Nondestructive Determination of Quality Management in Table Grapes using Near Infrared Spectroscopy (NIRS) Technique

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***Abstract*—Near infrared spectroscopy (NIRS) is a potential technique for nondestructive fruit quality management. The qualities of table grapes (*Vitis vinifera*) as soluble solid content (SSC), pH-value, titratable acidity (TA), firmness and seedlessness are the key parameters for consumer decision. This research was focused on using NIRS for quality management in table grapes as nondestructive determination. The sample spectra were acquired by NIR spectrometer (NIRSystem 6500) on interactance mode with fiber optic probe in wavelength range of 800-1,100 nm. To develop the calibration model, the relationship between NIR spectral data and all measured properties of table grapes were studied using Partial Least Square Regression (PLSR). The results showed the best models were the positive determination in Savitzky-Golay derivative 2nd of TSS, seedlessness and TA. There were coefficient of determination (R^2) of 0.980, 0.903 and 0.897, and standard error of calibration (SEC) of 0.430, 0.262 and 0.062, respectively. The full cross validation was analyzed, the standard error of cross validation (SECV) of 0.522, 0.570 and 0.103, and bias of -0.00272, 0.00205 and-0.00279, respectively. The R^2_{cal} and SEC of pH value of 0.632 and 0.352, and firmness of 0.661 and 0.685, respectively. Therefore, NIRS technique can be an efficiency nondestructive determination for quality management of table grapes in these key parameters.**

***Index Terms*—Nondestructive determination, Quality management, NIRS, Table grapes**

I. Introduction

Table grape (*Vitis vinifera*) is one of the most largely consumed fruits concerning with nice looking and good taste. The key quality parameters of table grapes are soluble solid content (SSC), titratable acid (TA) and pH-value [1]. The conventional methods for determination of grape quality are sample destruction, time consuming, complicated preparing and expensive.

Near infrared spectroscopy (NIRS) is a potential technique for nondestructive fruit quality management. It can evaluate the internal starch, soluble solids content, oil content, water content, dry matter content, acidity, firmness, stiffness factor and other physiological properties of fruit and vegetable products as citrus [2], mango [3], passion fruit [4] and paddy rice [5]. Chemometrics is developed to create the calibration and validation model from NIRS technique for quality management of fruit products. NIRS is a rapid and nondestructive technique requiring minimal sample process before analysis and coupled with chemometrics method it appears to be one of the most convenient and straight forward analytical tools for studying fruit quality and ripeness [6].

Good correlations were found between each of the physio-chemical indices and the spectra information. Coefficients of determination of TA were equal to 0.95 and 0.82 for white and red/black grapes, respectively whereas the relative values for SSC were 0.94 and 0.93 and for pH-value 0.80 and 0.90. Spectra information was not correlated with the sensory data [7]. The wine grape samples were determinate by NIRS (900-1,700 nm.). Their R^2 and SEP, respectively were 0.99 and 1.37%brix for sugar concentration, 0.98 and 3.88 g/L. for TA and 0.94 and 0.12 for pH-value. The obtained results present a good potential for a fast and reasonably inexpensive screening of these parameters in intact grapes [8]. NIRS is also capable to provide useful information about wine grape phytosanitary status. Quantitative analysis as Partial Least Square-Discriminant Analysis (PLS-DA) was applied on grape spectra in order to test the

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performance of Visible/NIR spectroscopy to classify healthy and infected bunches. The results obtained from PLS-DA models, in cross-validation, gave positive predictive values of classification between 89.8-91.1 % [9].

The aim of this study is to develop the nondestructive determination method for a rapid evaluation in table grapes for quality management by using NIRS technique.

II. Procedures

A. Sample preparing

The 'White Malaga' table grapes at Monsoon Valleys vineyard, Hua Hin, Prachub kirikhan, Thailand was prepared for both seedless and seeded grapes by Gibberellic acid applications (GA3). The 120 intact berries were collected for this experiment.

B. Materials and Methods

Interactance Spectra were collected using NIR spectrometer (FOSS NIRSystem 6500, Silver Spring, MD, USA) with fiber optic probe in wavelength range of 800-1,100 nm. with the resolution 2 nm. as in Fig. 1. For chemical analysis, reference data of each sample were obtained for SSC by refractometer (Atago, PAL-1, Tokyo, Japan), pH-value and TA by Automatic titrator (TitroLine, Camlab Co.Ltd., Cambridge, United Kingdom). The physical analysis as firmness was obtained by texture analysis (TA XT plus, Massachusetts, USA) and seedlessness by cutting & counting. Then, the chemometric was be analyzed. To develop the calibration and validation models, the relationship between NIRS data and all measured properties of table grapes samples were studied using Partial Least Square Regression (PLSR) with full cross validation by Unscrambler software v.10.5 (CAMO, Oslo, Norway).

