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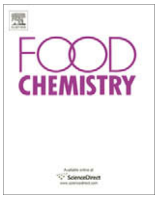

Analytical Methods

Rapid and non-destructive analysis of apricot fruit quality using FT-near-infrared spectroscopy

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ABSTRACT

A non-destructive optical method based on near-infrared spectroscopy has been used for the evaluation of apricot fruit quality. Diffuse reflectance measurements (800–2500 nm), physical, physiological and biochemical measurements were performed individually on 877 apricot fruits from eight contrasted cultivars harvested at different ripening stages. Relationships between spectral wavelengths and quality attributes were evaluated by application of chemometric techniques based on partial least squares (PLS) on fruit set divided randomly into two groups: 598 fruits for calibration and 279 for validation. Good prediction performance was obtained for soluble solids and titratable acidity with correlation coefficients of 0.92 and 0.89 respectively and root mean square errors of prediction of 0.98% Brix and 3.62 meq 100 g^{-1} FW respectively. For the other quality traits such as firmness, ethylene, individual sugars and organic acids, the prediction models were not satisfactorily accurate due to the high error of calibration and prediction.

1. Introduction

Quality fruit is characterised on the basis of size, colour, firmness, surface appearance and important traits related to the taste such as soluble solids and acidity. Most instrumental techniques measuring these properties are destructive and involve a considerable amount of manual work. Therefore, there is a demand for new and rapid analytical techniques for assessing fruit quality.

Optical visible/near-infrared spectroscopy (400–2500 nm) or only near-infrared spectroscopy (800–2500 nm) have been tested for non-destructive evaluation of firmness, dry matter, soluble solids, acidity and other physiological properties of many fruits and vegetables including apple (Liu & Ying, 2005; Peirs, Schenk, & Nicolaï, 2005; Zude, Herold, Roger, Bellon-Maurel, & Landahl, 2006), tomato (Shao et al., 2007), sweet cherry (Lu, 2001), stone fruit as peach, plum or nectarine (Carlomagno, Capozzo, Attolico, & Distante, 2004; Golic & Walsh, 2006; Peiris, Dull, Leffler, & Kays, 1998), prune (Slaughter, Thompson, & Tan, 2003), mandarin (Gomez, He, & Pereira, 2006), kiwi (McGlone, Jordan, Seelye, & Martinsen, 2002), watermelon (Ito et al., 2002), avocado (Clark, McGlone, Requejo, White, & Woolf, 2003). On apricot, Carlini, Massantini, and Mencarelli (2002) have shown the interest of wavelength selection methods and PLS (partial least square regression) for the evaluation of soluble solids in cherry and apricot. The main advantage of visible/near-infrared spectrometry is that, once models are established, it allows a non-destructive and individual characterisation of fruits, with simultaneous prediction of several quality traits. This technique appears to be useful to assist breeders in the selection of genotypes in breeding programs. Moreover it offers the possibility to screen fruits 'on-line' and estimate fruit quality which open new objective of market segmentation and fruit valorisation in a fresh or processed market.

The objective of this study was to evaluate the potential of near-infrared spectroscopy as a non-destructive method to predict apricot quality traits such as firmness, soluble solids, titratable acidity, ethylene production, sugar and acid contents through the comparison with standard techniques. The evaluation was performed on a large diversity of fruits covering genetic factor and physiological stages which was expected to be representative of the variability observed on the market. Samples belonging to eight cultivars harvested at different stages of ripening were used as a calibration set. The prediction models for each quality parameters were developed with partial least square technique.

Abbreviations: FT-NIR, Fourier transform near-infrared; SSC, soluble solids content; TA, titratable acidity; RMSEP, root mean square error of prediction; LV, latent variables; RMSEC, root mean square error of calibration; RMSEV, root mean square error of validation.

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2. Materials and methods

2.1. Selection of apricot fruit samples

Eight apricot cultivars or hybrids, named 'Moniqui', 'Goldrich', 'Bergeron', 'Iranien', 'Badami', 'A3844', 'A3759' and 'A4034' were chosen for their contrasted fruit quality traits such as colour, taste, physiological behaviour. To obtain a wide range of fruit composition, apricot fruits were collected from June 22 d to August 2 d, during the maturation period. A total of 877 fruits were collected. Fruits came from two INRA experimental orchards (Amarine (Gard) and Gotheron (Drôme), South of France) for 'Moniqui', 'Goldrich', 'Iranien', 'Badami', 'Bergeron' and 'A4034', and from a traditional private orchard (Donzère, Drôme, South of France) for 'A3844' and 'A3759'. At each picking date and for each cultivar, around 40 fruits were harvested. Non-destructive measurements were performed the day of picking 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 recorded on a multi-purpose analyser (MPA) spectrometer (Bruker Optics, Wissembourg, France) equipped with an integrating sphere to provide diffuse reflectance measurements and a TE-InGaAs detector. The MPA was completely software-controlled by the OPUS software Version 5.0 which was provided by Bruker Optics.

