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NEAR INFRARED TECHNOLOGY COUPLED WITH DIFFERENT SPECTRA CORRECTION APPROACHES FOR FAST AND NON-DESTRUCTIVE PREDICTION OF CHLOROGENIC ACID ON INTACT COFFEE BEANS

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The primary objective of this research was to utilise near-infrared reflectance spectroscopy as a swift, non-destructive method for identifying chlorogenic acid in whole coffee beans. Additionally, this investigation explored the efficacy of different spectral improvement techniques alongside partial least square regression to construct predictive models. NIR spectral data was gleaned from whole coffee beans spanning a wavelength range of 1000–2500 nm, while the chlorogenic acid content was ascertained via high-performance liquid chromatography procedures. Our findings revealed that the highest coefficient of determination reached for chlorogenic acid was 0.97, and the root mean square error for calibration was 0.31% when using the multiplicative scatter correction method. Furthermore, upon testing the model using an external validation dataset, a determination coefficient of 0.91 and a ratio error to range index of 11.56 with a root mean square prediction error at 0.51% was attained. From these results, it can be inferred that the near-infrared technology, coupled with an effective spectral enhancement process, can facilitate quick, non-invasive determination of chlorogenic acid in whole coffee beans.

Keywords: NIRS; spectrum; quality; agriculture; chemical properties

Coffee beans is one of the most important agricultural products cultivated in tropical counties. Beside served as leisure and social activity, coffee also used as a medical alternative beverage containing numerous potential health benefits. If consumed wisely with a significant dose, coffee can be benefited to human health as antioxidant and may help to prevent several chronic diseases, reducing in high risk diabetes, liver damage, and Alzheimer's disease (Lemos et al., 2022).

There are four major chemical properties that correspond to coffee qualities, namely caffeine, chlorogenic acids, cafestol, and kahweol (Farag et al., 2021). Other chemical properties like carbohydrates, lipids, nitrogenous compounds, vitamins, minerals, alkaloids, and phenolic compounds also can be found in coffee (Min et al., 2023). Caffeine is the main source of antioxidant diet and the major component in coffee, while chlorogenic acid (CGA) is the major polyphenol source which is important for antioxidant and reducing liver damage. On the other hand, cafestol and kahweol are the two chemical properties in coffee which are benefited to reduce diabetes by reducing insulin sensitivity and risk in cancer (Kulapichitr et al., 2022).

Chlorogenic acid is a natural compound that is found in abundance in coffee beans. It is a type of polyphenol, which is a class of plant compounds known for their antioxidant properties (Lemos et al., 2022). In addition to its taste, CGA in coffee beans also offers several health benefits. It has been studied for its potential to aid in mass loss by promoting fat metabolism and reducing the absorption of carbohydrates in the digestive system. Chlorogenic acid can also help regulate blood sugar levels by inhibiting an enzyme called glucose-6-phosphatase, which plays a role in sugar production in the body (Lemos et al., 2022). Overall, CGA in green coffee beans is considered to be one of the main bioactive compounds that may contribute to its potential health benefits, particularly in terms of mass management and antioxidant effects.

Several methods were employed to determine coffee quality parameters. Most of them are based on solvent extraction requiring complex laboratory procedures and involving other chemical materials (Tugnolo et al., 2021). To date, high-performance liquid chromatography (HPLC) is the main standard method used to measure and determine many coffee quality compositions, including chlorogenic acid concentration in coffee products, as well as in green bean and roasted coffee beans. Yet, this HPLC method has a number of limitations: expensive, requires a complex sample preparation, time consuming, and difficult to set up for online detection. Therefore, other alternative methods are required to overcome those limitations and to be applied directly for rapid and non-destructive assessment of coffee quality.

In recent decades, near infrared spectroscopy (NIRS) has become one of the most promising and increasingly applied for rapid, non-destructive, and simultaneous determination of chemical composition and quality attributes of foods and agricultural products (Pasquini, 2018). The principle behind NIRS involves the measurement of the intensity of NIR light before and after interaction with the sample. These measurements are typically made using a spectrometer detecting the intensity of light at different wavelengths. By comparing the intensity of incident NIR light with the intensity of reflected NIR light, the spectrum of the sample can be obtained (Pasquini, 2018). The main advantage of NIRS is that this method does not require a complicated sample preparation like extraction, is without involving chemical liquids and materials, is fast, non-destructive and most importantly, it can determine several quality parameters simultaneously using a single NIR spectrum (Munawar et al., 2022b). The NIRS records more information about sample characteristics and chemical properties, such as the basic molecular bonds of chemical components like C–H, N–H, C–H–O and O–H. It generates spectral data in the NIR wavelength region presenting a more detailed characterisation of the sample.

