

MASS SPECTROMETRY, PROTEOMICS AND POLYMER CHEMISTRY

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Elisa Robotti

University of Piemonte Orientale, Italy

BIOGRAPHY

Elisa Robotti gained her PhD in Chemical Sciences in 2005 at the University of Piemonte Orientale, Italy with the thesis on chemometric tools applied to the field of analytical chemistry. She won the Young Researcher Prize of the Division of Analytical Chemistry of the Italian Chemical Society in 2005. Currently she is Associate Professor of Analytical Chemistry and Chemometrics at the same University. Her research interests involve in the development and optimization of analytical methods (HPLC-MS/MS, GC-MS and ICP-MS), the development and application of multivariate strategies for the identification of biomarkers in health science (proteomics, metabolomics, lipidomics and genomics); food and environmental sciences, experimental design techniques which was also applied to the industrial optimization of products and processes. She is the co-author of more than 80 papers in national and international magazines (h-index Scopus: 23) and 11 book chapters. She is the editor of a volume on the analysis of 2D-PAGE maps. She was participated in several national and international congresses and also she is responsible for the research units in national and international projects.

elisa.robotti@uniupo.it

MULTIVARIATE STATISTICAL TOOLS FOR THE IDENTIFICATION OF BIOMARKERS: APPLICATION TO MASS SPECTROMETRY-BASED APPROACHES

Mass spectrometry based techniques, either coupled or not to a chromatographic separation, are high throughput methods providing a huge amount of information. These techniques are often exploited for the identification of markers of particular effects, e.g. comparing different groups of samples in health sciences applications (controls vs pathological, control vs drug-treated etc.) or in food science (samples stored in different conditions, exposed to different environmental effects, from different varieties/cultivars/geographical origins in authentication and traceability studies). The identification of biomarkers from complex data like these must be accomplished by multivariate statistical tools, able to take into consideration the relationships between the variables (protein counts, analyte signals or concentrations, m/z signals etc.), to identify pools of markers with the best predictive ability. To this purpose, pattern recognition methods (Principal Component Analysis etc.) and classification tools like PLS-DA, Linear Discriminant Analysis, SIMCA, Ranking-PCA are also coupled to variable selection methods, Support vector machines etc. can be successfully applied, with a particular attention towards two different aspects: The exhaustivity of the search for biomarkers, to identify all possible candidates providing exhaustive information that can be used to identify deranged pathways; the predictive ability of the models to identify pools of biomarkers that can be used as reliable diagnostic markers. Examples will be provided from different applications: health science, for the identification of biomarkers of disease or of drug treatment; food science, for the identification of markers of different storage conditions, of ripening effects, of geographical origin or variety in authentication studies. The examples will involve applications from LC-MS/MS, GC-MS and ICP-MS. Some hints will also be given on data fusion approaches and able to fuse together different sources of information.