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Non-Destructive Prediction of Chemical Content in Palm Oil Fruit Using Near-Infrared Spectroscopy and Artificial Neural Network

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Abstract

Oil and water content are important quality criteria of crude palm oil (CPO) resulted from palm oil fruit processing. Those contents are usually determined using chemical methods in the laboratory. This method is time consuming, long procedure, and destructive. Some efforts had been carried out to determine oil and water content of palm oil fruit non-destructively using some methods including Near-Infrared Spectroscopy (NIRS), but the results had not been satisfied. This research aims to assess Artificial Neural Network (ANN) and NIRS method to predict oil and water content of palm oil fruits non-destructively. The samples were palm oil fruits with ten maturity levels harvested from plantation in Bogor. The sample's reflectance was measured with spectrometer NIR-Flex 500 at wavelength of 1000-2500 nm. After that, oil and water content were determined using chemical method. Some pre-treatments of NIR spectra namely normalization, Savitzky-Golay first derivative, their combinations, and standard normal variation were applied. Multivariate analysis such as PLS were carried out and the results of Factor Component (FC) were input for ANN model. The result showed the best method to predict oil content was combination Savitzky-Golay first derivative and normalization pre-treatment using PLS-ANN with 20 FC (R^2=0.99; SEC= 0.55%; RPD=28.21; CV=2.31%). For water content, the best prediction was standard normal variate pre-treatment using PLS-ANN with 19 FC (R^2=0.99; SEC= 1.21%; RPD=15.51; CV=1.96%). The result shows that developed ANN and NIRS can predict oil and water content of palm oil fruit non-destructively.

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1. Introduction

Palm oil is one of the most important commodities in the world for vegetable oil production (ITPC, 2013). The quality of the produced oil is determined by essential parameters such as the ripeness, oil content and water content in the palm oil fruit. Typically, ripeness is predominantly carried out manually with human visual inspection, while the oil content and water content are analyzed in a

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laboratory through destructive testing. Laboratory tests are costly, time-consuming (as results take a considerable amount of time), demand substantial labor, and are prone to human errors. Therefore, there is a necessity to replace these approaches with rapid, non-destructive, and cost-effective techniques. Researchers have explored various non-destructive technologies to assess the quality of palm oil fruit, including methods based on electrical properties (Sinambela *et al.,* 2020), image analysis (Makky, 2016), and near-infrared spectroscopy (NIRS) (Makky and Soni, 2014; Novianty *et al.,* 2022).

NIR technology in agriculture offers advantages such as quick response time, low maintenance costs, and the ability to process large amounts of data (Blanco and Villarroya, 2002). Makky and Soni (2014) predicted the chemical content of palm oil fruit using the artificial neural network (ANN) calibration method with a VIS-NIR spectrometer. Novianty *et al.,* (2022) predicted the oil content of palm oil fruit using the NIRFlex N-500 spectrometer and EMD-ANN calibration method. According to the quality standards for oil content (crude palm oil) outlined in SNI 01-2901-2006, the maximum concentration allowable for water content and dirt is 5% (BSN 2006). However, the prediction of oil and water content in palm oil fruit using a combination of PLS-ANN methods and the NIRFlex N-500 spectrometer has not been explored, despite water content being a crucial quality component in palm oil fruit, alongside oil content. The PLS-ANN method is chosen for this research because it effectively manages complex data with numerous variables and also easier to understand, making it accessible for researchers. Integrating these methods improves prediction accuracy (Yu *et al.,* 2018). Overall, it's chosen for its balance between accuracy and simplicity in analyzing complex data. Therefore, this research aims to compare NIRS methods based on calibration of PLS-ANN and PLSR using the NIRFlex N-500 spectrometer to non-destructively predict the oil and water content in palm oil fruit.

2. Materials and methods

This research was conducted from June 2023 to November 2023 (Figure 1) at the Cikabayan Farm IPB Plantation, the Laboratory of Food and Agricultural Product Processing at IPB, and the Laboratory of Agricultural Industrial Engineering Testing at IPB, Bogor.

