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COMPARISON OF NIRS APPROACH FOR PREDICTION OF INTERNAL QUALITY TRAITS IN THREE FRUIT SPECIES

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Abstract: NIR Spectroscopy ability was investigated to assess the fruit structure effect (passion fruit, tomato and apricot) on prediction performance of soluble solids content (SSC) and titratable acidity (TA). Relationships between spectral wavelengths and SSC and TA were evaluated through the application of chemometric techniques based on partial least squares (PLS). Good prediction performance was obtained for apricot with correlation coefficients of 0.93 and 0.95 for SSC and TA and root mean square errors of prediction (RMSEP %) of 3.3% and 14.2% respectively. For the passion fruit and tomato, the prediction models were not satisfactorily accurate due to the high RMSEP. Results showed that NIR technology can be used to evaluate apricot internal quality, however, it was not appropriate to evaluate internal quality in fruits with thick skin, (passion fruit), and/or heterogeneous internal structure (tomato).

Keywords: near infrared; chemometrics; passion fruit; tomato; apricot; soluble solids content; total acidity.

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1. Introduction

In the food industry, evaluation of the quality of fruits and vegetables is an important issue. The assessment of ripeness, a major part of quality evaluation, depends on several factors such as soluble solid content (SSC), acidity, sugars, organic acids, ethylene rate, colour etc. Most of the methods used to measure these quality traits (i.e. analysis of the organic acids for HPLC or enzymatic method) are based on complex processing of samples, use of expensive chemicals, besides involving a considerable amount of manual work. In addition, these methods are destructive. Therefore, there is a need for fast, non-destructive techniques for the assessment of fruit internal quality, to ensure that all fruits meet a minimum level of acceptance (Cayuela & Weiland, 2010).

Near Infrared Spectroscopy (NIRS) is becoming an attractive analytical technique for measuring quality parameters in food, especially because it allows non-destructive analysis of food products, requires little or no sample preparation and is both flexible and versatile, i.e., it is applicable to multiproduct and multicomponent analysis. NIRS also allows testing of raw material and end products, and simultaneous measurement of several analytical parameters as well. Furthermore, NIRS generates no waste, is less expensive to run than conventional methods, since a single instrument can be used for a wide range of fruits species and parameters, and can be built into the processing line, enabling large-scale individual analysis and real-time decision making (Roberts, Stuth & Flinn, 2004).

NIR spectra are the result of the interaction of radiation with the sample, and their physical and chemical properties are reflected in it. The interactions occur with molecular groups associated with quality attributes such as the C–H group in sugars and acids and the O–H group in the water. Most of the NIR absorption bands associated with these groups are overtones or combination bands of the fundamental absorption bands in the near infrared region, which are themselves due to vibrational and rotational transitions (Nicolaï et al., 2007). Scattering from microstructures can indirectly indicate physical parameters (Nicolaï et al., 2007). The

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measurement modes most often used for the prediction of SSC and TA in intact fruits are reflectance, transmittance and interactance. Reflectance is the easiest operating mode to obtain measurements, since no contact with the fruit is required and light levels are relatively high. These spectra can then be manipulated using multivariate data analysis techniques to develop prediction models for each measured variable. Although the initially built model will require reference data based on the traditional destructive methods, a robust model can thereafter be used to predict the quality attributes non-destructively (Louw & Theron, 2010).

Previous research has demonstrated the potential of NIR spectroscopy for assessing soluble solid content (SSC), titratable acidity and/ or other physiological properties in intact fruits such as in prune (Slaughter, Thompson & Tan, 2003), stonefruit (Golic & Walsh, 2006) and apricot (Bureau et al., 2009). However, this successful use of NIR spectroscopy was restricted to fruits with homogeneous pulp and thin skin. Guthrie, Liebenberg & Walsh, (2006) obtained unsatisfactory results for melon fruit, similarly Guthrie & Walsh (1997) were not able to predict soluble solids content in pineapple. Lammertyn, Peirs, Baerdemaeker & Nicolai, (2000) pointed out that penetration of NIR radiation into fruit tissue is limited. For example, in apple, the penetration depth is up to 4mm in the 700–900 nm range and between 2 and 3mm in the 900–1900 nm range. In fact, in a later study, Nicolai and co-workers (2007) concluded that depending on the uniformity of the fruit, the determination of quality attributes is difficult. To our knowledge, no attempt has been made to compare the efficiency of NIR, with the same methodology, for structurally different fruits. Thus, we describe in this paper the use of near-infrared spectroscopy, as a non-destructive method, to predict quality traits, more specifically, soluble solids and titratable acidity, in three structurally different intact fruits: passion fruit (thick skin), tomato (heterogeneous internal structure) and apricot (homogeneous pulp and thin skin).

