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To cite this article: M Yulia and D Suhandy 2021 *J. Phys.: Conf. Ser.* **1751** 012079

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Simple analytical method based on UV-visible spectroscopy coupled with SIMCA method for authentication of Lampung robusta coffee with geographic indications (GIs)

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Abstract. Lampung Robusta coffee got a geographic indication (GIs) protection from Indonesian government since 2014 with certificate number of ID G 000 000 026. This GIs coffee come from three different geographic origins in Lampung province: Lampung Barat, Tanggamus and Way Kanan. In this research, we evaluate the possible application of simple analytical method based on UV-visible spectroscopy coupled with SIMCA (soft independent modelling of class analogy) for authentication of Lampung Robusta coffee with GIs. Two types of Lampung Robusta coffee were used: GIs coffee from Lampung Barat and non-GIs coffee from Pesawaran. Each type consists of 50 samples of ground roasted coffee with 1 gram weight. The all samples were extracted using a hot distilled water and 3 mL aqueous samples were pipetted into 10 mm quartz cuvette. UV-visible spectral data were recorded in the range of 190-1100 nm. The chemometrics (PCA and SIMCA) was performed using selected preprocessed spectral data in the range of 240-430 nm. The PCA result showed that GIs coffee and non-GIs coffee can be well separated. The SIMCA classification was accepted with 100% of correct classification.

1. Introduction

In 2007, Indonesian government officially announced Government Regulation No. 51 about Geographic Indication (GIs). According to this regulation, GIs can be defined as any indication which identifies goods and/or a product as originating from a particular region of which its geographical environment factors including nature, labor, or combination of both factors are attributable to a given reputation, quality, and characteristics of the produced goods and/or product [1]. In total up to May 2020, there are more than 60 Indonesian products which has been approved for GIs including several Indonesian Arabica and Robusta coffee such as Gayo Arabica and Lampung Robusta coffee [2].

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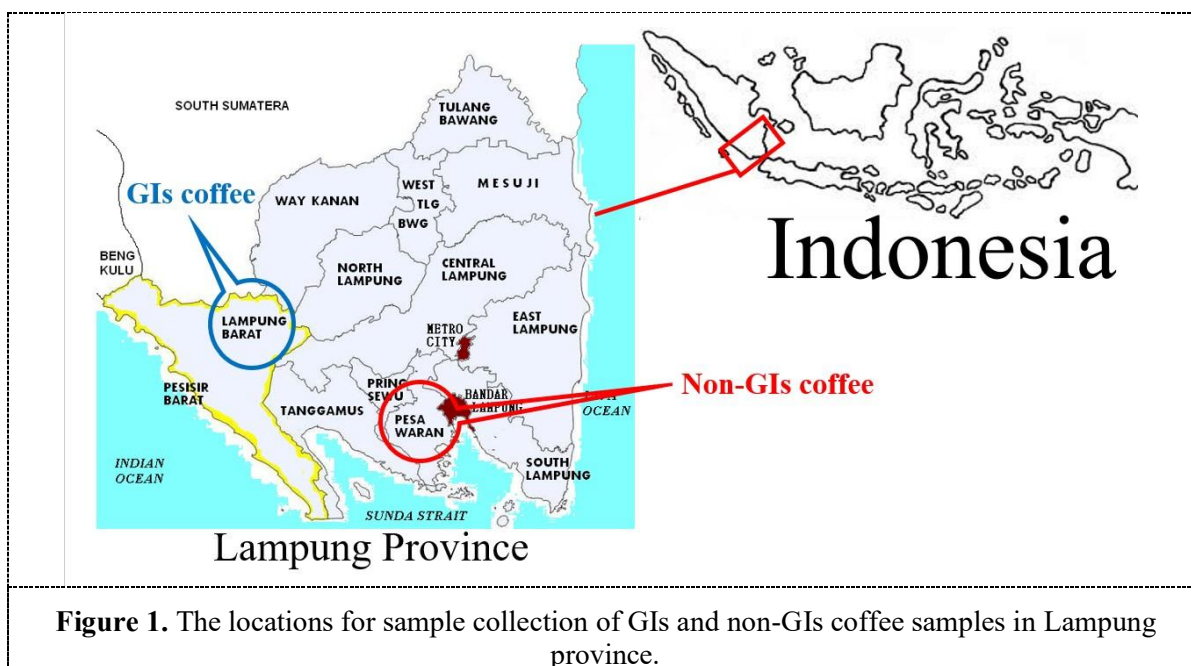
Lampung Robusta coffee got a geographic indication (GIs) protection from Indonesian government since 2014 with certificate number of ID G 000 000 026. This GIs coffee comes from three different geographic origins in Lampung province: Lampung Barat, Tanggamus and Way Kanan. However, several Robusta coffees in Lampung was also planted in other geographic area such as Pesawaran. Robusta coffee from this area for example, should be assigned as Lampung Robusta coffee non-GIs. In order to declare a true Lampung Robusta coffee with GIs, it is important to develop an authentication to discriminate Lampung Robusta coffee with GIs and non-GIs. This authentication is important to protect Lampung Robusta GIs coffee from any fraud trading.

