuses on improving processing technology [37,38], optimizing brewing conditions [39], extracting dietary fiber technology [40], analyzing taste components [41], and determining water content [42]. However, there is still little research on the analysis and evaluation of the quality of Yongchuan Xiuya tea. Yongchuan Xiuya tea contains dozens of contents, such as tea polyphenols, amino acids, caffeine, soluble sugar, gallic catechin, and epigallocatechin [43]. It is crucial to screen out one or more internal components closely related to quality. Therefore, this study attempts to combine traditional sensory evaluation methods, wet chemistry detection methods, and NIRS with chemometrics methods to analyze and assess Yongchuan Xiuya quality. Firstly, the sensory evaluation method is used to evaluate the quality of Yongchuan Xiuya tea. Then, the ingredient contents are determined by national standard methods, and principal component analysis (PCA) and correlation coefficient analysis are performed on the components to screen out representative ingredients and obtain the correlation between each component. Finally, NIRS combined with chemometrics methods are used to establish

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quality models, which are used to provide an accurate and fast new method to assess Yongchuan Xiuya tea quality.

2. Materials and Methods

2.1. Yongchuan Xiuya Samples

There are 100 Yongchuan Xiuya samples, 90 of which are from Chongqing Yunling Tea Industry Technology Co., Ltd., Chongqing Yulin Tea Industry Co., Ltd., and Chongqing Youyichun Tea Co., Ltd (Chongqing, China) (see Figure 1). The sample produced was from February 2023 to April 2023. Of the 90 samples, 60 were selected for the calibration set model (quality score range: 85.5–95.5) and 30 were used for validation (quality score range: 85.7–95.0), with a ratio of 2:1. Additionally, 10 samples purchased from the local market were used to test the effectiveness of the quality calibration model.



Figure 1. Samples of Yongchuan Xiuya.

2.2. Main Instruments

The HHS instrument model digital display constant temperature water bath pot was procured from Shanghai Boxun Industrial Co., Ltd. Medical Equipment Factory (Shanghai, China). The UV-2550 ultraviolet visible spectrophotometer was acquired from Shimadzu Corporation (Kyoto, Japan). The Milli-RO Plus 30 pure water machine was purchased from Millipore, France. The 2695 high-performance liquid chromatography (HPLC) and 2998 diode array detectors were procured from Waters, USA. The ODS C18 Inverted Column (250 mm \times 4.6 mm, 5 µm) was purchased from Phenomenex Corporation (Los Angeles, CA, USA). The electronic balance (PL203) was obtained from Mettler Toledo Instrument (Shanghai) Co., Ltd (Shanghai, China).

2.3. Methods

2.3.1. Sensory Evaluation Method

According to the national standard GB/T 23776-2018 [16], a precise amount of 3.0 g of Yongchuan Xiuya sample was accurately weighed using the quartering method and placed into a 150-mL evaluation cup. Then, the evaluation cup was quickly filled with boiling water, covered, and soaked for 4 min. Then, the tea infusion was drained into the evaluation cup at an equal speed in the order of brewing. Five senior tea sensory evaluation experts rated Yongchuan Xiuya tea quality with a maximum score of 100. The better the quality, the higher the scores. During the evaluation process, the reviewers are required to be physically healthy, have good personal hygiene conditions, and refrain from smoking throughout the entire process.

2.3.2. Component Determination Determination of Water Extracts [29]

An amount of 2 g of ground tea was placed into a 500 mL conical flask. 300 mL of boiling distilled water was added, and the flask was immediately transferred to a boiling water bath for extraction for 45 min. The flask was shaken every 10 min during the extraction process. After the completion of the extraction, the mixture was immediately filtered under pressure while still hot. The tea residue was washed several times with 150 mL of boiling distilled water. The tea residue, along with a known quantity of filter paper, was transferred into a drying dish and placed in a constant-temperature drying oven at 120 °C. It was dried for 1 h, cooled for 1 h, and then dried for another hour. Finally, it was immediately transferred into a dryer to cool to room temperature and weighed.

Determination of Tea Polyphenols [44]

In each test tube, 1.0 mL of gallic acid working solution, 1.0 mL of water, and 1.0 mL of tea sample test solution were transferred using a pipette. Subsequently, 5.0 mL of folinol reagent was added to each test tube and shaken thoroughly. After a reaction time of 3–8 min, 4.0 mL of 7.5% sodium carbonate solution were added, followed by the addition of water to reach the desired volume. The test tubes were then left at room temperature for 60 min. The absorbance was measured using a spectrophotometer at a wavelength of 765 nm with a 10 mm cuvette. After an additional hour, the samples were immediately transferred to a dryer to cool to room temperature and weighed.