2. Materials and Methods

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2.1. Selection of passion fruit, tomato and apricot

A total of 61 yellow passion fruits (*Passiflora edulis f. flavicarpa)*, in two different ripening stages (green-yellow and yellow) were harvested in 2011 in southern Brazil. For tomato, a total of 150 fruits of cultivar 'Levovil', in five different ripening stages (green, green-orange, orange-green, orange, red) were harvested in 2008 from an experimental greenhouse of INRA (Institut de la Recherche Agronomique) located in Southern France. 116 apricot fruits from three cultivars, named 'Bergeron', 'Iranien' and 'A4034' were harvested at two different stages of ripening: yellow (unripe) and orange (ripe) in INRA experimental orchards (Amarine and Gotheron), in South of France, in 2010.

Non-destructive measurements were performed on the day of picking for each fruit and conventional, destructive, measurements were carried out a few days later on frozen materials.

2.2. Near-infrared diffuse reflectance measurements (FT-NIR)

Spectra were collected for all samples in reflectance mode (log $1R^{-1}$) using a multi-purpose analyser (MPA) spectrometer (Bruker Optics). The instrument was equipped with an integrating sphere to provide diffuse reflectance measurements and a TE-InGaAs detector. The MPA was fully software-controlled (OPUS software Version 5.0, Bruker Optics).

The NIR spectrum for each sample was obtained from an average of 32 scans. NIR spectra were acquired between 800 and 2700 nm at 2 nm spectral resolution, with a scanner velocity of 10 kHz and a background of 32 scans. The time required to achieve a spectral measurement was 30 s. Intact tomato and apricot fruits were placed on an automated 30-position sample wheel, each position corresponding to an 18 mm diameter hole. The spectra for passion fruit were obtained in Brazil, an identical spectrometer was used (Bruker

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Optics) but without sample wheel. Fruits were placed at each–calyx axis set to the horizontal position. On each fruit, two opposite spectra were captured and the average of the two spectra was used (for the development of the models).

2.3. Determination of soluble solids content and titratable acidity through reference methods

Soluble solids content (SSC) was determined with a digital refractometer (PR-101 ATAGO, Norfolk, VA) with temperature compensation. SSC was expressed in °Brix. Titratable acidity (TA), determined by titration up to pH 8.1 with 0.1 N NaOH, was expressed in mmol H^+.100g^{-1} of fresh weight (FW).

2.4. Calibration and validation sets

PCA (principal component analysis) was initially performed using all available samples (n=61 for passion fruit; n=150 for tomato and n=116 for apricot) in order to evaluate the variability among the samples, to eliminate the aberrant spectra due to acquisition problems and to separate groups for calibration and internal validation. Samples to be used for both calibration and internal validation sets were selected solely on the basis of spectral data, following the method proposed by Shenk & Westerhaus (1991) which uses the pre- processing mean centering and ensures that all results will be interpretable in terms of variation around the mean. It is recommended for all practical applications (Nicolai et al., 2007).

Spectral preprocessing techniques were used to remove any irrelevant information that could not be handled properly by the regression techniques. Several preprocessing methods have been applied for this purpose. Smoothing techniques removed random noise from near infrared spectra, while MSC (multiple scatter correction) was used to compensate additive (baseline shift) and multiplicative effects in the spectral data, that are induced by physical effects, such as the non-uniform scattering throughout the spectrum as the

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dependence of scattering degree on radiation wavelength, particle size and refractive index (Nicolai et al., 2007).

In order to generate the prediction models for the quality traits of interest, the samples were grouped into two sets to have 80% samples for calibration and 20% for internal validation (Table 1). It is worthwhile to point out that internal validation samples were not utilized in calibration and cross validation steps, in order to avoid overfitting.

2.5. Chemometric treatment of the data

The MatLab software package (version 6.5, Mathworks USA.) and Origin 6.1® (OriginLab Inc., Northampton, USA) was used for the chemometric treatment of the data.

Partial least squares (PLS) regression models were built for the prediction of SSC and TA, using the spectral data (matrix X) and measurements carried out through the use of reference methods (matrix Y). In PLS, both the spectral matrix X and the reference data in the matrix Y were used for the calibration.

To determine the optimal number of latent variables (LV), internal cross-validation method was applied; through the routine "Leave one out". Root mean square error for cross validation (RMSECV) was obtained by comparing the predicted concentration with its experimental value. RMSECV was plotted against LVs to set the optimal number of LVs.

In order to identify anomalous samples (outliers) the *leverage* criterion and the Student residuals were used. The *leverage* criterion represents the influence of each sample in the regression model, with a threshold equal to 3 LV/n where n is the number of samples. The Student residual indicates if the sample is within a normal distribution, with a confidence level of 95%, assuming a threshold value of ± 2,5.

Afterwards, the models were tested to predict SSC and TA with validation set. The best calibration models were selected based on the highest correlation coefficient of validation (R^2) along with the lowest

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RMSECV and the lowest root mean square error of prediction (RMSEP). RMSEP was then expressed as %RMSEP corresponding to the percentage of error of prediction calculated with RMSEP divided by the mean values of measured quality parameters in fruits from the validation set (Duarte, Barros, Delgadillo, Almeida & Gil, 2002)

$$RMSEP = \sqrt{\frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{n}} \quad (1)$$

Where: y_i = known value; $\hat{y}_i$ = calculated or predicted value and n = number of samples in the validation set. This value represents the average error that can be expected for the prediction of future samples, with a confidence interval of 95%.

