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Calibration Model of %Titratable Acidity (Citric Acid) for Intact Tomato by Transmittance SW-NIR Spectroscopy

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***Abstract*—**The acidity (citric acid) is the one of chemical content that can be refer to the internal quality and it's a maturity index of tomato, The titratable acidity (%TA) can be predicted by a non-destructive method prediction by using the transmittance short wavelength (SW-NIR) spectroscopy in the wavelength range between 665-955 nm. The set of 167 tomato samples divided into groups of 117 tomatoes sample for training set and 50 tomatoes sample for test set were used to establish the calibration model to predict and measure %TA by partial least squares regression (PLSR) technique. The spectra were pretreated with MSC pretreatment and it gave the optimal result for calibration model as (R = 0.92, RMSEC = 0.03%) and this model obtained high accuracy result to use for %TA prediction in test set as (R = 0.81, RMSEP = 0.05%). From the result of prediction in test set shown that the transmittance SW-NIR spectroscopy technique can be used for a non-destructive method for %TA prediction of tomato.

***Keywords*—**Tomato, quality, prediction, transmittance, titratable acidity, citric acid.

I. Introduction

THE tomato (*Lycopersicon esculentum*) as in Fig. 1 is an important vegetable that grown worldwide and it is the second most consumed vegetable in the world, after the potato [1] in manufactory for food industry. Sorting of quality for tomatoes can be based on an external appearances such as size, color, maturity, and freshness etc. These are a visual inspection of tomatoes. The quality of finished products was related to the qualities of raw material [2]. On the other hand, the internal quality of tomato or an invisual inspection such as soluble solid content (SSC) and Titratable Acidity (TA) in this case is citric acid; it cannot be identified by visualization. The percentage of Titratable Acidity (%TA) measurement must be measured by a destructive method to access the values of it example manual titration method by individual tomato samples and it's a slow method to access the value and measurement and it has to be a destructive methods also. A destructive method is only used to access a few samples from a given batch of tomatoes [3] so the Transmittance SW-NIR Spectroscopy that it is a non-destructive method is interesting and suitable to use for identification and measure the percentage of Titratable Acidity as citric acid. From the previous studies, the NIR spectroscopy were used to determine the brix (^{o}Brix) value of intact apple, pear and persimmons fruits [4], to measure the durian sweetness/ripening examination [5], to evaluate of the taste quality for apple fruit [6], to analyze the quantitative contents of blueberry [7], to measure of Brix content in dragon fruit [8], to access to the soluble solid of sweet corn [9] and to evaluate of sugar concentration for sugarcane process [10]. In addition, the NIR spectroscopy non-destructive methods were used in pharmaceutical process, wood, fabric polymer process and Chemometrics, so this non-destructive method measured by using a Transmittance SW-NIR Spectroscopy technique can be used to predict and require the value of the percentage of titratable acidity (citric acid) of tomatoes as the aim of this study.

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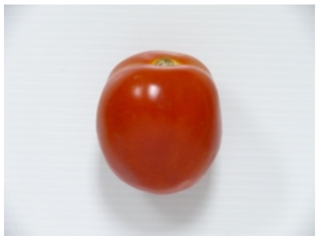

Fig. 1 The tomato that used in this research

II. Materials and Methods

A. Sample

A set of 167 fresh tomatoes were purchased from a local market in Thailand. All of samples were selected and chosen nearby size, color, maturity freshness and appearances.

B. Spectra Acquisition

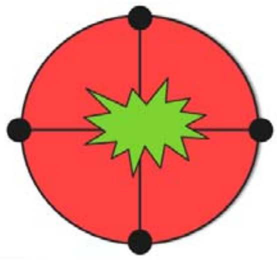

Fig. 2 The point of 4 positions for tomato scanning

The acquirement for spectra of tomatoes by each sample of tomato was scanned at 4 positions at equatorial points, at 90° interval, shown in Fig. 2 by using the Transmittance SW-NIR spectrophotometer (PureSpect, Saika TIF., Japan) in the wavelength range of 665-955 nm.

Each tomato was blended and filtered to obtain the tomato juice and measured the value of % Titratable Acidity by using an automatic titrator (METTLER TOLEDO T50) as Fig. 3 from 5 ml. tomato juice of each tomato was used for titration with 50 ml. of distilled water and 0.1N of sodium hydroxide (NaOH). The TA value was appeared in percentage.

Fig. 3 Citric acid titrator (METTLER TOLEDO T50)

C. Data Analysis

A set of 167 tomatoes for Titratable Acidity analysis, a set of 117 tomatoes were used for the training set and a set of 50 tomatoes were used for the test set. The average spectrum for each sample was calculated from the 4 individual measurements. The correlation coefficient (R) and the root mean squared error of calibration (RMSEC) were used to choose for the best of calibration model for spectral pretreatment in training set.

