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# Non-destructive assessment of quality traits in apples and pears using near infrared spectroscopy and chemometrics

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**Abstract -** The objective of this study was to evaluate the performance of a handheld NIR spectrometer for non-destructive quality analysis of apples and pears produced in the Brazilian Semi-arid region. NIR spectra were acquired with a portable spectrometer in the wavelength range of 750–1065 nm and reference analyses of dry matter content (DMC) and soluble solids content (SSC) were measured weekly during 10 weeks of storage at 0.5 °C. Spectra were pre-processed with standard normal variate and used to develop DMC and SSC models using partial least squares regression with full cross-validation. The models were validated using data not included in the calibration. Satisfactory prediction results were obtained for SSC in apples ($R^2$ = 0.58) and pears ($R^2$ = 0.55), and for DMC in apples ($R^2$ = 0.55) and pears ($R^2$ = 0.65). All prediction models showed a relative root mean square error of prediction lower than 8%. These findings indicate that the NIR spectrometer is a promising tool to be used for a rapid and non-destructive determination of internal quality traits in apples and pears.

**Index terms:** partial least squares regression, multivariate regression, fruit quality, soluble solids, dry matter.

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# Avaliação não destrutiva de atributos de qualidade em maçãs e peras usando espectroscopia no infravermelho próximo e quimiometria

**Resumo -** O objetivo deste estudo foi avaliar o desempenho de um espectrômetro portátil NIR na análise não destrutiva da qualidade de maçãs e peras produzidas na região semiárida brasileira. Os espectros NIR foram coletados com um espectrômetro portátil na faixa de comprimentos de onda de 750–1.065 nm, e as análises de referência de conteúdo de matéria seca (CMS) e conteúdo de sólidos solúveis (CSS) foram mensurados semanalmente durante 10 semanas de armazenamento a 0,5 °C. Os espectros foram pré-processados com a variação normal padrão e utilizados para desenvolver modelos de CMS e CSS usando a regressão dos quadrados mínimos parciais com validação cruzada completa. Os modelos foram validados externamente usando dados não incluídos na calibração. Resultados de predição satisfatórios foram obtidos para CSS em maçãs ($R^2$ = 0.58) e peras ($R^2$ = 0.55), e para CMS em maçãs ($R^2$ = 0.55) e peras ($R^2$ = 0.65). Todos os modelos de predição apresentaram raiz quadrada do erro médio quadrático de predição relativo menor que 8%. Estes resultados indicam que o espectrômetro NIR é uma ferramenta promissora para uma determinação rápida e não destrutiva dos atributos de qualidade interna de maçãs e peras.

**Termos para indexação:** regressão por quadrados mínimos parciais, regressão multivariada, qualidade do fruto, sólidos solúveis, matéria seca.

Apples and pears are temperate fruit that require chilling environmental conditions to break tree dormancy and produce flowers and fruit. Although apple and pear production is mostly located in the Southern region of Brazil, low chilling requirement cultivars associated with crop management techniques have allowed the production of these fruit species in warmer regions, such as the Northeastern region of Brazil (LOPES et al., 2013).

Sweetness is the major determinant of fruit quality for consumers (MUSACCHI; SERRA, 2018). In addition, fruit dry matter content (DMC) has also been suggested as an important quality index highly correlated with soluble (sugars) and insoluble (starch, cellulose, hemicellulose, pectin, and lignin) carbohydrates in the fruit (MUSACCHI; SERRA, 2018). Indeed, studies have shown that fruit with higher DMC have higher consumer acceptance (FREITAS et al., 2022). However, the methods used to measure DMC and SSC are destructive, time consuming, and require sample processing and manual labor (MARQUES et al., 2016; VILVERT et al., 2021). In this context, near infrared spectroscopy (NIRS) can be a precise, accurate, fast, reliable, and non-destructive tool for assessing internal quality (OLIVEIRA et al., 2014; LI et al., 2017; ANYIDOHO et al., 2021) in a wide range of fresh and processed fruit and vegetables (PISSARD et al., 2021).

The non-destructive measurement of fruit quality traits by NIR spectroscopy occurs by the interaction between infrared radiation and molecular groups such as C–H, C–O and O–H, key constituents of water, sugars and acids (OLIVEIRA et al., 2014). Recent studies have shown high precision in determining internal fruit quality with low-cost portable NIR spectrometers, which can be used at any point along the production chain, from farms to distribution centers around the world (WALSH et al., 2020). In Brazil, NIRS has been used to monitor mango DMC on-farm and in packing houses to guarantee high-quality fruit to consumers (FREITAS et al., 2022; MARQUES et al., 2016).

