

PREDICTION OF TOTAL SOLUBLE SOLIDS AND PH IN BANANA USING NEAR INFRARED SPECTROSCOPY

MAIMUNAH MOHD ALI*, RIMFIEL B. JANIUS,
NAZMI MAT NAWI, NORHASHILA HASHIM

Department of Biological and Agricultural Engineering, Faculty of Engineering,
University Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia
*Corresponding Author: maimunah_mohdali@gmail.com

Abstract

The potential application of near infrared (NIR) spectroscopy in the range of wavelength from 1000 to 2500 nm to non-destructively determine total soluble solids (Brix) and pH values of bananas were evaluated. Thirty banana samples were measured at five different maturity stages. Each banana sample was scanned at three different locations (top, middle and bottom). The Brix and pH values were associated with the absorbance spectral data for the model development which were split into prediction and calibration sets. The partial least squares (PLS) model was built based on both data sets of banana samples. The prediction model for the Brix values obtained a coefficient of determination of 0.81 and root means square error of predictions of 3.91 Brix. The prediction model for pH values had an R^2 of 0.69 and RMSEP of 0.36 pH. These findings proposed that near infrared spectroscopy has great potential to predict sugar content in bananas.

Keywords: Non-destructive, Near infrared spectroscopy, pH, Total soluble solids, Banana.

1. Introduction

Banana is one of the edible fruits in terms of consumer's choice and taste across the nation. The yield of the banana export commodity in 2012 achieved the highest statistical record of 16.5 million tons, which is a 7.3 percent increase from 2011 [1]. The rapid development of modern technologies using the non-destructive approach, especially for horticultural products has an implication on the satisfaction on the consumer's level of sugar or sweetness consumption. These alternative approaches are essential as an indicator to replace human assumption

Abbreviations

FAMA	Federal Agricultural Marketing Authority of Malaysia
LV	Latent variable
NIR	Near infrared
PLS	Partial least squares
R^2	Coefficient of determination
RMSEC	Root mean square of calibration
RMSEP	Root mean square of prediction
TSS	Total soluble solids
UV-VIS	Ultraviolet-visible

in the actual measurements. Sweetness, which is determined by sugar content, develops mostly during the ripening stage of the bananas. Delwiche et al. [2] stated that near infrared (NIR) soluble solids content (SSC) calibrations are recommended to NIR calibrations for the evaluation of the fruit's maturity regarding any individual sugars.

NIR spectroscopy is regarded as the most commonly used non-destructive technique in postharvest technology for the food quality of fruits and vegetables [3]. The advance method involving NIR spectroscopy has been evaluated using the portable device and on-line grading/sorting machines in order to determine the internal quality as well as external defects of the fruit [4]. For this reason, the massive demands in yield production and food quality measurements result in the expansion of feasible and real-time machine systems. The replacement of the conventional method is needed since the process is destructive, time-consuming, laborious, and manual loading [5]. Therefore, NIR spectroscopy technologies have been applied to overcome the limitation of the conventional methods without destroying the physicochemical properties in food and agricultural produce.

Various studies have expanded the non-destructive techniques to determine the internal parameters that involve other technologies, such as spectrophotometers, backscattering, and hyperspectral imaging systems. The application of the non-destructive method on fruits and vegetables using NIR spectroscopy is relatively new in Malaysia. NIR spectroscopy is utilized in the analysis of pharmaceutical products, fuels as well as agricultural products. Norris [6] used NIR spectroscopy in agricultural applications to measure moisture in grain for the preliminary study. The method was relatively inexpensive, rapid, non-destructive and was able to measure several components simultaneously.

The ripening process of banana also leads to the changes in the physicochemical, physical, and biochemical properties of the fruit. As a result, the colour of banana skin changes from green to yellow since the fruit ripens during the ripening stages. Subedi and Walsh [7] determined the soluble and insoluble forms of carbohydrates during the ripening process of mangoes and bananas using short-wave near-infrared spectroscopy. Delwiche et al. [2] investigated the reliability of NIR spectroscopy the changes of soluble solids content along with the fructose, glucose, and sucrose concentrations in mangoes. Bertone et al. [8] used NIR models to determine the firmness, starch content, and soluble solids content of apples according to the selected harvest date. The application of predictive modelling by considering the efficiency of non-linear regression models is essential in forecasting the quality changes of various agricultural produce [9, 10].

