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The Potential Application of Portable Spectrometer Equipped with Integrating Sphere and PLS-DA Method to Authenticate Indonesian Specialty Coffee

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Abstract. In this research, a potential application of using portable spectrometer equipped with an integrating sphere to authenticate Indonesian specialty coffee was described. 20 samples of specialty and normal ground roasted coffee was used as samples. Each sample has about 1.33 gram in weight and particle size of 297 micrometer. Spectral data in the range of 900-1657 nm was acquired in diffuse reflectance mode using a portable fiber optic NIR-Quest InGaAs spectrometer (Ocean Optics, USA) equipped with an integrating sphere (ISP-REF, Ocean Optics, USA) with 1.645 nm interval. The integrating sphere is coated with Spectralon® and installed a built-in tungsten-halogen light source. Partial least squares-discriminant analysis (PLS-DA) was used to classify the samples into two groups: specialty coffee (labelled as 1) and normal coffee (labelled as 0). The result demonstrated that the best PLS-DA model was obtained with $R^2_{cal}=0.97$ and $R^2_{val}=0.91$ for calibration and validation, respectively. This achievement suggested that the proposed NIR spectral acquisition using portable NIR spectrometer equipped with an integrating sphere is potential to establish an authentication system for ground roasted Indonesian specialty coffee in direct and fast measurement.

INTRODUCTION

High-quality or specialty coffee is the best quality of coffee bean with a long journey from farmers to baristas [1]. Specialty coffee bean is harvested at their peak of ripeness and selected with free of any defects. After harvesting, the quality of specialty coffee both in green and roasted bean is well monitored by coffee grader (Q-grader) by cupping test [1]. According to The Specialty Coffee Association of America (SCAA), in general specialty coffee is commonly defined by cupping score higher than 80 [2]. Since 13 May 2014, Lampung Robusta coffee certified as one of specialty coffee with geographical indication (GI) ID G 000 000 026 with the cupping score of 81.3 [3]. In order to protect specialty coffee from any adulteration, several analytical methods for coffee authentication has been developed [4-11].

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The high price of most bench top NIR spectrometer has been a big problem for NIR technology development in most developing countries, no exception Indonesia. To overcome this handicap, many instrument companies have developed a miniaturization and cost reduction of portable NIR spectrometers based on fiber-optic and semiconductor detector array technologies [12]. In general, portable spectrometer has characteristic of weigh less, smaller, typically cost less, and easier to handle than bench top spectrometer [13]. The affordability of portable spectrometer can be understood from several reported publication of using NIR portable devices during 2000-2016 from developing countries [14-19].

Portable spectrometer has been used recently for products authentication and quality control. In near infrared (NIR) region, portable micro-spectrometer (MicroNIR) was used to detect and quantify the adulteration in coffee, fuel, and palm oil [20-22]. Basri *et al*. [20] used microNIR and chemometrics (SIMCA and PLS regression) to establish qualitative and quantitative studies between pure and adulterated palm oil. Correia *et al.* [21] utilized microNIR and PLS method to determine the amount of biodiesel in diesel. The quantification of adulteration in Brazilian coffee with different types of adulterant (Robusta coffee, corn and peels/stick) was studied using microNIR and PLS and PCA method [22].

Extensive studies on coffee authentication in Indonesia has been conducted using low cost UV-visible spectrometer with acceptable result [23-31]. The need for fast measurement and avoids laborious sample preparation has motivated to establish specialty coffee authentication in Indonesia using low cost and portable NIR spectrometer. In this present work, we firstly report a feasibility study of using low cost and portable spectrometer for specialty coffee authentication coupled with PCA and PLS-DA.

MATERIALS AND METHODS

Specialty and Normal Coffee Samples

Specialty and normal coffees were obtained from Forest Women Farmer Group of HIMAWARI in Lampung province in green unroasted bean. All samples were roasted, grinded and sieved in same condition: medium roasting 200°C for 10 minutes, grinding at 234 rpm for 20 minutes and sieving using 50 mesh. The samples were placed on the sample holder and each sample has about 1.33 gram in weight and particle size of 297 micrometer (See Figure 1). Twenty samples of specialty and normal ground roasted coffee was prepared as samples.

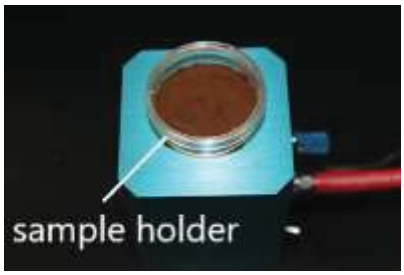

FIGURE 1. Sample holder for NIR diffuse reflectance spectral measurement.

