

Handling of uncertainty due to interference fringe in FT-NIR transmittance spectroscopy : performance comparison of interference elimination techniques using glucose-water system.

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Streszczenie

The applicability of two elimination techniques for interferences occurring in measurements with cells of short pathlength using Fourier transform near-infrared (FT-NIR) spectroscopy was evaluated. Due to the growing interest in the field of vibrational spectroscopy in aqueous biological fluids (e.g. glucose in blood), aqueous solutions of d-(+)-glucose were prepared and split into a calibration set and an independent validation set. All samples were measured with two FT-NIR spectrometers at various spectral resolutions. Moving average smoothing (MAS) and fast Fourier transform filter (FFT filter) were applied to the interference affected FT-NIR spectra in order to eliminate the interference pattern. After data pre-treatment, partial least squares regression (PLSR) models using different NIR regions were constructed using untreated (interference affected) spectra and spectra treated with MAS and FFT filter. The prediction of the independent validation set revealed information about the performance of the utilized interference elimination techniques, as well as the different NIR regions. The results showed that the combination band of water at approx. 5200cm^{-1} is of great importance since its performance was superior to the one of the so-called first overtone of water at approx. 6800cm^{-1} . Furthermore, this work demonstrated that MAS and FFT filter are fast and easy-to-use techniques for the elimination of interference fringes in FT-NIR transmittance spectroscopy.

Słowa kluczowe

FT-NIR spectroscopy, Interference fringe, water, Glucose, PLSR

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