Determination of Free Amino Acid [30]

To prepare the sample, 1 mL of the test solution was accurately drawn and injected into a 25-mL colorimetric tube. Subsequently, 0.5 mL of pH 8.0 phosphate buffer and 0.5 mL of 2% ninhydrin solution were added to the tube. The mixture was then heated in a boiling water bath for 15 min. After cooling, water was added to bring the volume to 25 mL. The solution was allowed to stand for 10 min before measuring the absorbance at a wavelength of 570 nm using a 5 mm colorimetric cuvette. A reagent blank solution was used as a reference.

Determination of Total Sugar [45]

An amount of 1.00 g of tea powder was accurately weighed and added to 40 mL of 80% ethanol. The mixture was then soaked in a water bath at 95 °C for one hour. After filtration, the filter residue was washed twice with 10 mL of 80% ethanol. The reagent was evaporated and dried, and the filter residue and filter paper were placed in a flask. One hundred milliliters of distilled water were added to the flask, and the mixture was soaked in a 100 °C water bath for one hour. After filtration, the filter residue was washed twice with 10 mL of hot distilled water. The filtrate was combined and centrifuged at 4000 r/min for 10 min. The supernatant was placed in a 100-mL volumetric flask and diluted to volume with distilled water. The solution was shaken well and set aside. One milliliter of the solution was accurately pipetted into a stoppered test tube, and 1 mL of distilled water was added as a blank. Four milliliters of anthrone sulfuric acid test solution were added to each tube, and the mixture was immediately shaken well. The test tubes were placed in a boiling water bath for 7 min and then cooled to room temperature with tap water. After 10 min, the absorbance was measured at a wavelength of 620 nm.

Determination of Flavone [46]

A total of 1.00 g of ground tea sample was weighed and placed into a 100-mL triangular flask. Next, 40 mL of boiling distilled water was added, and the mixture was extracted in a boiling water bath for 30 min. The resulting solution was then filtered into a 50-mL volumetric flask, and water was added to bring the volume up to 50 mL. The solution was thoroughly shaken to prepare the test solution. A volume of 0.5 mL of the test solution was drawn and mixed with 10 mL of a 1% aluminum trichloride aqueous solution. After

shaking well, the mixture was left to stand for 10 min. The absorbance was then measured using a 1 cm colorimetric cuvette at a wavelength of 420 nm, with 1% aluminum trichloride solution as the blank. The flavone content was calculated based on the absorbance of 1.00, which is equivalent to 320 μ g of flavonoid glycosides.

Determination of Gallic Acid, Caffeine, Catechin and Their Monomer Contents [47]

A total of 0.2 g of the sample were weighed and placed into a 50-mL test tube. Next, 10 mL of a 70% methanol solution preheated to 70 °C was added. The mixture was then extracted in a 70 °C water bath for 10 min and cooled to room temperature. Afterward, it was centrifuged at 3500 rpm for 10 min, and the supernatant was transferred to a 10 mL volumetric flask. The residue was extracted once more with 5 mL of a 70% methanol aqueous solution. The extraction solutions were combined into a constant volume of 10 mL, shaken well, and filtered through a 0.45 μ m membrane. A total of 2 mL of the solution was drawn by a pipette into a 10 mL volumetric flask, brought to the mark volume, and left to stand for testing.

Chromatographic column: C18 column (5 μ m × 250 mm × 4.6 mm); Column temperature: 35 °C; Injection volume: 10 μ L; Detector: UV detector; Detection wavelength: 278 nm; Mobile phase A: aqueous solution of acetic acid; Mobile phase B: acetonitrile; Mobile phase flow rate: 1 mL/min; Gradient condition: The mobile phase consisted of 100% A phase for the first 10 min, followed by a linear gradient to 68% A phase and 32% B phase over 15 min, which was maintained for 10 min, and finally returned to 100% A phase. After the flow rate and column temperature had stabilized, a 10 μ L mixed standard series working solution was drawn and injected into the HPLC system. A 10 μ L test solution was then injected under the same chromatographic conditions, and the peak area was calculated.

2.4. NIRS and Chemometrics Method

2.4.1. Spectra Acquisition

NIRS were collected by using a Thermo Antaris II Fourier transform (FT) NIR spectrometer (Waltham, MA, USA) with the reflectance mode, equipped with an InGaAs detector and an integrating sphere accessory. To obtain the spectral data, 10 g of the Yongchuan Xiuya tea were placed into the sample cup, which will rotate 360° when scanning. The spectral range is between 10,000 cm⁻¹ and 4000 cm⁻¹, with 3.857 cm⁻¹ intervals. Each sample was scanned three times, and the average spectrum (see Figure 2) of the three scans was used for subsequent analysis.



Figure 2. Near infrared average spectra of Yongchuan Xiuya samples.

2.4.2. Spectral Pretreatment

Before modeling, in order to effectively eliminate extraneous background and noise information and enhance model performance, various spectral preprocessing techniques were employed, including spectral free preprocessing (None), standard normal variable (SNV), first derivative (FD), second derivative (SD), multiple scatter correction (MSC), and their combined methods, to remove noise from the original spectra. After comparing the results, the optimal preprocessing method was determined.

