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Potential application of UV-visible spectroscopy and PLS-DA method to discriminate Indonesian CTC black tea according to grade levels

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Abstract. In this research, UV-visible spectroscopy combined with PLS-DA method was used to discriminate Indonesian CTC black tea with two different grade levels. A total of 20 CTC black tea samples (1 gram of each samples) were collected from PT Perkebunan VIII plantation in West Java province of Indonesia. The samples consisted of two different grade levels, Broken Pekoe or BP1 (10 samples) and FNGS II (10 samples). The extraction of tea samples was performed by using hot distilled water. The spectral data of aqueous tea samples were obtained using a UV-visible spectrometer in the range of 190-1100 nm. The result of PCA showed that the tea samples can be well clustered into two groups according to grade levels using two PCs which accounted for 99% of the total variance (PC1=89% and PC2=10%). The best PLS-DA model had coefficient of determination (R^2) of 0.99 with RMSEC = 0.043. The result of the PLS-DA model showed that with the moving average smoothing combined with mean normalization spectral pre-treatment samples from the two different grade levels could be 100% correctly discriminated. The results demonstrated that UV-visible spectroscopy with PLS-DA method could be successfully applied to discriminate Indonesian CTC black tea according to grade levels.

1. Introduction

There were many different tea species among the world. Green and black teas are the two most popular categories. Black tea is second to water as the most consumed beverage globally, with daily consumption of around 500 ml a day [1-2]. In 2013, the Food and Agriculture Organization of the United Nations (FAO) reported that world tea production reached 5.0639 million tons (more than 70% is black tea). China is the largest tea producing country accounting for more than 40 percent of the world tea production [3]. In Indonesia, average annual tea productivity is about 1.5 ton per hectares (ha) with five top central productions is located at West Java province (66.93% contribution), North Sumatera



province (6.23%), Central Java province (6.90%), West Sumatera province (5.27%) and East Java province (4.20%). More than 80% of Indonesian tea export is black tea [3].

The price of black tea is strongly depend on its quality and appearance. In other hand, the quality of black tea is influenced by several factors such as local growing conditions, climatic conditions, soil, harvesting time, as well as processing and preparation methods that influence the of final tea product [4]. In Indonesia, there are two tea processing methods for black tea namely orthodox and CTC (crush, tear and curl) methods. It is known that the aroma characteristics of the two tea are different [5].

In traditional way, the evaluation of quality of tea is currently graded manually by using trained tea testers, who evaluate tea samples based on the following: aroma, liquor color, texture, and morphological aspects [6]. There are several drawbacks of manual inspection: tedious, time consuming, and expensive and inconsistent (the results can be non-repetitive and subjected to physical and mental state of tea testers) [6]. Several analytical methods have been proposed to assess the quality of tea such as NIR spectroscopy [7-9], fluorescence spectroscopy [10], chemical analysis [11], high performance liquid chromatography (HPLC) [12], voltammetric analysis [13], and electronic nose and tongue [6]. However, most of these methods are destructive, expensive, and almost complicated.

Recently, a relatively cheap and simple spectroscopic method based on UV-visible spectroscopy has been used for food quality evaluation such as coffee [14-18], honey [19] and cocoa [20]. UV-visible spectroscopy has been used to discriminate several origin of green and black tea [21]. However, there is no report on the use of UV-visible spectroscopy for classification of CTC black tea according to grade levels. In this research, UV-visible spectroscopy with the aid of pattern recognition techniques (PCA and PLS-DA method) was attempted to identify different grades of Indonesian CTC black tea.

2. Materials and Methods

2.1. Tea samples

In this research, twenty CTC black tea samples (1 gram of each samples) were collected from PT Perkebunan VIII plantation in West Java province of Indonesia. The samples consisted of two different grade levels, BP1 (10 samples) and FNGS II (10 samples). The extraction of tea samples was performed by using hot distilled water.

2.2. Measurement of UV-Visible spectral data

The UV-Visible spectral data of aqueous tea samples from BP1 and FNGS II were obtained in the range of 190-1100 nm by using a UV-Vis spectrometer (Genesys™ 10S UV-Vis, Thermo Scientific, USA). This spectrometer was equipped with a quartz cell with optical path of 10 mm. The spectral acquisition was performed at spectral resolution of 1 nm at a room temperature (27-28°C). The raw spectra were pre-processed using mean normalization and moving averaging with seven segments.

