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Near Infrared Spectroscopy and Partial Least Squares Models for Cocoa Quality Analysis: Implications and Practical Use

Zulfahrizal[1*], Agus Arip Munawar[1], Daniel Moerlein[2]

[1] Department of Agricultural Engineering, Lab IE, DSAI Research Center, Pusmeptan Universitas Syiah Kuala, Banda Aceh 23111, Indonesia
[2] Department of Animal Sciences, Georg August University of Goettingen, Göttingen 37073, Germany

Corresponding Author Email: zulfahrizal@usk.ac.id

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ABSTRACT

This study aims to evaluate the feasibility of Near Infrared Spectroscopy (NIRS) technology for cocoa bean quality assessment and proposes a practical framework for farmer adoption. Combining NIRS with Partial Least Squares (PLS) regression models offers a non-destructive, rapid, and accurate alternative for determining key cocoa quality parameters: total phenol, theobromine, moisture, and caffeine content. The calibrated models demonstrated strong predictive performance, confirming NIRS as a reliable tool for quality control in cocoa farming. The adoption of NIRS technology enables farmers to make informed decisions regarding harvest timing, post-harvest processing, and quality control, ensuring that production meets market standards and secures higher prices. This not only improves farmers' financial stability but also enhances their market positioning and bargaining power, fostering a sustainable and prosperous cocoa industry. Detailed model performance metrics are reported in the results section.

1. INTRODUCTION

Cocoa farmers face a multitude of complex challenges when it comes to assessing the quality of their product, which significantly impacts their ability to compete in the global market and secure fair prices for their crops. Traditionally, quality assessment has heavily relied on subjective methods such as visual inspection and organoleptic evaluation, which, while valuable, are inherently inconsistent and susceptible to human error. This subjectivity leads to variability in quality determinations, making it difficult for farmers to standardize their processes or reliably compare their cocoa quality with that of other producers.

Furthermore, the lack of accessible, objective measurement tools on-site forces many farmers to depend on distant, centralized testing facilities. This not only incurs substantial costs but also introduces significant time delays in the quality assessment process, potentially leading to missed market opportunities or degradation of the cocoa before it can be properly evaluated. The situation is further exacerbated by the prohibitive expenses associated with advanced laboratory testing methods, which are often beyond the financial reach of small-scale and medium-sized cocoa farms. These farmers, who form the backbone of the cocoa industry in many regions, are thus at a distinct disadvantage when it comes to precisely determining and documenting the quality of their produce. Additionally, the cocoa industry's increasing emphasis on traceability and adherence to stringent international quality standards poses another layer of complexity. Many farmers lack the specialized training and equipment necessary to conduct the sophisticated analyses required to meet these standards, potentially limiting their access to premium markets and better prices.

The absence of rapid, on-site testing methods also hampers farmers' ability to detect and address quality issues early in the production process, often resulting in significant losses that could have been mitigated with timely intervention. This comprehensive set of challenges underscores the urgent need for innovative, cost-effective, and user-friendly quality assessment tools that can empower cocoa farmers to accurately evaluate their product quality, make informed decisions, and ultimately improve their economic outcomes in an increasingly competitive global marketplace. However, maintaining and enhancing the quality of cocoa beans remains a substantial challenge, particularly due to the limited access to advanced quality assessment technologies [1]. Traditionally, the assessment of cocoa beans relies on sensory evaluation and basic physical measurements, which are often subjective and inconsistent [2]. To address these challenges and improve the livelihood of cocoa farmers, integrating cost-effective, rapid, and reliable technologies for cocoa bean quality assessment is imperative. One such promising technology is Near Infrared Spectroscopy (NIRS) [3, 4].

NIRS is a rapid and non-destructive analytical technique that measures the absorption of near-infrared light by materials, providing detailed information about their molecular composition [5, 6]. This technology has been successfully applied in various agricultural domains, including the assessment of grain quality, meat freshness, and fruit ripeness. However, its application in the cocoa industry,

particularly for quality assessment of cocoa beans, is still in its nascent stages.

The NIRS operates in the wavelength range of 780 nm to 2500 nm, where the specific absorption patterns can be correlated with the chemical composition of the sample. The primary advantage of NIRS is its ability to analyze various chemical constituents simultaneously in a swift and non-invasive manner [7, 8]. NIRS has shown significant potential in assessing parameters such as moisture content, fat content, and protein levels in agricultural products, making it a highly versatile tool in food quality analysis [9, 10].

Studies on cocoa beans have started to explore the applicability of NIRS for quality determination. demonstrated that NIRS could be used to predict the fat content and acidity of cocoa beans, which are critical parameters influencing the beans' quality. Similarly, [11, 12] established that NIRS could accurately classify cocoa beans based on their genetic origin and post-harvest processing conditions. These findings suggest that NIRS could provide a comprehensive quality profile of cocoa beans, facilitating more objective and consistent quality assessment compared to traditional methods.

Recent advances from 2023 to 2024 in non-destructive analysis have further expanded the toolkit available for agricultural quality assessment. Complementary techniques such as Raman spectroscopy offer molecular fingerprinting capabilities; however, they are generally more expensive, require more stringent sample preparation, and exhibit greater sensitivity to fluorescence interference compared to NIRS [1]. Hyperspectral imaging and portable NIRS devices have emerged as particularly promising directions, enabling in-field, real-time quality monitoring without specialized laboratory infrastructure [13]. Furthermore, the integration of NIRS with AI-driven predictive models, including machine learning and deep learning approaches, has shown potential for enhancing prediction accuracy and generalizability across diverse cocoa origins and processing conditions [14]. These developments underscore the growing relevance of NIRS as a cornerstone technology in precision agricultural quality assurance.

Technological adoption among smallholder farmers can significantly influence their productivity and market access, ultimately enhancing their economic well-being [13, 14]. The introduction of NIRS for cocoa bean quality assessment holds promising prospects for such communities by ensuring better quality control and improved market prices. The reliability and speed of NIRS can provide farmers with immediate feedback on the quality of their produce, enabling them to make informed decisions regarding post-harvest processing and market timing [15].

One of the significant barriers to technology adoption among farmers is the initial cost and complexity of the technology. However, recent developments have made NIRS devices more affordable and user-friendly, increasing their accessibility for small-scale farmers [16, 17]. Moreover, the use of NIRS can foster greater transparency in the supply chain, as the quality of cocoa beans can be verified at multiple points from farm to factory. This transparency can lead to premium pricing for high-quality beans, directly improving farmers' income and promoting sustainable farming practices.

