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Development of Near-Infrared Models for Predicting Crude Fat and Moisture Content in *Arachis Hypogaea* Using PLSR Algorithm

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Abstract: *Groundnut is an economically important oil seed crop, and determining crude fat and moisture content is vital for assessing quality. However, standard laboratory methods for measuring these parameters are tedious and destructive. This study aimed to develop partial least squares regression (PLSR) models using near-infrared (NIR) spectroscopy for rapid prediction of crude fat and moisture in groundnut. A total of 69 groundnut samples were obtained and reference values for percentage crude fat (39.04 - 53.31%) and moisture (1.5 - 4.98%) were determined by Soxhlet extraction and gravimetric method respectively. NIR spectra (1000-2500 nm) of the powdered samples were obtained using FOSS DS2500 instrument. PLSR models were built correlating the spectra to reference data using 70% samples for calibration and 30% for validation. For crude fat, the model yielded an R^2 of 0.81, RMSEP of 1.51% and RPD of 2.27 while for moisture it showed R^2 of 0.79, RMSEP of 0.46% and RPD of 1.99. Results indicated good prediction abilities for both quality parameters. This demonstrates the potential of NIR spectroscopy coupled with multivariate calibration to rapidly and non-destructively analyze crude fat and moisture content in groundnut for quality control applications. Further model improvement is possible by expanding the sample datasets.*

Keywords: *Near-infrared, Model, Crude fat, Moisture content, Partial least squared regression, Groundnut.*

INTRODUCTION

Groundnut (*Arachis hypogaea*) is an oil-seed legume that has been described as a multi-purpose plant because of its many benefits (Akram *et al*., 2018). In Nigerian major languages, Groundnut is known as Gyada in Hausa language, Epa in Yoruba language and Ntụ ọka in Igbo language. The World production figure of groundnut in 2019 was 48.8 million tons from 29.6 million hectares with average production of 1647 kg ha-1 (FAO, 2021).

The main agro-ecological zones for groundnut production in Nigeria are Sahel, Sudan, northern guinea and most of the southern guinea and derived savannah (Vabi *et al*., 2019). In the Northern part of Nigeria, groundnut are processed into various products which include groundnut paste popularly known as peanut butter, groundnut cake, salted groundnut and groundnut soup. Groundnut has contributed extremely to the development of the Nigerian economy through the sales of seeds, cakes, oil and haulms (Olorunju *et al.,* 1999).

Assessing quality parameters like crude fat and moisture content in groundnut is critical for determining nutritional value, ensuring food safety, and monitoring processing suitability (Alhassan *et al*., 2017). However, conventional analytical techniques like Soxhlet extraction for fat and oven drying for moisture are tedious, destructive, time consuming, and require hazardous chemicals (Chen *et al*., 2013; Kaur *et al*., 2016). There is a need for rapid, non-invasive analytical methods to efficiently analyze these quality attributes.

A non-destructive and rapid method like near-infrared spectroscopy (NIRS) can provide real-time analysis without compromising sample integrity. Developing and validating an NIRS model for crude fat and moisture content analysis in groundnut samples will enhance quality control practices in the food industry, leading to improved product consistency, reduced costs, and increased customer satisfaction (Xue *et. al*., 2020; Singh *et al.*, 2023).

This research seek to develop and validate a near-infrared spectroscopy (NIRS) model for the analysis of crude fat and moisture content in groundnut samples, offering a rapid and non-destructive approach for quality control in the food industry.

MATERIALS AND METHOD

Sample Collection and Processing

A total of 69 groundnut samples comprising of three varieties (SAMNUT 24, SAMNUT 25 and SAMNUT 27) were obtained at the Centre for Dryland Agriculture's archive situated in Bayero University Kano.

About 250g of each groundnut seed samples were crushed in a grinder (Knifetec KN295, FOSS). The ground samples were store in an airtight container for further analysis.

Fat Content Determination

The percentage crude fat of the groundnut seeds sample were determined using Soctex 8000 Extraction System following the protocol of the manufacturer: the crude fat of the grounded samples were extracted using petroleum ether as solvent and the Randall modification of the soxhlet method. 1 gram of the ground groundnut seed samples was weighed into thimbles.