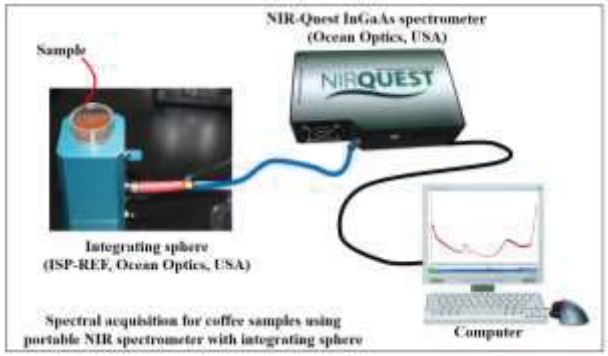

FIGURE 2. Spectral acquisition set up of coffee samples using portable spectrometer equipped with integrating sphere.

NIR Spectral Data Acquisition

Spectral data of 20 coffee samples in the range of 900-1657 nm was acquired in diffuse reflectance mode using a portable fiber optic NIR-Quest InGaAs spectrometer (Ocean Optics, USA) equipped with an integrating sphere (ISP-REF, Ocean Optics, USA) with 1.645 nm interval. The integrating sphere is coated with Spectralon® and installed a built-in tungsten-halogen light source as depicted in Figure 2. Spectral acquisition was done in room temperature in a dark environment (no external light). Original spectra of sample ($S(\lambda)$) were calculated based on equation 1 [32]:

$$S(\lambda) = \frac{S_{meas1}(\lambda) - S_{meas2}(\lambda) - D(\lambda)}{S_{ref}(\lambda) - D(\lambda)} \quad \text{.....(1)}$$

where $S_{meas1}(\lambda)$ is intensity of the original reflection data of sample with sample holder, $S_{meas2}(\lambda)$ is intensity of the original reflection data of sample holder without sample, $D(\lambda)$ is the intensity of dark (no light) and $S_{ref}(\lambda)$ is intensity of the spectrum obtained using a white reflectance standard [32]. A certified reflectance standard WS-1-SL (Labsphere, North Sutton, NH, USA) made of Spectralon™ was used as the white reference standard. These dark and reference measurements were performed before each sample measurement.

Chemometrics

Original spectra were modified using two preprocessing algorithms: moving average with 13 point (MA 13s) and standard normal variate (SNV). Signal noise to ratio (SNR) of portable spectrometer can be significantly increased by using moving average algorithm [33]. SNV algorithm may cancel the influence of high scattering effect coming from particle size and density of ground roasted coffee sample [34].

Principal component analysis (PCA) is one of the unsupervised classifications which has been applied frequently in coffee authentication [24]. PCA was applied on preprocessed spectra (MA 13s+SNV) using informative spectral region at 950-1450 nm. Score plot of PC1 and PC2 was used to evaluate the ability of PCA to cluster the samples into two classes: specialty and normal coffee class. Partial least squares-discriminant analysis (PLS-DA) has been widely used for supervised classification purpose [24]. PLS-DA was developed using PLS1 algorithm and full-cross validation with Y variable is type of coffee as categorical variables. Here, the label for each class was determined: Y=1 for specialty coffee class and Y=0 for normal coffee class. The PLS-DA model was evaluated based on coefficient of determination both in calibration and validation (R^2_{cal} and R^2_{val}). The threshold of ±0.5 was used to classify the samples [24]: below 0.5 is belong to normal coffee while above 0.5 is belong to specialty coffee. The chemometrics (spectral preprocessing, PCA and PLS-DA) was calculated by using The Unscrambler 9.7 (64-bit) (Camo Software AS, Oslo, Norway).

RESULTS AND DISCUSSION

NIR Spectral Data Analysis of Specialty and Normal Coffee

Figure 3 shows average spectral data of specialty coffee (red line) and normal coffee (blue line) samples preprocessed by 13 points of moving average (MA 13s) and SNV. There are several peaks observed in two spectral windows in 1100-1200 nm and 1400-1500 nm which was corresponding to the second, and first overtones, respectively [22]. The interval of 1100–1200 nm was corresponded to the 2nd overtone of the C-H functional group [35]. In this interval, the highest peak was observed at 1150 nm. This peak was also contributed to 2nd overtone of C-H vibration [35]. The spectral valley around 1180 nm was also observed in the interval 1100-1200 nm. This wavelength might be related to 2nd overtone of C–H in CH2 groups [35].