Despite its advantages, the adoption of NIRS technology in the cocoa industry faces challenges. The initial investment in NIRS equipment, along with the need for training and calibration specific to cocoa beans, represents a significant hurdle. Additionally, integrating NIRS into the existing quality control infrastructure requires cooperation among various stakeholders, including farmers, cooperatives, and processing companies.

However, with ongoing advancements in portable NIRS devices and reductions in costs, these barriers are gradually diminishing. Government and non-governmental organizations (NGOs) can play a pivotal role in facilitating the dissemination of NIRS technology through subsidies, training programs, and awareness campaigns. Multi-stakeholder collaboration can enable the development of standardized protocols for NIRS application in cocoa bean assessment, ensuring consistency and reliability in quality evaluation across the supply chain. This presented work aimed to employ and adopt NIRS technology for rapid and simultaneous assessment of cocoa beans quality parameters in the form of total phenol, theobromine, moisture and caffeine contents.

2. MATERIALS AND METHODS

2.1 Cocoa beans

A total of 59 bulk samples of cocoa beans, with 60 g per bulk, were collected from different locations in East Java and Aceh region during the peak growth season. The sample size of 59 was determined to represent the typical variability in cocoa bean quality across the two major growing regions, ensuring sufficient diversity in chemical composition for robust model calibration. A preliminary power analysis confirmed that this number provides adequate statistical power (> 0.80) for Partial Least Squares (PLS) regression with the number of latent variables considered.

Upon receipt, the cocoa beans were first subjected to a cleaning process to remove foreign materials such as dirt, stones, and plant debris. This was done manually using sieves and air blowers. Post-harvest processes, specifically fermentation and drying, were standardized to reduce variability in the quality assessment. Beans were fermented in wooden boxes for six days, turning them every 48 hours to ensure uniform fermentation [18, 19].

After fermentation, the beans were sun-dried then homogenized. This involved mixing the beans thoroughly to ensure consistent sampling. Any damaged or moldy beans were discarded during this process. For the NIRS analysis, intact beans and ground samples were prepared. Grinding was essential to analyze the internal composition accurately [20, 21]. Beans were ground using a commercial grinder to produce fine, homogeneous powder. The grinder was cleaned between samples to prevent cross-contamination.

2.2 Near infrared spectral acquisition

Absorbance spectral data in the near infrared (NIR) wavelength range region was acquired by means of a self-developed portable sensing device PSD NIRS i16 instrument (*NIRS iKakao*) equipped with a NIR sensor capable of measuring wavelengths ranging from 1000 to 2500 nm [20, 21]. This spectral range was specifically chosen due to its sensitivity to key functional groups such as O-H, C-H, and N-H, which are inherently linked to cocoa quality parameters like moisture content, fat content, and protein levels, as well as compounds such as theobromine and caffeine. The cocoa beans samples were prepared, ensuring proper cleanliness of

the sample surface to minimize any potential interference in the spectral measurements as illustrated in Figure 1. Each prepared cocoa bean sample was filled within the samples holder as cylindrical cup with diameter of 6 cm, consistently covering the entire measurement area. The raw spectral data obtained from the instrument for each bulk cocoa beans sample was acquired and recorded as an average of 32 scanning with optical gain 4×.

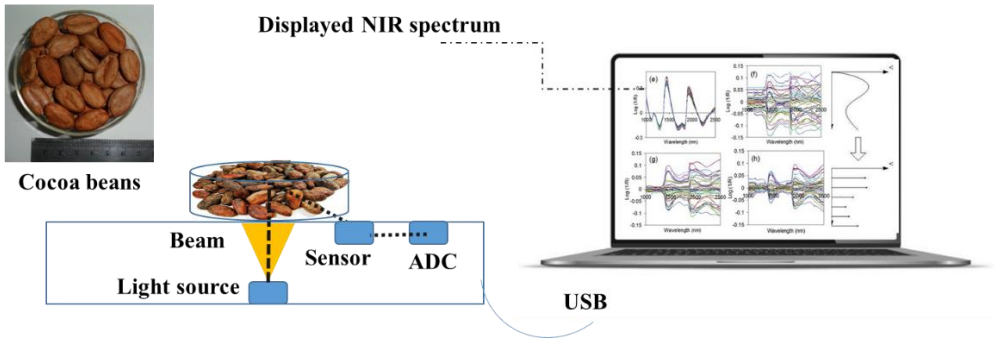


Figure 1. Near infrared (NIR) spectral data acquisition of intact cocoa bean samples in the near infrared region

2.3 Cocoa quality measurements

To accurately measure the total phenolic content in cocoa samples, the Folin-Ciocalteu method is employed due to its reliability and widespread use in food science. Initially, cocoa samples, either as intact beans or ground into a fine powder, are prepared. For ground samples, approximately 1 gram is weighed and placed into a centrifuge tube [13]. To extract the phenolic compounds, 10 mL of methanol is added to the tube, followed by thorough mixing using a vortex mixer for about 5 minutes. The mixture is then centrifuged at 4000 rpm for 10 minutes, and the clear supernatant is carefully collected for analysis. To perform the Folin-Ciocalteu assay, 0.1 mL of the cocoa extract is transferred into a test tube, to which 0.5 mL of the Folin-Ciocalteu reagent is added. The mixture is vortexed and allowed to react for 3 to 5 minutes at room temperature. Subsequently, 2 mL of a 20% aqueous sodium carbonate solution is added, and the mixture is vortexed again to ensure thorough mixing [22].

The reaction mixture is then diluted with 7.4 mL of distilled water to achieve a final volume of 10 mL and incubated in the dark at room temperature for 60 minutes to facilitate color development. The absorbance of the resulting blue-colored solution is measured at 765 nm using a UV-Vis spectrophotometer, calibrated with a blank solution prepared under the same conditions but without the cocoa extract. A calibration curve is generated using gallic acid standard solutions with known concentrations, ranging from 0.1 mg/mL to 1 mg/mL, and plotting absorbance against concentration. The total phenolic content of the cocoa extract is determined using the equation derived from the gallic acid standard calibration curve, and the results are expressed as milligrams of gallic acid equivalents (GAE) per gram of sample (mg GAE/g). The calculation involves the concentration of phenols in the extract, the volume used, and the mass of the sample. To ensure accuracy and reproducibility, each sample and standard are run in triplicate, and quality control samples with known phenolic content are included throughout the assay.