Many researchers have investigated the principles of near infrared spectroscopy in assessing the internal parameters of horticultural products by using non-destructive techniques. Among the commodities tested in NIR spectroscopy were pears [11], mangoes [2, 12-14], watermelons [15-17], olives [18-20], and bayberry fruit [21]. Apart from that, Subedi and Walsh [7] applied NIR spectroscopy to predict the accuracy of the models of mango and banana, according to its ripening stages. Besides, the principles and applications of NIR were almost similar to mid-infrared and ultraviolet-visible (UV-VIS) execution. However, no effort has been made to evaluate the total soluble solids and pH of banana according to different scanning locations using NIR spectroscopy. Hence, the aim of this study is to determine the ability of near infrared spectroscopy in determining the Brix and pH values of bananas at five different ripening stages obtained by spectroscopic and conventional methods. The prediction models of the fruit quality were also determined to improve the application of NIR spectroscopy as a reliable and rapid method along the fruit ripening process.

2. Material and Method

2.1. Sample preparations

A total of thirty 'Berangan' bananas (*Musa acuminata*) were procured at different ripening stages which vary from ripening stage 3 (unripe) to stage 7 (overripe) which are in accordance with the maturity standard established by the Federal Agricultural Marketing Authority of Malaysia (FAMA). The samples were obtained from Taman Pertanian Universiti (TPU), Universiti Putra Malaysia, Serdang, Selangor and stored at an ambient temperature in the Power and Energy Systems Laboratory for three weeks. As the banana matured, six bananas from each stage were randomly selected for spectroscopic and conventional measurements of Brix and pH values. For each sample, the spectroscopic measurement was taken first, followed immediately by the conventional method.

2.2. Spectral acquisition

Thirty bananas samples were measured using Spectrum 100N FT-NIR spectrometer (Model: PerkinElmer, USA) to acquire absorbance spectra in the range of wavelength from 1000 to 2500 nm. A total of 810 scans which included three scanning locations of the absorbance data, were recorded in this study. The measurement was carried out by placing the sample in a black box (20 cm × 15 cm × 15 cm) to avoid light interruption from the area of surroundings (Fig. 1). The probe was made to touch the banana samples and scanning was done at three different locations, i.e., (top, middle and bottom) to determine the variation between the scanning locations as shown in Fig. 2. The accumulated absorbance spectra data were extracted using Essential FTIR software (version 3.10, build 41, USA) in order to get the conversion of the spectrum. Three replications of each location were averaged and later used for further statistical analysis.

2.3. Total soluble solids (TSS)

Samples of banana (ten grams per sample) were blended with 40 ml of distilled water using a fruit juicer (Model: Philips Juicer HR1871, USA). The TSS values were determined using a digital refractometer (Model: Atago PAL-a Alpha Digital, Tokyo, Japan). The measurement was performed with three replications

to get the average values. The measurement was conducted at room temperature ($\pm 28^{\circ}\text{C}$) after spectral acquisition process.

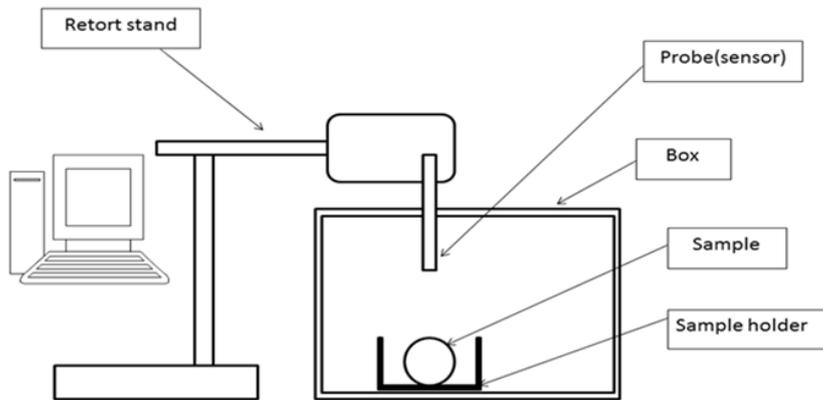


Fig. 1. Schematic diagram of absorbance measurement inside the black box.