Numerous studies have been investigated and reported related to NIRS applications in food and agricultural products such as assessing quality parameters on intact fruits (Hayati et al., 2020), rapid adulterations and fraudulence detections on agricultural products (Chen et al., 2018; Vieira et al., 2021), rapid quality detection of plant diseases (Mireei et al., 2017), and soil quality assessment (Jaconi et al., 2019; Wang et al., 2021). Furthermore, for coffee itself, NIRS has been used to determine caffeine, theobromine, and theophylline contents in coffee products. In addition, NIRS is also employed for discrimination between the Arabica and Robusta coffee variety in blends (Catelani et al., 2018; Correia et al., 2018; Santos et al., 2012). Real time monitoring of the coffee roasting process by means of NIRS has been investigated as well. For CGA concentration, to the best our knowledge, it is still scarce. Hence, the presented study reports the use of NIRS to determine CGA content on intact green coffee beans by establishing accurate and robust prediction models using NIR spectral data with various machine learning algorithms.

Material and methods

Samples

A total of 108 bulk of intact green beans from various geographical origins in Indonesia (West Java, West Sumatera, Southwest Nusa, North Sumatera, and Aceh Province) were used in this study. Each bulk contains an amount of 60 g for spectral data acquisition and is further used for actual chlorogenic acids measurement. Samples were split into two datasets, namely calibration dataset (n = 72) used to establish prediction models for predicting CGA, and validation dataset (n = 36) used to test the model performance based on its prediction accuracy. All the samples were collected directly from the coffee farmers in those mentioned areas and stored for 2 days in room temperature 26 °C to equilibrate prior to spectral data acquisition and CGA analysis.

NIR spectral data acquisition

The spectral data of intact coffee bean samples were acquired and recorded in near infrared wavelength region from 1000 to 2500 nm by means of NIRS instrument (Thermo Nicolet Antaris TM II, Thermo Fisher Inc., USA). Each bulk of coffee sample was scanned 32 times and rotated during scanning. Spectral data for each sample was the average of these 32 scans and used for developing calibration models and further data analysis (Munawar et al., 2022a).

Actual chlorogenic acid (CGA) measurement

After the completion of spectral data acquisition for coffee bean samples, CGA contents were determined using a standard high performance liquid chromatography (HPLC) method. The coffee bean samples were grounded and extracted with water : methanol mixture in a 6 : 4 ratio. Then, they were stirred and left undisturbed for 5 minutes. The resulting supernatant was then subjected to HPLC. The mobile phase consisted of 70% methanol, with a flow rate of 0.5 mL·min^{-1}, and the UV detector was set to 324 nm. Approximately 10 mL of the supernatant was injected for analysis. The CGA of the samples was determined by measuring the peak area and comparing it to a calibration graph, constructed using 4 pure CGA solutions, which exhibited a correlation coefficient of 0.999. The primary CGA groups identified in the green coffee bean represented the total isomers of CGA (Klikarová et al., 2022; Shan et al., 2014).

Spectral data corrections

Techniques for spectral correction in NIRS serve to boost data quality, decrease noise interference, and augment the precision and dependability of ensuing analyses. A range of correction algorithms for spectra are utilised across numerous NIRS applications, founded on the principles of smoothing, baseline adjustment, standardisation, and transformation. For the purposes of this investigation, several distinct methods for spectral correction were evaluated and applied. In this study, we attempted to employ different spectra correction methods, namely smoothing with Savitzky-Golay algorithm (SGS), second order de-trending (DT-2), de-resolve (DR), peak normalisation (PN), multiplicative scatter correction (MSC), baseline correction (BSC), and standard normal variate (SNV) (Nicolai et al., 2007; Pasquini, 2018). The influence of these methods on CGA prediction performance was compared. Different spectra corrections provide a particular algorithm, and they have specific advantage that can enhance spectral data. For instance, the MSC correction effect is multiplicative, affecting both the slope and offset of the spectrum, and the same for all samples. This allows it to correct for both multiplicative and additive effects. The MSC works by standardising each spectrum to have the same mean and variance, effectively reducing the scatter effect and increasing the consistency between samples (Pasquini, 2018). Mathematically, this is represented by the following equation:

$$Y_{corrected} = \left(\frac{(Y - B)}{A} \right) \quad (1)$$

where: $Y_{corrected}$ – spectral data after MSC correction; Y – refers to raw spectrum before correction; B – indicates the intercept of the best fitted line; while A – the slope of the best fitted line

The corrected spectrum compensates for both additive (B) and multiplicative (A) scatter effects. By minimizing the scatter effects, MSC reduces spectral variability and enhances prediction performance. This makes it particularly effective in agricultural applications like the evaluation of food and feed materials by NIR spectroscopy where physical properties of the sample can vary widely.

