Rapid and non-destructive prediction of mango sweetness and acidity using near infrared spectroscopy

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Abstract: The study aimed on evaluating the feasibility of NIRS to predict sweetness and acidity of intact mango fruit in form of soluble solids content (SSC) and titratable acidity (TA) through calibration modeling. Diffuse reflectance spectra in NIR wavelength range of 1000 – 2500 nm were acquired for a total of 58 mango samples. PCR and PLSR were used to develop SCC or TA prediction models respectively. Multiplicative scatter correction (MSC) and standard normal variate (SNV) were applied to the spectra prior to prediction model development. The result showed that the best model for SSC prediction was achieved when PLSR is applied in combination with SNV spectra (r of calibration = 0.82) and PLSR-MSC for TA prediction (r of calibration = 0.98). These results indicated that NIRS was feasible to predict sweetness and acidity of intact mango fruit and might be considered as one of the rapid and non-destructive method of an automatic sorting and grading system based on imaging technology.

1 Introduction

In last few decades, the application of near infrared reflectance spectroscopy (NIRS) as a non-destructive technique in food and agricultural product industries is gaining more attentions both in term of instrumental design and spectra data analysis. NIRS, covered by definition of spectra wavelength range from 780 to 2500 nm, works based on the principle of electromagnetic radiation interaction with biological objects [Ni07]. It is considered to be suitable for determining the inner quality of foods and agricultural products since this method is characterized by low labour costs, simple sample

preparation, non-destructive, pollution free and high speed of analysis. NIRS also allows several constituents to be evaluated at the same time. Chemometrics is required to extract the information about quality attributes buried on near infrared spectra through a process called multivariate calibration from which a mathematical relationship between NIR spectra and the measured quality parameter will be revealed to determine desired quality attributes [Ni07]. Therefore, the main objective of this study is to develop a multivariate calibration model of NIR spectra to predict sweetness in form of soluble solids content (SSC) and acidity in form of titratable acidity (TA) in intact mango fruit in a non-destructive manner through chemometrics.

2 Methodology

2.1 Spectra acquisition

NIR spectra of intact mangoes were acquired for a total of 58 samples using FT-NIR instrument (Nicolet Antaris, USA). Each fruit in every measurement was hand placed right to the incoming holes (1 cm of diameter) of the light source to ensure direct contact and eliminate noise as shown in Figure 1.

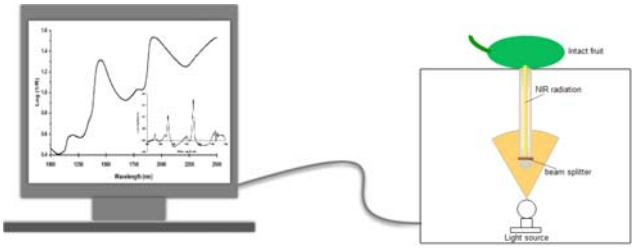

Figure 1: NIR spectra acquisition for one intact mango.

Diffuse reflectance (Log 1/R) spectra in wavelength range of 1000 – 2500 nm were obtained 64 times and averaged. The spectra of each sample were measured in 6 different points and the mean values of these measurements were noted as 'real' spectra.

2.2 Soluble solid content and titratable acidity measurement

After collecting and recording the spectra, each sample fruit was sliced and the pulp was taken. SSC and TA measurement were carried out by making juices from 20 grams of pulp sample and maximum 100 ml distilled water. A little filtered juice was squeezed and dropped into a hand-held analog refractometer (model HRO32, Krüss Optronic GmbH) to record SSC in form of ^{o}Brix whilst automatic titration method (Titroline 96, Schott) with 0.1 N NaOH to an end point of pH 8.1 was used to measure TA expressed in mg·100g^{-1} fresh mass.

