Contents lists available at ScienceDirect



Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy



Rapid and non-destructive discrimination of special-grade flat green tea using Near-infrared spectroscopy



SPECTROCHIMICA

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ARTICLE INFO

ABSTRACT

Article history: Received 14 May 2018 Received in revised form 27 July 2018 Accepted 30 July 2018 Available online 01 August 2018

Keywords: Near-infrared spectroscopy Sensory quality Green tea Specific spectral region Sensory-related chemical compounds Special-grade green tea is a premium tea product with the best rank and high value. Special-grade green tea is normally classified by panel sensory evaluation which is time and sample costly. Near-infrared spectroscopy is considered as a promising rapid and non-destructive analytical technique for food quality evaluation and grading. This study established a discrimination method of special-grade flat green tea using Near-infrared spectroscopy. Full spectrum was used for partial least squares (PLS) modelling to predict the sensory scores of green tea, while specific spectral regions were used for synergy interval-partial least squares (siPLS) modelling. The best performance was achieved by the siPLS model of MSC + Mean Centering pretreatments and subintervals from 15 intervals. The optimal model was used to discriminate special-grade flat green tea with the prediction accuracy of 97% and 93% in the cross-validation and external validation respectively. The chemical compositions of green tea samples were also analyzed, including polyphenols (total polyphenols, catechins and flavonol glycosides), alkaloids and amino acids. Principal components analysis result showed that there is potential correlation between specific spectral regions and the presence of polyphenols and alkaloids. Thus, NIR technique is a practical method for rapid and non-destructive discrimination of special-grade flat green tea with chemical support. © 2018 Elsevier B.V. All rights reserved.

1. Introduction

Green tea is one of the popular non-alcoholic beverages over the word. The consumption of green tea is generally increasing due to its health benefits such as anti-oxidation, anti-senescence and other functions against cardiovascular disease [1]. China is the biggest green tea market and producer in the world. Green tea accounts for above 50% of total tea products consumption in China and the production of green tea has excessed 1.524.000 tons in 2016 [2]. The export of green tea is around 270,000 tons, which accounts for 82% of total tea export in China [2]. Special-grade green tea is the premium tea products with the highest grade. It is characterized by super-excellent appearance features, bright and green tea infusion, high and pleasant aroma, and umami taste due to its rigorous harvesting standard of fresh tea leaf and delicate processing. Special-grade green tea in China is manually harvested only in spring season with the harvesting standard of one bud or one bud with one leaf [3] leading to the high production cost. In 2016, special-grade tea accounted for 44% of total tea production in China, while the production value of special-grade tea excessed 69% of total production value of tea [2].

Special-grade green tea is difficult to be discriminated from other grades of green tea only based on dry tea appearance. The sensory

* Corresponding authors. E-mail addresses: FangyFan@zju.edu.cn (F. Fan), shuygong@zju.edu.cn (S. Gong). evaluation is necessary to identify the special-grade green tea. To date, tea sensory evaluation in China is carried out by professional human panel test according to the National standardized method, demanding specific and qualified room, specific brewing tea sets and methods, which is time costly and inconvenient. Besides, it takes long time to train a sensory evaluation expert, and the sensory evaluation results are likely to be influenced by environment, individual and even the emotion of panel member, which results in a low repeatability of results and a low comparability of samples evaluated by different panel or different spatio-temporal batch.

Therefore, a rapid, feasible and repeatable method is in need for classification of special-grade green tea and sensory quality assessment. Near-infrared spectroscopy (NIR) technique, with the advantages of rapid, accuracy and non-destruction, has been used for food quality evaluation, such as grape seeds and skins [4], Chinese rice wine [5] and coffee [6]. NIR is based on different chemical bonds absorb or emit light at different wavenumbers, and prominent absorption bands are related with some hydrogen-based functional groups like C—H, C—O, O—H, N—H et al. [7]. There are various sensory-related chemical compounds present in tea leaves, mainly including tea polyphenols (e.g. catechins and flavonol glycosides), alkaloids and amino acids [1]. These chemical constituents have their specific related absorbance regions on NIR spectrum [8,9]. NIR was used for quantitative measurement of total polyphenol content ($R_p = 0.9382$) [10], major catechins ($R_p = 0.9760$ for EGCG; $R_p = 0.9763$ for ECG) [11], caffeine ($R_p = 0.9471$)

