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Fast and contactless assessment of intact mango fruit quality attributes using near infrared spectroscopy (NIRS)

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Abstract. In recent decades, the development of fast, non-destructive and robust methods to determine agricultural products quality parameters become interesting and gaining more attentions in term of their potential applications in many field. One of those methods is near infrared spectroscopy (NIRS) which is works based on the interaction of biological matter with light radiation. The main purpose of this present study is to employ the NIRS method in assessing mango fruit quality parameters in form of soluble solids content (SSC) and vitamin C. Spectra data of absorbance NIR were acquired in wavelength range from 1000 to 2500 nm with optical gain 4x and resolution windows 0.02 nm. Prediction models were developed using partial least square regression (PLSR) followed by 10-fold cross validation. The results showed that both SSC and vitamin C of mango fruit can be determined simultaneously with maximum correlation coefficient are 0.88 and 0.87 for SSC and vitamin C respectively. Judging from its predictive abilities, it may conclude that NIRS can be used as fast and contactless method in assessing mango fruit quality parameters like SSC and vitamin C.

1. Introduction

Mango (Mangifera indica) is one of the most popular tropical fruit worldwide due to its nutritional benefits and taste. Originally, mango fruit comes from South Asia and has spread to many tropical countries including Indonesia [1], [2]. Besides its delicious taste, mangoes are rich in health benefits for the body. Even this one fruit is also believed to be able to prevent various dangerous diseases. Mango fruit contains low calories and high fiber. Mango is a source of vitamins A, C and E. It also has folate, B6, iron, to calcium [3], [4]. This one fruit is also a good source of antioxidants, containing phytochemicals that are good for human health. Mangoes are safe for consumption for everyone, both children and adults. Even many processed foods and beauty products that include mangoes as one of the basic ingredients. In addition to the distinctive aroma, mangoes can provide benefits for the skin [5].

Soluble solids content (SSC) and vitamin C are two among other mango quality attributes that are important and plays an important role in maintaining human health. Mangoes have high vitamin C and SSC which can help to reduce bad cholesterol levels. This tropical fruit is also rich in potassium which is needed by the body. Potassium functions to balance body fluid cells to control blood pressure and heart rate. Mango is believed to reduce cholesterol and improve heart health [6], [7].

In order to determine mango quality attributes, several methods were widely used and applied. However, most of those methods are destructive, required chemical materials, complicated procedures and time consuming [8], [9]. Therefore, it is unsuitable to be used in horticulture industries. In recent decades, the development of fast, non-destructive and robust methods to determine agricultural products quality parameters become interesting and gaining more attentions in term of their potential applications in many field. One of those methods is near infrared spectroscopy (NIRS) which is works based on the interaction of biological matter with light radiation [10], [11].

Numerous studies have been reported related to NIRS applications in many field including agriculture such as fruit and horticulture [12], [13], meat and dairy products quality evaluation [14],

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[15], soil macro and micro nutrients [16]–[18], and other agricultural crops quality [19]–[23]. Therefore, the main purpose of this present study is to employ the NIRS method in assessing mango fruit quality parameters in form of soluble solids content (SSC) and vitamin C.

2. Material and Methods

2.1 Spectra data

Near infrared spectra data of intact mango fruits were obtained using a portable sensing device (PSD-FTNIR i16) in wavelength range from 1000 to 2500 nm. Optical gain was set to 4x and resolution windows was 0.02 nm. Spectra data were then recorded as absorbance or Log (1/R) in form of csv and spa extension file formats [9], [24].

2.2 Spectra correction

To obtain more accurate and robust prediction results, spectra data were corrected and enhanced using several algorithms namely mean normalization (MN) and smoothing. Corrected spectra data were used to construct prediction models form SSC and vitamin C determination of intact mango fruit.

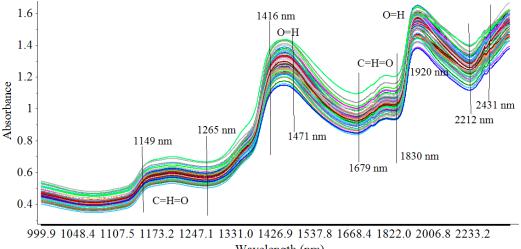
2.3 SSC and vitamin C prediction

Mango quality attributes as SSC and vitamin C were determined by constructing prediction models with partial least square regression (PLSR) approach. Spectra data (X variables) were regressed with actual SSC and vitamin C (Y variables) to obtain more correlated models. To avoid overfittings, 10-fold cross validation was applied during calibration models development and the results is compared. Prediction performances were evaluated by means of several statistical indicators, namely: correlation coefficient (r) between the predicted and actual results, root mean square error (RMSE) in calibration and validation, and also ratio prediction to deviation index (PRD) of the predicted values [25]–[27].