2.4.3. Partial Least Squares Regression Method

Partial least squares regression (PLSR) is a classic method for multiple data regression. It is particularly effective when the variables exhibit high internal linearity. PLSR combines the advantages of principal component analysis, canonical correlation analysis, and multiple linear regression analysis to extract maximum information that reflects data variation. It can also avoid issues such as non-normal distribution of data, factor uncertainty, and model failure, resulting in a reliable prediction function [48].

2.4.4. Backpropagation Artificial Neural Network Method

Backpropagation artificial neural network (BP-ANN) has emerged as a research hotspot in the field of artificial intelligence in recent years. It abstracts the neural network of the human brain from the perspective of information processing, forms different networks according to different connection modes, and is composed of a large number of neurons connected with each other. Each node represents a specific transfer function. By establishing the connection between input data and output data, a prediction model can be established [49]. Using the first three principal components as input variables and the quality score of Yongchuan Xiuya tea as output values, the BP-ANN model for the quality of Yongchuan Xiuya tea was established by continuously adjusting the number of hidden layers on the Matlab 2012 software platform. The BP-ANN model achieved the best prediction results when the number of hidden layers was five. During the establishment process of the BP-ANN model, the learning speed was set to 0.1, the allowable error was 0.0001, the maximum number of iterations was 1000, and the transfer function was the tanh function. The BP-ANN model began to converge after 35 iterations.

2.4.5. Data Analysis

Correlation coefficient analysis was conducted using SPSS 19.0 software [50]. The PCA method was performed using the Matlab 2012a software package to establish PLS and BP-ANN models [51]. The results were evaluated based on the coefficient of determination of cross validation (Rc2), coefficient of determination of prediction (Rp2), root mean square error of cross validation (RMSECV), and root mean square error of prediction (RMSEP) [52]. A higher R2 and a lower RMSEP indicate better prediction performance. The equations used to calculate RMSECV, RMSEP, and R2 are provided.

RMSECV was computed as follows:

$$\text{RMSECV} = \sqrt{\frac{\sum_{i=1}^{n} (y'_i - y_i)^2}{n}}$$
(1)

where *n* is the number of samples in the calibration set, y_i is the true value for sample *i*, and y'_i is the theoretical value for sample *i* predicted from the calibration set. RMSEP was computed as follows:

$$\text{RMSEP} = \sqrt{\frac{\sum_{i=1}^{n} (y_i - y'_i)^2}{n}}$$
(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.

R² was computed as follows:

$$R^{2} = 1 - \frac{\sum_{i=1}^{n} (y'_{i} - y_{i})^{2}}{\sum_{i=1}^{n} (y'_{i} - \overline{y})^{2}}$$
(3)

where y_i and y_i' are the true value and predicted value of sample *i*, respectively, and \overline{y} is the average true value of all samples.

3. Results and Discussion

3.1. The Quality and Component Contents

After sensory evaluation experts rated the quality, national standard methods were used to test the components in the tea. The results were shown in Table 1.

Index	Max	Min	Average	SD
Scores	95	85.5	87.42	2 14
GA/mg/g	1.86	0.64	0.72	0.29
CAF/%	3.56	1.42	1.73	0.52
GC/mg/g	0.34	0.19	0.25	0.04
EGC/%	0.36	0.09	0.21	0.09
C/%	0.10	0.05	0.06	0.03
EC/%	0.12	0.04	0.07	0.02
EGCG/%	5.25	3.12	3.74	0.65
GCG/mg/g	0.26	0.14	0.19	0.08
ECG/%	0.42	0.13	0.21	0.18
CG/%	0.26	0.12	0.16	0.03
TC/%	15.66	10.43	11.67	2.13
TP/%	34.36	27.82	30.31	3.75
AA/%	3.25	1.24	1.76	0.83
F/%	2.83	1.75	2.44	0.35
WE/%	43.52	38.85	40.53	3.66
TS/%	5.12	2.70	3.73	2.52

Table 1. Scores and inclusions contents of Yongchuan xiuya tea.

Note: Max: maximum; Min: minimum; SD: standard deviation; GA: Gallic acid; CAF: Caffeine; GC: Gallocatechin; EGC: Epigallocatechin; C: Catechin; EC: Epicatechin; EGCG: Epigallocatechin gallate; GCG: Gallocatechin gallate; ECG: Epicatechin gallate; CG: Catechin gallate; TC: Total catechins; TP: Tea polyphenols; AA: Amino acid; F: Flavone; WE: Water extracts; TS: Total sugar.