Calibration and validation

The main task in NIRS application is to establish prediction models for the chemical constituents of samples through the calibration process. Two regression approaches were applied in calibration, namely principal component regression (PCR) and partial least square regression (PLSR), and the results are compared. A total of 74 datasets consisting of NIR spectral data and actual CGA concentration were used in this calibration process. The *k*-fold cross validation algorithm was also employed during calibration, where *k* is set to 10 segments. To ensure NIRS-based model's generalisability and avoid overfitting, external validation using independent dataset was performed. A total of 29 data were used to validate the model and quantify prediction's performance. Beside R^2 and RMSE, the performance of external validation was also quantified using the range to error ratio (RER). All of those data analyses, including various spectra correction and regression methods, were performed using The Unscrambler X 10.3 software (CAMO, Oslo, Norway).

Prediction performance

To justify the model performance, several statistical indicators were used, namely the coefficient of determination (R^2), root mean square error (RMSE, it measures the average difference between the actual and predicted values). A lower RMSE is preferable since it indicates a better predictive performance. Ratio prediction to deviation (RPD) index was also used to quantify model performance. It provides an indication of the quality and reliability of predictions made by the model. The RPD value is calculated as the ratio of the standard deviation of reference data to the standard deviation of the difference between predicted and reference values. The higher the RPD value, the better the prediction performance of the model. The RPD values greater than 2 are generally considered acceptable, with higher values indicating more accurate and reliable predictions (Lazaar et al., 2020; Walsh et al., 2020).

Results and discussion

NIR spectral features of coffee beans

As presented in Fig. 1, the spectra features of intact coffee bean samples are quite similar between Arabica and Robusta bean samples. Certain vibrations of the molecular bands like O–H, C–H, C–H–O, and N–H revealed the chemical properties in the sample. The wavelength that appears in all

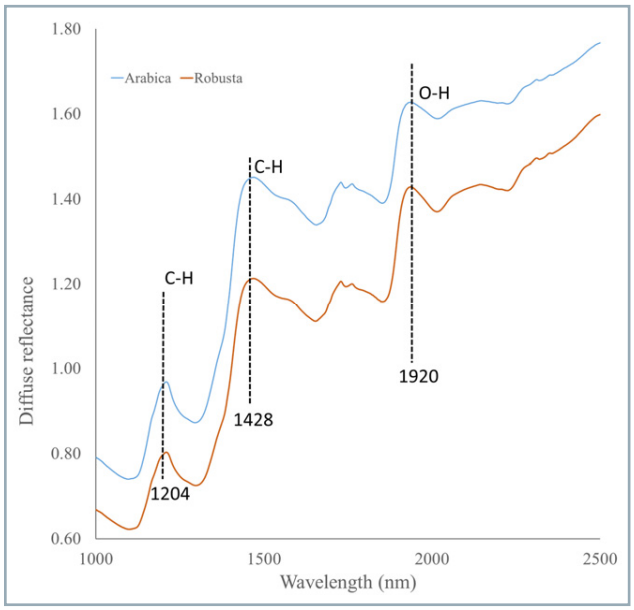


Fig. 1 Spectra features of intact green coffee bean samples in the NIR region

the spectra around 1920 nm is the combination wavelength of O–H vibration in water molecules.

The wavelengths around 1428 nm and 1204 nm correspond to C–H molecule vibrations with respect to the first and second overtones. These distinct characteristics provide evidence of significant changes that occur in beans when they were roasted (Souza et al., 2022). Roasting involves the evaporation of water and the initiation of chemical reactions, particularly involving C–H bonds, as depicted in Fig. 1. These reactions likely involve the prominent organic compounds, such as carbohydrates, proteins, trigonelline, and chlorogenic acids. Through the analysis of the spectral map behaviour of complete coffee bean samples, a more comprehensive understanding of the chemical and physical transformations that occur during roasting can be acquired.

Overtones, in the context of coffee beans, refer to higher frequency vibrations or sounds that accompany the fundamental frequency of an object or substance. In the case of coffee beans, overtones represent specific acoustic frequencies or vibrations that arise from certain processes or conditions. Coffee is composed of various organic molecules, including caffeine, chlorogenic acid and its derivatives, trigonelline, polysaccharides, sucrose, proteins, and lipids. In the near-infrared (NIR) wavelength region, chlorogenic acid exhibits distinctive absorption bands and peaks. By measuring the intensity of these absorption peaks, it is possible to quantify the presence and concentration of chlorogenic acid in a green coffee bean sample. This chemical information is embedded in NIR spectra and can be revealed by establishing calibration models based on NIR spectral data.