To measure and analyze the *theobromine content* in cocoa samples, high performance liquid chromatography (HPLC) is employed due to its precision and effectiveness in separating and quantifying alkaloids [23, 24]. The process begins with the preparation of cocoa samples, which are either in the form of intact beans or ground into a fine powder. For analysis, approximately 1 gram of the ground cocoa sample is weighed and placed into a clean centrifuge tube. To extract theobromine, 10 mL of a solvent mixture (typically a combination of methanol and water, often 70:30 v/v) is added to the tube. The mixture is then sonicated for 30 minutes to ensure thorough extraction of theobromine from the cocoa matrix. Post sonication, the sample is centrifuged at 4000 rpm for 10 minutes to separate the solid residues from the liquid extract. The clear supernatant is carefully collected and filtered through a 0.45 µm polytetrafluoroethylene (PTFE) syringe filter to remove any particulate matter that could clog the HPLC column [25].

The HPLC system, equipped with a reversed-phase C18 column (typically 150 mm × 4.6 mm i.d., 5 µm particle size), is used for the separation of theobromine. The mobile phase commonly consists of a mixture of acetonitrile and water with 0.1% formic acid, and is delivered at a flow rate of 1.0 mL/min. The column temperature is maintained at 25 °C. An aliquot of 20 µL of the filtered cocoa extract is injected into the HPLC system for analysis. The elution of theobromine is monitored using an ultraviolet (UV) detector set at a wavelength of 272 nm, as this wavelength optimizes the absorption characteristics of theobromine.

For quantification, a series of theobromine standards with known concentrations ranging from 1 µg/mL to 100 µg/mL are prepared and analyzed under the same HPLC conditions to generate a calibration curve. The actual and reference concentration of theobromine content in the cocoa samples is determined by comparing the peak areas in the sample chromatograms with those in the standard calibration curve. The results are expressed as a triplicate average in milligrams of theobromine per gram of cocoa sample (mg/g) [23, 26, 27].

On the other hand, the moisture content in cocoa samples were determined by means of the gravimetric method. This procedure begins with the preparation of the cocoa samples, which should be representative of the batch being analyzed. The cocoa beans are first cleaned to remove any debris and then ground into a uniform powder using a commercial grinder. A sample of the ground cocoa, typically weighing about 2-5 grams, is accurately weighed using an analytical balance (precision of 0.001 g) and placed in a pre-weighed, clean, and dry moisture dish or crucible [28].

The moisture dish containing the cocoa sample is then placed in a drying oven set at 105 °C. The sample is dried for a predetermined period, usually 16-18 hours, to ensure complete removal of moisture. During this period, the oven

maintains a consistent temperature, and proper ventilation is ensured to allow moisture to escape. After drying, the moisture dish is carefully removed from the oven using tongs, cooled in a desiccator to prevent moisture absorption from the atmosphere, and reweighed promptly once it reaches room temperature [29, 30]. The moisture content is calculated by determining the weight loss of the sample, which represents the water evaporated during drying.

Moreover, caffeine content was also determined using HPLC method. The analysis begins with the preparation of cocoa samples, which may be in the form of ground cocoa powder or extracts. A representative amount of the sample, typically around 1-2 grams, is accurately weighed and placed into a clean centrifuge tube. To extract caffeine, a suitable solvent such as a mixture of methanol and water is added to the tube [31-33]. The mixture is then sonicated for efficient extraction, ensuring that the caffeine is completely dissolved into the solvent. After sonication, the sample is centrifuged to separate the solid residues, and the clear supernatant containing the extracted caffeine is collected for analysis.

The HPLC system is utilized for the separation and quantification of caffeine in the sample extract. The system comprises a column, often a C18 column, where the separation of compounds occurs based on their chemical properties. The mobile phase, usually a combination of water and acetonitrile, is pumped through the column at a specific flow rate, with the gradient adjusted to elute caffeine at a specific retention time. An aliquot of the filtered sample extract is injected into the HPLC system, and the elution is monitored using a UV-Vis detector set at an appropriate wavelength for caffeine detection, commonly around 272 nm.

2.4 Spectral data correction

Noises due to light scattering and amplifications were corrected by means of multiplicative scatter correction (MSC). While other preprocessing techniques such as Standard Normal Variate (SNV) and de-trending can also address scattering effects, MSC was selected for its specific advantages in this context. SNV may overcorrect spectra by normalizing each spectrum independently without considering the overall dataset structure, potentially distorting chemical information. De-trending primarily corrects baseline drifts but may not adequately address the complex scattering effects present in heterogeneous samples like cocoa beans. MSC, in contrast, uses an ideal reference spectrum derived from the dataset to correct each individual spectrum, preserving chemical information while effectively reducing scatter-related noise. This approach is particularly beneficial for samples where particle size and surface characteristics significantly affect spectral data. A comparison of spectral data before and after MSC correction is presented in Figure 2.

The primary purpose of the MSC approach is to enhance the quality of spectral data by mitigating unwanted variability caused by scattering effects and other sources of systematic variation. This method aims to remove or reduce the impact of undesired variation in spectral measurements, ensuring that the true underlying chemical information in the data is more clearly revealed [34]. By applying MSC, the spectral data is corrected to minimize the influence of factors such as particle size variations, instrumental noise, baseline shifts, or other forms of unwanted variability that can obscure the relevant information in the spectra [35]. Ultimately, the MSC approach facilitates more accurate, reliable, and interpretable spectral analysis, enabling researchers and analysts to extract meaningful insights and make informed decisions based on the corrected data. Comparison of spectral data before and after correction using the MSC approach is presented in Figure 2.

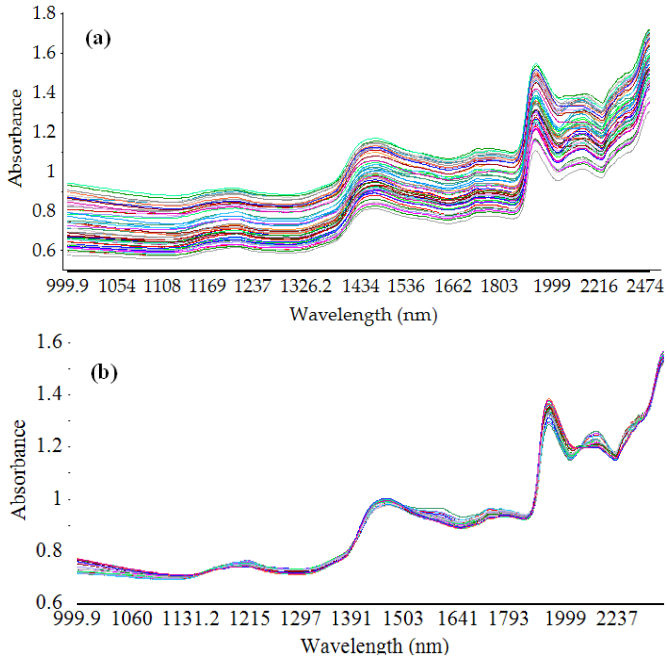


Figure 2. Spectral data before correction (a) and after correction using multiplicative scatter correction (MSC) approach (b)

