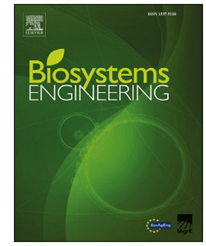
Available online at www.sciencedirect.com

ScienceDirect

journal homepage: www.elsevier.com/locate/issn/15375110



Research Paper

Development of calibration models for the evaluation of pomegranate aril quality by Fourier-transform near infrared spectroscopy combined with chemometrics

Ebrahiema Arendse [a], *Olaniyi A. Fawole* [b], *Lembe S. Magwaza* [c], *Helene H. Nieuwoudt* [d], *Umezuruike L. Opara* [b,*]

[a] *Postharvest Technology Research Laboratory, South African Research Chair in Postharvest Technology, Department of Food Science, Stellenbosch University, Private Bag X1, Stellenbosch 7602, South Africa*
[b] *Postharvest Technology Research Laboratory, South African Research Chair in Postharvest Technology, Department of Horticultural Science, Stellenbosch University, Private Bag X1, Stellenbosch 7602, South Africa*
[c] *Department of Crop Science, School of Agricultural, Earth and Environmental Science, University of KwaZulu-Natal, Private Bag X01, Scottsville, 3209, Pietermaritzburg, South Africa*
[d] *Institute for Wine Biotechnology, Department Viticulture and Oenology, Stellenbosch University, Private Bag X1, Matieland 7602, South Africa*

ARTICLE INFO

Article history:
Received 15 February 2017
Received in revised form
10 April 2017
Accepted 13 April 2017

Keywords:
Punica granatum L.
Fruit quality
Near infrared
Partial least squares
Chemometrics

A Fourier transform NIR (FT-NIR) method was developed combining chemometrics for prediction of organoleptic and phytochemical parameters of pomegranate arils using two different FT-NIR acquisition methods; namely, an integrating sphere (IS) and an emission head (EH) used over a spectral region 800–2500 nm. Several pre-processing methods were investigated. Pre-processing methods that yielded higher coefficient of determination (R^2) and residual predictive deviation (RPD), lower root mean square error estimation (RMSEE) and root mean square error of prediction (RMSEP) values were used for model development. Model development using the EH gave the best prediction of total soluble solids (R^2 = 87.55, RMSEP = 0.30%), pH (R^2 = 85.18, RMSEP = 0.10), titratable acidity (R^2 = 85.59, RMSEP = 0.10%), BrimA (R^2 = 83.43, RMSEP = 0.43), aril hue (R^2 = 88.59, RMSEP = 4.19), total phenolic concentration (R^2 = 86.48, RMSEP = 0.11 g l^{-1}), total anthocyanin concentration (R^2 = 70.50, RMSEP = 0.13 g l^{-1}) and vitamin C concentration (R^2 = 84.86, RMSEP = 0.09 g l^{-1}), while the IS provided the best results for TSS:TA (R^2 = 82.20, RMSEP = 1.03), aril firmness (R^2 = 68.40, RMSEP = 6.71 N), aril colour components (a^* (R^2 = 73.54, RMSEP = 1.67) and Chroma (R^2 = 78.37, RMSEP = 2.31)). Good prediction was observed for both the models based on EH and IS data acquisition methods. However, better prediction performance was obtained with the model based on EH data acquisition

* *Corresponding author*. Fax: +27 21 808 3743.
E-mail address: opara@sun.ac.za (U.L. Opara).
http://dx.doi.org/10.1016/j.biosystemseng.2017.04.004

method, resulting in accurate predictions of 8 quality parameters. This study demonstrated that FT-NIR and associated chemometric analysis can holistically evaluate the quality parameters of pomegranate arils.

