NIR spectroscopy application for determination caffeine content of Arabica green bean coffee

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Abstract. Caffeine is considered as an important quality indicators of coffee. Caffeine content in green coffee bean influence the flavour and price of coffee. Commonly, percentage of caffeine content is determined by chemical method, which is known time consuming, destructive and expensive, so it is not suitable for a real time coffee content prediction system. The objective of this study was to develop a PLS model based on NIR-Spectroscopy to predict caffeine content of Indonesia coffee beans nondestructively. The wavelength used in this study was 1000-2500 nm and the caffeine content of samples were determined by LCMS method. Several data pretreatments such as multiple scatter correction (MSC), first derivative (dg1), combination of dg1+MSC, with PLS factors variation were applied to obtain the best prediction of caffeine content by NIR. The best prediction was obtained using MSC and 6 PLS factors indicated by a high coefficient correlation value which was \( >0.9 \). NIR method can be used for predicting the caffeine content of green bean coffee nondestructively.

1. Introduction

At present, Indonesia is number four of the coffee exporter countries in the world after Brazil, Vietnam and Colombia, and About 67% of total produced coffee is exported [1]. Ensuring the quality and customer satisfaction is important for the continuation of coffee business. Quality of coffee is influenced by the chemical compositions of coffee, one of which is the caffeine content. Then, it is important to know the percentage of caffeine content in coffee beans. Commonly, it is known that caffeine has a bitter characteristic. However, caffeine is only responsible for no more than 10% of the bitterness of coffee beverages [2].

There are several methods that is commonly used to determine the chemical content of coffee bean such as chemical method and also nondestructive method. However, the chemical method is destructive, expensive and time consuming. Therefore, the nondestructive method such Near Infrared Spectroscopy (NIRS), which is simple, fast and cheap, is widely developed to determine the chemical content of coffee beans. NIR spectroscopy had been successfully applied in predicting the caffeine content of coffee powder
[3], coffee beans [4] and coffee beverages [5], and also in determining the caffeine content in Java Preanger coffee [6]. In this study, NIR spectroscopy method was used to determine the caffeine content in several Indonesian green bean coffee.

2. Material and Methods

2.1. Samples Measurement

The coffee samples were collected from three regions, namely Gayo, Java Preanger and Mandheling coffee beans. Total of 240 samples (water content 12-14%) were weighed in amount of 96 grams, then put in a petri dish in 4 layers for NIR spectra measurement [4]. The NIR spectra measurement was conducted using NIR spectrometer type NIRFlex N-500 (BUCHI Labotechnic AG. Switzerland) in the wavelength of 1000-2500 nm. After that, the coffee samples were measured using LC-MS 2020 (Shimadzu, Kyoto, Japan) to determine the caffeine content.

2.2. NIR Data Pretreatment and Analysis

NIR data were pretreated using several data pretreatment namely first (dg1) and second (dg2) derivative of Savitzky-Golay, multiple scatter correction (MSC), combination of dg1+MSC and combination of dg2+MSC. After that, the calibration and validation model of NIR and reference data were developed using partial least square (PLS) method with several variations of factors. Accuracy of NIR model were determined by the value of coefficient correlation (r), standard error calibration (SEC), standard error prediction (SEP), consistency (%), and ratio of standard deviation to SE (RPD) [6].

3. Result and Discussion

Figure 1 showed the reflectance data of Indonesia green bean coffee which were known as the result of diffuse reflectance of NIR light. Moreover, the spectra data were influenced by the chemical content of each coffee beans.

![Figure 1. Reflectance data of coffee beans](image-url)
Caffeine content of the samples is shown in Table 1. Result showed that the caffeine content from different coffee origin is different, and it is influenced by the geographical indication.

| Coffee origin | Mean (%) | Min (%) | Max (%) | Standard Deviation (%) |
|---------------|----------|---------|---------|------------------------|
| Gayo          | 1.258    | 1.139   | 1.390   | 0.063                  |
| Java Preanger | 1.315    | 1.184   | 1.412   | 0.053                  |
| Mandheling    | 0.988    | 0.909   | 1.097   | 0.052                  |

Table 2 shows the result of calibration and validation of NIR spectra and the reference (chemical) data using PLS method. The best calibration was obtained using the MSC method and 6 factors of PLS indicated by the high correlation coefficient value ($r$) of 0.936, high RPD of 2.146 and consistency of 88%. This research showed that a wider range of data could simplify the obtained NIR calibration model, compared to the result of [6] with a small range of data, that the best calibration model was obtained using combination of dg1 and MSC data pretreatment.

In this research, MSC data pretreatment were applied to remove the multiplicative interference and fix the multiplicative and additive scatter effects of the data, which could reduce the effect of each coffee beans gap while spectra measurement [7].

| Data Pretreatment | PLS Factors | r     | SEC (%) | SEP (%) | RPD   | Consistency |
|-------------------|-------------|-------|---------|---------|-------|-------------|
| Original          | 6           | 0.914 | 0.067   | 0.072   | 1.965 | 92,838      |
| MSC               | 4           | 0.891 | 0.075   | 0.081   | 1.758 | 92,786      |
| MSC               | 5           | 0.909 | 0.069   | 0.080   | 1.785 | 86,431      |
| MSC               | 6           | 0.936 | 0.058   | 0.066   | 2.146 | 87,925      |
| dg1               | 4           | 0.922 | 0.058   | 0.082   | 1.734 | 71,151      |
| dg1               | 5           | 0.947 | 0.053   | 0.073   | 1.950 | 73,103      |
| dg1               | 6           | 0.959 | 0.047   | 0.066   | 2.156 | 70,879      |
| dg1+MSC           | 4           | 0.928 | 0.062   | 0.077   | 1.848 | 80,075      |
| dg1+MSC           | 5           | 0.952 | 0.050   | 0.068   | 2.110 | 74,658      |
| dg1+MSC           | 6           | 0.967 | 0.042   | 0.065   | 2.207 | 64,893      |

4. Conclusion
Result showed that NIR spectroscopy can be used to determine the caffeine content in Indonesian Arabica coffee beans indicated by a high correlation coefficient ($r$) value of 0.936, high RPD value of 2.146 and consistency more than 87%.

References
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