Table 1 shows that the maximum quality score was 95 points, the minimum score was 85.5 points, the average score was 87.42, and the standard deviation was 2.14. The differences in tea infusion quality scores were minimal. Additionally, Table 1 presents the contents of 16 components, including caffeine, EGCG, total catechin, tea polyphenols, water extracts, amino acids, and total sugar, which were found in higher concentrations. Conversely, GA, GC, EGC, C, EC, GCG, CG, and ECG were present in relatively lower concentrations. The components in tea are interrelated and play a role in determining tea quality; however, their contributions to tea quality vary. To identify the components that significantly contribute to the quality of Yongchuan Xiuya tea, principal component analysis (PCA) and correlation coefficient analysis were conducted on the aforementioned components.

3.2. Principal Component Analysis and Correlation Coefficient Analysis

PCA was applied to 16 kinds of internal components, and the results are shown in Table 2.

Index	Eigenvectors								
mucx	PC1	PC2	PC3	PC4	PC5				
GA	0.3092	-0.1684	0.2143	-0.1344	0.0987				
CAF	0.2700	0.0092	0.0920	-0.1380	0.3366				
GC	0.2363	-0.0505	0.2820	-0.1056	-0.0874				
EGC	0.0387	0.4508	-0.0529	0.3573	0.7270				
С	0.1029	0.3163	0.0912	-0.5467	-0.1461				
EC	0.2227	0.3625	-0.3097	-0.2095	0.1042				
EGCG	0.5567	-0.2150	-0.0203	0.0991	-0.0177				
GCG	0.2658	-0.3010	0.0691	0.0890	-0.1915				
ECG	0.3883	0.4862	-0.1006	-0.0258	0.0201				
CG	0.2863	-0.1253	-0.2899	0.0788	-0.0880				
TC	0.4024	0.1010	-0.1016	-0.1390	0.0539				
TP	0.4612	0.3161	0.1659	0.2979	0.0307				
AA	-0.0513	0.2736	0.6230	0.1107	0.0159				
F	-0.1244	0.3345	-0.3926	0.0217	0.1383				
WE	0.6299	-0.0458	0.1857	0.3510	-0.0671				
TS	0.1348	0.0780	-0.2124	0.4611	-0.4856				
Eigenvalues	13.14	2.30	0.20	0.13	0.06				
Contribution rates/%	82.13	14.36	1.24	0.83	0.38				
Accumulated contribution rate of PC1-PC3/%		97.73		Accumulated contribution rate of PC4–PC5/%	1.21				

Table 2. Eigenvectors and variance contribution rates of principal components.

Note: GA: Gallic acid; CAF: Caffeine; GC: Gallocatechin; EGC: Epigallocatechin; C: Catechin; EC: Epicatechin; EGCG: Epigallocatechin gallate; GCG: Gallocatechin gallate; ECG: Epicatechin gallate; CG: Catechin gallate; TC: Total catechins; TP: Tea polyphenols; AA: Amino acid; F: Flavone; WE: Water extracts; TS: Total sugar; PC: principal component.

Table 2 demonstrates that the cumulative variance contribution rate of the first five principal components (PCs) was 98.94%, while the cumulative variance contribution rate of the first three PCs was 97.73%. According to the principle of principal component analysis (PCA) [52], the first three PCs can effectively explain the vast majority of information regarding the ingredients present in Yongchuan Xiuya tea. Specifically, PC1 and PC2 can explain 82.13% and 14.36% of the information in the 16 internal components, respectively, resulting in a total interpretation rate of 96.49%. Table 2 illustrates that PC1 comprehensively reflects the information of EGCG, catechin, tea polyphenols, and water extracts, which are crucial factors affecting the concentration and bitter taste of tea infusion. Therefore, it is defined as the bitter taste factor. PC2 comprehensively reflects the information of EGC and ECG, which generally exhibit the characteristics of refreshing aftertaste and weak convergence. Thus, they are defined as refreshing factors. PC3 mainly reflects the total amount of amino acids in tea. Generally, the more total amino acids in tea, the fresher the taste of the tea infusion. Therefore, it is defined as the freshness factor. The scores of the first three PCs were showed in Table 3, and score1 vs. score2 in Figure 3 showed good clustering performance among samples, indicating the efficiency of PCA in extracting sample information. However, a small number of samples had relatively long spatial distances in the figures, which may be due to differences in the content of components between these Yongchuan Xiuya samples and other samples. This also indicates that the selected samples in this experiment have a certain representativeness and universality.

