



CING BIOINFORMATICS WORKSHOP #2

On

Mass Spectrometry-based omics: Data production, analysis and perspectives

Venue: The Cyprus Institute of Neurology and Genetics, Amphitheatre

Date: July 6, Thursday, 9:00-13:00

Potential Attendees: CING Scientists and CSMM Students

Registration: Free

Certificate of Attendance: It will be given to the registered attendees after the end of the Workshop.

Lecturers: Kyriacos Kyriacou (CING Electron Microscopy and Molecular Pathology Department), Kleitos Sokratous (CING Bioinformatics Group), Anastasis Oulas (CING Bioinformatics Group), George Spyrou (CING Bioinformatics Group)

Program

9:00-9:30 **Lecture 1.** Welcome Session and Introduction (Kyriacos Kyriacou)

Recent advances in mass spectrometry based proteomics and metabolomics technologies, offer a great promise in the understanding and treatment of the molecular basis of disease. Proteins are the work horses of cellular processes and the ability of studying dynamic protein expression, post-translational modifications, protein-protein interactions, is driving the identification of many disease-related biomarkers and actionable drug targets. It is anticipated that in addition to the increasing research applications in medical/biomedical research, proteomic and metabolomic profiling will become standard practice in the clinical laboratory. Indeed a major challenge that remains in more fully understanding the human genome, is the identification of the human proteome and metabolome. Proteins are structurally and functionally more diverse, and complicated to investigate, compared to genes. Moreover, proteins have a large dynamic range, are more transiently expressed and cannot be amplified like genes. The organization of this workshop, is both necessary and timely and it follows in the footsteps of the first Bioinformatics workshop. The aims are: to highlight the recent advances in proteomics and metabolomics, to discuss the applications that are available, as a result of the infrastructure established at the department of EM/MP, and showcase the essential link between these omics and Bioinformatics.

9.30-10:15 **Lecture 2.** Mass spectrometry-based omics: Proteomics and Metabolomics (Kleitos Sokratous)

Mass spectrometry (MS) has become an indispensable analytical technique for studying the proteome and metabolome profile of very complex biological samples. Multiple sample preparation methods as well as a variety of MS strategies can be employed, depending on the question under investigation. Here, the most commonly used MS-based methodologies that are currently used in proteomics and metabolomics, both targeted and untargeted, will be presented.

10:15-11:00 **Lecture 3.** Bioinformatics Functional Analysis of Proteomics Data (Anastasis Oulas)

Following proteomics analysis, the functional analysis of the relevant differential proteins may unmask pathways, interactions, post-translational modifications (PTM's) relevant for the biological question of interest. This in silico approach can be used to formulate new hypothesis that could be eventually used to further interrogate the biological system under investigation.

COFFEE BREAK (11:00-11:30)

11:30-12:15 **Lecture 4.** Structural analysis of biomolecules using mass spectrometry methods (Kleitos Sokratous)

Mass spectrometry (MS) has emerged as a powerful analytical tool for analysing biomolecules and biomolecular complexes. In addition, MS is becoming increasingly popular in the field of structural biology for studying protein structures and for mapping protein-protein interactions. Various MS techniques have been developed over the years to provide insights into the structural properties of proteins and protein complexes. In this session, the following structural MS techniques will be presented: native MS, ion mobility MS (IM-MS), Hydrogen Deuterium Exchange MS (HDX-MS) and cross-linking MS (XL-MS) as well as computational modelling using MS results.

12:15-13:00 **Lecture 5.** Structural Bioinformatics (George Spyrou)

A critical aspect in the bioinformatics analysis of biomolecules concerns their structure because it is strongly related to their function. In this session an introduction to structural bioinformatics will take place covering topics such as (1) biomolecular structure data formatting, (2) structure visualization and management tools, (3) computational modelling and simulations.