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Rapid and comprehensive grade evaluation of Keemun black tea using efficient multidimensional data fusion

Luqing Li [a,1], Yurong Chen [a,1], Shuai Dong [a], Jingfei Shen [a], Shuci Cao [a], Qingqing Cui [a], Yan Song [b], Jingming Ning [a,*]

[a] State Key Laboratory of Tea Plant Biology and Utilization, Anhui Agricultural University, 130 Changjiang West Road, Hefei 230036, China
[b] School of Engineering, Anhui Agricultural University, Hefei 230036, China

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ABSTRACT

To develop a comprehensive evaluation method for Keemun black tea, we used micro-near-infrared spectroscopy, computer vision, and colorimetric sensor array to collect data. We used support vector machine, least-squares support vector machine (LS-SVM), extreme learning machine, and partial least squares discriminant analysis algorithms to qualitatively discriminate between different grades of tea. Our results indicated that the LS-SVM model with mid-level data fusion attained an accuracy of 98.57% in the testing set. To quantitatively determine flavour substances in black tea, we used support vector regression. The correlation coefficient for the predicted sets of gallic acid, caffeine, epigallocatechin, catechin, epigallocatechin gallate, epicatechin, gallocatechin gallate and total catechins were 0.84089, 0.94249, 0.94050, 0.83820, 0.81111, 0.82670, 0.93230, and 0.93608, respectively. Furthermore, all compounds exhibited residual predictive deviation values exceeding 2. Hence, combining spectral, shape, colour, and aroma data with mid-level data can provide a rapid and comprehensive assessment of Keemun black tea quality.

1. Introduction

Keemun black tea is highly appreciated by consumers because of its intense aroma and unique flavour and quality. Tea are typically graded depending on the quality of freshly picked leaves and other sensory criteria. However, sensory evaluations are subjective (Zhi et al., 2017). To ensure the objectivity of tea evaluations, many studies have employed methods such as gas chromatography–mass spectrometry and liquid chromatography–mass spectrometry to determine the chemical compounds in tea. However, these methods are complex, highly susceptible to environmental factors, and costly (Wang et al., 2021a). To overcome these limitations, researchers have used a series of objective and smart nondestructive testing techniques to evaluate the quality of tea. These techniques provide information on the colour, shape, aroma, and flavour of tea for the comprehensive analyses of tea samples.

Near-infrared spectroscopy (NIRS) primarily relies on low-energy electronic transitions and stretching vibrations in hydrogen-containing groups, such as in C—H, N—H, O—H, P—H, and S—H (Arslan et al., 2020). Due to the presence of hydroxyl-containing compounds like catechins and amino acids in tea leaves, near-infrared spectroscopy can be employed to detect these components. Firmani et al. (2019) used NIRS in conjunction with partial least squares discriminant analysis (PLS-DA) and soft independent modelling of class analogies to distinguish Darjeeling tea with protected geographical indication from other varieties of adulterated Darjeeling tea. Although benchtop NIR spectrometers provide accurate and objective results, they are difficult and expensive to use in complex environments outside the laboratory. Therefore, micro-NIR spectrometers have been integrated into smartphones to achieve low cost and portability. micro-NIR spectrometers provide results similar to those of benchtop NIR instruments (Wang et al., 2020). Li et al. (2021) used smartphone-based micro-NIR technology to classify black tea, achieving an accuracy of 100 % for the calibration set and 94.29 % for the prediction set. Although NIRS enables qualitative and quantitative assessments of key quality components in tea leaves (Chen et al., 2018), it cannot capture the visual characteristics of tea leaves. By contrast, a computer vision system (CVS) can extract information such as colour, texture, and shape from images of tea samples and can objectively reproduce the visual characteristics of

* Corresponding author.
E-mail address: ningjm1998009@163.com (J. Ning).
[1] These authors contributed equally to this work.

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tea leaves. This technique can distinguish between colour change patterns of tea samples and predict the concentrations of colour-related compounds (Ren et al., 2021). Wang et al. (2023) used a CVS to extract colour variables from images of tea samples and to monitor the fermentation process of black tea. The results of this approach play a major role in the pricing and sale of tea leaves. Ren et al. (2021) used a CVS to extract six shape features from images of tea samples. Using these morphological features, they developed a prediction model with an accuracy of 100 % for evaluating the quality of black tea. However, none of these methods can detect components related to the aroma of tea leaves. By contrast, colorimetric sensor array (CSA) simulate the operating principle of the human sense of smell, enabling the acquisition of aroma information from tea samples. Its principle is to use the response pattern of sensor array cross-reactivity to obtain specific fingerprint information for differentiation of the substances to be measured. Studies have reported that porphyrin materials produce cross-responses to volatile gases such as alcohols, amines, ethers, thioethers and thiols, aromatics, halocarbons, and ketones (Li et al., 2022). Unlike electronic noses (e-noses), CSA is minimally affected by environmental conditions, such as temperature and humidity. Li et al. (2023) used the characterization information obtained from CSA to achieve rapid quantitative prediction of major volatile organic compounds during black tea fermentation. Therefore, when a single technique is employed, only one aspect of tea samples is evaluated, which provides limited information for determining the quality of tea.

Multiple technologies have been integrated to evaluate tea samples from different perspectives. Some studies have highlighted the benefits of integrating different sources of information for the comprehensive evaluation of tea samples. For instance, Liu et al. (2022) used NIRS in conjunction with a CVS to quantitatively predict moisture during green tea processing. They combined low- and mid-level data and discovered that mid-level data fusion yielded more favourable results. Zhou et al. (2023) used a CVS in conjunction with an e-nose to obtain colour and aroma information, and through data fusion, they detected the fermentation degree of black tea. Their results indicated that mid-level data fusion outperformed low-level data fusion. Overall, the quality of black tea is determined by its colour, shape, aroma, and flavour. To overcome the limitations associated with the use of a single technique, additional comprehensive sensor data should be analysed, and other data fusion strategies should be implemented to evaluate the quality of black tea.

Black tea has various chemical components, of which catechins are one of the most crucial. During the production of black tea, catechins are gradually transformed into aromatic aldehydes, ketones, theaflavins, and thearubigins, which influence the aroma, flavour, and colour of black tea (Hua et al., 2021). These compounds have a substantial effect on the mouthfeel and flavour of black tea, thereby affecting its overall quality (Chen et al., 2018). In terms of sales, the quality of tea leaves influences the price of the final tea product, with higher-quality tea being more expensive than lower-quality tea. Therefore, to ensure the correct grading and pricing of tea leaves during the sale process, a rapid, accurate, and reliable method is required for evaluating tea quality.