3. Results

3.1. Characterization of the spectral data

The general shapes of the spectra for the three fruit types were quite similar, though the spectra for the passion fruit showed weak absorption intensity and a slight displacement, possibly due to the thickness of the skin (Figure 1). The main absorption peaks coincided for all three fruits. The peak at 1190 nm corresponds to the second and third C–H overtone regions, associated with sugar (Osborne, Fearn & Hindle, 1993). The peak at 1500 nm overlaps with the first O-H overtone region related to organic acids (Roberts, Stuth & Flinn, 2004). In general, the absorbance patterns seen here can be loosely related to the functional groups associated with water and sugars. Indeed, most fruits contain 80–90% of water and show a rising

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sugar content throughout ripening. The spectra obtained here for apricot and tomato can be compared to other studies, apricot (Bureau et al., 2009) and tomato (Sirisomboon, Tanaka, Kojima & Williams, 2012). To the best of our knowledge, no study was published for passion fruit.

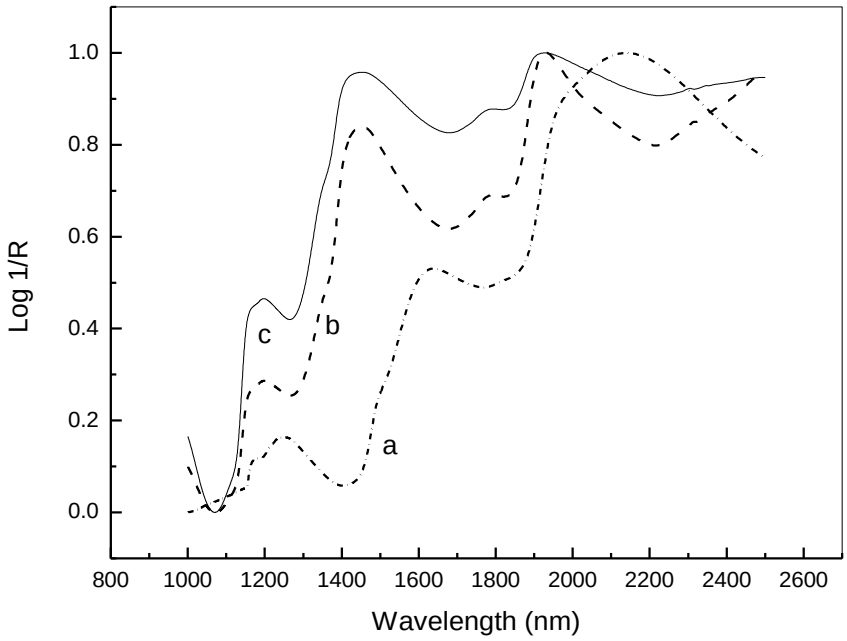

Figure 1. Typical normalized NIR spectra (mean) performed on intact fruits of passion fruit (a), tomato (b) and apricot (c)

The samples showed a large variability of SSC and TA for fruits of the three species used in this trial. These results confirm that selected fruits were in different ripening stages. Statistical analysis for the calibration and validation sample sets, i.e., data ranges, means, standard deviations (SD) and number of samples for SSC and TA are shown on Table 1.

Table 1: Range, mean and standard deviation (SD) of the passion fruit, tomato and apricot quality traits in both calibration and validation sample sets

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Fruit	Parameter	Sample set	Range	Mean	Standard Deviation	Number of samples
Passion fruit	SSC (°Brix)	Calibration set	9.0 – 16.0	13.3	±1.8	49
		Validation set	12.1 – 14.2	14.2	±1.3	12
	TA (mmol H^+.100g^{-1} FW)	Calibration set	24.7 – 110.4	68.9	±14.35	48
		Validation set	34 – 83.8	63.6	±12.90	11
Tomato	SSC (°Brix)	Calibration set	3.7 - 6.4	4.8	±0.49	118
		Validation set	3.9 - 6.1	4.7	±0.54	32
	TA (mmol H^+.100g^{-1} FW)	Calibration set	3.5 - 7.4	5.6	±0.81	118
		Validation set	3.9-7.0	5.8	±0.63	32
Apricot	SSC (°Brix)	Calibration set	11.3 - 20.4	15.2	±2.3	92
		Validation set	11.6 - 20.1	15.3	±2.1	24
	TA (mmol H^+.100g^{-1} FW)	Calibration set	3 - 24.5	11.5	±6.5	92
		Validation set	5.2-20.7	10.5	±5.1	24

3.2. Prediction of soluble solids content

For fruits from the three different plant species used in this trial, different calibration models were calculated. The spectra pre-processing and the number of factors were both taken into consideration to determine the best models. As a result of variable selection, it is possible to establish models that are more robust, simpler to interpret and with a better accuracy. Only the best model for each fruit is shown on Table 2.

