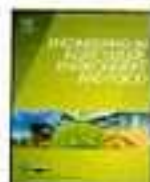




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Research paper

## Chlorogenic acid (CGA) determination in roasted coffee beans by Near Infrared (NIR) spectroscopy<sup>a\*</sup>



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## Research paper

Chlorogenic acid (CGA) determination in roasted coffee beans by Near Infrared (NIR) spectroscopy<sup>☆</sup>Jiajie Shan<sup>☆, \*</sup>, Tetsuhito Suzuki<sup>☆</sup>, Diding Suhandy<sup>☆</sup>, Yuichi Ogawa<sup>☆</sup>, Naoshi Kondo<sup>☆</sup><sup>☆</sup> Graduate School of Agriculture, Kyoto University, Kitashinrake-cho, Sakyo-ku, Kyoto 606-8502, Japan<sup>☆</sup> Department of Agricultural Engineering, Lampung University, Jl. Soemantri Brojonegoro No. 1 Gedungmang Bandar Lampung, Lampung, Indonesia

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## ABSTRACT

Roasting can potentially affect the functional properties of the resulting coffee. For instance, antioxidant phenolic chlorogenic acids (CGA) are known to be thermally labile. In this study, we develop a new NIR spectroscopic method to measure CGA concentration found in the coffee beans. High performance liquid chromatography (HPLC) was used to determine standard reference values of CGA concentration. A partial least squares regression (PLSR) with full cross-validation method was employed for the development and the validation of the regression model. The resultant model accuracy of  $R_{CV}^2 = 0.76$  and RMSECV = 1.16% with preprocessing of the spectra by MSC and SNV is thought to be accurate enough for the rapid and non-destructive determination of CGA concentration in roasted coffee beans.

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## 1. Introduction

In international trade, coffee is the second most important raw material traded, and the most important foreign exchange earner for many developing countries. For this reason coffee is an attractive source of tax revenue. As a consequence, in this highly competitive market, ensuring premium quality and customer satisfaction is of utmost importance to the continued success of the coffee business. One of the functional quality characteristics of coffee which are attracting increasing interest is its antioxidant properties.

Within this class of antioxidant phenolic compounds, chlorogenic acid (CGA) has been proved to play an important role in human health, as well as contribute to the acidity and overall quality of the final cup of coffee, such as bitterness (Tfouni et al., 2012). However, CGA is thermally unstable, which means it can undergo thermal degradation during the roasting stage. As a result, the content of CGA in roasted coffee beans could be several times less than that in the green coffee beans (Perrone et al., 2010). The effect of roasting on the CGA composition of coffee has been studied (Trugo and Macrae, 1984b) with it being well-established that CGA progressively degrades with increasing roasting severity. These studies, however, used time-consuming and laborious methods, so

it is necessary to develop a method that can detect CGA concentration quickly.

At present, high-performance liquid chromatography (HPLC) is the standard method used to quantify CGA concentration in instant coffee (Trugo and Macrae, 1984a), as well as in green and roasted coffee beans (Trugo and Macrae, 1984b). However, this HPLC method has a number of limitations: it requires a complex sample preparation, it is time consuming, and difficult to set up for online detection.

In contrast, spectroscopy has been increasingly used for rapid determination of chemical composition of agricultural products recently. Compared to traditional methods, such as HPLC, spectroscopic methods usually require little sample preparation and less measurement time. While, UV-Vis spectrometry has been used to determine CGA concentration in aqueous solutions of coffee (Belay and Gholap, 2004), the caffeine, however, has to be extracted with dichloromethane before CGA concentration can be determined in the solution. A direct nondestructive determination of CGA in coffee beans without extraction is impossible, due to its spectral overlap with caffeine in the UV-Vis region. Absorption in the UV-Vis region is a result of electronic transition motions. UV-Vis spectroscopy is commonly used for special compound (such as a conjugated system with special functional groups) identification because most compounds don't have absorption in the UV-Vis region.