Calibration model to predict CGA

The main part in NIR spectroscopy is to develop prediction models used to determine quality parameters like CGA concentration through the calibration process. It is a mathematical algorithm that relates the NIR spectral data

Table 1 Calibration results using PCR and PLSR methods for CGA prediction

Calibration method	Statistical indicators			
	R^2	*r*	RMSEC	RPD
PCR	0.773	0.879	0.624	2.247
PLSR	0.905	0.952	0.441	3.179

from a sample to a known CGA reference value obtained from laboratory measurement. Firstly, we establish the models based on raw NIR spectral data by means of PCR and PLSR approaches. The prediction performance obtained from both regression approaches was compared, and the best one was chosen for further calibrations. PCR is a method that combines PCA and linear regression to analyse the relationship between NIR spectral data and actual CGA values obtained from laboratory analysis. The CGA prediction performance using PCR is described in Table 1.

On the other hand, PLSR is a technique similar to PCR, finding the relationship between NIR spectra and reference or actual CGA values. However, unlike PCR, PLSR takes into consideration the structure and covariance between predictors and response in the original space. PLSR decomposes both the predictor and response variables into latent variables known as factor. They were generated by maximising the covariance between NIR spectral data and CGA values. In this work, maximum 7 factors were involved in constructing the models. Based on the factors, PLSR constructs a regression model that relates NIR spectral data to actual CGA concentrations. The model is developed by iteratively estimating the regression coefficients. The CGA prediction performance using PLSR is also described in Table 1.

Both PCR and PLSR provided good prediction performance, whereas the maximum achieved R^2 coefficient is 0.905 using the PLSR approach which means that around 90.5% of the CGA can be predicted accurately by means of NIR spectral data. Moreover, the ratio prediction to deviation (RPD) index from both regression methods was above 2, which is categorized as good prediction performance (2.247) for PCR and excellent performance (3.179) for PLSR, respectively.

Based on obtained results, the PLSR calibration model provides better prediction accuracy than the PCR model because it considers the covariance structure between NIR spectral data and actual CGA contents. The PLSR can handle multi-collinearity and capture complex relationships between variables. NIRS spectra often contain highly correlated information, making traditional regression models unstable or ineffective. PLSR performs well in such scenarios as it considers the covariance structure between spectral data and CGA concentrations. PLSR effectively handles multi-collinearity, ensuring robust model development.

Moreover, NIR spectral data can have complex relationships, including nonlinear and interactive effects. PLSR is commonly designed to capture such complexity by constructing latent variables or factors of PLSR components that explain the covariance between NIR data as predictors and actual CGA as the response. This allows PLSR to model intricate patterns in spectral data, leading to improved prediction accuracy. Nonetheless, both PCR and PLSR are popular methods for developing calibration models in NIRS applications. They enable the prediction of properties or components of interest based on NIR spectra, facilitating quality control, process optimisation, and rapid analysis in various industries. The scatter plots derived from PCR and PLSR for CGA prediction are presented in Fig. 2.

Further calibration was attempted to investigate the impact of various spectra correction algorithms on the prediction accuracy of CGA determination. The models were constructed using the PLSR method as previously founded it is better than PCR, with achieved maximum R^2 and RPD indexes 0.905 and 3.179, respectively, by means of raw NIR spectra data. In NIRS, spectra corrections are essential preprocessing steps to enhance data quality, remove unwanted variations, and improve the accuracy of subsequent analysis. The first approach employed to spectral data is de-trending 2nd order (DT-2) algorithm. It seeks to remove systematic variations or trends in spectra caused by factors like instrument drift or changes in experimental

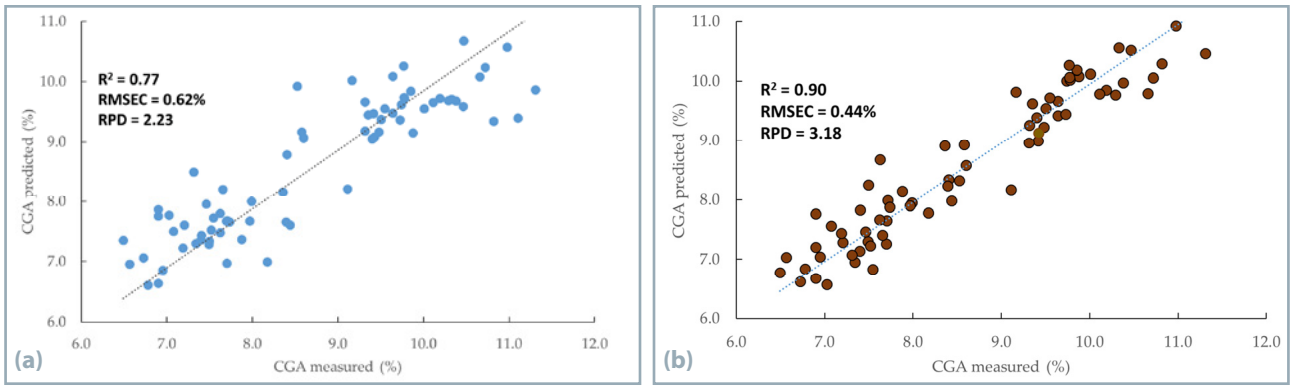


Fig. 2 Prediction performance using PCR (a) and PSLR (b) for CGA determination on intact green coffee beans using raw spectral data

