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Evaluation of a handheld ultra-compact NIR spectrometer for rapid and non-destructive determination of apple fruit quality

Audrey Pissard [a,*], Emanuel José Nascimento Marques [b], Pierre Dardenne [a], Marc Lateur [c], Celio Pasquini [d], Maria Fernanda Pimentel [e], Juan Antonio Fernández Pierna [a], Vincent Baeten [a]

[a] *Knowledge and Valorization of Agricultural Products Department, Walloon Agricultural Research Centre (CRA-W), Gembloux, Belgium*
[b] *Department of Fundamental Chemistry, Federal University of Pernambuco (UFPE), Recife, PE, Brazil*
[c] *Life Sciences Department, Walloon Agricultural Research Centre (CRA-W), Gembloux, Belgium*
[d] *Institute of Chemistry, University of Campinas (UNICAMP), Campinas, SP, Brazil*
[e] *Department of Chemical Engineering, Federal University of Pernambuco (UFPE), Recife, PE, Brazil*

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ABSTRACT

Benchtop and portable devices based on near infrared (NIR) spectroscopy are increasingly used to evaluate the quality parameters of fruits. This study aims to compare the analytical performance of a benchtop spectrometer (XDS) and a handheld ultra-compact spectrometer (MicroNIR) and to investigate calibration transfer between these devices for quality parameters of apples (soluble solids content, titratable acidity, pulp firmness, and starch-iodine index). Regression analyses were performed on a subset of apples measured with both spectrometers. The coefficient of determination (R^2) and the root mean square error of cross-validation (RMSECV) values obtained with Partial Least Squares (PLS) models were similar, which suggests that MicroNIR offers similar performance to the XDS device. For example, for soluble solids content, it was observed a $R^2 = 0.89$ with a RMSECV = 0.62 and a $R^2 = 0.91$ with a RMSECV = 0.57 for XDS and MicroNIR respectively. For the transfer, calibration models were built using XDS spectra and different regression methods. The best performances were obtained with Least Squares Support Vector Machines (LS-SVM). The Direct Standardization method was applied to achieve calibration transfer. Only two transfer samples were enough to significantly reduce the root mean square error of prediction (RMSEP) values with a relative reduction varying from 74 % to 93 % for PLS and Multiple Linear Regression (MLR) models respectively. It showed the potential of a simple calibration transfer method to allow the use of historical database registered with benchtop instrument.

1. Introduction

Apples are the third most cultivated and consumed fruit in the world, only behind bananas and watermelons. Almost 86 million tons of apples were produced in 2018, with China accounting for 46 % of world production, followed by the United States (5 %), Poland (5 %), Turkey (4 %) and Iran (3%) (FAOSTAT, 2020).

The consumer market for apples is highly demanding in terms of quality, which requires an efficient system of quality control allowing a careful selection of fruits. Thus, before going out to the market, fruit must meet minimum quality requirements for external characteristics, such as size, shape, and color, as well as internal requirements, such as sugar content, acidity, and firmness (Peng and Lu, 2008). The evaluation of these attributes is important, as they directly affect the taste and

texture of the fruit and, consequently, consumer acceptance. In particular, sugar, acidity and firmness determine whether an apple is sweet and crisp; and therefore whether the apple is appealing to customers.

The use of NIR spectroscopy to determine the quality of agricultural products, such as vegetables and fruits, has been extensively investigated during the last decades (Nicolaï et al., 2007, 2014; Wang et al., 2015; Walsh et al., 2020). A large number of authors have reported on the use of NIR spectroscopy to determine apple quality parameters, such as soluble solids content (Park et al., 2003; Sanchez et al., 2003; Zude et al., 2006; Liu et al., 2007; Paz et al., 2009; Bobelyn et al., 2010; Ouyang et al., 2012; Pissard et al., 2012; Liu and Zhou, 2013; Pissard et al., 2013; Giovanelli et al., 2014; Kumar et al., 2015; Guo et al., 2016), acidity, pulp firmness (Park et al., 2003; Zude et al., 2006; Paz et al., 2009; Bobelyn et al., 2010; Shi et al., 2011; Giovanelli et al., 2014;

Kumar et al., 2015), maturity indexes, dry matter content (Giovanelli et al., 2014; Kumar et al., 2015), shelf-life (Paz et al., 2009), indexes related to the antioxidant capacity (Giovanelli et al., 2014), polyphenols and vitamin C (Pissard et al., 2012, 2013). NIR spectroscopy has the advantages of being rapid, non-destructive and does not require sample preparation or the use of chemical reagents. Thus, this analytical technology is aligned with Green Chemistry concepts (Armenta et al., 2008; Gałuszka et al., 2013).

The use of NIR spectroscopy under field conditions has been limited for many years due to restrictions imposed by the size and low robustness of the instruments available on the market. A significant reduction in size and cost of these instruments has been possible thanks to the development of new technologies used in the construction of NIR (Fernández Pierna et al., 2010; O'Brien et al., 2012; Lutz et al., 2014; Marques et al., 2016). As reported by Walsh et al. (2020), a range of alternative detector technologies (*i.e.* light dispersion technologies such as the linear variable filter) has been released. So, handheld NIR spectrometers are gaining interest for rapid quality prediction of fresh fruits (dos Santos Neto et al., 2017; Escribano et al., 2017; Malegori et al., 2017; Toivonen et al., 2017; Donis-González et al., 2020; Gabriëls et al., 2020) and represent an attractive and viable alternative for both agro-industries and small producers to monitor the quality of the apples either at the orchard during the harvest or during the process before going to market. Handheld instruments have been recently reviewed by Pasquini (2018). He reported that a lot of portable instruments have been evaluated for applications in several areas where conventional bench spectrophotometers were originally employed.

A key concern in application of NIR and other non-destructive technologies is that the prediction results are influenced by the types of instruments which makes a model based on one instrument could not be used in other instrument (Xiao et al., 2017). This issue also relates for the handheld NIR devices released on the market regarding the use of historical databases and/or calibration models previously built using benchtop spectrometers. Repetition of the whole procedure including samples acquisition and calibration would generally require significant time and investment.