Samples were extracted at 90 ^oC for 1 hour 8 minutes; boiling for 20 minutes, followed by rinsing for 40 minutes and then recovery of the solvent set at 8 minutes. Crude fats were recovered into a pre-weighed extraction cups. The extraction cups were dried in an oven and allowed to cool in a desiccator before being weighed.

Moisture Content Determination

Moisture content was determined using a digital moisture analyzer (OHAUS MB25) following the protocol of the manufacturer: a sample pan (A round aluminum tray that is 10 cm in diameter) was placed in the analyzer to tare the initial weight. 1 gram of ground groundnut seed was spread on the sample pan, a temperature of 105 ^{o} C was set to heat up the sample to a constant weight and weight loss due to evaporation was measured and displayed on the screen as the moisture content of the groundnut sample.

Near Infrared (NIR) Spectroscopy

Near infrared (NIR) spectra of each groundnut samples were obtained using FOSS DS25000. The ring cup was filled with the groundnut samples and placed in the scanning chamber. The recorded spectra range was from 400–2500 nm, every 0.5nm. Each spectrum was an average of 32 scans. The spectra were exported to the WinISI spectral analytical software version 4.0 (Chadalavada *et al*., 2022) .

Chemometrics: The multivariate (partial least squared regression) and statistical data analyses were carried out using The UNSCRAMBLER 10.4 software (Camo software, Oslo, Norway) and Microsoft Excel.

Calibration and Validation: The results from the percentage crude fat and moisture contents of the groundnut samples were used as reference values, and were computed together with their respective spectrum for the calibration and validation of PLSR model (Chadalavada *et al*., 2022)

The spectral data of 69 samples extracted were then split at random into calibration and validation datasets. For a sizeable dataset with normal distribution, random selection is acceptable since it reduces user bias . 49 samples (70% of the total dataset) was used in model calibration and 20 datasets (30% of the total datasets) was used as validation set.

Evaluation: Different statistical parameters which includes coefficient of determination (R^2), the root mean squared error of calibration (RMSEC), the root mean squared error of prediction (RMSEP) and the residual predictive deviation (RPD) were used to evaluate the performance of the partial least squared regression model (Chadalavada *et al*., 2022).

Results and Discussions

Assessing the quality and shelf life of groundnut, it is critical to accurately determine the crude fat and moisture content. This study attempted to create partial least squared regression (PLSR) models that could quickly estimate the percentages of crude fat and moisture in groundnut samples.

Table 1: Descriptive Statistic of the Groundnut

PARAMETER	RANGE	MEAN	STANDARD DEVIATION
% Crude Fat	39.04 - 53.31	44.86	3.29
% Moisture	1.5 - 4.98	3.57	0.73

The mean and standard deviation of groundnut samples analysed indicate there is variation for the percentage of crude fat and moisture content.

The reference samples were measured by standard chemical methods and the range of crude fat content in the groundnut samples was found to be between 39.04 - 53.31% as shown in table 1. These values are consistent with the nutritional composition reported by Olayinka *et al*. (2022) who reported the percentage crude fat in 8 cultivars of groundnut with SAMNUT 11 having the lowest value of 45.51% and SAMNUT 23 49.98%. Alhassan *et al*. (2017) who analyzed the proximate analysis of 10 new groundnut accessions in Ghana reported the percentage crude fat of the samples to be within the range of 31 - 46%. Musa *et al*. (2010) who investigated the proximate composition of groundnut in some selected varieties and reported the crude fat to be within the range of 32.7 - 53.1%. These consistencies showed that the developed model is versatile, in the sense that the range of values used in model development covers the ranges of groundnut's crude fats reported my several studies.

The assessment of moisture content in the groundnut samples indicated levels ranging from 1.5 - 4.98% as presented in table 4.2. These values are within the range of moisture content of groundnut as reported by Olayinka *et al*. (2022) who conducted a study on the moisture content of 8 groundnut varieties and obtained a low of 4.28% and high of 5.28% for moisture content. Ayola *et al* (2012) also reported a moisture content range of 1-7%. However, the result recorded by Musa *et al* (2010) reported moisture content to be between 6.6 to 8.9% in groundnut. This indicates that the datasets used for the model of the moisture contents needs to be upgraded to cover more range so as to have an improved accuracy.

Low moisture content is pivotal in preventing microbial growth and extending the shelf life of the groundnuts (FAO, 2018). The observed low moisture content in this research underscores proper post-harvest handling and storage practices, which are crucial in maintaining product quality (Pokhrel, 2020).