Table 2: Results of performance of NIR models for non destructive quality assessment of passion, tomato and apricot fruits

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Fruit	Parameter [a]	Spectral range (nm)	Mathematic treatement	Factor (LV)	RMSECV	RMSEP	RMSEP %	R^2
Passion fruit	SSC	2500-1000	MSC	5	1.62	1.66	9.82	0.631
	TA	2500-1000	1 st derivative	5	14.69	12.88	11.42	0.497
Tomato	SSC	2500-1000	MSC	10	0.13	0.53	8.85	0.525
	TA	2500-1000	MSC	8	0.35	0.73	10.43	0.514
Apricot	SSC	2500-2000	MSC +smoothing	6	0.85	0.69	3.32	0.930
	TA	2000-800	MSC +smoothing	6	2.00	1.82	14.21	0.951

[a] SSC values expressed in ° Brix and TA values expressed in mmol H^+.$100g^{-1}$ FW.

Initially, very different trends were observed for the evolution of the calibration error (RMSECV), according to the number of LVs, between the three species (Figure 2). For passion and tomato fruits, evolution of RMSECV with number of LVs showed no consistent trend (Figure 2a). The behavior of the unstressed calibration error for the passion and tomato fruits was characterized by low correlation coefficients between predicted and measured values. The best PLS model developed for the passion fruit used pre-processing multiple scatter correction (MSC) and 5 LVs which provided the lowest cross validation error of 1.62 °Brix. When the model was applied to predict the 12 internal validation samples, a low correlation (R^2 = 0.63) and a high error of prediction (RMSEP% = 9.8%) were found (Figure 2b). For tomatoes, results were similar to the results found for passion fruits (Figure 2c). The lowest cross validation error (0.13 °Brix) was observed for models using 10 LVs and MSC pre-processing. When the model was used to predict the 32 internal validation samples, the prediction error was 8.85% and the correlation coefficient was 0.52 (Figure 2d). However, in apricot, the relationship between RMSECV and number of LVs followed a regular profile, and a good correlation was found (Figure 2e). The same ratio was observed by Camps & Christen (2009). The lowest cross validation error (0.69 °Brix) was observed for models using 6 LVs and MSC pre-processing followed by smoothing. A high correlation coefficient (R^2 = 0.93) and a low

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prediction error (RMSEP 3.3%) were observed, when the model was used to predict the 24 internal validation samples (Figure 2f).