2.3 Model calibration and validation

NIR spectra data were analyzed using The Unscrambler® X version 10.1 (CAMO software AS, Oslo-Norway). Principal component analysis (PCA) was firstly applied to the untreated raw spectra in order to explore the spectra in details and detect outliers by subjecting Hotelling T^2 ellipse [C04]. Prior to calibration model development, spectra pre-processing was performed to eliminate noise and spectra scattering. Multiplicative scatter correction (MSC) and standard normal variate transformation (SNV) algorithms were used to correct additive and multiplicative effects in the spectra [LSO10]. Calibration models were established by principal component regression (PCR) and partial least squares regression (PLSR) to predict SSC and TA simultaneously using treated NIR spectra. Full cross validations with ten segments were applied during calibration to quantify model performance in predicting desired quality attributes and prevent over fitting of the prediction model. The performances of the models were evaluated by using the following statistical parameters: the coefficient of determination (R^2), coefficient of correlation (r) between predicted and measured quality attributes, the root mean square error of calibration (RMSEC), root mean square error of cross validation prediction (RMSECV), the difference between RMSEC and RMSECV, and the residual predictive deviation or RPD, defined as the ratio between standard deviation (SD) and RMSECV. The higher the value of RPD the greater probability of the model to predict desired chemical constituent in samples set accurately [JKC06].

3 Results and discussion

Typical diffuse reflectance spectra of intact mango are shown in Figure 2a from which the presence of strong water absorbance bands were observed at around 1460 nm and 1930 nm because of O-H tone combination and first overtone of water.

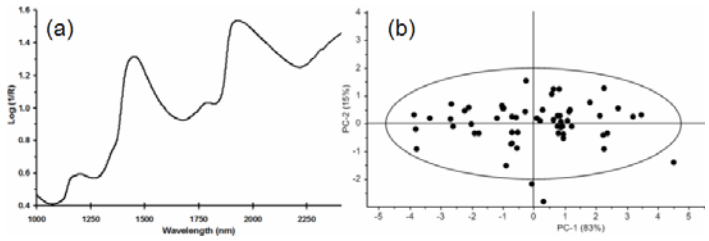

Figure 2: Typical diffuse reflectance spectra of intact mango (a) and PCA with Hotelling T^2 ellipse analysis for outlier detection (b).

Moreover, the absorption bands in the range of 2200 - 2300 nm related to C-H-O structures such as glucose, fructose, vitamin A and C; whilst absorption bands at around 1400, 1800 and 2100 nm are associated with organic acid [CH07]. PCA with Hotelling T^2 ellipse was applied to detect outliers prior to prediction model development (Figure 2b) from which three samples were detected and removed due to their bad influence potential to the model performance.

It was observed that the best model for SSC prediction was achieved when PLSR is applied in combination with SNV spectra, presented in the scatter plot Figure 3a, (r calibration=0.82, RMSECV=1.42 ^{o}Brix and RPD=1.68). On the other hand, PLSR based on MSC spectra calibration model was found to be the best model in predicting TA (r calibration=0.98, RMSECV=26.94 mg·100g^{-1} and RPD=4.73). Scatter plot drawn from this selected model (Figure 3b) indicate that slope of the curve is near to ideal of 45o and imply that predicted TA may be near to measured ones.

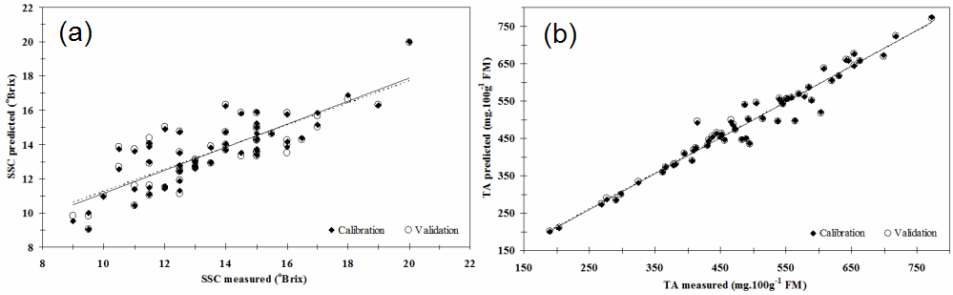

Figure 3: Predicted SSC based on PLSR-SNV model vs. measured SSC (a) and predicted TA based on PLSR-MSC model vs. measured TA (b).

4 Conclusion

In this present study, the feasibility of NIRS for the prediction of sweetness and acidity of intact mango was demonstrated. Thus, NIRS combined with proper multivariate analysis could become an alternative for rapid and non-destructive method for determining inner quality attributes of mango fruit.

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