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Analytical Methods

Rapid and non-destructive determination of quality parameters in the 'Tommy Atkins' mango using a novel handheld near infrared spectrometer



Emanuel José Nascimento Marques ^{a,*}, Sérgio Tonetto de Freitas ^b, Maria Fernanda Pimentel ^c, Celio Pasquini ^d

- ^a Department of Fundamental Chemistry, Federal University of Pernambuco (UFPE), 50670-901 Recife, PE, Brazil
- ^b Embrapa Tropical Semi-Arid, Brazilian Agricultural Research Corporation, 56302-970 Petrolina, PE, Brazil
- ^c Department of Chemical Engineering, Federal University of Pernambuco (UFPE), 50670-901 Recife, PE, Brazil
- ^d Institute of Chemistry, University of Campinas (UNICAMP), 13084-971 Campinas, SP, Brazil

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ABSTRACT

The objective of this study was to evaluate the potential of a new handheld ultra-compact near infrared (NIR) spectrometer, based on the linear-variable filter (LVF) technology for rapid and non-destructive quality control analysis of the 'Tommy Atkins' mango. Multivariate calibration models were built using the Partial Least Squares (PLS) regression method to determine soluble solids (SS), dry matter (DM), titratable acidity (TA) and pulp firmness (PF). Different spectral pre-processing techniques were tested. Coefficient of determination and root mean square errors of prediction (RMSEP) values were, respectively: 0.92 and 0.55 °Brix for SS, 0.67 and 0.51% for DM, 0.50 and 0.17% citric acid for TA, 0.72 and 12.2 N for PF. The predictive models allowed monitoring physico-chemical changes in each fruit during ripening. The results show the feasibility of using the new NIR handheld spectrometer to determine quality parameters in the 'Tommy Atkins' mango.

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1. Introduction

Mango (*Mangifera indica* L.) is a climacteric fruit cultivated in tropical and subtropical regions in the world and its production is increasing each year following consumer demand (Jahurul et al., 2015; Schmilovitch, Mizrach, Hoffman, Egozi, & Fuchs, 2000). In 2013, mango production worldwide reached 40 million tons, moving more than 25 billion dollars in the producing countries (FAOSTAT., 2013). India, China, Thailand, Indonesia, Mexico, Pakistan and Brazil are the largest mango producers, accounting for about 75% of world production (FAOSTAT, 2013).

Although mango production is an important activity worldwide, problems related to fruit quality limit the consumption of this fruit. One of the main problems is marketing fruits with different maturity stages and consumer quality in the same batch (Kienzle et al., 2011). This problem is due to low precision of the visual parameters used to determine the maturity stage at harvest and to monitor fruit consumer quality during storage and marketing (Kienzle et al., 2011; Thangaraj & Irulappan, 1989). In addition, destructive

* Corresponding author.

E-mail address: emanueljn@gmail.com (E.J.N. Marques).

methods often used to estimate quality of the fruit sent to the market are labor-intensive, expensive, due to fruit sampling, and may not be representative of the commercial batch. Therefore, the development of non-destructive, reliable, accurate, fast and robust methods is essential to ensure a better quality of fruit delivered to consumers.

In the past decades, near infrared (NIR) spectroscopy has proven to be a reliable analytical technique for qualitative and quantitative analyses of a great variety of compounds present in different agricultural and food products (Cen & He, 2007; Nicolaï et al., 2007; Norris, 1964). The technique has the advantages of being rapid and non-destructive, precise, with no sample preparation requirements. These characteristics make NIR spectroscopy an important tool for fruit quality control.

Previous studies have demonstrated the potential of NIR spectroscopy for nondestructive determination of quality parameters in mango, such as soluble solids, dry matter, titratable acidity, pulp firmness, starch content and other physico-chemical properties (Betemps, Fachinello & Galarça,2011; Delwiche, Mekwatanakarn, & Wang, 2008; Guthrie & Walsh, 1997; Jha et al., 2012, 2014; Mahayothee, Leitenberger, Neidhart, Mühlbauer, & Carle, 2004; Saranwong, Sornsrivichai, & Kawano, 2001, 2003, 2004;

Schmilovitch et al., 2000; Subedi & Walsh, 2011; Subedi, Walsh, & Owens, 2007; Valente, Leardi, Self, Luciano, & Pain, 2009). Some of these studies have also shown that handheld NIR spectrometers can be suitably used for the determination of quality parameters in mango, providing performance similar to the benchtop NIR spectrometers for this kind of application (Betemps, Fachinello, & Galarça, 2011; Jha et al., 2012, 2014; Saranwong et al., 2003).

In recent years, the development of new technologies used in the construction of NIR spectrometers has resulted in a significant reduction in the size and cost of these devices. An important example is the spectrometers using the linear variable filter (LVF) technology which requires no moving parts, consequently leading to smaller and more rugged devices (Lutz, Bonn, Rode, & Huck, 2014; O'Brien et al., 2012). This makes the LVF based instruments more suitable for use outside of the laboratory for fruit quality analysis in the field or in storage.

The main objective of this study was to evaluate the potential of a new handheld ultra-compact NIR spectrometer, containing the LVF technology, for rapid and non-destructive determination of mango fruit quality. The specific objectives were to (1) determine the penetration depth of NIR radiation into mango fruit tissue, (2) develop accurate calibration models, and (3) use the calibration models for non-destructive individual fruit quality analysis during ripening.

