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## The Feasibility of Geographical Origin Discrimination of Lampung Robusta Coffee Using UV-Visible Spectroscopy and Chemometric Methods

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# The Feasibility of Geographical Origin Discrimination of Lampung Robusta Coffee Using UV-Visible Spectroscopy and Chemometric Methods

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**Abstract.** In this study, UV-visible spectroscopy and partial least squares-discriminant analysis (PLS-DA) method was used to discriminate the origin of Lampung robusta coffee. Total 40 Lampung robusta coffee samples with two origins (Lampung Barat and Tanggamus) were used. Each samples has 1 gram weight and was extracted using hot distilled water. UV-visible spectral data of the all aqueous coffee samples were obtained using a UV-visible spectrometer in transmittance mode in the range of 190-1100 nm. The performance of the developed PLS-DA model was evaluated based on coefficient of determination ( $R^2$ ), root mean square error of calibration (RMSEC), and residual prediction to deviation (RPD). Using Savitzky-Golay 1<sup>st</sup> derivative and moving average spectra, PLS-DA model was developed with the following results:  $R^2 = 0.97$  for calibration and  $R^2 = 0.88$  for validation, RMSEC = 0.089421 and RMSECV=0.178384. The performance of prediction was quite good with RMSEP = 0.215303 and RPD = 2.83. This results show that UV-visible spectroscopy and PLS-DA method is a promising analytical method to discriminate geographical origin of Lampung robusta coffee.

## 1. Introduction

In 2016, the area of robusta coffee production in Indonesia was estimated at about 0.912 million hectares (ha). Comparing to 2001, there was a significant decreasing of the area of robusta coffee production at rate about 26%. Up to now, the central productions of robusta coffee in Indonesia are in Sumatera, Java, and Sulawesi. In 2016, the average of national coffee production is about 725 kg per ha [1].

Lampung province is one of the important robusta coffee production area in Indonesia with average production about 0.117 million tons (about 18.35% of national contribution up to 2016). In Lampung province, robusta coffee was planted in low, middle and high land. Low land of Lampung robusta coffee production is in Pesawaran, Pringsewu, Lampung Utara and Way Kanan regency with total production about 24 thousand tons/year. Middle land of Lampung robusta coffee production is in Tanggamus



regency with total production about 17.5 thousand tons/year. High land of Lampung robusta coffee production is in Lampung Barat regency with total production about 42.7 thousand tons/year [1].

Several previous studies have reported the relationship between environmental factors (such as altitude or elevation, shading etc.) and quality of coffee [2]. Avelino *et al.* (2005) reported that chlorogenic acids (CGA) was accumulated with an increase in altitude [3]. Total lipid content was reported to decrease with increasing altitude [4]. In Lampung, several robusta coffees were planted with different altitude or elevation. For example, in Lampung Barat the average altitude was 1000 m above sea level (high land) while in Pesawaran was 150 m above sea level (low land). Therefore, the quality of Lampung robusta coffee is highly influenced by its origin due to different of elevation or altitude. For this reason, it is important to develop an analytical method that is able to discriminate the origin of Lampung robusta coffee in order to develop an authentication for Lampung robusta coffee. The authenticity of coffee with respect to its geographical origin of Lampung robusta coffee (low, middle and high land) is quite important for both producers and consumers.

In the previous study, several analytical methods have been used for the authentication of origin of coffee and other agricultural products. For example, Ossa *et al.*, (2018) used HRMS-based metabolomics to assess the origin of Colombian coffees [5]. Several analytical methods based on spectroscopic techniques have been employed to study and classify coffee. Brazilian coffee from different origins and farming systems was evaluated by proton transfer reaction mass spectrometry (PTR-MS) and near infrared spectroscopy (NIRS) [6]. Classification of coffee mainly by quality has also been achieved using FTIR analysis of the dry extract of coffee originating from various countries [7]. Evaluation of coffee based on the geographical origin (Brazil, Kenya, Ethiopia, Yemen and Colombia) has been successfully achieved using a combination of FTIR and PCA method [8]. Fluorescence spectroscopy and SIMCA method has been used for discrimination of several Indonesian specialty coffees [9]. NIR spectroscopy in tandem with chemometrics has been utilized to detect and quantify the adulteration in ground roasted Indonesian palm civet coffee [10].

UV-visible spectroscopy is simpler and cheaper spectroscopic method. It has been used for coffee authentication recently. Suhandy and Yulia (2018) used UV-visible spectroscopy and PLS-DA method for peaberry coffee authentication [11]. The quantification and discrimination of adulteration in Indonesian palm civet coffee has been conducted using UV-visible spectroscopy along with chemometrics methods [12-13]. In recent works, UV-visible spectroscopy has been used for discrimination and identification of decaffeinated coffee [14], fresh and expired ground roasted coffee [15] and Gayo wine coffee [16]. In this research, we apply PLS-DA method on UV-visible spectral data to discriminate the origin of Lampung robusta coffee (middle and high land Lampung robusta coffee).

