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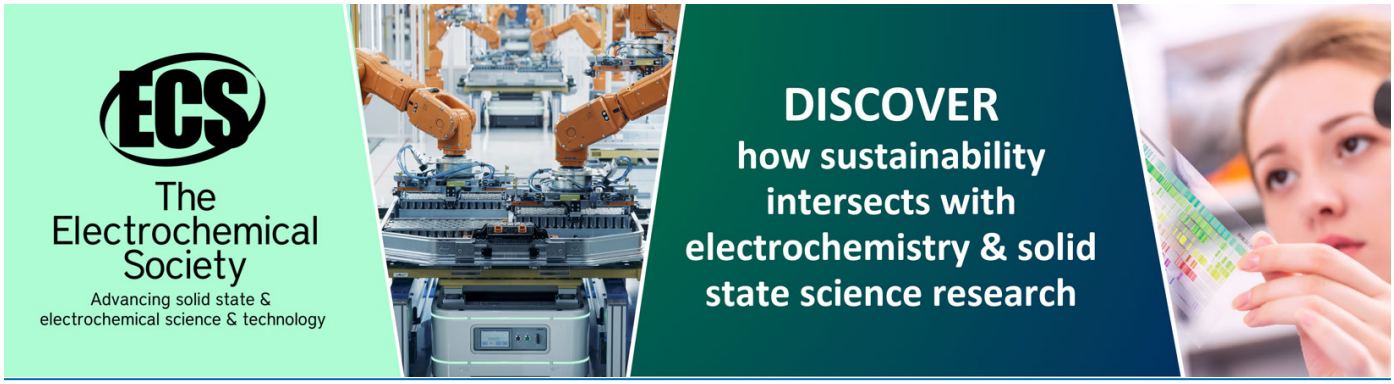

Application of NIRS adaptive technology for prediction of in vitro digestibility parameters of feed ingredients from Fermented Cocoa Pods

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Abstract. Near Infrared Reflectance Spectroscopy (NIRS) is an alternative method that can be applied in the evaluation of feed ingredients. The purpose of this study was to evaluate the in vitro digestibility value of fermented cocoa pods using the NIRS method of feed analysis. This study used 18 samples of fermented cocoa shell waste, where the material used was fermented cocoa pod skin (KBK) then in vitro analysis was carried out. Samples were acquired spectrum by Thermo Integrative. Chemical analysis is intended to compare the data from chemical analysis and the NIRS method. The parameters analyzed were pH, dry matter digestibility (KCBK), and organic matter digestibility (KCBO). Spectrum data were processed using PLS with the pre-treatment methods of multiplicative scatter correction (MSC) and DeTrending (DT). Based on the analysis that has been carried out using the NIRS method with a prediction model that has been built on pH parameters, KCBK has a good predictive model with the DT pre-treatment method and KCBO has a good predictive model with the MSC method where (pH = LV: 8, r: 0 .79, R2: 0.62, RMSEC: 0.04 and RPD: 2.00; KCBK= LV: 8, r: 0.86, R2: 0.74, RMSEC: 1.30 and RPD: 2.02 ; KCBO= LV: 8, r: 0.88, R2: 0.78, RMSEC: 1.39 and RPD: 2.21). Rough predictions for pH were obtained with Non pre-treatment and MSC pre-treatment (pH and MSC = LV: 8, r: 0.74, R2: 0.55, RMSEC: 0.05, RPD 1.58) and rough predictions on KCBK were obtained with Non Preatment (KCBK=LV: 8, r: 0.83 R2:0.70, RMSEC: 1.30, and RPD 1.87).

1. Introduction

Cocoa pods contain nutrients that can be used as animal feed ingredients. However in the cocoa pods, there are several limiting factors such as the high content of crude fiber, tannins and theobromine alkaloids. Theobromine and tannins have a strong affinity for proteins and carbohydrates, so they become a limiting factor in the use of cocoa husks for animal feed, because they can inhibit the growth of rumen microbes [1]. To reduce crude fiber and increase nutritional value, a fermentation technology process is needed. In the preparation of the ration, the feed ingredients used, such as fermented cocoa pods, need accuracy in analysis so that in the preparation ration, precise and accurate results are obtained according to the needs of livestock [2]. So far, the measurement method that is often used is an analysis using various chemicals (wet analysis) such as proximate analysis or dry matter and organic digestibility using the two-stage analysis method. This conventional method requires a long time, high cost, uses hazardous chemicals, and is not environmentally friendly [3]. Therefore, it is necessary to have an alternative method that can provide a faster and more efficient method in the analysis feed ingredients. One alternative method that can be applied in the evaluation of feed ingredients, one of which is the Near Infrared Reflectance Spectroscopy (NIRS) method or also called