Figure 1. NIR spectrometer (FOSS NIRSystem 6500)

Moreover, in this study, the model's efficiency was determined by the following static values Coefficient of Determination (R^2), Standard Error of Calibration (SEC), Standard Error of Cross Validation (SECV) which are defined in the following equations:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - x_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} \quad (1)$$

$$SEC, SECV = \sqrt{\frac{\sum_{i=1}^{n_p}(x_i - y_i)^2}{n_p - 1}} \quad (2)$$

III. Results and Discussion

A. Raw Spectra

In Fig. 2 are shown the 120 raw interactance spectra of homogenized samples of 'White Malaga' table grape berries. The whole dataset which used to select the best pre-treatments for each quality parameter. The 5 pre-treatments which were developed are Original, the first Savitzky-Golay derivative, the second Savitzky-Golay derivative, Multiplicative Scatter Correction (MSC) and Orthogonal Signal Correction (OSC).

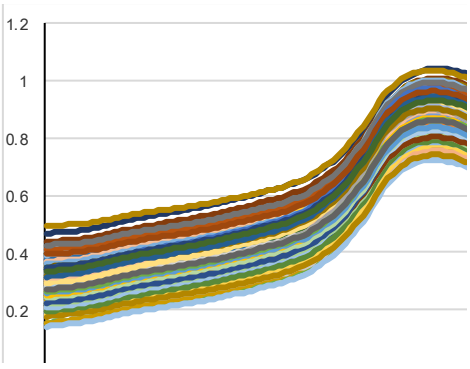


Figure 2. Interactance Spectra (Raw spectra) of homogenized samples of 'White Malaga' table grapes berries (800-1,100 nm)

B. Chemometric Analysis

Chemometric analyze all spectra by Unscrambler software and remove outlier 5% out of sample group. Then, based on the highest R^2 and lowest SEC and factor, the second Savitzky-Golay derivative was the best transformation for all pre-treatments. TSS, seedlessness and TA show the best performance and their coefficient of determination (R^2) of 0.980, 0.903 and 0.897, and

standard error of calibration (SEC) of 0.430, 0.262 and 0.062, respectively. The full cross validation was analyzed, the standard error of cross validation (SECV) of 0.522, 0.570 and 0.103 and bias of -0.00272, 0.00205 and -0.00279, respectively. The R^2_{cal} and SEC of pH value of 0.632 and 0.352, and firmness of 0.661 and 0.685, respectively as in Fig. 3 and Table I.

TABLE I. INTERACTANCE SPECTRA OF 'WHITE MALAGA' TABLE GRAPE BERRIES ON WAVELENGTH 800-1,100 NM.

