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# Classification and quantitation of milk powder by near-infrared spectroscopy and mutual information-based variable selection and partial least squares

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**Abstract:** Milk is among the most popular nutrient source worldwide, which is of great interest due to its beneficial medicinal properties. The feasibility of the classification of milk powder samples with respect to their brands and the determination of protein concentration is investigated by NIR spectroscopy along with chemometrics. Two datasets were prepared for experiment. One contains 179 samples of four brands for classification and the other contains 30 samples for quantitative analysis. Principal component analysis (PCA) was used for exploratory analysis. Based on an effective model-independent variable selection method, i.e., minimal-redundancy maximal-relevance (MRMR), only 18 variables were selected to construct a partial least-square discriminant analysis (PLS-DA) model. On the test set, the PLS-DA model based on the selected variable set was compared with the full-spectrum PLS-DA model, both of which achieved 100% accuracy. In quantitative analysis, the partial least-square regression (PLSR) model constructed by the selected subset of 260 variables outperforms significantly the full-spectrum model. It seems that the combination of NIR spectroscopy, MRMR and PLS-DA or PLSR is a powerful tool for classifying different brands of milk and determining the protein content.

Keywords: Near-infrared; Milk; Feature selection; PLS-DA

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