Quantitative Analysis of Total Soluble Solids and Titratable Acidity of Sweet Tamarind by SW-NIRS

S. Suktanarak and S. Teerachaichayut

***Abstract*—Quality of sweet tamarind ('Prakaytong'variety) must be acceptable as customer needs. Total soluble solids (TSS) and titratable acidity (TA) are important indexes for consideration of quality. Short wavelength near infrared spectroscopy (SW-NIRS) in transmittance mode ranged 665-955 nm was investigated to use for detection of total soluble solids and titratable acidity in sweet tamarind. A set of 209 samples (137 samples for a calibration set and 72 samples for a prediction set) was used for total soluble solids determination. A set of 163 samples (104 samples for a calibration set and 59 samples for a prediction set) was used for titratable acidity determination. Partial least squares regression (PLSR) was used to develop the calibration models. Smoothing (Savitsky–Golay) spectral pretreatment obtained good results of a calibration model for total soluble solids (R=0.90, RMSEC=1.71) and obtained accuracy for screening in the prediction set (R=0.86, RMSEP=1.91). Smoothing (Savitsky–Golay) combined with first derivative spectral pretreatment obtained accepted results for the calibration model for titratable acidity (R=0.87, RMSEC=0.29) and obtained accuracy for screening in the prediction set (R=0.83, RMSEP=0.33). All results indicated that it is possible to use SW-NIRS for nondestructive prediction of total soluble solids and titratable acidity in sweet tamarind.**

***Index Terms*—Sweet tamarind, total soluble solids, titratable acidity, near infrared spectroscopy.**

I. Introduction

Sweet tamarind (Tamarindus indica L.) is one of important fruit in Thailand. It grows in many provinces of Thailand such as Phetchabun, Lampang, Chiangmai, Nakhonratchasima and Ubonratchathani [1]. In between 2007-2011, the export value of sweet tamarind has been increased [2]. However, consumers buy sweet tamarind on the basis of quality using sugar content and acid content as indicators.

In recent years, near infrared spectroscopy has been a nondestructive method to detect qualities in fruits such as mangosteen [3], apple [4] and orange [5]. Advantages of NIRS are nondestructive, fast and reliable. The objective of this work is to study a feasibility of using SW-NIRS for determination of total soluble solids and titratable acidity in sweet tamarind.

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II. Materials and Method

A. Sample

Sweet tamarinds ('Prakaytong' variety) were divided into 2 groups. They were used for total soluble solids analysis and titratable acidity analysis. A set of 209 sweet tamarinds was used for determination of total soluble solids and a set of 179 sweet tamarinds was used for determination of titratable acidity. All samples were purchased from auction market in Thailand. Good appearances of samples were sorted before using in this research.

B. Spectral Acquisition

The short wavelength near infrared spectrophotometer (PureSpect, Saika TIF., Japan) was used for a nondestructive measurement. The SW-NIR spectra were acquired by transmittance mode in the wavelength range 665-955 nm. Scanning was done at the center of seed pods in each sample.

C. Data Analysis

The spectral pretreatments were investigated in order to obtain the best result of calibration. The calibration models were developed using partial least squares regression (PLSR). Statistical analysis was performed by using the Unscrambler (CAMO, Oslo, Norway).

D. Reference Analysis

For total soluble solids determination, 230 samples were divided into 2 sets which were used for the calibration set (137 samples) and the prediction set (72 samples). For titratable acidity determination, 163 samples were divided into 2 sets which were used for the calibration set (104 samples) and the prediction set (59 samples). After spectral measurements, juice was squeezed from sweet tamarind flesh. Total soluble solids content of samples was measured using a digital refractometer (PR101, Palette Series, Atago Co., Ltd., Tokyo, Japan) and titratable acidity was analyzed using auto titrator (METTLER TOLEDO, T50).