Table 4 shows that the quality score was highly significantly positively correlated with EGC (0.09–0.36%), EGCG (3.12–5.25%), and ECG (0.13–0.42%) (p < 0.01). EGC, EGCG, and ECG are monomers of catechin, which have strong antioxidant activity, can eliminate free radicals in the body, and have anti-aging effects. During the processing of Yongchuan Xiuya, the enzyme activity is quickly inactivated through high-temperature sterilization, fully retaining tea polyphenol content and avoiding the occurrence of oxidation reactions

in the leaves, which can affect the quality of Yongchuan Xiuya [43]. With the rolling of Yongchuan Xiuya, the mesophyll cells were destroyed, and the contents of the cells penetrated the surface of the leaves. The tea polyphenols had a preliminary oxidation reaction, producing some catechin, which were refreshing and irritant ingredients of the tea and were conducive to the quality improvement. The Yongchuan Xiuya tea quality score was positively correlated with the contents of catechin (10.43–15.66%), tea polyphenols (27.82–34.36%), and water extracts (38.85–43.52%) (*p* < 0.01). Tea polyphenols are a mixture of polyphenols existing in tea plants. Its main components are flavanols with catechin as the main component, which mainly present an astringent taste in tea infusion. A large amount of tea polyphenols is not conducive to improving the quality of tea. Yongchuan Xiuya, as a famous and high-quality green tea, is processed from tender fresh tea leaves, and the distribution of polyphenols in the tea plant is mainly concentrated in the vigorous growth part of the new shoots; therefore, the content in fresh leaves is relatively high. As tea polyphenols contain a large number of -OH chemical bonds, they are very likely to be oxidized and denatured into other substances when Yongchuan Xiuya is rolled, resulting in a large reduction in tea polyphenol content, which can reduce the astringency of tea. At the same time, some of the retained tea polyphenols also have antioxidant, antiviral, and bactericidal effects. Water extract of tea infusion is a general term for various substances soluble in water and is a comprehensive indicator of tea quality. The amount of water extract is positively correlated with tea quality; that is, the better the quality of tea, the higher the content of water extract [53]. Generally speaking, the water extract content of young leaves is higher than that of old leaves; spring tea has a higher content of water extracts than other seasons. Therefore, in this study, the quality of Yongchuan Xiuya processed in spring was significantly positively correlated with the water extract content, and a higher water extract content was beneficial for improving tea quality. There is a highly significant positive correlation between the quality score and the amino acid content (2.70-5.12%) (*p* < 0.01). Amino acids in tea infusions are the main component of the fresh and refreshing taste of green tea, and there is a certain correlation with the sweetness of the tea [54]. In addition, amino acids are also a component of the tea aroma. When conducting tea evaluation, the Yongchuan Xiuya tea infusion contained a faint aroma, which was conducive to improving the quality. Table 4 also shows that the total amount of EGCG, ECG, catechin, and tea polyphenols had a very significant positive correlation (p < 0.01), and they have played a positive role in each other, jointly affecting the quality of Yongchuan Xiuya tea. In addition, the correlation between GA (0.64 mg/g-1.86 mg/g) and the quality score was the largest with -0.20; however, there was no significant correlation between them (p > 0.05). Although the contribution values of caffeine (1.42–3.56%) and flavonoids (1.75–2.83%) were also significant, with correlation coefficients of -0.19 and 0.17, respectively, these two substances mainly present a bitter taste and are not conducive to improving the quality; however, there was no significant correlation between them and the quality scores (p > 0.05). And there is no inevitable relationship between the ingredient content and the tea quality. A high content of ingredients may not necessarily contribute significantly to the quality, while a low content of ingredients may not necessarily contribute significantly to the quality. It can also be seen from Table 3 that the correlation coefficients between the score of Yongchuan Xiuya tea and the total amount of EGC, EGCG, ECG, catechin, tea polyphenols, amino acids, and water extracts were 0.51, 0.57, 0.53, 0.63, 0.56, 0.70, and 0.54, respectively. The order of contribution of these seven ingredients to the quality of tea was: amino acids, total catechin, EGCG, tea polyphenols, water extracts, ECG, and EGC. So, after conducting PCA and correlation analysis on the internal components of Yongchuan Xiuya tea, seven types of internal components that contributed significantly to the quality can be effectively selected from a large number of internal components. It not only reduced the workload of detection, with detection indicators accounting for 43.75% of the original detection indicators, but also laid a solid foundation for evaluating Yongchuan Xiuya tea quality.

 Table 3. The scores of PC1, PC2, and PC3.

