Evaluation of sapodilla fruit quality using near-infrared spectroscopy

Kusumiyati [1]*, Syariful Mubarok[1], Jajang Sauman Hamdani [1], Farida [1], Wawan Sutari [1], Yuda Hadiwijaya [2] , Ine Elisa Putri [2] and Tino Mutiarawati [1]

[1]*Lecturer, *[2]*Alumni of Agrotechnology Studies Program, Agriculture Faculty, Padjadjaran University, Jl. Raya Jatinangor km 21 Bandung, West Java, Indonesia-45363. *e-mail: kusumiyati@unpad.ac.id, kusumiyati@yahoo.com*

Abstract

Fruit quality detection using near-infrared spectroscopy is a fast, accurate, and non-destructive method. Hence the fruits can still be marketed after the measurement. The purpose of this study was to analyze the quality of sapodilla fruit using near-infrared spectroscopy. The study was conducted in March to August 2017 at the Plant Production Technology Laboratory of Horticulture Division, Agriculture Faculty of Padjadjaran University, Jatinangor. The method used in this study was multivariate data analysis of chemometrics. The spectra data were obtained using portable near-infrared spectrometer (NirVana AG410, Integrated Spectronics Pty, Ltd, Australia) with wavelength range of 312-1050 nm. Calibration and prediction models were acquired using partial least square (PLS). The results revealed that non-destructive method using near-infrared spectrometer was able to measure sapodilla fruit quality such as, firmness, total dissolved solids, and color values including L^*, a^*, b^*, h^o, and C^*.

Key words: Calibration, prediction, root mean square errors of calibration, sapodilla.

Introduction

Sapodilla (*Achras zapota* L.) is a long-lived tree native to tropical America. It was introduced to the country of Philippines by Spanish. Nowadays, it spreads through some Asian countries especially Southeast Asia and India, moreover now it is found growing throughout warm areas over the world.

Postharvest researchers and producers describe the quality of fruits by certain characteristics such as sugar content, firmness and color [24]. In general, quality assessment of fruit can be performed by visual assessment, tasting the fruit itself or destructive analysis at the laboratory. Visual assessment will not be able to assess the internal quality, while tasting fruit itself and destructive analysis will damage the fruit. Destructive analysis also requires some hazardous chemicals. Hence, this method is calculated to be cost and time-consuming, also requiring materials and laboratory analysis[10, 21].

Near-infrared spectroscopy has been used to predict fruit quality since 1990s [12]. This is an alternative technique that saves time and labor. Near-infrared spectroscopy method can be used to measure the quality of fresh commodities quickly, accurately and environmental friendly [3]. Near-infrared spectrometer record spectra data consists of physical and chemical information from irradiated samples such as total dissolved solids (TDS), firmness, and internal defects [19, 26]. There has been a lot of researches done to predict fruit quality using near-infrared spectroscopy as performed in prune fruit [25], mango [23], fuji apple [17], apricot[7], apple [4, 18] and jujube[27, 28]. This method was also used to detect some fruit-vegetable commodities such as tomato [13, 14] and bitter gourd [15]. Therefore, this work aimed to analyze total dissolved solids (TDS), firmness, and fruit color of sapodilla fruit using near-infrared spectroscopy.

Materials and Methods

Sample collection: Samples of 300 sapodillas cv. Sukatali were all harvested from the orchard, located in Situraja, Sumedang with the same criteria 90 days after flowering. Then, the fruits were brought to the laboratory for further analysis.

Spectra data acquirement: Six separate measurements using the NirVana AG410 spectrometer with wavelength range of 312-1050 nm were taken out of each sapodilla at six point's scaterred along the axial region, with three points located on each side of the fruit (Fig.1). Hence, the total spectral data was 1800 which then be picked for calibration and prediction set. The spectral data were obtained by positioning the near-infrared spectrometer directly on the fruit skin.
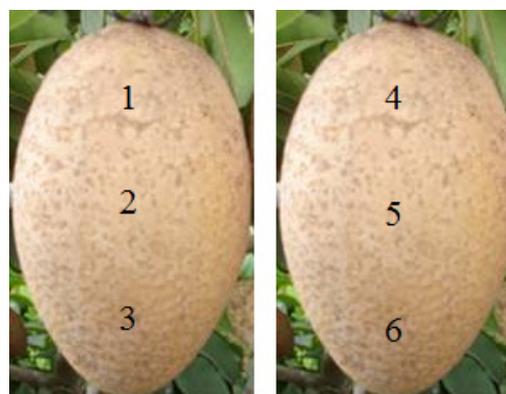

Figure 1. Irradiated points on each side by near-infrared spectrometer.