In respect to low-cost and simple spectroscopy method, Suhandy and co-workers recently has developed an authentication for Indonesian ground roasted specialty coffee using UV-visible spectroscopy along with several chemometrics methods including authentication of peaberry and normal coffee, discrimination between civet and non-civet coffee, authentication of organic coffee and etc. [3-7]. In present research, we evaluate the possible application of simple analytical method based on UV-visible spectroscopy coupled with SIMCA (soft independent modelling of class analogy) for authentication of Lampung Robusta coffee with GIs. SIMCA is a popular and widely used classification methods for coffee authentication due to its several advantages such as working well with few numbers of samples with no restriction on the number of variables [8-10]. Two types of Lampung Robusta coffee were used: GIs coffee from Lampung Barat and non-GIs coffee from Pesawaran.

2. Research methodology

2.1. Coffee samples

The all coffee samples were Robusta coffee (*Coffea canephora*) and collected from two locations with different elevation in Lampung province: Lampung Barat (1156 meters above sea level) for GIs coffee samples and Pesawaran (534 meters above sea level) for non-GIs coffee samples (see Figure 1). All samples were processed by dry method. Each type of coffee (GIs and non-GIs) consists of 50 samples of ground roasted coffee with 1 gram weight. The all samples were extracted using a 10 mL of hot distilled water and diluted with distilled water according to previous reported researches [5, 11-12]. Three mL aqueous samples were pipetted into 10 mm quartz cuvette for spectral acquisition.



2.2. Spectral acquisition of GIs and non-GIs coffee samples

The spectral data of GIs and non-GIs coffee samples were acquired using a low-cost benchtop UV-Vis spectrometer (Genesys™ 10S UV-Vis, Thermo Scientific, USA) in transmittance mode in the range of 190-1100 nm with spectral resolution of 1 nm at a room temperature (about 28-29°C). The original spectral data was preprocessed using several spectral preprocessing techniques. The best preprocessing was obtained for MSC (multiplicative scatter correction) and followed by SGD1 (Savitzky-Golay first derivative with 9 points and polynomial order 2). The chemometrics analysis was performed using the preprocessed spectral data using selected spectral window at 240-430 nm.

2.3. Chemometrics analysis

Two chemometrics were used in this research: unsupervised classification of principal components analysis (PCA) and supervised classification of soft independent modelling of class analogy (SIMCA). For SIMCA, samples were divided into three set: calibration (52 samples), validation (32 samples) and prediction (16 samples). SIMCA model for GIs and non-GIs coffee was developed using calibration and validation sample set in each class (GIs and non-GIs). The prediction performance of SIMCA was evaluated by using Cooman's plot. The PCA and SIMCA calculation including spectral preprocessing techniques was done using The Unscrambler X version 10.4 (64-bit) (Camo Software AS, Oslo, Norway).