Therefore, based on our experience, the best option would be to use a calibration transfer procedure for correction of the instrumental and/or environmental differences (Fernández Pierna et al., 2010; Grelet et al., 2015, 2017). This would make spectral data coming from the handheld instrument compatible with the calibration models developed using the benchtop instrument. This is especially valuable for NIR spectroscopy for the fruit and vegetable sector as large NIR datasets are required for robustness purposes (Nicolaï et al., 2007). As reported by Fan et al. (2019) several strategies have been proposed and widely used to transfer a calibration model between different conditions or spectral instruments including direct standardization (DS), piecewise direct standardization (PDS) (Wang et al., 1991), orthogonal signal correction (OSC) (Sjöblom et al., 1998), Shenk-Westerhaus (Fearn, 2001) and Rank-Kennard-Stone-PDS (Liang et al., 2016). Some of these methods have been successfully used in calibration transfer for fruit internal quality detection. A calibration model for the soluble solids content (SSC) of apples developed on a Fourier transform-based spectrophotometer was successfully transferred to a diode array (DA) spectrophotometer using the Piecewise Direct Standardization (PDS) method (Alamar et al., 2007). More recently, Xiao et al. (2017) showed the feasibility of calibration transfer between a benchtop Fourier transform (FT) spectrometer and a portable grating scanning spectrometer for a single grape berry using a modified PDS method, and Pu et al. (2018) investigated calibration transfer from a handheld micro NIR spectrometer to desktop hyperspectral imaging for predicting SSC in bananito.

The objectives of this study were: (1) to compare the analytical performance of a benchtop NIR spectrometer and a handheld ultra-compact NIR spectrometer for rapid and non-destructive determination of quality parameters of apples, and (2) to evaluate whether a spectral calibration transfer between these two spectrometers can enable the use of historical databases and/or calibration models, thereby offering opportunities for faster direct analysis of apples at the orchard with the use of robust models.

2. Materials and methods

2.1. Fruit samples

The samples used in this study were harvested in Belgium during the period from 2008 to 2014, corresponding to eight hundred sixty-six ($n = 866$) apples from forty-eight ($n = 48$) varieties harvested at different maturity stages. These samples were used for the building of a historical database containing the results of the reference analyses (using classical wet chemistry methods) and the spectra recorded in the Vis-NIR region with a benchtop spectrometer (see section 2.2).

To cope with the objectives of this work, a subset of 93 apples from 2 varieties analyzed in 2014 using both spectrometers (benchtop NIR spectrometer and a handheld ultra-compact NIR spectrometer) was used for study 1 (aiming to compare the analytical performance of a benchtop and a handheld spectrometer) and the remaining samples ($n = 773$) were used in study 2 to build the multivariate calibration models used for the calibration transfer between instruments.

2.2. Spectral data acquisition

Spectra were recorded from 2008 to 2014 according to the harvest time of apple varieties. Spectra of all apples were recorded at $22 \pm 1\ °C$ using a benchtop NIR spectrometer (XDS Rapid Content Analyzer, FOSS, Hillerød, DK). In 2014, a set of 93 apples were measured with a handheld ultra-compact NIR spectrometer (MicroNIR 1700, VIAVI, CA, USA) in addition to the benchtop spectrometer. The scans were acquired at 4 equidistant points distributed along the equatorial region of each fruit. Calibration models were constructed using the mean spectra of the fruits.

Spectra acquisition for the XDS spectrometer was performed in reflectance mode (log 1/R), in the spectral range between 400 and 2500 nm with a nominal spectral resolution of 2 nm. The integration time was approximately 1 s, with each recorded spectrum corresponding to an average of 32 scans, resulting in a measurement time of approximately 32 s.

Spectra acquisition for the MicroNIR spectrometer was performed in reflectance mode (log 1/R), in the spectral range between 950 and 1650 nm with a nominal spectral resolution of 6.2 nm. For data treatment, the range was trimmed to $1100-1600$ nm. The integration time was approximately 12 ms, with each recorded spectrum corresponding to the average of 800 scans, resulting in a measurement time of approximately 9.6 s.

2.3. Reference analyses

Intact fruits were individually analyzed by reference methods after NIR measurements. The quality parameters analyzed are the soluble solids content (SSC), titratable acidity (TA), pulp firmness (PF), and starch-iodine index (SII). First, the fruits were used to determine pulp firmness (PF). Later, each apple was cut into small pieces, discarding the core with the seeds. A fraction of these pieces was randomly chosen and then pressed by means of a manual juice extractor. The resulting liquid fraction was used to determine soluble solids content (SSC) and titratable acidity (TA). The maturity stage of some apples was evaluated through the starch-iodine index (SII). The procedures used to carry out the reference analyzes are detailed below (sections 2.3.1 to 2.3.5).

2.3.1. Soluble solids content (SSC)

SSC was determined using a digital refractometer model PAL-1 (Atago, Tokyo, Japan) with automatic temperature compensation. Measurements were performed using 1 mL of fruit juice. The results

were expressed in percentage (%).

2.3.2. Titratable acidity (TA)

TA was determined in 10 mL of juice diluted in 50 mL of distilled water. Titration was accomplished with an automated titrator (Titroline Easy, Schott instruments). A standard solution of NaOH 0.1 mol L^{-1} was used as titrant (Vaysse and Landry, 2004). The analyses were performed in duplicate and the mean values were used for the construction of the calibration models. The results were expressed in milli-equivalents of malic acid per liter of juice (mEq malic acid L^{-1}).

2.3.3. Pulp firmness (PF)

PF was determined using a Magness-Taylor style penetrometer probe (Fruit Pressure Tester FT 327, Facchini srl, Italy) equipped with an 11 mm diameter stainless probe. This parameter was determined on the whole fruit and the results represent the necessary force to effect 10 mm of penetration of the probe through the pulp of the fruit. Two measurements were performed per fruit, on opposite sides of the equatorial region, after the removal of a small area of the epidermis (−1 cm^2), and the mean values were used to build the calibration models. The results were expressed in kilograms per square centimeter (kg cm^{-2}).

2.3.4. Starch-iodine index (SII)

The maturity stage of some apples was evaluated through the starch-iodine index (SII). SII was determined using the whole fruit cut lengthwise and one of the halves was sprayed with a solution prepared by the addition of 10 g of iodine and 40 g of potassium iodide in 1 L of distilled water (Vaysse and Landry, 2004). Afterwards, the half of the fruit was kept at rest for 10 min. After this period, the coloring of the fruit surface was compared with the colors of a suitable table for this purpose. The results were expressed using a scale with values from 1 to 10, with intervals of one unit. In this case, the value 1 on the scale corresponds to unripe fruits, in which no starch degradation occurred, and the value 10 corresponds to fruits with advanced maturation, in which all starch has been degraded.