## 2. Materials and Methods

### 2.1. Lampung robusta coffee samples with different origin

Two types of Lampung robusta coffees were used in this study. Twenty samples of ground roasted coffee samples from Lampung Barat (high land at about 1000 m above sea level) and twenty samples from Tanggamus (middle land at about 450 m above sea level) were prepared with 1 gram weight for each samples. The all samples were subjected to extraction procedure using hot distilled water [11]. For PLS-DA analysis, the samples were randomly divided into two groups: calibration set (30 samples) and prediction set (10 samples).

### 2.2. Measurement of UV-Visible spectral data

The UV-Visible spectral data of aqueous coffee samples from Tanggamus and Lampung Barat 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 subjected to several spectral pre-treatments (Savitzky-Golay first derivative and moving averaging). These modified spectral data were used for further analysis.

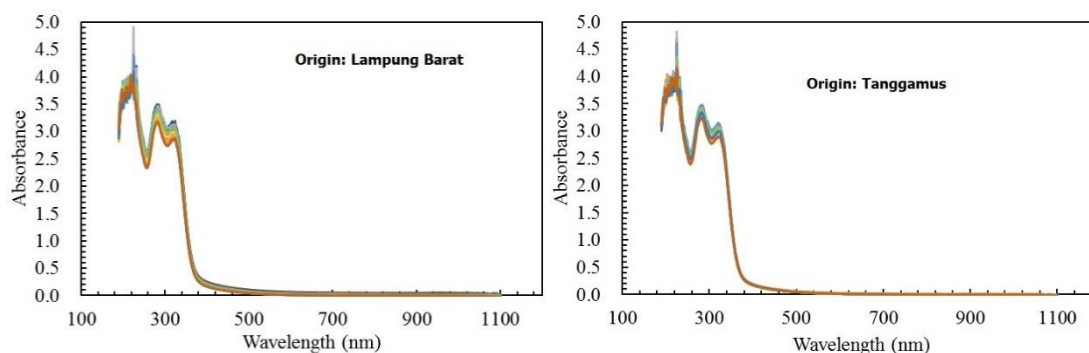
### 2.3. Partial least squares-discrimination analysis (PLS-DA)

PLS-DA is one the popular and widely used chemometrics for discrimination purposes [11]. It is based on a PLS regression algorithm with a dummy variable as a reference value (variable Y). Here, we set Lampung Barat coffee = 1 and Tanggamus coffee = 0. The following parameters were used to evaluate the performance of PLS-DA model in calibration step: coefficient of determination ( $R^2$ ), RMSEC (root mean square error of calibration) and RMSECV (root mean square error of cross-validation). In the prediction step, two parameters namely RMSEP (root mean square error of prediction) and RPD (residual prediction to deviation) were used [11, 17]. In this research, a threshold of  $\pm 0.5$  was used to classify the coffee samples. A coffee sample was classified as Lampung Barat coffee if its value was above 0.5 and classified as Tanggamus coffee if the value was below 0.5 [11].

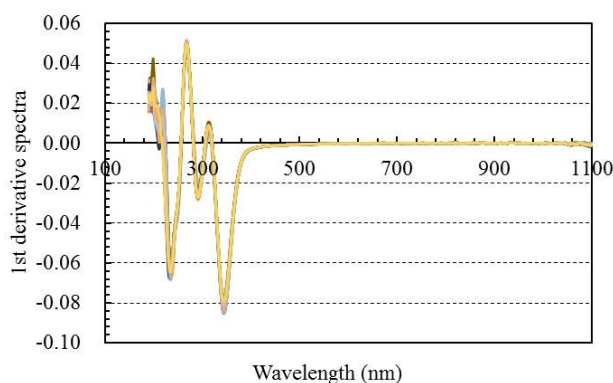
## 3. Results and Discussion

### 3.1. Spectral analysis of Lampung robusta coffee with different origin

Figure 1 shows the original spectral data of coffee samples with different origin, Lampung Barat (left side) and Tanggamus (right side) in the range of 190-1100 nm. It can be seen that both spectra (Lampung Barat and Tanggamus) are almost similar in the shape of spectra and intensity of absorbance. It is not easy to see any differences between the two. We can also notice some noisy spectral information around 190-225 nm both for Lampung Barat and Tanggamus. To improve the quality of the calibration model, two spectral pre-treatments namely smoothing moving average and first derivation of Savitzky-Golay were applied. Figure 2 shows the spectral data of Lampung robusta coffee with different origin after applying smoothing and derivation.



