

Title Prediction of titratable acidity, malic acid, and citric acid in bayberry fruit by near-infrared spectroscopy

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Abstract

An experiment was conducted to simultaneously measure titratable acidity, malic acid, and citric acid of bayberry fruit in a nondestructive manner using near-infrared (NIR) transmittance spectroscopy and chemometrics. The sampling set included different cultivars that were obtainable from different areas in China. Calibration models using partial least squares (PLS) regression were developed based on GB 12293-90 of China and with high-performance liquid chromatography (HPLC) as reference methods. Different preprocessing methods and different wave bands were applied. The correlation coefficient of calibration (r_c), root-mean-square error of calibration (RMSEC), and root-mean-square error of prediction (RMSEP) of the best model for titratable acidity was 0.8959, 2.24, and 2.89 g/L, respectively, with the range of 10,000–5405 cm^{-1} . R_c , RMSEC, and RMSEP values for malic acid and citric acid were 0.6689, 0.32, 0.47 and 0.8970, 1.51, 2.12 g/L, respectively. The prediction accuracies could not be improved by using first and second derivative pretreatment methods. Due to the short time consumption and low monitoring cost, NIR spectroscopic technique has its potential for the rapid and nondestructive prediction of titratable acidity and citric acid in bayberry fruit in a temperature-controlled room, although the accuracy was not high.