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A Discrimination of Dry and Wet Processing Lampung Robusta Coffee using UV Spectroscopy and PLS-DA

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Abstract. Postharvest treatment of coffee, including processing coffee cherry into a green bean, highly influenced the coffee's final flavor. In general, two types of coffee cherry processing have existed: dry (unwashed) and wet (washed) processing. This research aims to evaluate a possible application of UV spectroscopy and PLS-DA for the discrimination of dry and wet processing Lampung robusta coffee. A total of 50 samples were used as samples. All samples were roasted, ground, and sieved with mesh 50. An aqueous sample was prepared by using a water-based extraction procedure. The spectral data were measured in transmittance mode using a benchtop UV-visible spectrometer from 190 nm to 400 nm. The PCA and PLS-DA were used to discriminate between dry and wet processing coffee samples. PLS-DA models were developed based on UV spectroscopic data in the selected window from 220 nm to 350 nm for original and preprocessed spectra. The PLS-DA models were able to classify samples according to different bean processing methods with an acceptable result. This application could help identify and develop a certification of Lampung robusta coffee according to their bean processing method.

Keywords: dry processing, PCA, PLS-DA, UV spectroscopy, wet processing

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1. Introduction

Coffee is one of the most popular beverages in the world, with an annual consumption of more than 400 billion cups [1]. Three popular coffee varieties are traded in Indonesia: Arabica, Robusta, and Liberica. In coffee berry processing, there are two popular processing methods in practice: wet processing (washed) and dry processing (natural or unwashed). The overall quality and chemical composition of the coffee beans are greatly influenced by the two parameters of the coffee variety (Arabica, Robusta, or Liberica) and the method used to process the coffee cherries (dry and wet) [2]. For example, in the wet process, the fermentation of coffee beans has a significant impact on coffee quality, as reported in some previous reports, such as strong aroma and pleasant acidity [3-6]. In general, wet-processed coffee, especially Indonesian coffee, is more expensive than that dry-processed coffee.

Recently, several methods have been developed to evaluate the quality of coffee variety and its processing methods to control and avoid coffee adulteration. Buratti et al. [1] used multiple analysis



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methods including spectroscopic and electronic nose to discriminate between Arabica (washed and natural) and Robusta coffees. Lyman et al. [7] utilized ATR-FT-IR spectroscopy to investigate the correlation between coffee cherry processing variables and the flavor of brewed coffee. Discrimination of Arabica washed coffee from several growing areas in Rwanda was performed using the combination of electronic nose and electronic tongue [6]. Those methods are accurate and have the potential for fast online and routine analysis. However, they are time-consuming in sample preparation, high cost for the device, and requirement for a highly trained person to do the analysis.

Suhandy and co-workers have developed a simple authentication of ground roasted coffee and tea using a low-cost UV-visible spectrometer associated with different chemometric methods [8-13]. For example, Suhandy and Yulia [12] utilized UV-visible spectroscopic data and PCA-DA (principal component analysis-discriminant analysis) to classify Arabica Gayo wine coffee with an acceptable result. In this present study, we evaluated possible UV-visible spectroscopy applications coupled with the PLS-DA method to distinguish between dry and wet processing Lampung Robusta coffee.

2. Materials and methods

2.1 Coffee beans with different processing

Fifty coffee samples of fine Robusta coffee from Sumberjaya, West Lampung (elevation: 1000 m) were directly collected from farmers. The samples were processed into two different bean processes: 25 samples from wet processing (washed coffee) and 25 samples from dry processing (natural coffee). All samples were subjected to medium roasting at a temperature of 200°C for 10 minutes then ground and sieved using 50 mesh (297 micrometers of coffee particle size) [14]. Coffee extraction including dilution was conducted for each sample according to previous work [15].

2.2 UV-visible spectral data acquisition

A benchtop and low-cost UV-Vis spectrometer model Genesys™ 10S from Thermo Scientific, USA was used to generate UV spectra from 190 nm to 400 nm. The interval of 1 nm was used. This spectrometer is equipped with one reference and five sample holders (dual-beam spectrometer). The spectral acquisition of 3 mL of distilled water for reference and 3 mL of aqueous coffee samples was made at the same time using 10 mm of quartz cell.

2.3 PCA and PLS-DA

PCA (unsupervised) and PLS-DA (supervised) were applied for both original and preprocessed spectra. Original spectra were obtained directly from the spectrometer without any spectral preprocessing. In contrast, preprocessed spectra were calculated by using two preprocessing algorithms simultaneously: moving average smoothing with 7 segments (MAS 7) and standard normal variate (SNV). In PCA, the result of PC scores of PC1 and PC2 was plotted to map the samples into several possible clusters. In PLS-DA, the matrix **X** is the predictor variable containing UV-vis spectral data matrix. The matrix **Y** is the response variable containing information about the sample class in binary code 'zero' for dry coffee class and 'one' for wet coffee class [16]. In the PLS-DA model development, the samples (n=50) were divided into calibration (n=30) and testing sets (n=20). Using PCA with the NIPALS (non-linear iterative partial least squares) algorithm, the **X** and **Y** matrices are breakdown simultaneously into the matrix of scores and loadings. The multivariate software of Unscrambler ver. 9.7 and 10.4 (CAMO, Norway) was used to calculate the spectral preprocessing, PCA, and PLS-DA.