The primary purpose of the MSC approach is to enhance the quality of spectral data by mitigating unwanted variability caused by scattering effects and other sources of systematic variation. This method aims to remove or reduce the impact of undesired variation in spectral measurements, ensuring that the true underlying chemical information in the data is more clearly revealed. By applying MSC, the spectral data is corrected to minimize the influence of factors such as particle size variations, instrumental noise, baseline shifts, or other forms of unwanted variability that can obscure the relevant information in the spectra. While other preprocessing techniques like SNV and de-trending can also address scattering effects, MSC was chosen for its specific advantages in this context. SNV is effective in removing multiplicative effects but may overcorrect the spectra, potentially distorting the chemical information by normalizing each spectrum independently without considering the overall dataset structure. Detrending, on the other hand, primarily corrects for baseline drifts and polynomial variations but may not adequately address the complex scattering effects present in heterogeneous samples like cocoa beans. MSC, in contrast, uses an ideal spectrum derived from the data itself to correct each individual spectrum, thereby preserving the chemical information while effectively reducing scatter-related noise. The MSC corrected spectra show reduced baseline variation and improved signal-to-noise ratio compared to the raw spectra, facilitating more reliable extraction of chemical information.

This approach is particularly beneficial when dealing with samples where particle size and surface characteristics can significantly affect the spectral data. The choice of MSC was also influenced by its proven effectiveness in similar agricultural applications, where it has demonstrated superior

performance in enhancing the accuracy and robustness of predictive models. Ultimately, the MSC approach facilitates more accurate, reliable, and interpretable spectral analysis, enabling researchers and analysts to extract meaningful insights and make informed decisions based on the corrected data.

2.5 Calibration model

The NIRS calibration was performed to create a predictive model that correlates the spectral data as X-variables with the cocoa quality properties: total phenol, theobromine, moisture and caffeine contents as Y-variables in the cocoa samples using PLS. It constructs a latent variable space that captures the maximum covariance between X and Y by iteratively deriving a set of orthogonal latent variables that are linear combinations of the original X variables [35, 36].

Evaluation of predictive model performance is crucial in assessing its accuracy and model reliability. Cross-validation was employed using a leave one out (LOO) strategy, where each sample is sequentially excluded from model training and used as the test sample. This approach provides an unbiased estimate of prediction performance while making full use of the available 59-sample dataset. Model performance was evaluated using the coefficient of determination (R^2), root mean squared error (RMSE), ratio of performance to deviation (RPD), and range to error ratio (RER).

3. RESULTS AND DISCUSSION

The near infrared spectral features of intact cocoa bean samples in the wavelength region from 1000 to 2500 nm provide crucial insights into their chemical composition. This spectral range is particularly sensitive to the overtones and combination bands of molecular vibrations, primarily related to functional groups such as O-H, N-H, and C-H bonds. In the context of cocoa beans, the NIR spectra typically exhibit several key absorption features. Around 1450 nm and 1940 nm, prominent absorption peaks are observed, which are attributed to the O-H stretching vibrations associated with moisture content. These water-related bands are crucial for assessing the moisture levels in cocoa beans, which significantly impact their quality and storage properties.

Additionally, the absorption bands near 1710 nm can be linked to the C-H overtone stretching vibrations, which correlate with the fat content in the beans. Cocoa beans are rich in fats, and the intensity of these bands can provide quantitative information about the lipid content, which is a critical quality parameter. Another significant feature in the region around 2100-2200 nm is the combination band of C-H stretching and C-H deformation, offering further insights into the fat profile and the presence of volatile organic compounds that influence the beans' flavor profile.

Prior to model development, the distribution of each quality parameter was assessed to understand the data characteristics and inform interpretation of the calibration results. The Shapiro-Wilk test was applied to each variable. As shown in Table 1, the near-zero skewness values for Total Phenol (0.08) and Caffeine (-0.14) indicate approximately symmetric, near-normal distributions. Theobromine shows modest left-skewness (-0.28), while Moisture content exhibits a right-skewed distribution (0.87), suggesting a concentration of samples at lower moisture values. The kurtosis values, all negative or near zero, indicate platykurtic distributions with lighter tails than a normal distribution, implying fewer extreme outliers. These distributional characteristics are typical for agricultural samples and are consistent with the heterogeneous nature of field-collected cocoa beans. The broad range of values across all four parameters confirms that the dataset captures sufficient variability for robust PLS calibration.

Furthermore, the absorption features around 2300-2350 nm can be associated with the N-H and C-H stretching vibrations, indicative of protein content and overall amino acid composition [9, 16]. This information is vital for understanding the nutritional and processing qualities of cocoa beans. The broad and overlapping nature of these spectral features often necessitates the use of chemometric techniques like PLS regression to de-convolute the data and establish accurate predictive models for cocoa quality properties. Descriptive statistics of measured cocoa quality properties inform of total phenol, theobromine, moisture and caffeine contents is presented in Table 1.

Table 1. Descriptive statistics of measured cocoa bean quality properties

Statistical Indicators	Total Phenol	Theobromine	Moisture Content	Caffeine
n	59	59	59	59
Mean	8.04	2.36	8.12	0.95
Max	10.88	3.56	11.26	1.65
Min	5.57	1.01	6.50	0.16
Range	5.31	2.55	4.76	1.49
Std. Dev.	1.43	0.83	1.16	0.44
Variance	2.06	0.68	1.35	0.19
RMS	8.17	2.50	8.20	1.05
Skewness	0.08	-0.28	0.87	-0.14
Kurtosis	-0.81	-1.40	0.00	-1.13
Median	7.99	2.54	7.78	1.01
Q1	6.94	1.60	7.23	0.61
Q3	9.03	3.11	8.70	1.32

Prior to model development, the distribution of each quality parameter was assessed. The near-zero skewness values for Total Phenol (0.08) and Caffeine content (-0.14) indicate approximately symmetric, and also near-normal distributions. Theobromine shows modest left-skewness (-0.28), while Moisture content exhibits a right-skewed distribution (0.87). on the other hand, the kurtosis values, all negative or near zero, indicate platy distributions with lighter tails than a normal distribution, implying that fewer extreme outliers. These distributional characteristics are typical for agricultural samples.