For the evaluation of prediction, the values of The correlation coefficient (R) and the root mean squared error of prediction (RMSEP) were considered and The Unscrambler program (CAMO, Oslo, Norway) was used for statistical analysis in this study.

III. Results and Discussion

The average original absorbance of SW-NIR spectra of samples in each group as a high, medium and low level of %TA were compared and shown in the Fig. 4 and it can conclude that the percentages of %TA content were related to the absorbance, the higher %TA was appeared in the higher of the absorbance and followed by the medium level and low level of %TA respectively. The description of tomato samples in training set and test set were shown in Table I. From this Table, training set that was built for equation and model creating contains a set of 117 tomatoes that has the minimum and maximum %TA in the set, the range of %TA between 0.29 to 0.62%.

The test set was built for equation testing, the prediction model contains a set of 50 tomatoes and shows the range of %TA between 0.31 to 0.60%, the value of %TA content for the test set must not be lower and exceed to the minimum and maximum value of %TA content in the training set.

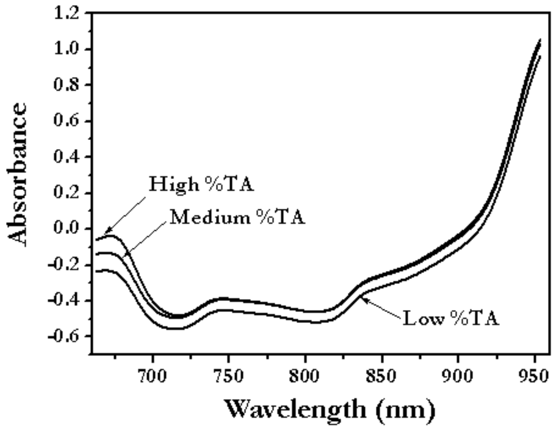

Fig. 4 The average original absorbance spectra in the different levels of %TA

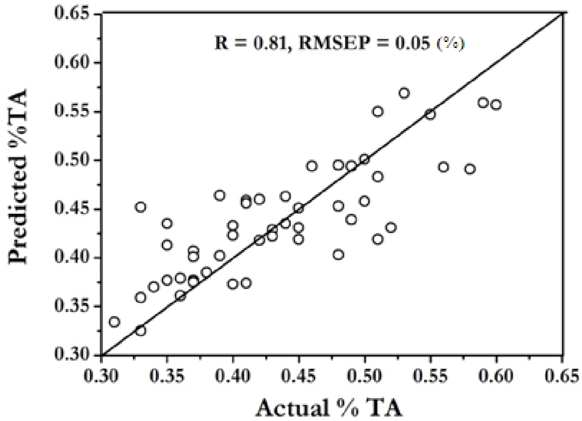

Fig.5 The scattered plots between an actual and predicted value of %TA in test set

Table II, shows the results of %TA content of tomato classification obtained for the training set from PLSR models generated using different spectral pretreatment conditions. Each spectral pretreatment gave the difference the value of the correlation coefficient (R). From the Table III was shown the result of partial least squares regression (PLSR) for %TA of tomato prediction and it can investigated that the MSC spectral pretreatment obtained the optimal result as the correlation coefficient is (R = 0.92) and the root mean square standard error of calibration is (RMSEC = 0.03%) and after that this calibration model was used for %TA content prediction in the test set, from the result in the Table III can conclude that, the model it can use to predict and obtained the good prediction result as in the test set as the correlation coefficient is (R = 0.81) and the root mean square standard error of prediction is (RMSEP = 0.05%).

TABLE I
THE DESCRIPTION AND CHARACTERISTIC OF TOMATO SAMPLES IN TRAINING SET AND TEST SET

Sample set	N	Unit	Range	Mean	SD
Training	117	%	0.29-0.62	0.44	0.08
Test	50	°%	0.31-0.60	0.44	0.08