2.4. Study 1: comparing analytical performance between benchtop and handheld spectrometers

In this study, the analytical performance of the XDS and MicroNIR spectrometers were compared for the determination of quality parameters from a set of 93 apples measured in 2014.

Initially, different spectral preprocessing techniques were evaluated: Standard Normal Variate (SNV), first and second derivative with Savitzky-Golay filter using second order polynomial and 15-point window. Calibration models were built using Partial Least Squares (PLS) regression. The spectral range from 1100 to 1600 nm was used for MicroNIR spectra while for XDS spectra, two spectral ranges (400−2500 nm and 1100−1600 nm) were used for calibration models. It must be mentioned that only these spectral ranges were used and that the influence of the spectral window on the calibration performance was not evaluated here.

The number of latent variables maintained in the calibration models was determined according to the root mean square error of cross-validation (RMSECV), using full cross-validation. According to the reduced number of samples (n = 93), the predictive performance of the models was evaluated in the internal validation step, considering the values of the RMSECV, R^2 (coefficient of determination) and bias.

Outliers were identified and removed using the values of Hotelling and the Quadratic Sum of the Residuals, which allowed identification of extreme values and samples that were not well represented by the regression equation. The calculations related to the pre-processing and the multivariate calibration models building were performed using the Unscrambler software version 9.8 (CAMO, Oslo, Norway).

2.5. Study 2: calibration transfer between benchtop and handheld spectrometers

This study was carried out in two steps. In a first step, calibration models were developed using the XDS spectrometer spectra of 773 fruits. Different multivariate calibration techniques were used to determine the quality parameters of apples. In a second step, the feasibility of calibration transfer between the XDS and MicroNIR spectrometers was evaluated, using the sample set from study 1 (n = 93) that was analyzed by both instruments.

For the first step, i.e. the development of calibration models, the 773 samples were divided into calibration and validation (prediction) sets using the SPXY algorithm (Sample set Partitioning based on joint X–Y distances) (Galvão et al., 2005) for each quality parameter evaluated. Calibration models were built by means of the Multiple Linear Regression (MLR), Partial Least Squares (PLS) and Least Squares Support Vector Machines (LS-SVM) regression methods, using the spectral range from 1100 to 1600 nm. The influence of the spectral window on the calibration performance was not evaluated here. In all cases, spectral preprocessing was performed using the SNV technique since it gave rise to the best results in the first part of the study (study 1). The SPA algorithm (Successive Projections Algorithm) (Araújo et al., 2001) was used to perform the variable selection for the models built using MLR. In the case of the models developed by the PLS regression, the number of latent variables was determined according to the RMSECV values in the internal validation step. In this step, the systematic "venetian blinds" method was used to select the internal validation subsets, using 10 % of the samples from each subset to perform the predictions. For the models developed by the LS-SVM regression, the values of the gamma (γ) and quadratic sigma (σ^2) parameters were optimized in order to achieve the minimum value of RMSECV. Compression of the original spectral data was performed using the PLS regression with different numbers of latent variables. The Support Vector Machine (SVM) used was the "Epsilon-SVR" type, using a Radial Basis Function (RBF) as core function. Outliers were identified and removed using the values of Hotelling T^2 and the Quadratic Sum of the Residuals. Predictive performance of the calibration models, built using the MLR, PLS and LS-SVM methods was evaluated in the validation (prediction) step, using a set of independent samples, considering the values of the Root Mean Square Error of Prediction (RMSEP), R^2 and bias. Scatter plots between reference and predicted values of the parameters were constructed to assist in the results visualization.

For the second step, i.e, the calibration transfer step, the Direct Standardization (DS) method was used (Wang et al., 1991). It consists of directly relating the response of a sample measured with one instrument to its response obtained on another instrument. This linear relationship is described by a transformation matrix F (Feudale et al., 2002). The benchtop spectrometer (XDS) was treated as the primary instrument (master) and the handheld spectrometer (MicroNIR) as secondary (slave). Therefore, the spectra of the handheld instrument were transformed (standardized) in order to use the models previously developed using the spectra from the benchtop instrument.

Ninety-three (93) apples (the samples set from study 1), whose spectra were recorded in the two spectrometers, were used in this step. The SPXY algorithm (Galvão et al., 2005) was used to select transfer samples (n = 30) and prediction samples (n = 63 for SSC, TA and SII; n = 43 for PF).

It was necessary to perform a wavelength interpolation procedure, because the number of wavelengths in the same spectral range (1100−1600 nm) were different for the two spectrometers. Thus, the spectra obtained from the XDS spectrometer, corresponding to 251 wavelengths registered at 2 nm intervals, were transformed to 82 wavelengths registered at 6.3 nm intervals, exactly matching the spectra obtained from the MicroNIR spectrometer. This procedure was necessary to determine the RMSEP^S_P values (RMSEP values obtained by the prediction set of the secondary instrument using the model build for the

primary instrument).

Calculations were performed using the MATLAB software version 2010a (Mathworks, Natick, MA, USA) and the PLS_Toolbox version 8.2 (Eigenvector Research, Manson, WA, USA). The graphical interface for MATLAB "SPA_GUI" (available at http://www.ele.ita.br/~kawakami/eng) was used to perform the variables selection by the SPA algorithm.

3. Results and discussion

3.1. Characterization of the spectral data

Fruits are composed of around 80–90 % water and the remaining fraction is composed of different compounds, such as carbohydrates, proteins, organic acids and other minor constituents (Gómez et al., 2006). Therefore, their spectra in the NIR region show wide and complex absorption bands, resulting from the overlapping of bands corresponding to overtones and combinations of fundamental vibrational modes, mainly attributed to the O—H, C–H and NH— bonds (Golic et al., 2003; Magwaza et al., 2012). These characteristics can be visualized in Fig. 1, which shows the VIS-NIR absorption spectra (raw data) from the 866 intact apples, recorded in the range between 400 and 2500 nm using the XDS spectrometer. The highlighted region corresponds to the spectral range recorded by the MicroNIR spectrometer, between 1100 and 1600 nm.