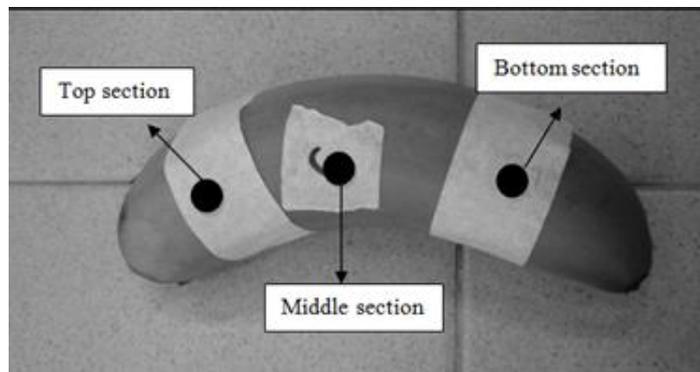


Fig. 2. Three locations for scanning (Top, Middle, Bottom).

2.4. pH

The measurement of pH values was conducted using a digital pH meter (Model: Mettler Toledo FE20, Singapore) with an accuracy range of 0.01. Likewise, the measurement of pH was similar to the Brix measurement. The pH values were determined from the same spots on the banana samples, which were similar to the location of the spectral acquisition execution.

2.5. Data analysis and model development

The absorbance spectral data were analysed by using partial least squares (PLS) in spite of the development of the prediction and calibration models for both Brix and pH values. The pre-processing of the spectrum and the model developments for Brix and pH values were executed using the Unscrambler software (version 9.7, Camo Software AS, Oslo, Norway). The absorbance spectral data of reference versus predicted Brix and pH for the calibration and prediction models were plotted to examine the nature of the absorbance spectral distribution. On the

whole, thirty samples were utilized for the model development of prediction and calibration process.

PLS is a regression model, used for predicting a future value from a measurement. From this, a model is developed based on the number of factors for the purpose of calibration. About 75% of the banana samples were randomly selected for calibrating the NIR models. Meanwhile, the other 25% of the banana samples which consists of the remainders were used for determining the prediction model. The overall range of NIR absorbance spectra was divided into small groups of 100 wavelengths to find the best models for calibration and prediction.

3. Results and Discussion

3.1. Descriptive statistics of banana samples

Table 1 illustrates the statistical details of the samples based on the Brix and pH in the banana, according to its maturity stages. The variation of Brix and pH values increased along the maturity stages. For the pH values, the results show that the banana samples were in the acidic ranges from 5.2 to 6.3. On the other hand, the Brix values increased significantly from 6.5 to 24.1. The trend of increasing Brix and pH values indicated that the higher maturity stage had a high sugar content. The Brix and pH values progressively increased during the maturity stage which showed an obvious increment in the last stage of the ripening process. Meanwhile, the ranges, means and standard deviations of Brix and pH values of the whole banana samples are presented in Table 2.

Table 1. Statistical details of stages used in the data analysis.

Stages	Parameter	Minimum	Maximum	Mean	Standard deviation
3	Brix	6.47	10.60	8.94	1.55
	pH	5.23	5.73	5.50	0.22
4	Brix	6.47	10.30	8.22	1.54
	pH	5.26	6.31	5.52	0.41
5	Brix	15.60	20.37	18.21	1.69
	pH	5.49	5.99	5.80	0.23
6	Brix	16.33	21.93	18.41	2.20
	pH	5.64	6.07	5.91	0.15
7	Brix	15.80	24.10	20.82	3.00
	pH	6.12	6.24	6.17	0.04

Table 2. Statistical details of the samples used in the data analysis.

Parameter	Minimum	Maximum	Mean	Standard deviation
Brix	6.47	24.10	14.92	5.69
pH	5.23	6.31	5.78	0.34

3.2. Spectral acquisition

Absorbance spectral curves in the range from 1000 to 2500 nm for stage 3 until stage 7 show an insignificant trend of curves between the peaks and valleys (Fig.