1. The table presents a thorough statistical analysis cocoa quality properties: total phenol, theobromine, moisture content, and caffeine properties in a dataset comprising 59 samples. The descriptive statistics reveal the central tendencies and variability within the dataset. The mean values indicate the average concentrations, with total phenol at 8.04, theobromine at 2.36, moisture content at 8.12, and caffeine at 0.95.
2. The maximum and minimum values show the range of observed data, with Total Phenol ranging from 5.57 to 10.88, Theobromine from 1.01 to 3.56, Moisture content from 6.50 to 11.26, and Caffeine from 0.16 to 1.65. The range, calculated as the difference between the maximum and minimum values, provides an overview of the data spread: 5.31 for Total Phenol, 2.55 for Theobromine, 4.76 for Moisture content, and

1.49 for Caffeine.

3. The standard deviation and variance metrics measure the dispersion around the means. Total Phenol has a standard deviation of 1.43 and variance of 2.06, suggesting moderate variability. In contrast, Theobromine shows a lower standard deviation 0.83 and variance 0.68, indicating less variability. Moisture content has a standard deviation of 1.16 and variance of 1.35, showing a slightly more spread out distribution. Caffeine presents a relatively small standard deviation 0.44 and variance 0.19, pointing to less variability in the caffeine content across samples.

The root mean square (RMS) values provide another measure of the data's central tendency and magnitude, with figures closely aligning to the mean values for each property, reinforcing their average concentrations within the dataset. Skewness and kurtosis provide insights into the data distribution's shape. Total Phenol 0.08 and Caffeine -0.14 exhibit near-zero skewness, indicating near-symmetric distributions, while Theobromine -0.28 suggests a slight left tail and Moisture content 0.87 indicates a right-skewed distribution. The kurtosis values show all properties have distributions close to normal, with Total Phenol -0.81, Theobromine -1.40, Moisture content 0.00 suggesting zero excess kurtosis, and Caffeine -1.13, indicating platy-kurtic distributions with lighter tails than a normal distribution.

The median and quartile values describe the data's central tendency and dispersion in more detail. For instance, the median values closely match the means, implying symmetric distributions for Total Phenol, Theobromine, Moisture, and Caffeine. The first and third quartiles (Q1 and Q3), capturing the 25th and 75th percentiles, help understand the data spread, showing that the central 50% of the data lies between 6.94 to 9.03 for Total Phenol, 1.60 to 3.11 for Theobromine, 7.23 to 8.70 for Moisture, and 0.61 to 1.32 for Caffeine.

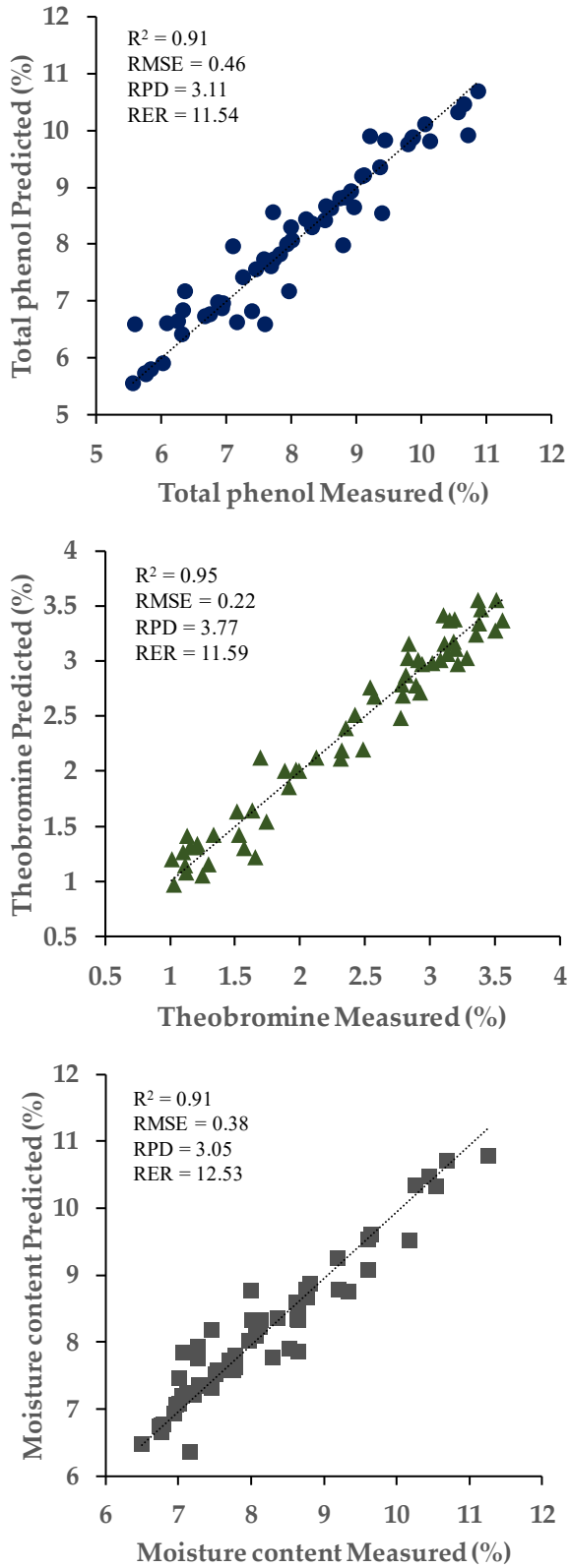
Calibration models used to determine quality properties of cocoa beans were developed using raw uncorrected spectra and also using the MSC corrected spectral data. The prediction performance of raw spectra in determining cocoa quality properties is shown in Table 2. It presents a detailed performance analysis of the chosen statistical indicators for total phenol, theobromine, moisture, and caffeine properties. The impressive coefficient of determination (R^2) values ranging from 0.91 to 0.95 across all properties signify strong relationships between the spectral data and the actual content levels, indicating that approximately 91% to 95% of the variance in the properties can be explained by the models. The high R^2 value (0.98) indicates that the model can reliably predict theobromine content, critical for assessing flavor attributes in cocoa products.

