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Determination of main fruits in adulterated nectars by ATR-FTIR spectroscopy combined with multivariate calibration and variable selection methods

Determination of fruits in adulterated nectars by ATR-FTIR and PLS

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Abstract

Grape, orange, peach and passion fruit nectars were formulated and adulterated by dilution with syrup, apple and cashew juices at 10 levels for each adulterant. Attenuated total reflectance Fourier transform mid infrared (ATR-FTIR) spectra were obtained. Partial least squares (PLS) multivariate calibration models allied to different variable selection methods, such as interval partial least squares (iPLS), ordered predictors selection (OPS) and genetic algorithm (GA), were used to quantify the main fruits. PLS improved by iPLS-OPS variable selection showed the highest predictive capacity to quantify the main fruit contents. The selected variables in the final models varied from 72 to 100; the root mean square errors of prediction were estimated from 0.5 to 2.6 %; the correlation coefficients of prediction ranged from 0.948 to 0.990; and,