3). From the findings, the spectral curves have no identical trend and identical patterns regardless of their maturity stages. The graph shows three significant peaks at 1200 nm, 1450 nm, and 1950 nm, which located randomly for different maturity stages. The curves of the spectra were not in order along the maturity stages, even though they were in the same phase. The observed trend according to the maturity stage is not quite uniformly distributed due to the fruit ripening of bananas. For this reason, it can be denoted that the absorbance spectra are not dependent on the maturity stages.

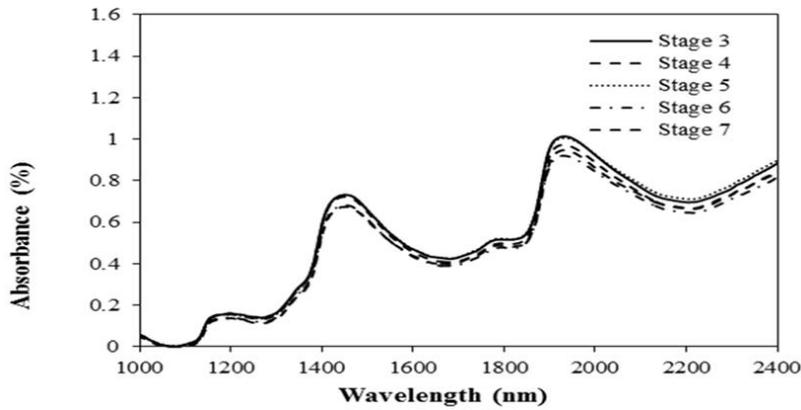


Fig. 3. NIR absorbance spectral curves at five maturity stages.

The spectral curves for three different scanning locations (top, middle and bottom) also illustrate an insignificant trend of curves between the peaks and valleys (Fig. 4). The graph shows three absorbance peaks at 1200 nm, 1450 nm, and 1950 nm. The peaks and valleys of NIR absorbance spectral curves indicated that the correlation between the internal qualities of the bananas and the appropriate wavelengths detected at certain peaks were established. Nevertheless, there are no major differences recorded between the three scanning locations. Although the quality measurement was not performed according to the scanning locations in this study, the variation of spectral data was described to show the differences between each scanning location.

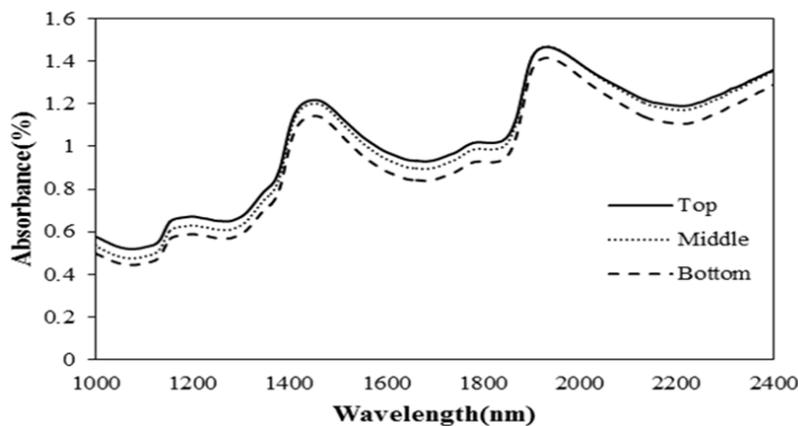


Fig. 4. NIR absorbance spectral curves at three scanning locations.

The development of PLS models was built to calibrate the absorbance spectral data with Brix and pH values in the calibration and prediction sets. Table 3 shows that the accuracy of calibration and prediction models for banana was within the acceptable range with all coefficients of determination (R^2) values above 0.80 excluding the prediction model of pH in banana. Besides, the calibration accuracy obtained R^2 values of 0.98 for Brix and 0.92 for pH. On the contrary, the interpretation of prediction models for Brix was accepted with $R^2 = 0.81$ whereas for pH it was slightly off from the acceptable range with R^2 values of 0.69.

Table 3. PLS model performances of banana for absorbance measurement.