In this study, we investigated the use of multiple sensor technologies in conjunction with multivariate statistical analysis and data fusion strategies for the nondestructive, objective, and accurate measurement of black tea quality for the purpose of black tea classification. First, we used multiple sensor technologies, such as NIRS, computer vision, and colorimetric sensor array, to obtain spectral, shape, colour, and aroma data. Second, we developed qualitative discrimination models based on these spectral, shape, colour, and aroma data and evaluated the effects of low-, mid-, and high-level data fusion on black tea classification. Third, we developed customised smartphone software for NIRS for obtaining spectral data and build quantitative models for relevant flavour substances in black tea. Fourth, we compared individual spectral, shape, colour, and flavour data with other detection results after data fusion.

2. Materials and methods

2.1. Sample materials

Keemun black tea samples were obtained from Xiangyuan Tea (Anhui, China). Based on their sensory evaluation, they were divided into seven grades: Grade 1, Grade 2, Grade 3, Grade 4, Grade 5, Grade 6, and Grade 7.

2.2. Artificial sensory evaluation

Based on the GB/T 23776–2018 "Tea sensory evaluation method", nine tea assessors carried out an organoleptic assessment of the tea samples. The total tea sensory evaluation score is calculated as follows:

Total sensory score = appearance × 25 % + liquor colour × 10 % + aroma × 25 % + flavor × 30 % + infused leaf × 10 %.

2.3. Spectrum acquisition

A smartphone-compatible micro-NIR spectrometer was used to collect spectral data from seven varieties of Keemun black tea. Spectral data were collected using a NIR-S-R2 spectrometer (InnoSpectra Corporation, Taiwan, China) with a spectral range of 900–1700 nm and a scanning resolution of 7.03 nm. Six scans were averaged to obtain the final spectrum, resulting in a total of 228 data points (spectral variables) per spectrum. Approximately 50 g of tea was collected from each cultivar and ground into powder. This powder was then sieved through an 80-mesh sieve (with a mesh diameter of less than 0.180 mm) to obtain the samples. A total of 30 samples were prepared for each tea variety, which were used for spectral data collection. The spectral data were then saved in CSV format on the smartphone and uploaded to a computer for further processing and analysis.

2.4. Image acquisition

The imaging signals acquired in this study primarily consisted of colour and shape signals. The colour signals were acquired using a self-developed portable recording system consisting of a dark box, a digital camera, and a laptop. For image acquisition, approximately 10 g of black tea was accurately weighed in a Petri dish. The laptop was then used to extract the hue, saturation, and value (HSV) of each tea leaf image. Subsequently, the HSV colour channels were individually quantised to create feature vectors. The following methods were used to partition the HSV colour channels of each tea leaf image:

$$H=\begin{cases}0 & h\in[0,15]\cup(345,360]\\1 & h\in(15,25]\\2 & h\in(25,45]\\3 & h\in(45,55]\\4 & h\in(55,80]\\5 & h\in(80,108]\\6 & h\in(108,140]\\7 & h\in(140,165]\\8 & h\in(165,190]\\9 & h\in(190,220]\\10 & h\in(220,255]\\11 & h\in(255,275]\\12 & h\in(275,290]\\13 & h\in(290,316]\\14 & h\in(316,330]\\15 & h\in(330,345]\end{cases}, \tag{1}$$

$$S=\begin{cases}0 & s\in(0,0.15]\\1 & s\in(0.15,0.4]\\2 & s\in(0.4,0.75]\\3 & s\in(0.75,1]\end{cases}, \tag{2}$$

$$V = \begin{cases} 0 & v \in (0, 0.15] \\ 1 & v \in (0.15, 0.4] \\ 2 & v \in (0.4, 0.75] \\ 3 & v \in (0.75, 1] \end{cases}. \tag{3}$$

The quantised results of the HSV colour channels were combined into a one-dimensional feature vector, *F*, as follows:

$$F = L_S L_V H + L_V S + V \tag{4}$$

where L_S is the number of quantisation levels for the S component, and L_V is the number of quantisation levels for the V component. Equations (1), (2), (3), and (4) are used to obtain the feature vector *F* with values in the range of [0, 255]. The entire colour space is represented as a feature vector with 256 levels. To calculate the frequency of each feature vector, a histogram of colour features is created for denoting a colour feature.

The shape signals were acquired using a self-developed image acquisition system consisting of an industrial camera (MV-U500, with a resolution of 2592 × 1944 pixels), a backlight, a roller sieve, a linear motion module, and a carrier platform. After the images were uploaded to the computer, shape feature parameters were extracted. Leaf width (*d*) is defined as the average width of a leaf, leaf length (*l*) is defined as the length of the leaf skeleton, leaf area (*S*) is defined as the number of pixels occupied by the leaf, and leaf perimeter (*C*) is defined as the number of pixels occupied by the outer contour of the leaf. The length-to-width ratio (*N*) represents the rectangularity of a single leaf, which is calculated as $N = l/d$. Rectangularity (*R*) represents the degree of filling of the bounding rectangle, which is calculated as $R = S/(l \times d)$. In this study, after the feature parameters were extracted, each feature was distributed within a specific range. For instance, the leaf length was distributed within the range of 0–36 mm with a step size of 3 mm. The leaf width was distributed within the range of 0–5 mm with an increment of 0.5 mm. The leaf area was divided into intervals of 500 pixels within the range of 0–6000 pixels. The leaf perimeter was divided into intervals of 50 pixels within the range of 0–650 pixels. The length-to-width ratio was distributed within the range of 0.1–1 with an increment of 0.1. Rectangularity was distributed within the range of 0–31 with a step size of 5. The frequency of each feature was calculated, and a histogram of all shape features was created for denoting a shape feature.

2.5. Aroma acquisition

The selection of the materials in the study was based on our team's previous working study, which found a strong response to the volatile components produced in tea.

In this experiment, a CSA was developed to obtain aroma information from tea samples. To determine the optimal substrate and dabbing method for the sensor array, we examined the RGB response values of a CSA consisting of various combinations of C2 reversed-phase silica gel plates, filter papers, and Research Plus multichannel and microcapillary pipettes. We then compared the RGB response values of each dye dot in the sensor array to evaluate the performance of each combinations.

As shown in Fig. S1, a CSA was fabricated using porphyrin. Chemically reactive dyes were dissolved in *N*,*N*-dimethylacetamide solution and sonicated for 30 min to obtain a concentrated solution of 2 mg/mL porphyrin. A C2 reversed-phase silica gel plate was then used as a substrate for the CSA. Subsequently, a microcapillary pipette was used to draw 5 μL of the prepared dye solution and to deposit it on the silica gel plate, resulting in dye spots with a diameter of 3 mm. Finally, the CSA was allowed to dry in a ventilated fume hood for 15 min and then sealed for further use.