3. Results and discussion

3.1 Analysis of UV-vis spectra

Figures 1 and 2 show the original and preprocessed spectra of 50 samples of dry and wet coffee samples from 190 nm to 400 nm. Spectral data of dry and wet-processed coffee are similar in shapes and absorbance intensity. For original and preprocessed spectra, wavelengths at around 250 nm, 280 nm, and 320 nm showed high absorbance intensities. Previously, it has been shown that the absorbance of caffeine in aqueous coffee samples was identified at the wavelengths of 250 nm and 280 nm [17-20]. Direct investigation of UV-visible spectra to distinguish the difference between dry and wet-processed coffee samples was difficult. Therefore, multivariate analysis (MVA) of PCA and PLS-DA was used to extract the spectral information. To minimize noise information (very high or very low absorbance), further analysis was performed on the specific wavelength range of 220-350 nm.

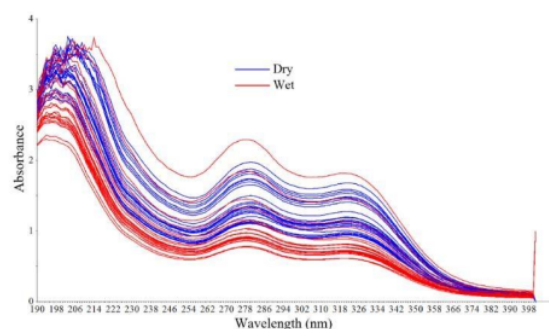


Figure 1. The plot of wavelength versus absorbance intensity (original) of 50 samples of dry and wet coffee samples in the wavelength of 190-400 nm.

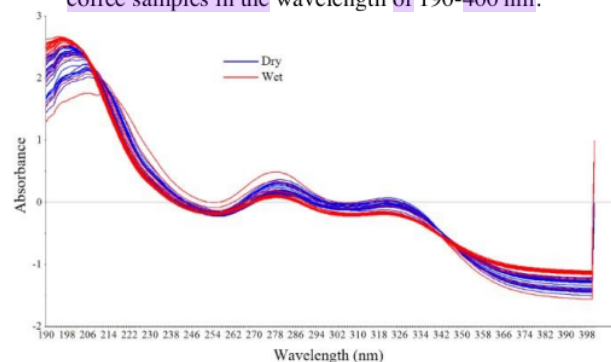


Figure 2. The plot of wavelength versus absorbance intensity (preprocessed) of 50 samples of dry and wet coffee samples in the wavelength of 190-400 nm.

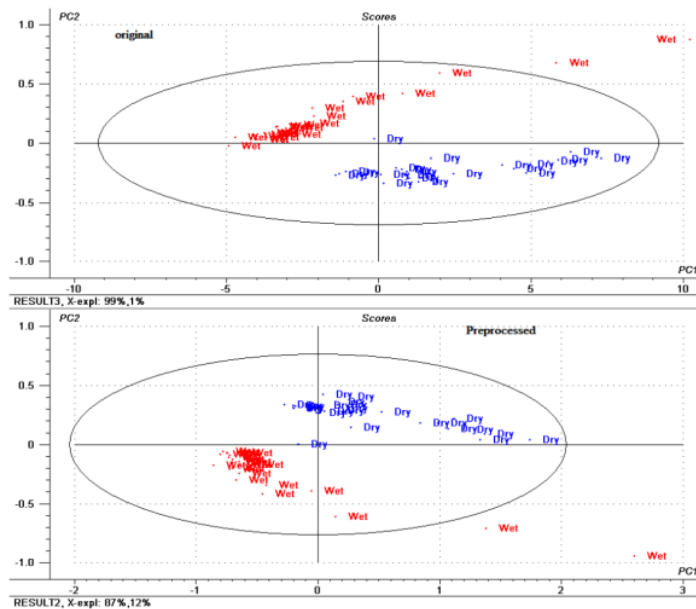


Figure 3. The scores plot of PCA (PC1xPC2) for original and preprocessed spectral data from 220 nm to 350 nm.

3.2 PCA results

The plot of PCA scores for the PC1 and PC2 for original and preprocessed spectra using selected intervals from 220 nm to 350 nm was demonstrated in Figure 3. Ellipse represents Hotelling T^2 with 95% confidence in the PCA score plots. Two samples of wet-processed coffee were laid outside the 95% Hotelling T^2 ellipse and indicated potential outliers. It can be seen that the separation of the dry and wet coffee samples was mainly driven by the value of PC1 (along the x -axis) both in original and preprocessed spectra. Most wet-processed coffee samples were scattered on the left of PC1, and most dry samples were on the right of PC1.