Parameter	LVs	Maximum		Mean	
		R^2	RMSEC	R^2	RMSEP
Brix	10	0.98	1.13	0.81	3.90
pH	10	0.92	0.13	0.69	0.36

*LVs: latent variables; R^2 : coefficient of determination; RMSEC: root mean square error of calibration; RMSEP: root mean square error of prediction

3.3. Total soluble solids (TSS)

The three absorbance spectra were collected from the top, middle and bottom of one banana sample at the scanning distance; 0 cm was averaged. This average spectral data was measured for calibration model aligned with the Brix values of the corresponding banana sample. The interpretations of the calibration and prediction data set for absorbance spectral data are illustrated in Figs. 5 (a) and (b). The value of R^2 was 0.98, whereas the value of RMSEC values was 1.13 % Brix for the values obtained in the calibration model. Meanwhile, the value of R^2 was 0.81 and a high RMSEP value of 3.90 Brix as recorded in the prediction model. Another result ($R^2 = 0.78$) has been reported by Jaiswal et al. [22], which may differ due to variation in sugar content of banana samples after baseline correction and Nawi et al. [23] on sugarcane ($R^2 = 0.88$; RMSEP=1.19 %Brix). Based on the finding, the NIR absorbance spectra data are directly correlated to the Brix of bananas. In this case, the total soluble solids are also associated with the concentration of chemical attributes such as starch of soluble sugars and water content in the fruit tissue. The results showed that the NIR and PLS models were feasible as an alternative approach for predicting the sugar content of bananas.

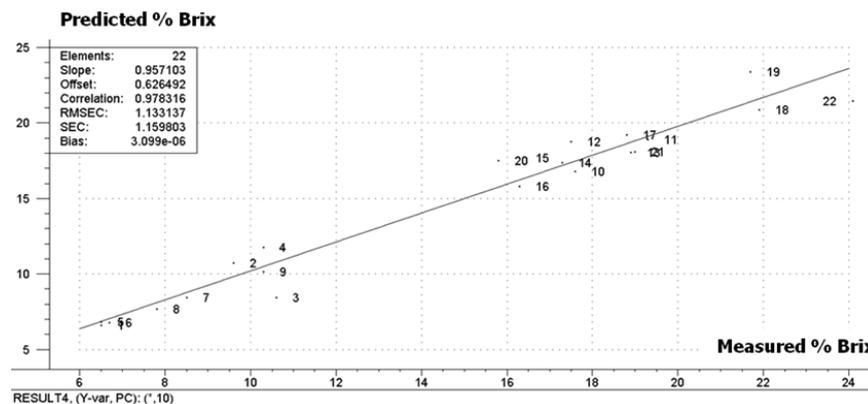


Fig. 5 (a). Calibration model of % Brix for NIR absorbance spectra.

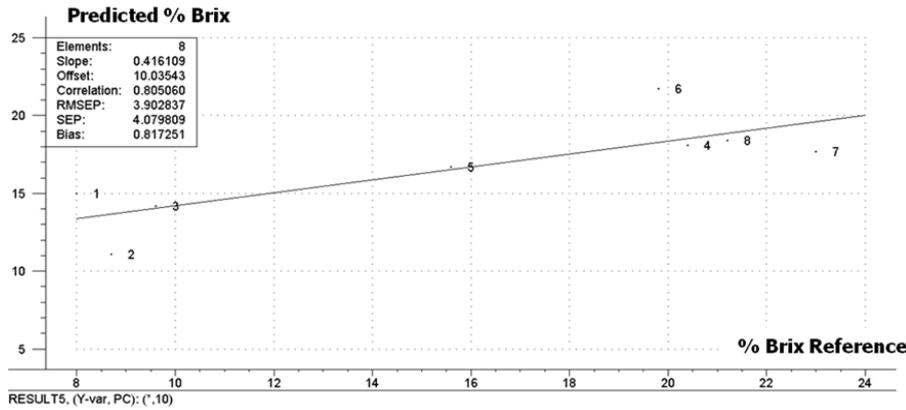


Fig. 5 (b). Prediction model of % Brix for NIR absorbance spectra.

