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Detection of Butter Adulteration with Lard by Employing ¹h-NMR Spectroscopy and Multivariate Data Analysis

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ABSTRACT

The use of proton Nuclear Magnetic Resonance (1 H-NMR) spectroscopy allows the analysis of butter adulteration with lard by simultaneously quantification of all proton bearing compounds and consequently all relevant sample classes. Since the spectra obtained were too complex to be analyzed visually by the naked eyes, the classification of spectra was carried out using multivariate data analysis. The spectroscopic data of butter adulterated with lard samples were chemometrically evaluated and calibrated using the partial least square (PLS) algorithm. The multivariate calibration of PLS model for the prediction of adulterant was developed for quantitative measurement. The model yielded a highest regression coefficient (R^{2}) = 0.998 and the lowest root mean square error calibration (RMSEC) = 0.0091 and root mean square error prediction (RMSEP) = 0.0090, respectively. Cross validation testing evaluates the predictive power of the model. PLS model was shown as good models as the intercept of $R^{2}Y$ and $Q^{2}Y$ were 0.0853 and -0.309, respectively.

Keywords: Butter, Lard, ¹H-NMR, Multivariate data analysis, Adulteration, Chemometric