Postharvest Biology and Technology 111 (2016) 345–351

Contents lists available at ScienceDirect

Postharvest Biology and Technology

journal homepage: www.elsevier.com/locate/postharvbio

# Robust PLS models for soluble solids content and firmness determination in low chilling peach using near-infrared spectroscopy (NIR)

Paloma Andrade Martins Nascimento[a], Lívia Cirino de Carvalho[a], Luis Carlos Cunha Júnior[b], Fabíola Manhas Verbi Pereira[c], Gustavo Henrique de Almeida Teixeira[d,*]

[a] Universidade Estadual Paulista (UNESP), Faculdade de Ciências Farmacêuticas (FCFAR), Campus de Araraquara. Rod. Araraquara- Jaú, km.1 s/n, Araraquara, SP, Brazil
[b] Universidade Federal de Goiás (UFG), Escola de Agronomia (EA), Setor de Horticultura, Avenida Esperança s/n – Campus Universitário, 74.690-000, Goiânia, GO, Brazil
[c] Universidade Estadual Paulista (UNESP), Instituto de Química (IQ), Campus de Araraquara, Rua Prof. Francisco Degni, 55, Araraquara, SP, Brazil
[d] Universidade Estadual Paulista (UNESP), Faculdade de Ciências Agrárias e Veterinárias (FCAV), Via de acesso Prof. Paulo Donato Castellane s/n, Jaboticabal, SP, CEP 14.870-900, Brazil

A R T I C L E  I N F O

*Article history:*
Received 3 June 2015
Received in revised form 6 August 2015
Accepted 11 August 2015
Available online 4 October 2015

*Keywords:*
*Prunus persica* L
Aurora 1
Maturity stages
Chemometrics
PLS

A B S T R A C T

The objectives of this study was to develop partial least square (PLS) models using NIR spectroscopy for the determination of SSC and firmness in intact low chilling 'Aurora-1' peach fruit, and verify the influence of maturity stage and harvest season on the models to be developed (robustness). FT-NIR spectra were obtained as log 1/R with fruit harvested in 2013 at 3 maturity stages and in 2014. The spectra were collected on the background and blush colour skin areas of the each fruit. Model performance was evaluated based on the values of root mean square error for prediction ($RMSE_P$) and coefficient of determination ($R_P^2$) obtained from validation fruit set (Kennard-Stone), and prediction fruit set (2014). PCA could not group the fruit based on blush and background skin colour, maturity stages, and harvest season. The model constructed using the external validation method obtained a $RMSE_{VE}$ of 1.08 % with 11 latent variables ($LV_S$) and a $R_{VE}^2$ of 0.59. The prediction set, independent data, resulting in a less accurate model ($RMSE_P$ 1.04 %, $R_p^2$ 0.45 and 11 $LV_S$). The same trend happened for determining firmness with the external validation resulting in better model with $RMSE_{VE}$ 9.51 N and $R_{VE}^2$ of 0.40 and the prediction set with $RMSE_P$ of 13.2 N, $R_P^2$ 0.40 with 7 $LV_S$. The NIR spectroscopy showed to be a potential analytical method to determine SSC and firmness of intact low chilling 'Aurora 1' cultivar. However, it is necessary to optimize the models in other to reduce the prediction errors.



## 1. Introduction

In temperate regions peach trees (*Prunus persica* L.) require exposure to chilling temperatures during the winter to overcome the rest period, after which normal bud break and development can occur (Campoy et al., 2011; Viti et al., 2010). The duration of chilling length required to bud break of a given cultivar is known as the chilling requirement of that particular cultivar (Wagner Júnior et al., 2013), and it varies greatly from 1050 h in 'Contender' to 600 h in 'LaFeliciana' (Parker and Werner, 2015). On the other hand, in subtropical and tropical regions the cultivation of peach trees is possible due to agronomic innovations and the development of low chilling cultivars, which require low exposure to chilling temperatures (100 to 200 h).

In Florida, USA, Ferguson et al. (2015) reported various low chilling cultivars, such as, 'Flordaprince' and 'Tropicalbeauty' with 150 h estimated chilling units, and 'UFSun' with 100 h. In subtropical regions of Brazil the cultivation of peach trees is carried out also with low chilling cultivars originated from local breading programs, for example the cultivar Aurora 1 (Ojima et al., 1989). The cultivar Aurora-1 requires less than the 100 h of chilling period to bud break. Its fruit has oblong shape, weights around 100 g, and presents a red blush colour (80% color over yellow background), and the fruit has also excellent sensory quality, with

* Corresponding author. Fax: +55 16 32092668.
*E-mail addresses:* gustavo@fcav.unesp.br, teixeiragha@yahoo.com.br (G.H.d.A. Teixeira).

http://dx.doi.org/10.1016/j.postharvbio.2015.08.006
0925-5214/

firm flesh, yellow pulp, and high soluble solids content (SSC), approximately 14% (Cunha Junior et al., 2007; Donadio, 2010).

Peach quality is greatly affected by the soluble solids content and it influences the acceptance of peach fruit by the consumers. Crisosto et al. (2013) reported 70% consumer acceptance when 'Elegant Lady' peach had 13% of SSC, on the other hand, when SSC were less than 11% there was little receptivity by consumers. Consumers also evaluate the firmness as an important quality parameter. Kader (2002) reported that fruit with a firmness of 27–36 Newton (N) can be considered "ready-to-buy" and with 9 to 13 N considered ripe "ready-to-eat".