3. Results and discussions

3.1. Analysis of spectra of GIs and non-GIs coffee samples

Original (left) and preprocessed spectra (right) of average GIs and non-GIs coffee samples was depicted in Figure 2. The spectral data in the range of 190-240 nm was highly noisy due to low intensity of lamp. The spectral data in the range of 430-1100 nm was very low in absorbance. For this reason, we selected spectral window in the range of 240-430 nm for chemometrics calculation. In general, GIs coffee spectrum has higher absorbance comparing to that of non-GIs coffee. It may be due to different in concentration of chemical compound in GIs and non-GIs coffee.

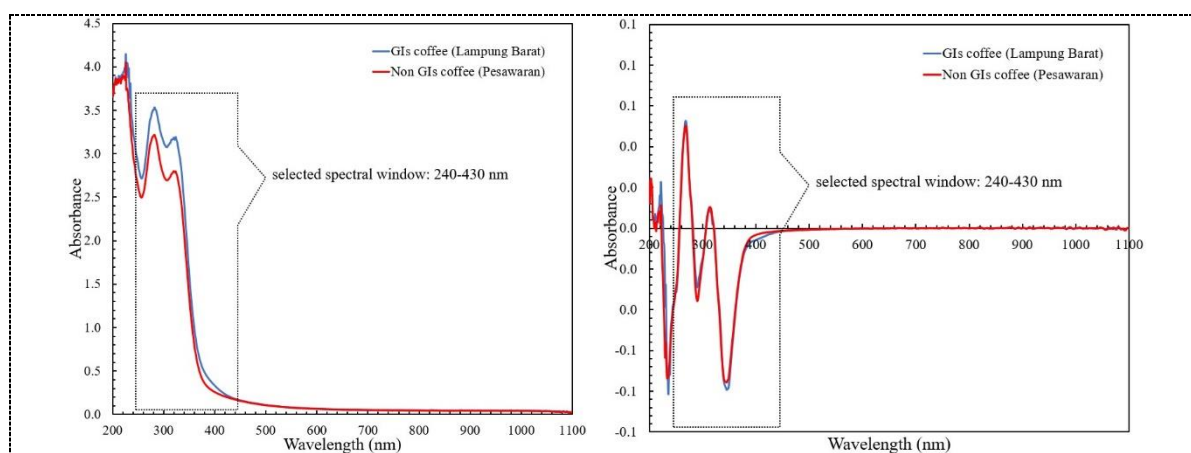


Figure 2. Average spectra of GIs and non-GIs coffee samples for original (left) and preprocessed spectra (right).

3.2. Results of PCA

The first three principal components (PC1, PC2 and PC3) was plotted for original and preprocessed spectra as depicted in Figure 3. The total explained variance for the first three PCs for original and preprocessed spectra was 99% and 71%, respectively. It can be seen that a clear separation was observed between GIs and non-GIs coffee especially for preprocessed spectral data. Most of GIs coffee samples were located at positive PC1 (along x-axis) ($PC1 > 0$) and all non-GIs coffee samples

were in negative PC1 (PC1<0). In Figure 4 we plotted a relation between wavelengths and its corresponding *x*-loading values for first four PCs (PC1, PC2, PC3 and PC4) using preprocessed spectral data in the range of 240-430 nm. Wavelengths with high *x*-loadings highly contributed to the separation of coffee samples. High *x*-loadings was observed at interval 260-280 nm and 320-340 nm. Those intervals were corresponding with absorbance of caffeine and chlorogenate (CGA) acid in coffee [5,13-16].