[10], and free amino acid ($R_p = 0.958$) [12] in tea leaf. These chemical compounds have considered being responsible for sensory quality of green tea [13]. Thus, NIR has the potential for assessing green tea sensory quality.

In the present study, NIR was used to establish a model for nondestructive discrimination of special-grade green tea from other grade green tea. Flat tea was used for NIR analysis so as to eliminate the detection error due to the interspace between tea leaves. To elevate the prediction accuracy of the model, modelling results using full spectrum and specific spectrum regions of NIR were compared, and the correlation with sensory-related chemical compounds including catechins, flavonol glycosides, alkaloids, amino acids and total polyphenols were discussed.

2. Materials and Methods

2.1. Collection of Commercial Green Tea Samples and Chemicals

A total of 279 flat green tea samples were collected from tea market in Zhejiang province, including 127 special-grade tea and 152 other grades samples. Details of samples are shown in Appendix A. All the samples were stored in sealed plastic bags at -20 °C before NIR spectroscopy measurement, sensory evaluation and chemical compounds determination.

The reference compounds of individual catechins, (-)-epicatechin (EC, \geq 98%), (–)-epigallocatechin (EGC, \geq 98%), (–)-epicatechin gallate (ECG, \geq 98%), (-)-epigallocatechin 3-gallate (EGCG, \geq 98%), (-)gallocatechin (GC, \geq 98%), and (-)-gallocatechin gallate (GCG, \geq 98%), individual purine alkaloids caffeine (CAF, ≥98%), theobromine (TB, ≥98%) and theophylline (TP, ≥98%), individual flavonol glycosides Quercetin 3 o glucoside (Que-glu, \geq 98%), Quercetin 3 o galactoside (Que-gala, $\geq 98\%$), Quercetin 3 o rutinoside (Que-rut, $\geq 98\%$), Myricetin 3 o glucoside (Myr-glu, ≥98%), Myricetin 3 o galactoside (Myr-gala, \geq 98%), Myricetin 3 *o* rhamnoside (Myr-rha, \geq 98%), Kaempferol 3 o glucoside (Kae-glu, ≥98%), and Kaempferol 3 o rutinoside (Kae-rut, ≥98%), individual free amino acids Aspartic acid (Asp, ≥98%), Glutamic acid (Glu, ≥98%), Asparaginate (Asn, ≥98%), Serine (Ser, ≥98%), Glutamine (Gln, ≥98%), Histidine (His, ≥98%), Glycine (Gly, ≥98%), Threonine (Thr, $\geq 98\%$), Arginine (Arg, $\geq 98\%$), Alanine (Ala, $\geq 98\%$), γ Aminobutyric acid (Gaba, \geq 98%), Theanine (Thea, \geq 98%), Tyrosine (Tyr, ≥98%), Valine (Val, ≥98%), Tryptophan (Trp, ≥98%), Phenylalanine (Phe, \geq 98%), Isoleucine (Ile, \geq 98%), Leucine (Leu, \geq 98%) and Lysine (Lys, ≥98%) were purchased from Shanghai Yuanye Bio-Technology Co., Ltd. (Shanghai, China). And the other chemical reagents used were of analytical grade purchased from Sinopharm Chemical Reagent Co. Ltd. (Shanghai, China). The ultra-pure water (>18 M Ω cm) was prepared by Milli-Q[™] reference system (Merck Millipore, Milford, MA, USA).