Compared to the UV-Vis region, near-infrared spectroscopy (NIRS) records more information about sample characteristics, such as basic molecular bonds of chemical components, such as C–H,

<sup>☆</sup> Partly presented at the Sensing Technologies for Biomaterial, Food and Agriculture Conference in April 2013.

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and O–H bonds, generating a spectrum that presents a more detailed characterization of the sample. In addition, it also has the potential for online processing. Thus, if NIR spectroscopy could be applied for CGA analysis, it would offer a number of advantages. To date, NIRS has been used to determine caffeine, theobromine and theophylline in coffee, and CGA in plant samples with wavelet transform preprocessing (Hock et al., 2005; Shao and Zhuang, 2013). In addition, it has been used to evaluate the quality of various sensory properties (Esteban-Diez et al., 2004). FT-NIR spectroscopy has been used to discriminate roasted green tea according to geographical origin (Chen et al., 2009). The FT-IR/ATR method has been applied to analyze brewed coffee characteristics (Esteban et al., 2004). However, to date, there has been no research on quantifying CGA concentration of coffees based on NIR spectroscopy.

This paper investigates the potential for using NIR spectroscopy to measure CGA concentration in roasted coffee beans. Various roasting temperatures and times were used to obtain different grades of roasted coffee. NIR diffuse reflectance spectra of green roasting degrees of coffee were obtained from ground coffee powder. Diffuse reflectance spectroscopy measures not only reflectance from the coffee surface, but also information from below the coffee surface.

Next, the effect of different particle sizes on the obtained diffuse reflectance spectra was evaluated. Prior to the NIR spectral analysis, the CGA concentration of all samples was determined by high performance liquid chromatography (HPLC). In this report, partial least squares regression (PLSR) was used to calibrate the concentration of CGA model with NIR diffuse reflectance spectra. Multiple scattering correction (MSC) was used to remove baseline effects and full cross validation was used to develop and validate the performance of the calibration and validation models.

## Materials and methods

### 1. Sample preparation and chemicals

A batch of Arabica green coffee originating from Antigua Island was purchased from a supermarket. In order to obtain a wide range of CGA concentration to develop a universal model, the Arabica green coffee beans were divided into 65 sub-samples and each sample was roasted at a different time and temperature. More specifically, 38 of these green coffee bean samples were roasted in a coffee roaster (Gene Café, CBR-101A) at 5 °C intervals from a temperature of 65 °C to 250 °C for 15 min; and 22 of the other green coffee bean samples were roasted at 5 min intervals from 10 min to 120 min at 170 °C and 200 °C, respectively. Another 5 reference green coffee bean samples were not processed. After being roasted, each sample was ground in an electric coffee grinder (Cuisinart, C944). Particle sizes were not uniform in the ground coffee powder. In order to check the effect of particle sizes on diffuse reflectance spectra, coffee powder from a green coffee sample was separated into different particle sizes (200 µm, 300 µm, 500 µm, 600 µm, 700 µm, 1000 µm) by sieving through successively finer sieves in ascending order of particle size. The sieving conditions were the same for every sample class. These experiments were performed at room temperature (around 20 °C).

### 2. Near infrared spectroscopy (NIRS)

The NIR diffuse reflectance spectra were recorded by a UV-NIR spectrometer (V-670, JASCO Co.), equipped with an integrating sphere beside the detector (HISN-729, JASCO Co.) which is connected to the spectrometer by an optical fiber. Light is first generated by a grating, and then guided by optical fiber to the