the infrared reflection method. The NIRS method has the potential to analyze feed quickly, thoroughly, economically, effectively, and efficiently, without chemicals, and can analyze feed without damaging the product [4–6]. the application of the NIRS method in the field of animal feed is still limited. Therefore, it is necessary to research to compare the accuracy of the data from NIRS analysis and chemical analysis, so that the data obtained can enrich the application of NIRS in the field of animal feed.

2. Materials and Methods

2.1 Research Materials and Tools

The material used in this study is research, consisting of 18 samples of cocoa pod waste that has been fermented using lingzhi mushrooms that have been tested in vitro. Sampling was carried out on the internet of think using the Thermo Nicolet Antaris II tool and The Unscrambler X version 10.4 software which was used to process spectrum data.

2.2 Measurement of the KBK NIRS Spectrum

The measurement of the NIRS spectrum is done by reflecting near infrared light or what is often called infrared on the KBK sample. Spectrum measurements are carried out to obtain the initial spectrum of the sample. The wavelength used is in the range of 1000-2500 nm [7,8]. Spectrum measurements were carried out on 18 KBK samples respectively. So 18 waves were obtained that represent each sample. The results obtained from the reflection of infrared light on the sample are in the form of an initial spectrum (raw spectrum) that forms wave peaks. The wave peaks obtained from the results of the spectrum measurements show that there are differences in each sample which indicates the variety of characteristics in each sample treatment that can be read by NIRS.

3. Results and Discussion

3. 1 Chemical Analysis

Fermented KBK waste is the sample used in this study. There were 18 samples with different curing times, namely 15, 30, and 45 days of curing. At each curing time, there are 6 samples each. Prior to calibration using the Nears Infrared Reflectance Spectroscopy (NIRS) method, the sample has been chemically analyzed in the form of in vitro digestibility analysis in the laboratory on the 3 parameters studied, namely Dry Matter Digestibility (KCBK), Organic Matter Digestibility (KCBO), pH.

Table 1. Summary of Data Chemical Analysis pH KCBK, KCBO (n=18)

Parameter	Maximum	Minimum	Average	Standard Deviation
PH	7,06	6,76	6,86	0,08
KCBK	39,09	30,10	34,77	2,62
KCBO	33,51	23,79	29,14	3,07

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in each sample which indicates the variety of characteristics in each sample treatment that can be read by NIRS [7]. The fermented KBK sample at NIRS consisted of 18 samples with the results of the initial spectrum waves being shown in Figure 1.