Effective calibration model was defined by the correlation coefficient (R_{cal}) between predicted and measured values of each observation and root mean square errors of prediction. The effective models were defined by R_{cal} of 0.71 or higher showing rough screening ability, and are preferable for further prediction[31]. Then, the effective calibration models were used to predict the values of another sapodilla fruits (prediction set) in order to test their prediction feasibility. Each model was evaluated according to its accomplishment and prediction accuracy by using the R between values of predicted model and values of measured values (R_{pre}).

Root mean square error of calibration (RMSEC) is the difference in values between predicted value calibration and reference value of calibration set. Root mean square error of prediction (RMSEP) is the difference in values between predicted value prediction and reference value of prediction set. The calculations of RMSEC and RMSEP are described in the following equations [32]:

$$RMSEC = \sqrt{\frac{1}{n_c}\sum_{i=1}^{nc}(\hat{y}i - yi)^2} \quad (1)$$

$$RMSEP = \sqrt{\frac{1}{n_p}\sum_{i=1}^{np}(\hat{y}i - yi)^2} \quad (2)$$

where $\hat{y}i$ = predicted value of the i observation, yi = measured value of the i observation, n^c = number of observations in the calibration set, n^p = number of observations in the prediction set.

Effective model should provide a high correlation coefficient of calibration (R_{cal}) and coefficient of determination (R^2) of prediction and low values of RMSEC and RMSEP, nevertheless both root mean square errors either calibration or prediction should not have a high degree of difference from each other [21].

The RPD is the relationship between standard deviation (SD) of reference data using destructive method to the standard error (SE) in the prediction set [30]. RPD was originally used to assess how well the calibration model was built between the reference value and the predicted value of NIR [29]. RPD value higher than 3 can be used for screening, while RPD values over than 5 are useful for quality control and RPD values greater than 8 are useful for any application [1]. RPD can be used to assess NIR's ability to predict soil properties [6]. The RPD was classified into 3 categories: category A: RPD > 2.0, category B: RPD 1.4 - 2.0, category C: RPD < 1.4. RPD is defined in the following equation:

$$RPD = \frac{SD}{SE} \quad (3)$$

Measurement of firmness: Fruit firmness was determined by using a digital tension gauge (AD-4932A-50N, Taiwan) with measurement range from 0.0 to 50.0 N. Measurement was done by puncturing the fruit at one time. The results were expressed as N (Newton).

Measurement of total dissolved solids: Total dissolved solids were determined with a digital refractometer model PR-101α (alpha) (Atago, Model 41325, Japan) with measurement range from 0.0 to 45.0% Brix. Measurements were obtained using sapodilla fruit extract. The results were expressed as %Brix.

Color measurement: Color is the basis for sorting many products into commercial grades, but concentration of pigments or other specific constituents might provide a better quality index [16]. Color parameters relate directly to consumer assessment of appearance, pigment concentrations are usually more related to maturity levels, and the concentrations of other certain constituent are related to flavour. The color of the object can be illustrated by several color coordinate systems [8, 9, 11, 20]. The most common used notations is the CIE $L^*a^*b^*$ color space (Fig. 2) designed in 1976 to afford more color differences in relation to human perception of color.
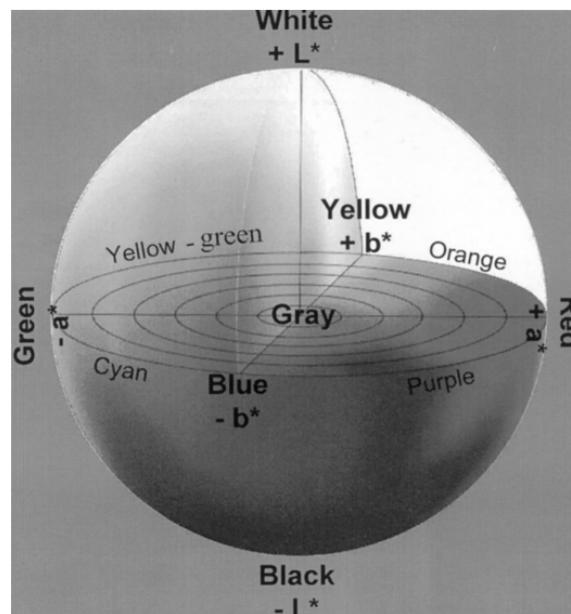

Figure 2. CIE $L^*a^*b^*$ color space [22].

