Achieving robustness to temperature change of a NIRS-PLSR model for intact mango fruit dry matter content

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Abstract

Temperature impacts the extent of H bonding in water and thus impacts near infrared (NIR) spectra of fruit and influences the robustness of models between spectra and attributes such as dry matter content (DMC). Temperature correction methods including external parameter orthogonalisation (EPO), generalised least square weighting (GLSW), bias correction, repeatability file, calibration wavelength optimization and global modelling were applied to reduce the impact of sample temperature change on DMC prediction of intact mango fruit using a calibration data set of 1392 samples and a validation set of 660 samples of variable sample temperatures, drawn from 15 populations sourced from separate harvests. All methods except bias correction reduced bias corrected root mean square error of prediction (RMSEP) and increased coefficient of determination (R^2). For a global model, it is recommended that at least 2.4 % of samples in the model be scanned at different temperatures. However, the EPO method is recommended overall, as it returned the lowest RMSEP and highest R^2 (1.05 % w/w, and 0.82 compared with the control result of 1.43 % and 0.68, respectively), in prediction of the population with spectra acquired at three temperatures. A residual of ± 0.10×$\hat{y}$, where $\hat{y}$ is the reference value, was associated with a confidence interval of 92.4 and 77.4 % for the EPO corrected and original models, respectively. The results have significance for the practical implementation of NIRS-DMC estimation of fruit in field conditions.