Table 2. Prediction performance of cocoa quality properties using raw spectral data

Properties	Statistical Indicator				
	R^2	r	RMSE	RPD	RER
Total Phenol	0.91	0.95	0.46	3.11	11.54
Theobromine	0.95	0.97	0.22	3.77	11.59
Moisture	0.91	0.95	0.38	3.05	12.53
Caffeine	0.93	0.96	0.14	3.14	10.64

Note: determination (R^2), root mean squared error (RMSE), ratio of performance to deviation (RPD), and range to error ratio (RER)

The high correlation coefficient (r) values of 0.95 to 0.97 further affirm the positive linear relationship between predicted and actual values, demonstrating the accuracy of the models in capturing the variability in the properties. The RMSE values, which range from 0.14 to 0.46, are relatively low, indicating the models' precision in predicting the content levels of total phenol, theobromine, moisture, and caffeine. The RPD values, varying from 3.05 to 3.77, suggest that the models perform satisfactorily, with moderate to high predictive capabilities considering the variability in the data. Scatter plot derive for cocoa quality prediction using NIRS spectral data before correction is presented in Figure 3.



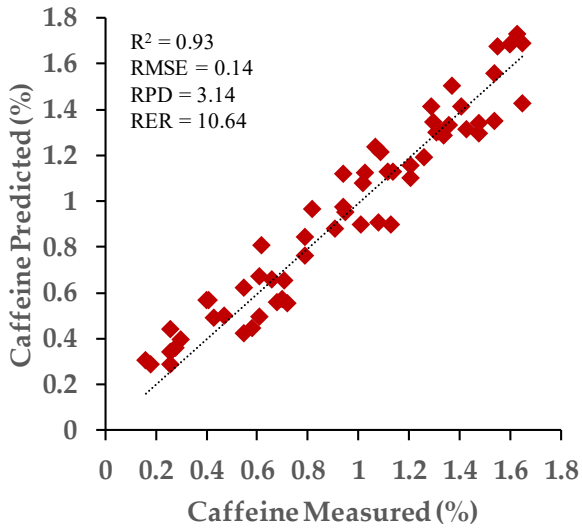


Figure 3. Prediction performance of cocoa quality properties using raw uncorrected spectral data

Additionally, the RER values ranging from 10.64 to 12.53 demonstrate the models' efficiency in estimating the properties relative to the data variation. The results presented may be attributed to the complex interactions between the spectral data and the chemical composition of the samples. The high R^2 and r values could be a result of the strong relationship between the specific patterns in the spectral data and the characteristic absorption features of Total Phenol, Theobromine, Moisture, and Caffeine.

The low RMSE values indicate that the models have a small average error in predicting the content levels, which could stem from the effective capture of key spectral features related to the properties of interest. The moderate to high RPD values suggest that the models offer reliable predictive performance, translating spectral information into accurate estimations of the properties. The RER values further reinforce the efficiency of the models in providing precise predictions relative to the data variability, showcasing their robustness and effectiveness in analyzing and predicting Total Phenol, Theobromine, Moisture, and Caffeine content in the samples.

Beside using uncorrected spectra, calibration models were also established using the MSC corrected spectra. The prediction performance is presented in Table 3. The comparatively lower performance of raw spectral data relative to MSC-corrected data (Table 3) can be explained by the presence of unmitigated light scattering effects. In solid agricultural samples such as cocoa beans, variations in particle size, surface texture, and sample packing introduce multiplicative and additive scatter components that overlay the chemically relevant absorption features. These scattering effects increase baseline variability and reduce the signal-to-noise ratio, thereby weakening the correlation between spectral features and the chemical constituents of interest. As a result, the PLS models built on raw spectra capture some variance attributable to physical sample heterogeneity rather than purely chemical composition, which explains the lower R^2 and higher RMSE values compared to the MSC-corrected models.

The presented table provides a comprehensive statistical analysis of the model performance for predicting total phenol, theobromine, moisture, and caffeine content in cocoa samples using MSC corrected spectral data. For Total Phenol, the coefficient of determination (R^2) of 0.94 and correlation coefficient (r) of 0.97 indicate that the model explains 94% of the variance in Total Phenol content, demonstrating a very strong linear relationship between the predicted and actual values. The low RMSE of 0.41 highlights the model's accuracy, with minimal average prediction error. Additionally, the RPD of 3.49 implies that the model is quite robust, with good predictive capability relative to the variability in the data. The RER value of 12.95 further supports the model's efficiency in predicting Total Phenol content.

Table 3. Prediction performance of cocoa quality properties using multiplicative scatter correction (MSC) corrected spectral data

Properties	Statistical Indicator				
	R^2	R	RMSE	RPD	RER
Total Phenol	0.94	0.97	0.41	3.49	12.95
Theobromine	0.98	0.99	0.18	4.61	14.17
Moisture	0.93	0.96	0.35	3.31	13.60
Caffeine	0.97	0.98	0.11	4.02	13.55

Note: determination (R^2), root mean squared error (RMSE), ratio of performance to deviation (RPD), and range to error ratio (RER)

These results are consistent with those of previous studies employing NIRS combined with PLS regression for rapid, simultaneous prediction of multiple quality parameters in agricultural products [6, 14, 22, 27, 32]. The high RPD values (> 3.0) indicate that the models are suitable for practical quality screening applications, while RER values above 10 confirm robustness across the full range of sample variability.

For Theobromine, the model performance is exceptional, as indicated by an R^2 of 0.98 and r of 0.99, meaning the model accounts for 98% of the variance and almost perfectly correlates with actual values. The RMSE of 0.18 is very low, signifying high prediction accuracy. The RPD value of 4.61 reflects excellent model performance, and the high RER value of 14.17 indicates that the model predictions are not only precise but also efficient relative to the data's range.