2.1 Sample Preparation and NIR Measurement

Sample palm oil fruit from Cikabayan Farm, IPB, were used for this research. The samples that were used for NIR measurement were Tenera varieties (*Elaeis guineensis* Jacq. Var. tenera). Data absorbance for this research was collected from 408 samples of palm oil fruit were grouped by maturity age as follows, 3 months, 4 months, 4 months 1 week, 4 months 2 weeks, 4 months 3 weeks, 5 months, 5 months 1 week, 5 months 2 weeks, 5 months 3 weeks, and 6 months. NIR spectrum data acquisition was carried out using the NIRFlex N-500 spectrometer (manufactured by BUCHI Labortechnic AG, Switzerland) by shooting the Transflectance adapter at the palm oil fruit, measured at 3 points in the wavelength range of 10,000-4,000 cm^{-1} or 1,000-2,500 nm. However, this research

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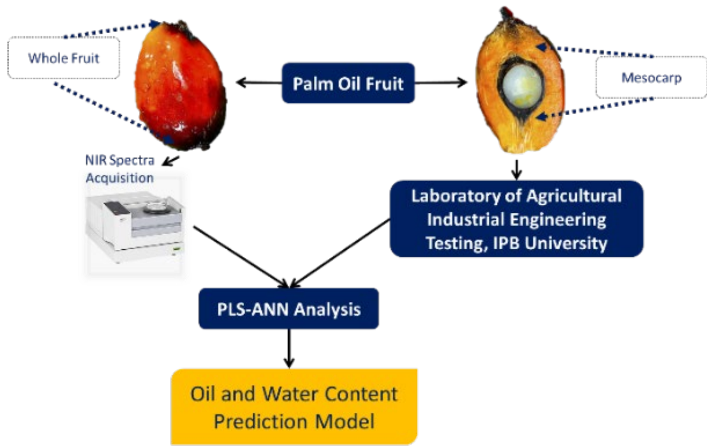

Figure 1. Research framework.

analysis focuses on the wavelength range of 10,000-6,666.7 cm^{-1} or 1,000–1,500 nm. Based on preliminary research, the NIR signals with this wavelength range have minimal visual overlap compared to other regions and helps reduce the computational burden as the number of wavelengths has been reduced during the initial steps of signal processing (Novianty *et al.*, 2022). The energy reflected by the palm oil fruit samples was captured by the detector as reflectance data or spectrum data, which was then recorded using the NIRFlex N-500 Fiber Optic Solids.

2.2 Destructive Measurement (Chemical Content)

Oil and water content were determined according to the Indonesian National Standard (SNI) 01-2891-1992, using Equation 1 for oil content and Equation 2 for water content (BSN 1992).

$$\% \text{ Oil Content} = \frac{W - W_1}{W_2} \times 100\% \quad (1)$$

$$\% \text{ Water Content} = \frac{W_3}{W_4} \times 100\% \quad (2)$$

Where: W= Sample weight in grams (g), W_1= Weight of fat before extraction in grams (g), W_2= Weight of fat flask after extraction in grams (g), W_3= Weight of sample before drying in grams (g), W_4= Weight loss after drying in grams (g)

2.3 Spectra Pre-treatment and The Development of Calibration Models Using the ANN Method

The chemical data utilized in this research comprise 120 datasets acquired from 3 palm oil fruits for each chemical dataset (with ages ranging from 3 months to 5 months) and 4 palm oil fruits for each chemical dataset (with ages ranging from 5 months 1 week to 6 months). Consequently, a total of 408 palm oil fruits were employed for the 120 chemical datasets. Similarly, regarding the NIR data, one NIR dataset is derived from the average of 3 NIR datasets from palm oil fruits (aged 3 months to 5 months), and one NIR dataset is derived from the average of 4 NIR datasets from palm oil fruits (aged

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5 months 1 week to 6 months). Thus, the 408 NIR datasets are averaged to yield 120 NIR datasets. This indicates that the input utilized for the predictive method consists of one chemical dataset paired with one NIR dataset. The data are divided into a ratio of 70:30, where 70% of the data constitutes the calibration set and 30% of the data comprises the validation set.

Input for creating an ANN model using absorbance spectra data that has been given pre-treatment and continuing to PLS (Partial Least Squares) analysis. Pre-treatment is carried out to improve the spectra for easier identification of chemical content within them. Four types of spectral pre-treatment are performed, namely, normalization (N01), first derivative Savitzky-Golay (SG1), combination 1 (SG1-N01), and standard normal variate (SNV).