Color is measured in common by chromameters to acquire the value of L^*, a^* and b^* in which the sensors are filtered to respond identically to the human eye. L^* value defines the brightness of the color, where 0 is for black and 100 white. a^* value denotes the type of green - red, where negative a^* is green, and positive a^* is a red color. The b^* describe the blue-yellow type, and the negative b^* is blue, whereas the positive b^* is yellow. Fruit color measurements were carried out from two different sides of the fruit, whereas in each side measured at the top, middle and bottom of the sapodilla fruit. The upper part is the part affixed to the stem of the fruit.

Hue is location around the circumference of circle and chroma is the gap from center. The calculations of Hue (h^0) and Chroma (C^*) are defined in the following equations :

$$h^0 : tg^{-1}\left(\frac{b^*}{a^*}\right) \quad (4)$$

$$C^* : \sqrt{a^{*2} + b^{*2}} \quad (5)$$

Multiple regression analysis: Regression is a statistical measure to predict the value of a variable in relation to other variables through linear regression equation. Those variables are divided into two types called dependent and independent variable. When the regression model contains only one dependent and one independent variable, this model is called simple linear regression. The simple linear regression equation is as follows [22]:

$$Y = \beta_0 + \beta_1 X_1 \quad (6)$$

While Y is dependent variable, X is independent variable, whereas β_0 is called the regression constant (y-intercept), β_1 is coefficient regression of variable X_1 (slope)

Multiple linear regression is a linear regression involving more than one independent variables [22]. The equation of multiple linear regression is as follows:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + ... + \beta_n X_n + \varepsilon \tag{7}$$

where Y is dependent variable, X is the independent variable, β_0 is called the y-intercept and $\beta_1, \beta_2, \beta_n$ are called as slopes and ε is random error.

Results and Discussion

Destructive data analysis on sapodilla: Measured data of sapodilla using destructive method would be used as reference data for the development of calibration model. The quality parameters were firmness, total dissolved solids (TDS) and color including L^*, a^*, b^*, h^0, C^*. The success of value prediction of sapodilla quality using near-infrared spectroscopy was determined by the measured data of destructive method. Destructive data of sapodilla in both calibration and prediction set are presented in Table 1.

Near-infrared data analysis of sapodilla: Data analysis of sapodilla was measured by reflectance and NIR absorbance data using multivariate data analysis with partial least square (PLS). Total samples used were 300 fruits. Each fruit was irradiated by 6 points as illustrated in Fig 1. Therefore, the total spectra data was 1800 which would then be selected for calibration and prediction set. Calibration and prediction models by partial least square (PLS) using near-infrared spectral data of sapodilla fruits are presented in Table 2.

Firmness assessment: In callibration set the firmness assessment used 604 and 600 data for prediction set with wavelength 312-

1050 nm. Correlation coefficient (R_{cal}) for firmness assessment of sapodilla was 0.94 means high (close to 1). This showed that the NIR prediction was close to the measured value using destructive method. The calibration and prediction models of firmness using PLS analysis are visualized in Fig. 3.
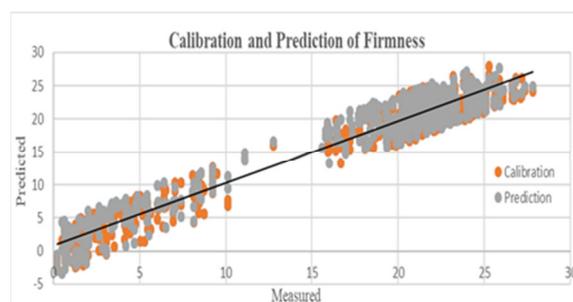

Figure 3. Calibration and prediction models of firmness using PLS analysis.

The root mean square error of calibration (RMSEC) was 1.93. Considering the standard error values in the calibration set, it could be presumed that the calibration model was good due to the error value was close to zero (0). To examine the accuracy of regression equation of calibration set, it is necessary to perform the prediction set.

Prediction set of firmness assessment used different samples and spectra data from the calibration set. The amount data used was 600 both from spectra data and measured data. Correlation coefficient of prediction (R_{pre}) was 0.93 which means the near-infrared prediction was close to the measured data. RPD value for firmness assessment was 3.94.

The level of accuracy in the prediction set based on calibration modellargely determined by the root mean square errors of prediction (RMSEP). Based on the result of the prediction set, it could be examined that the RMSEP generated was 2.04.

Table 1. Measured data of destructive method in calibration and prediction set of sapodilla fruits.