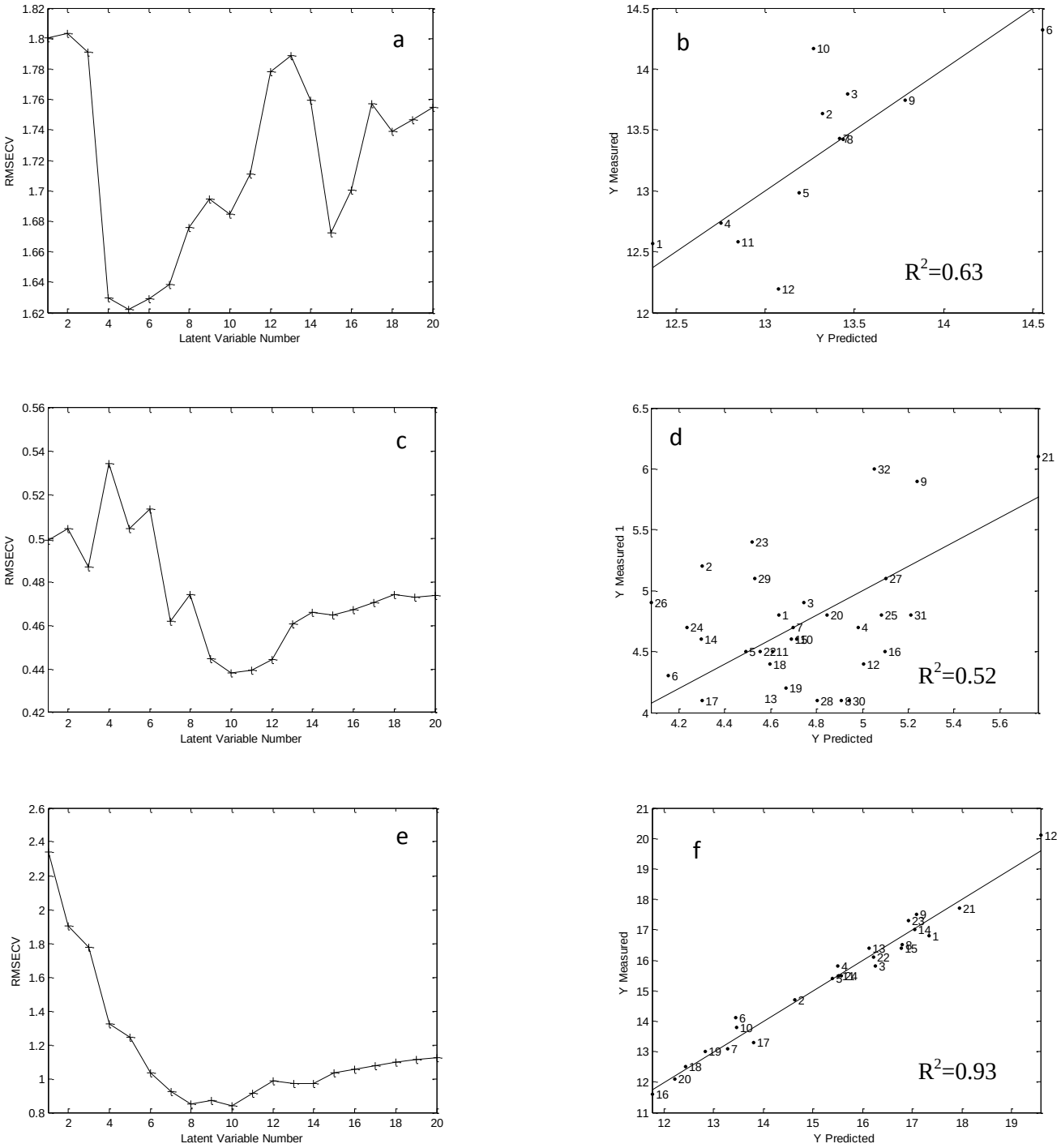

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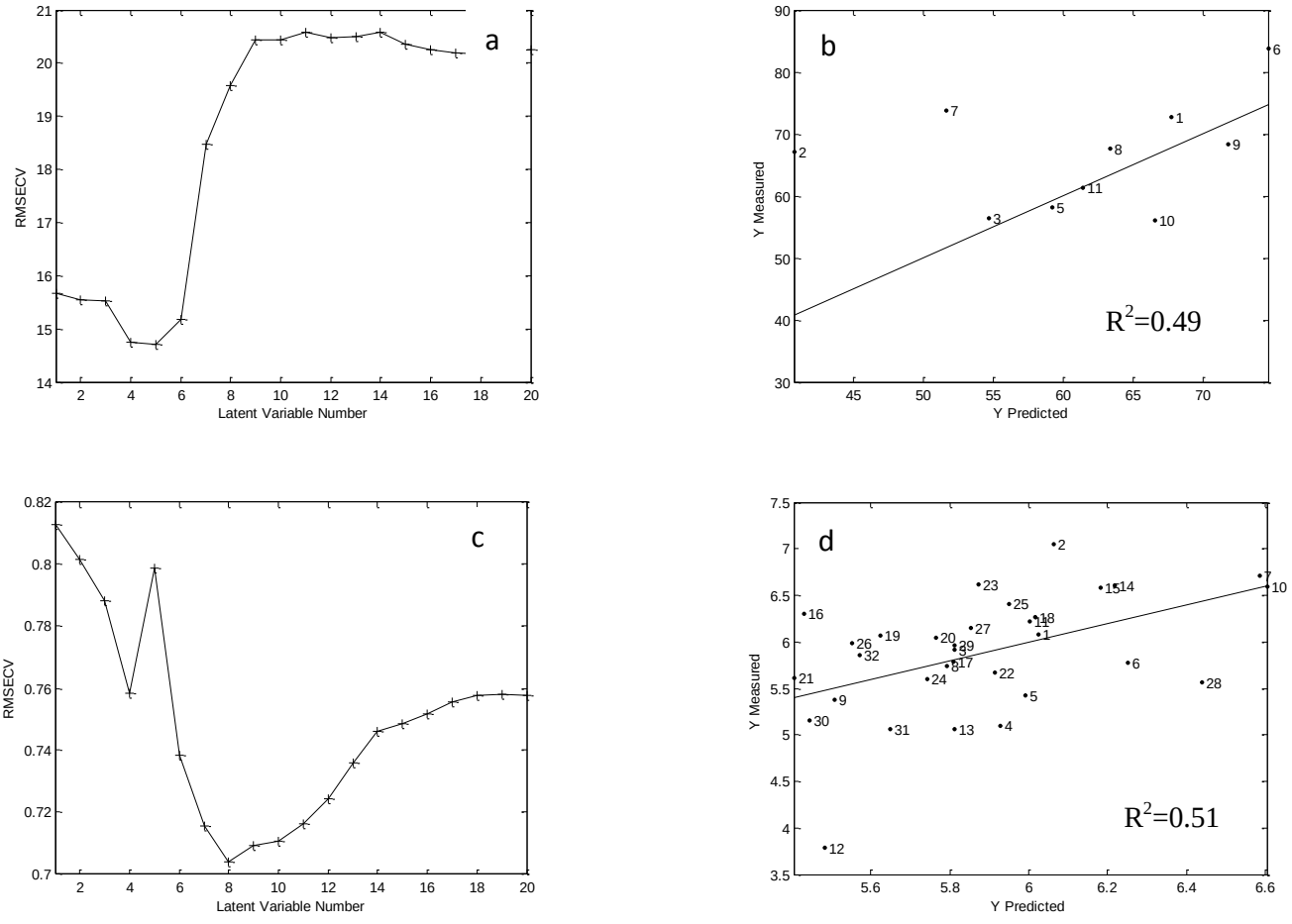
Figure 2. Change of the RMSECV values versus the number of LVs and the scatterplot between predicted and measured values of SSC for passion fruit (a) (b), tomato (c) (d) and apricot (e) (f)

3.3. Prediction of titratable acidity

Measurement of acidity-related parameters in intact fruits is notoriously difficult (Flores, Sánchez, Pérez-Marín, Guerrero & Garrido-Varo, 2009). Such difficulties can be observed in Figure 3. Similarly to what was found for the soluble solids content, when the cross validation error was plotted against the number of LVs for passion fruit and tomato (Figure 3a and 3c), the correlation coefficients were below 0.49 and 0.51 respectively, indicating a poor relationship between measured and predicted values for titratable acidity.