2.3. Principal component analysis (PCA) and partial least squares-discriminant analysis (PLS-DA)

PCA is unsupervised chemometric analysis which is commonly applied in the field of analytical chemistry and process analytical technology (PAT) [22]. It is a suitable technique for an initial data screening and evaluation. In PCA, original data (spectral data) values are projected onto principal components (PCs) for cluster analysis. PLS-DA is a supervised model. It is based on PLS regression with a dummy variable as a reference value (variable Y). In the case of PLS-DA, the y variable contains the identification of classes (in this case, tea grade levels classes). In this research, the response variable y is composed of 0's and 1's, where the value 1 is assigned to BP1 samples and the value 0 to FNGS II samples. To evaluate the performance of PLS-DA model, the coefficient of determination (R^2), root mean square error of calibration (RMSEC) and root mean square error of cross-validation (RMSECV) are used in this research [23]. It is expected to have ideal models with lower RMSEC and RMSECV as well as higher R^2 . In most reported studies, a threshold of ± 0.5 was used to classify the PLS-DA samples. Here, a tea sample was classified as BP1 levels if its value was above 0.5 and classified as FNGS II levels if the value was below 0.5 [11]. All chemometrics analysis were performed using the Unscrambler

9.7 (CAMO AS, Oslo, Norway).

3. Results and Discussion

3.1. Spectral data of Indonesian CTC black tea with different grade levels

Figure 1 shows the pre-processed spectral data of tea samples with different grade levels, BP1 and FNGS II in the range of 190-1100 nm. In general, it is hard to see the difference between BP1 and FNGS II spectral data. Here, we can see a noisy spectral data in the range of 190-230 nm. In the range of 450-1100 nm, the intensity of absorbance is almost close to zero. For this reason, the spectral data in the range of 230-450 nm was used for further analysis (PCA and PLS-DA). In this range, we can see one peak of absorbance at wavelength around 285 nm and one valley of absorbance at wavelength around 250 nm. Those wavelengths may contain valuable information on differentiation between BP1 and FNGS II tea samples. Based on previous reported study, those wavelengths may refer to the absorbance of phenolic compounds presented in the tea extractions [24].

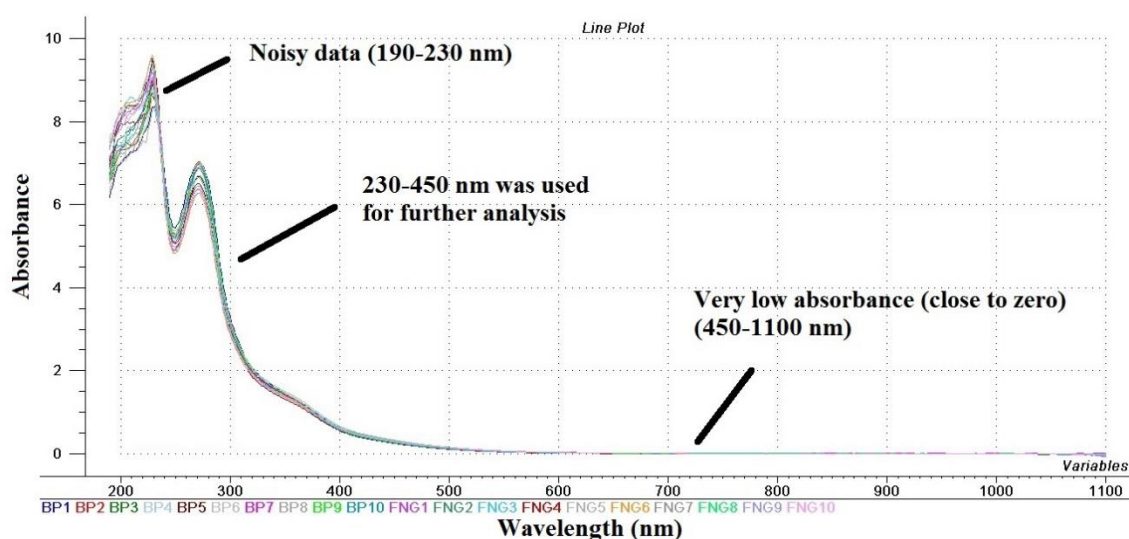


Figure 1. Plot of absorbance versus wavelength of pre-processed spectra of tea samples with two grade levels (BP1 and FNGS II) in the range of 190-1100 nm.

