

WINTER WORKSHOP ON BIOLOGICAL INTERPRETATION OF METABOLOMICS AND LIPIDOMICS DATA

LOCATION: DLR 131 & 134

DATE: FEBRUARY 16 & 17

FEBRUARY 16TH

DATA FOUNDATIONS, LIPID STRUCTURE, AND METABOLIC CONTEXT

- 9:00 - 9:45: **Understanding the Structure and Information in Metabolomics and Lipidomics Datasets** - *Priyanka Ramesh*
 - How datasets are organized (sample metadata, feature tables, annotation fields)
 - Types of variables: intensities, identifiers, metadata
 - Interpreting raw vs. processed data structures
- 9:45 - 10:45: **Lipid Structure, Properties, and Roles - Part 1** - *Christina R. Ferreira*
 - Fundamentals of lipid classification and diversity
 - Linking chemical structure to physical properties
- 10:45 - 11:00: **Coffee/Tea Break**
- 11:00 - 12:00: **Lipid Structure, Properties, and Roles - Part 2** - *Christina R. Ferreira*
 - Biological functions of lipid classes
 - Case examples in health and disease contexts
- 12:00 - 13:00: **Lunch**
- 13:00 - 14:00: **Approaches to biological interpretation of lipid profiles generated using MRM analysis: Case studies** - *Theresa Casey*
 - Data reshaping for pathway analysis, interpreting lipid turnover and flux, and case studies
- 14:00 - 15:00: **Feature Selection and Feature Engineering in Mass Spectrometry: Finding the Signals That Matter** - *Bartek Rajwa*
 - Overview of ML approaches for lipidomics
 - Feature selection, classification, and predictive modeling
 - Examples from disease development studies
- 15:00 - 15:15: **Coffee/Tea Break**
- 15:15 - 16:15: **Small Molecule Profiling Analysis in Toxic Insult Models** - *Jonathan Shannahan*
 - Biomarkers of toxic exposure, integration into toxicology workflows, and dose-response interpretation
- 16:15 - 16:45: **Day 1 Wrap-up and Open Q&A**

FEBRUARY 17TH

SPATIAL AND INTEGRATIVE BIOLOGICAL INTERPRETATION

- 9:00 - 9:45: **Lipid Ontology** - *Christina Ferreira*
 - Ontology systems for lipid annotation, classification consistency, and data integration
- 9:45 - 10:30: **Overlay of Morphological and Chemical Data in Spatial Analysis** - *Weiwei Zhang*
 - Integrating histology with metabolomics/lipidomics to interpret spatial patterns
- 10:30 - 11:15: **Specific Pathway Analysis Using Spatial Metabolomics** - *Wagner Tamagno*
 - Pathway-level interpretation from spatial metabolomics datasets
 - Mapping metabolic flux and localization in tissues
- 11:15 - 11:30: **Coffee/Tea Break**
- 11:30 - 12:00: **Cardinal MS Application to Spatial Metabolomics Data Analysis** - *Julie Brothwell*
 - Spatial metabolomics workflows and applying Cardinal MS to lipidomics data
- 12:00 - 12:45: **High-Throughput Profiling: Biological Insights from Automated DESI-MS** - *Nicolás Morato*
 - Profiling diseases and biological condition markers in a biologically meaningful context.
- 12:45 - 13:45: **Lunch**
- 13:45 - 14:15: **Integrative Panel Discussion: From Data to Biological Insight**
 - All speakers; linking molecular data to biological meaning
- 14:45 - 15:15: **Guided Group Exercise: Full Interpretation Workflow**
 - Teams analyze a case dataset combining untargeted, targeted, and spatial data
- 15:15 - 15:30: **Coffee/Tea Break**
- 15:30 - 16:00: **Workshop Synthesis & Closing Remarks**
 - Summary of key points, feedback, and networking