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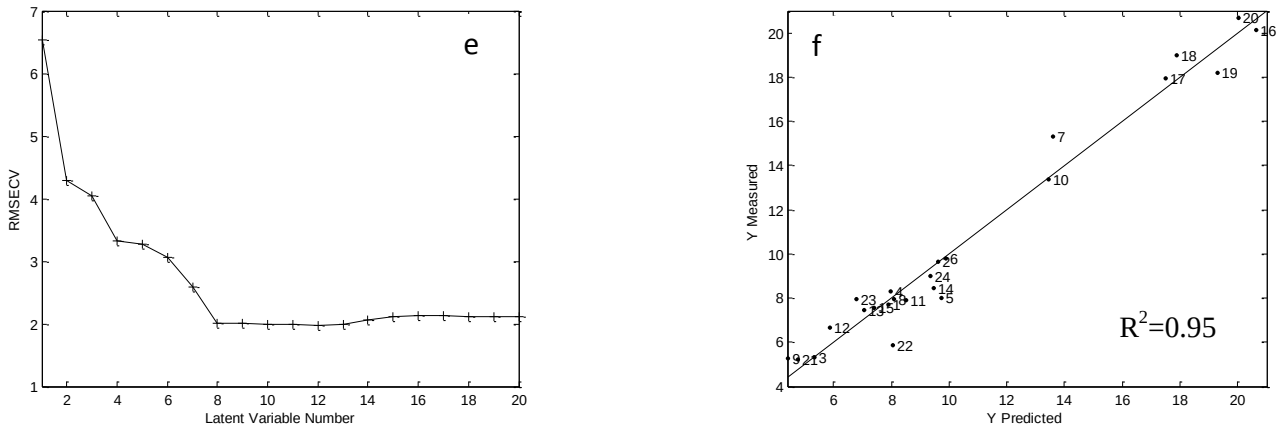

Figure 3. Change of the RMSECV value versus the number of LVs and the scatterplot between predicted and measured values of TA for passion fruit (a) (b), tomato (b) (c) and apricot (e) (f)

The best PLS model developed for the passion fruit used pre-processing first derivative and 5 LVs, which resulted in a cross validation error of 14.69 mmol H^+.100g FW^{-1}. When the model was used to predict the 11 internal validation samples, a low correlation (R^2 = 0.49) and a high value for the error of prediction (RMSEP% = 11.4%) were found (Figure 3b).

For tomatoes, a minor cross validation error (0.35 mmol H^+.100g FW^{-1}) was observed for a model using 8 LVs and MSC pre-processing. When the model was used to predict the 32 internal validation samples, a prediction error of 10.43% and a correlation coefficient of 0.51 were found. One possible reason leading to the difficulty for predicting fruit acidity could be due to the low titratable acidity, which ranges from 3.5 to 7.4 mmol H^+.100g FW^{-1} in tomato (Table-1).

Similarly to what was found for SSC, higher correlation coefficients were found for apricot, when compared to passion fruits and tomatoes. The best model for TA in apricot used 6 LVs and MSC pre-processing, followed by smoothing. This model yielded a cross validation error of 2.00 mmol H^+.100g FW^{-1}. When the model was used to predict the 24 internal validation samples, a high correlation coefficient (R^2 = 0.95) was obtained, along with a prediction error of 14.21%.

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4. Discussion

There are several potential limitations in NIR assessment that make it difficult to predict quality in some fruits. These limitations can be intrinsic to the spectral range used: NIR is not a high sensitivity method. NIR spectra of fruit and vegetables are dominated by water absorption bands and the typical low acid concentration (compared to sugar) found in fruit cannot be well measured (Nicolaï et al., 2007). Other limitations are linked to the physical nature of the fruits and the properties of NIR radiation, notably the depth of penetration of NIR radiation into fruit tissue (Nicolai et al., 2007; Lammertyn et al., 2000). Some limitations can be linked to the fruit themselves: variation in quality traits (Long & Walsh, 2006), and fruit sampling location (Guthrie et al., 2006; Long & Walsh, 2006). Finally, other limitations are related to experimental design, such as the robustness of the calibration models (Golic & Walsh, 2006) depending on properly chosen sample sets, with a maximum variability and limited internal correlations. In this work, we tested the effectiveness of the use of NIR technology for the prediction of SSC and TA in fruits presenting anatomical features expected to interfere with the penetration of NIR radiation into fruit tissue.