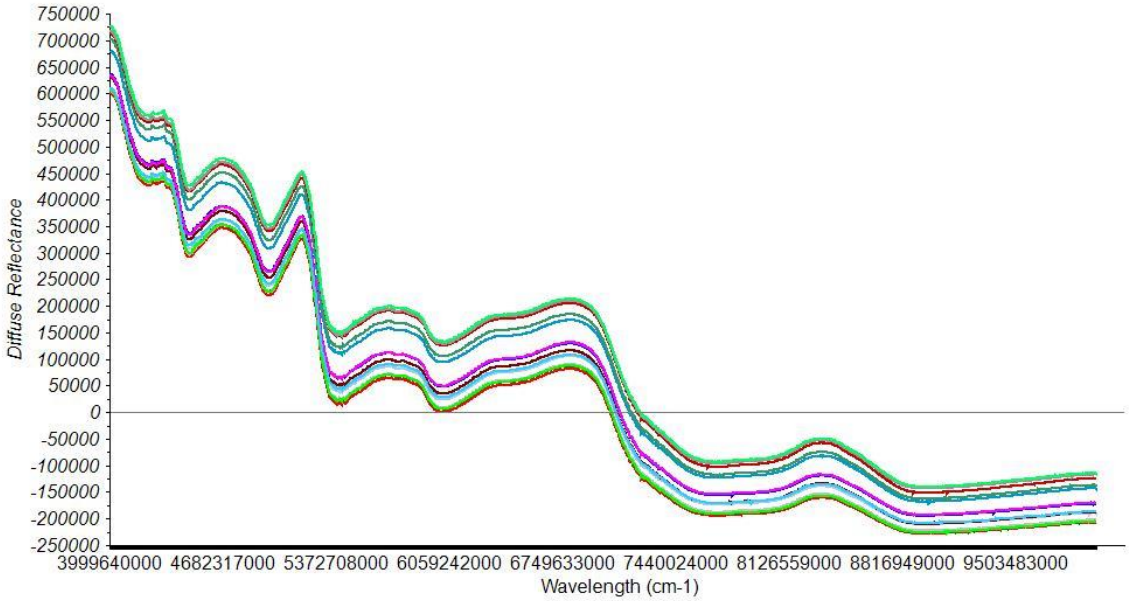


Figure 1. Initial Spectrum Waves of Cocoa Fruit Peel

The initial spectrum (raw spectrum) obtained from the infrared reflection results in the sample then still needs to be treated using principal component analysis (PCA). PCA serves to eliminate spectrum data (outlier removal) that is not a sample group due to interference with the spread of light. Outlier removal is done by projecting spectrum data using PCA and then the Hotelling T2 ellipses method is applied to the PCA projection results. As presented in picture 2

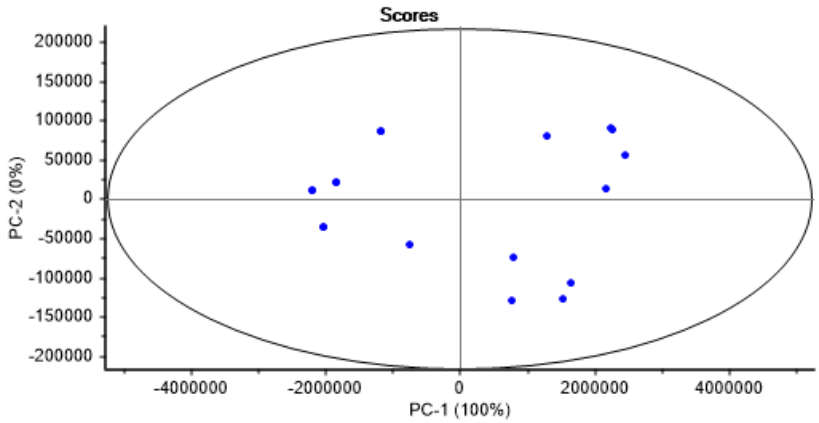
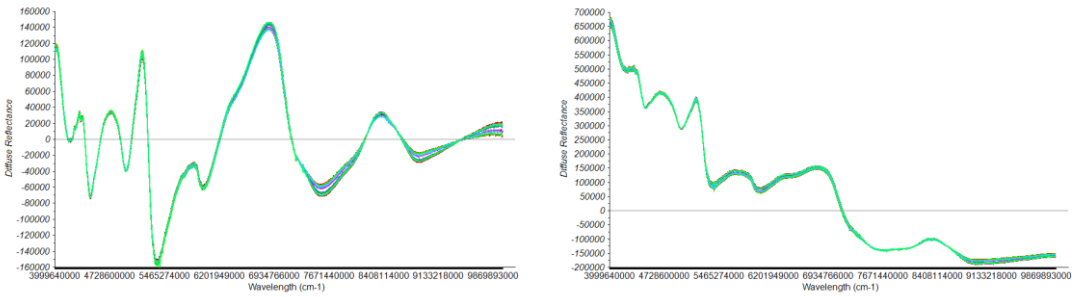


Figure 2. The use of PCA on the initial spectrum

The results obtained from the application of the Hotelling T2 ellipse method to the PCA projection results show that there is no large amount of data outside the ellipse. This indicates that outlier removal is not necessary because the combination of NIRS and PCA has been able to classify samples well.

3.3 NIRS Spectrum Pretreatment

The NIRS raw spectrum obtained still needs further pretreatment to correct the noise problem due to frequency interference during reflection. In addition, pretreatment needs to be carried out to overcome the problem of light scattering when reflecting NIRS data as well as the possibility of environmental disturbances. Thus, the spectrum that is read is the sample spectrum information, not other data content. Spectrum pretreatment methods that can be used include Multiplicative Scatter Correction (MSC) and De-Trending (DT) [9–12]. The corrected and corrected spectrum using MSC and DT methods can be seen in Figure 3.



a b

Figure 3. (a) Initial spectrum of cocoa pod husk + DT waste, (b) Initial spectrum of cocoa pod husk + MSC waste