III. Result

A. Calibration Model for Total Soluble Solids Determination

Samples were classified into three groups as low total soluble solids (53.3-64.16), medium total soluble solids (65-69.1) and high total soluble solids (70-78.8). The features of averaged original spectra of sweet tamarinds based on total soluble solids were shown in Fig. 1 a). Due to sweet tamarinds contained with a hard stone in each pod, the noise occurred in spectra. Spectral pretreatment using smoothing (Savitsky–Golay) was applied and obtained the features of

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averaged smoothing spectra as shown in Fig. 1 b).

TABLE I: STATISTICAL CHARACTERISTICS OF SAMPLES IN THE CALIBRATION SET AND PREDICTION SET FOR TOTAL SOLUBLE SOLIDS DETERMINATION

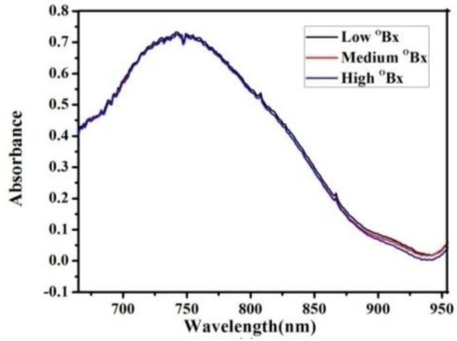
Items	Calibration set	Prediction set
Number of sample	137	72
Range	53.3-78.3	57.5-77.8
Mean	67.69	68.02
Standard deviation	4.0	3.85
Unit	°Brix	°Brix
Wavelength	665-955 nm	665-955 nm

In Table I, it showed the standard deviation of total soluble solids of samples is quite similar in the calibration and prediction set. As well as, a range of total soluble solids in the prediction set were in the range of the calibration set. Spectra pretreatments were investigated as shown in Table II. It showed that smoothing (Savitsky–Golay, 3-point fit) spectral pretreatment obtained the best result (R=0.74, RMSEP = 2.77). Therefore, smoothing (Savitsky–Golay, 3-point fit) spectral pretreatment was used for establishment a calibration model for total soluble solids in this study. In Table 3, the calibration model for total soluble solids was developed and cross-validated (R=0.90, RMSEC=1.71) while results of prediction in the prediction set obtained good accuracy (R=0.86, RMSEP=1.91). The scatter plots between actual total soluble solids and predicted total soluble solids in the calibration set and the prediction set were shown in Fig. 2 (a) and Fig. 2 (b), respectively.

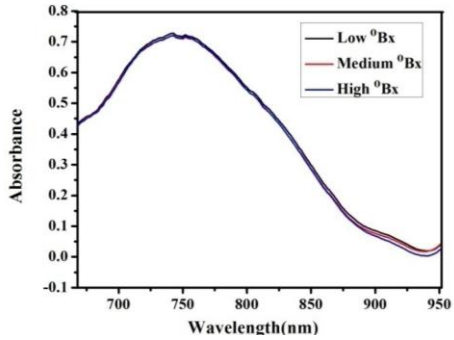
TABLE II: STATISTICAL RESULTS OF VARIOUS SPECTRAL PRETREATMENTS

Spectral Pretreatments	F	N	RMSEP	R
Original	13	137	2.85	0.72
Smoothing	15	137	2.77	0.74
1st derivative	12	137	2.92	0.71
2nd derivative	16	137	3.21	0.66
MSC	11	137	2.88	0.71
Mean	13	137	2.85	0.72
SNV	12	137	2.87	0.72
Smooth + 1st derivative	11	137	2.99	0.68
Smooth + 2nd derivative	17	137	3.05	0.69
MSC + Smoothing + 1st derivative	12	137	2.93	0.70
MSC + Smoothing + 2nd derivative	13	137	3.06	0.66
mean + Smoothing + 1st derivative	11	137	2.00	0.68
mean + Smoothing + 2nd derivative	17	137	3.05	0.69
SNV+ Smooth + 1st derivative	13	137	2.94	0.71
SNV+ Smooth + 2nd derivative	12	137	3.09	0.64

F = Factors
N = number of sample
Smoothing = Savitzky-Golay smoothing
1st derivative = Savitzky-Golay first derivative
2nd derivative = Savitzky-Golay second derivative
MSC = multiplicative scatter correction pretreatment
Mean = mean center
SNV = standard normal variate transformation



a). Original spectra.