No.	PC1	PC2	PC3	No.	PC1	PC2	PC3
1	1.775	-3.9385	-0.8617	46	-1.6018	1.0217	0.1246
2	-0.5805	-1.9684	-1.0791	47	-0.6848	1.0424	0.3529
3	3.036	-3.6361	-0.5471	48	-0.3122	0.3511	0.5925
4	0.3416	-1.9419	0.2925	49	-2.6226	0.1124	-0.5502
5	1.9355	-3.7638	-0.1638	50	-1.804	-0.7823	-0.2341
6	0.7175	-0.474	1.2196	51	0.1521	1.2412	-0.3517
7	-1.4983	-2.1944	0.6161	52	-0.9203	1.0401	-1.6748
8	-1.3936	-0.7726	-0.435	53	3.2586	2.1336	-0.2424
9	-0.4868	-1.2719	0.4365	54	-0.5582	0.9662	-2.2403
10	-1.6856	-1.4367	0.7026	55	8.6524	0.2162	0.4486
11	-1.1042	-0.7088	1.1916	56	-1.2403	0.8776	1.5701
12	-1.3511	-0.36	1.2587	57	-1.7705	1.1294	2.3058
13	1.9368	-0.5548	0.6023	58	-1.8578	-0.3888	0.337
14	-2.7788	-0.9177	1.675	59	-1.2806	0.7363	0.1073
15	-1.926	-1.2402	1.3203	60	-0.3502	2.5421	-0.487
16	-1.3358	-2.9497	-0.7029	61	1.4713	1.2027	-0.8319
17	-0.4809	-1.9466	-1.0661	62	1.679	0.921	0.355
18	2.3096	-2.6868	0.8809	63	-3.2776	-0.2199	-2.3119
19	-0.0364	-1.2208	0.2805	64	3.6238	-1.0214	0.7686
20	-1.3692	-0.9329	0.105	65	-0.856	1.0487	-0.1566
21	6.4563	2.4076	1.0552	66	3.4822	0.6847	-1.016
22	-1.1998	-0.0999	1.1245	67	-1.9691	1.267	-1.9004
23	1.3245	-0.6896	1.0234	68	-2.618	0.1019	1.0843
24	1.536	-0.5213	2.5202	69	-2.7939	-0.4014	1.3374
25	-0.9508	2.0737	1.536	70	-1.6442	-0.4213	-0.8723
26	-3.5698	-1.1139	-1.972	71	3.8298	1.6497	-1.9752
27	0.1921	1.7773	1.0972	72	1.4916	1.0777	1.1331
28	5.9119	-2.8599	-2.5312	73	-0.7033	1.212	-0.0083
29	-1.5615	-0.4516	-1.8843	74	-0.8629	-0.8127	0.7028
30	-1.4591	0.0522	-0.0647	75	-0.5721	-1.0933	1.4466
31	-2.403	0.2643	0.577	76	-0.606	-0.2355	-0.2221
32	1.6636	2.1569	0.1681	77	-3.0995	0.1555	-1.2727
33	-0.8841	3.1177	-0.9166	78	-0.6562	0.8468	-1.3858
34	-3.0552	0.4802	1.698	79	-0.0721	1.5898	1.2834
35	0.9055	0.7643	-1.6245	80	0.6024	0.5936	0.8527
36	0.9089	0.6691	0.3768	81	0.4541	1.4327	-0.3668
37	3.1934	0.0564	-0.1861	82	-0.4966	0.4367	0.3332
38	1.8949	-0.3699	1.1487	83	-1.7236	1.7501	0.1776
39	0.4785	0.2402	-0.0766	84	-0.8348	1.1868	0.4829
40	-2.6544	0.4731	-2.6383	85	-0.3491	0.3818	0.7866
41	4.5366	0.1026	0.4665	86	-2.8626	0.0101	-0.509
42	-1.7693	0.3486	0.2686	87	-2.504	-0.6591	-0.1861
43	3.9881	1.047	-1.3119	88	0.0562	1.812	-0.4681
44	-0.8125	0.6777	-1.6815	89	-1.2035	1.1401	-2.758
45	-0.9541	0.2529	-0.2702	90	3.6786	2.3452	-0.1724



Figure 3. Samples spatial distribution of PC1 vs. PC2.

Table 4. The correlation between the components and quality scores of Yongchuan. Xiuya tea.

Indexes	s S	GA	CAF	GC	EGC	С	EC	EGCG	GCG	ECG	CG	TC	ТР	AA	F	WE	TS
S	1.00																
GA	-0.20	1.00															
CAF	-0.19	0.56 **	1.00														
GC	0.03	0.40 *	0.34 **	1.00													
EGC	0.51 **	0.05	0.04	0.02	1.00												
С	0.02	0.18	0.09	0.15	-0.16	1.00											
EC	-0.11	0.13	0.32 **	0.23 *	-0.01	0.34 **	1.00										
EGCG	0.57 **	0.61 **	0.46 **	0.35 **	0.06	-0.08	0.29 **	1.00									
GCG	-0.10	0.45 *	0.30 **	0.37 **	0.02	-0.07	0.06	0.70 **	1.00								
ECG	0.53 **	0.57 **	0.51 **	0.37 **	0.05	0.22	0.51 **	0.73 **	0.45 *	1.00							
CG	-0.11	0.40 **	0.38 **	0.28 **	0.14	0.09	0.24 *	0.51 **	0.41 *	0.65 **	1.00						
TC	0.63 **	0.58 **	0.51 **	0.44 **	0.12	0.42 **	0.67 **	0.75 **	0.49 *	0.93 **	0.61 **	1.00					
TP	0.56 **	0.41 **	0.38 **	0.27 **	0.08	0.19	0.32 **	0.37 **	0.19	0.54 **	0.22 *	0.52 **	1.00				
AA	0.70 **	-0.06	-0.03	0.06	0.01	0.17	-0.10	-0.24 *	-0.14	-0.12	-0.25 *	-0.11	0.16	1.00			
F	0.17	0.38 **	-0.08	-0.30 **	-0.07	0.04	0.26 *	-0.41 **	-0.35 *	-0.20	-0.16	-0.18	0.04	-0.03	1.00		
WE	0.54 **	0.01	0.13	0.13	-0.05	0.09	0.32 **	0.17	0.01	0.28 *	0.04	0.28 *	0.58 **	0.31 **	0.19	1.00	
TS	-0.03	0.09	0.01	0.11	0.03	0.02	0.15	0.19	0.16	0.24 *	0.35 **	0.23 *	0.32 **	0.06	-0.02	0.16	1.00