Pretreatment using MSC can correct spectrum data by reducing offset effects (additive and chemical) as well as accumulation of data on the spectrum (amplication) so that the spectrum looks closer to the mean value and coincides (Figure a) when compared to the previous raw spectrum in Figure 1. [7] the use of the MSC method was able to increase the RPD value to predict the total insoluble solids in persimmon fruit. Besides MSC, DT pretreatment applications can also be used for spectrum correction. As shown in (Figure b), the DT pretreatment shows the concavity or curvature of the spectrum waves where DT serves to remove nonlinear trends in the spectral data to reduce noise. [8] DT pretreatment can improve the performance of PLS as indicated by the increase in the RPD value. So that it is clear the difference in the spectrum waves between pretreatment and non-pretreatment. The pretreatment application in this study functions so that the absorbance data information obtained is correct from the sample spectrum and then processed into numerical data.

3.4. Evaluation of NIRS Prediction Model With Calibration and Validation

The calibration results presented in Table 2 show the values of the statistical parameters. The results of pH calibration with nonpretreatment and MSC pretreatment treatment showed a rough evaluation value, where the RPD value of nonpretreatment and MSC obtained a value close to 2 and was still classified as a rough prediction, while the pretreatment Dt value showed good results [13,14] RPD values between 1.5-1.9 indicates that the prediction is still rough and still needs improvement in calibration. RPD values between 2-2.5 indicate a fairly good predictive model. While the RPD value between 2.5-3 or more indicates the accuracy of the prediction model is good and very good, the value of the latent variable used is 8, and the value of the good latent variable is below 9. The value of r is classified a good prediction because it is close to 1 (one) and the best value was obtained in pretreatment Dt with a value of 0.79. The value of the coefficient of determination (R2) on the Nonpretreatment and pretreatment MSC is 0.55 and

Dt is 0.62 which indicates the predictive model can read the height and the low of the wave [12,13]. For the overall treatment, the RMSEC value was obtained which was already good because the RMSEC value was lower than the RPD value and was also close to 0.

Table 2. Results of Calibration of KBK Waste pH Levels with the PLS Method

Treatment	Latent Variable	r	R^2	RMSEC (%)	RPD
Non-pretreatment	8	0,74	0,55	0,05	1,58
MSC	8	0,74	0,55	0,05	1,58
DT	8	0,79	0,62	0,04	2,00

The calibration results presented in Table 3 show the values of the statistical parameters. The results of the calibration of KCBK with non-pretreatment treatment show a rough evaluation value, where the RPD value of Non Preatment is 1.87, and the RPD Preatment MSC and DT values have shown a good evaluation value with an RPD MSC value of 2.00, Dt 2.02. explained that the RPD value between 1.5-1.9 indicates a rough prediction and still needs improvement in calibration. RPD values between 2-2.5 indicate a fairly good predictive model. While the RPD value between 2.5-3 or more indicates the accuracy of the prediction model is good and very good, the value of the latent variable used is 8, and the value of the good latent variable is below 9. The best value of r is obtained in pretreatment MSC and Dt with a value of 0.86. The value of R2 in MSC and Dt pretreatment also shows that the model can predict quantitatively roughly. R2 values ranging from 0.66-0.81 indicate that the predictive model can estimate quantitative values. The RMSEC value is still relatively high, this is due to the high chemical analysis SD. the RMSEC value below the SD value for chemical analysis can be categorized as good.

Table 3. Results of Calibration of KBK Levels in KCBK Waste with the PLS

Treatment	Latent Variable	r	R^2	RMSEC (%)	RPD
Non - retreatment	8	0,83	0,70	0,40	1,87
MSC	8	0,86	0,73	0,31	2,00
DT	8	0,86	0,74	0,30	2,02

The calibration results presented in Table 4 show that the value of the KCBO parameter with nonpretreatment and pretreatment treatment shows a fairly good evaluation value, for the RPD value of nonpretreatment the value is 2.11 while the MSC treatment is 2.21 and Dt is 2.14. RPD values between 1.5-1.9 indicate that the prediction is still rough and still needs improvement in calibration. RPD values between 2-2.5 indicate a fairly good predictive model. While the RPD value between 2.5-3 or more indicates the accuracy of the prediction model is good and very good. The latent variable value used is 8, a good latent variable value is below 9. The r value is classified a good prediction because it is close to 1 (one) and the best value is obtained in MSC pretreatment with a value of 0.78. The value of R2 in MSC and Dt pretreatment also shows that the model can predict quantitatively roughly. R2 values ranging from 0.66-0.81 indicate that the predictive model can estimate quantitative values. The RMSEC value is still relatively high, this is due to the high chemical analysis SD.the RMSEC value is smaller than the standard deviation, meaning the data is classified as good.