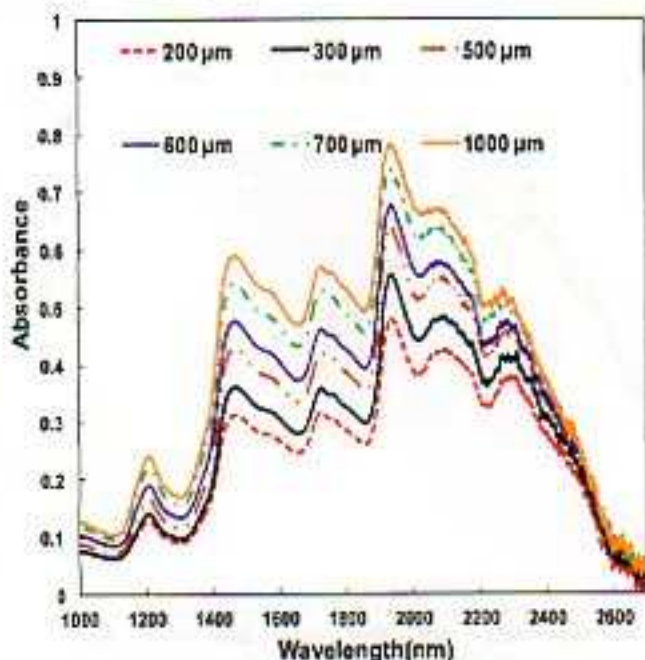


Fig. 1. NIR absorbance spectra of the same green coffee sample with different particle sizes.

integrating sphere. Diffuse reflection light from the coffee powder sample is then integrated and detected. An integrating sphere is an optical component consisting of a hollow spherical cavity with its interior covered with a diffuse white reflective coating, with small holes at the entrance and exit ports. As a consequence, the integrating sphere has a uniform scattering or diffuse effect.

The NIR instrument was controlled by a compatible Windows XP system, and Spectra Manager (V-670, JASCO Co.) was used to acquire spectra data. The size of the light spot in the instrument was 4 cm in diameter. A 4 cm by 4 cm square sample holder was used; with care taken to ensure every sample (weight of approx. 2.45 g) was placed into the sample holder and the sample surface kept flat. Each spectrum was measured from 1000 to 2700 nm, with a bandwidth of 8.0 nm, and a scan speed of 400 nm/min. All experiments were conducted at room temperature (around 20 °C), and the baseline was repeatedly measured every five samples to guarantee that the device was operating correctly.

### 2.3. High performance liquid chromatography analysis

After NIR diffuse reflectance spectra were taken, the actual reference concentrations of CGA in the coffee beans were measured by a standard high performance liquid chromatography (HPLC) procedure. The HPLC system was equipped with an autosampler (Model SIL-20AC, SHIMADZU, Japan), a UV-Vis detector (Model SPD-20A, SHIMADZU, Japan), and a shim-pack VP-ODS column (SHIMADZU, Japan). HPLC sample preparation consisted of extracting the ground coffee with a water and methanol mixture solution (6:4 volume ratio). The mixture containing the ground coffee powder was stirred, and then allowed to stand for 5 min. After that, the supernatant was used for subsequent HPLC analysis. The mobile phase was 70% methanol and the flow rate was 0.5 mL/min. The UV detector was set to 324 nm and the volume of sample injected was 10 µL. Quantification was achieved by peak area measurement and compared to the calibration graph, which was plotted from four pure CGA solutions with a correlation coefficient of 0.999. The main CGA groups in the green coffee beans included:



Table 1  
CGA concentration in the sampled coffee beans.

The number of sample	Range (%)	Mean (%)	Standard deviation (%)
16	1.7–10.3	4.78	2.06

caffeoylquinic acid, dicaffeoylquinic acid and feruloylquinic acid. In this study, the total isomers of CGA were used.

#### 2.4. Data analysis

The whole spectra data (within the wavelength range 800–2700 nm) and the CGA concentration variables were entered into the Unscramble software v9.8 (CAMO, Norway), and sequentially treated mathematically and finally analyzed statistically. Several pre-treatments were applied to find the best relationship between the NIR spectra and CGA concentration. Partial least squares regression (PLSR) was employed to develop a calibration model. Full cross-validation was then used to test the performance of the calibration model, taking into account the number of samples. The signal to noise ratios (SNR) of the spectra decreased after 2200 nm due to the instrument properties. Consequently, only the spectra between 1000 and 2200 nm were used in the subsequent studies.