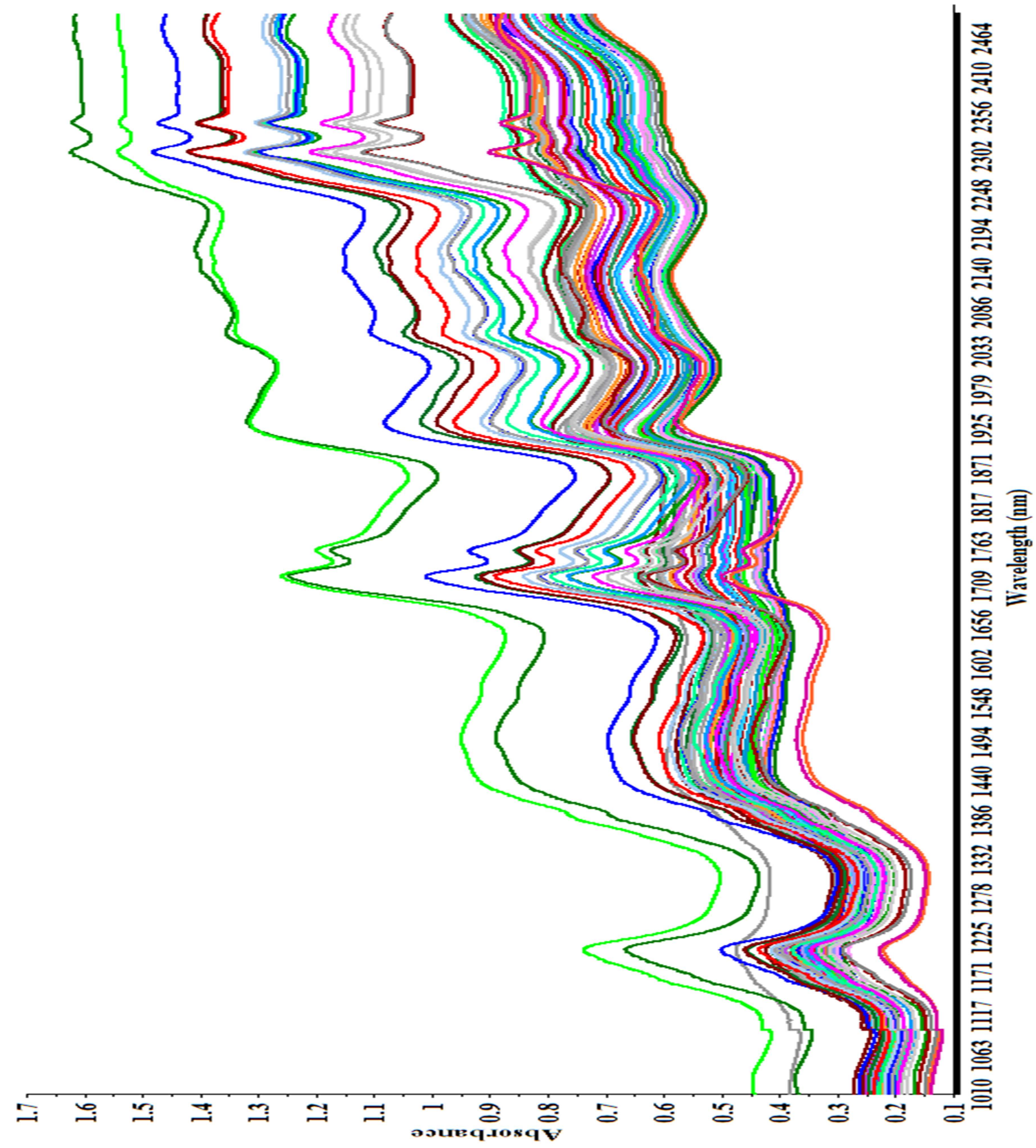


Fig. 1 Illustrating the wavelength of near-infrared absorbance bands for crude fat (overtones and combinations of C–H) and moisture content (overtones and combinations of O–H) for the groundnut seeds.