			No. of Calibration	Factor	CAL				VAL			
					SEC	R^2	R	Bias	SECV	R^2	R	Bias
1	TA(%)	Original	114	7	0.090	0.778	0.882	-0.000001	0.097	0.743	0.860	0.000405
		Derivative1	114	6	0.087	0.794	0.891	0.000000	0.095	0.756	0.867	-0.000260
		Derivative2	114	5	0.062	0.897	0.947	0.000000	0.103	0.716	0.846	-0.002794
		MSC	114	7	0.084	0.803	0.896	-0.000001	0.092	0.769	0.875	-0.000906
		OSC	114	6	0.124	0.584	0.764	0.000000	0.133	0.527	0.721	0.000804
2	pH	Original	106	6	0.479	0.297	0.545	0.000001	0.517	0.196	0.439	-0.003448
		Derivative1	106	7	0.356	0.611	0.781	0.000000	0.417	0.476	0.688	0.002922
		Derivative2	106	2	0.352	0.632	0.795	0.000000	0.395	0.547	0.734	0.000111
		MSC	106	7	0.444	0.396	0.629	-0.000001	0.492	0.272	0.519	0.000024
		OSC	106	7	0.469	0.341	0.584	0.000186	0.527	0.182	0.437	-0.001023
3	SSC(%)	Original	114	7	0.449	0.977	0.989	0.000013	0.493	0.973	0.986	-0.003792
		Derivative1	114	5	0.408	0.981	0.991	0.000000	0.447	0.978	0.989	-0.002806
		Derivative2	114	3	0.430	0.980	0.990	0.000000	0.522	0.971	0.985	-0.002717
		MSC	113	6	0.397	0.983	0.991	0.000025	0.427	0.981	0.990	-0.002062
		OSC	114	6	1.484	0.763	0.874	-0.000677	1.625	0.721	0.847	-0.015813
4	Firmness(N.)	Original	114	6	0.829	0.526	0.725	-0.000481	0.900	0.452	0.668	0.006356
		Derivative1	114	5	0.827	0.523	0.723	0.000000	0.902	0.442	0.661	0.004964
		Derivative2	114	3	0.685	0.661	0.813	0.000000	0.872	0.460	0.678	0.006405
		MSC	114	5	0.837	0.517	0.719	0.000000	0.889	0.465	0.677	0.003307
		OSC	114	5	0.901	0.407	0.638	0.000093	0.955	0.345	0.581	0.003544
5	No. of seed	Original	114	3	0.550	0.574	0.758	0.000000	0.570	0.551	0.738	0.002053
		Derivative1	114	4	0.540	0.590	0.768	0.000000	0.574	0.544	0.733	0.003724
		Derivative2	114	7	0.262	0.903	0.951	0.000000	0.570	0.551	0.751	0.002046
		MSC	114	1	0.593	0.518	0.720	-0.000001	0.605	0.507	0.706	0.002476
		OSC	114	1	0.678	0.354	0.595	-0.000015	0.694	0.335	0.569	0.003160

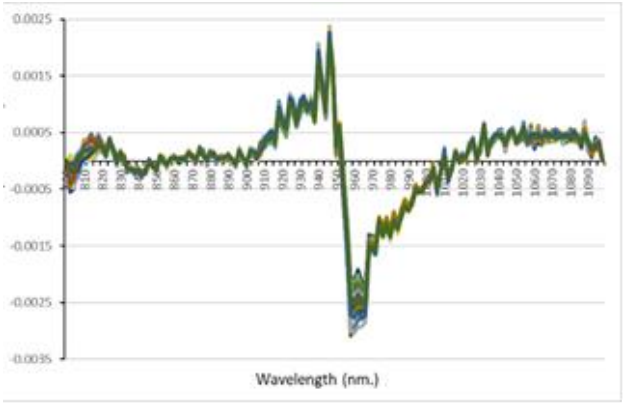
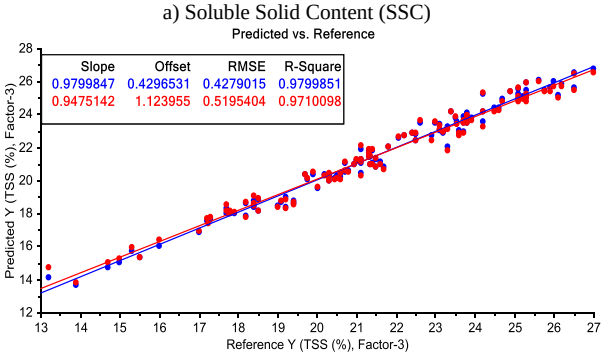


Figure 3. Interactance Spectra (Savitzky-Golay derivative2) of homogenized samples of 'White Malaga' table grapes berries (800-1,100 nm.)

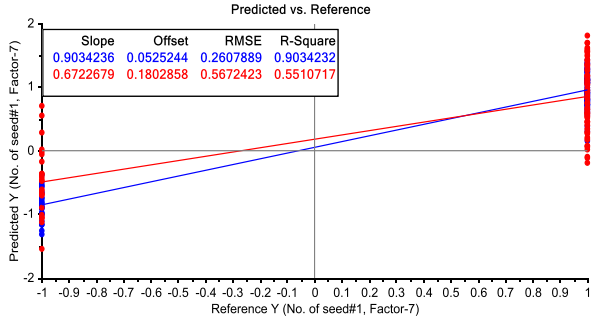
Model for predicting SSC presented a very satisfactory performance, with a calibration values of R^2_{cal}, RMSEC and $slope_{cal}$ of 0.980, 0.428, and 0.980, while the validation values of R^2_{val}, RMSECV and $slope_{val}$ of 0.971, 0.520, and 0.948, respectively. The prediction model of seedlessness, with a calibration values of R^2_{cal}, RMSEC, and $slope_{cal}$ of 0.903, 0.261, and 0.903, while the validation values of R^2_{val}, RMSECV and $slope_{val}$ of 0.551, 0.567, and 0.672 respectively. The prediction model of TA, with a calibration values of R^2_{cal}, RMSEC and $slope_{cal}$ of 0.897, 0.061, and 0.897 while the validation values of R^2_{val}, RMSECV and $slope_{val}$ of 0.716, 0.103, and 0.765 respectively as in Fig. 4.