In spectral window of 1400-1500 nm, peak and valley was observed at wavelength of 1350 nm and 1450 nm. The spectral peak around 1350 nm was contributed to 1st overtone of C–H combination bands [36]; the spectral valley around 1450 nm was contributed to 1st overtone of O-H stretching [37]. The spectral window of 1400-1500 nm is corresponding to the absorbance of chlorogenic acids, water, alcohols, and especially carbohydrate in ground roasted coffee [22]. This result showed us the importance of spectral window at 1100-1200 nm and 1400-1500 nm for coffee authentication. For this reason, the next analysis of PCA and PLS-DA was conducted using preprocessed spectra involved the two spectral windows of 1100-1200 and 1400-1500 nm (950-1450 nm).

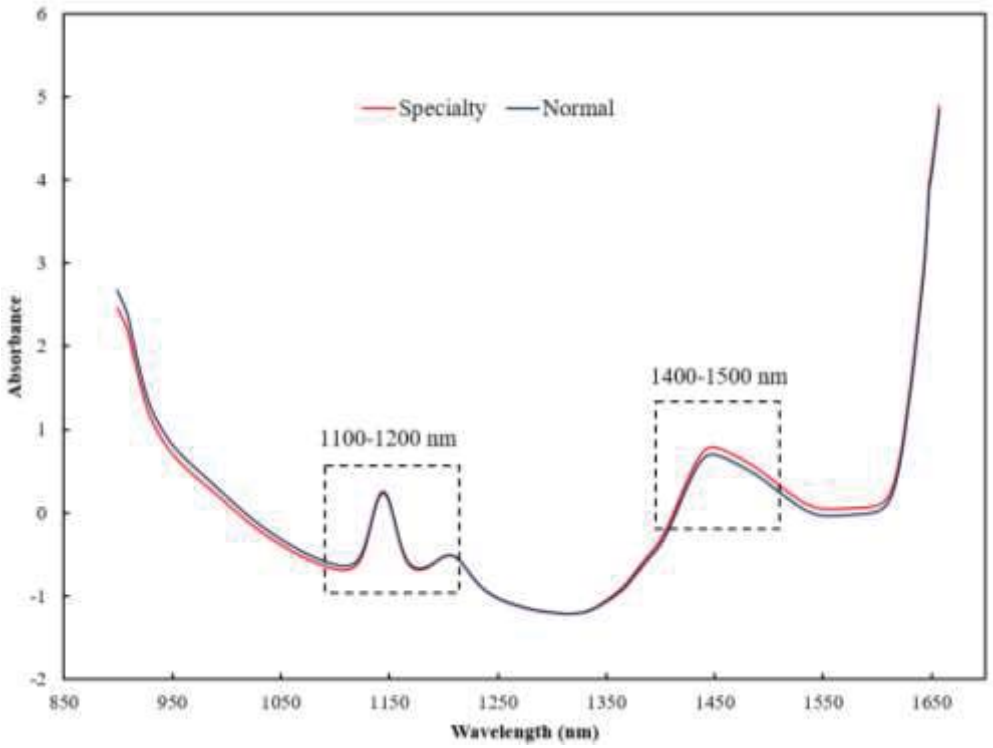

FIGURE 3. The average absorbance NIR preprocessed spectral data (MA 13s+SNV) of specialty and normal coffee samples in the range of 899-1657 nm.

The Result of Unsupervised Classification Using PCA

To authenticate the specialty coffee, a PCA was performed for specialty and normal coffee samples using preprocessed spectral data in the range of 950-1450 nm. The PC1xPC2 score plot with a total of 95% of explained variance was demonstrated in Figure 4. As seen in Figure 4, a clear separation between specialty coffee and normal coffee can be obtained. All normal coffee samples were clustered in positive PC1 (PC1>0) while all specialty coffees were in negative PC1 (PC1<0).

