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Investigation of plasticizer aggregation problem in casein based biopolymer using chemical imaging

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Abstract

This work aims to investigate the emergence of aggregates caused by redundant plasticizers in the protein matrix of casein based biopolymers using chemical imaging techniques. Near infrared (NIR) images (950 – 1671 nm) were first acquired and the spatial variations on macroscale with a pixel size of 0.4 mm × 0.5 mm were visualized. The introduction of plasticizers resulted in a strong hydrogen bonding matrix in the protein polymeric film as evidenced by analysis of Fourier transform near infrared (FT-NIR) spectral profiles in the range of 7500 – 4000 cm^{-1}. Attenuated total reflectance Fourier transform infrared (ATR-FTIR) images (4000 – 650 cm^{-1}) coupled with principal components analysis (PCA) and multivariate curve resolution alternating least squares (MCR-ALS) analysis suggested the existence of sorbitol re-crystallization after 5 months storage in the ambient condition. Raman images with a higher pixel size of 1.2 μm × 1.2 μm indicated an uneven film surface caused by sorbitol migration and re-crystallization. A partial least squares (PLS) regression model was developed to predict plasticizer concentration based on the mean spectra of FT-NIR hypercubes, producing coefficient of determination in calibration ($R^2{}_{Cal}$) of 0.93, cross-validation ($R^2{}_{CV}$) of 0.92 and prediction ($R^2{}_{P}$) of 0.89. Visualization of aggregates in the