2. Materials and methods

2.1. Fruit samples

Four hundred 'Tommy Atkins' mangoes (*M. indica* L.) were harvested at maturity stages 1 to 2 (Santos, Pereira, Vieira, & Lima, 2008) from a commercial orchard located in Juazeiro, Bahia, Brazil (latitude 9°24'S, longitude 40°21'W). After harvest, the fruits were transported to the Postharvest Laboratory at the Embrapa Tropical Semi-Arid in Petrolina, PE, Brazil. The fruits were then washed, dried and stored at 24 °C (±1 °C) for 18 days.

2.2. Spectral data acquisition

The NIR spectral data were obtained with the handheld ultra-compact MicroNIR 1700 spectrometer. The instrument has a linear-variable filter (LVF) developed by VIAVI (Santa Rosa, CA, USA), which is directly attached to a linear Indium gallium arsenide (InGaAs) array detector. The system has two small tungsten light bulbs and a USB interface coupled for power and data transfer. The MicroNIR 1700 has a 128-pixel detector array, recording data with a spectral nominal resolution of 6.25 nm with a wavelength range between 950 and 1650 nm. The spectrometer's dimensions are 45 mm in diameter and 42 mm in height, weighting about 60 g.

Spectra acquisition was accomplished in the reflectance mode ($\log 1/R$) in the spectral range between 950 and 1650 nm. The integration time was 10 ms and each collected spectrum was the average of 50 scans, resulting in a measurement time of 0.50 s.

2.3. NIR radiation penetration into mango pericarp tissue

Mango fruit was cut into two thick pericarp slices so that the seed was not used. The spectra were taken by positioning the spectrometer on the skin side and a polyethylene plate on the opposite side of the fruit slice. Initially, two spectra were obtained from the whole slice. Afterwards, a ~ 1 mm slice of pericarp tissue was removed from the side opposite to the skin using a sharp knife and again two spectra were taken on the skin side. The two spectra obtained for each slice were averaged to provide a mean spectrum.

This procedure was repeated for different mango pericarp slices with thicknesses ranging from 31.0 to 0.7 mm. The thickness of each slice was determined using a digital caliper (King-Tools, China) before each measurement.

2.4. Development of multivariate calibration models

Two hundred and fifty 'Tommy Atkins' mangoes were randomly divided into 10 groups of 25 fruit. NIR spectral data and reference data were obtained at harvest and every two days during storage for 18 days at 24° C ($\pm 1^{\circ}$ C).

For spectra acquisition, six separate measurements using the MicroNIR 1700 spectrometer were carried out on each mango at six points distributed along the axial region, with three points located on each side of the fruit. The measurements were performed by positioning the spectrometer directly on the fruit skin. The six spectra were averaged to provide a mean spectrum for each fruit

Reference analyses were accomplished using the fruit regions corresponding to the area previously used for the NIR spectra acquisition. First, 2 mm of the fruit skin was removed to determine pulp firmness. Later, a $5 \times 2 \times 1$ cm pulp sample was extracted from each side of the fruit, cut into small pieces, mixed and divided into 2 fractions: (1) used for dry matter measurement, and (2) used for soluble solids (SS) and titratable acidity (TA) measurement, using conventional methods. Fraction 2 was pressed in a manual juicer and the juice used for SS and TA quantification.

2.4.1. Reference analyses

2.4.1.1. Soluble solids. Soluble solids (SS) were determined with a digital refractometer model PAL-1 (Atago, Tokyo, Japan) with automatic temperature compensation and operating range from 0 to 53 °Brix. Measurements were performed using 1 mL of fruit juice. The results were expressed as °Brix.

2.4.1.2. Dry matter. Dry matter (DM) was determined by the mass difference between the fresh sample and the dry sample. The sample was dried until it reached a constant weight using an oven at 65 $^{\circ}$ C (AOAC, 1995). The results were expressed as percentage of DM

2.4.1.3. Titratable acidity. Titratable acidity (TA) was determined in 1.00 mL of juice diluted in 50 mL of distilled water. Titration was accomplished with a digital burette model Digitrate Pro (Jencons, Franklin, KY, USA). Phenolphthalein was used as the titration indicator and NaOH 0.1 mol L⁻¹ as the titrant (AOAC, 1995). The results were expressed as percentage (m/v) of citric acid.

2.4.1.4. Pulp firmness. Pulp firmness (PF) was determined with a texture analyzer model TA.XT Plus (Extralab, Jarinu, SP, Brazil) equipped with a 6 mm diameter stainless probe. Analyses were accomplished on both fruit sides by previously removing 2 mm (thickness) of skin tissue. The measurements were performed on opposite sides located in the equatorial region of the fruit. The results represent the maximum force required for the probe to penetrate 10 mm into the fruit pulp. Data were expressed in Newtons (N).

2.5. Non-destructive monitoring of individual mango fruit ripening

Twenty-two 'Tommy Atkins' mangoes were stored at $24\,^{\circ}$ C ($\pm 1\,^{\circ}$ C) for 14 days. Spectral data were collected from each individual fruit at harvest and twice a day during storage. Fruit ripening was monitored only non-destructively by means of NIR spectroscopy. Spectra acquisition was accomplished using the same procedure described above. At each evaluation, spectra data of all

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