Simultaneous measurement of two enzyme activities using infrared spectroscopy: A comparative evaluation of PARAFAC, TUCKER and N-PLS modeling

Enzymes are used in many processes to release fermentable sugars for green production of biofuel, or the refinery of biomass for extraction of functional food ingredients such as pectin or prebiotic oligosaccharides. The complex biomasses may, however, require a multitude of specific enzymes which are active on specific substrates generating a multitude of products. In this paper we use the plant polymer, pectin, to present a method to quantify enzyme activity of two pectolytic enzymes by monitoring their superimposed spectral evolutions simultaneously. The data is analyzed by three chemometric multiway methods, namely PARAFAC, TUCKER3 and N-PLS, to establish simultaneous enzyme activity assays for pectin lyase and pectin methyl esterase. Correlation coefficients $R_{pred2}$ for prediction test sets are 0.48, 0.96 and 0.96 for pectin lyase and 0.70, 0.89 and 0.89 for pectin methyl esterase, respectively. The retrieved models are compared and prediction test sets show that especially TUCKER3 performs well, even in comparison to the supervised regression method N-PLS.

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