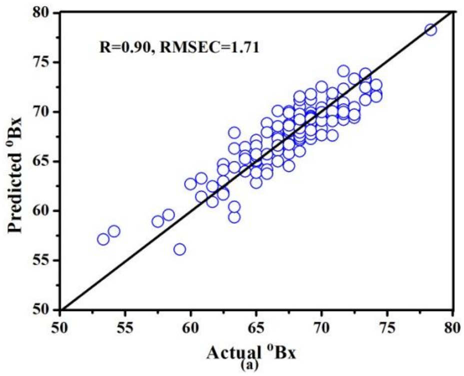
b). Smoothing spectra .

Fig. 1. Averaged spectra of sample with different total soluble solids.

TABLE III: RESULTS OF THE PLSR MODEL FOR TOTAL SOLUBLE SOLIDS DETERMINATION IN THE CALIBRATION SET AND PREDICTION SET

Items	Calibration set	Prediction set
Pretreatment	Smoothing	Smoothing
F	15	15
N	137	72
R	0.90	0.86
RMSEC/RMSEP	1.71	1.91

F = Factors
N= number of sample
R= coefficients of correlation
RMSEC= root mean square error calibration
RMSEP= root mean square error prediction



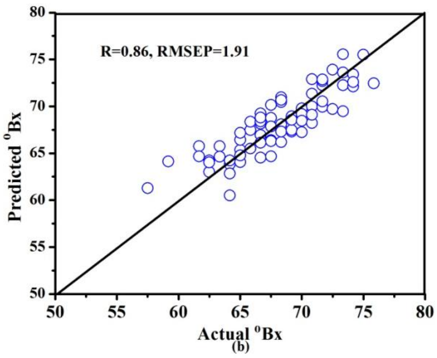


Fig. 2. Scattered plots of actual total soluble solids and predicted total soluble solids: (a) Calibration set (b) Prediction set.

B. Calibration Model for Titratable Acidity Determination

TABLE IV: STATISTICAL CHARACTERISTICS OF CALIBRATION SET AND PREDICTION SET FOR TITRATABLE ACIDITY DETERMINATION

Items	Calibration set	Prediction set
Number of sample	104	58
Range	0.26-3.59	0.27-3.44
Mean	2.12	2.09
Standard deviation	0.61	0.62
Unit	%TA	%TA
Wavelength	665-955 nm	665-955 nm

In Table VI, the statistical characteristics of the calibration set and the prediction set were used for titratable acidity determination in this study. Averaged original spectra of sweet tamarind groups having different titratable acidity (0.26-2.09 for a group of low titratable acidity, 2.10-2.57 for a group of medium titratable acidity and 2.61-3.59 for a group of high titratable acidity) were shown in Fig. 3.

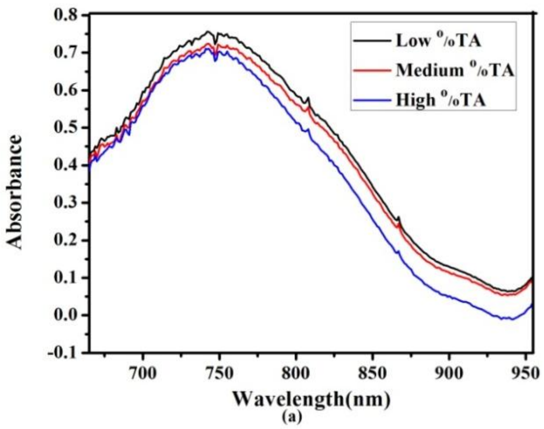


Fig. 3. Averaged original spectra of samples with different titratable acidity.