Then, after pre-treatment next to PLS analysis that extracts predictors for the analysis of dependent and independent variables (Abdi, 2010) and generates factor components (FC) as representations of new data related to the original data. FC were used to summarize information from the dataset in statistical analysis as input for ANN model that can enhance the performance of the calibration model, especially when multiple variables are correlated (Perera *et al.*, 2021; Liu *et al.*, 2022). Moreover, a calibration model employing PLS-Regression was implemented to compare with the PLS-ANN method, with the goal of illustrating that the utilization of Artificial Neural Networks (ANN) can produce better outcomes than relying solely on the PLSR method.

ANN is a tool for modeling non-linear statistical data where complex relationships between various inputs and outputs are modeled for pattern recognition (Hamdani *et al.*, 2023). In this research, ANN utilizes a feed-forward neural network trained by a back propagation algorithm (multi-layer perceptron) to build the calibration model. The input layer in this study includes variations of optimum factor components from the pre-treated NIRS spectra data of palm oil fruit. The hidden layer in this research has 1 piece with 2 neurons. The output layer represents the oil or water content that is predicted by the ANN. The ANN model from this research is in Figure 2. In this research, The Unscrambler X software was employed for preprocessing spectra and implementing the PLSR method, while RapidMiner was utilized for analyzing artificial neural networks (ANN).

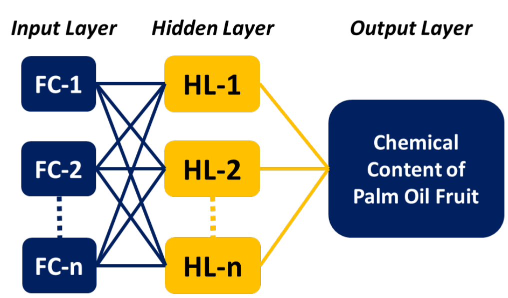

Figure 2. ANN model

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2.4 Model Evaluation

The statistical parameters used to evaluate predictive models include the coefficient of determination (R^2), standard error of calibration set (SEC), standard error of prediction set (SEP), coefficient of variation (CV), residual predictive deviation (RPD), and consistency. A good model's validity can be assessed based on the following statistical parameters, such as R^2 value ≈ 1, SEP ≈ SEC, RPD ≥ 2, consistency values within the range of 80-110%, and CV < 10% (Nicolai *et al.,* 2007; Monge *et al.,* 2019).

3. Result and discussion

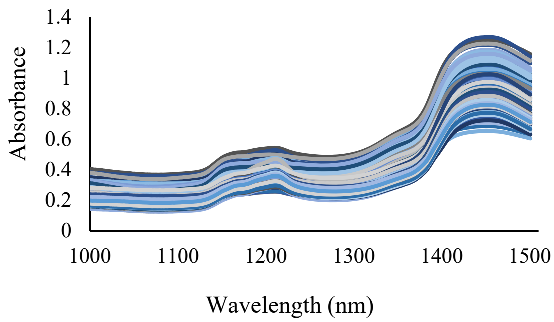
3.1 NIR Spectra of Palm Oil Fruit

Figure 3(a) illustrates the original absorbsance spectra obtained from NIRS measurements on palm oil fruit. The spectral shape is affected by dominant chemical components in samples that measured. The wavelength range of 1,100 – 1,220 nm suspected as oil content, at wavelength interval there is a dominance of CH, CH_2, and CH_3 bonding arrangements, which are components constituting oil content (Osborne *et al.,* 1993). Meanwhile, for water content is identified through C-O and O-H were distinguished within the wavelength range of 1,408-1470 nm (Osborne *et al.,* 1993; Lengkey *et al.,* 2013; Iqbal *et al.,* 2014).

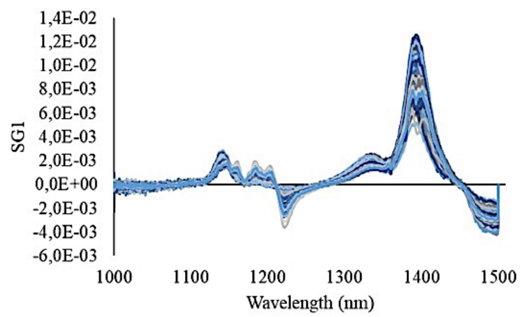
The results of the spectrum refinement process with the first derivative Savitzky-Golay pre-treatment (SG1) can be seen in Figure 3(b). Palm oil fruit spectra after correction with SG1 form a slenderer pattern with clearer peaks and valleys compared to the original spectra. This is because the first derivative functions as a separator for chemical components that experience overlapping (Lengkey *et al.,* 2013).