Table 2 Prediction performance of PLSR models coupled with various spectra corrections

Spectra correction method	Statistical indicators			
	R^2	*r*	RMSE	RPD
De-trending	0.95	0.98	0.40	3.51
De-resolve	0.87	0.94	0.51	2.75
Peak normalisation	0.94	0.97	0.41	3.42
Multiplicative scatter correction	0.97	0.98	0.31	4.52
Baseline shift correction	0.95	0.97	0.39	3.59
Standard normal variate	0.93	0.96	0.43	3.26

conditions. Achieved result by DT-2 is slightly improved compared to raw spectra, with R^2 and RPD indexes increased to 0.95 and 3.51, respectively.

Other spectra corrections also improved the accuracy and robustness. Yet, the de-resolve algorithm seems to be lower than raw spectra. Probably this is because some relevant information related to CGA was removed during the correction process. Overall, the R^2 coefficient and RPD index of the models are acceptable and categorised as good model performance. The prediction performance of CGA

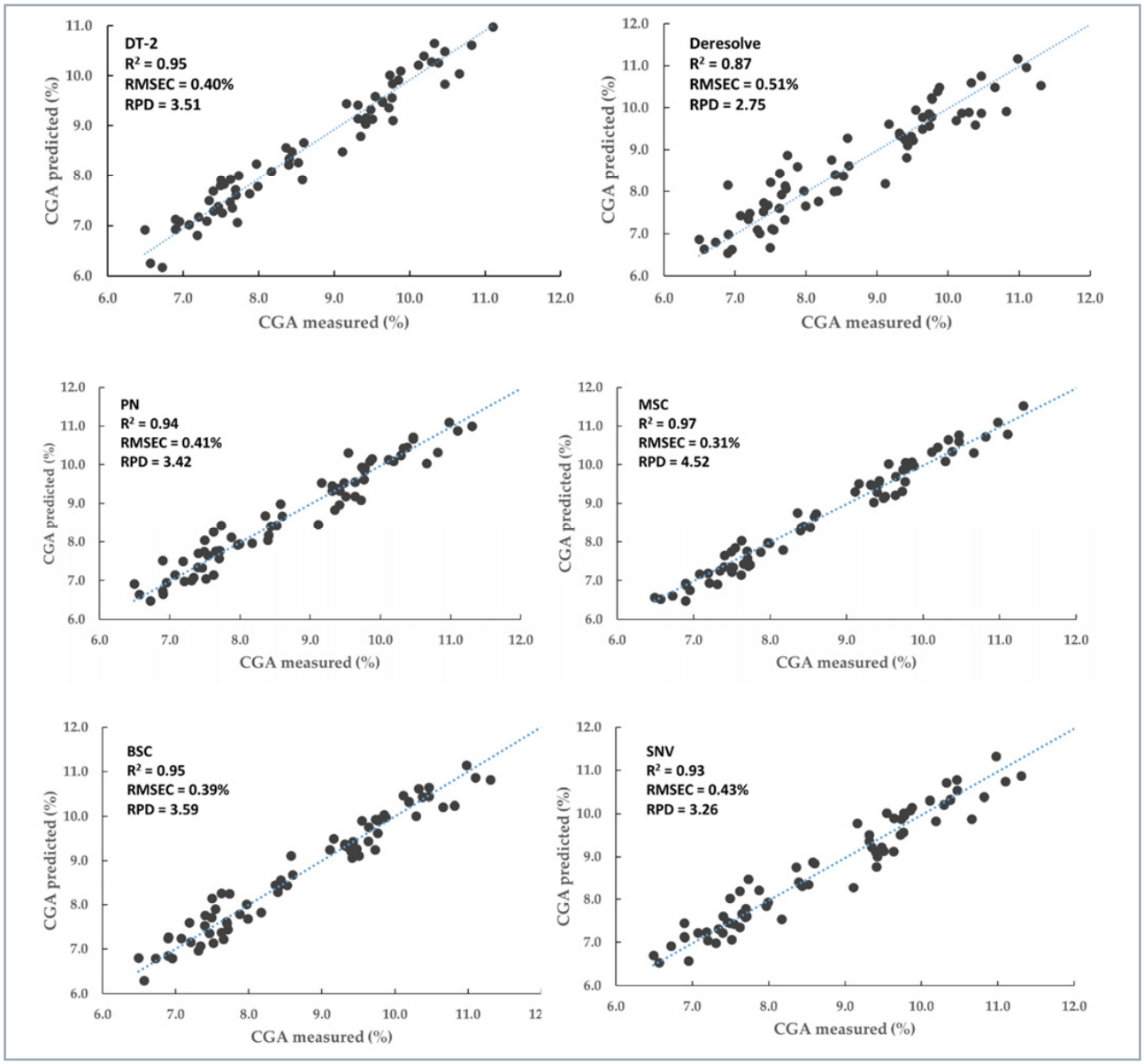


Fig. 3 Prediction performance of various spectra corrections coupled with PLSR for CGA determination on intact green coffee beans

determination using PLSR coupled with various spectral data corrections is presented in Table 2 and Fig. 3. The choice and application of spectral corrections depend on the specific characteristics of NIRS data and analytical objectives. Applying appropriate corrections helps eliminate noise, baseline variations, and confounding factors, improving the reliability and accuracy of subsequent chemometric analysis techniques like PLSR, PCR, or others.