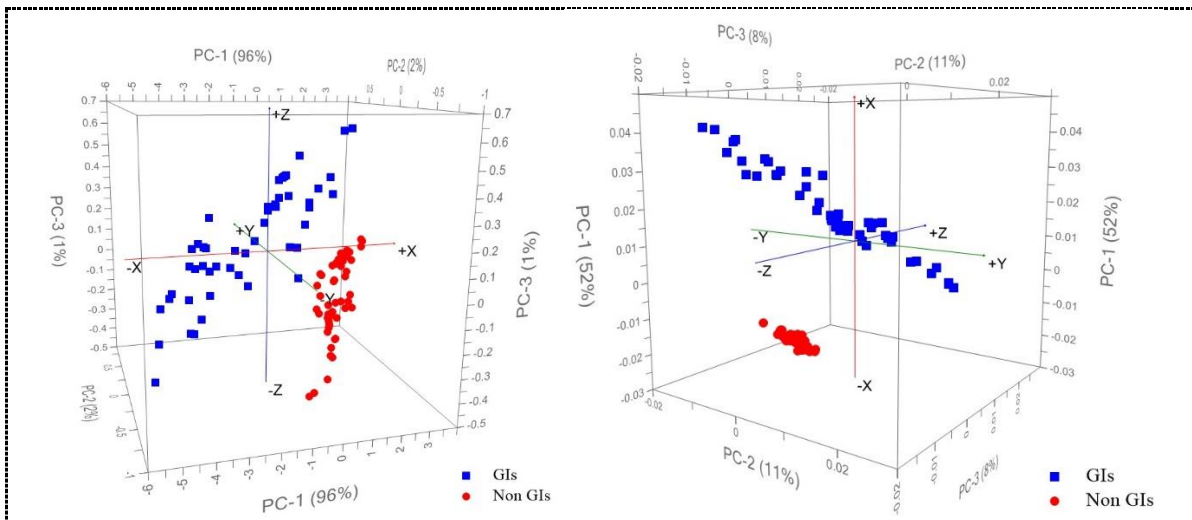


Figure 3. PCA score plot of GIs (square blue color) and non-GIs (circle red color) coffee samples calculated based on original (left) and preprocessed (right) spectra in the range of 240-430 nm.

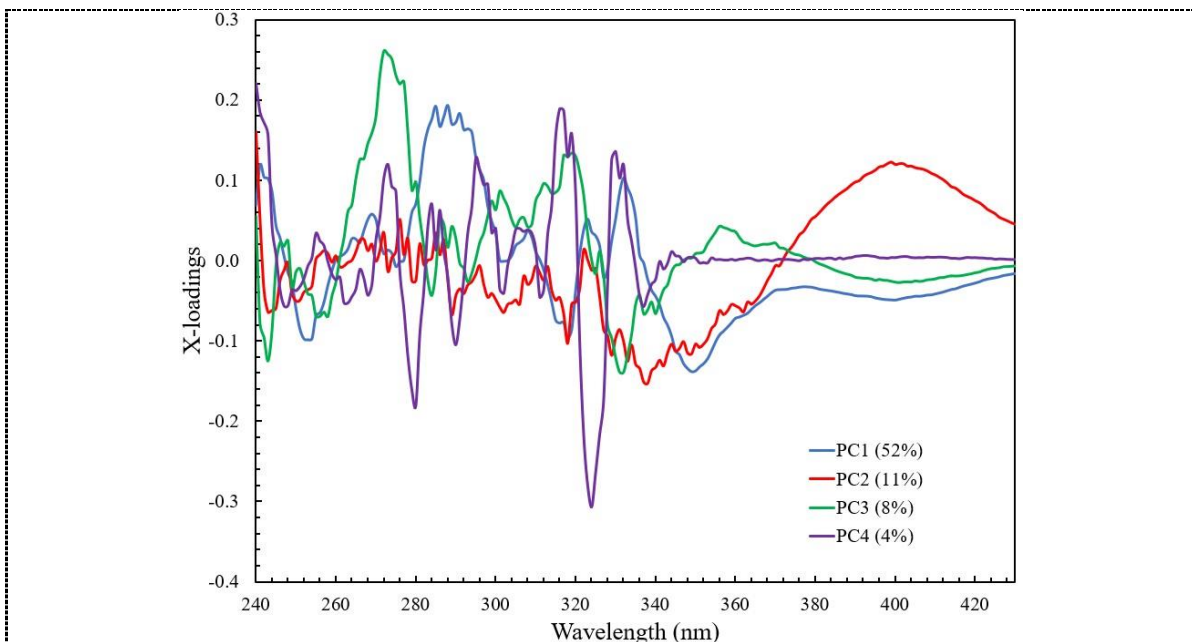
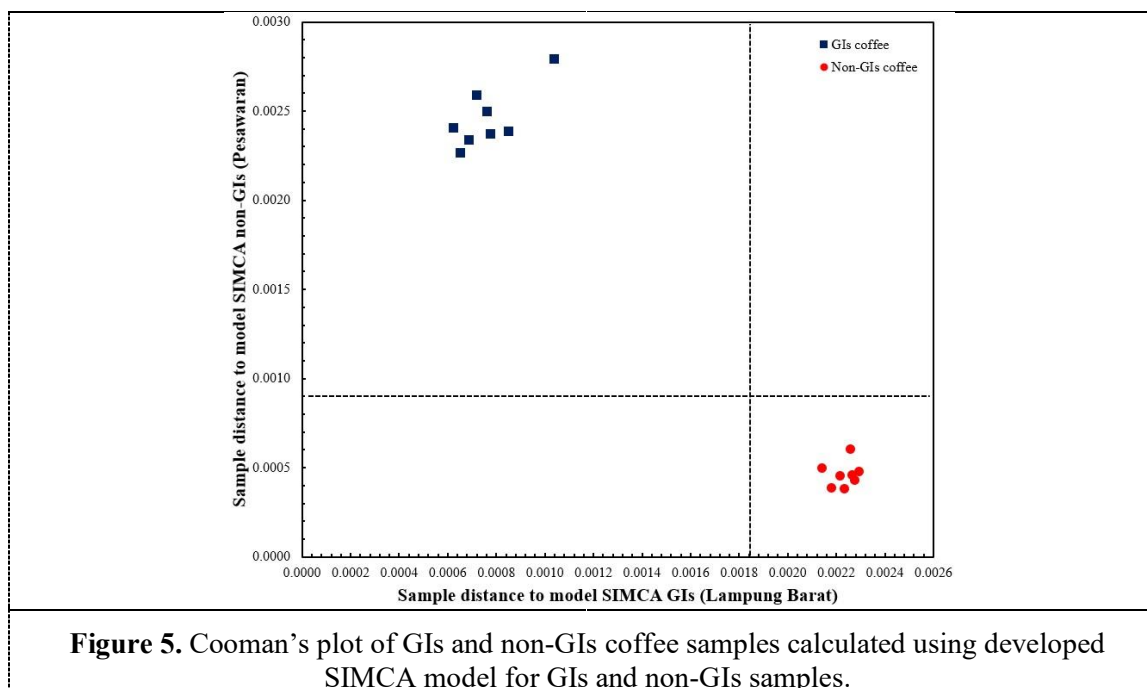