The determination of SSC and firmness are based on simple analytical methods (AOAC, 1997), but both determinations are destructive, time consuming, and are not adequate to monitor peach quality in modern grading lines. One alternative method is the use of near infrared (NIR) spectroscopy as this method has been used to determine internal quality attributes of various fruit (Nicolaï et al., 2007; Mariani et al., 2014; Viegas et al., 2016). Regarding peach fruit, Golic and Walsh (2006) developed a combined model for several peach and nectarine cultivars to determine SSC. Golding et al. (2006) used a portable NIR to predict SSC in peach fruit at different maturity stages. The development of models to predict SSC in peach fruit is the most common use of NIR spectroscopy (Ying et al., 2005; Shao et al., 2011), but firmness (Fu et al., 2008; Lafuente et al., 2015) and flesh colour (Slaughter et al., 2013) were also studied. Although various studies can be found regarding the use of NIR spectroscopy evaluating peach fruit quality, the developed models were built based on cultivars with high chilling requirements and with fruit produced in temperate regions. These models cannot be used in subtropical and/or tropical regions to monitor peach quality, as the cultivars and environment are very different, thus, it is necessary the development of models for peach fruit produced in these conditions.

Therefore, the objectives of this study was to develop partial least square (PLS) models using NIR spectroscopy for the determination of SSC and firmness in intact low chilling 'Aurora-1' peach fruit, and verify the influence of maturity stage and harvest season on the models to be developed (robustness).

## 2. Materials and methods

### 2.1. Fruit material

Peach fruit were harvest in commercial orchards of Val Frutas, located at Vista Alegre do Alto, São Paulo, Brazil, (21°10′14″ S latitude, 48°37′45″ W longitude, and 700 m altitude). A total of 539 intact peach fruit of the low chilling cultivar Aurora 1 were collected in 2013 and 2014. The fruit were harvest in three maturity stages, as such: physiological mature (100–115 hue angle), ripe (106–80 hue angle), and over-ripe (hue angle lower than 80) based on the recommendations of Cunha Junior et al. (2007). The fruit were also harvested at the beginning, in the middle and at the end of the crop season in 2013 to build the calibration and validation models, and at the beginning of the harvest season in 2014, to build the prediction model (Table 1).

### 2.2. FT-NIR spectra acquisition

The spectra were collected using a FT-IR Spectrum 100N (PerkinElmer, Shelton, CT, USA). The spectrometer was equipped with Near Infrared Reflectance Accessory (NIRA), an integrating sphere and InGaAs detector. The light source was a halogen lamp. Diffuse reflectance spectra were obtained over the range of 4000–0,000 $cm^{-1}$ (1000–2500 nm) at a spectral resolution of 8 $cm^{-1}$ with 64 scans per spectra. The log 1/R spectra were referred as absorbance spectra for convenience.

Fruit were set onto the NIRA and two spectra were collected on the equator of both sides of each fruit (blush and background color), equidistant from proximal and distal ends (Subedi et al., 2007). Each spectrum was used as individual sample in the models. After spectra acquisition, fruit were subjected to analytical determinations, considering the same areas of spectral analysis.

### 2.3. Reference analysis

#### 2.3.1. Colour

L*, a* and b* colour coordinates were determined using a Minolta colorimeter CR 400 (Minolta, Osaka, Japan). L measures luminosity, while a* and b* values index the red–green and yellow–blue space, respectively. Determinations were taken on the two sides of each fruit (blush and background colour) at the same areas where the NIR spectra were acquired. It was also calculated the hue angle, arc tangent of (b */a *), and chromaticity, (C *) ([(a *) × 2 + (b *) × 2] × 0.5) according to the method described by McGuire (1992). Fruit were reclassified according to the maturation stages by the hue angle according to Cunha Junior et al. (2007), physiological mature (100–115°), ripe (106–80°) and over-ripe (hue angle of <80°).

#### 2.3.2. Firmness

Firmness was determined using a penetrometer Bishop FT 327, Italy, using an 8 mm tip. The results were expressed in Newton (N), on the same two positions where the NIR spectra were acquired. The laboratory error for this determination was 4.02 N.

#### 2.3.3. Soluble solids content (SSC)

The fruit parts where the NIR spectra were collected were also used to analysed the soluble solids content according to the reference method 920.151 reported by AOAC (1997). It was used a refractometer (Alpha, Atago Co., Ltd, Japan). The measurements were carried out in duplicate and the results were expressed in percentage (%). The laboratory error for this determination was 0.4%.

### 2.4. Chemometrics

The Unscrambler version 10.3 (Camo, Oslo, Norway) was used for data analysis. Spectra were pre-processed using Standard Normal Variate, (SNV), Multiplicative Scatter Correction (MSC), SNV+ De-Trend, second polynomial order of the first ($d^1A$) of Savitzky–Golay with smoothing window five points (2 + 2).

**Table 1**
Descriptive statistics of the calibration and validation set (2013), and the prediction set (2014) classified with the classic Kernnard-Stone selection algorithm.

| | | Soluble Solids Content (SSC—%) | | | | Firmness (Newton - N) | | | |
|---|---|---|---|---|---|---|---|---|---|
| Group | N[a] | Mean | SD[b] | Maximum | Minimum | Mean | SD | Maximum | Minimum |
| Calibration | 340 | 11.2 | 1.66 | 17.6 | 6.6 | 44.1 | 14.7 | 111.7 | 4.9 |
| Validation | 90 | 11.4 | 1.68 | 16.0 | 6.3 | 42.1 | 12.2 | 78.4 | 10.8 |
| Prediction | 109 | 12.7 | 1.38 | 17.0 | 9.2 | 53.9 | 13.9 | 84.3 | 15.7 |

[a] N = number,
[b] SD = standard deviation.