To understand the reaction pattern and response time of the sensor array, the CSA was exposed to Keemun black tea samples as the reaction substrate. This step was conducted for examining the response of the CSA to the reaction substrate over an exposure period of 28 min, with RGB images of the sensor array acquired every 2 min, starting from the beginning of the reaction. This process enabled the generation of difference images, illustrating the temporal variations in the reaction. Through the analysis of these difference images, the optimal reaction time was identified, which could be applied in further experiments.

During the procedure, 3 g of each black tea sample was placed in a clean Petri dish. The CSA was then positioned over different black tea samples, and the reaction proceeded at room temperature. RGB images of the CSA were captured using a flatbed scanner before and after the reaction.

2.6. Chemical analysis

The catechin content in various black tea samples was determined using the method outlined in the national standard titled "Determination of Tea Polyphenols and Catechins in Tea" (GB/T 8313-2018). Fig. 1 shows the experimental workflow employed in this study.

2.7. Data fusion strategy

Four algorithms, namely support vector machine (SVM), least-squares SVM (LS-SVM), extreme learning machine, and PLS-DA, were used to qualitatively differentiate between the grades of black tea. Support vector regression (SVR) was also used to quantitatively identify the flavour substances of black tea.

Data fusion is a method for integrating information from diverse sources to enable a more comprehensive assessment. Typically, data fusion is classified into three levels: low, middle, and high. In low-level data fusion, data obtained from each sensor are simply merged, ensuring that all information is preserved. In mid-level data fusion, feature information is extracted from various sensor data and combined to eliminate redundancy and enhance computational efficiency. In high-level data fusion, individual regression models are constructed and the final predictions are generated by using the results of the model data from each sensor in combination. Consequently, the prediction results of each model can be analysed, and integrated decisions can be made. Fig. S2 shows the data fusion strategy used in this study.

2.8. Self-developed software

This research is based on the Java programming language and utilizes Google's official Integrated Development Environment tool, Android Studio, for software development. The main functions of the software include spectral scanning and model prediction. The acquired data is first transmitted via Bluetooth and stored on a mobile device. Subsequently, the data is preprocessed and feature extracted, and then the predictive models are used to classify the samples and calculate the catechin content.

3. Results

3.1. Sensory evaluation

As shown in Table S1, when the quality of black tea decreased, the total score decreased. Other scores also demonstrated similar decreasing trends. In terms of appearance, the degree of uniformity of black tea gradually decreased when the sample colour shifted from black to grey. In terms of liquor colour, the degree of redness gradually decreased. In terms of aroma and flavour, the degree of sweetness decreased. In infused leaves, the degrees of both redness and tenderness decreased.

Overall, the sensory quality of black tea is influenced by several factors. Generally, black teas with good raw material tenderness also have higher sensory quality (Zhang et al., 2011). In terms of raw material for Keemun black tea, higher-quality tea samples typically consist of leaves with greater plucking tenderness. Therefore, higher-quality black tea has greater sensory quality than lower-quality black tea.

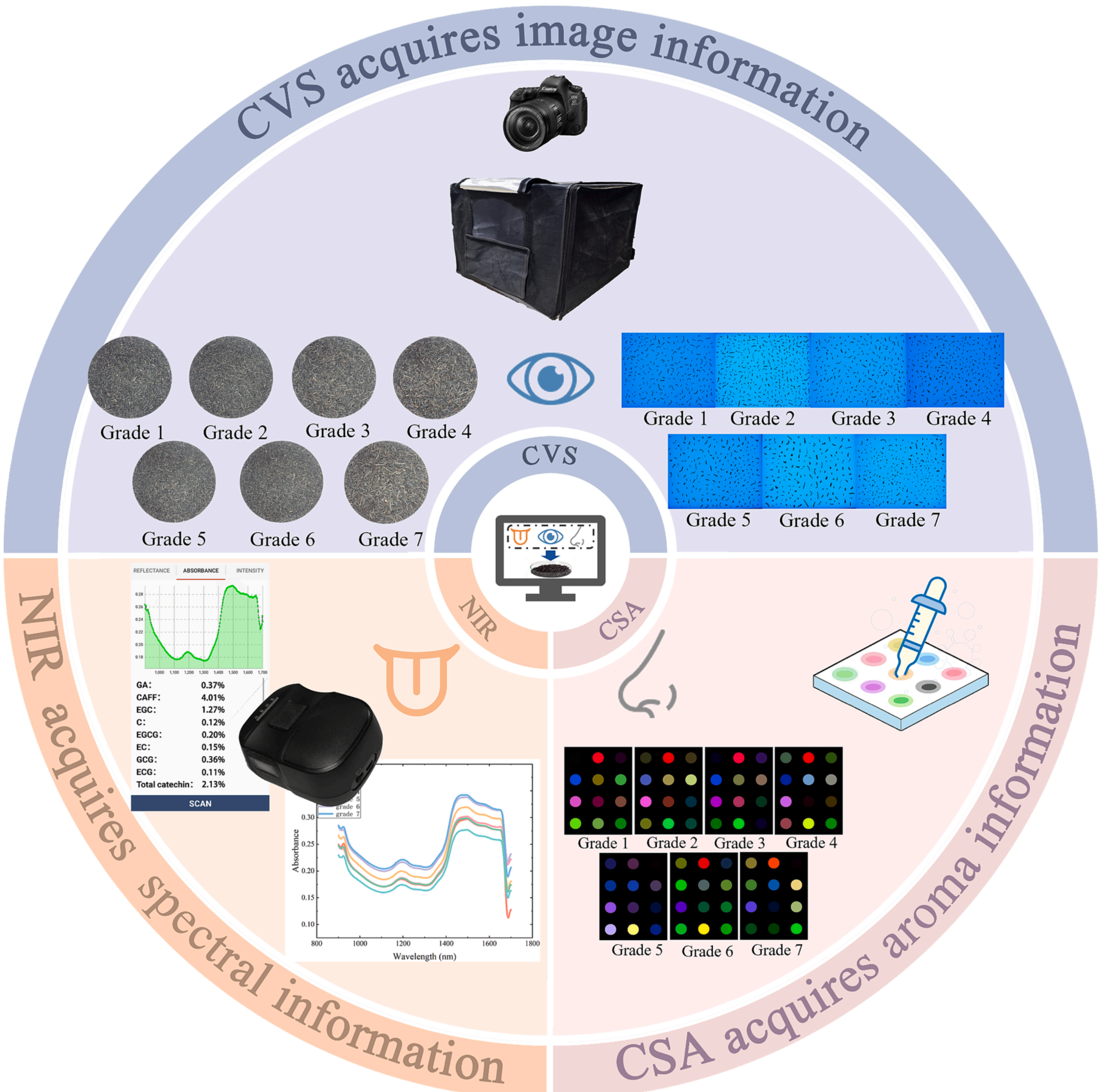

Fig. 1. Experimental flowchart.