Another pre-treatment, namely normalization (N01), can be observed in Figure 3(c). Normalization pre-treatment forms a pattern that is similar to the original spectra but with a narrower range between spectra values. Normalization pre-treatment serves to reduce the range of reflectance values into the range of 0-1, thereby minimizing the effect of sample particle size differences (Lengkey *et al.,* 2013).

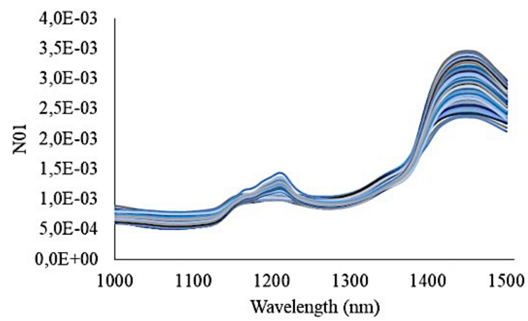
Meanwhile, Figure 3(d) and Figure 3(e) represent combination of the first derivative Savitzky-Golay followed by normalization (SG1-N01) and standard normal variation (SNV) pre-treatment. It can be observed from Figure 3(d), spectra with combination pre-treatment that they are more influenced by the SG1 pre-treatment, resulting in similar spectral outcomes. Meanwhile, SNV pre-treatment aims to reduce the interference of noise waves, resulting in a smoother and denser spectrum as Figure 3(e) (Nurhasanah *et al.,* 2019).



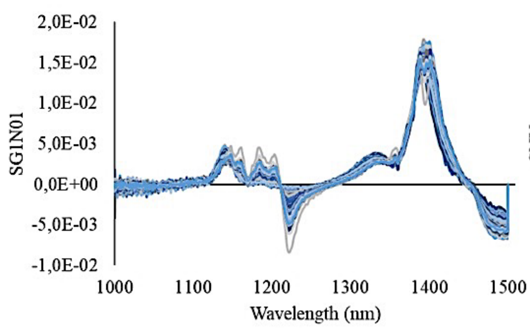
(a)



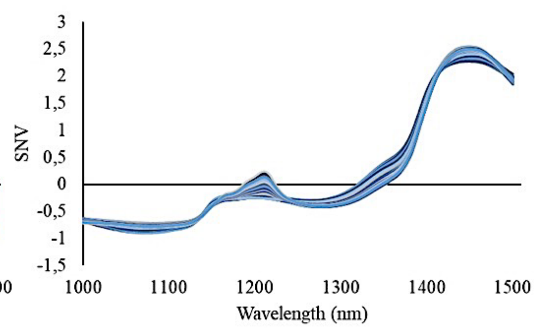
(b)



(c)



(d)



(e)

Figure 3. Spectra (a) Original; (b) SG1; (c) N01; (d) SG1-N01; and (e) SNV

3.2 Oil and Water Content in Palm Oil Fruit

The oil content of palm fruit varies for each level of maturity (10 maturity levels) (Figure 4). The same is also indicated by the moisture content at 10 maturity levels. From Figure 4, it can be observed that as the maturity level increases, the oil content also increases. In contrast, for moisture content, as the maturity level increases, the moisture content in palm fruit tends to decrease. It can be concluded that the moisture content and oil content exhibit different trends as the age of the palm fruit increases.

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The quantity of chemical data utilized in this research differs across parameters. Specifically, for oil content analysis, 96 out of 120 data were employed due to the identification of inaccurate oil data, particularly concerning data at the 4th month harvesting age. In contrast, for water content analysis, the full complement of 120 out of 120 data was utilized, as the obtained moisture data were deemed accurate.