Parameters		Calibration set				Prediction set			
		n	Range	Mean	Standard deviation	n	Range	Mean	Standard deviation
Firmness (N)		604	0.23 – 27.81	16.67	8.25	600	0.23 – 27.81	16.90	8.04
TDS (%Brix)		606	7.5 – 33.8	22.53	4.68	605	10.5 – 32.1	22.01	4.20
Color	L^*	618	31.89 – 66.53	54.88	5.12	601	37.3 – 64.01	55.01	4.67
	a^*	682	-3.88 – 12.72	5.26	3.03	608	-2.25 – 11.34	5.25	2.66
	b^*	687	5.96 – 34.55	23.52	5.46	630	10.22 – 32.78	23.46	5.07
	h^0	641	47.95 – 89.80	75.14	8.58	600	56.30 – 89.47	76.18	7.60
	C^*	602	8.01 – 35.01	23.92	5.15	600	12.48 – 33.34	24.22	4.66

Table 2. Calibration and prediction models by partial least square (PLS) using near-infrared spectral data of sapodilla fruits.

Parameters		R_{cal}	RMSEC	R_{pre}	RMSEP	RPD	Calibration & Prediction	
							R	RMSE
Firmness		0.94	1.93	0.93	2.04	3.94	0.93	1.99
TDS		0.85	1.66	0.78	2.05	2.04	0.81	1.88
	L^*	0.90	1.46	0.91	1.27	3.67	0.90	1.37
	a^*	0.90	0.90	0.90	0.84	3.16	0.90	0.88
Color	b^*	0.91	1.56	0.91	1.48	3.42	0.91	1.52
	h^0	0.92	2.28	0.92	2.02	3.76	0.92	2.16
	C^*	0.91	1.47	0.90	1.33	3.50	0.91	1.40

R_{cal}-correlation coefficient of calibration; RMSEC-root mean square errors of calibration; R_{pre}-correlation coefficient of prediction; RMSEP-root mean square errors of prediction; RPD-ratio performance to deviation; R-coefficient calibration; RMSE-root mean square errors.

Total dissolved solids assessment: Calibration set of the TDS assessment used 606 and 605 data for prediction set. Correlation coefficient of calibration (R_{cal}) and prediction (R_{pre}) for TDS assessment of sapodilla were 0.85 and 0.78, respectively, with the RPD value as 2.04. This result implied that the near-infrared spectroscopy showed the good performance to predict total dissolved solids. The calibration and prediction models of total dissolved solids using PLS analysis are visualized in Fig. 4.
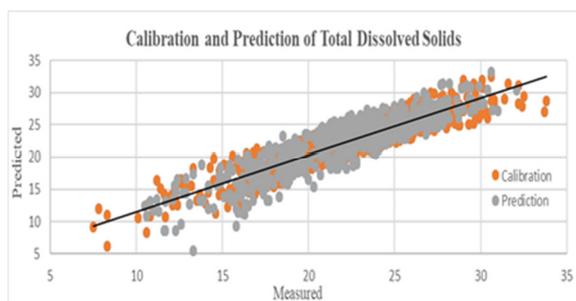

Figure 4. Calibration and prediction models of total dissolved solids using PLS analysis.

RMSEC and RMSEP for both calibration and prediction were 1.66 and 2.05, respectively. Considering the standard error value in calibration and prediction set, it could be assumed that the calibration and prediction models have been built well because the default error value were close to zero (0).

L^* value assessment: The amount of measured and spectra data used for both calibration and prediction set of L^* assessment were 618 and 601, respectively with R_{cal} as 0.90 and R_{pre} as 0.91 which mean close to 1. RMSEC and RMSEP of L* assessment were 1.46 and 1.27, respectively. RPD value was 3.67 which indicated the good performance of near-infrared prediction. The calibration and prediction models of color including L^*, a^*, b^*, h^0, C^* using PLS analysis are visualized in Fig. 5.

a^* value assessment: In calibration set the assessment of a^* used 682 and 608 data for prediction set with wavelength 312-1050 nm which had 0.90 for R_{cal} and also 0.90 for R_{pre}. The root mean square error of calibration (RMSEC) was 0.90. Considering the standard error values at the calibration set, it can be assumed that the calibration regression that has been built was acceptable due to the default error value close to zero (0). To analyze the accuracy of regression equation of calibration it is necessary to perform the prediction set.

