

MASS SPECTROMETRY-BASED METABOLOMICS

OVERVIEW

- Metabolomics is an emerging -omic science aimed to analyze the metabolome in complex biological systems by the combination of sensitive analytical techniques such as mass spectrometry (MS) and multivariate data analysis.
- The metabolome is defined as the set of low molecular weight metabolites present in a biofluid, cell, tissue or organism at a qualitative/quantitative level as consequence of certain physiological conditions, such as genetic modifications, pathological states or responses to external stimulus.
- Changes in the metabolome are considered to be the best reflection of the activities of the cell at a functional level.

Metabolomic analysis provides a unique tool to examine cell function and to investigate the biochemical mechanisms involved and related to the observed phenotype responses.

APPROACHES

- Untargeted approach: simultaneous detection as many metabolites as possible to obtain a profile to identify key metabolites that are differently expressed in cases vs. controls.
- Targeted approach: qualitative and quantitative study of one or a small group of predeterminated metabolites chemically similar involved in the problem of interest.

APPLICATIONS IN SYSTEMS BIOLOGY

- Informative metabolomics: characterization and identification of targeted or untargeted metabolites to obtain intrinsic sample information.
- Predictive metabolomics: create a predictive model corresponding to the phenotype of a given organism or biological sample.
- Discriminant metabolomics: identification of Biomarkers for classification.

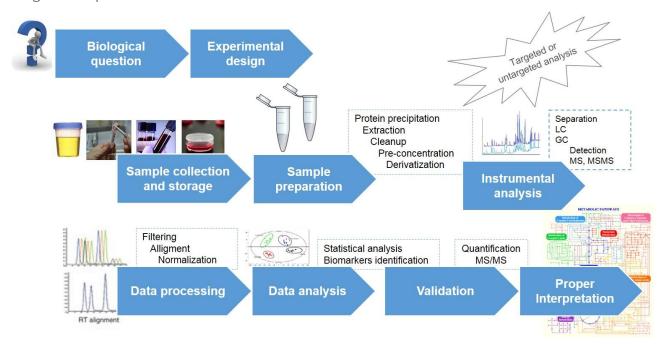
MS-Based Metabolomic Strategy Q-TOF analysis (Scan) TQ analysis (MRM) RP and HILIC chromatography.. Т Multivariate Data Analysis (PCA, PLSDA..) Target Metabolite list: T R Key metabolites of relevant pathways G ➤ Metabolite Class E G Т E List of detected T metabolites D D Metabolite identification. List of potential biomarkers Metabolite Ouantification **Biomarker Validation** Quantification **Biochemical interpretation**



WORKFLOW

A comprehensive analysis of metabolomic data requires a proper workflow strategy that integrates all stages from the experimental design, sample preparation, instrumental analysis, data analysis and biological interpretation.

Three main research interdisciplinary disciplines, bioscience, analytical chemistry and informatics, are essential for successful metabolomics work.



BIOMEDICAL APPLICATIONS

Basic and clinical research: Identify metabolites correlated with disease states providing key information on biological systems.

Pharmaceutical: Identify signatures and biomarkers of pharmacological actions and toxicity for drug development.

Environmental: Identify metabolites related to the effects of chemicals on a biological system.

Nutrition: proof of concept of nutraceuticals.

Metabolomics: Gate to precision medicine and personalized health care

SERVICES

- Assistance to the experimental design.
- Development of metabolic profiling studies using LC-MS (ESI+/-) and GC-MS analysis platforms.
- Discovery of biomarkers by comprehensive metabolic profiling and multivariate data analysis.
- Specific oriented platforms (lipids, oxidative damage, etc.)
- Standardized targeted quantitative analysis of biomarkers in biological samples