Based on the performance obtained, it was found that MSC in conjunction with the PLSR approach, was the most effective method for spectral correction. The achieved R^2 and RPD coefficients were the highest, 0.97 and 4.52, respectively. Similar findings have also been noted in previous research, demonstrating that the implementation of MSC leads to greater accuracy and robustness when predicting the quality attributes of agricultural products. The basic principle of MSC is to divide each spectrum by this reference spectrum to reduce the unwanted scatter-related variations. It is employed to mitigate the scattering effects caused by sample inhomogeneity, particle size variations, or differences in sample thickness. Scattering occurs when light interacts with intact coffee bean's physical structure, causing the measured spectra to be perturbed with additional noise and variations. These scattering effects can obscure or distort spectral information and hinder accurate analysis and interpretation. MSC correction aims to normalise the spectra by scaling each spectrum to a reference spectrum or normalisation factor that represents the average scatter across all spectra.

To evaluate and test the model, external validation was performed using a total of 29 data from validation dataset. It is crucial to ensure the reliability and generalisability of NIRS models. It helps in assessing the model's ability to provide accurate predictions for unseen samples and to identify any potential biases or limitations. Selected prediction model MSC-PLSR was used to determine the CGA concentration of this dataset. Spectral data were automatically subjected for MSC corrections to enhance the spectra quality, and CGA was predicted and compared with actual ones. Prediction performance on this external validation shows a good prediction accuracy with coefficient R^2 0.915 and prediction error RMSEP 0.512%, as presented in Fig. 4.

Hence, the achieved ratio error to range (RER) index is 11.563, which is categorised as a good prediction accuracy

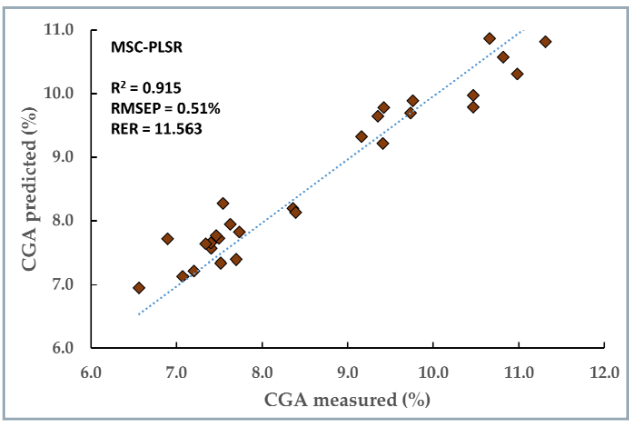


Fig. 4 CGA prediction performance using external validation dataset based on the MSC-PLSR model

and more reliable model. It provides an indication of the quality and performance of the NIRS model in relation to the variability of reference values. A commonly accepted threshold for an acceptable RER index varies depending on the specific application and the properties being measured. However, in general, a RER value greater than 10 or 20 is often considered as a reasonable benchmark for a well-performing NIRS model in many applications.

The use of this method resulted in the highest coefficients of determination (R^2) and ratio of performance to deviation (RPD) values, surpassing those reported in comparable studies such as Shan et al. (2014), who utilised BSC with PLSR and found the RPD and R^2 values being 3.014 and 0.884, respectively. The extensibility of the MSC-PLSR model was further demonstrated with the R^2 coefficient of 0.915 and root mean square error of prediction (RMSEP) of 0.512% when applied to an external validation dataset of 29 samples for the prediction of CGA concentration. This study thereby aligns with current shift in the industry towards harnessing the rapidity and non-destructive nature of NIRS, particularly when combined with effective spectral correction and regression techniques for the determination of quality parameters such as CGA concentration in products like green coffee beans. This continues the work of numerous researchers who have promoted the benefits of NIRS in the agricultural sector.

