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Identification and Classification of Fiber-Fortified Semolina by Near-Infrared Spectroscopy (NIR)

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Abstract : Food fortification is the intentional addition of a nutrient in a food matrix and has been widely used to overcome the lack of nutrients in the diet or increasing the nutritional value of food. Fortified food must meet the demand of the population, taking into account their habits and risks that these foods may cause. Wheat and its by-products, such as semolina, has been strongly indicated to be used as a food vehicle since it is widely consumed and used in the production of other foods. These products have been strategically used to add some nutrients, such as fibers. Methods of analysis and quantification of these kinds of components are destructive and require lengthy sample preparation and analysis. Therefore, the industry has searched for faster and less invasive methods, such as Near-Infrared Spectroscopy (NIR). NIR is a rapid and cost-effective method, however, it is based on indirect measurements, yielding high amount of data. Therefore, NIR spectroscopy requires calibration with mathematical and statistical tools (Chemometrics) to extract analytical information from the corresponding spectra, as Principal Component Analysis (PCA) and Linear Discriminant Analysis (LDA). PCA is well suited for NIR, once it can handle many spectra at a time and be used for non-supervised classification. Advantages of the PCA, which is also a data reduction technique, is that it reduces the data spectra to a smaller number of latent variables for further interpretation. On the other hand, LDA is a supervised method that searches the Canonical Variables (CV) with the maximum separation among different categories. In LDA, the first CV is the direction of maximum ratio between inter and intra-class variances. The present work used a portable infrared spectrometer (NIR) for identification and classification of pure and fiber-fortified semolina samples. The fiber was added to semolina in two different concentrations, and after the spectra acquisition, the data was used for PCA and LDA to identify and discriminate the samples. The results showed that NIR spectroscopy associate to PCA was very effective in identifying pure and fiber-fortified semolina. Additionally, the classification range of the samples using LDA was between 78.3% and 95% for calibration and 75% and 95% for cross-validation. Thus, after the multivariate analysis such as PCA and LDA, it was possible to verify that NIR associated to chemometric methods is able to identify and classify the different samples in a fast and non-destructive way.

Keywords : Chemometrics, fiber, linear discriminant analysis, near-infrared spectroscopy, principal component analysis, semolina
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