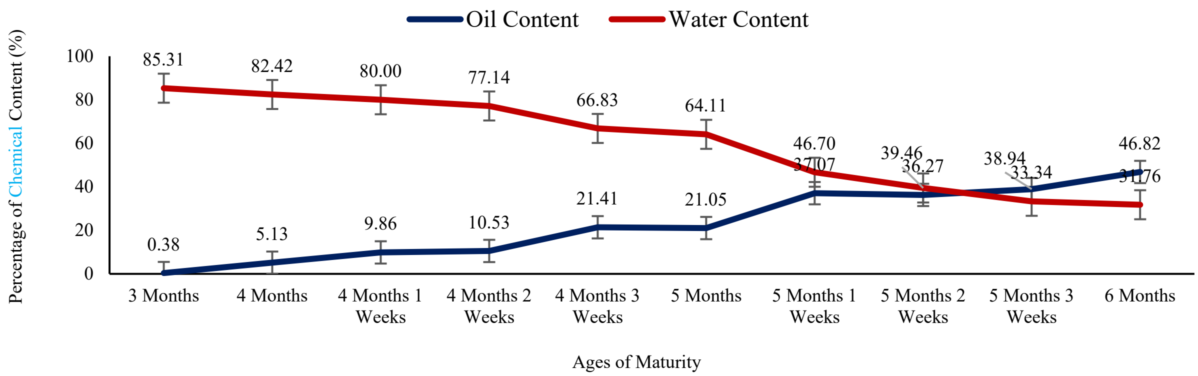

Figure 4. Change in oil and water content of palm oil fruit along maturity level.

3.3 Calibration and Prediction Results for Oil and Water Content

Table 1 shows that both the PLSR and PLS-ANN methods have a high coefficient of determination (R^2) ≈ 1 for predicting oil content. However, PLSR has a standard error calibration (SEC) range of 0.6 to 4.4, while the PLS-ANN model achieves lower SEC values within the range of 0.6 to 2.9. Similarly, for water content (Table 2), the PLSR method has a SEC value range of 1.4 to 7.4, whereas PLS-ANN achieves a lower SEC in the range of 0.8 to 1.9. Standard Error (SE) is employed for comparing NIR predictions with conventional methods. A smaller SEC and SEP denote a more accurate model (Lengkey *et al.*, 2013). The comparison demonstrates that calibration with ANN enhances the accuracy of the model in predicting the oil and water content of palm fruit, resulting in a lower SEC than PLSR.

The best model for predicting the oil content of palm fruit is achieved through the PLS-ANN method with pre-treatment combination of the first derivative Savitzky-Golay and normalization (SG1-N01) 20 PLS factor components (Figure 5(a)). The decision to utilize 20 factor components was prompted by the observation that the consistency of the 21th factor no longer satisfied the criteria, suggesting the presence of overfitting. Following this, the decision was taken to select the optimum number of PLS factor with the highest qualification, but still meet the criteria of good model. Figure 5(a) explains the plot of predicted oil content and the chemically tested of oil content. The high coefficient of determination (R^2) value of 0.99, SEC value of 0.55%, CV value of 2.31%, and RPD value of 28.21 indicate that this model is excellent at predicting oil content in palm oil fruit. This finding

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aligns with previous research by Lengkey *et al.*, (2013), which identified the combination of the first derivative Savitzky-Golay and normalization as the best pre-treatment for predicting oil content. The effectiveness of this combination in predicting oil content is attributed to the relatively high percentage of oil content in the palm fruit studied. Additionally, the normalization function plays a collaborative role by narrowing the spectral range, enhancing the linearity of the relationship between chemical content and spectra after normalization.

Table 1. Analysis results for the oil content of palm fruit using PLSR and PLS-ANN.

