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The potential application of UV-visible spectroscopy and chemometrics for discrimination of Lampung robusta coffee with different fermentations

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Abstract. Coffee is one of the important agricultural products in Indonesia. In this present work, we evaluate the potential application of UV-visible spectroscopy and principal component analysis (PCA) to discriminate Lampung robusta coffee with different fermentation. Total of 300 samples was used with three fermentation conditions: 100 samples belong to F0 or ORI (no fermentation), 100 samples belong to F2 (fermented 2 days using special microbial fermentation), and 100 samples belong to F4 (fermented 4 days using special microbial fermentation). A hot distilled water was used to extract the coffee samples. The extraction procedure including dilution was performed based on several previous reported studies. The spectral data acquisition was done by using a UV-visible spectrometer in the range of 190-1100 nm (full-spectrum) with 1 nm of interval. The result showed that using an unsupervised classification of principal component analysis (PCA) using modified spectral data of standard normal variate (SNV) and moving average, the samples can be well clustered into three different groups of fermentation. Our results highlight the potential of UV-visible spectroscopy combined with chemometrics as a green and relatively fast analytical method to discriminate Lampung robusta coffee based on fermentation.

1. Introduction

Coffee is one of the important agricultural products in Indonesia. In 2017, coffee ranks next after palm oil, rubber, and coconut as Indonesia's most valuable agricultural export [1]. The current total coffee production in Indonesia is about 668.68 thousands ton with productivity of 731.34 kg/ha in 2018 [1]. Nowadays, the world specialty coffee market is growing significantly, providing high quality coffee. One of the types of specialty coffee from Indonesia is coffee with special fermentation. For example, a special production of Gayo Arabica coffee from Takengon, Aceh with several times of fermentation called Gayo Wine coffee is becoming popular. This coffee has a unique taste and high in price. The popularity and limited supply of Gayo Wine coffee makes it very vulnerable to fraudulent [2]. In Lampung, a special coffee fermentation is done using special microbial fermentation with different lengths of fermentation (2, 4, 6 and 9 days of fermentation). The difference in length of fermentation



resulted in a different and unique taste of coffee. However, in practice, it is not easy to discriminate Lampung robusta coffee with different in fermentation, especially for ground roasted coffee.

In order to support the fair trade of specialty coffee, it needs to develop an analytical method to ensure the authenticity of specialty coffee. In previous works, several reported studies have been published on the development of analytical methods for coffee authentication such as methods based on mass spectrometry and chromatography [3-5] and methods based on vibrational spectroscopy [6-8].

A simpler and cheaper analytical method based on electron transition spectroscopy (UV-visible spectroscopy) has been widely used for coffee authentication [9–18]. However, there is no report on the use of UV-visible spectroscopy for classification of ground roasted Lampung robusta coffee with different fermentation. Therefore, the objective of this present research is to investigate the application of UV-visible spectroscopy combined with principal component analysis (PCA) to classify ground roasted Lampung robusta coffee according to their length of fermentation.

2. Materials and Methods

2.1. *Coffee samples and spectral acquisition*

Total 300 samples (1 gram each sample) with same particle size (297 micrometers) was used with three fermentation conditions: 100 samples belong to F0 (no fermentation), 100 samples belong to F2 (fermented 2 days using special microbial fermentation), and 100 samples belong to F4 (fermented 4 days using special microbial fermentation). A hot distilled water was used to extract the coffee samples. The extraction procedure including dilution was performed based on several previous reported studies [9-18]. The spectral acquisition was performed using an aqueous coffee sample by pipetting 2 mL of coffee aqueous samples into a quartz cell with an optical path of 10 mm. The spectral data of aqueous coffee samples were measured in the range of 190-1100 nm by using a UV-Vis spectrometer (Genesys™ 10S UV-Vis, Thermo Scientific, USA) with a spectral resolution of 1 nm and room temperature about 27-28°C. The analysis of spectral data was done using original and modified spectra with a full and selected spectrum.

2.2. *Principal component analysis (PCA)*

Principal component analysis (PCA) is one of the most popular and widely used unsupervised methods for dimensionality reduction by converting a number of correlated variables into fewer variables called principal components (PCs) [2]. In this study, PCA was utilized to unsupervised classify the ground roasted Lampung robusta coffee samples based on their fermentation. Before performing PCA analysis, original spectral data was transformed into modified spectral data using standard normal variate (SNV) and moving average smoothing with 9 segments algorithms. PCA analysis was done using original and modified spectral data. The acceptance of the PCA result was evaluated based on the cumulative percentage of variance (CPV) of the calculated PC. To accept the PCA result, the CPV of more than 70%-85% is required [17]. The calculation of PCA was performed using the multivariate software of the Unscrambler 9.7 (CAMO Software AS, Oslo, Norway).

