Title: Multi-omics in food analysis: the role of chemometrics in biomarkers identification and authentication

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Abstract:

The multi-omic characterization of food is increasingly widespread and is gaining more and more relevance in the field of food control. The huge amount of information provided by such highthrougput approaches makes it necessary the application of multivariate chemometric tools to extract the useful information and identify the effects played by the studied factors. Here, different examples will be provided, focusing on the statistical data treatment, involving the multi-omic characterization of food by proteomics, lipidomics and metabolomics. The case studies involve two different applications: 1) the identification of an illicit conservation treatment (a Cafodos-like solution) applied to fresh fish (sea bass); 2) the study of an ancient wheat filiera, from grain to bread, for the authentication of the product.

The study on sea bass involved four groups of samples: controls stored on ice in the fridge for 3 hours; controls stored under the same conditions for 24 hours; treated with a solution of hydrogen peroxide and citric acid for 3 hours; and treated with the same solution for 24 hours (these last two groups, while they are kept on ice in the fridge). Different parts of each fish (eye, muscle, skin, gills) were sampled by a sampling procedure based on the use of polymeric strips functionalized with adsorptive beads. The method, originally developed for the non-invasive sampling of cultural heritage, was exploited as a tool that can be easily applied in the field. The strips were then extracted with different media according to the final multi-omic analysis.

The study on the "San Pastore" wheat filiera involved: 1) the study of the differences between the historical San Pastore variety versus other hystorical and modern varieties; 2) the study of mixtures of San Pastore flour with other varieties for a possible application in food authentication, 3) the study of bread produced by San Pastore flour to verify if changes to the receipt (flour mixture, type of oil, type of yeast) can be detected.

In both these case studies, the samples were characterized by proteomics (by UHPLC-HRMS), lipidomics (by UHPLC-HRMS) and metabolomics (by GCxGC-MS).

The collected data were processed using multivariate statistical techniques of pattern recognition (PCA, ASCA, MFA, artificial neural networks) and classification (PLS-DA, SIMCA, Artificial neural networks), coupled to data fusion approaches, to identify the effect

played by the studied factors: effect of the illicit treatment (fish), differences between the cultivars (wheat), effect played by the receipt (flour mixture, oil and yeast) on bread.

References

[1] Benedetto, A. *et al.* Multi-omics approaches for freshness estimation and detcetion of illicit conservation treatments in Sea Bass (Dicentrarchus Labrax): data fusion applications" *International Journal of Molecular Sciences,* **2024,** 25(3), 1509. https://doi.org/10.3390/ijms25031509

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Biography

Elisa Robotti is Associate Professor of Analytical Chemistry and Chemometrics at the University of Piemonte Orientale, Italy. She is co-author of more than 100 articles in national and international journals (200; Scopus h-index: 30) and more than 10 book chapters. She is and has been involved in several European and national/international projects. In 2005 she has been awarded the Young Researcher Award of the Division of Analytical Chemistry of the Italian Chemical Society. Her areas of expertise cover:

- Development, optimization and validation (ISO17025) of analytical methods (HPLC-UV, HPLC-MS / MS, GC-MS, ICP-MS) for the determination of analytes in food, environmental and clinical matrices
- Development and application of biomarker identification methods based on shotgun proteomics, metabolomics and lipidomics;
- Exploitation of chemometric tools in different fields: cultural heritage preservation, industrial quality control, food chemistry, environmental applications