The prediction model of pH-value and firmness were presented acceptable performance. The pH-value has the calibration values of R^2_{cal}, RMSEC and $slope_{cal}$ of 0.632, 0.350 and 0.632, while the validation values of R^2_{val}, RMSECV and $slope_{val}$ of 0.547, 0.393, and 0.557 respectively. The firmness has the calibration values of R^2_{cal}, RMSEC and $slope_{cal}$ of 0.661, 0.682 and 0.661, while the validation values of R^2_{val}, RMSECV and $slope_{val}$ of 0.460, 0.868, and 0.523 respectively as in Fig. 5.

a) Soluble Solid Content (SSC)



b) Seedlessness



c) Titratable Acid (TA)

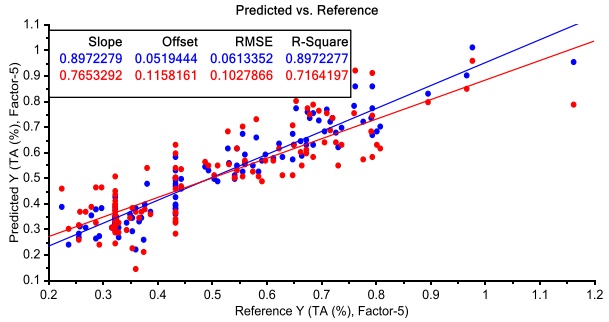


Figure 4. Performance of linear regression model of prediction by optimal pre-treatment. (blue is Calibration and red is Validation)

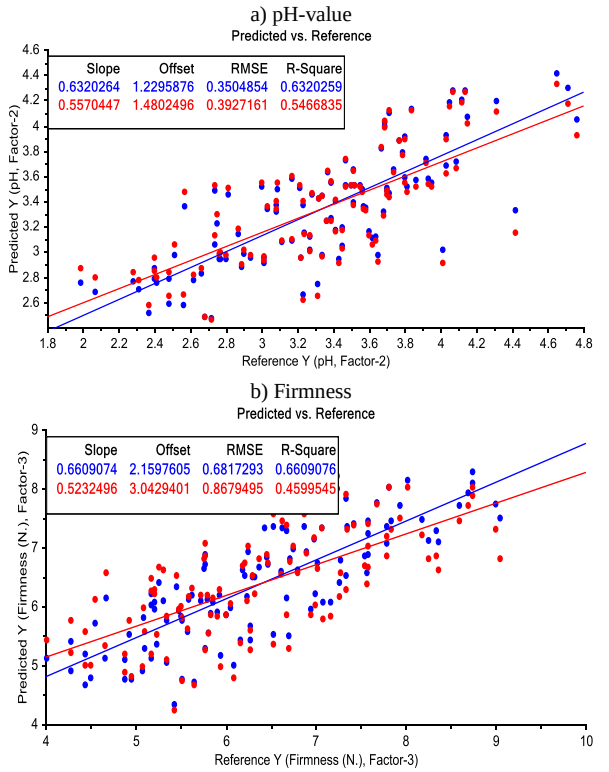


Figure 5. Performance of linear regression model of prediction by pre-treatment. (blue is Calibration and red is Validation)

C. Loading Weight

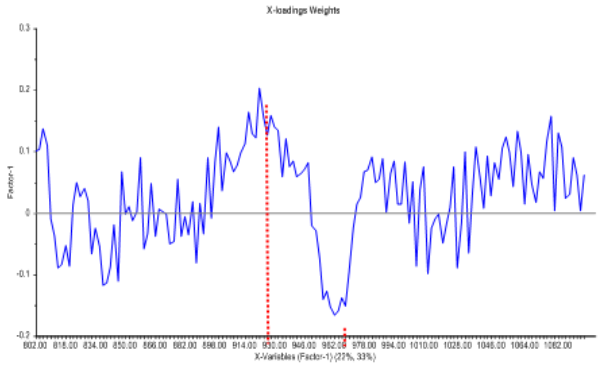


Figure 6. The loading graph of seedlessness of table grape between wavelength 800-1,100 nm

The peak loading of seedlessness by Savitzky-Golay derivative2 are as 922 and 962 nm. which should be the best absorption as in Fig. 6. The main reason should be concerning with organic substances of table grape seed which mostly are cellulose and phenolic compounds. These substances can mostly absorb NIRS on these wavelengths [10]. Therefore, we can do this nondestructive determination of table grape seedlessness by this technique.