4.1. Fruit specificities

The three species used in this trial have distinct physical (Figure 4) and biochemical (Table 1) characteristics. Regarding chemical composition, passion fruit pulp is characterized by high acidity. Tomato has usually low SSC and acidity, and may contain over 95% water. In apricot, SSC is higher than the acidity. A broad range of values was recorded in this work for SSC and TA in all of the three fruits. This finding is likely due to the fact that sampling was, as experimentally designed, carried out during different ripening stages, and it is well known that during ripening, sugars accumulate and acidity decreases, the later,

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as a result of the consumption of the predominant acids during fruit respiration. Values of the SSC and TA in this work were within the range found in literature for passion fruit (Jiménez, Sierra, Rodríguez-Pulido, González-Miret, Heredia & Osorio, 2011), tomato (Scibisz et al., 2011) and apricot (Bureau et al., 2009; Camps & Christen, 2009).

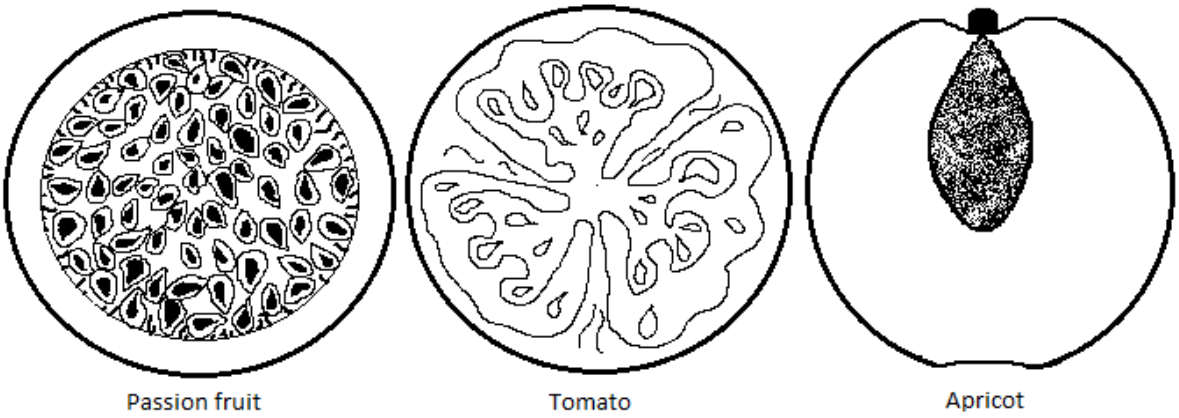

Figure 4. Schematic representation of the fruit anatomy of the three species used in this trial. Equatorial sections are presented for passion fruit and tomato, and a transverse section for apricot

The passion fruit is a fleshy, berry type fruit, with a thin pericarp (peel) that can be lignified. The passion fruit mesocarp thickness ranges from 0.5 to 4.0 cm, and the endocarp (pulp) contains seeds with fleshy aril (Vasconcellos, Savazaki, Grassi, Busquet & Mosca, 2001). The tomato is a fleshy berry, with at least two locular cavities. The locular cavities contain the seeds, within a more or less abundant gel. They are enclosed by a parenchyma that forms a sub-epidermal layer of 0.2 to 1 cm, radial septa that separate the locules, and a collumella. The pericarp is protected to the outside by an epidermis covered with a waxy cuticle, presenting many hairs, stomata and lenticels (Hobson & Davies, 1971). The composition of these different tissues is not homogeneous. Cheng, Wang, Chen & Lin, (2011), in particular, showed that sugar concentrations in the placenta and close to the calix were consistently low relative to the outer pericarp, collumella, and locular

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cavity. Apricot is a stone fruit that consists of three parts: a thin skin, a fleshy mesocarp which encloses the seeds. The thickness and shape of the mesocarp vary according to different cultivars (Romani & Jennings, 1971).

The three fruits used in this trial present different structures which seems to affect the depth of near infrared radiation penetration. In passion fruit, NIR radiation only should penetrate in tissue that is clearly distinct from the edible part. In tomato, NIR radiation may interact with edible tissues, but they present variable compositions. Positioning of the beam relative to septa or locules means it will encounter different compositions. Apricot on the other hand presents a relatively homogeneous tissue.

4.2. NIR prediction results

For apricot, excellent results were found, showing that NIR technology can be effectively used for the quantification of the soluble solid content and titratable acidity for apricot. The best PLS model for apricot used three varieties, involving higher variability of fruit quality traits. This can be the cause of the high value of the prediction error for TA (14%). Our model presented a lower predictive performance when compared to the model developed by Camps & Christen (2009), for three varieties of apricot (‘Bergerouge’, ‘Harostar’ and ‘Kioto’), tough the varieties used in that trial were not the same used in our trial and those author also used a Visible-NIR spectrometer (650–1200 nm), instead of a NIR spectrometer. The model developed by Camps & Christen presented a R^2 of 0.9 and a RMSEP 9.6%. Bureau et al., (2009) developed prediction models that presented a correlation coefficient of 0.88 and a prediction error of 15% for eight apricot cultivars or hybrids. Measuring SSC and TA have been reported also using reflectance ant has shown excellent correlation for various fruits such as prune, plums and peaches (Slaughter, Thompson & Tan, 2003; Louw & Theron, 2010; Pérez-Marín, Sáncheza, Paza, Sorianoc, Guerrero & Garrido-Varo, 2009). All of these fruit share with apricot similar anatomical features such as thin skin and homogeneous pericarp.