3.2. Feature selection

3.2.1. NIRS feature selection

Fig. 2 A (a) and 3 A (b) show the original and averaged spectral curves obtained using micro-NIR spectroscopy. As indicated by these curves, the spectral trends of different grades of tea were similar. Prominent absorption peaks were observed in the wavelength ranges of 920–930, 1190–1200, 1490–1500, and 1650–1660 nm. The absorption peak observed near 930 nm was ascribed to the second overtone of O—H vibration in water molecules. The peak observed within the range of 1165–1180 nm was ascribed to the second overtone of –CH═CH in free amino acids and C—H vibration in catechins. The absorption peak observed near 1500 nm corresponded to the first overtone of O—H vibration in water molecules. The peak observed near 1650 nm was ascribed to the second overtone of C—H and S—H vibration in caffeine (Wang et al., 2021).

3.2.2. CVS feature selection

Fig. 2 B (a) depicts the images of different grades of black tea acquired using the self-developed portable acquisition system. Fig. 2 B (b) shows the resulting histograms after the distribution of various features within specific ranges. As indicated by the graphs, the features of higher-grade tea leaves were mainly distributed in the range of 125–175, whereas those of lower-grade tea leaves were mainly distributed in the range of 25–75. When the tea grade increased, the overall frequency of feature vectors demonstrated an initial increase followed by a decrease. Typically, feature vectors represent the quantification of hue, saturation, and brightness components, with higher frequency values indicating

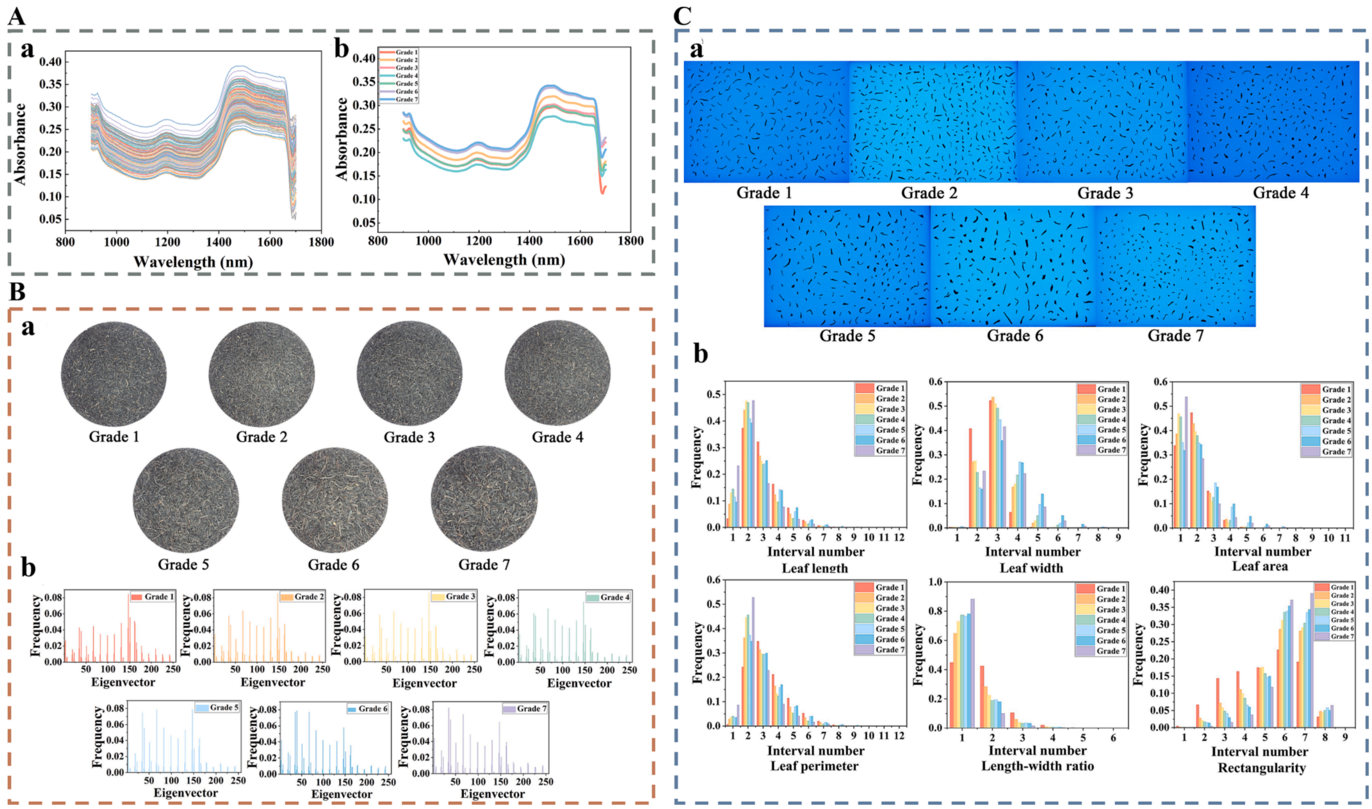

Fig. 2. A (a) Raw data and A (b) average data of spectral curves of different grades of Keemun black tea. B (a) Computer vision acquisition of colour images and B (b) Colour feature histogram of different tea grades. C (a) Computer vision acquisition of shape images and C (b) Shape feature histogram of different tea grades.

stronger interactions between these components, resulting in more distinct colour characteristics. Hence, higher-grade tea leaves have a brighter and more vivid colour, whereas lower-grade tea leaves have a darker and less vivid colour. These findings were consistent with our sensory evaluation results. Overall, these findings may be ascribed to the high stem content in low-grade tea leaves, which affects the overall colour.

Fig. 2 C (a) depicts the images of different grades of black tea acquired using the self-developed image acquisition system. Fig. 2 C (b) shows the resulting histograms after features were distributed with specific ranges. As indicated by the graphs, the distribution of shape features varied across different tea grades. However, relatively small differences in certain intervals were observed for adjacent tea grades. For instance, the leaf length was mainly distributed in the second interval, demonstrating an overall increasing trend followed by a decreasing trend. The leaf width was mainly distributed in the third interval, indicating wider leaves for tea of lower grades. The leaf area was mainly distributed in the first and second intervals, with smaller areas found for higher-grade tea leaves. The leaf perimeter was mainly distributed in the second and third intervals, demonstrating an overall increasing trend followed by a decreasing trend. The length-to-width ratio was mainly distributed in the first interval, indicating a gradual decrease in length as the tea grade decreased. Rectangularity was mainly distributed in the sixth and seventh intervals, demonstrating a gradual increase as the tea grade decreased.

Higher-grade tea leaves are selected from fresh leaves comprising one bud and one or two leaves, whereas lower-grade tea leaves typically consist of one bud and three or four leaves. This distinction in leaf composition may result in higher-grade tea leaves exhibiting a finer and longer appearance than their lower-grade counterparts. However, certain characteristics of Grade 7 tea leaves deviate from this pattern. This deviation can be attributed to the fact that Grade 7 tea leaves have low quality requirements. To minimise costs and prevent the wastage of raw materials, manufacturers can combine leftover materials from other grades to produce Grade 7 tea leaves (Song et al., 2021).