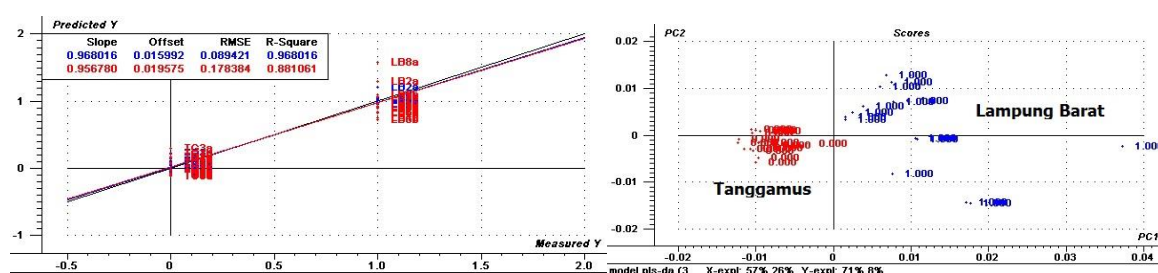
**Figure 1.** Typical original absorbance spectra of Lampung robusta coffee samples from Lampung Barat and Tanggamus in the range of 190-1100 nm.



**Figure 2.** The pre-processed spectra of Lampung Barat and Tanggamus coffee (smoothing moving average and 1st derivation of Savitzky-Golay spectra) in the range of 190-1100 nm.

### 3.2. PLS-DA model development

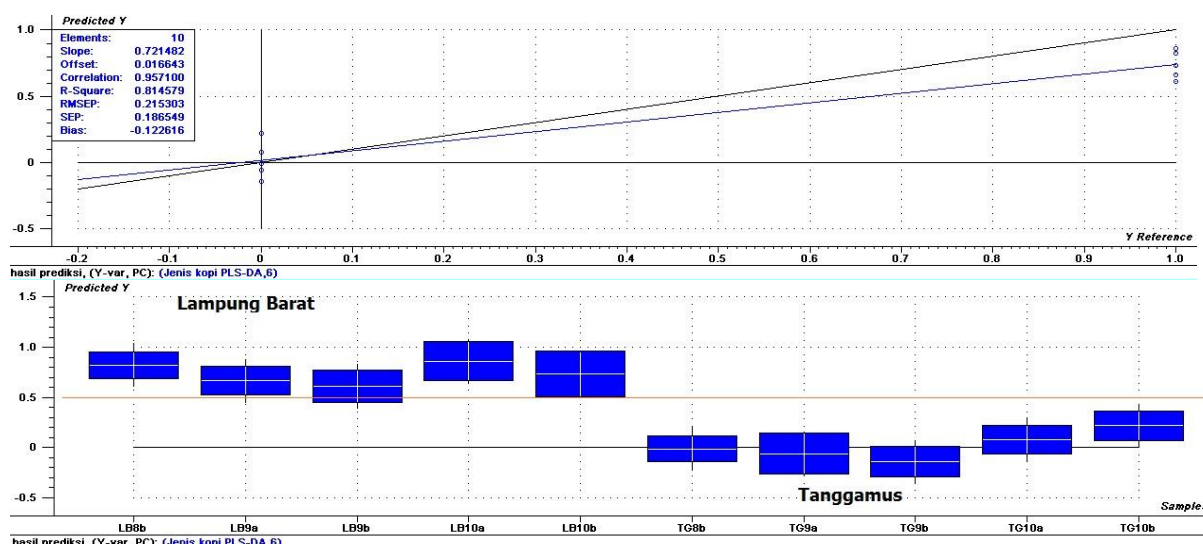
Figure 3 (left) shows the calibration model developed by using PLS-DA method using pre-processed spectra with all wavelengths in the range of 190-1100 nm. This calibration model has high coefficient of determination ( $R^2$ ) for calibration and acceptable  $R^2$  for validation. The both values of RMSEC and RMSECV were low. This result indicated that UV-visible spectroscopy along with PLS-DA method has potential to discriminate the origin of Lampung robusta coffee. The developed PLS-DA model was able to separate Lampung Barat coffee and Tanggamus coffee as seen in Figure 3 (right). Most of Tanggamus coffees were situated in the negative of PC1 and most of Lampung Barat coffees were located at the positive of PC1.



**Figure 3.** The PLS-DA model developed using pre-processed spectra in the range of 190-1100 nm.

### 3.3. Evaluation of PLS-DA model for prediction

Figure 4 demonstrated the result of prediction using the developed PLS-DA model. The quality of prediction was good with  $R^2_{pred} = 0.82$  and RMSEP = 0.215303. The RPD was 2.83. Using the threshold of  $\pm 0.5$ , we can see that all predicted samples were properly classified. This result shows that the calibration model based on UV-visible spectroscopy and PLS-DA method for discrimination the origin of Lampung robusta coffee could be well developed.



**Figure 4.** The result of prediction using PLS-DA calibration model developed using spectral data in the range of 190-1100 nm.

## 4. Conclusion

In this research, UV-Vis spectroscopy combined with PLS-DA method was used to discriminate two origin of Lampung robusta coffees: Lampung Barat (high land) and Tanggamus (middle land). It was concluded that the developed PLS-DA model has very good quality and the prediction resulted in acceptable result with all prediction samples were properly classified. This result may open a possibility

to establish a simple and relatively cheap analytical method for authentication of Lampung robusta coffee.

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