3. Result and discussion

3.1 Spectra feature of intact mango fruits

Typical absorbance spectra data of intact mango fruits is shown in Figure 1. It describes a specific wavebands region of several chemical moleule bonds vibrated due to light radiations. When the incident light in near infrared region penetrates onto mango fruit, some of those light are absorbed, reflected and transmitted.







As shown in Figure 1, C-H-O bands related to soluble solids content were vibrated in wavelength range 1149 - 1265 nm, and 1679 - 1830 nm respectively. Other quality attributes related to C-H-O

molecular structures were aslo to be believed vibrated in those wavelength regions. Water content, which is mostly found on mango and other fruits were vibrated in wavelength range 1416 - 1471 nm, and 1920 nm.

Actual measuements of SSC and vitamin C of mango fruits were determined using stabdard laboratory procedures. For SSC content, the refraction index method was applied and the SSC was expressed as ^oBrix. On the other hand, actual vitamin C was determined using a titration method with the addition of indophenol 2.5 solutions. Descriptive statistics of SCC and vitamnin C composition of mango fruits is presented in Table 1.

Statistical parameters	SSC	Vitamin C	
Mean	13.40	32.21	
Max	20.00	35.66	
Min	9.00	28.93	
Range	11.00	6.73	
Std. Deviation	2.43	1.31	
Variance	5.91	1.71	
Skewness	0.43	0.14	
Kurtosis	-0.03	1.12	
Median	13.00	32.13	
Q1	11.50	31.59	
Q3	15.00	32.74	

SSC: soluble solids content, Q1: first quartile, Q3: third quartile.

All of these spectra data, actual data of SSC and vitamin C were combined and prohected onto the PLSR approach to establish predictionn models used to assess quality attributes. Partial least square regssion was chosen as a regression approach since this method is preferable and commonly used in NIRS applications.

3.2 SSC and vitamin C prediction of intact mango fruits

The main part on NIRS application is to develop prediction models used to determine inner quality parameters of intact mango fruits. First of all the models are constructed to determine SSC content of mango fruit. Raw spectra data withour correction was used as X data variable. Prediction perfromance of SSC using raw spectra dat is shown in Figure 2.

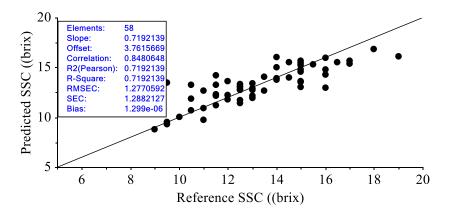


Figure 2. Prediction performance of SSC using raw spectra data.

Obtained result shows that correlation coefficient achieved for SSC prediction of intact mango fruits using raw spectra data is 0.85 and RMSE is 1.27. Moreover, the ratio prediction to deviation (RPD) is 1.91 which is categorized as sufficient performance. Beside using raw spectra data, SSC prediction models were also developed using corrected spectra data by means of mean normalization (MN) and smoothing. Prediction performance of SSC using MN spectra data is presented in Figure 3.

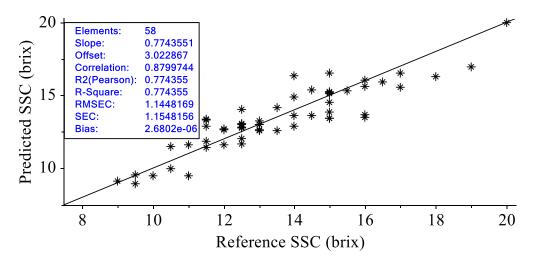


Figure 3. Prediction performance of SSC using MN spectra data.

The prediction performance is better when the model is constructed using corrected spectra. Mean normalization seeks to normalize and compensate spectra data to its average and thus remove some other irrelevant background information. The correlation coefficient is increased to 0.88 whilst prediction error RMSE is reduced to 1.14. Therefore, the RPD index is increased to 2.14 which is categorized as good model performance. Moreover, predictive abilities were also comparable when the model is constructed using smoothing spectra data as presented in Figure 4.

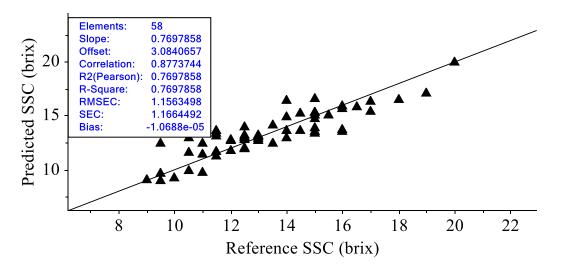


Figure 4. Prediction performance of SSC using Smoothing spectra data.

Based on obtained results, smoothing and MN spectra data clearly improved the prediction performance of SSC on intact mango fruits. Similar findings also noted by other researchers reported

that corrected and enhanced spectra data can improve and generate a better prediction results of several quality attributes on intact horticultural products [17], [28]. Thus, it is strongly recommended to correct and enhance spectra data prior to prediction models development.