2.2. NIR Spectral Measurement and Pretreatment

The NIR spectra of green tea samples were recorded by a NIR Spectrometer (Büchi N-200, Flawil, Switzerland) in diffuse reflection mode at room temperature, with a resolution of 2 cm⁻¹ and a wavenumber range of 10,000 cm⁻¹-4000 cm⁻¹. The reflectance was detected by Indium Gallium Arsenide (InGaAs). Ten grams of whole dry tea leaves were placed into a glass Petri dish. All tea samples were measured in triplicate and the average spectra were processed. Raw spectra were processed by the specific spectral pretreatment methods including multiplicative signal correction (MSC), Mean Centering, Savitzky-Golay filter with 9 point and differentiation (first derivation and second derivation). The spectral pretreatment and processing were carried out by Büchi NIRCal 5.4 software (Büchi, Flawil, Switzerland).

2.3. Sensory Evaluation

Sensory evaluation of green tea was carried out according to the National Standard of China (GB/T23776-2009), which was in corresponded to international norm ISO 3103:1980. The sensory evaluation panel included 6 members (4 women and 2 men). All of them were professional and trained expert sensory assessors. Sensory evaluation included 5 terms of dry leaf appearance, color and taste of tea infusion, aroma and infused tea leaf. For dry leaf appearance, the factors of shape, maturity, color, and uniformity were assessed. For tea infusion, 3 g tea was weighed and extracted with 150 mL boiling water in 4 min, and the tea infusion was collected for color (brightness and clarity), aroma (flavor, strength, purity and permanency) and taste (body, umami and astringency) assessments. Besides, the infused leaf was inspected for the assessment of tea leaf maturity and color. Dry leaf appearance (x_1) , tea infusion color (x_2) , aroma (x_3) , taste (x_4) and infused leaf appearance (x_5) were scored based on a total point of 100. A higher score represented a better sensory property. The total sensory quality was calculated according to Eq. (1):

$$Score = \sum_{i=1}^{5} w_i x_i \tag{1}$$

 X_i (i = 1, 2, 3, 4, 5) is the score of 5 sensory terms and w_i is the weight coefficient of each sensory term ($w_1 = 0.25, w_2 = 0.1, w_3 = 0.25, w_4 = 0.3, w_5 = 0.1$). Special-grade green tea was differentiated from other grade green tea by total sensory score above 90 point.

2.4. Establishment of NIR Models

All the green tea samples were divided into two subsets. The calibration set (185 samples) was used for model development and cross validation, while the validation set (94 samples) was used to test the practical utility of the established models. To avoid the bias, the division was made as follows: all the samples were sorted according to their total sensory scores, then two samples were selected from every three samples into the calibration set [5]. Both subsets constituted covered similar sensory score ranges (calibration set: 72.85–95.60, validation set: 73.40–94.98) and means (calibration set: 88.05, validation set: 87.89). Calibration set covered the full range of sensory scores and the RSD values of the means of two subsets were 1.94%. It indicated that samples distribution in calibration and validation sets were uniform and satisfactory, and could impose quite a challenge to estimate strong models.

Full spectrum and specific spectral regions were used for model establishment. Full spectrum with the wavenumbers of 10,000 cm⁻¹– 4000 cm⁻¹ was used for predicting sensory scores using partial least squares (PLS) regression. Specific spectral regions were selected by synergy interval PLS (siPLS) in order to improve PLS model performance. The siPLS models were built with specific spectral regions divided from the full spectrum divided into 10, 12, 15, 17, 20 and 30 equal intervals. Then all possible combinations of 4 intervals were used for modelling by PLS methods. The accuracy of model was evaluated based on correlation coefficient (R) combined with root mean square error (RMSE) and ratio prediction deviation (RPD). The correlation coefficient is defined as follows [14]:

$$\mathbf{R} = \sqrt{1 - \frac{\sum \left(y_{pred} - y_{ref}\right)^2}{\sum \left(y_{pred} - y_{ref}\right)^2}}.$$

The RMSE and RPD are:

$$\text{RMSE} = \sqrt{\frac{\sum \left(y_{pred} - y_{ref}\right)^2}{N}}$$

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