Analytical Authentication of Butter Using Fourier Transform Infrared Spectroscopy Coupled with Chemometrics

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Abstract : Fourier Transform Infrared (FT-IR) spectroscopy coupled with chemometrics was used to distinguish between butter samples and non-butter samples. Further, quantification of the content of margarine in adulterated butter samples was investigated. Fingerprinting region (1400-800 cm^{-1}) was used to develop unsupervised pattern recognition (Principal Component Analysis, PCA), supervised modeling (Soft Independent Modelling by Class Analogy, SIMCA), classification (Partial Least Squares Discriminant Analysis, PLS-DA) and regression (Partial Least Squares Regression, PLS-R) models. PCA of the fingerprinting region shows a clustering of the two sample types. All samples were classified in their rightful class by SIMCA approach; however, nine adulterated samples (between 1% and 30% w/w of margarine) were classified as belonging both at the butter class and at the non-butter one. In the two-class PLS-DA model's (R^2 = 0.73, RMSEP, Root Mean Square Error of Prediction = 0.26% w/w) sensitivity was 71.4% and Positive Predictive Value (PPV) 100%. Its threshold was calculated at 7% w/w of margarine in adulterated butter samples. Finally, PLS-R model (R^2 = 0.84, RMSEP = 16.54%) was developed. PLS-DA was a suitable classification tool and PLS-R a proper quantification approach. Results demonstrate that FT-IR spectroscopy combined with PLS-R can be used as a rapid, simple and safe method to identify pure butter samples from adulterated ones and to determine the grade of adulteration of margarine in butter samples.

Keywords : adulterated butter, margarine, PCA, PLS-DA, PLS-R, SIMCA