The objective of this study was to evaluate the performance of a handheld NIR spectrometer for non-destructive quality analysis of apples and pears produced in the Brazilian Semi-arid region.

A total of 100 'Eva' apples and 100 'Triunfo' pears were harvested from an experimental orchard in Petrolina, PE, Brazil (9°09' S latitude, 40°22' W longitude, and an altitude of 365.5 m). The climate of the region is BSh (semi-arid), according to Köppen's climate classification.

The fruit were harvested at physiological maturity, washed, dried, and stored at 0.5 °C and 90% RH. Every week, 10 fruit of both species were taken for measurement of spectral data and reference analysis.

The NIR spectral data were registered using a handheld NIR spectrometer F-750 Produce Quality Meter (Felix Instruments, Portland, USA). Spectral acquisition was performed on the equatorial region of each fruit by positioning the spectrometer directly on the fruit skin. The measurements were taken at three different temperatures (2° C, 10° C, and 20 °C) (Figure 1).

Reference analyses were performed on the same fruit region used for spectra acquisition. Two samples of 2 × 2 × 1 cm per fruit were used for reference analysis, one for determination of soluble solids content (SSC) by refractometry, and the other for dry matter content (DMC) determination after drying the samples at 65 °C.

Multivariate calibration models were developed using the spectral range from 750 to 1065 nm. Standard normal variate (SNV) transformation was applied to the spectral data to eliminate radiation scattering effects. The samples were divided into two independent groups, being 70% for calibration and 30% for validation. The models for the prediction of DMC and SSC were built through partial least squares (PLS) regression.

The optimal number of latent variables (LV) was determined according to the root mean square error of cross-validation (RMSECV), using full cross-validation. The identification and removal of anomalous samples (outliers) were performed considering the limit values set automatically by the software, based on the graph of the Hotelling $T^2$ *versus* the quadratic sum of the residuals (Q) (MARQUES; FREITAS, 2020).

The performance of the multivariate models for predicting quality traits in apples and pears was evaluated by the RMSECV, the root mean square error of prediction (RMSEP), and the coefficient of determination ($R^2$). Relative RMSEP (or $RMSEP_r$, in percentage) was calculated by dividing RMSEP by mean values of reference analysis.

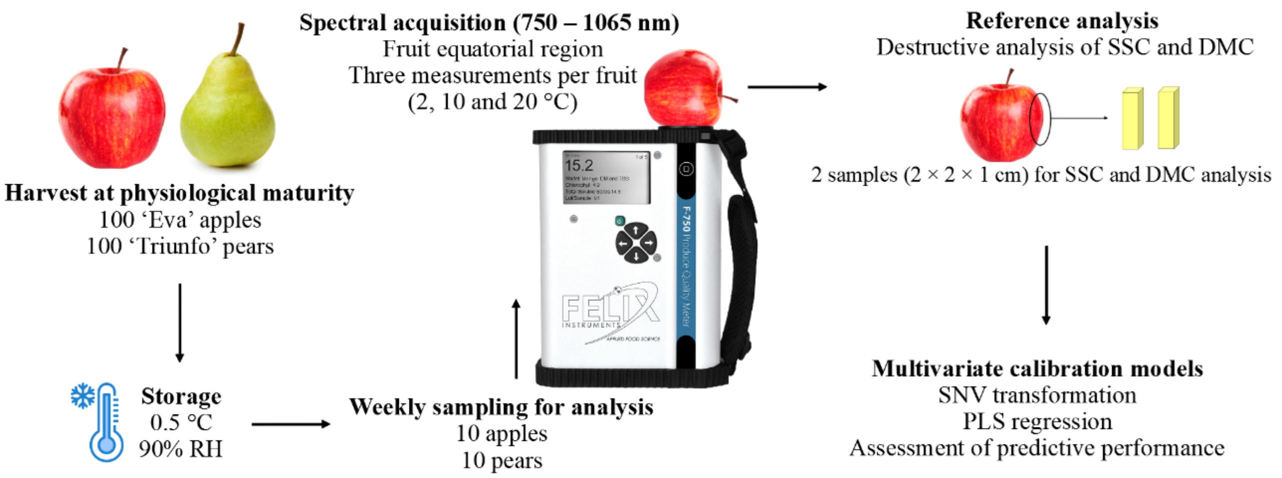


**Figure 1**. Schematic representation of spectra acquisition and data analysis.

Raw spectra and SNV pretreated spectra for all the apple and pear samples are shown in Figure 2. Intense absorption bands were found in the range of 920–1050 nm, which corresponds to the water absorption bands, related to the second overtone of the O–H stretch (XIAOBO et al., 2010). The NIR spectra absorption band around 970 nm reflects the high moisture content in apples (BOBELYN et al., 2010; IGNAT et al., 2014) and pears (TRAVERS et al., 2014; LEE; HAN, 2016).