The water absorption bands are normally wide and centered at approximately 970, 1450 and 1940 nm. Indeed, in the spectral range used in this study, it is possible to observe all these characteristic water absorption bands. The bands centered around 1450 and 970 nm are related to the first and second overtones of the O—H stretch, respectively. The band centered near 1940 nm is related to the combination of the asymmetric stretch and bending of the water molecules (Weyer and Lo, 2002) (Fig. 1).

Organic acids usually present bands related to the O—H group. These bands are centered near 1445 nm, 1000 nm and 800 nm and correspond to the first, second and third overtones, respectively (Weyer and Lo, 2002). In this case, these bands are also overlapped with bands attributed to water (Fig. 1). In addition, the organic acids exhibit a characteristic band centered in the vicinity of 1890 nm, which is associated with the combination between the stretching of O—H and C=O bonds.

Starch and sugars found in fruit, such as sucrose, glucose and fructose, have absorption bands difficult to visualize because they are very close to the regions where the water has a strong absorption (Fig. 1) (Delwiche et al., 2008). In general, these bands come from the second (920 nm) and third (720 nm) overtones of O—H stretching vibrations, and third (910 nm) and fourth (750 nm) overtones of C—H stretching vibration (Golic et al., 2003). Additionally, the absorption band centered around 1190 nm corresponds to the second C—H overtone

regions and is associated with the presence of sugars (Osborne et al., 1993).

3.2. Reference analyses

The samples used in this study showed variability for the quality parameters evaluated, which can be attributed to the different stages of ripening and the great number of apple varieties. Statistical parameters of the reference data of apple fruit samples are described in Table 1.

An important factor that must be evaluated prior to the building of the calibration models is the existence of correlation between the different quality parameters determined through the reference analyses. Indirect determination of one or more parameters through another may occur due the correlations between these parameters, leading to possible misinterpretations about the predictive models. In this study, the Pearson correlation coefficient was used to check the possible correlations. No significant correlation was found (data not show).

3.3. Study 1: comparing analytical performance between benchtop and handheld spectrometers

Initially, a study was carried out to evaluate the feasibility of the handheld spectrometer to estimate quality parameter of apples. For comparison purposes, models were also built using the data set acquired from the benchtop instrument in two spectral ranges: one covering the visible and NIR range (400−2500 nm) and the other covering the same range as the handheld (1100−1600 nm). The same set of apples ($n = 93$, from 2 different varieties) was analyzed using both instruments (XDS and MicroNIR). Multivariate calibration models were built using PLS regression for the determination SSC, TA, PF, and SII. Prediction performances of the all models in the internal validation step were satisfactory, in terms of the RMSECV and R^2 values (Table 2). Additionally,

Table 1

Statistical parameters of the quality parameters Soluble Solids Content (SSC), Titratable Acidity (TA), Pulp Firmness (PF), and Starch-Iodine Index (SII) of apple fruit samples used in this study.

Parameter	Min.[a]	Max.[b]	Mean[c]	Std[d]
SSC	7.8	24.1	12.3	2.0
TA	0.9	28.4	6.7	2.9
PF	1.5	12.7	7.3	2.1
SII	2	10	8	2

[a] Minimum value for the parameter.
[b] Maximum value for the parameter.
[c] Mean value for the parameter.
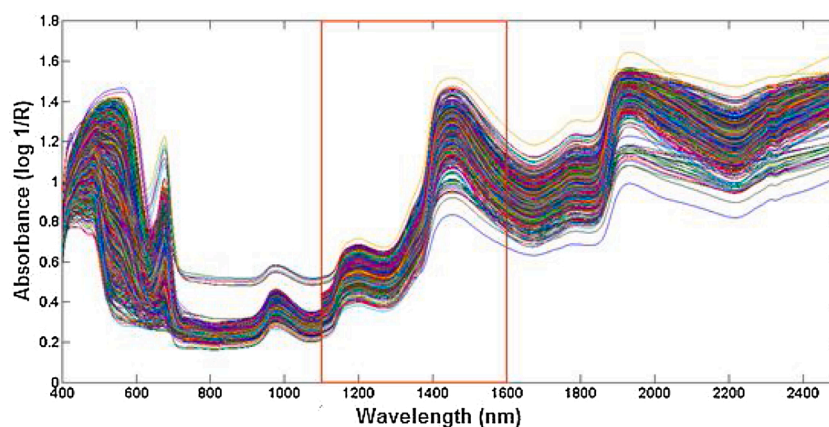[d] Standard deviation for the parameter.

Fig. 1. Raw Vis-NIR absorption spectra of 866 intact apples fruit in the 400 and 2500 nm region, recorded using the XDS spectrometer. The highlighted region corresponds to the spectral range recorded by the MicroNIR spectrometer.

Table 2

Internal validation step results for the PLS models developed to predict Soluble Solids Content (SSC), Titratable Acidity (TA), Pulp Firmness (PF), and Starch-Iodine Index (SII) in apples using the XDS (in two different spectral ranges) and MicroNIR spectrometers and SNV as pre-processing method.

Parameter	Instrument / Spectral range	Internal Validation							
		Min.[a]	Max.[b]	n[c]	Outliers[d]	LV[e]	RMSECV	R²	Bias
SSC	XDS 400−2500 nm	9.4	16.2	91	2 (2.2)	5	0.56	0.91	−0.005
	XDS 1100−1600 nm	9.4	16.2	90	3 (3.3)	7	0.62	0.89	0.010
	MicroNIR 1100−1600 nm	9.4	17.1	90	3 (3.3)	6	0.57	0.91	0.016
TA	XDS 400−2500 nm	4.5	12.1	87	6 (6.9)	10	0.83	0.76	0.012
	XDS 1100−1600 nm	4.5	12.1	88	5 (5.7)	9	0.88	0.71	0.016
	MicroNIR 1100−1600 nm	4.5	11.1	87	6 (6.9)	9	0.80	0.76	0.025
PF	XDS 400−2500 nm	5.80	10.45	69	4 (5.8)	10	0.58	0.69	−0.002
	XDS 1100−1600 nm	5.80	10.10	72	1 (1.4)	9	0.49	0.74	0.010
	MicroNIR 1100−1600 nm	5.80	10.45	70	3 (4.3)	9	0.50	0.75	−0.020
SII	XDS 400−2500 nm	4.5	12.1	87	6 (6.9)	10	0.83	0.76	0.012
	XDS 1100−1600 nm	4.5	12.1	88	5 (5.7)	9	0.88	0.71	0.016
	MicroNIR 1100−1600 nm	4.5	11.1	87	6 (6.9)	9	0.80	0.76	0.025

[a] Minimum value for the parameter.
[b] Maximum value for the parameter.
[c] Number of samples used.
[d] Number of anomalous samples and percentage in relation to the total number of samples.
[e] Number of latent variables used in the PLS models.

low bias values were observed, showing no evidence of systematic errors in the models (Table 2). The best results were obtained using SNV as preprocessing. Therefore, only the results with this method are shown.