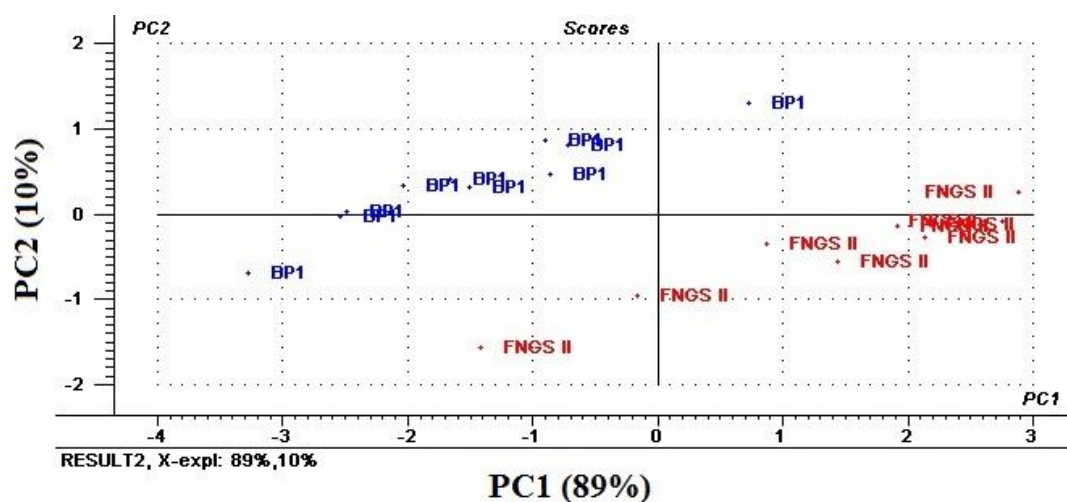


Figure 2. The result of PCA (PC1 versus PC2) using pre-processed spectra (mean normalization and smoothing moving average) in the range of 230-450 nm.

3.2. The result of PCA analysis

In order to see the initial clustering of the samples, PCA was performed using all samples (20 samples) using pre-processed spectral data in the range of 230-450 nm. The result of PCA was depicted in Figure 2. The total of PC1 and PC2 can explain 99% of the total variance of original data. We can see that the PCA resulted in good separation between BP1 and FNGS II samples. Tea samples from BP1 grade levels were clearly separated from FNGS II tea samples. The BP1 samples were laid in the negative of PC1 and most of FNGS II samples was located at the positive of PC1.