Note: * p < 0.05; ** p < 0.01; S: Score; GA: Gallic acid; CAF: Caffeine; GC: Gallocatechin; EGC: Epigallocatechin; C: Catechin; EC: Epicatechin; EGCG: Epigallocatechin gallate; GCG: Gallocatechin gallate; ECG: Epicatechin gallate; CG: Catechin gallate; TC: Total catechins; TP: Tea polyphenols; AA: Amino acid; F: Flavone; WE: Water extracts; TS: Total sugar.

3.3. Establishment of NIRS Model

3.3.1. Screening of Spectral Pretreatment Methods and Establishment of PLS Model

Figure 2 shows that the spectra exhibit multiple absorption peaks in the long wave band (4000–7000 cm⁻¹), primarily due to the presence of water -OH and various components of varying quality in Yongchuan Xiuya tea NIRS absorption information. Prior to model building, nine spectral preprocessing methods were employed to pretreat the NIR spectra of Yongchuan Xiuya tea with varying quality scores. Subsequently, PLS was utilized to construct NIRS models. The performance of the models was evaluated using RMSECV and Rc2, with higher Rc2 and lower RMSECV indicating better pretreatment methods. The results of all the pre-treatment models are presented in Figure 4.

In Figure 4, among the nine models, the NIRS models built with the original spectra yielded the worst results (Rc2 = 0.5374, RMSECV = 1.5102). The models with a single preprocessing method, specifically the SD pretreatment method, showed better results (Rc2 = 0.6598, RMSECV = 1.3423); however, the prediction results were still inferior to

those obtained with combined pre-treatment methods. The NIRS model built using the (MSC + FD) combined method produced the best results (Rc2 = 0.8268, RMSECV = 1.1265), representing a 53.85% increase in Rc2 and a 25.40% decrease in RMSECV compared to the original spectra of the NIR model. Therefore, it is crucial to pretreat the original spectra before building NIRS models, which is consistent with previous findings. In this study, the best spectral pretreatment method was the combination of MSC + FD, and the Rc2 and RMSECV of the best calibration model built using the PLS method were 0.8268 and 1.1265, respectively. When the 30 prediction samples were used to verify the robustness, the Rp2 and RMSEP were 0.7955 and 1.2263, respectively (see Figure 5). However, the performance was still unsatisfactory, and there is still ample room for improvement in the results.



Figure 4. The performances of nine different pretreatment methods.



Figure 5. Prediction results of Yongchuan Xiuya tea quality by PLS model.

3.3.2. Establishment of BP-ANN Model

Principal Component Analysis

Before building the BP-ANN model for the quality of Yongchuan Xiuya tea, it was required to input as little data as possible, and the PCA should be carried out on the pretreated spectra first. And the cumulative contribution rate of the first five PCs is shown in Table 5.

Table 5. Cumulative contribution rate of the first five PCs.

Principal Components (PC)	PC1	PC(1–2)	PC(1–3)	PC(1-4)	PC(1–5)
Cumulative contribution rate/%	80.35	92.55	96.25	98.14	99.04

It can be seen from Table 5 that the contribution rate of the first five PCs decreases rapidly. The contribution rate of PC1 was 80.35%, the cumulative contribution rate of PC1-PC5 was 99.04%, and the cumulative contribution rate of the first three PCs was 96.25%. According to the PCA principle, the information of the first three PCs can represent all the information of the spectra.

BP-ANN Model

The results of the BP-ANN model are shown in Figures 6 and 7.



Figure 6. The results of quality score of Yongchuan Xiuya tea by BP-ANN calibration set model.