3. Results and Discussion

3.1. *Spectral analysis of coffee samples with different fermentation*

The original spectra of 300 coffee samples with different fermentation (0, 2 and 4 days of fermentation) in the range of 190-1100 nm were demonstrated in Figure 1. In the range of 190-250 nm, the spectral data is very noisy and should not be used for further analysis. In the range of 450-1100 nm, the absorbance value is close to zero. It means almost all light is transmitted in this wavelength range (no information). Figure 2 showed the modified spectral data in the range of 250-450 nm. Several peaks are identified at 256 nm, 280 nm, and 322 nm. Those wavelengths are well correlated to the absorbance of some chemical composition of coffee such as caffeine, chlorogenic acids and trigonelline [18].

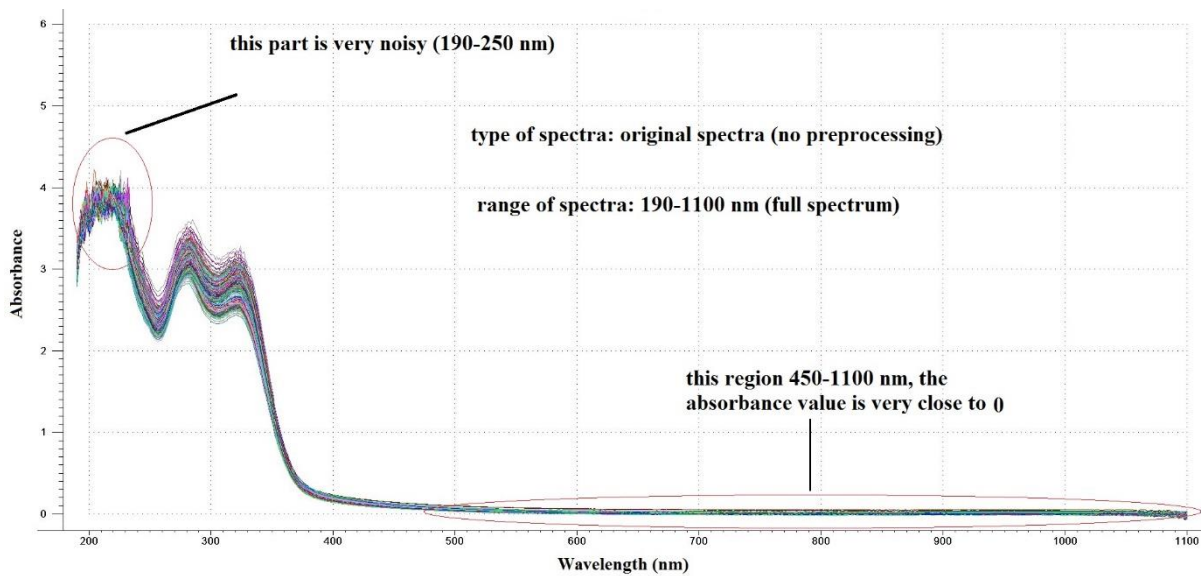


Figure 1. The original spectra of 300 samples of Lampung robusta coffee with different fermentation in the range of 190-1100 nm.