### 3. Results and discussion

#### 3.1. Scattering effect of different particle sizes

NIR absorbance spectra of coffee powder with different particle sizes are shown in Fig. 1. All these different particle sizes of coffee powder were obtained from one green coffee sample. Different absorbance spectra were observed for the different particle sizes of the same coffee sample. From Fig. 1, it can be seen that absorbance intensity increased as particle size increased. The reason for this is that the space between particles increases as particle size increases. As a consequence, the light absorbed in the increased space between particles contributes to a higher absorbance. For samples with the same particle size, absorbance is the same. Therefore, in an attempt to reduce the effect of different particle sizes, and keep CGA as the only variable, we chose to use coffee powder of a certain particle size in this study. Coffee samples with larger particle sizes have a lower absorbance, and vice versa. The particle size distribution might differ among samples because they have different moisture content. But as I did not measure the moisture content and the particle distribution, I chose 600  $\mu\text{m}$  to eliminate sample particle size effect.

#### 3.2. CGA concentration analysis

The total concentration of CGA in the unroasted green coffee beans was around 10%, and the concentration decreased to around 5% during roasting, which has been reported to be due to the thermal breakage of carbon-carbon covalent bonds (Perrone et al., 2010). The CGA concentration range of the coffee samples is shown in Table 1.

#### 3.3. Observations on the NIR spectra

The original absorbance spectra of the different roasted coffee bean samples are shown in Fig. 2. The overall shape of the roasted coffee bean spectra was qualitatively examined in order to extract the influence of roasting on the spectral profiles. Differences in absorbance spectra intensity were related to roasting degrees (different roasting temperature and time). The most significant spectra

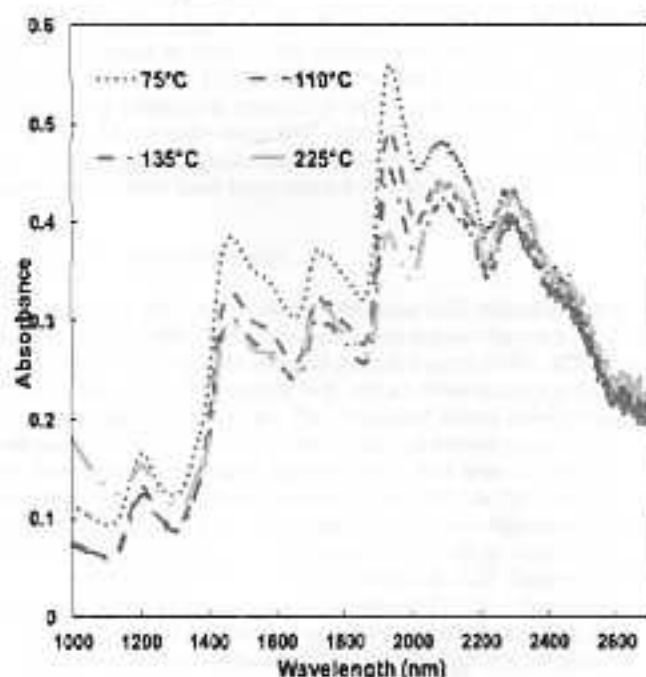


Fig. 2. NIR absorbance spectra of roasted coffee at different roasting temperatures.

differences appeared around 1200–1350 nm, 1450–1850 nm, and 1900–2050 nm. This is thought to be due to structural changes in the chemical composition during roasting (Ribeiro et al., 2011).