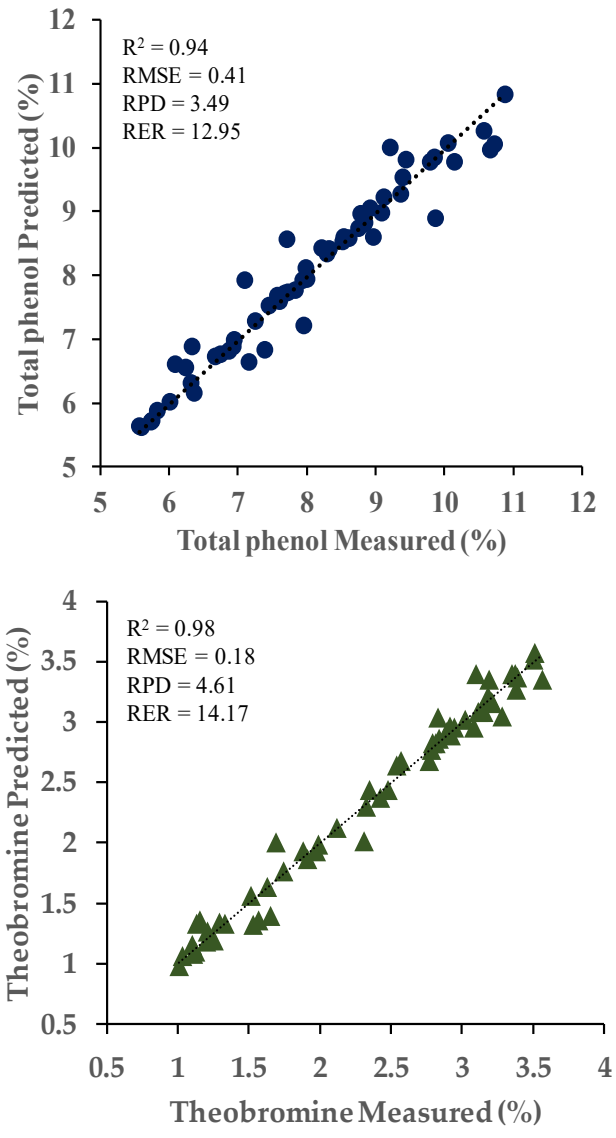
However, the widespread adoption of this technology is not without practical limitations. With respect to sample preparation requirements, NIRS analysis of intact beans can be performed with minimal preparation, primarily ensuring clean sample surfaces, which is a significant advantage over destructive laboratory methods. Yet, achieving optimal prediction accuracy for ground samples requires consistent grinding fineness and homogeneity, which may be challenging in field conditions. Furthermore, the current NIRS calibration models were developed using samples from East Java and Aceh; their applicability to cocoa beans from other growing regions may require local recalibration, representing an additional operational consideration.

With respect to equipment costs and accessibility for small-scale farmers, the initial investment in laboratory-grade NIRS equipment which is typically USD 15,000–50,000 is indeed prohibitive for individual smallholder farmers. This cost barrier is disproportionately felt by small-scale operators who lack access to credit or cooperative purchasing arrangements. Strategies to mitigate this include: (i) cooperative ownership models where groups of farmers share a single device; (ii) government-subsidized demonstration units operated by agricultural extension services; and (iii) the emerging market for portable, low-cost NIRS devices (USD 2,000–5,000), which, while offering somewhat reduced accuracy, may provide a practical entry point for smaller operations. The integration of NIRS with mobile platforms and IoT

infrastructure represents a longer-term pathway to democratizing access.

However, the widespread adoption of this technology is not without practical limitations. With respect to sample preparation requirements, NIRS analysis of intact beans can be performed with minimal preparation, primarily ensuring clean sample surfaces, which is a significant advantage over destructive laboratory methods. However, achieving optimal prediction accuracy for ground samples requires consistent grinding fineness and homogeneity, which may be challenging in field conditions. Furthermore, the current NIRS calibration models were developed using samples from East Java and Aceh; their applicability to cocoa beans from other growing regions may require local recalibration, representing an additional operational consideration.

Moisture content prediction also exhibits strong performance, with an R^2 of 0.93 and r of 0.96, indicating that the model explains 93% of the variance and maintains a strong correlation with actual values. The RMSE is low at 0.35, underscoring the model's accuracy. The RPD value of 3.31 shows solid predictive capability, and the RER value of 13.60 confirms the model's efficiency and reliability in predicting moisture content. Scatter plot derive for cocoa quality prediction using NIRS spectral data after correction is presented in Figure 4.



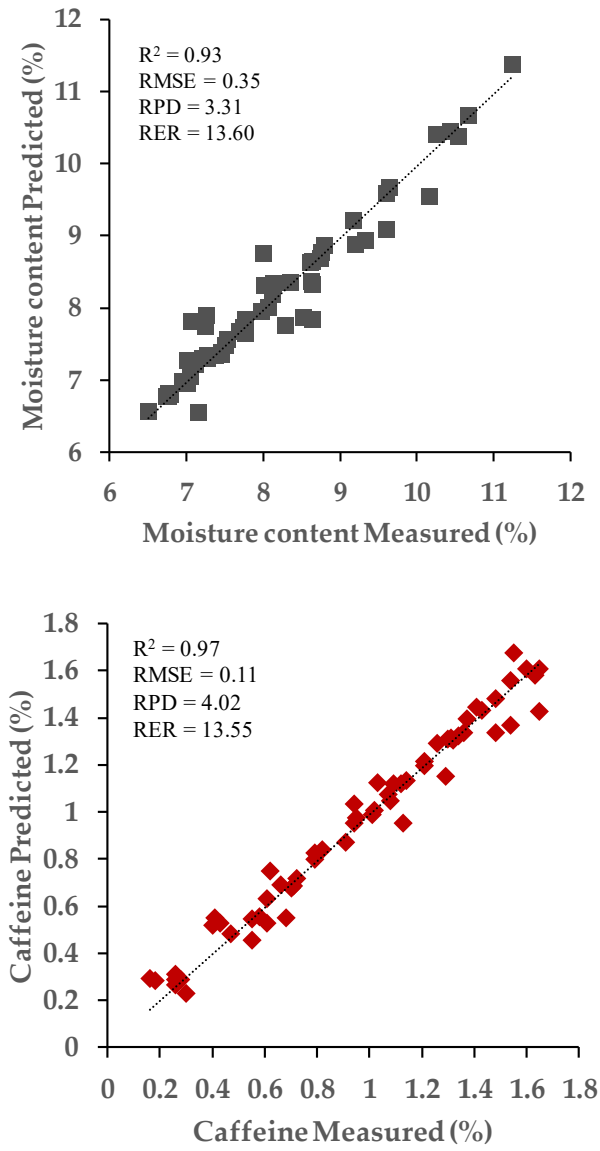


Figure 4. Prediction performance of cocoa quality properties using multiplicative scatter correction (MSC) corrected spectral data

Caffeine prediction shows similarly high performance, with an R^2 of 0.97 and r of 0.98, indicating the model explains 97% of the variance with a very strong linear relationship to the actual values. This also in agreement with previous works [6, 14, 22, 27, 32] mentioning that NIRS in tandem with PLSR can be used for rapid and simultaneous prediction of several quality parameters on agricultural products. The extremely low RMSE of 0.11 highlights the model's high accuracy. Furthermore, an RPD of 4.02 suggests an excellent predictive model, while the RER value of 13.55 demonstrates the model's substantial efficiency and robustness in caffeine prediction.