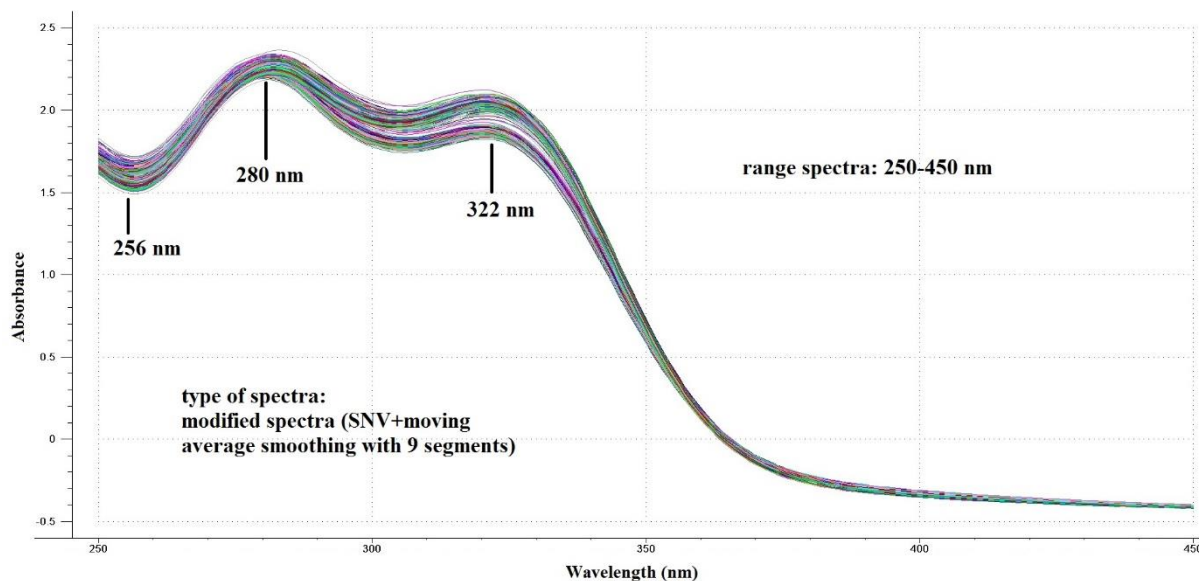


Figure 2. The modified spectra of 300 samples of Lampung robusta coffee with different fermentation in the range of 250-450 nm..

3.2. The result of PCA: mapping of samples

The result of PCA analysis in the term of plot scores using original and modified spectra was depicted in Figure 3 and Figure 4. It can be seen that both original and modified spectra in the range of 190-1100 nm (full-spectrum) and 250-450 nm (selected spectrum) resulted in a separation of coffee samples according to their length of fermentation. However, using two PCs (PC1 and PC2), modified spectra in the range of 250-450 nm resulted in higher cumulative percentages of variance (CPV = 98%) comparing to that of original spectra in the range of 190-1100 nm (CPV = 89%).

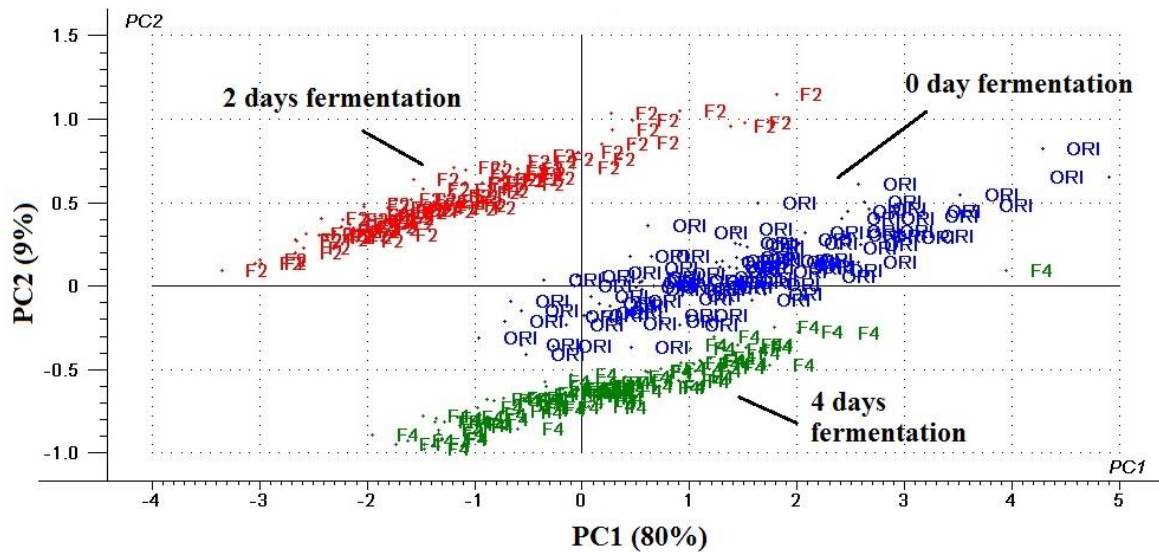


Figure 3. The result of the PCA analysis of coffee samples with different fermentation using original spectra in the range of 190-1100 nm.