TABLE V: STATISTICAL RESULTS OF VARIOUS SPECTRAL PRETREATMENTS

Spectral Pretreatments	F	N	RMSEP	R
Original	6	104	0.44	0.69
Smoothing	3	104	0.43	0.62
1st derivative	14	104	0.44	0.71
2nd derivative	3	104	0.48	0.62
MSC	12	104	0.45	0.69
Mean	6	104	0.44	0.69
SNV	6	104	0.48	0.63
Smooth + 1st derivative	5	104	0.43	0.71
Smooth + 2nd derivative	4	104	0.49	0.60
MSC + Smoothing + 1st derivative	4	104	0.47	0.64
MSC + Smoothing + 2nd derivative	4	104	0.49	0.60
mean + Smoothing + 1st derivative	5	104	0.47	0.65
mean + Smoothing + 2nd derivative	4	104	0.49	0.60
SNV+ Smooth + 1st derivative	6	104	0.50	0.62
SNV+ Smooth + 2nd derivative	4	104	0.48	0.62

F = Factors
N= number of sample
Smoothing = Savitzky-Golay smoothing
1st derivative = Savitzky-Golay first derivative
2nd derivative = Savitzky-Golay second derivative
MSC = multiplicative scatter correction pretreatment
Mean = mean centerresult
SNV = standard normal variate transformation

Table V showed spectral pretreatment using smoothing combined with first derivative obtained the best result (R=0.71, RMSEP=0.43). Therefore, smoothing and first derivative spectral pretreatments were used to develop the calibration model for titratable acidity in this study. In Table 6, the calibration model for titratable acidity was cross-validated (R=0.87, RMSSEC=0.29) and used for determination of titratable acidity in the prediction set (R=0.83, RMSEP=0.33). The scatter plots between actual titratable acidity and predicted titratable acidity in the calibration set and the prediction set were shown in Fig. 4 (a) and Fig. 4 (b), respectively.

TABLE VI: RESULTS OF THE PLSR MODEL FOR TITRATABLE ACIDITY DETERMINATION IN THE CALIBRATION SET AND PREDICTION SET

Items	Calibration set	Prediction set
Pretreatment	Smoothing+ first derivative	Smoothing+ first derivative
F	5	5
N	104	59
R	0.87	0.83
RMSEC/RMSEP	0.29	0.33

F = Factors
N= number of sample
R= coefficients of correlation
RMSEC= root mean square error calibration
RMSEP= root mean square error prediction

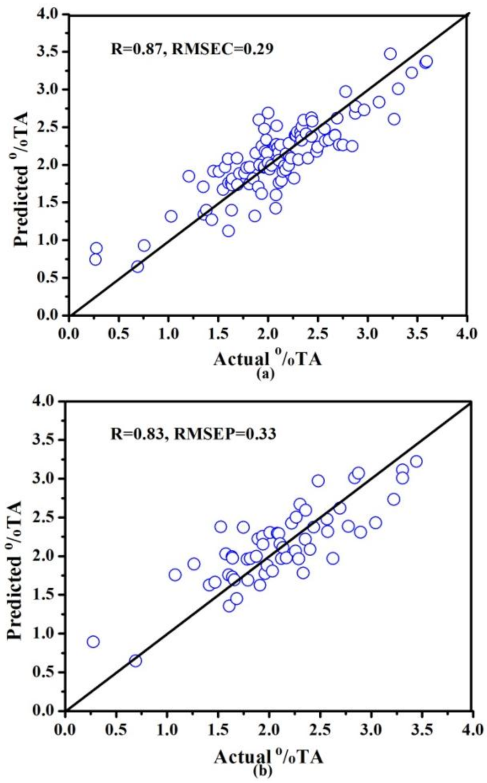


Fig. 4. Scattered plots of actual tritrable acidity and predicted tritrable acidity: (a) Calibration set (b) Prediction set.

IV. CONCLUSION

In this study, the results indicated that spectral pretreatments were required for calibration models. SW-NIRS is possible to use as a non-destructive technique for prediction of total soluble solids and titratable acidity of intact sweet tamarind.

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