The level of accuracy in the prediction set based on calibration model largely determined by the root mean square errors of prediction (RMSEP). Based on the result of the prediction set obtained, it can be examined that the root mean square errors prediction (RMSEP) generated was 0.84.

b^* value assessment: Calibration set of the b^* assessment used 687 spectra data and 630 for prediction set with wavelength 312 - 1050 nm. Correlation coefficient of calibration (R_{cal}) and prediction (R_{pre}) for b^* value assessment were 0.91 and 0.91, respectively, with the RPD value was 3.42, which indicated that the near-infrared prediction was sufficiently good for predicting b^* value of sapodilla.
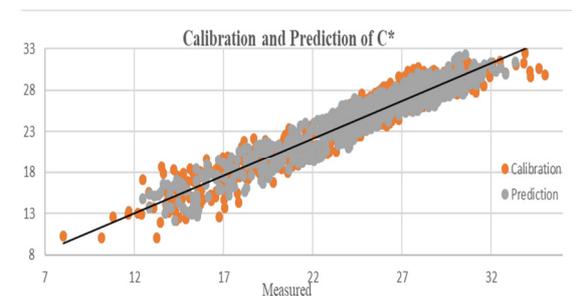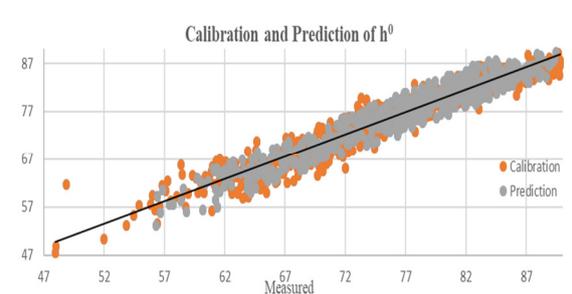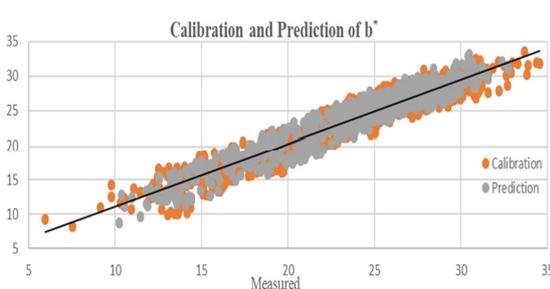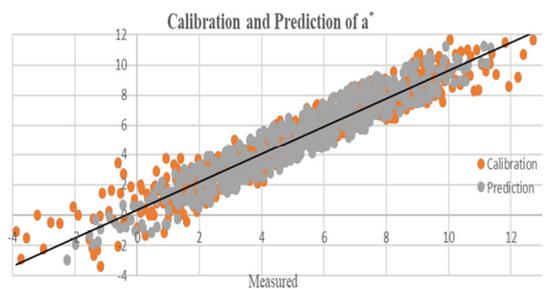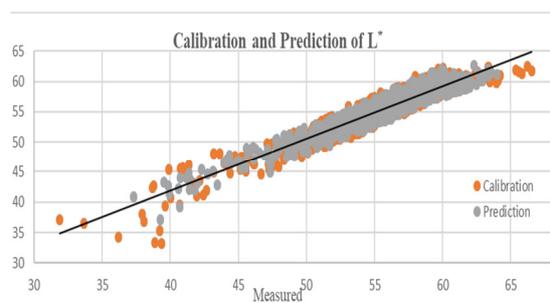

Figure 5. Calibration and prediction models of color including L^*, a^*, b^*, h^0, C^* using PLS analysis.

In calibration set, the root mean square errors of calibration (RMSEC) was 1.56. The root mean square errors prediction (RMSEP) generated was 1.48. Considering the standard error values in the calibration and prediction set, it can be assumed that the calibration model shave been built well due to the default error close to zero (0).

Hue value assessment: The number of measured data and spectra data used for calibration and prediction set of h^0 assessment were 641 and 600, respectively. R_{cal} and R_{pre} of h^0 value assessment were 0.92 and 0.92, respectively, with 3.76 for RPD value which implied the good performance of near-infrared spectroscopy. RMSEC was 2.28 and 2.02 for RMSEP. Considering the RMSEC and RMSEP value, it can be presumed that the calibration and prediction models that have been developed were adequately good due to the default error close to zero (0).

Chroma value assessment: Calibration set of the TDS assessment used 602 and 600 data for prediction set. R_{cal} and R_{pre} for chroma assessment of sapodilla were 0.91 and 0.90, respectively, with the RPD value as 3.50. This result denoted that the near-infrared spectroscopy showed the good performance to predict Chroma value of sapodilla.

Root means square error of calibration and root means square error of prediction were 1.47 and 1.33, respectively. Considering the standard error value in calibration and prediction set, it could be assumed that the calibration and prediction models have been built well because the error value were close to zero (0).

Conclusions

Evaluation of sapodilla quality using near-infrared spectroscopy was able to measure firmness, total dissolved solids and color values with high accuracies and low errors.

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