A comparison was accomplished between the RMSECV values provided by the models for each quality parameter evaluated. The comparison was performed considering the two instruments and their respective spectral range, as well as the different preprocessing techniques employed. As observed in Table 2, the coefficient of determination and the RMSECV values obtained with the PLS models were similar regardless of the instrument (XDS or MicroNIR) or spectral range for each quality parameter analyzed. Therefore, we concluded that the MicroNIR spectrometer offers similar performance to the XDS spectrometer for determining the quality parameters of apples evaluated in this study. Malegori et al. (2017) also highlighted the suitability of MicroNIR for monitoring chemical parameters (titrable acidity and ascorbic acid) in acerola fruit and showed comparable results of models developed using the benchtop FT-NIR and the portable instrument. However, the results of this study related to laboratory application

where vibration and ambient conditions were kept under control. Spectral analyses in the field (or on-tree) are more complicated because they are potentially sensitive to diurnal changes of sunlight and temperature conditions that can influence instrument performance and lead to inferior predictive performance compared to laboratory conditions, as highlighted by Fan et al. (2020). Further work should be focused on on-tree applications of the MicroNIR to confirm its good performance to determine the quality parameters of apples in practical situations *i.e.* for pre-harvest in-field measurements.

3.4. Study 2: Calibration transfer between benchtop and handheld spectrometers

The results obtained in this study were divided into two sections (3.4.1 and 3.4.2) corresponding to the two steps described in materials and methods.

Table 3

Statistical parameters related to the calibration and external validation steps for the determination of SSC, TA, PF, and SII using SNV as spectral preprocessing and the PLS, SPA-MLR and LS-SVM regression methods for build the multivariate calibration models.

Parameter/ Method	Range	Calibration								External validation (prediction)					
		n[a]	Outliers[b]	V[c]	γ	σ^2	R²	RMSEC	Bias	n[d]	Outliers	R²	RMSEP	Bias	RMSEPr[e]
Soluble Solids Content (%)															
PLS		396	16 (3.9)	6	–	–	0.61	1.0	0.000	176	1 (0.6)	0.65	1.0	0.006	6.3
SPA-MLR	7.8 - 24.1	411	1 (0.2)	12	–	–	0.64	0.8	0.000	176	1 (0.6)	0.70	0.9	0.003	5.6
LS-SVM		408	4 (1.0)	15	10	0.01	0.81	0.7	0.040	176	1 (0.6)	0.73	0.7	0.098	4.4
Titratable acidity (mEq malic acid L^{-1})															
PLS		407	13 (3.1)	6	–	–	0.18	1.79	0.000	169	8 (4.5)	0.24	1.03	−0.055	14.4
SPA-MLR	0.90 - 13.40	405	15 (3.6)	30	–	–	0.58	1.24	0.000	172	5 (2.8)	0.53	1.00	−0.042	14.0
LS-SVM		405	15 (3.6)	12	10	0.1	0.95	0.44	0.026	175	1 (0.6)	0.68	0.89	0.126	12.4
Pulp Firmness (kg cm^{-2})															
PLS		402	13 (3.2)	10	–	–	0.56	1.47	0.000	177	2 (1.1)	0.52	1.38	0.046	18.6
SPA-MLR	2.1 - 12.7	415	0 (0)	21	–	–	0.59	1.43	0.000	179	0 (0)	0.55	1.23	−0.080	16.6
LS-SVM		413	2 (0.5)	12	3.16	0.01	0.94	0.54	−0.005	179	0 (0)	0.74	0.99	0.084	13.4
Starch-Iodine Index															
PLS		213	12 (5.3)	8	–	–	0.44	1.19	0.000	99	1 (1)	0.37	1.30	−0.543	21.7
SPA-MLR	3−9	225	0 (0)	22	–	–	0.57	1.03	0.000	100	0 (0)	0.56	1.18	−0.327	19.7
LS-SVM		225	0 (0)	16	10	0.01	0.72	0.83	0.075	100	0 (0)	0.73	0.84	−0.332	14.0

[a] Number of samples used in the calibration step excluding the outliers.
[b] Number of anomalous samples and percentage in relation to the total number of samples.
[c] Number of variables used: for PLS represents the number of latent variables, for SPA-MLR represents the number of spectral variables, and for LS-SVM represents the number of latent variables in the PLS model used for data compression.
[d] Number of samples used in the external validation stage, excluding outliers.
[e] Relative RMSEP calculated in relation to the mean value of the range for the quality parameter evaluated, expressed in percentage.

3.4.1. Multivariate calibration using the XDS spectrometer

In this study, a set of apples ($n = 773$) from 48 varieties analyzed by means of the XDS spectrometer was used to build the multivariate calibration models using the PLS, SPA-MLR and LS-SVM regression methods. The quality parameters evaluated were SSC, TA, PF, and SII. The models were built using the spectral range between 1100 and 1600 nm and SNV as preprocessing technique. Statistical parameters related to the calibration and external validation (prediction) steps are shown in Table 3.

Calibration models developed using the PLS, SPA-MLR and LS-SVM for SSC determination presented satisfactory predictive performance, with RMSEPr values (relative RMSEP, calculated in relation to the mean value of the range of the quality parameter) ranging from 4.4 % for LS-SVM up to 6.3 % for PLS. The values of R^2 were also satisfactory, ranging from 0.73 for LS-SVM to 0.65 for PLS. Predicted *versus* reference plot for SSC is shown in Fig. 2 A, B, C. The comparison of the prediction statistics between models showed that LS-SVM gave rise to the higher R^2 and the lowest error or prediction. Therefore, the model developed by LS-SVM showed a better predictive performance compared to the models developed by PLS and SPA-MLR. It must be mentioned that performances of current calibration models for SSC were poorer that those obtained in previous study (Pissard et al., 2013).