Table 4. Results of Calibration of KBK Levels in KCBO Waste with the PLS Method

Treatment	*Latent Variable*	r	R^2	RMSEC (%)	RPD
Non - *pretreatment*	8	0,83	0,70	1,40	1,87
MSC	8	0,86	0,73	1,31	2,00
DT	8	0,86	0,74	1,30	2,02

4. Conclusion

The prediction model of the NIRS method in analyzing the in vitro digestibility of fermented KBK is classified as being able to predict the parameter values of pH, KCBK, and KCBO. The predicted value for KCBO is the highest where RPD, LV, RMSEC, R2, and r are 2.21, 8, 1.39, 0.78 and 0.88 then KCBK with values 2.02, 8, 1.30 , 0.74 and 0.86 then pH with a value of 2.00, 8, 0.4, 0.62 and 0.79. The use of the Dt spectrum pretreatment is the best in increasing the accuracy of the calibration predictions and the validation of the parameter values of RPD, LV, RMSEC, R2 and r when compared to MSC pretreatment and non-pretreatment.

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References

[1] Rodionova O Y, Fernández Pierna J A, Baeten V and Pomerantsev A L 2021 Chemometric non-targeted analysis for detection of soybean meal adulteration by near infrared spectroscopy *Food Control* **119**

[2] Mohamed H, Nagy P, Agbaba J and Kamal-Eldin A 2021 Use of near and mid infra-red spectroscopy for analysis of protein, fat, lactose and total solids in raw cow and camel milk *Food Chem.* **334** 127436

[3] Yao S, Qin H, Wang Q, Lu Z, Yao X, Yu Z, Chen X, Zhang L and Lu J 2020 Optimizing analysis of coal property using laser-induced breakdown and near-infrared reflectance spectroscopies *Spectrochim. Acta - Part A Mol. Biomol. Spectrosc.* **239** 118492

[4] Samadi, Wajizah S and Munawar A A 2020 Near infrared spectroscopy (NIRS) data analysis for a rapid and simultaneous prediction of feed nutritive parameters *Data Br.* **29** 105211

[5] Cozzolino D 2014 An overview of the use of infrared spectroscopy and chemometrics in authenticity and traceability of cereals *FRIN* **60** 262–5

[6] Comino F, Aranda V, García-Ruiz R, Ayora-Cañada M J and Domínguez-Vidal A 2018 Infrared spectroscopy as a tool for the assessment of soil biological quality in agricultural soils under contrasting management practices *Ecol. Indic.* **87** 117–26

[7] Samadi, Wajizah S and Munawar A A 2020 Near infrared spectroscopy (NIRS) data analysis for a rapid and simultaneous prediction of feed nutritive parameters *Data Br.* **29**

[8] Munawar A A, Yunus Y, Devianti and Satriyo P 2020 Calibration models database of near infrared spectroscopy to predict agricultural soil fertility properties *Data Br.* **30**

[9] Marques E J N, De Freitas S T, Pimentel M F and Pasquini C 2016 Rapid and non-destructive

determination of quality parameters in the “Tommy Atkins” mango using a novel handheld near infrared spectrometer *Food Chem.* **197** 1207–14

[10] Arendse E, Fawole O A, Magwaza L S and Opara U L 2018 Non-destructive prediction of internal and external quality attributes of fruit with thick rind: A review *J. Food Eng.* **217** 11–23

[11] Deng Y, Wang Y, Zhong G and Yu X 2018 Simultaneous quantitative analysis of protein, carbohydrate and fat in nutritionally complete formulas of medical foods by near-infrared spectroscopy *Infrared Phys. Technol.* **93** 124–9

[12] Pasquini C 2018 Near infrared spectroscopy: A mature analytical technique with new perspectives – A review *Anal. Chim. Acta* **1026** 8–36

[13] Piñeiro G, Perelman S, Guerschman J P and Paruelo J M 2008 How to evaluate models: Observed vs. predicted or predicted vs. observed? *Ecol. Modell.* **216** 316–22

[14] Nordey T, Joas J, Davrieux F, Chillet M and Léchaudel M 2017 Robust NIRS models for non-destructive prediction of mango internal quality *Sci. Hortic. (Amsterdam).* **216** 51–7