TABLE II
THE PLSR RESULTS FOR THE CLASSIFICATION OF SAMPLES IN THE TRAINING SET AND TEST SET USING MULTIPLE MODELS

	Training set			Test set	
Spectral pretreatment	N	Factor	R	N	R
Original	117	14	0.92	50	0.78
Smoothing	117	14	0.89	50	0.73
Median	117	14	0.91	50	0.73
Moving Average	117	14	0.89	50	0.70
MSC	117	13	0.92	50	0.81
SNV	117	14	0.92	50	0.79
Center & Scale	117	14	0.92	50	0.78
1st derivative	117	5	0.79	50	0.68
2nd derivative	117	5	0.84	50	0.68
Smoothing + 1st derivative	117	11	0.89	50	0.72
Smoothing + 2nd derivative	117	5	0.82	50	0.70
SNV + 1st derivative	117	8	0.88	50	0.76
SNV + 2nd derivative	117	5	0.83	50	0.67
MSC + 1st derivative	117	8	0.89	50	0.32
MSC + 2nd derivative	117	5	0.83	50	0.67
SNV + Med + 1st derivative	117	8	0.86	50	0.70
SNV + Med + 2nd derivative	117	3	0.82	50	0.69
MSC + Med + 1st derivative	117	8	0.86	50	0.20
MSC + Med + 2nd derivative	117	3	0.82	50	0.71
SNV + Smoothing + 1st derivative	117	11	0.91	50	0.74
SNV + Smoothing + 2nd derivative	117	5	0.82	50	0.71
Mean + Smoothing	117	14	0.88	50	0.71

TABLE III
THE PLSR RESULT OF %TA PREDICTION FOR TOMATOES

	Training set				Test set		
Spectral pretreatment	N	Factor	R	RMSEC	N	R	RMSEP
MSC	117	13	0.92	0.03	50	0.81	0.05

The relationship between an actual value and predicted value of %TA for tomato samples that it was predicted by calibration model in test set was scattered and shown in Fig. 5.

V. CONCLUSION

In this study, the absorbance spectra that pretreated by MSC spectra pretreatment can be used to be the calibration model of % TA prediction of tomato. The model obtained the good and rather accurate results for %TA prediction as R=0.81, therefore from this study it can conclude that the transmittance SW-NIR spectroscopy can be a non-destructive technique to predict and evaluate the chemical value as %TA of tomato. This calibration model can be improved and possibly apply in the sorting line process of tomato for manufactory in the future.

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REFERENCES

[1] J. Chen, M.A. Arnold and G.W. Small, "Comparison of Combination and First Overtone Spectral Regions for Near-Infrared Calibration Models for Glucose and Other Biomolecules in Aqueous Solutions", *Analytical Chemistry*, 2004; 76: 5405-5413.

[2] S. Teerachaichayut, K. Petcharaporn and S. Suktanarak, "Calibration Model of Soluble Solid Content for Intant Tomato by Transmittance SW-NIR Spectroscopy" *The 3rd Asian Near-Infrared Symposium*, Bangkok, Thailand, May 14-18, p.120-121(2012).

[3] K. Flores, M.T. Sanchez, D.P. Marin and J.E. Guerrero, "Feasibility in NIRS Instruments for Predicting Internal Quality in Intact Tomato", *Journal of Food Engineering*, 2009; 91: 311-318.

[4] P. Jannok, S. Ratree, K. Uchida and S Kawano, "Development of a universal NIR calibration model for determining the brix value of intact apple, pear and persimmon fruits", *The 3rd Asian Near-Infrared Symposium*, Bangkok, Thailand, May 14-18, p.50-51(2012).

[5] C. Bangweak, O. Jitham and J. Phumprasert, "Durian sweetness/ripening examination by non-destructive technique: NIRS", *The 3rd Asian Near-Infrared Symposium*, Bangkok, Thailand, May 14-18, p.54-55(2012).
[6] J. Y. Chen, Y. Miao, J. Ma, H. Inoue and H. Zhang "Nondestructive evaluation of the Taste Quality for Apple Fruit Using Near Infrared Spectroscopy", *The 3rd Asian Near-Infrared Symposium*, Bangkok, Thailand, May 14-18, p.134-135(2012).
[7] K. Mitsuki, N. Yoshimura, M. Takayanagi, H. Hoshino and I. Ogiwara "Quantitative Analysis of Contents of Blueberry by Near Infrared Spectroscopy", *The 3rd Asian Near-Infrared Symposium*, Bangkok, Thailand, May 14-18, p.158-159(2012).
[8] W. Thanapase, A. Janhiran and S. Kasemsumran. "Nondestructive Measurement of Brix in Dragon Fruit by Transmittance Mode and Interactance Mode NIR Instrument", *The 3rd Asian Near-Infrared Symposium*, Bangkok, Thailand, May 14-18, p.172-173(2012).
[9] P. Noimanee, D. Boonyakiat and P. Theanjumpol, "Assessment of Soluble Solid of Sweet Corn Using NIR Technique", *The 3rd Asian Near-Infrared Symposium*, Bangkok, Thailand, May 14-18, p.188-189(2012).
[10] E. Taira, Y. Miyahira, M. Ueno and K. Saengprachatanarug, "Rapid Evaluation of Sugar Concentration Using NIR for Sugarcane Process control", *The 3rd Asian Near-Infrared Symposium*, Bangkok, Thailand, May 14-18, p.204-205(2012).