259
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Title:L-ascorbic acid prediction in aqueous solution based on FTIR-ATR terahertz spectroscopy
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Abstract:The feasibility of using attenuated total reflectance-terahertz (ATR-THz) spectroscopy for quantification of L-ascorbic acid (L-AA) in aqueous solutions was investigated. The spectra of 55 samples of L-AA solution ranging in concentration from 0-21% were acquired using Terahertz-based Fourier transform infrared (THz-FTIR) spectrometer. Spectral absorbance in the range 20 to 400 cm⁻¹ was used in this analysis. Full spectrum partial least squares (FS-PLS) regression was used to develop and validate the calibration model for determination of L-AA. The result showed that using the pre-processing of Savitzky-Golay first derivative spectra, prediction resulted in the lowest root mean square error of prediction (RMSEP) = 2.791%. A ratio of standard deviation to prediction error (RPD) value of 4.48 was obtained.
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Controlled terms:Forecasting - Fourier transform infrared spectroscopy - Mean square error - Molecular structure - Molecular vibrations - Spectrometers - Terahertz spectroscopy - Terahertz waves
Uncontrolled terms:Calibration model - First derivative - Fourier transform infrared - FS-PLS regression - FT-IR-ATR - Full spectrum - Intermolecular vibrations - Intra-molecular vibration - L-ascorbic acid - Partial least square (PLS) - Pre-processing - Prediction errors - Root-mean-square error of predictions - RPD value - Savitzky-Golay - Spectral absorbance - Standard deviation
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