Title Nondestructive measurement of internal quality in pear using genetic algorithms and FT-NIR spectroscopy

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Abstract

An improved genetic algorithms (GAs) is used to implement an automated wavelength selection procedure for use in building multivariate calibration models based on partial least squares regression. The methods also allow the number of latent variables used in constructing the calibration models to be optimized along with the selection of the wavelengths. Studies are performed to characterize the signal and noise characteristics of the spectral data, and optimal configurations for the GAs are found for each data set through experimental design techniques. The experiments tested in this method were sugar content (SC), titratable acidity (TA) and valid acidity (pH).

Despite the complexity of the spectral data, the GAs procedure were found to perform well (RMSEP = 0.395, 0.0195, 0.0087 for SC, TA and pH respectively), leading to calibration models that significantly outperform those based on full-spectrum analyses (RMSEP = 0.512, 0.0198, 0.0111 for SC, TA and pH respectively). In addition, a significant reduction in the number of spectral points required to build the models is realized and all of the numbers of wavelengths for building the calibration models can reduce by 84.4%. This work proved that the GA could find optimal values for several disparate variables associated with the calibration model and that the PLS procedure could be integrated into the objective function driving the optimization.