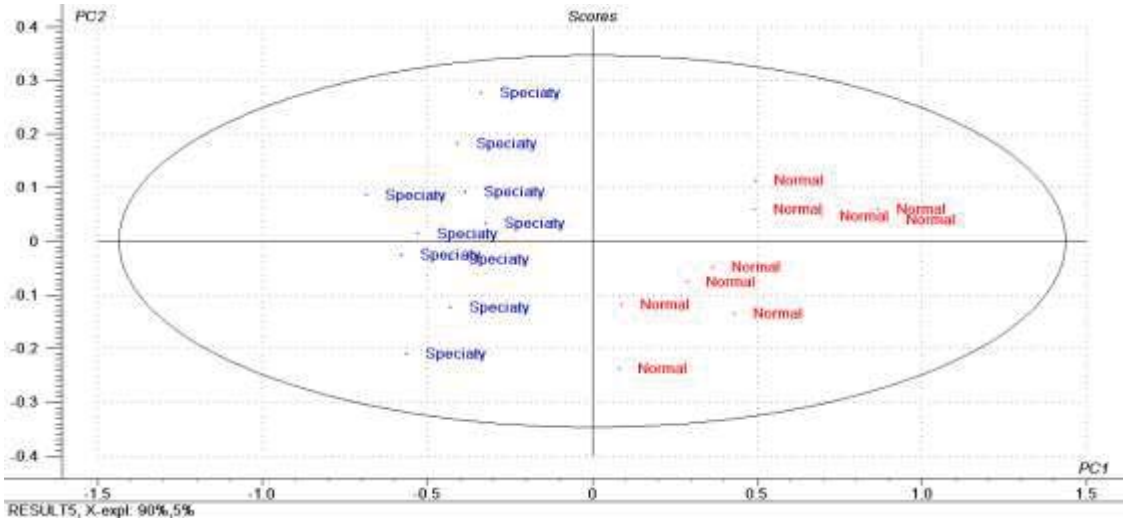

FIGURE 4. PC1xPC2 score plot of specialty and normal coffee calculated using PCA based on preprocessed spectral data (MA 13s+SNV) in the range of 950-1450 nm.

The Result of Supervised Classification Using PLS-DA

The PLS-DA model for classification of specialty and normal coffee was depicted in Figure 5. The model has coefficient of determination very close to 1 (R^2_{cal}=0.97 and R^2_{val}=0.91) indicated that the developed PLS-DA model could established a strong relationship between type of coffee and spectral data. Using 0.5 threshold, all samples can be classified properly into specialty and normal coffee resulted a 100% of accuracy in calibration and validation samples as demonstrated in Figure 6.

