APPLICATION OF VIS–NIR HYPERSPECTRAL IMAGING FOR PREDICTION OF FLAVONOIDS, ANTHOCYANINS AND SOLUBLE SOLIDS CONTENT IN TABLE GRAPES

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Introduction

Grapes are one of the most spread fruits in the world as fresh fruit, wine, grape juice and raisins. According to the International Organization of Vine and Wine statistics, approximately 42% of world grape production is used as fresh fruit (OIV, 2018). A great number of studies have shown that the ripening indices such as the changes in skin color, softening, titratable acidity, soluble solids content and flavonoids compounds are traditionally used to select the right commercial ripeness time. Furthermore, color is considered as one of the most important physical properties of agro-food products and it plays a fundamental role in the assessment of external quality in food industries (Abdullah et al., 2001). However, these quality attributes change during postharvest storage and thus influence the hedonistic and nutritional value of table grapes. In this context, it may be important to evaluate the content of these secondary metabolites in grapes. Nevertheless, conventional techniques and methods are normally sample-destructive, induce laborious sample preparation steps, are time-consuming, and generate chemical waste, thereby limiting their utility in online/in-line quality monitoring. Recently, the research has focused on the development of non-destructive techniques suitable to increase the samples analyzed and the number of determinations for each single sample, thus providing real-time information of fruits physiological evolution and a most robust statistical data analysis (Costa et al., 2009). Hyperspectral imaging (HSI) has been widely used in food analysis, and it has showed great potential in the grape industry. This technique provides a new detection method that integrates imaging and spectral techniques into a single system (Cen et al., 2014), simultaneously providing information on spectral response values and spatial location for each pixel in the hyperspectral image. This paper reports on the application of hyperspectral imaging technique for predicting the soluble solid content (SSC), total anthocyanins (TA) and total flavonoids (TF) of different table grape cultivars.

Materials and Methods

2.1. Samples

Three white table grapes (Sugarone Superior Seedless, Thompson Seedless and Victoria) and four red/black table grapes (Sable Seedless, Alphonse Lavallée, Lival and Black Magic) were purchased from local fruit markets at commercial harvest ripeness.

2.2. Collecting spectral data

The hyperspectral images were firstly corrected with a white (W) and a dark (D) reference. The samples were separated from the background as the regions of interest (ROIs) to reduce redundancy. In total, 350 average spectra representing all the tested berries were recorded.

2.3. Determination of chemical reference

Each berry was weighed, manually peeled and the juice was collected separately. SSC was measured by a portable refractometer. TA and TF were quantified as reported by Fracassetti et al. (2017).

2.4. Spectral data analysis and building the calibration models

The partial least squares (PLS) analysis between one attribute (TA, TF, and SSC) and the spectral data was conducted using XLStat software 2019. The input spectra were preprocessed using Standard Normal Variate (SNV); 1st derivative and 2nd derivative methods. To reduce the probability of an over fitting of the experimental data, PLS models with 1-25 latent factors were fitted, and the model with a number of PLS factors that maximized the coefficient of determination (R^2_{cal}) for the calibration and minimized the root mean square error of calibration ($RMSE_{Cal}$) was selected. An external validation set (116 berries), were used to calculate the root mean square error of prediction ($RMSE_{val}$), the coefficient of determination (R^2_{val}), the Range Error Ratio (RER), and the Ratio Performance Deviation (RPD) of the PLS predictive models.

Results and Discussion

The PLSR method was applied to build the predictive model for the total anthocyanin and flavonoids and soluble solid content of table grape with the raw pretreated spectral data, covering the wavelength range of 400–1000 nm. The optimal number of latent factors corresponded to the minimal root mean square error (RMSE) that ensured good generalization of the predictive model. **Table 1** shows the statistical data of the predicted results with different spectral pre-treatments using the PLSR model. The best performance using the PLSR predictive model for TF, TA and SSC was obtained after SNV pre-treatment. The predictive model PLSR+SNV provides the highest determination coefficient and the lowest minimum root mean square error in both calibration and validation sets for the quality attributes evaluated. The number of latent factors (LVs) to predict TF, TA, and SSC were fifteen, four, and twenty factors, respectively.

Attribute	Data pretreatment	No. LVs	Calibration		Validation			
			R^2_{cal}	$RMSE_{cal}$	R^2_{val}	$RMSE_{val}$	RER	RPD
TF	PLSR+1st DER	12	0.9604	109.5	0.9387	137.6	17.7	4.1
TF	**PLSR+SNV**	**15**	**0.9642**	**107.5**	**0.9512**	**123.0**	**19.8**	**4.5**
TF	PLSR+2nd DER	5	0.9298	147.0	0.9188	158.9	15.4	3.5
TA	PLSR+1st DER	5	0.9370	56.5	0.9246	62.4	15.5	3.5
TA	**PLSR+SNV**	**4**	**0.9492**	**49.9**	**0.9493**	**52.7**	**18.3**	**4.2**
TA	PLSR+2nd DER	4	0.9168	63.8	0.8942	74.6	13.0	3.0
SSC	PLSR+1st DER	12	0.9732	0.657	0.9351	0.99	16.5	3.9
SSC	**PLSR+SNV**	**20**	**0.9796**	**0.584**	**0.9482**	**0.90**	**18.2**	**4.3**
SSC	PLSR+2nd DER	15	0.9769	0.614	0.9071	1.19	13.8	3.3

Table 1. *Performance of PLS models and data pretreatments. TF: total flavonoids; TA: total anthocyanins; SSC: soluble solid content; RMSE: root mean square error; RER: range error ratio; RPD: ratio performance deviation.*

Table 1 shows that the model was very accurate for predicting TF content with R^2 of 0.964 and 0.951 for training and validation sets, respectively. The RMSE was 107.5 and123 for calibration and validation sets, respectively. TA was predicted with R^2 of 0.949 and RMSE of 49.9 for the calibration set. The accuracy of the model in the validation set for predicting TA was with R^2 of 0.949 and RMSE of 52.7. The SSC was predicted with R^2 of 0.979 and RMSE of 0.58 for the calibration set and R^2 of 0.948 and RMSE of 0.90 resulted from the validation sets. It is obvious for the three attributes of that study that the validation tests gave similar results as the calibration set indicating good performance of the models for predicting these quality components nondestructively. Furthermore, the PLSR + SNV predictive model for TF, TA and SSC shows the highest values of RPD (4.5, 4.2 and 4.3 for TF, TA and SSC respectively) and RER (19.8, 18.3 and 18.2 for TF, TA and SSC respectively) indices. The RPD is defined as the ratio of the standard deviation of the validation set samples divided by the $RMSE_{val}$. When the RPD is equal to one then the $RMSE_{val}$ is equal to the standard deviation of the reference data meaning that the model is not predicting the reference values. Higher values (greater than 2.5) for the RPD suggest increasingly accurate models (Petisco et al., 2009). RER is equal to

the range in the compositional values (i.e. the maximum value minus the minimum value) divided by the $RMSE_{val}$. According to AACC International Approved Methods 39-00.01(1999), RER > 4 the calibration is suitable for sample screening, RER > 10 the calibration is acceptable for quality control, and for an RER > 15 the calibration is good for quantification.

Conclusion

The Vis-NIR hyperspectral imaging technique has showed the ability to predict table grape quality attributes. The model based on SNV data pretreatment showed the best prediction performance for Total Flavonoids, Total Anthocyanins and soluble solid content. Furthermore, the PLSR+SNV model provided the highest values of RER and RPD meaning that the model is able to quantify the chemical references.

Reference

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