3.2.3. CSA feature selection

Fig. 3(a) presents the comparison results of the response differences of arrays constructed using various combinations of C2 reversed-phase silica gel plates, filter papers, and Research Plus multichannel and microcapillary pipettes. Under the same conditions, the response differences of the sensor arrays varied. Specifically, the combination of C2 reversed-phase silica gel plates and microcapillary pipettes exhibited higher RGB response values than other combinations. Therefore, this combination was selected as the optimal method for the sensor array in the subsequent experiment.

Fig. 3(b) shows the comparison results of the optimal response time. At the beginning of the experiment, a substantial colour change was observed in the dye spots. However, with the reaction time, the intensity of colour change gradually diminished, until it reached saturation at approximately 22 min. Consequently, in subsequent experiments, an optimal response time of 22 min was selected.

Fig. 3(c) depicts RGB difference images of the response array before and after the reaction for various grades of tea samples. Because of differences in raw materials, each grade of black tea contains distinct volatile flavour substances. After interaction with these chemical components, the porphyrin dyes in the response array exhibited characteristic colour changes. The number and brightness of the reaction spots clearly revealed distinct colour change patterns for different tea grades. Additionally, the similarity in colour change patterns obtained from difference images in parallel experiments using the same tea grade suggested favourable reproducibility of the experiment. Notably, the colour changes of the reaction spots were similar for Grades 1, 2, 3, and 4 and for Grades 6 and 7, indicating similar volatile flavour substances in adjacent tea grades.

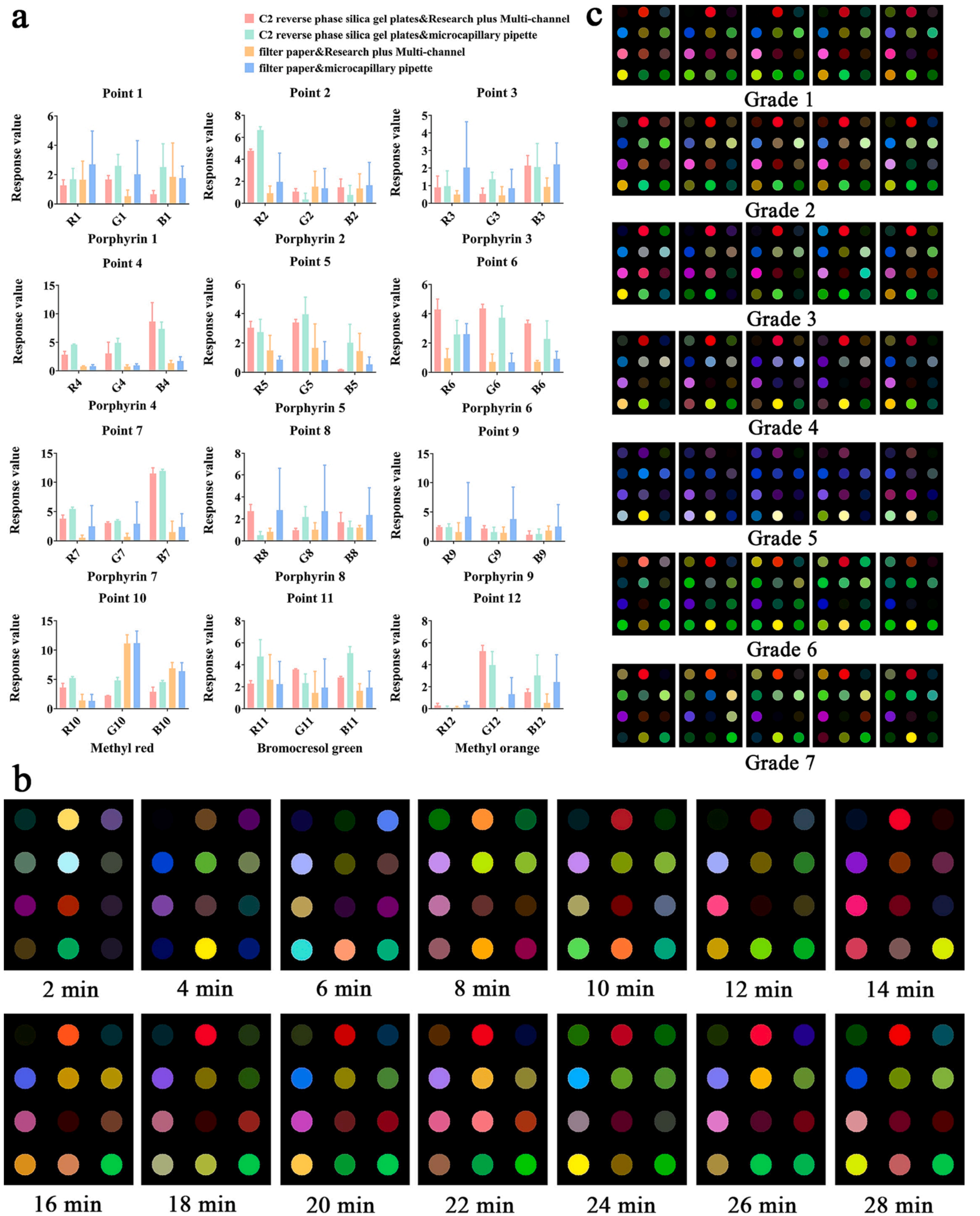

Fig. 3. (a) Comparison of bar charts of the optimal base plate and point board method. (b) Comparison of optimal response time difference images. (c) Difference images of finished products for different black tea grades in a CSA.

3.2.4. Data analysis of quality components

Fig. 4 presents the concentrations of various flavour substances in each grade of black tea. As the tea grade increased, the concentration of gallic acid (GA) initially decreased, then increased, and decreased again. As the tea grade increased, the concentration of caffeine (CAFF) initially increased, then decreased, then increased again, and finally decreased. As the tea grade increased, the concentrations of catechins initially increased, then decreased, and then increased again. Particularly, the concentration of epigallocatechin (EGC) was high. These findings can be attributed to the extensive degradation of epigallocatechin gallate (EGCG), epicatechin gallate (ECG), and epicatechin (EC) during the fermentation of black tea, leading to decreases in their concentrations. During the fermentation process, the hydrolysis of galloylated catechins may have produced some non-galloylated catechins, such as EGC (Zhang et al., 2019).

3.3. Prediction models for data from a single sensor

The K-S sample partitioning algorithm was utilized to randomly divide the samples into training and prediction sets in a 2:1 ratio. Table S2 presents the prediction results of various algorithms for Keemun black tea grading.

