

# International Summit on Current Trends in Mass Spectrometry

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### Mass spectrometry-based approach for clinical proteomics

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Today, mass spectrometry-based (MS) approach is the leading approach employed in high-throughput analysis. Moreover, the investigation of complex biological samples requires the development of computational tools for processing and handling the great amount of data produced by MS experiments. The recent development of gel-free proteomics approach is allowing a significant improvement over gel-based analysis. Specifically, at ITB-CNR proteomics laboratory, the gel-free MudPIT (Multidimensional Protein Identification Technology) proteomic methodology is used for biomarker discovery and developing clinical methods. Our workflow involves user-friendly tools for characterization of biomarkers and proteotypic peptides, useful for validation step. Specifically, to perform a rapid comparison of protein lists and estimation of differentially expressed proteins, MAProMa home-built software has been developed. It is based on a label-free quantitative approach and it allows the visualization of data in a format more comprehensible to biologists and clinicians. Moreover, the correlation of proteomic data by unsupervised learning algorithms is evaluated; for example, hierarchical cluster groups the protein lists based on information found in the data that describes the objects (proteins) and their relationships. It will be presented technologies and tools to perform clinical proteomics studies involving different biological samples, for investigating human diseases, such as cardio-respiratory, degenerative and tumor diseases.

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### Ambient ionization MS for new insights in coffee science

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Coffee is one of the most consumed beverage and an important commodity for many developing countries. Its quality is generally related to good agriculture and handling practices. Geographic origin also plays a central role and discussions about terroir are common nowadays. Chemical investigations of coffees usually deal with low number of analytes using elaborated or time-consuming protocols and do not allow high-throughput analysis. The development of new, simple and fast methods for coffee analysis and quality control is still required. Ambient ionization MS comprises a set of techniques where the ionization process occurs outside the mass spectrometer, in open-air environment. Generally, they are simple and provide direct analyses. Here, ambient ionization techniques (Paper Spray, EASI and DESI-Imaging) are described to study and discriminate coffees. Coffee Spray ionization, where a bean slice is used as both sample and substrate to perform electrospray, is also introduced. Paper Spray fingerprinting combined with multivariate statistics was successfully employed as a fast and simple way to discriminate coffee origin. EASI-MS was used to study intact coffee beans submitted to different post-harvest treatments and wax components related to stomach irritations were easily detected. DESI-Imaging of a cross-sectioned bean revealed different spatial distribution of important phenolic compounds present in coffee. All these ambient ionization techniques proved to be very useful in coffee science. They can be employed to study a single bean or for high-throughput analysis, while preserving its integrity. Besides, with the improvements of portable MS, they have potential to be used in field studies.

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