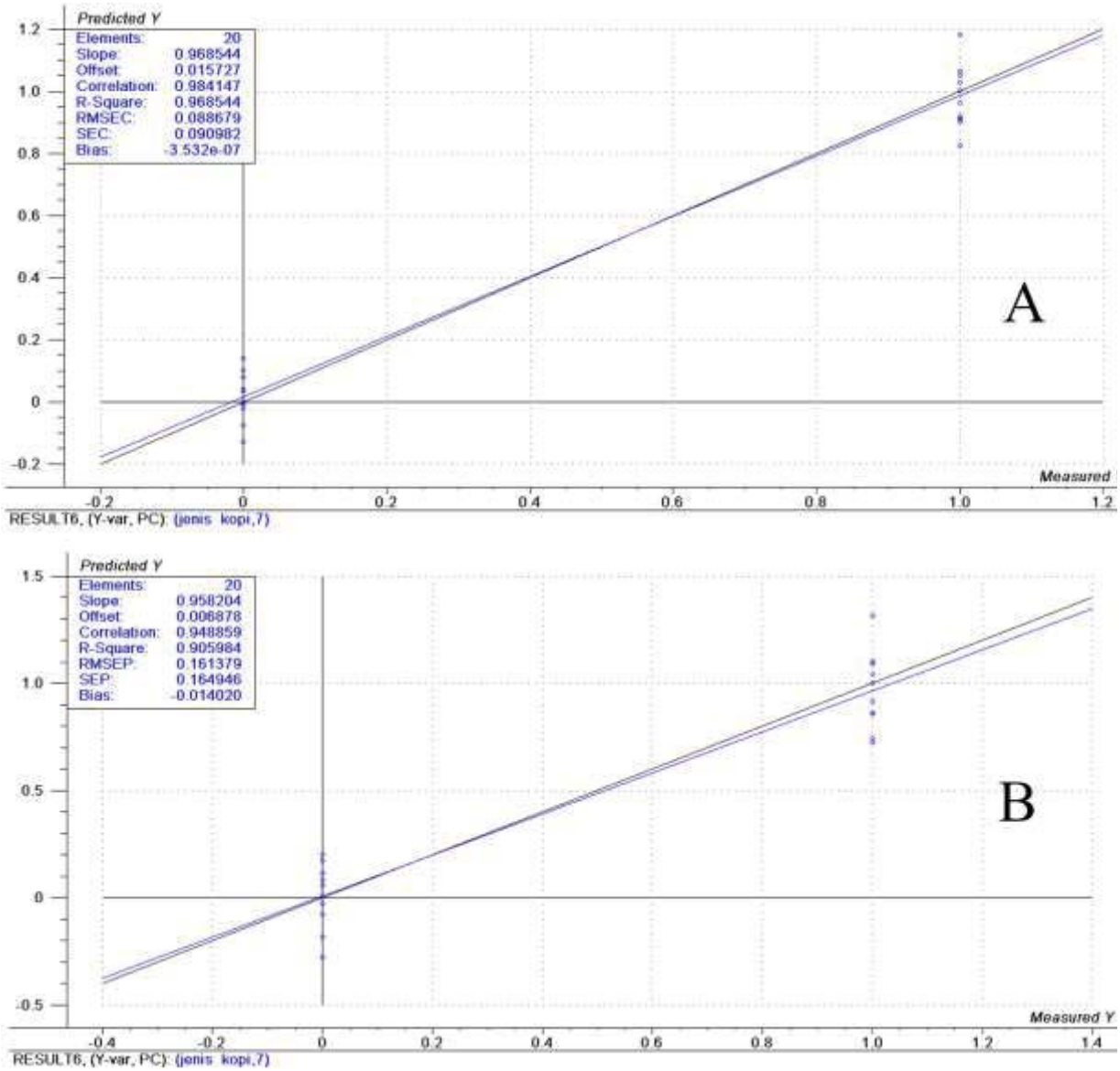

FIGURE 5. Scatter plot of PLS-DA model developed using preprocessed spectra in the range of 950-1450 nm for calibration (A) and validation (B).

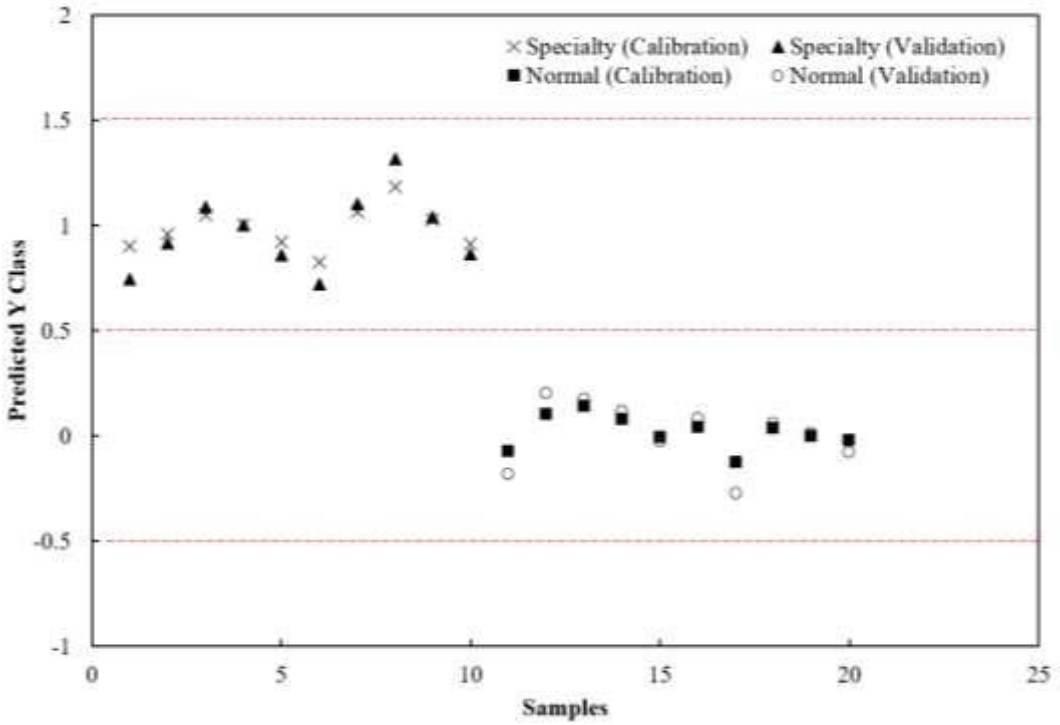

FIGURE 6. Plot of samples versus predicted Y class for calibration and validation using preprocessed spectra in the range of 950-1450 nm.

SUMMARY

In this work, a feasibility of specialty coffee authentication using low cost and portable NIR spectrometer equipped with an integrating sphere was presented. No extraction was involved and after grinding and sieving, coffee samples can be directly placed on NIR spectral measurement. The result of unsupervised and supervised classification was acceptable with a clear separation between specialty and normal coffee. The best PLS-DA classification model was determined with R^2_{cal}=0.97 and R^2_{val}=0.91 for calibration and validation. This result suggested that low cost and portable NIR spectrometer coupled with chemometrics is suitable for specialty coffee authentication with fast and little sample preparation.

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