

Short communication

Determination of total polyphenols content in green tea using FT-NIR spectroscopy and different PLS algorithms

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Abstract

This paper attempted the feasibility to determine content total polyphenols content in green tea with near infrared (NIR) spectroscopy coupled with an appropriate multivariate calibration method. Partial least squares (PLS), interval PLS (iPLS) and synergy interval PLS (siPLS) algorithms were performed comparatively to calibrate regression model. The number of PLS components and the number of intervals were optimized according to root mean square error of cross-validation (RMSECV) in calibration set. The performance of the final model was evaluated according to root mean square error of prediction (RMSEP) and correlation coefficient (R) in prediction set. Experimental results showed that the performance of siPLS model is the best in contrast to PLS and iPLS. The optimal model was achieved with $R = 0.9583$ and $RMSEP = 0.7327$ in prediction set. This study demonstrated that NIR spectroscopy with siPLS algorithm could be used successfully to analysis of total polyphenols content in green tea, and revealed superiority of siPLS algorithm in contrast with other multivariate calibration methods.

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1. Introduction

Tea polyphenols substance is of great interest due to its beneficial medicinal properties [1]. There is increasing evidence that polyphenols substances found in tea can enhance general health. Recently, many researches have suggested that antioxidants found in polyphenols substances, may have an important role to prevent cardiovascular disease [2], chronic gastritis [3,4] and some cancers [5,6,7]. Additionally, polyphenols compounds are mainly responsible for the characteristic astringent and bitter taste of tea brews [8]. In recent years, many methods of analysis have been employed to determine total polyphenols content in tea, such as colorimetric measurements and titration method with potassium permanganate [9]. However, these methods are all time-consuming. Near infrared reflectance spectroscopy is a fast, accurate and non-destructive technique that can be employed as a replacement of time-consuming chemical method.

Near infrared (NIR) spectroscopy has been proved to be a powerful analytical tool used in the agricultural, nutritional, petrochemical, textile and pharmaceutical industries [10–19]. Since 1990s, attempts have been made to simultaneously predict alkaloids and phenolic substance in green tea leaves using near infrared spectroscopy [20,21]. Some studies on the quantitative analysis of total antioxidant capacity in green tea by NIR are also reported in 2003 and 2004 [22,23]. Recently, Some researchers applied near infrared spectroscopy to analyze simultaneously the content of free amino acids, caffeine, total polyphenols and amylose in green tea [24–27].

For these works mentioned above, near infrared spectral data calibrations are often made with the classical multivariate calibration analysis, for example, partial least squares (PLS) regression and artificial neural net (ANN). Many spectral pre-treatment methods have been developed to reduce the effects of variations in the spectral data that are not related to the chemical variations in the samples [24,25]. These methods often improve the calibrations, but they do not take into account that there might be spectral regions that do not contain any information about the chemical variations in the samples [28]. In fact, one of the major problems in multivariate data analysis is to select appropriate

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spectral region in order to achieve the best performance. Some researchers have constructed PLS models in different spectral regions to quantify compositions content in tea, however, these regions were selected manually [27]. Spectral regions selected manually might as well weaken the performance of the calibration model without prior experienced knowledge about NIR spectroscopy.

In recent years, both theoretical and experimental evidence have been published that spectral region selection can significantly improve the performance of these calibration techniques [29,30]. It is so important to select specific regions where contain much information that generate more stable models with superior interpretability, and this will produce the lowest prediction error. Some methods have been recently described in the literature to implement spectral region selection and have used PLS for multivariate calibration in each subset [30].

A graphically oriented local modeling procedure called interval partial least squares (iPLS) was presented for usage on NIR spectral data [30,31]. It has shown that selective optimum interval in the spectral data could give precision prediction models. Norgaard et al. (2000) also proposed a method called Synergy Interval PLS (siPLS) to select several intervals spectra data which could split the data set into a number of intervals (variable-wise) and calculates all possible PLS model combinations of two, three or four intervals.