Among the four models, the SVM model consistently outperformed the other models in terms of spectral, shape, colour, and aroma data. For micro-NIR spectral data, the SVM model achieved an accuracy of 100 % on the training set and 91.43 % on the prediction set. For colour and shape data, the SVM model also achieved an accuracy of 100 % and 99.29 %, respectively, on the training set and 90.00 % and 85.71 %, respectively, on the prediction set. However, for aroma data, the SVM model achieved an accuracy of 95 % on the training set and only 77.14 % on the prediction set. Because implementing a single technique captures only one aspect of the characteristics of a sample, the discriminatory accuracy of these models is relatively low. Therefore, these models should be integrated to comprehensively evaluate tea quality from multiple perspectives.

3.4. Discriminant models for multilevel data fusion

The data obtained from various techniques are typically multidimensional and may contain a large amount of irrelevant information. If all of this information is used for modelling, the prediction accuracy of the model used may decrease. Therefore, for modelling, variable selection methods are required to select highly relevant feature variables from all variables. Table S3 presents the prediction results of classification models for Keemun black tea grading with different variable selection methods, including competitive adaptive reweighted sampling, particle swarm optimisation (PSO), successive projections algorithm, and variable combination population analysis. For spectral, colour, and shape data, the PSO model outperformed the other models, achieving identification rates with an accuracy of 99.29 %, 100.00 %, and 95.71 %, respectively, on the training set and 94.29 %, 92.86 %, and 87.14 %, respectively, on the prediction set, thereby yielding satisfactory results. However, for aroma data, the performance of the variable selection methods was lower than that for the original data. This discrepancy may be attributed to fewer variables in the aroma data and because the variable selection methods may have eliminated useful information along with useless information.

In this study, data fusion was used to integrate spectral, colour, shape, and aroma data obtained using NIRS, CVS, and CSA techniques, with low-, mid-, and high-level data fusion. The mid-level fusion data consisted of the four types of single-sensor data from obtained after PSO-based variable selection, whereas the high-level fusion data consisted of the model calculation results of the four types of single-sensor data obtained using PLS-DA. Table 1 presents the discrimination results obtained by applying four models to the fused data. Among all models, the LS-SVM model exhibited the highest performance. In low-level fusion, the discrimination accuracy of 100 % on the training set and with four misclassified samples out of 70 in the prediction set, resulting in an accuracy of 94.29 %. Among all fusion methods, mid-level fusion exhibited the highest overall performance, with a discrimination accuracy of 100 % on the training set and with only one misclassified sample in the prediction set, resulting in an accuracy of 98.57 %.

3.5. Quantitative prediction of the concentrations of chemical components

An SVM regression model was constructed using spectral data combined with the measured concentrations of flavour substances. The model results are listed in Table 2. In terms of predicting the concentrations of CAFF, catechin (C), and EC, the SVR models constructed using preprocessed data achieved the highest prediction performance among all models. For these three-component prediction models, The correlation coefficient for the training sets (Rc) were all greater than 0.9,

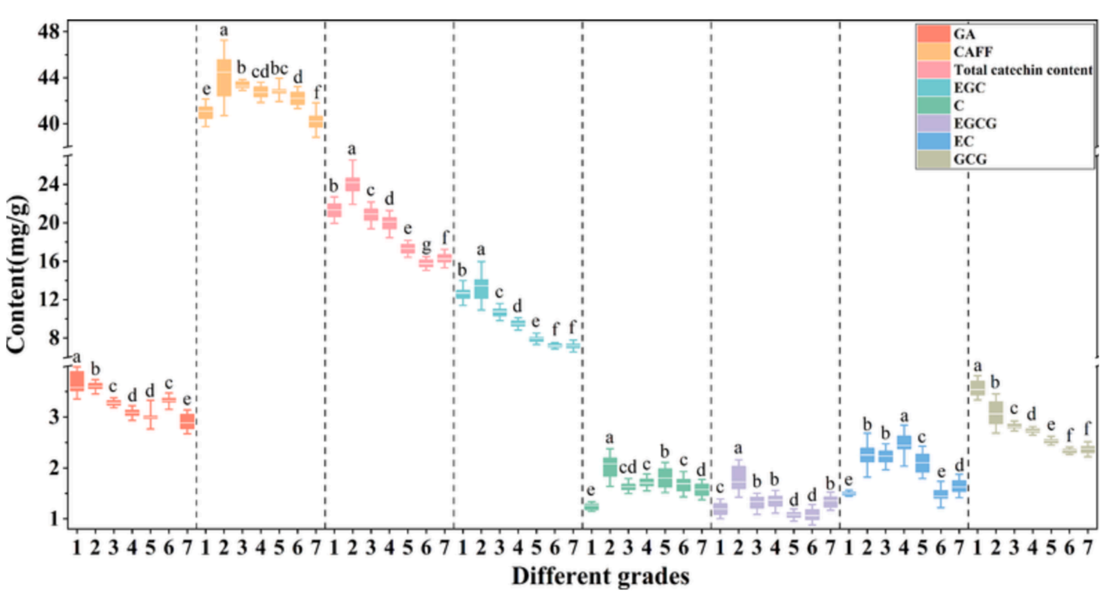

Fig. 4. Concentrations of flavour substances in different Keemun black tea grades. *Letters in Fig. 4 represent significant differences in flavour substances in different grades of tea.

Table 1
Model discrimination results based on multi-layer fusion information.

Data	Model	NVs	Parameter	Calibration set		Prediction set	
				Result	CCR	Result	CCR
Low-level	SVM	591	c = 12.126, g = 0.009	139/140	99.29 %	49/70	70.00 %
	LS-SVM	**591**	σ^2 **= 259.450,** γ**= 333.070**	**140/140**	**100.00 %**	**66/70**	**94.29 %**
	ELM	591	n = 53	121/140	86.43 %	42/70	60.00 %
	PLS-DA	591	LVs = 3	55/140	39.29 %	26/70	37.14 %
Middle-level	SVM	304	c = 194.012, g = 0.016	140/140	100.00 %	50/70	71.43 %
	LS-SVM	**304**	σ^2 **= 934.417,** γ **= 53.067**	**140/140**	**100.00 %**	**69/70**	**98.57 %**
	ELM	304	n = 53	115/140	82.14 %	38/70	54.29 %
	PLS-DA	304	LVs = 2	54/140	38.57 %	26/70	37.14 %
High-level	SVM	4	c = 0.001, g = 0.082	127/140	90.71 %	63/70	90.00 %
	LS-SVM	**4**	σ^2 **= 1.846,** γ **= 3.795**	**129/140**	**92.14 %**	**66/70**	**94.29 %**
	ELM	4	n = 33	119/140	85.00 %	55/70	78.57 %
	PLS-DA	4	LVs = 4	109/140	77.86 %	57/70	81.43 %

and the correlation coefficient for the predicted sets (Rp) were all greater than 0.8, thereby indicating the high prediction accuracy of the models. However, after variable selection, the prediction performance of the three components decreased, presumably because of the removal of crucial feature wavelengths during the selection process.