The statistical indicators in the table reveal that the models for all four cocoa properties are highly accurate and reliable, with strong predictive capabilities. The high R^2 and r values, coupled with low RMSE, high RPD, and high RER, collectively indicate that these models are well-suited for practical applications in cocoa quality assessment, ensuring consistent and accurate predictions of key chemical components. Comparison performance of raw and MSC corrected spectral in determining four quality properties in term of RMSE is shown in Figure 5.

The accurate prediction of these properties directly relates

to the technology adoption practices for cocoa farmers. By integrating advanced techniques such as NIRS technology combined with robust predictive models, farmers can rapidly and non-destructively assess the quality of their cocoa beans. This empowers them to make informed decisions about harvest timing, postharvest processing, and quality control, which are crucial for maximizing the value of their produce. Improved quality assessment helps farmers meet market standards and fetch premium prices for high-quality beans, thereby enhancing their income.

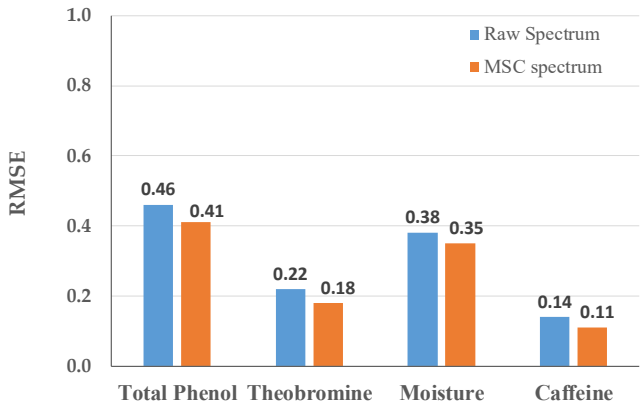


Figure 5. Comparison between raw and multiplicative scatter correction (MSC) spectral data in determining cocoa quality properties

Additionally, the use of these technologies can streamline supply chain processes, ensuring transparency and consistency in quality evaluation from farm to market. As farmers adopt these modern practices, they can achieve better yields and product quality, leading to improved market access and bargaining power. Ultimately, the widespread adoption of such technologies can drive economic prosperity among cocoa farming communities by enabling more efficient and profitable farming practices, fostering sustainable agriculture, and improving the overall livelihood of farmers. The adoption of these technologies also brings opportunities for enhanced supply chain transparency and efficiency. By providing reliable and immediate quality metrics, these tools enable better communication and trust between farmers, processors, and buyers. This can lead to improved logistics, reduced losses, and better alignment with market demands [9, 18, 21]. Furthermore, the ability to rapidly assess and respond to quality parameters can facilitate certification processes, aiding farmers in accessing niche markets that offer premiums for certified high quality or sustainably produced cocoa.

NIRS technology facilitates better resource management and reduces the reliance on subjective methods, leading to more consistent cocoa quality and reduced losses. This reliability increases the farmers' bargaining power in the supply chain, fostering fairer trade practices and potentially reducing exploitation by middlemen. The efficiency of NIRS also aligns with sustainable agricultural practices, as precise quality assessments can guide appropriate use of fertilizers and resources, lowering costs and environmental impact [19, 33].

Additionally, the dissemination of NIRS technology can create new employment opportunities, ranging from technical roles in operating and maintaining the equipment to positions in data analysis and agronomic advisory services. Training programs and support from governmental and NGOs can further enhance farmers' skills, fostering a more knowledgeable and empowered farming community.

However, the widespread adoption of this technology is not without challenges. Initial costs of NIRS equipment and training can be prohibitive for cocoa small-scale farmers. Moreover, there is a need for widespread training programs to ensure that farmers and cooperative managers are proficient in using these technologies. Support from government bodies, NGOs, and private enterprises in the form of subsidies, training workshops, and demonstration projects related to the applications of advanced technologies will be crucial in overcoming these barriers.

Future opportunities lie in the development of more affordable and user friendly NIRS devices for smallholder cocoa farmers. Innovations aimed at integrating NIRS technology with mobile platforms and Internet of Things can further democratize access, allowing farmers to conduct quality assessments using smartphones or portable devices. Additionally, advancements in data analytics and artificial intelligence can enhance the predictive models' accuracy and usability, making them even more valuable tools for farmers.

This broader access can catalyze overall rural development by improving educational outcomes and living standards through increased household income. Hence, the successful implementation of NIRS technology promises significant socio-economic benefits for cocoa farmers, transforming agricultural practices, improving market access, and fostering sustainable development within the cocoa farming communities.

While challenges exist, the adoption of advanced spectroscopic techniques like NIRS and robust predictive models offers promising pathways for enhancing the prosperity of cocoa farmers. By employing and managing these technologies, farmers can achieve better quality control, access premium markets, and ultimately improve their livelihood. Continued innovation and supportive policies will be essential to fully realize these benefits and foster a more sustainable and prosperous cocoa farming industry.

4. CONCLUSION

The integration of NIRS with PLS regression models represents a transformative approach to cocoa bean quality assessment. The MSC-corrected calibration models demonstrated high predictive accuracy for total phenol, theobromine, moisture, and caffeine content, with R^2 of 0.93-0.98, RMSE of 0.11-0.41, RPD of 3.31-4.61, and RER of 12.95-14.17, confirming their suitability for practical quality screening applications.

From a practical standpoint, the adoption of NIRS technology can directly improve cocoa bean market accessibility for farmers. By providing rapid, objective quality data, NIRS enables farmers to document and demonstrate the quality of their produce, supporting access to premium markets and fair-trade certification schemes that reward high-quality beans with premium prices. Cooperatives equipped with shared NIRS devices could serve as quality hubs, offering testing services to member farmers and fostering collective bargaining power. To facilitate cost-effective adoption, the following strategies are recommended: (i) establishment of government-subsidized NIRS units at cooperative and extension service centers; (ii) development of user-friendly, multilingual NIRS operating software tailored for non-specialist users; (iii) training programs for farmers and

cooperative managers on NIRS operation and data interpretation; and (iv) investment in research to develop and validate low-cost portable NIRS devices suitable for field deployment.

While challenges related to initial costs and technical training remain, particularly for small-scale farmers, concerted support from government bodies, NGOs, and private enterprises can overcome these barriers. Future research should prioritize the integration of NIRS with mobile platforms and AI-driven predictive models to further improve accessibility and accuracy, as well as the benchmarking of PLS models against machine learning and deep learning approaches to fully characterize the performance advantages of each methodology.

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