Most absorption bands in the near-infrared region are overtones or combination bands of the fundamental absorption bands, which include the C–H bond, N–H bond and O–H bond. Decreases in spectral intensity can be observed in Fig. 2 as roasting temperature increased. During roasting, complex chemical reactions occur, such as the Maillard reaction and pyrolysis, resulting in the release of water and volatiles. Thus, water loss and chemical change, such as the formation of flavor compounds, could explain the observed changes in absorbance intensity. As we expected, the water bond intensity around 1450 nm (first overtone of O–H stretching), and at 1940 nm (a combination band of O–H stretching and O–H deformation) decreased gradually with darker roasting of the coffee beans (higher temperature or longer time). However, the molecular overtone and combination bands (C–H, O–H, N–H) in the NIR region are very broad and complex, and it is difficult to assign specific features to specific chemical components. Thus, multivariate calibration techniques are generally used with NIR spectra.

#### 3.4. Regression model of CGA concentration

Outliers in spectral data were identified by the Hotelling's T-square statistic method using the score plot of the PLS model. Hotelling's T-square statistic is a measure of the variation of a sample within a PLS model and a high T-square level for a certain sample indicates a high influence of the sample on the model. The confidence interval was defined by Hotelling's T-square ellipse with a 95% confidence level. Three samples were identified as outliers in this experiment.

The capability of the prediction model was evaluated by using several parameters, including the root mean square error of cross validation (RMSECV), determination coefficient of cross validation ( $R_{CV}^2$ ), and ratio prediction to deviation (RPD). The results obtained when using the PLSR to model CGA concentration on the basis of NIR spectra in combination with different preprocessing methods,

Table 2  
Validation models developed by PLSR based on NIR preprocessed

LVs	Cross Validation	
	$R_{CV}^2$	RMSECV (%)
0	0.72	1.16
1	0.59	1.43
2	0.45	1.65
3	0.72	1.17
4	0.76	1.10
7	0.71	1.20

Standard normal variate.

used to select the most suitable latent variables (LVs) of each (see Table 2). Multiple scatter correction (MSC) was first and then other preprocessing methods were applied on the

The results indicate that the best regression model for the prediction of CGA concentration in roasted coffee beans was obtained when seven LVs were taken into account in the calibration model in combination with MSC and SNV preprocessed spectra. The calibration model had a  $R_{CV}^2$  of 0.76, and RMSECV of 1.10%. It was usually applied on NIR spectra to remove scatter effect. From the results, we could conclude that scattering was creating noise interfering with the PLSR model's accuracy. Besides, CGA has been considered to have five groups of isomers. After roasting, considerable changes in the CGA composition were observed. Some CGA isomers decreased sharply, while others decreased gradually, while yet others increased due to a transition from one isomer to another. Thus, the different isomer states will interfere with the results. This was considered to be a part of the error of the model. However, the model still exhibits a high predictive ability. Fig. 3 shows the scatter plot of reference values of CGA concentration vs. prediction values of CGA concentration obtained from the

PLSR model in combination with MSC and SNV pretreatments. This can also be used to display the goodness of the final regression model.  $R_{CV}^2$  was 0.76, RMSECV was 1.10% and RPD was 2.01, which indicates the calibration model can accurately predict CGA concentration. The results show that NIR spectroscopy is a suitable method for the quantitative determination of CGA concentration in coffee beans which have been roasted to different degrees.

#### 4. Summary and conclusions

In this study, NIRS was used to determine CGA concentration in ground coffee powder. In order to remove the scatter effect associated with different particle sizes, we used a specific particle size (600  $\mu\text{m}$ ) for all samples when obtaining NIR diffuse reflectance spectra of powdered coffee bean samples. The developed model development used spectra from 1000 to 2200 nm. In the subsequent analysis, MSC was first applied to remove baseline shift, and then several preprocessing approaches were applied on the spectra. The best calibration results,  $R_{CV}^2 = 0.76$  and RMSECV = 1.10%, were obtained from a PLSR model with MSC and SNV preprocessed NIR spectra. The results from this paper indicate NIRS, combined with chemometric methods, can be used to accurately determine CGA concentration in coffee samples. It can also be used to optimize the roasting process so as to retain the greatest amount of CGA with the appropriate roasting temperature and time. More studies (such as with different coffee varieties, particle sizes, more sophisticated mathematical methods and so on) should be investigated for future online application.

