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WP009: Application of targeted and untargeted ^{1}H NMR spectroscopy in cheese analysis

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Introduction

Cheeses that are labelled with PDO, or Protected Designation of Origin are regarded as possessing high quality and belong to the higher price segment of the market. It is not surprising that these products are often imitated or mislabelled, thus, development of robust and reliable analytical techniques is required to differ such products from one another. In the recent years Nuclear Magnetic resonance (NMR) spectroscopy has gained significant popularity in food analysis and we have decided to apply this method to discrimination of cheeses.

Methods

We have used proton NMR spectroscopy using both targeted and untargeted approaches to discriminate cheeses based on geographical origin and preparation technologies. The freeze-dried samples were extracted either by water or chloroform and each dataset was treated separately. Quantitative (targeted) analysis included identification of signals and assignment of these to specific metabolites, integration, and referral to external standard in aqueous extracts and calculation of relative molar concentrations of groups of compounds in chloroform extracts. Untargeted profiling consisted in binning (bucketing) the entire spectrum and subjecting the resulting bucket table to multivariate statistical methods such as principal component analysis (PCA).

Results

We have used the NMR approach in two case studies. The first case was the dataset containing two Italian PDO cheeses and several non-PDO competitor varieties. Both aqueous and chloroform extracts demonstrated that after the statistical analysis (Random Forest approach) the PDO cheese can be discriminated from others with 92-93% predictivity. The second case consisted in nutritional value study of cheeses enriched with blackcurrant and Cornelian Cherry. Here, the targeted NMR results indicate that it is possible to differ the blackcurrant-modified cheeses (that turned out to possess increased bioactive potential) from the others.

Innovative aspects

- NMR spectroscopic analysis of cheeses as a promising technique in mislabelling detection
- Can also be used for differentiating cheeses made with different production technology
- Both targeted and untargeted analysis, as well as both aqueous and lipid extracts are applicable

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