'Eva' apples had a mean SSC of 14.91% (Table 1), close to previous results observed by Miranda et al. (2015) in the same cultivar. 'Triunfo' pears showed a mean SSC of 12.28% (Table 1), which is consistent with a previous report of the same cultivar and growing conditions (SANTOS et al., 2019).

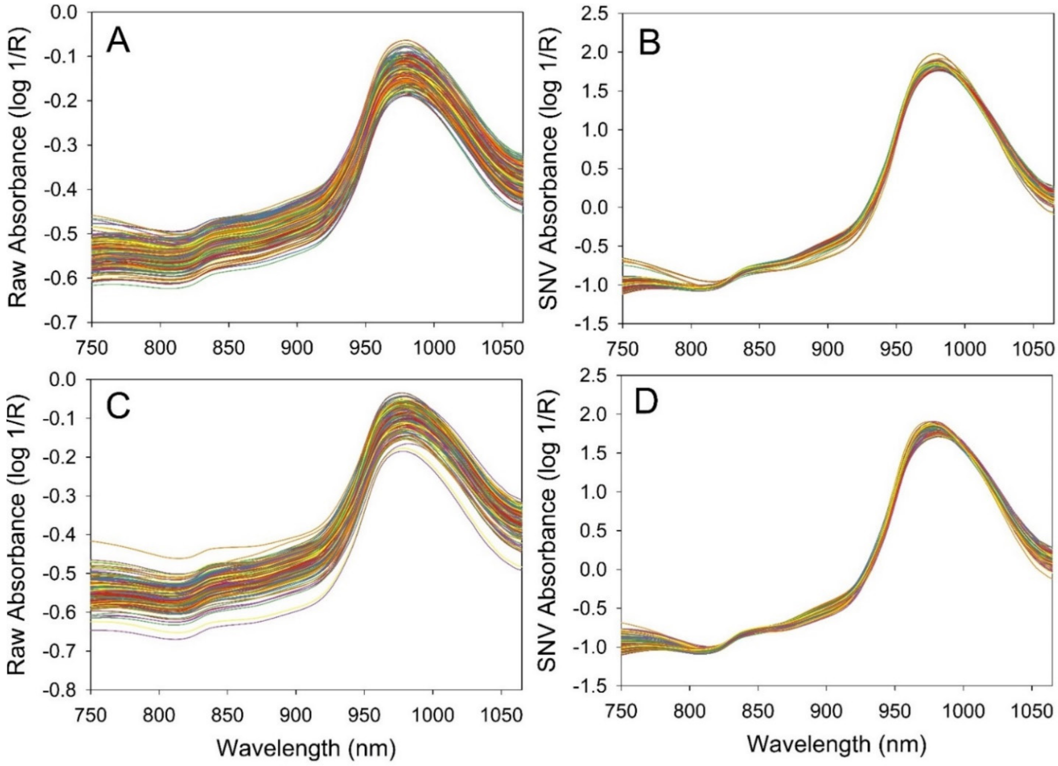


**Figure 2.** Raw spectra (on the left) and spectra pre-processed with standard normal variate (SNV) (on the right) obtained from apple (A and B) and pear (C and D) samples. Each line represents the absorbance spectra of a sample (one fruit) collected with the spectrometer.

**Table 1.** Statistical parameters related to the calibration and validation steps for the models developed to determine SSC and DMC in apples and pears, using SNV as spectral pre-processing method and the PLS regression to build the multivariate calibration models.

| Parameter | Mean | Range | SD | Calibration | | | | | Validation | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | n | Outliers | LV | $R^2$ | RMSECV | n | $R^2$ | RMSEP | $RMSEP_r$ |
| **Apple** | | | | | | | | | | | | |
| SSC (%) | 14.91 | 10.30–18.80 | 2.01 | 120 | 0 (0) | 6 | 0.70 | 1.19 | 51 | 0.58 | 1.13 | 7.6 |
| DMC (%) | 20.07 | 17.27–24.75 | 1.51 | 200 | 0 (0) | 9 | 0.71 | 0.83 | 88 | 0.55 | 0.94 | 4.7 |
| **Pear** | | | | | | | | | | | | |
| SSC (%) | 12.28 | 9.70–15.30 | 0.98 | 205 | 5 (2.4) | 10 | 0.78 | 0.48 | 96 | 0.55 | 0.59 | 4.8 |
| DMC (%) | 14.11 | 11.79–17.97 | 1.01 | 239 | 1 (0.4) | 10 | 0.78 | 0.51 | 108 | 0.65 | 0.50 | 3.5 |

Range: minimum and maximum values for the quality trait; SD: standard deviation; n: number of samples; Outliers: number of anomalous samples and percentage in relation to the total number of samples; LV: number of latent variables; RMSECV: root mean square error of cross-validation; RMSEP: root mean square error of prediction; RMSEPr: relative RMSEP calculated in relation to the mean value of the range for the quality parameter evaluated, expressed in percentage.