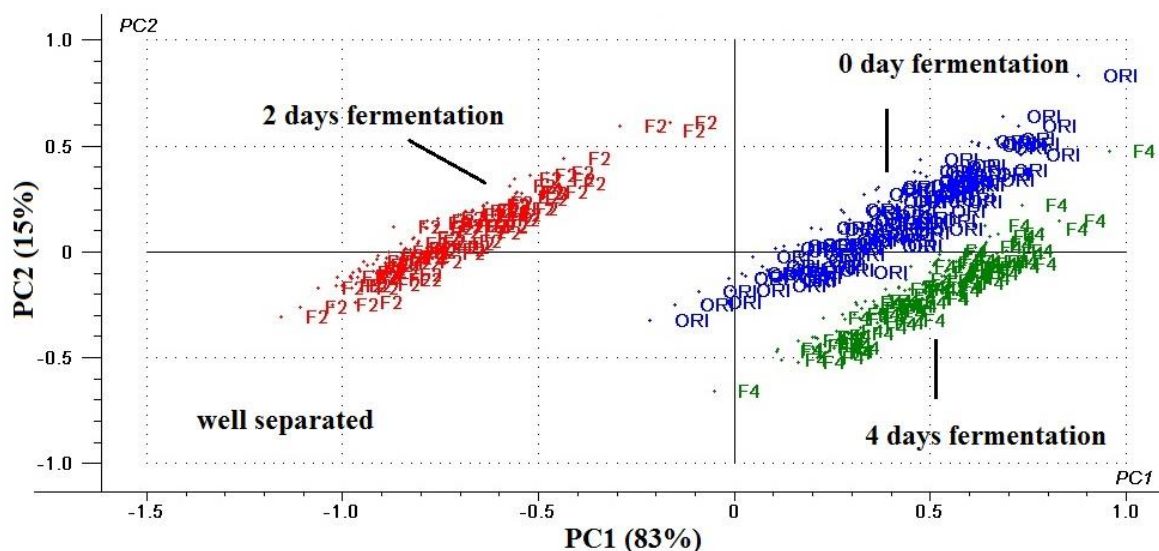


Figure 4. The result of the PCA analysis of coffee samples with different fermentation using modified spectra in the range of 250-450 nm.

3.3. The result of PCA: mapping of variables

To identify the most important variables that are highly responsible for the separation of coffee samples according to their length of fermentation, the plot of X-loading versus wavelength was demonstrated in Figure 5. X-loadings of PCA describe the data structure in terms of variable contributions and correlations. Higher X-loading means important variables. From Figure 5, it can be seen that the highest X-loadings was identified at a wavelength of 320 nm. This wavelength is related to the absorbance of trigonelline in coffee [18]. It can be said that the separation of Lampung robusta coffee based on fermentation mostly driven by the different content in trigonelline. However, further analysis must be performed to clarify this finding.

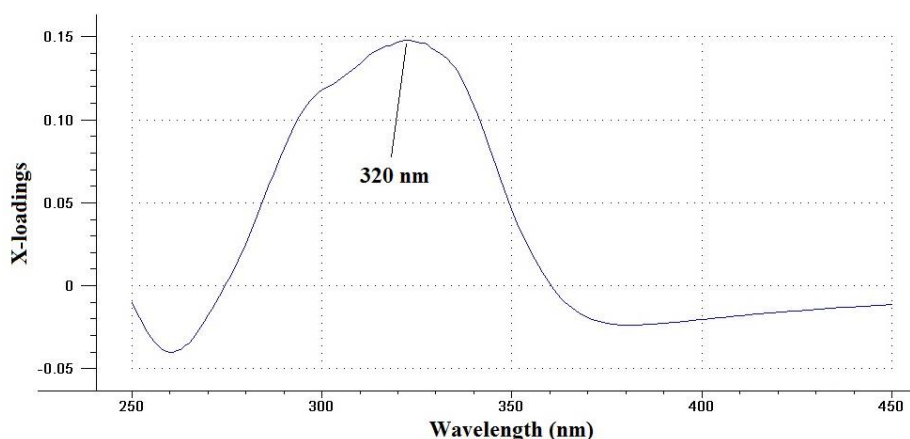


Figure 5. The X-loadings versus wavelength plot from PCA analysis using modified spectra in the range of 250–450 nm.

4. Conclusion

Our results highlight the potential of UV-visible spectroscopy combined with chemometrics as a green and relatively fast analytical method to discriminate Lampung robusta coffee based on fermentation. Both original full-spectrum and modified selected-spectrum spectral data resulted in a clear separation of coffee samples according to the length of fermentation. The highest X-loadings were identified at a wavelength of 320 nm. This wavelength is related to the absorbance of trigonelline in coffee. It can be concluded that the separation of Lampung robusta coffee based on fermentation mostly driven by the different content in trigonelline.

Acknowledgment

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