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The lowest correlation for both parameters SSC and TA was found for passion fruit. Passion fruit contains similar soluble solids content and high amounts of acids (range 24.70 – 110.42 mmol H^+.100g FW^{-1}), when compared to apricot. However, the thick skin in passion fruit acts as a barrier and prevents the penetration of the infrared radiation to the pulp. Indeed, Guthrie et al., (2006) determined the total soluble solids in intact melon and observed a correlation coefficient lower than the correlation coefficient found for other fruits, being the difference attributed to the heterogeneity of SSC distribution within the fruit and the poor penetration of light through the irregular fruit skin. Dull, Birth, Smittle & Leffler, (1989) used two wavelengths to assess SSC in sliced melon 'cantaloupes' (913 nm and 884 nm) and in intact melon (896 nm and 860 nm). The correlation coefficient for sliced melon and intact melon were 0.968 and 0.600, respectively, while RMSEP was 1.56 and 2.18, respectively for sliced melon and intact melon. Those results clearly demonstrated that NIR can be more effectively used for the prediction of SSC in sliced melon when compared to intact melon. Flores, Sanchez, Perez-Marin, Lopez, Guerrero, & Garrido-Varo, (2008) evaluated SSC in cut and intact watermelons and melons using a NIR diode array spectrometer. The results of SSC prediction for cut watermelons and melons were much better than those of intact watermelons and melons (cut watermelons: R^2 = 0.92, RMESCV = 0.49; intact watermelons: R^2 = 0.81, RMSECV = 0.93; cut melons: R^2 = 0.94, RMSECV = 0.60, intact melons: R^2 = 0.87, RMSECV = 0.98). For passion fruit, the thick skin prevents the use of NIR to predict the composition of the internal pulp.

In tomato, prediction of models for non-destructive measurement by spectroscopic methods has generally been poor (Walsh, Golic & Greensill, 2004). Tomatoes combine low concentrations (SSC and TA) and heterogeneous composition. They are internally divided into different compartments so they cannot be considered as a homogeneous sphere. Each juicy compartment, with liquid and seeds, is surrounded by a flesh wall construction (Li, Yao, Yang & Li, 2006), and this structure can interfere with the NIR radiation penetration. Chen (2008) determined soluble solids content and titratable acidity in two tomato varieties ('DRK 453' and 'Trust') in five different stages of maturity and found values remarkably low (R^2 = 0.03 and

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0.49; RMSEP 0.15°Brix and 0.43 mg/ml respectively). On the other hand, He et al., (2005) found excellent results (R^2= 0.9 and 0.83, and RMSEP = 0.19°Brix) using Vis/NIR spectroscopy, one tomato variety (Heatwave) at a single maturity stage. Sirisomboon et al., (2012) observed a high correlation for SSC of R^2= 0.8 and RMSEP of 0.21 °Brix for a single variety of tomato (Momotaro) at three different stages of maturity (mature green, pink, and red). However in these last two cases, prediction heavily relied on the internal correlation in the sample set, as a given variety has a defined genetic program that coordinates color evolution and sugar accumulation during maturation.

It is important to note that for commercial purposes a major determinant for internal quality in fruit is their sweetness, since this is the major parameter affecting consumer acceptance or rejection and thus influencing the market value of the fruit (Li et al., 2006). So, even the correlation coefficients for the passion fruit and tomatoes were below 0.63 and 0.52, the prediction error was lower than 10% (9.8% for passion fruit and 8.85% for tomato). This findings demonstrate that NIR technology can be used for sorting (between low, medium and high levels of sweetness) fruits on arrival to the industry. In addition, since NIR is a non destructive technology, it would allow increased sampling for each batch, ensuring a more precise and accurate guarantee of specific quality.

5. Conclusion

The applicability of NIR spectroscopic technique to determine the soluble solids content and titratable acidity was tested in three fruits with different characteristics (passion fruit, tomato and apricot). The calibration and prediction performance of PLS models developed with different spectral regions and pretreatment methods was also investigated. The analysis of the best models shows that the physical features of the fruit directly affect the results. The low correlation values for passion fruit were attributed to the low penetration of infrared radiation due the thick skin of the fruit. For tomatoes, internal characteristics

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(heterogeneity) and high water contents led to weak correlations. On the other hand, good and robust prediction results were observed for apricot, which is a fruit with thin skin and homogeneous pulp.

From the results obtained in this work, it can be pointed out that NIR spectroscopy can be used to predict the soluble solids content and titratable acidity with excellent accuracy in intact homogeneous fruits, as apricot. However, a poor performance was obtained to intact passion fruit and tomato, where NIR was not adequate to establish quality traits due to the physical structure of these species. Therefore, it is worthwhile to note that there are specific limitations to each fruit type, as observed for passion fruit and tomato, that should be considered in NIR spectroscopy applications.

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