Conclusion

The conclusions drawn from this study founded that multiplicative scatter correction (MSC) together with partial least squares regression (PLSR) stands as the most effective strategy for spectral amendment in NIRS application. Prediction performance exhibited by the MSC-PLSR model resulted in the top coefficients of determination (R^2) and the ratio of performance to deviation (RPD) values, implying paramount precision and robust capability in forecasting the quality aspects of agricultural merchandise. Emphasised in this research is the application of the MSC-PLSR model to another validation dataset consisting of 29 samples, which demonstrated considerable prediction exactitude, with the R^2 coefficient of 0.915 and root mean square error of prediction (RMSEP) of 0.512% for the estimation of CGA concentration. The achieved range to error ratio (RER) index of 11.563 further attests to notable prediction precision and a reliable model. Hence, NIRS, when paired with corresponding spectral rectification and regression solutions, can effectively be harnessed to gauge CGA concentration along with other quality parameters swiftly and non-invasively on whole green coffee beans.

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References

CATELANI, T. A. – SANTOS, J. R. – PÁSCOA, R. N. M. J. – PEZZA, L. – PEZZA, H. R. – LOPES, J. A. 2018. Real-time monitoring of a coffee roasting process with near infrared spectroscopy using multivariate

statistical analysis: A feasibility study. In Talanta, vol. 179, pp. 292–299. DOI: https://doi.org/10.1016/j.talanta.2017.11.010

CHEN, H.– LIN, Z. – TAN, C. 2018. Fast quantitative detection of sesame oil adulteration by near-infrared spectroscopy and chemometric models. In Vibrational Spectroscopy, vol. 99, pp. 178–183. DOI: https://doi.org/10.1016/j.vibspec.2018.10.003

CORREIA, R. M. – TOSATO, F. – DOMINGOS, E. – RODRIGUES, R. R. T. – AQUINO, L. F. M. – FILGUEIRAS, P. R. – LACERDA, V. – ROMÃO, W. 2018. Portable near infrared spectroscopy applied to quality control of Brazilian coffee. In Talanta, vol. 176, pp. 59–68.
DOI: https://doi.org/10.1016/j.talanta.2017.08.009

FARAG, M. A. – VON BERGEN, M. – SALEH, B. M. – HOMSI, M. N. – ABD EL-AL, M. S. 2021. How do green and black coffee brews and bioactive interaction with gut microbiome affect its health outcomes? Mining evidence from mechanistic studies, metagenomics and clinical trials. In Trends in Food Science and Technology, vol. 118, part B, pp. 920–937. DOI: https://doi.org/10.1016/j.tifs.2021.11.004

HAYATI, R. – MUNAWAR, A. A. – FACHRUDDIN, F. 2020. Enhanced near infrared spectral data to improve prediction accuracy in determining quality parameters of intact mango. In Data in Brief, vol. 29, article no. 105571.
DOI: https://doi.org/10.1016/j.dib.2020.105571

JACONI, A. – VOS, C. – DON, A. 2019. Near infrared spectroscopy as an easy and precise method to estimate soil texture. In Geoderma, vol. 337, pp. 906–913.
DOI: https://doi.org/10.1016/j.geoderma.2018.10.038

KLIKAROVÁ, J. – ŘEHÁKOVÁ, B. – ČESLOVÁ, L. 2022. Evaluation of regular and decaffeinated (un)roasted coffee beans using HPLC and multivariate statistical methods. In Journal of Food Composition and Analysis, vol. 114, article no. 104841.
DOI: https://doi.org/10.1016/j.jfca.2022.104841

KULAPICHITR, F. – BOROMPICHAICHARTKUL, C. – FANG, M. – SUPPAVORASATIT, I. – CADWALLADER, K. R. 2022. Effect of post-harvest drying process on chlorogenic acids, antioxidant activities and CIE-Lab color of Thai Arabica green coffee beans. In Food Chemistry, vol. 366, article no. 130504.
DOI: https://doi.org/10.1016/j.foodchem.2021.130504

LAZAAR, A. – MOUAZEN, A. M. – EL HAMMOUTI, K. – FULLEN, M. – PRADHAN, B. – MEMON, M. S. – ANDICH, K. – MONIR, A. 2020. The application of proximal visible and near-infrared spectroscopy to estimate soil organic matter on the Triffa Plain of Morocco. In International Soil and Water Conservation Research, vol. 8, no. 2, pp. 195–204. DOI: https://doi.org/10.1016/j.iswcr.2020.04.005

LEMOS, M. F. – DE ANDRADE SALUSTRIANO, N. – DE SOUZA COSTA, M. M. – LIRIO, K. – DA FONSECA, A. F. A. – PACHECO, H. P. – ENDRINGER, D. C. – FRONZA, M. – SCHERER, R. 2022. Chlorogenic acid and caffeine contents and anti-inflammatory and antioxidant activities of green beans of conilon and arabica coffees harvested with different degrees of maturation. In Journal of Saudi Chemical Society, vol. 26, no. 3, article no. 101467.
DOI: https://doi.org/10.1016/j.jscs.2022.101467