In terms of predicting the concentrations of GA, EGC, EGCG, gallocatechin gallate (GCG), and total catechins, the SVR models constructed using preprocessed and variable-selected data achieved the highest prediction performance among all models. The Rc and Rp values were all greater than 0.8. The preprocessing of most of the data resulted in improved prediction performance, suggesting that data preprocessing can aid in retaining useful information while eliminating interfering factors, such as noise. In addition, all models exhibited residual predictive deviation (RPD) values greater than 2.0, indicating their high accuracy for the quantitative prediction of the concentrations chemical components among different tea grades.

4. Discussion

Keemun black tea is primarily graded depending on its colour, aroma, flavour, and shape. Computer vision can be used to obtain information on the shape and colour of black tea. Each grade of black tea has a certain shape. However, the shape variations between adjacent grades are small. These findings are consistent with those of Song et al. (2021). In terms of colour, higher-grade tea leaves have a vibrant and bright colour, whereas lower-grade tea leaves tend to have a less vibrant and darker colour. Colorimetric sensor array is used to obtain information on the aroma of black tea. Each grade of black tea has a distinct content of volatile aroma substances. However, the colour variations between adjacent grades are small. These findings are consistent with those of Huo et al. (2014). NIRS is used to obtain information on the aroma and flavour of black tea. Several grades of tea exhibit similar NIRS spectra, indicating similar flavour attributes. These findings are consistent with those of Wang et al. (2021b).

Table S4 presents the results of some studies on the quality of different grades of tea. According to the results of traditional sensory evaluation methods, higher-grade tea has higher overall sensory quality scores, with the concentrations of flavour substances serving as the material basis for high-quality tea (Pang et al., 2022). However, traditional sensory evaluation methods are subjective. Han et al. (2022) and Zeng et al. (2023) have used liquid chromatography quadrupole time-of-flight mass spectrometry and gas chromatography–mass spectrometry to objectively analyse tea leaves. These techniques, however, are associated with high costs and complex operation. Therefore, more convenient nondestructive testing techniques have been introduced. Liu et al. (2019) used NIR technology to identify different grades of green tea, achieving an accuracy of 100 %. However, the use of a single technology detects only specific quality characteristics. Therefore, data fusion has been introduced to improve model accuracy. Xu et al. (2019) reported that the integration of an e-nose and computer vision technology increased the accuracy of tea quality identification in comparison with the use of a single sensor. Similarly, Ren et al. (2020) successfully differentiated between black tea grades by combining spectral and image information. However, in these studies, no comprehensive analyses of tea samples were conducted. Given the small differences between adjacent grades of Keemun black tea and the potential for confusion, combining multiple sensory technologies is necessary to comprehensively capture the quality characteristics of black tea and to achieve precise and objective quality assessments. In this study, we combined spectroscopy with shape, colour, and aroma data to classify tea grades, providing a more comprehensive approach. We also implemented different data fusion strategies, including low-, mid-, and high-level fusion strategies.

Most of the aforementioned studies have focused on the qualitative discrimination of tea grades. In this study, we applied micro-NIRS technology to quantitatively evaluate flavour substances in different grades of Keemun black tea. In the future, we intend to develop a mobile app for the rapid identification of the grade of Keemun black tea, and we will integrate it into an online detection system. Compared with traditional detection techniques, our technique is faster, nondestructive, and capable of rapidly monitoring a large number of samples. These capabilities lay the foundation for the development of online monitoring tools. This simple yet efficient method, which requires minimal operation, can be useful for protecting consumer rights and regulating the market.

5. Conclusion

In this study, we examined the feasibility of integrating spectroscopy with shape, colour, and aroma data for evaluating the quality of different grades of Keemun black tea. Using multiple data fusion strategies, including low-, mid-, and high-level data fusion, we developed a discrimination model that is more accurate than models based on a single method. Among all models, the LS-SVM model combined with mid-level data fusion achieved the highest accuracy (98.57 %) on the test set. We also used spectroscopic data to quantitatively determine flavour substances in black tea. For GA, CAFF, EGC, C, EGCG, EC, GCG, and total catechins, the Rc values were 0.96767, 0.96165, 0.96606, 0.91554, 0.83693, 0.99827, 0.96288, and 0.98500, respectively, and the Rp values were 0.84089, 0.94249, 0.94050, 0.83820, 0.81111, 0.82670, 0.93230, and 0.93608, respectively. All RPD values were greater than 2. In summary, we developed a comprehensive strategy for evaluating the quality of different grades of Keemun black tea, thereby overcoming the limitations of single-sensor data. This strategy can be widely implemented to predict the concentrations of flavour substances in different grades of black tea.

Table 2
Prediction model results of Keemun black tea flavour substances based on SVR.