Pre-Treatment	Methods	Factor Component	Calibration (n= 67)			Validation (n= 29)			Consistency (%)
			R^2	SEC (%)	CV (%)	SEP (%)	CV (%)	RPD	
Ori	PLSR	20	0.99	0.99	4.17	5.40	25.13	3.09	18.25
		12	0.96	3.56	15.04	4.79	22.29	3.49	74.29
		11	0.95	3.91	16.55	4.58	21.34	3.64	85.36
	PLS-ANN	22	0.99	1.16	4.91	1.89	8.81	8.82	61.31
		20	0.99	1.51	6.37	2.15	10.60	7.76	66.15
		19	0.99	1.76	7.44	2.15	10.01	7.76	81.79
SG1	PLSR	17	0.99	0.61	2.58	5.02	23.36	3.33	12.15
		7	0.96	3.53	14.92	4.86	22.62	3.43	72.60
		6	0.95	4.09	17.31	4.98	23.18	3.35	82.20
	PLS-ANN	20	0.99	0.62	2.60	0.73	3.41	22.80	84.13
		19	0.99	0.76	3.20	0.99	4.62	16.82	76.17
		18	0.99	0.89	3.77	1.05	4.90	15.85	84.66
N01	PLSR	20	0.99	1.06	4.49	4.49	20.90	3.72	23.62
		11	0.96	3.70	15.64	4.63	21.57	3.60	79.78
		10	0.95	4.06	17.15	4.63	21.57	3.60	87.50
	PLS-ANN	20	0.99	1.43	6.05	1.94	9.03	8.60	73.68
		15	0.99	2.92	8.86	2.74	12.76	6.09	76.45
		14	0.98	2.50	10.58	2.92	13.58	5.72	85.73
SG1N01	PLSR	13	0.99	1.17	4.95	4.11	19.13	4.06	28.48
		6	0.95	3.81	16.11	5.10	23.73	3.27	74.71
		5	0.94	4.37	18.47	5.11	23.79	3.27	85.46
	PLS-ANN	20	0.99	0.55	2.31	0.59	2.75	28.21	92.14
		19	0.99	0.65	2.74	0.63	2.93	26.54	103.10
		18	0.99	0.93	3.94	1.02	4.74	16.38	91.43
SNV	PLSR	19	0.99	1.17	4.94	3.93	18.28	4.25	29.76
		11	0.96	3.41	14.43	4.96	23.09	3.36	68.77
		10	0.95	3.85	16.27	4.28	19.93	3.90	89.87
	PLS-ANN	20	0.99	1.50	6.34	1.62	7.53	10.32	92.71
		18	0.99	1.79	7.59	1.59	7.41	10.49	112.76
		17	0.99	1.88	7.94	1.71	7.97	9.75	109.57

Note: Green Block = Best Result

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Table 2. Analysis results for the water content of palm fruit using PLSR and PLS-ANN

Pre-Treatment	Methods	Factor Component	Calibration (n= 84)			Validation (n= 36)			Consistency (%)
			R^2	SEC (%)	CV (%)	SEP (%)	CV (%)	RPD	
Ori	PLSR	15	0.99	1.75	2.83	4.48	7.76	5.23	39.18
		11	0.99	2.48	4.00	3.46	5.99	6.78	71.82
		10	0.98	2.73	4.41	3.16	5.48	7.41	86.50
	PLS-ANN	20	0.99	1.12	1.81	1.57	2.72	14.93	71.64
		19	0.99	1.22	1.97	1.42	2.46	16.51	86.00
		18	0.99	1.25	2.02	1.51	2.61	15.54	82.90
SG1	PLSR	6	0.98	2.97	4.79	3.92	6.80	5.97	75.72
		5	0.98	3.42	5.51	3.89	6.75	6.02	87.76
		1	0.89	7.43	11.98	7.14	12.38	3.28	104.07
	PLS-ANN	15	0.99	1.19	1.92	1.73	3.01	13.51	68.68
		13	0.99	1.34	2.16	1.76	3.05	13.33	76.28
		12	0.99	1.67	2.69	2.05	3.55	11.45	81.65
N01	PLSR	17	0.99	1.48	2.39	4.58	7.93	5.12	32.41
		12	0.99	2.59	4.17	3.79	6.58	6.17	68.22
		11	0.98	2.78	4.48	3.43	5.95	6.83	81.06
	PLS-ANN	17	0.99	1.47	2.37	2.06	3.57	11.39	71.50
		16	0.99	1.62	2.61	2.06	3.57	11.39	78.54
		15	0.99	1.87	3.01	2.20	3.81	10.65	84.91
SG1N01	PLSR	12	0.99	1.46	2.36	4.32	7.49	5.42	33.91
		6	0.98	3.02	4.88	3.83	6.65	6.11	78.87
		5	0.98	3.39	5.46	4.10	7.10	5.72	82.71
	PLS-ANN	20	0.99	0.84	1.36	1.14	1.98	20.47	73.76
		13	0.99	1.34	2.17	1.70	2.95	13.76	78.92
		12	0.99	1.72	2.77	2.11	3.66	11.10	81.48
SNV	PLSR	15	0.99	1.44	2.32	4.10	7.10	5.72	35.09
		10	0.99	2.42	3.91	3.29	5.70	7.13	73.70
		9	0.99	2.59	4.17	3.00	5.21	7.80	86.03
	PLS-ANN	22	0.99	0.79	1.28	1.11	1.93	21.02	71.12
		21	0.99	0.96	1.55	1.32	2.28	17.78	73.03
		19	0.99	1.21	1.96	1.51	2.62	15.51	80.35