Nomenclature

FT-NIR	Fourier transform near infrared
PLS	Partial least squares
PCA	Principal component analysis
R^2	Coefficient of determination
RMSEE	Root mean square error estimation
RMSEP	Root mean square error of prediction
RPD	Residual predictive deviation
CV	Coefficient of variation
LV	Latent variables
FD	First derivative
SD	Second derivative
MSC	Multiplicative scattering correction
SNV	Vector normalisation
MPA	Multi-Purpose Analyser
IS	Integrating sphere
EH	Emission head
TSS	Total soluble solids
TA	Titratable acidity

1. Introduction

Pomegranate (*Punica granatum* L.) has gained global recognition and has been extensively documented for its potential health benefits such as antioxidant, anti-hypertension, anti-mutagenic and anti-inflammatory activities (Fawole, Makunga, & Opara, 2012a; Ismail, Sestili, & Akhtar, 2012; Seeram, Zhang, Reed, Krueger, & Vaya, 2006). Scientific evidence has linked these potential health benefits to active polyphenolic compounds derived from fruit consumption (Seeram et al., 2006; Miguel, Neves, & Antunes, 2010; Fawole, Opara, Theron, & 2012b). Furthermore, pomegranate fruit contains considerable amounts of soluble solids, organic acids, vitamins, polysaccharides, mineral elements, fatty acids and vitamin C content (Opara, Al-Ani, & Al-Shuaibi, 2009). Despite the nutritional and health benefits, consumption is still limited due to the difficulties of extracting the arils. Therefore, minimally processed fresh pomegranate arils have become popular due to their convenience to consumers, increasing both prospects of production and consumption (Ayhan & Eştürk, 2009; Caleb, Opara, & Witthuhn, 2012; Arendse, Fawole, Magwaza, & Opara, 2016a). The growing pomegranate industry requires non-invasive methods that allow accurate, rapid and cost effective analysis of fruit quality. Non-invasive assessment of fruit quality can contribute in the implementation of suitable management strategies to predict and control desired pomegranate quality attributes such as sugar content, acidity, colour and content of phytochemical components.

Several non-destructive techniques have been used for the assessment of internal and external quality of fresh fruit. These include visible to near infrared spectroscopy (Vis/NIRS, Magwaza et al., 2012a; Ghosh et al., 2016), Vis/NIRS-based systems such as multispectral and hyperspectral imaging (Khodabakhshian, Emadi, Khojastehpour, Golzarian, & Sazgarnia, 2016), nuclear magnetic resonance imaging (NMR/MRI; Zhang & McCarthy, 2013), and X-ray computed tomography (CT; Magwaza & Opara, 2014; Arendse, Fawole, Magwaza, & Opara, 2016b). Amongst the non-destructive methods, NIRS combined with chemometric techniques are the most widely used due to its accuracy, rapidity and cost effectiveness for quantification of chemical constituents (Huang, Yu, Xu, & Ying, 2008; Magwaza, Naidoo, Laurie, Laing, & Shimelis, 2016; Magwaza et al., 2012a; Nicolaï et al., 2007). NIR spectroscopy is appropriate for the measurement of compounds containing polar functional groups such as–OH, C–O, and N–H (Blanco & Villarroya, 2002) and provides a non-invasive alternative for predicting the presence and/or concentration of specific chemical constituents in fruit and vegetables without prior sample preparation (Musingarabwi, Nieuwoudt, Young, Eyéghè-Bickong, & Vivier, 2016). To our knowledge, there is no reported use of Fourier transform near infrared (FT-NIR) spectroscopy in the analysis of pomegranate aril quality. The ability to assess pomegranate aril composition using high-throughput technologies such as FT-NIR spectroscopy would support the practical implementation of comprehensive analysis for predicting aril quality for on-line grading and sorting systems in commercial pack-houses. The objective of this study was to develop a FT-NIR method for accurate prediction of organoleptic and phytochemical quality parameters of pomegranate arils.

2. Materials and methods

2.1. *Fruit sampling*

Pomegranate fruit (cv. Wonderful) used in this study were obtained from Sonlia commercial packhouse (33°34′851″S, 19°00′360″E), located in the Western Cape Province, South Africa. Production unit's code was used to identify orchards, 200 fruit were obtained from Heinrich Frederich Schaefer (HFR) orchard while another set of 100 fruit was obtained from Portville to add orchard location variability. Procured fruit were packed in open-top telescopic carton boxes and immediately transported to Postharvest Technology facility at Stellenbosch University, South Africa. On arrival, fruit were equilibrated at ambient temperature before sorting by removing any fruit with external damage. Fruit were processed at 23 ± 3 °C by separating the arils from the husk. Surface moisture on the arils were removed by gently applying sterile paper towels after which 100 g of arils were weighed using an electronic scale (Mettler Toledo, Switzerland, 0.01 g).