Flavour substances	Model	N	Parameter	Calibration set		Prediction set		
				Rc	RMSEC	Rp	RMSEP	RPD
GA	raw-SVR	228	c = 64, g = 0.25	0.78215	0.02843	0.64750	0.03748	7.80
	MSC-SVR	228	c = 1.3195, g = 1024	0.98675	0.00248	0.83273	0.02673	10.93
	SNV-SVR	228	c = 1.3195, g = 2.2974	0.98533	0.00275	0.83596	0.02640	11.07
	detrend-SVR	228	c = 6.9644, g = 337.7940	0.98849	0.00223	0.81270	0.02984	9.79
	SNV-CARS-SVR	16	c = 21.1121, g = 0.0825	0.78296	0.03606	0.78430	0.03273	8.93
	SNV -PSO-SVR	**115**	**c = 1.3195, g = 4**	**0.96767**	**0.00604**	**0.84089**	**0.02613**	**11.18**
	SNV -SPA-SVR	6	c = 12.1257, g = 2.2974	0.87309	0.02165	0.79316	0.03597	8.12
CAFF	raw-SVR	228	c = 588.1336, g = 0.7579	0.66633	1.46282	0.59004	1.63990	0.97
	MSC-SVR	228	c = 6.9644, g = 1024	0.95767	0.21426	0.79430	0.92299	1.72
	SNV-SVR	**228**	**c = 4, g = 4**	**0.96165**	**0.19628**	**0.94249**	**0.78878**	**2.01**
	detrend-SVR	228	c = 6.9644, g = 1024	0.93994	0.30974	0.70611	1.29427	1.23
	SNV-CARS-SVR	9	c = 6.9644, g = 21.1121	0.76536	1.10858	0.69325	1.30098	1.22
	SNV-PSO-SVR	120	c = 6.9644, g = 4	0.95855	0.20941	0.77918	0.98670	1.61
	SNV-SPA-SVR	20	c = 337.7940, g = 1.3195	0.69636	1.34749	0.70343	1.30542	1.22
EGC	raw-SVR	228	c = 1024, g = 4	0.96378	0.48084	0.88055	1.44331	1.76
	MSC-SVR	228	c = 1024, g = 4	0.94672	0.69236	0.89541	1.27572	1.99
	SNV-SVR	228	c = 1024, g = 0.0090	0.94483	0.71573	0.89422	1.29048	1.97
	detrend-SVR	228	c = 588.1336, g = 21.1121	0.96289	0.50830	0.90451	1.21140	2.10
	detrend-CARS-SVR	**34**	**c = 337.7940, g = 337.7940**	**0.96606**	**0.46023**	**0.94050**	**0.75619**	**3.37**
	detrend-PSO-SVR	131	c = 337.7940, g = 111.4305	0.98135	0.26957	0.90792	1.18229	2.15
	detrend-SPA-SVR	4	c = 194.0117, g = 1024	0.89033	1.35514	0.86096	1.65931	1.53
C	raw-SVR	228	c = 6.9644, g = 12.1257	0.85907	0.01976	0.73203	0.03718	7.26
	MSC-SVR	228	c = 6.9644, g = 36.7583	0.82991	0.02219	0.76947	0.03201	8.44
	SNV-SVR	228	c = 6.9644, g = 0.0825	0.82604	0.02261	0.76833	0.03222	8.38
	detrend-SVR	**228**	**c = 0.4353, g = 1024**	**0.91554**	**0.01273**	**0.83820**	**0.02452**	**11.01**
	detrend-CARS-SVR	25	c = 6.9644, g = 194.0117	0.79905	0.02718	0.73156	0.03668	7.36
	detrend-PSO-SVR	94	c = 6.9644, g = 1024	0.98744	0.00180	0.79834	0.02719	9.93
	detrend-SPA-SVR	14	c = 1.3195, g = 1024	0.79382	0.02699	0.70170	0.03983	6.78
EGCG	raw-SVR	228	c = 588.1336, g = 0.7579	0.86638	0.02183	0.69835	0.03245	7.78
	MSC-SVR	228	c = 1.3195, g = 588.1336	0.95801	0.00708	0.71035	0.03229	7.82
	SNV-SVR	228	c = 1.3195, g = 1.3195	0.95394	0.00778	0.71145	0.03210	7.87
	detrend-SVR	228	c = 36.7583, g = 12.1257	0.83063	0.02856	0.70293	0.03246	7.78
	detrend-CARS-SVR	**17**	**c = 6.9644, g = 2.2974**	**0.83693**	**0.02440**	**0.81111**	**0.02215**	**11.40**
	detrend-PSO-SVR	113	c = 2.2974, g = 1.3195	0.93329	0.01102	0.72003	0.03069	8.23
	detrend-SPA-SVR	4	c = 588.1336, g = 0.0825	0.70227	0.04106	0.42659	0.03841	6.57
EC	raw-SVR	228	c = 1024, g = 0.1436	0.79936	0.06240	0.82348	0.05998	7.08
	MSC-SVR	228	c = 21.1121, g = 36.7583	0.87562	0.04074	0.80499	0.06280	6.76
	SNV-SVR	228	c = 6.9644, g = 0.1436	0.84719	0.04924	0.79949	0.06449	6.59
	detrend-SVR	**228**	**c = 4, g = 1024**	**0.99827**	**0.00066**	**0.82670**	**0.05907**	**7.19**
	detrend-CARS-SVR	28	c = 6.9644, g = 1024	0.85763	0.04621	0.82105	0.05803	7.32
	detrend-PSO-SVR	107	c = 1.3195, g = 588.1336	0.81701	0.05894	0.79832	0.06819	6.23
	detrend-SPA-SVR	5	c = 36.7583, g = 337.7940	0.72687	0.08128	0.68969	0.09393	4.52
GCG	raw-SVR	228	c = 588.1336, g = 1.3195	0.97191	0.01014	0.90149	0.03423	12.40
	MSC-SVR	228	c = 6.9644, g = 588.1336	0.99974	0.00010	0.93071	0.02610	16.26
	SNV-SVR	228	c = 6.9644, g = 1.3195	0.99974	0.00010	0.93098	0.02605	16.29
	detrend-SVR	228	c = 588.1336, g = 1.3195	0.94119	0.02181	0.87707	0.04159	10.21
	SNV-CARS-SVR	**26**	**c = 2.2974, g = 6.9644**	**0.96288**	**0.01321**	**0.93230**	**0.02400**	**17.69**
	SNV-PSO-SVR	112	c = 4, g = 2.2974	0.99912	0.00033	0.91524	0.03052	13.91
	SNV-SPA-SVR	1	c = 1.3195, g = 194.0117	0.89673	0.03547	0.87179	0.04309	9.85
Total catechins	raw-SVR	228	c = 1024, g = 2.2974	0.94186	1.11227	0.84704	2.5337	1.18
	MSC-SVR	228	c = 64, g = 111.4305	0.98007	0.37653	0.90168	1.66529	1.79
	SNV-SVR	228	c = 64, g = 0.2500	0.97849	0.40774	0.90173	1.66452	1.79
	detrend-SVR	228	c = 337.7940, g = 194.0117	0.99999	0.00010	0.88199	2.13100	1.40
	SNV-CARS-SVR	**28**	**c = 21.1121, g = 12.1257**	**0.98500**	**0.26878**	**0.93608**	**1.13169**	**2.64**
	SNV-PSO-SVR	109	c = 337.7940, g = 0.2500	0.98711	0.23312	0.88995	1.88097	1.59
	SNV-SPA-SVR	11	c = 337.7940, g = 0.7579	0.95425	0.82753	0.81030	3.52120	0.85

Ethical statements

Participants gave informed consent via the statement “I am aware that my responses are confidential, and I agree to participate in this sensory evaluation” where an affirmative reply was required to enter the sensory evaluation. They were able to withdraw from the sensory evaluation at any time without giving a reason. The tea products evaluated were safe for consumption.

CRediT authorship contribution statement

Luqing Li: Formal analysis, Methodology, Investigation, Writing – review & editing, Project administration, Funding acquisition. **Yurong Chen:** Conceptualization, Methodology, Investigation, Formal analysis, Data curation, Writing – original draft. **Shuai Dong:** Formal analysis, Writing – review & editing. **Jingfei Shen:** Data curation. **Shuci Cao:** Validation, Supervision. **Qingqing Cui:** Validation, Supervision. **Yan Song:** Validation, Supervision. **Jingming Ning:** Resources, Project administration, Funding acquisition.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The authors do not have permission to share data.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.fochx.2023.100924.

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