Calibration models developed by the three methods for TA determination showed similar predictive performance, with RMSEPr values varying from 12.4 % for LS-SVM to 14.4 % for PLS. R^2 values of prediction were also similar for LS-SVM (0.68) and SPA-MLR (0.53), but lower for the PLS model (0.24). The predicted *versus* reference plot for TA is shown in Fig. 2 D, E, F. As observed in Table 3, the RMSEP values from the different calibration methods used for TA determination were very similar.

The calibration model developed for the determination of PF by LS-SVM presented satisfactory predictive performance, showing RMSEPr with a value of 13.4 %, whereas this parameter presented higher values for the models developed by PLS (18.6 %) and SPA- MLR (16.6 %). R^2 values were similar for PLS (0.52) and SPA-MLR (0.55), and higher for LS-SVM (0.74), indicating the better ability of this regression method to explain the total data variance. Again, the comparison of the statistics of prediction between models showed that LS-SVM gave rise to the higher

R^2 and the lowest error of prediction, suggesting its better predictive performance for the determination of PF.

The employment of SNV to perform preprocessing of the spectral data used to build the calibration models for PF prediction should be noted. Since this parameter corresponds to a physical property of the sample, initially the raw spectra were used for the modeling to avoid the removal of information of a physical nature contained in the spectra. The predictive performance of the model developed, however, was better when SNV was used as preprocessing. This fact suggests that the PF is possibly being determined indirectly by means of information concerning, predominantly, the chemical composition of the samples. Although relevant, a detailed explanation of the observed fact is beyond of the scope of this study and should be explored in future studies. Non-invasive techniques to measure the fruit firmness have been investigated by Subedi and Walsh (2009) where they evaluated a sound velocity technique and visible-shot wave near infrared spectroscopy for the assessment of fruit firmness.

The calibration model developed for SII determination using LS-SVM method showed satisfactory predictive performance. The RMSEPr value was 14.0 %, whereas this parameter presented higher values for the models developed by the PLS (21.7 %) and SPA- MLR (19.7 %) methods. The R^2 values of prediction increased as follows: 0.37 for PLS, 0.56 for SPA-MLR and 0.73 for LS-SVM. The high values of RMSEPr provided by the PLS and SPA-MLR models will probably make their practical applications unfeasible. A similar situation was found by Marques et al. (2016) with mango samples. In that study, calibration models built for TA and PF determination in mango failed to predict these parameters during the fruit ripening. This fact was attributed to high values of the relative prediction errors (RMSEPr about 20 %).

The comparison between the RMSEP values obtained by the different calibration methods used for SII determination showed higher values with PLS and SPA-MLR compared to LS-SVM. Therefore, the model developed by LS-SVM had better predictive performance compared to the models developed by PLS and SPA-MLR.

Regarding the bias, the samples were generally well distributed along the regression line and there was no evidence of significant systematic errors in the models built for the determination of SSC, TA and PF, considering the three regression method employed. For the
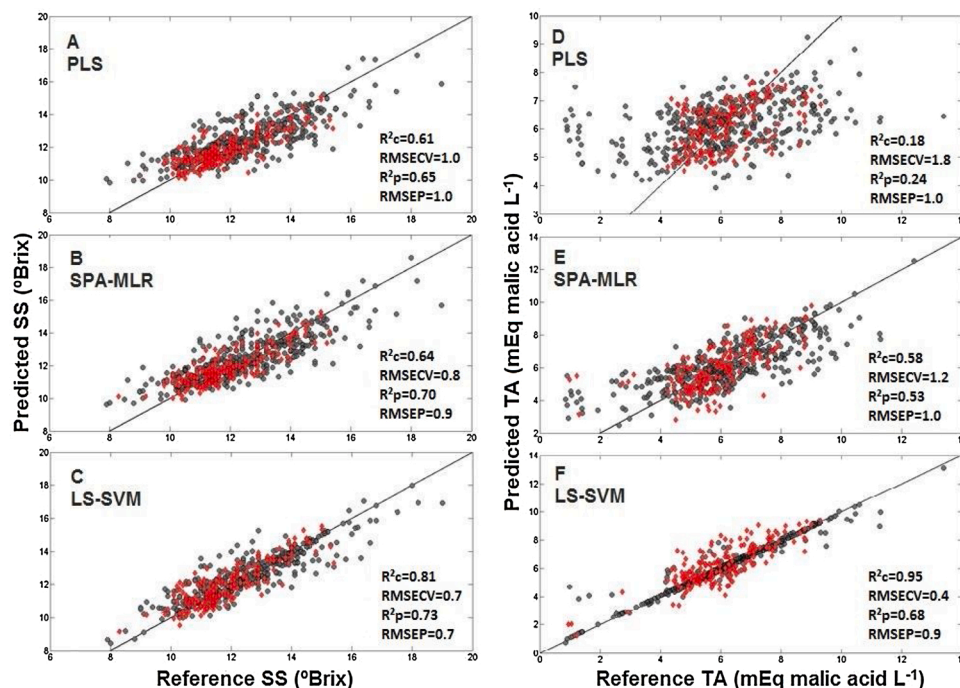

Fig. 2. Predicted *versus* reference plots from calibration (black symbols) and external validation (red symbols). The solid line is the bisectrix. (A), (B) and (C) correspond to the Soluble Solids Content (SSC) determination using the PLS, SPA-MLR and LS-SVM methods, respectively. (D), (E) and (F) correspond to the Titratable Acidity (TA) determination using the PLS, SPA-MLR and LS-SVM methods, respectively. R^2c = coefficient of determination of calibration; R^2p = coefficient of determination of prediction. (For interpretation of the references to colour in the Figure, the reader is referred to the web version of this article).

parameter SII, however, higher bias value was observed.