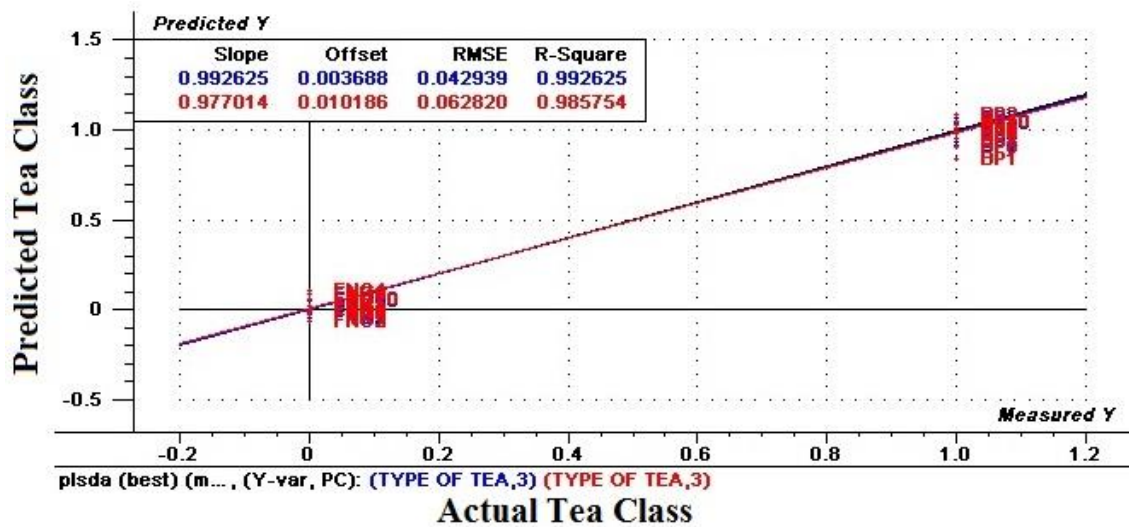


Figure 3. The best PLS-DA model developed using pre-processed spectra in the range of 230-450 nm.

3.3. The result of PLS-DA model development

Figure 3 showed the result for model development using PLS-DA method. The best PLS-DA model was obtained with very high coefficient of determination ($R^2 = 0.99$) for both calibration and validation. The $RMSEC = 0.043$ and $RMSECV = 0.063$. The quality of our PLS-DA model was comparable to that of previous reported studies in the field of tea authentication. For example, Chen *et al.* (2014) investigated the use of near-infrared spectroscopy and chemometrics on discrimination of white tea and albino tea and developed the best PLS-DA model with coefficient of correlation $r = 0.86519$, $RMSEC$ value of 0.247 and $RMSEP$ value of 0.201 [23].

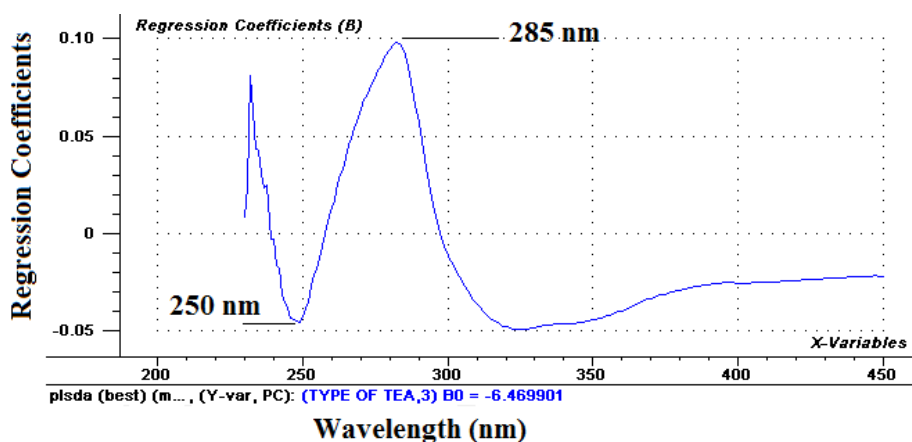


Figure 4. Plot of wavelengths versus regression coefficients for the best PLS-DA model developed using spectral data in the range of 230–450 nm.

3.4. Investigation of important wavelengths

In order to investigate the important wavelengths, plot of wavelength versus regression coefficient of the developed PLS-DA model was depicted as seen in Figure 4. There are two wavelengths with very high regression coefficients. First, wavelength at around 250 nm with negative regression coefficient of -0.05. The second wavelength was at around 285 nm with positive regression coefficient of 0.10. From here, we can see that the developed PLS-DA model for discrimination of BP1 and FNGS II tea samples were highly influenced by these two important wavelengths.

4. Conclusion

The current research has suggested that UV-visible spectroscopy coupled with chemometrics can serve as a reliable and effective tool to discriminate the grade levels (BP1 and FNGS II) of Indonesian CTC black tea. The separation and classification of BP1 and FNGS II samples were well achieved using PCA and PLS-DA method. In our research, the solvent for tea extraction is only water which are simpler (avoiding laborious sample preparation), environment friendly (free chemical waste) and cheaper (no additional operational costs). For this reason, in the near future, this result may open an authentication and quality evaluation of Indonesian CTC black tea based on UV-visible spectroscopy.

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