Note: Green Block = Best Result

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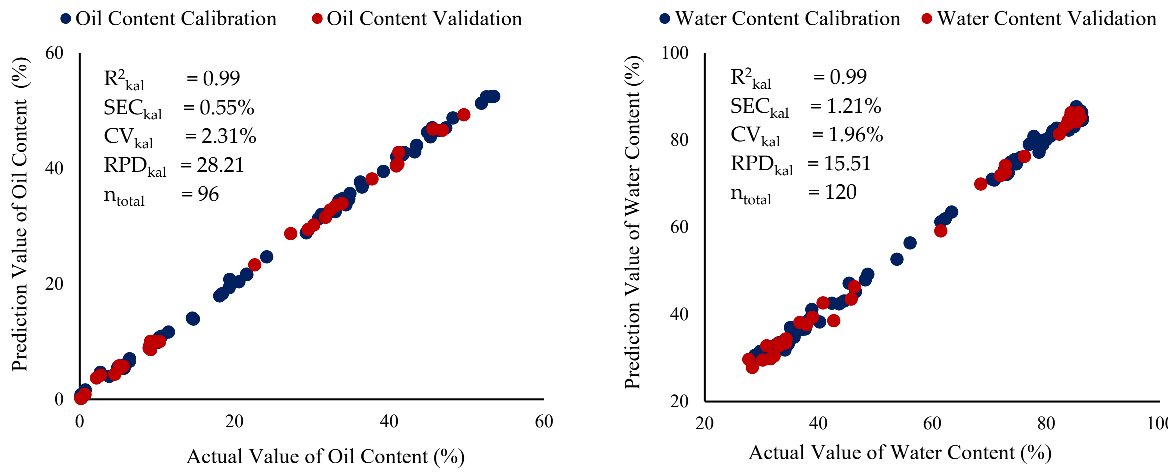

(a) (b)

Figure 5. Actual and prediction values (a) oil content; (b) water content.

The optimal model for predicting water content is achieved through the PLS-ANN method with pre-treatment combination of the standard normal variate and 19 PLS factor components (Figure 5(b)). The decision to select 19 factor components was made due to consistency in the 20th factor no longer meeting the criteria, indicating overfitting. Therefore, the highest qualifying result within the domain of criteria for reliable model was chosen. The plot in Figure 5(b) illustrates the relationship between predicted water content and chemically tested water content. The high coefficient of determination (R^2) value of 0.99, SEC value of 1.21%, CV value of 1.96%, and RPD value of 15.51 collectively indicate that this model excels in predicting water content in palm oil fruit. SNV pre-treatment is effective in predicting water content due to the notably high average water content in this study. The SNV pre-treatment widens the spectral range from the original spectra to a wider range, effectively minimizing noise wave interference. As a result, this leads to a smoother and denser spectrum, thereby enhancing the linearity of the relationship between chemical content and spectra after the application of SNV.

In PLS-ANN analysis, the number of PLS factors may exceed that of PLSR due to the combined flexibility of artificial neural networks and the complexity of the relationships being modeled. This enhanced capability of PLS-ANN to uncover intricate patterns may necessitate a different number of factors for effective modeling. Consequently, a larger number of factors may be required for accurate modeling in PLS-ANN compared to traditional PLSR.

4. Conclusion

NIR spectroscopy and the PLS-ANN calibration method from combination first derivative Savitzky-Golay and normalization spectra with 20 FC can accurately predict oil content in palm oil fruit

(R^2=0.99, SEC=0.55, CV=2.31%, RPD=28.21). For predicting water content, the best model is obtained from standard normal variate spectrum data using the PLS-ANN calibration with 19 FC (R^2=0.99, SEC=1.21, CV=1.96%, RPD=15.51). The research results indicate that NIRS can be used as a rapid and non-destructive method for determining oil and water content in palm oil fruit.

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