Accepted Manuscript

Comparing the analytical performance of near and mid infrared spectrometers for evaluating pomegranate juice quality

Ebrahiema Arendse, Olaniyi Amos Fawole, Lembe Samukelo Magwaza, Helene Nieuwoudt, Umezuruike Linus Opara

PII: S0023-6438(18)30057-4

DOI: 10.1016/j.lwt.2018.01.035

Reference: YFSTL 6799

To appear in: *LWT - Food Science and Technology*

Received Date: 26 September 2017

Revised Date: 16 December 2017

Accepted Date: 13 January 2018

Please cite this article as: Arendse, E., Fawole, O.A., Magwaza, L.S., Nieuwoudt, H., Opara, U.L., Comparing the analytical performance of near and mid infrared spectrometers for evaluating pomegranate juice quality, *LWT - Food Science and Technology* (2018), doi: 10.1016/j.lwt.2018.01.035.

Comparing the analytical performance of near and mid infrared spectrometers for evaluating pomegranate juice quality

Ebrahiema Arendse[1], Olaniyi Amos Fawole[2], Lembe Samukelo Magwaza[3], Helene Nieuwoudt[4], Umezuruike Linus Opara[2]*

[1]*Postharvest Technology Research Laboratory, South African Research Chair in Postharvest Technology, Department of Food Science, Stellenbosch University, Private Bag X1, Stellenbosch 7602, South Africa*

[2]*Postharvest Technology Research Laboratory, South African Research Chair in Postharvest Technology, Department of Horticultural Science, Stellenbosch University, Private Bag X1, Stellenbosch 7602, South Africa*

[3]*Department of Crop and Horticultural Science, School of Agricultural, Earth and Environmental Science, University of KwaZulu-Natal, Private Bag X01, Scottsville, 3209, Pietermaritzburg, South Africa*

[4]*Institute for Wine Biotechnology, Department Viticulture and Oenology, Stellenbosch University, Private Bag X1, Matieland 7602, South Africa*

* Corresponding author: (UL Opara) opara@sun.ac.za

Tel: +27 21 808 4064 Fax: +27 21 808 3743

Abstract

Near infrared (NIR) and mid infrared (MIR) spectral acquisition modes were compared for predicting organoleptic and phytochemical quality attributes of pomegranate juice. Three Fourier transform infrared (FT-IR) spectrometers namely, a FT-NIR spectrometer, FT-MIR spectrometer in attenuated total reflection mode and FT-MIR spectrometer in transmission mode were used. Calibration models were constructed by subjecting the spectral data to partial least squares regression analysis. The models were assessed based on their overall performance (lower root mean square error of prediction, the number of latent variables and residual predictive deviation). The predictive abilities of the instruments for juice quality attributes were statistically compared using Bland and Altman, and Passing-Bablok. The outcomes are critically discussed, which showed the suitability of the FT-MIR spectrometer in transmission mode for predicting selected quality attributes of pomegranate juice.

Keywords: *Punica granatum* L., Juice quality, Near infrared, Mid infrared, Partial least squares, Chemometrics, Bland and Altman, Passing-Bablok

1. Introduction