

Chemometric detection of acetaminophen in pharmaceuticals by infrared spectroscopy combined with pattern recognition techniques : comparison of attenuated total reflectance-FTIR and Raman spectroscopy.

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Streszczenie

This paper presents and discusses the building of discriminant models from attenuated total reflectance (ATR)-FTIR and Raman spectra that were constructed to detect the presence of acetaminophen in over-the-counter pharmaceutical formulations. The datasets, containing 11 spectra of pure substances and 21 spectra of various formulations, were processed by partial least squares (PLS) discriminant analysis. The models found in the present study coped greatly with the discrimination, and their quality parameters were acceptable. A root mean square error of cross-validation was in the 0.14-0.35 range, while a root mean square error of prediction was in the 0.20-0.56 range. It was found that standard normal variate preprocessing had a negligible influence on the quality of ATR-FTIR; in the Raman case, it lowered the prediction error by 2. The influence of variable selection with the uninformative variable elimination by PLS method was studied, and no further model improvement was found.

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