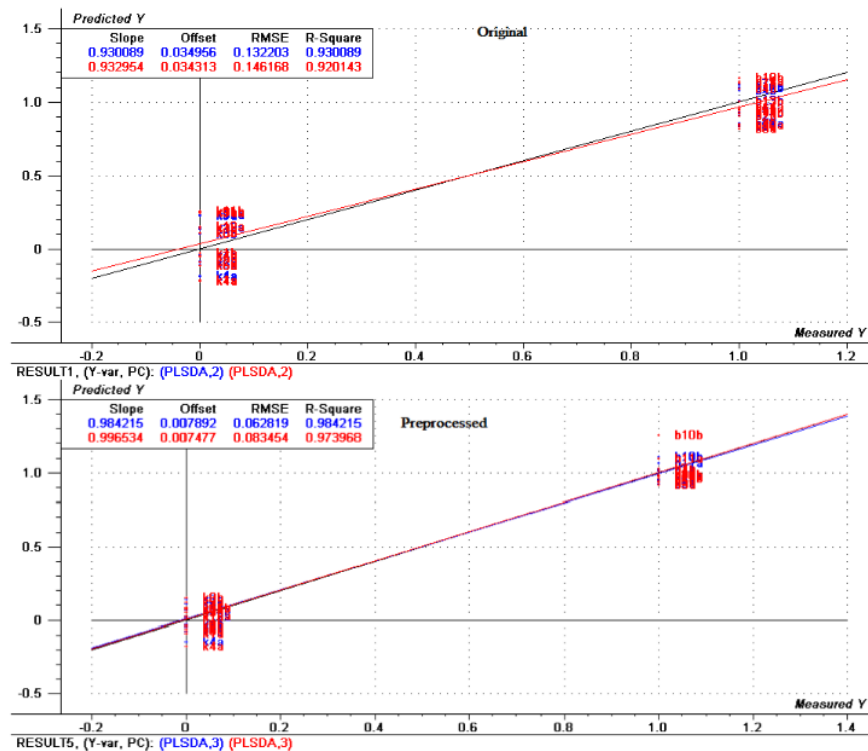


Figure 4. The plot of actual and predicted class values developed using PLS regression for original and preprocessed spectra from 220 nm to 350 nm.

3.3 PLS-DA results

The plot of actual and predicted class values developed using PLS regression was depicted in Figure 4 for original and preprocessed spectra from 220 nm to 350 nm ($y=0$ for dry coffee samples and $y=1$ for wet coffee samples). The PLS-DA models were developed using calibration set samples (total 30 samples for both wet and dry coffee samples) with the full-cross validation method. Using original spectra, the coefficient of determination (R^2) was 0.93 for calibration and 0.92 for validation. It was improved for preprocessed spectral data with R^2 0.98 for calibration and 0.97 for validation. The high R^2 obtained in this study indicating the satisfactory effectiveness of the PLS-DA models. It can also be said that the applied preprocessing algorithms were successfully improved the quality of PLS-DA models.

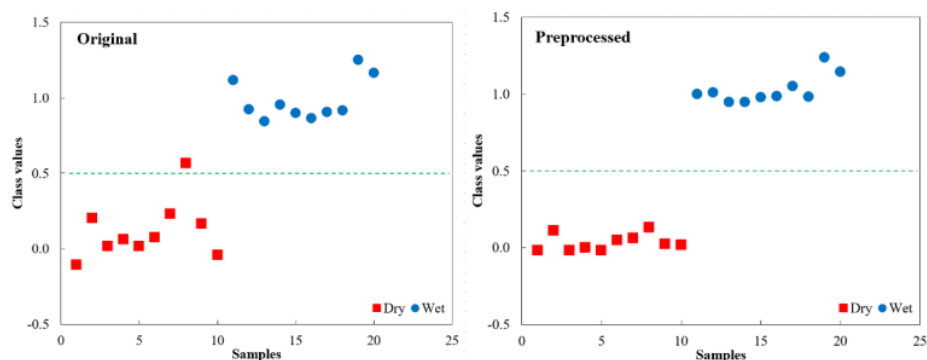


Figure 5. Classification result of the testing set samples using PLS-DA model of original (left) and preprocessed spectra (right).

PLS-DA model's ability to distinguish between dry and wet-processed coffee samples was conducted using 20 samples of the testing set. The result was demonstrated in Figure 5. Using a threshold of ± 0.5 , using PLS-DA of original spectra, one sample of dry-processed coffee was misclassified as a wet coffee class. However, a better performance was achieved using the PLS-DA of preprocessed spectra. All samples were classified with a 100% correctness into dry and wet classes.

4. Conclusion

Significant improvement of the chemometrics results was achieved after applying appropriate spectral preprocessing. The developed PLS-DA model was improved using preprocessed spectroscopic data in terms of R^2 value from 0.93 to 0.98 in calibration and 0.92 to 0.97 for validation. The PLS-DA model of preprocessed spectra was better than that of the original spectra with no misclassified samples detected. This study shows the application of UV-visible spectroscopy and chemometric with the appropriate spectral preprocessing for discrimination between dry and wet-processed coffee samples. This result may help us to develop a simple and low-cost Lampung specialty Robusta coffee certification system based on the coffee berry processing method.

Acknowledgments

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