DMC averaged 20.07% and 14.11% for apples and pears, respectively (Table 1). There are no previous studies reporting DMC for ‘Eva’ apples and ‘Triunfo’ pears. Apple mean DMC found in this study is comparable to that found in ‘Red Delicious’ (20.15%) and higher than that in seven other apple cultivars (13.87–17.04%) evaluated by Zhang et al. (2019). Travers et al. (2014) assessed ‘Clara Frijis’ pears and reported a mean DMC (14.90%) slightly higher than that found in our study.

According to the results, there was a high variability in DMC and SSC of the samples used for the calibration and validation processes in our study (Table 1). The SSC ranged from 10.30% to 18.80% and 9.70% to 15.30% in apples and pears, respectively. The DMC ranged from 17.27% to 24.75% and 11.79% to 17.97% in apples and pears, respectively. The observed high variability in quality traits was possibly due to the widely different ripening stages of the fruit used in our study, which was important to guarantee the robustness, reliability, and reproducibility of the prediction models (LI et al., 2017).

The predicted *versus* reference plot for assessment of SSC and DMC in apples and pears is shown in Figure 3. Calibration models developed for SSC determination presented satisfactory predictive performance, with $RMSEP_r$ values of 7.6% (apple) and 4.8% (pear) and $R^2p$ of 0.58 and 0.55 for apples and pears, respectively.

Pissard et al. (2021) reported $RMSEP_r$ and $R^2p$ values of 6.3% and 0.65, respectively, when developing a calibration model for SSC in apples also using the PLS regression method. Bobelyn et al. (2010) evaluated the performance of a NIR spectrometer working in the spectral range of 800–1690 nm for SSC determination in apples of six commercial