MIN, J. – CAO, Z. – CUI, L. – LI, F. – LU, Z. – HOU, Y. – YANG, H. – WANG, X. – XU, C. 2023. The association between coffee consumption and risk of incident depression and anxiety: Exploring the benefits of moderate intake. In Psychiatry Research, vol. 326, article no. 115307.
DOI: https://doi.org/10.1016/j.psychres.2023.115307

MIREEI, S. A. – AMINI-POZVEH, S. – NAZERI, M. 2017. Selecting optimal wavelengths for detection of insect infested tomatoes based on SIMCA-aided CFS algorithm. In Postharvest Biology and Technology, vol. 123, pp. 22–32.
DOI: https://doi.org/10.1016/j.postharvbio.2016.08.009

MUNAWAR, A. A. – DEVIANTI – SATRIYO, P. – BAHARI, S. A. 2022a. Near infrared spectroscopy: rapid and simultaneous approach to predict the fixed carbon, volatile matter and ash contents in biochar produced from agricultural residues. In Acta Technologica Agriculturae, vol. 25, no. 1, pp. 1–6.
DOI: https://doi.org/10.2478/ata-2022-0001

MUNAWAR, A. A. – ZULFAHRIZAL – MEILINA, H. – PAWELZIK, E. 2022b. Near infrared spectroscopy as a fast and non-destructive technique for total acidity prediction of intact mango: Comparison among regression approaches. In Computers and Electronics in Agriculture, vol. 193, article no. 106657.
DOI: https://doi.org/10.1016/j.compag.2021.106657

NICOLAÏ, B. M. – BEULLENS, K. – BOBELYN, E. – PEIRS, A. – SAEYS, W. – THERON, K. I. – LAMMERTYN, J. 2007. Nondestructive measurement of fruit and vegetable quality by means of NIR spectroscopy: A review. In Postharvest Biology and Technology, vol. 46, pp. 99–118. DOI: https://doi.org/10.1016/j.postharvbio.2007.06.024

PASQUINI, C. 2018. Near infrared spectroscopy: A mature analytical technique with new perspectives – A review. In Analytica Chimica Acta, vol. 1026, pp. 8–36.
DOI: https://doi.org/10.1016/j.aca.2018.04.004

SANTOS, J. R. – SARRAGUÇA, M. C. – RANGEL, A. O. S. S. – LOPES, J. A. 2012. Evaluation of green coffee beans quality using near infrared spectroscopy: A quantitative approach. In Food Chemistry, vol. 135, no. 3, pp. 1828–1835.
DOI: https://doi.org/10.1016/j.foodchem.2012.06.059

SHAN, J. – SUZUKI, T. – SUHANDY, D. – OGAWA, Y. – KONDO, N. 2014. Chlorogenic acid (CGA) determination in roasted coffee beans by Near Infrared (NIR) spectroscopy. In Engineering in Agriculture, Environment and Food, vol. 7, no. 4, pp. 139–142.
DOI: https://doi.org/10.1016/j.eaef.2014.08.003

SOUZA, J. C. – PASQUINI, C. – HESPANHOL, M. C. 2022. Feasibility of compact near-infrared spectrophotometers and multivariate data analysis to assess roasted ground coffee traits. In Food Control, vol. 138, article no.109041.
DOI: https://doi.org/10.1016/j.foodcont.2022.109041

TUGNOLO, A. – GIOVENZANA, V. – MALEGORI, C. – OLIVERI, P. – CASSON, A. – CURATITOLI, M. – GUIDETTI, R. – BEGHI, R. 2021. A reliable tool based on near-infrared spectroscopy for the monitoring of moisture content in roasted and ground coffee: A comparative study with thermogravimetric analysis. In Food Control, vol. 130, article no. 108312.
DOI: https://doi.org/10.1016/j.foodcont.2021.108312

VIEIRA, L. S. – ASSIS, C. – DE QUEIROZ, M. E. L. R. – NEVES, A. A. – DE OLIVEIRA, A. F. 2021. Building robust models for identification of adulteration in olive oil using FT-NIR, PLS-DA and variable selection. In Food Chemistry, vol. 345, article no. 128866.
DOI: https://doi.org/10.1016/j.foodchem.2020.128866

WALSH, K. B. – MCGLONE, V. A. – HAN, D. H. 2020. The uses of near infra-red spectroscopy in postharvest decision support: A review. In Postharvest Biology and Technology, vol. 163, pp. 111139.
DOI: https://doi.org/10.1016/j.postharvbio.2020.111139

WANG, Q. – ZHANG, H. – LI, F. – GU, C. – QIAO, Y. – HUANG, S. 2021. Assessment of calibration methods for nitrogen estimation in wet and dry soil samples with different wavelength ranges using near-infrared spectroscopy. In Computers and Electronics in Agriculture, vol. 186, article no. 106181.
DOI: https://doi.org/10.1016/j.compag.2021.106181