Characteristics of the NIR Spectrum

The various absorption peaks and valleys observed in Figure 1 spectra data were based on the groundnut samples' chemical component properties. The primary strong bands were seen at wavelengths of 1206, 1474, 1722, 1946, and 2300 nm. The strong band detected at approximately 1206 nm was associated with the second overtone's C–H stretching in different groups (-CH_2). A band relating to the CO stretching of the third overtone (-CO) and the O-H stretching of the first overtone (water) was discovered at around 1474 nm. The second overtone of the N-H stretching in amides and aromatic amines was observed at approximately 1506 nm. Furthermore, as noted by Xu *et al*., (2017), a second strong band was detected at 1722 nm, which was linked to the C–O of oil and the C–H stretching of the first overtone, -CH_2. A vibrational stretching associated with the C-H of oil and the C-H of the -CH_2 first overtone was detected at 1758 nm. The combination absorbance of C-H stretching and the deformation of CH_2, which is associated to oil, is the peak about 2306 nm. Another significant peak was seen near 1950 nm, which was potentially due to the O-H bending of the second overtone (water). The range of 2000–2250 nm was attributed to the over lapping of combination absorbance of C=O stretching, the deformation of –CO–NH–, the combination absorbance of N–H stretching, and the deformation of –CO–NH–. The spectra of groundnut were almost parallel to the spectra of sesame reported by Tsegay *et al.,* (2023).

Fat displays distinct absorption bands in NIR spectra, appearing as unique duplets around 1700 nm and 2300 nm, with the left branch standing out more. The information from other components can be occasionally be swamped or hidden by water absorption bands since they are such broad, dominating features in the NIR spectra. The enlargement and broadening of the moisture bands is noticed as the water content increases in the sample.

Statistical Chemometrics of Partial Least Squared Regression (PLSR) Model

Chemometrics of the partial least squared (PLSR) model of the percentage Crude fat and moisture content of the sample are presented in table 2.

Table 2: Statistical Chemometric Results

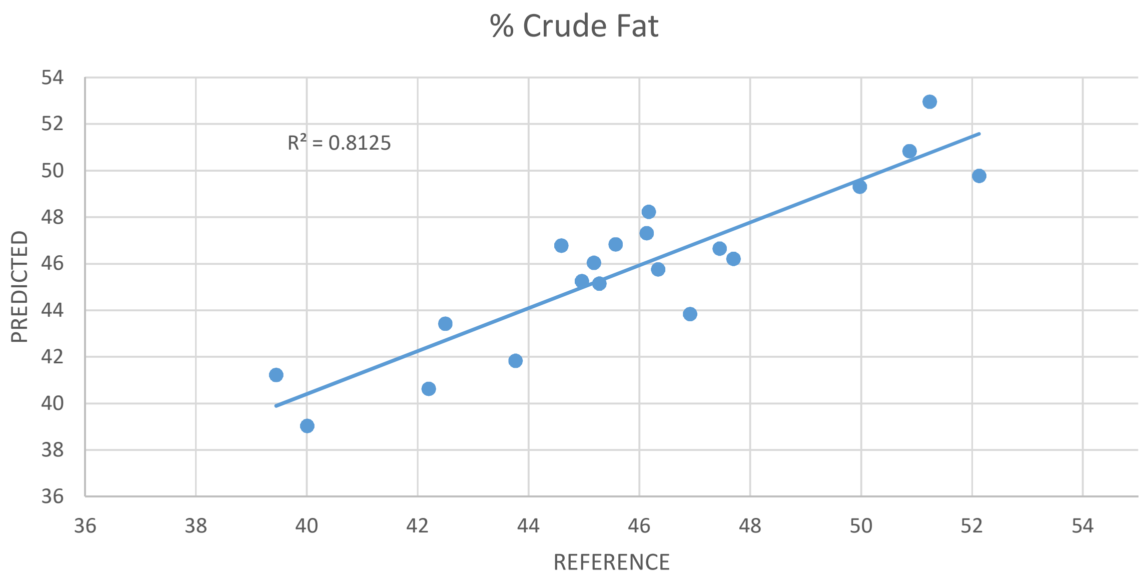
PARAMETERS	R^2	RMSEC	RMSEP	RPD
% Crude Fat	0.81	2.30	1.51	2.27
% Moisture	0.79	0.59	0.46	1.99

Key: R^2 = Co-efficient of determination, RMSEC = Root mean squared error of Calibration, RMSEP = Root mean squared error of prediction, RPD = Residual predictive deviation

Model Evaluation

The coefficient of determination (R^2) indicates how well the spectral data correlates to the reference values, with higher values representing stronger correlations (Romeo, 2020). The R^2 of 0.81 for fat and 0.79 for moisture suggests reasonably good correlation, however, as noted by Di Bucchianico (2007), the coefficient of determination with higher values does not always mean the model is a good fit. Other evaluation means should be put into account.