In Figures 6 and 7, the BP-ANN calibration model of the Yongchuan Xiuya tea quality score had good prediction results. The Rc² and RMSECV of the model were 0.9617 and 0.6053, respectively. It means that the RMSECV has been significantly decreased by 46.27% compared with the RMSECV of the PLS model, greatly improving the prediction accuracy. When 30 samples in the prediction set were applied to check the calibration set model's robustness, the Rp² and RMSEP were 0.9315 and 0.6787, respectively, and the RMSEP significantly decreased by 44.65% compared with the RMSEP of the PLS model. So, the quality score model of Yongchuan Xiuya tea established by the BP-ANN method had the best results and higher prediction accuracy. It may be due to the fact that fresh tea leaves are products of photosynthesis, and their internal components are extremely rich. After processing, fresh tea leaves produce up to hundreds of internal components. However, due to the limitations of current detection methods, there may be other internal components that have not been detected yet, and there are still a lot of interactions between the internal components. Among the seven components selected in this study that were closely related to Yongchuan Xiuya tea quality, the catechin monomers, total catechin, and tea polyphenols were highly significantly related, and the interaction was obvious. The relationship between each component was not simple linear but significant non-linear. Therefore, when the Yongchuan Xiuya tea quality score model was built, although the R_p^2 of the linear PLS model also reached more than 0.82, the prediction errors were still larger. However, when the nonlinear BP-ANN method was applied to build a prediction model for the quality of Yongchuan Xiuya tea, the obtained results were the best, which has also indirectly verified the significant nonlinear relationship between the seven components in the tea.



Figure 7. The results of quality score of Yongchuan Xiuya tea by BP-ANN prediction set model.

3.3.3. Verification of the Practical Application Effect of the BP-ANN Model

The BP-ANN model was applied to predict the quality scores of 10 external Yongchuan Xiuya samples that were not involved in the modeling, and the actual application effect of the model was tested. The results were shown in Figure 8.

Figure 8 illustrates a strong correlation between the true values and the predicted values obtained from the optimal BP-ANN model used to predict the quality of 10 external Yongchuan Xiuya tea samples. The R2 and RMSEP values were 0.9579 and 0.6086, respectively, which were comparable to the results obtained from the BP-ANN calibration model. These findings suggest that the nonlinear BP-ANN method is highly suitable for establishing a quality evaluation model for Yongchuan Xiuya tea. The model exhibits robustness and has demonstrated good performance in predicting the quality of external samples. However, upon examining the specific prediction results of the 10 external samples, it was observed that samples with a quality score of less than 92 had a predicted score greater than the true quality score, while samples with a quality score. This indicates that the predicted quality score of the samples tends to converge toward the center.



Figure 8. Result of quality score for 10 external Yongchuan Xiuya samples.

4. Conclusions

Based on the detection of the intrinsic components in the Yongchuan Xiuya tea, PCA and correlation analysis methods were applied to select the intrinsic components closely related to the tea quality; then, the linear PLS method and the nonlinear BP-ANN method were respectively used to establish the digital evaluation model of tea quality, and the evaluation of tea quality was initially realized. The main research conclusions were as follows:

(1) PCA was conducted on the components, and the cumulative variance contribution rate of the first three PCs was 97.73%. Among them, PC1, PC2, and PC3 mainly reflected the bitter, refreshing, and refreshing taste factors of tea infusion, respectively. After correlation analysis, seven components closely related to tea quality were screened out, which were amino acids, total catechin, EGCG, tea polyphenols, water extracts, ECG, and EGC, respectively.

(2) The Rc^2 and RMSECV in the Yongchuan Xiuya tea quality prediction model established by the PLS method were 0.8268 and 1.1265, respectively, and the Rp^2 and RMSEP were 0.7955 and 1.2263, respectively.

(3) The quality model built by the BP-ANN method was the best. The Rc² and RMSECV of the calibration set model were 0.9617 and 0.6053, respectively. The Rp² and RMSEP of the prediction set model were 0.9315 and 0.6787, respectively. When the BP-ANN model was applied to predict the quality of 10 external samples, the R² and RMSEP were 0.9579 and 0.6086, respectively, indicating that the model had good robustness. The BP-ANN method was very suitable for establishing a quality evaluation model in this paper, and it has been achieved to assess Yongchuan Xiuya tea quality rapidly, accurately, and digitally. However, there are still some shortcomings in this study, such as insufficient diversity in sample collection. In future practical applications, it is recommended to further supplement the collection of Yongchuan Xiuya samples with different qualities, especially those with poor quality and samples from different years. This will expand the quality score range of the samples and make the experimental data more representative and comprehensive. Only then can the established quality evaluation model have a wider range of uses, and only then can we more accurately predict the quality of Yongcuan Xiuya tea.

Author Contributions: Conceptualization, Y.Z. (Ying Zang), J.W. and X.W.; methodology, R.C. and Y.W.; software, H.L.; validation, Y.Z. (Yingfu Zhong) and Q.W.; writing—original draft preparation, Y.Z. (Ying Zang) and J.W.; writing—review and editing, Z.C. and M.D.; funding, Z.C. and M.D. All authors have read and agreed to the published version of the manuscript.

Funding: This work was supported by the municipal financial special project of Chongqing Academy (cqaas2023sjczzd002), the National Key R&D Program of China (2022YFD1601401), the Chongqing Modern Agricultural Industry Technology System (CQMAITS202308).

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: The data are available from the corresponding author.

Conflicts of Interest: The authors declare no conflict of interest.

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