In general, the models developed by means of the LS-SVM regression showed better predictive performance in comparison to the models developed using the PLS regression and SPA-MLR. The LS-SVM method showed significantly lower RMSEP values for most quality parameters evaluated. The superiority of SVM compared to PLS has already been demonstrated for quality parameters of apples (Liu and Zhou, 2013; Pissard et al., 2013). It has also been highlighted in the quality analysis of other fruit, *i.e.* for the evaluation of acerola fruit quality (Malegori et al., 2017), for the determination of total soluble solids content in grapes (Xiao et al., 2017) and for sugar content of mango (Al-Sanabani et al., 2019). Chauchard et al. (2004) also compared classical linear regression techniques (PLSR and MLR) and LS-SVM regression for the prediction of total acidity in fresh grapes. LS-SVM regression produced a more accurate prediction. The overall performance of the calibration models developed by the LS-SVM over those developed by the PLS and SPA-MLR can be attributed to the ability of this method to describe nonlinear relationships between spectral data and the reference values of the evaluated parameters. It is likely that the large number of samples and varieties of apples (characterizing a complex data set) used in this study resulted in considerable deviations from linearity in the relationship between the independent (X) and dependent (Y) variables. In general, deviations from linearity are expected in spectroscopic analyses of complex matrices, such as foods, plant tissues and soils (Souza et al., 2012).

3.4.2. Calibration transfer

Calibration models previously described (in Section 3.4.1) and a set of independent samples ($n = 93$, not used for building these models) were used in this study. This set was divided into transfer samples ($n = 30$) and prediction samples ($n = 63$ or $n = 43$, depending on the quality parameter evaluated) by means of the SPXY algorithm. SNV was applied for spectral preprocessing.

Calibration models developed using the SPA-MLR method were more sensitive to changes in the instrumental responses when compared to the models developed using the PLS and LS-SVM methods (Table 4). This fact can be verified due to the high $RMSEP^S_P$ (RMSEP value obtained by the prediction set of the secondary instrument using the model build for the primary instrument) values, when compared to the $RMSEP^P_P$ (RMSEP value obtained by the prediction set of the primary instrument using the model built for this instrument) values for the SPA-MLR method. In contrast, the models developed by the LS-SVM method were less sensitive, so that $RMSEP^P_P$ and $RMSEP^S_P$ showed close values. This behavior can be attributed to the high generalization capacity, which is an intrinsic characteristic of the Support Vector Machines (Ferrão et al., 2007). Thus, calibration models developed by the LS-SVM method generally have a reasonably predictive performance for samples not belonging to the calibration and/or validation sets, and, in the present case, for spectra obtained by a different instrument.

Results for the calibration transfer procedure using the DS method can be visualized in Fig. 3. In these graphs, the values of $RMSEP^{S-DS}_P$ (RMSEP value obtained by the prediction set of the secondary instrument standardized by the DS method, applied to the model calculated in the primary instrument – represented by the solid black line) are presented as function of the number of transfer samples ($n = 2$ to $n = 30$). The dashed green line located at the bottom of the graphs represents the value of $RMSEP^P_P$. The dashed red line located at the top of the graphs represents the value of $RMSEP^S_P$.

It is possible to observe that two transfer samples were already sufficient to significantly reduce the RMSEP values for the models built using the PLS and SPA-MLR methods for all quality parameters (Fig. 3). In this case, the relative reductions between the two procedures (with and without calibration transfer) varied from 74 % for SII determination by the PLS method to 93 % for TA determination by the SPA-MLR method. In general, the $RMSEP^{S-DS}_P$ values for the models built using the PLS and SPA-MLR methods stabilized after the use of six transfer

RMSEP	PLS	SPA-MLR	LS-SVM
Soluble Solids Content (%)			
$RMSEP^P_P$ [a]	1.10 (6)[e]	1.10 (12)[f]	0.90 (15)[g]
$RMSEP^S_P$ [b]	7.70	11.30	2.00
$R^{2\ P}_{\ \ P}$ [c]	0.70	0.78	0.81
$R^{2\ S}_{\ \ P}$ [d]	0.38	0.49	0.62
Titratable acidity (mEq malic acid L^{-1})			
$RMSEP^P_P$	1.55 (6)	1.67 (30)	1.75 (12)
$RMSEP^S_P$	9.38	35.06	2.41
$R^{2\ P}_{\ \ P}$	0.30	0.65	0.78
$R^{2\ S}_{\ \ P}$	0.24	0.40	0.55
Pulp Firmness (kg cm^{-2})			
$RMSEP^P_P$	1.25 (10)	1.52 (21)	1.24 (12)
$RMSEP^S_P$	22.73	12.20	1.38
$R^{2\ P}_{\ \ P}$	0.50	0.56	0.77
$R^{2\ S}_{\ \ P}$	0.33	0.42	0.54
Starch-Iodine Index			
$RMSEP^P_P$	1.88 (8)	1.73 (22)	1.42 (16)
$RMSEP^S_P$	9.20	16.71	2.63
$R^{2\ P}_{\ \ P}$	0.40	0.52	0.70
$R^{2\ S}_{\ \ P}$	0.28	0.36	0.51

[a] RMSEP value obtained by the prediction set of the primary instrument using the model calculated in this instrument.

[b] RMSEP value obtained by the prediction set of the secondary instrument using the model calculated in the primary instrument.

[c] R^2 value obtained by the prediction set of the primary instrument using the model calculated in this instrument.

[d] R^2 value obtained by the prediction set of the secondary instrument using the model calculated in the primary instrument.

[e] Number of latent variables in the PLS model.

[f] Number of spectral original variables used in the SPA-MLR model.

[g] Number of latent variables in the PLS model used for the data compression in the LS-SVM model.

samples, remaining very close to $RMSEP^P_P$ values.

In the case of the calibration models developed by the LS-SVM method, the $RMSEP^{S-DS}_P$ values also showed fewer oscillations after the use of about 20 transfer samples (Fig. 3). However, the reductions in the RMSEP values were not very significant in comparison to the values obtained without applying the calibration transfer procedure. The relative reductions between the two procedures ranged from 10 % for PF determination to 60 % for SSC determination. This fact was expected, since the calibration models developed using the LS-SVM method presented a much better predictive performance than the models developed using the PLS and SPA-MLR methods without prior application of the calibration transfer procedure. This fact was confirmed through the low $RMSEP^S_P$ values obtained, which were very similar to the $RMSEP^P_P$ values.