In this research, we investigate and compare the results provided by PLS, iPLS and siPLS procedures for NIR quantitative analysis of total polyphenols content in green tea. We systematically studied the different steps that have to be gone through in model calibration. The number of PLS factor and the number of regions intervals were optimized according to the root mean square error of cross-validation (RMSECV) in calibration set. The performance of the final model was evaluated according to the root mean square error of prediction (RMSEP) and the correlation coefficient (R) in prediction set.

2. Materials and methods

2.1. Sample preparation

All tea samples came from different provinces in China, and they were all already on stock within 4 months period. Taking into consideration the heterogeneity of tea samples, the samples would be ground before analysis. For the grinding, the whole tealeaves were put into a small electric coffee mill and ground during 10 s. After this procedure, the powders are sieved with a mesh width 500 μm and these sieved powders are used for the further analysis.

2.2. Chemical analysis

Total polyphenols content were reference measured by a photometric Folin-Ciocalteu assay according to a proposed international standard method [9]. Absorbance (E) at 540 nm of the reaction solution is determined in a 1 cm light-path cell by a Lengguang-752 spectrophotometer (Lengguang Optical Instru-

ment Ltd. Co., Shanghai, China). The calibration standard is gallic acid.

2.3. Spectra collection

The NIR spectra were collected in the reflectance mode using the Antaris. Near infrared spectrophotometer (Thermo Electron Co., USA) with an integrating sphere. Each spectrum was the average spectrum of 32 scans. The range of spectra is from 10,000 to 4000 cm^{-1} , and the data were measured in 3.856 cm^{-1} intervals, which resulted in 1557 variables.

The standard sample accessory holder was used for performing the tea spectra collection. The sample accessory holder is sample cup specifically designed by Thermo Electron Co. For each tea sample, 10 ± 0.1 g of dry tealeaves were filled into the sample cup in the standard procedure depending upon the bulk density of materials. The corresponding amount of dry tea powders was densely packed into the sample cup and then compressed by closing it. When spectra collecting, tea sample was collected one times every rotating the cup 120° angle, thus, each sample was collected three times. The average of the three spectra, which were collected from the same tea sample, was used in the next analysis. The temperature was kept around 25°C and the humidity was kept at a steady level in the laboratory.

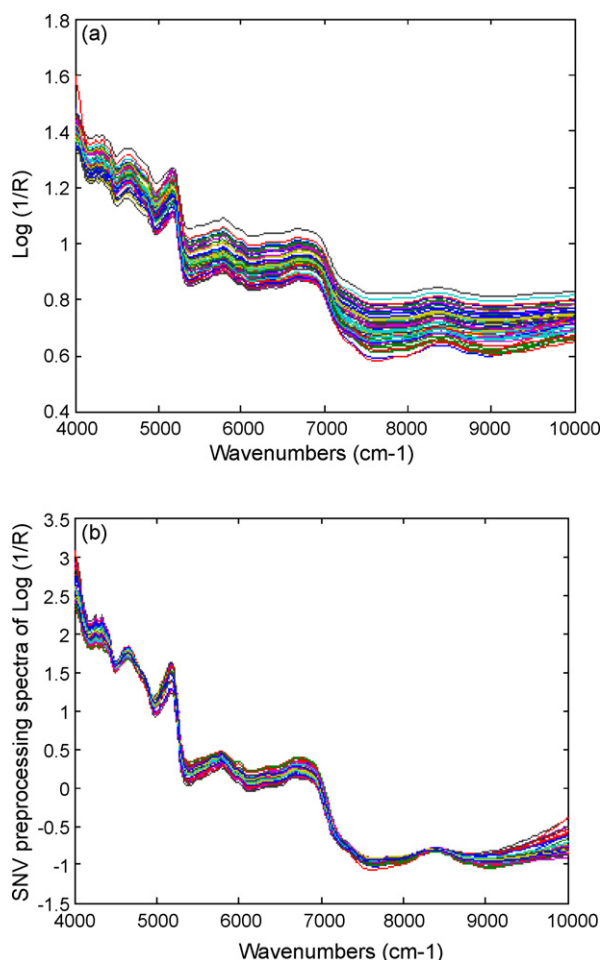


Fig. 1. Spectra of tea obtained from (a) raw data and (b) SNV preprocessing data.

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