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

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1 Comparing the analytical performance of near and mid infrared spectrometers for 2 evaluating pomegranate juice quality

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19 20 **Abstract**

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

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

34 35 **1. Introduction**

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