A



B

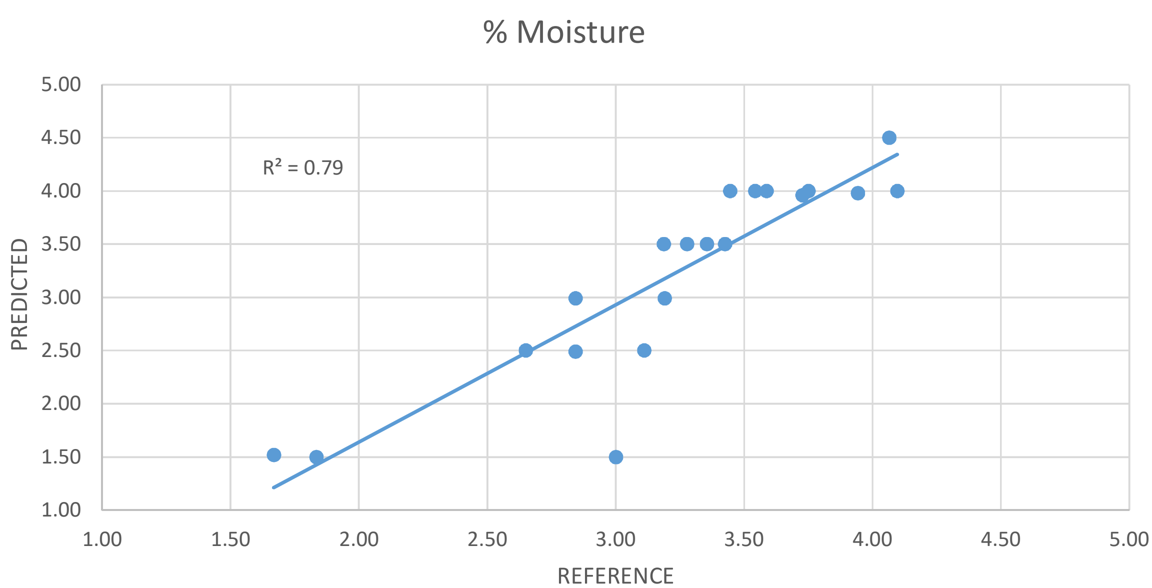


Fig. 2 A plot of correlation between predicted and reference value for crude fat (A) and moisture content (B) of the groundnut.

The root mean squared error of calibration (RMSEC) quantifies the accuracy of the model to the calibration data. Lower values for RMSEC suggests that the model fits well with the calibration data used as reference for the model. The RMSEC for both percentage crude fat and moisture content obtained are 2.30% and 0.49% respectively.

The root mean squared error of prediction (RMSEP) determines model accuracy by comparing predicted versus actual reference values, with lower values indicating greater precision (Zhan *et al.*, 2017). The RMSEP of 1.51% for fat and 0.46% for moisture suggests a decent correlation between the NIR spectra and the reference values determined by standard chemical methods which implies reasonably good quantitative prediction abilities but potential for enhancement.

According to Williams (2010), an RPD value below 1.5 suggests unreliable calibration. A value ranging from 1.5 to 2.0 indicates the model's ability to differentiate between high and low values. When the value falls within 2.0 to 2.5, it signifies the model's capability to provide approximate quantitative predictions. A value within the range of 2.5 to 3.0 indicates strong quantitative prediction, while a value exceeding 3.0 suggests outstanding quantitative prediction. From this, it is deduced that model developed in this research can be used to make a fair quantitative prediction of groundnut's crude fat and moisture content.

Conclusion

The study demonstrates the use of PLSR and NIR spectroscopy for quick groundnut quality parameter prediction. Efficient PLSR models using NIR absorbance spectra was developed, offering comparable performance to traditional methods, eliminating hazardous chemicals, and saving time. The research aims to improve quality control, process optimization, and value addition in groundnut processing, contributing to sustainability efforts in the food industry.

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper**.**

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