The NIR spectrum of each sample was obtained by taking the average of 32 scans. It was acquired between 800 and 2700 nm at 2 nm spectral resolution, with scanner velocity of 10 kHz and a background of 32 scans. The time required to achieve a spectral measurement was 30 s. The intact apricots were placed on an automated 30-position sample wheel, each position corresponding to an 18 mm diameter hole. Apricots were placed at each position with their stem–calyx axis horizontal. On each apricot, a diffuse reflectance spectrum was measured on two opposite sides, the first on the blushed side and the second on the un-blushed side.

2.3. Determination of quality traits using reference analyses

Fruit firmness was determined by the pressure (kPa) required to achieve a 3% deformation of fruit height with a multi-purpose texture analyser (Pénélaup®, Serisud, Montpellier, France). The skin colour (un-blushed and blushed sides) was determined using a CR-400 chromameter (Minolta, Osaka, Japan) and expressed in the CIE 1976 $L^*a^*b^*$ colour space (illuminant D65, 0° view angle, illumination area diameter 8 mm). Ethylene rate (nmol kg^{-1} h^{-1}) was measured by gas chromatography after 1 h of confinement in a jar (Chambroy, Souty, Jacquemin, Gomez, & Audergon, 1995). Then fruits were cut and frozen at −20 °C for a few days until biochemical analyses. Fruit pieces were homogenised with an Ultraturrax T25 equipment (Ika Labortechnik, Staufen, Germany) to obtain a puree. Soluble solids content was determined with a digital refractometer (PR-101 ATAGO, Norfolk, VA) and expressed in % Brix at 20 °C. Titratable acidity was determined by titration up to pH 8.1 with 0.1 N NaOH and expressed in meq 100 g^{-1} of fresh weight using an autotitrator (Methrom, Herisau, Switzerland). Sugars (glucose, fructose, sucrose) and organic acids (malic and citric acids) were quantified using an enzymatic methods with kits for food analysis (Boehringer Mannheim Co., Mannhein, Germany) and expressed in g 100 g^{-1} of fresh weight for sugars and meq 100 g^{-1} of fresh weight for acids. These measurements were performed with an automatic analyser BM-704 (Hitachi, Tokyo, Japan).

2.4. Statistical treatment of data

Several pre-processing techniques were tested and just the SNV (standard normal variate) correction was retained. Each spectrum was separately normalised to null mean value and unit variance.

Principal component analysis (PCA) was used to investigate sample spectra and eliminate the defective spectra (aberrant spectra due to a problem of acquisition). The PLS regression method was used to develop models for predicting the composition of apricot fruits. In PLS, both the spectral matrix X and the reference data in the data matrix Y are used for the calibration. The X and Y matrices are reduced to a few factors (latent variables) using all of the available information.

In order to carry out a validation test, the data set was randomly split into two subsets with 598 apricots (two thirds of fruits) used for calibration and 279 apricots (one third of fruits) used for validation. The spectral measurements used for validation might deviate from the calibration samples as they correspond to different fruits for each harvesting date and cultivars. For each quality trait, analysis of the NIR data involved 10 separate modelling/validation exercises. Each exercise used a different random split of the fruits. Repeating the analysis across 10 separate modelling/validation exercises makes possible to examine the stability of the model with variation of the fruit selection. In this work, different wavelength intervals were tested, starting with the full interval between 800 and 2400 nm (Fig. 1). The non-informative regions were tentatively purged and the resulting performances were estimated.

The performance of the calibration models and the number of latent variables (up to a maximum of 15) were evaluated by the root mean square error of calibration (RMSEC), the root mean square error of prediction (RMSEP) and the correlation coefficient r between the predicted and the measured parameters. Acceptable models should have low RMSEC and RMSEP, high r and small differences between RMSEC and RMSEP. Large differences indicate the introduction of too many PLS factors (latent variables) in the model.

The pre-processing and calculations were carried out under SAISIR environment (Bertrand, 2007) and DESIR interface (Lecomte, 2007) in MatLab software package (version 7.2, MathWorks, USA).

3. Results and discussion

The general profile of the absorption spectra for apricot (Fig. 1) is very similar to that of other plant materials as mandarin (Gomez et al., 2006), apple (Liu & Ying, 2005) or tomato (Pedro & Ferreira, 2005). These spectra are in fact dominated by water absorption bands with overtone bands of the OH-bonds at 970, 1190 and 1450 nm and a combination band at 1940 nm (Nicolaï et al., 2007).

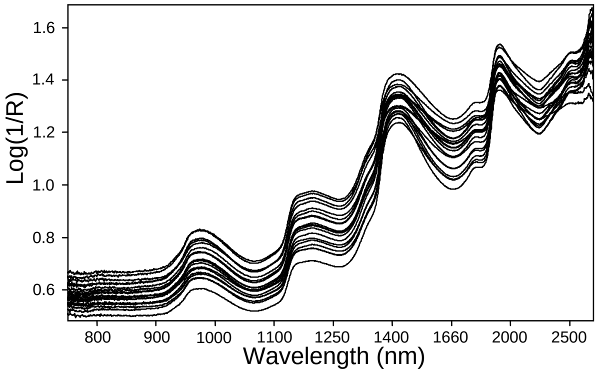

Fig. 1. Typical original spectra (Log(1/R)) for 20 apricot fruits issued from different cultivars and ripening stages.