IV. Conclusion

The results of this study confirm the efficiency of using NIRS technique in table grapes. The interactance mode of wavelength 800-1,100 nm. is well suited for evaluating the internal quality parameters. Good prediction models were achieved for SSC, seedlessness and TA, and promising results were also obtained for pH-value and firmness, which may be further modified and improved. This technique should be suitable for nondestructive determination in the vineyard for farmer decision about quality management and harvesting in near future.

Acknowledgment

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References

[1] F. Piazzolla, M. Amodio, and G. Colelli, "Spectra evolution over on-vine holding of Italia table grapes: prediction of maturity and discrimination for harvest times using a Vis-NIR hyperspectral device," *Journal of Agricultural Engineering*, vol. 639, pp. 109-116, 2017.

[2] A. Gomez, Y. He, and G. Pereira, "Non-destructive measurement of acidity, soluble solids and firmness of Satsuma mandarin using Vis/NIR-spectroscopy techniques," *Journal Food Engineering*, vol. 77, pp. 313-319, 2006.

[3] S. Saranwong, J. Sornsrivichai, and S. Kawano, "Prediction of ripe-stage eating quality of mango fruit from its harvest quality measured nondestructively by near infrared spectroscopy," *Postharvest Biology Technology*, vol. 31, pp. 137-145, 2004.

[4] P. Maniwara, K. Nakano, D. Boonyakiat, S. Ohashi, M. Hiroi, and T. Tohyama, "The use of visible and near infrared spectroscopy for evaluating passion fruit postharvest quality," *Journal of Food Engineering*, vol. 143, pp. 33-43, 2014.

[5] P. Siriphollakul, S. Kanlayanarat, R. Rittiron, J. Wanitchang, T. Suwonsichon, P. Boonyaritthongchai, and K. Nakano, "Pasting properties by near-infrared reflectance analysis of whole grain paddy rice samples," *Journal of Innovative Optical Health Sciences*, vol. 8, no. 6, p. 8, 2015.

[6] R. Guidetti, R. Beghi, and L. Bodria, "Evaluation of grape quality parameters by a simple Vis/NIR system," *American Society of Agricultural and Biological Engineers*, vol. 53, no. 2, pp. 477-484, 2010.

[7] A. Baiano, C. Terracone, G. Peri, and R. Romaniello, "Application of hyperspectral imaging for prediction of physio-chemical and sensory characteristics of table grapes," *Computers and Electronics in Agriculture*, vol. 87, pp. 142-151, 2012.

[8] J. Bueno, J. Hernandez-Hierro, F. Rodriquez-Pulido, and F. Heredia, "Determination of technological maturity of grapes and total phenolic compounds of grape skins in red and white cultivars during ripening by near infrared hyperspectral image: A

preliminary approach," *Food Chemistry*, vol. 152, pp. 586-591, 2014.
[9] V. Giovenzana, R. Beghi, L. Brancadoro, and R. Guidetti, "Classification of wine grape based on different phytosanitary status by using Vis/NIR spectroscopy," *Chemical Engineering Transactions*, vol. 58, pp. 331-336, 2017.
[10] F. Rodriguez-Pulido, D.F. Bardin, S. Da-Wen, G. Belen, G. M. Lourdes, and H. Francisco, "Grape seed characterization by NIR hyperspectral imaging," *Postharvest Biology and technology*, vol. 76, pp. 74-82, 2013.

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1. H. Nuredin, K. Chaorai, L. Visooth, W. Jim, and R. John, "Detection of grapevine viruses in wine grape vineyards in Thailand and India," in *Proc. 3th International Symposium on Tropical Wine*, Chiangmai, Thailand, 2011, p. 11.
2. B. Peter, K. Chaorai, M. Inge, and P. Alain, "Development of ochratoxin a during Robusta (coffea canephora) coffee cherry drying," *Journal of Agricultural and Food Chemistry*, vol. 48, pp. 1358-1362, 2000.