3.4. pH

The interpretation of the PLS models in predicting pH values is demonstrated in Figs. 6 (a) and (b). The value of R^2 was 0.92 and the value of RMSEC was 0.13 pH. On the contrary, the values for the prediction model were $R^2 = 0.69$ and $RMSEP = 0.36$ pH. As a result, these prediction accuracies were lower than the findings stated from the mean of absorbance spectral data for the calibration model. It was also found that the accuracy of the prediction model in this finding ($R^2 = 0.69$) was slightly lower as compared to the results by Jha et al. [24] in predicting the pH of mangoes ($R^2 = 0.50$ pH). The low R^2 value obtained for the pH can be partially related to the chemical properties of the fruit based on the unpredictable changes of the malic and citric acids.

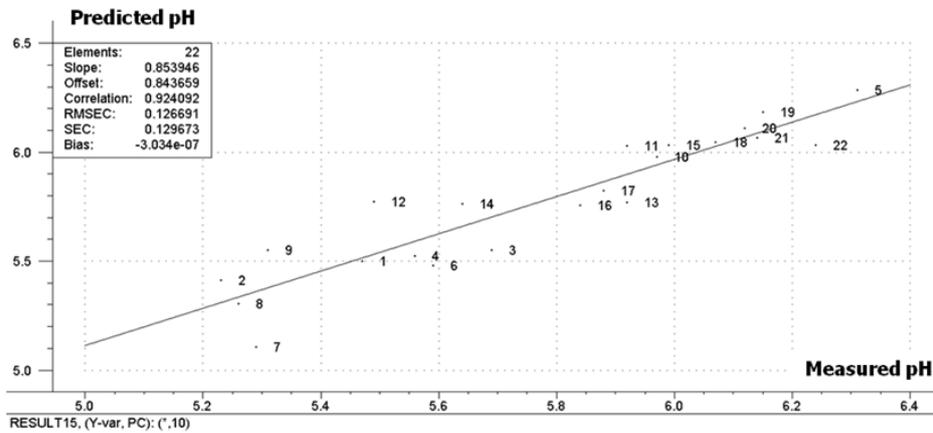


Fig. 6(a). Calibration model of pH for NIR absorbance spectra.

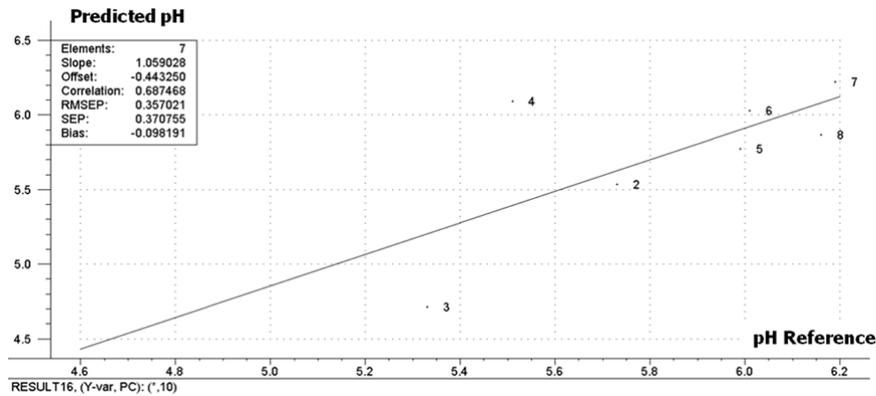


Fig. 6(b). Prediction model of pH for NIR absorbance data.

4. Conclusions

The principle and application of NIR spectroscopy in predicting the Brix and pH values of bananas, at different maturity stages were evaluated in the range from 1000 to 2500 nm. The main conclusions from the present research work can be summarized as follows:

- The PLS models showed a good correlation between the reference and predicted Brix values with the R^2 values of 0.81 and RMSEP values at 3.90.
- For the prediction accuracy of pH values, the absorbance spectra associated with the pH acquired the R^2 values of 0.69 and RMSEP values at 0.36.

These findings suggest that NIR spectroscopy is applicable to non-destructively predict sugar content in bananas. The non-destructive approach used to evaluate fruit quality during maturity stage could overcome the problem of the conventional analysis and avoid postharvest losses. Apart from that, the prediction models are beneficial in developing portable online machine system for sorting/grading process of various agricultural produce. Furthermore, more work is to be done before the proposed methods can be implemented for experimental and non-destructive use.

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