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#### References

- Balay A, Ghisla AV. Characterization and determination of chlorogenic acid (CGA) in coffee beans by UV-Vis spectroscopy. *Int J Food Appl Chem* 2004;3:234–40.
- Chen QS, Zhao J, Liu B. Study on discrimination of mast green tea according to geographical origin by FT-NIR spectroscopy and supervised pattern recognition. *Spectrochim Acta Part A* 2009;72:845–50.
- Esteban-Diez I, Gonzalez-Sala JM, Pizarro E. Prediction of sensory properties of espresso from roasted coffee samples by near-infrared spectroscopy. *Anal Chim Acta* 2004;525:171–82.
- Hashimoto A, Mori H, Kanou M, Yamazaki A, Kameoka T. Mid-infrared spectroscopic analysis on brewed coffee characteristics. In: 10th Asia-Pacific Conference of Chemical Engineering; 2004.
- Huck CW, Guggenbichler W, Bonn CE. Analysis of caffeine, theobromine and theophylline in coffee by near infrared spectroscopy (NIRS) compared to high-performance liquid chromatography (HPLC) coupled to mass spectrometry. *Anal Chim Acta* 2005;538:195–203.
- Perreze D, Donangelo R, Donangelo CM, Farah A. Modeling weight loss and chlorogenic acids content in coffee during roasting. *Agro Food Chem* 2010;58:12230–43.
- Ribeiro J, Ferreira MMC, Salva TG. Chemometric models for the quantitative descriptive sensory analysis of Arabica coffee beverage using near infrared spectroscopy. *Talanta* 2011;22:1352–6.
- Shan XC, Zhuang YD. Determination of chlorogenic acid in plant samples by using near-infrared spectrum with wavelet transform preprocessing. *Anal Sci* 2004;20:451–4.
- Turpo LC, Maciel R. Chlorogenic acid composition of instant coffee. *Analyst* 1984;109:263–6.
- Trope IC, Mattar B. A study of the effect of roasting on the chlorogenic acid composition of coffee using HPLC. *Food Chem* 1984;15:219–27.
- Youni SW, Senise CS, Carneiro LR, Camargo MKR, Trilles CRM, Gonalves KMVAR, et al. Effect of roasting on chlorogenic acid, caffeine and polyphenolic hydrocarbons levels in two coffee cultivars: coffee *Arabica* cv. *Int J Food Sci Technol* 2012;47:405–15.

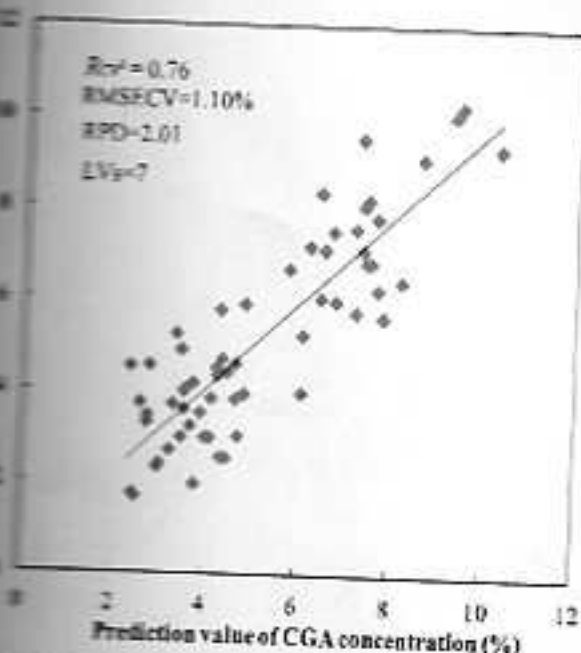


Fig. 3. Plot of reference CGA concentration values vs. prediction CGA concentration values obtained from cross validation model.