Another quality attribute prediction on intact mangos namely vitamin C or sometimes is called as ascorbic acid, was also determined simultaneously by means of those mentioned spectra data. (raw, MN and smoothing). Prediction performance of vitamin C on intact mango fruits by means of raw spectra data is shown in Figure 5.

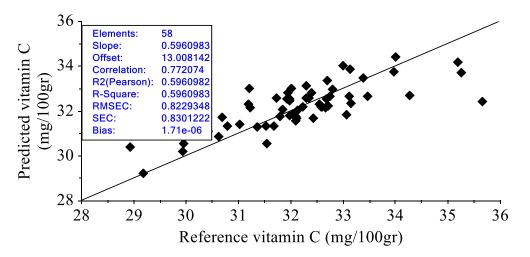


Figure 5. Prediction performance of vitamin C using raw spectra data.

Constructed prediction models achieved a correlation coefficient 0.77 with prediction error RMSE is 0.822 and RPD index is 1.59 which is categorized as sufficient performance. A better predictive results were achieved when the models are developed using enhanced spectra data either with MN or smoothing spectra data. Prediction performance of vitamin C using MN spectra data is presented in Figure 6.

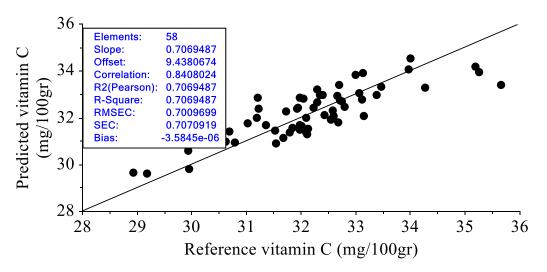


Figure 6. Prediction performance of vitamin C using MN spectra data.

Judging from prediction performance by using MN spectra data, it clearly showed that prediction accuracy and robustness were improved. It seems that irrelevant background information were

eliminated and removed when spectra corrections are employed to the spectra datasets. Based on obtained prediction results, it show that the ability of enhanced spectra data combined with PLSR regression approach can be used to determine vitamin C on intact mango fruits accurately. Prediction performance of smoothing spectra for vitamin C assessment is presented in Figure 7.

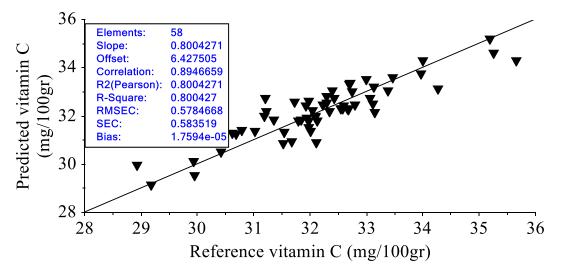


Figure 7. Prediction performance of vitamin C using smoothing spectra data.

The predictive abilities of near infrared spectroscopic model are also improved when it constructed using smoothing data. It achieved 0.89 of correlation coefficient and RPD index is increased to 2.30 which is clustered as good model performance. The summarize of prediction performance using NIRS for SSC and vitamin C assessment on intact mango fruits are presented in Table 2 and Table 3.

Spectrum		Statistical indicators			
	\mathbb{R}^2	r	RMSE	RPD	
Raw	0.72	0.85	1.27	1.92	
MN	0.77	0.88	1.14	2.14	
Smoothing	0.77	0.87	1.15	2.12	

Table 2. Prediction performance for SSC on intact mango fruits using NIR spectra data.

r: correlation coefficient, R^2 : coefficient of determination, RMSE: root mean square error *RPD*: ratio prediction to deviation, MN: mean normalization.

Table 3. Prediction performance for vitamin C on intact mange	fruits using NIR spectra	data.
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Spectrum	Statistical indicators			
	\mathbb{R}^2	r	RMSE	RPD
Raw	0.60	0.77	0.82	1.59
MN	0.71	0.84	0.70	1.87
Smoothing	0.80	0.89	0.57	2.30

r: correlation coefficient, R^2 : coefficient of determination, RMSE: root mean square error *RPD*: ratio prediction to deviation, MN: mean normalization.

Near infrared spectroscopy (NIRS) considered as a non-destructive tool that uses a specific photodiode sensor that is sensitive to light so it does not require sample preparation or hazardous

chemicals, fast and reliable for quantitative and qualitative analysis. NIRS is ideal for rapid identification of raw materials and is also a powerful and robust method for multi-component quantitative analysis. The existence of FT-NIR tools can make it easier to identify the content contained in a raw material such as solids, liquids, gases, powders and syrups. The results obtained have a high degree of accuracy through wavelet transforms and have been tested in the laboratory.

4. Conclusion

Based on achieved prediction results, we may conclude that near infrared spectroscopy is able to be used in assessing quality parameters of intact mango fruits in form of soluble solids content (SSC) and vitamin C. Predictive abilities were improved when the models are constructed using enhanced spectra datasets with maximum achieved correlation coefficient are 0.88 for SSC and 0.87 for vitamin C prediction respectively.

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