Figure 4. Wavelength versus *x*-loadings of the first four PCs plot calculated using preprocessed spectra in the range of 240-430 nm.

3.3. Result of SIMCA

The developed SIMCA model for GIs and non-GIs samples were used to predict class membership of prediction sample set. Figure 5 showed the result of prediction in Cooman's plot. The dashed vertical and horizontal lines were membership threshold for GIs and non-GIs coffee samples which was calculated using 90% confidence level. It can be seen that there were no any samples belong to both class (GIs and non-GIs) as no samples were located in the left lower part of Cooman's plot. All samples were classified correctly into its corresponding class resulting a 100% of correct classification for GIs and non-GIs samples.



4. Conclusion

This research was conducted to evaluate the possible application of UV-visible spectroscopy for simple authentication of Lampung Robusta coffee with geographic indications (GIs coffee). PCA was used to separate the GIs and non-GIs samples. A clear separation was observed between GIs and non-GIs samples especially using preprocessed spectral data in the range of 240-430 nm. Cooman's plot of GIs and non-GIs coffee samples were generated using the developed SIMCA model in each class (GIs and non-GIs). All prediction samples can be classified properly into GIs and non-GIs classes resulted in a 100% of correct classification. This result demonstrated that UV-visible spectroscopy has the potential for simple analytical method for authentication of Lampung Robusta coffee with geographic indications (GIs).

Acknowledgment

This research was supported by the Ministry of Research and Technology/National Agency for Research and Innovation, Republic of Indonesia (PKPT 2020-2021). The authors highly acknowledge Laboratory of Bioprocess and Postharvest Engineering, Faculty of Agriculture, The University of Lampung, Bandar Lampung, Lampung, Indonesia for permission to use the UV-visible spectrometer.

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