Results obtained in this study showed that the DS method was successful as transfer method. DS is one of the most used methods for data standardization. Xiao et al. (2017) proposed a modified piecewise direct standardization (PDS) to solve the problem of transfer between different instruments of different types as well as with different number of wavelengths. They concluded that linear interpolation-PDS can solve the difficulty caused by resolution difference and performed better than the traditional wavelengths-reserved method. Hayes et al. (2016) also obtained good results with PDS in a similar transfer between photodiode array instruments for total soluble solids measurement in intact apple fruit. Pu et al. (2018) tested different standardization methods and showed that PDS performed better than DS. In this study, only DS was used to test the feasibility of transferring calibration models between the benchtop and a handheld spectrometer. It is possible that standardization methods based on another algorithm would give even more effective results than those achieved with a simple DS algorithm. In addition, regarding the spectral pre-processing, the SNV pre-treatment was used in this study without testing any other one. However, the use of
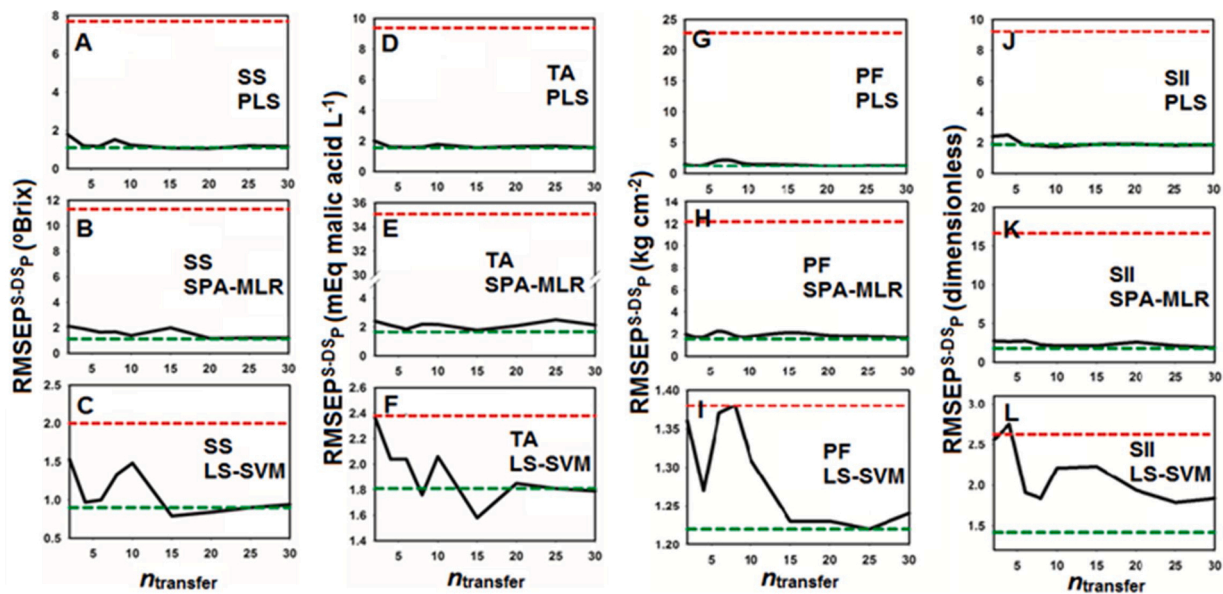
Fig. 3. $RMSEP^{S-DS}_P$ values (continuous black line) obtained as a function of the number of transfer samples ($n = 2$ to $n = 30$). Graphs (A), (B) and (C) refer to calibration models for Soluble Solids Content (SSC) determination, (D), (E) and (F) for Titratable Acidity (TA) determination, (G), (H) and (I) for Pulp Firmness (PF) determination, (J), (K) and (L) for Starch-Iodine Index (SII) determination. Calibration models were built using the PLS, SPA-MLR and LS-SVM methods. The dashed green line located at the bottom of the graphs represents the value of $RMSEP^P_P$. The dashed red line located at the top of the graphs represents the value of $RMSEP^S_P$. (For interpretation of the references to colour in the Figure, the reader is referred to the web version of this article).

appropriate spectral pre-processing can make calibration models more transferable (Soldado et al., 2013). Further investigations could be focused on considering more standardization methods and more advanced spectral pre-treatments to improve the transfer performance.

4. Conclusion

In the first study presented, a comparison between the analytical performance of the benchtop (XDS) and handheld (MicroNIR) spectrometers for the determination of soluble solids content, titratable acidity, pulp firmness, and starch-iodine index in apples was accomplished. It was found that the predictive performance of the calibration models developed were similar, since the RMSECV values were comparable. Therefore, the MicroNIR spectrometer offered equivalent performance to the benchtop spectrometer for the determination of the quality parameters evaluated.

In the second study presented, calibration models were developed using different regression methods (PLS, SPA-MLR and LS-SVM) for determining apple quality using a historical and very large database acquired using the benchtop spectrometer. Models developed using the LS-SVM method presented better predictive performance, showing significantly lower RMSEP values for most of the quality parameters evaluated. Additionally, the possibility of calibration transfer between the benchtop and handheld spectrometers was evaluated in the context of the determination of quality parameters in apples. Here, the Direct Standardization method was used successfully to perform the calibration transfer procedure. This method enabled a significant reduction of the RMSEP values for both the PLS and SPA-MLR models. However, the reduction of the RMSEP values was not so evident for the LS-SVM models. This fact was attributed to the high generalization capacity of this regression method, which made it possible to obtain closer $RMSEP^S_P$ and $RMSEP^P_P$ values, even without the application of the calibration transfer methods.

In general, it was found that a simple calibration transfer method was able to allow the data recorded using the handheld spectrometer to be used in the models developed by the benchtop spectrometer. In this way, the historical database registered over several years with the benchtop instrument could be used, eliminating the need to acquire a new

database and, thereby offering opportunities for faster direct analysis of apples at the orchard with the use of robust models.

CRediT authorship contribution statement

Audrey Pissard: Investigation, Formal analysis, Writing - original draft, Writing - review & editing. **Emanuel José Nascimento Marques:** Investigation, Formal analysis, Writing - original draft. **Pierre Dardenne:** Supervision. **Marc Lateur:** Resources. **Celio Pasquini:** Conceptualization, Methodology, Supervision, Project administration. **Maria Fernanda Pimentel:** Conceptualization, Methodology, Supervision, Project administration. **Juan Antonio Fernández Pierna:** Methodology, Supervision, Formal analysis, Writing - review & editing. **Vincent Baeten:** Conceptualization, Methodology, Supervision, Project administration.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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