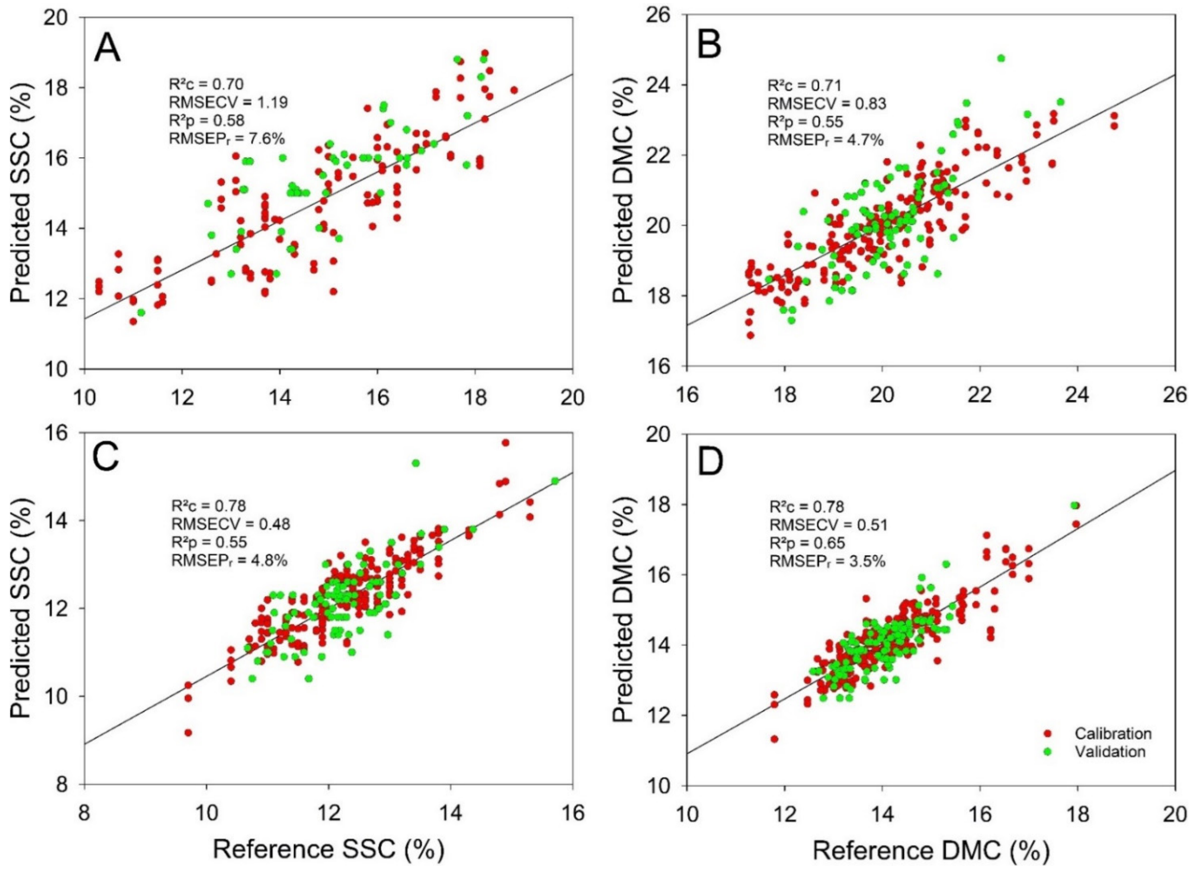


**Figure 3.** Predicted *versus* reference plots from calibration and validation models for determination of SSC (on the left) and DMC (on the right) in apples (A and B) and pears (C and D). The solid line is the bisectrix.

$R^2c$: coefficient of determination of calibration; RMSECV: root mean square error of cross-validation; $R^2p$: coefficient of determination of prediction; $RMSEP_r$: relative root mean square error of prediction.

cultivars from eight different regions. These authors observed that the best prediction model was obtained for 'Golden Delicious' apples, with a high $R^2p$ (0.86) combined with a low $RMSEP_r$ (3.6%). Ignat et al. (2014) used two instruments, VIS-NIR (340–1014 nm) and short-wavelength near-infrared (SWIR) (850–1888 nm) spectrometers, to evaluate 'Granny Smith', 'Pink Lady', and 'Starking' apples and found $RMSEP_r$ and $R^2p$ values of 5.6–6.2% and 0.82–0.86, respectively.

The model for SSC determination in pears was comparable to those developed by Travers et al. (2014) in 'Clara Frijis' pears ($R^2$ = 0.61–0.65, $RMSEP_r$ = 5.8–6.1%), whose spectral data were collected between 680 and 1000 nm. Machado et al. (2012) employed a VIS-NIR spectrometer working in the spectral range between 600 and 1000 nm to determine SSC in pears of three cultivars. The $RMSEP_r$ and $R^2$ ranges found were 2.59–32.86% and 0.85-0.94, respectively.

For DMC, the model prediction performance was satisfactory, showing $RMSEP_r$ of 4.7% and 3.5% for apples and pears, respectively. The $R^2p$ for DMC was 0.55 for apple and 0.65 for pear models. The F-750 spectrometer was also tested for DMC determination in eight apple cultivars by Zhang et al. (2019), which developed models with a $RMSEP_r$ range of 0.3–3.4% and $R^2$ values between 0.49 and 0.88. Goke et al. (2018) evaluated the F-750 spectrometer in the development of DMC models for pears and found $RMSEP_r$ of 3.0% and $R^2$ of 0.81 for 'Bartlett', as well as $RMSEP_r$ of 4.0% and $R^2$ of 0.90 for 'd'Anjou'.

The models developed for non-destructive determination of SSC and DMC in apples and pears had $RMSEP_r$ values lower than 10% associated with a coefficient of determination greater than 0.50, which are recommended for high precision analysis (PRATIM ROY et al., 2009). Many variables can affect the performance of a predictive model, including those related to environmental conditions (temperature, solar radiation, precipitation, seasonal variation), fruit variability (species, cultivar, harvest time, maturity), and chemometric treatments (preprocessing technique, regression model) (WALSH et al., 2020). Thus, model robustness can be significantly improved by the addition of new samples, from different seasons, cultivars, and maturity stages (BOBELYN et al., 2010; XIAOBO et al., 2010).

This is the first report on the use of a NIR spectrometer for non-destructive quality analysis of apples and pears produced in the Brazilian Semi-arid region. The models developed allow using the NIR spectrometer to determine SSC and DMC in apples and pears with a good prediction performance.

The NIR spectrometer is a promising tool to be used by growers, shippers, and retailers for a rapid and non-destructive determination of internal quality traits in apples and pears. Further investigations with more advanced spectral pre-treatment techniques and model development are recommended in order to improve the predictive performance of the models.

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