

TWO-DAY COURSE, Saturday and Sunday

Introduction to MALDI and DESI Mass Spectrometry Imaging: Principles, Protocols, Applications and Data Analysis

INSTRUCTORS



Georgia Charkoftaki
Yale University



Peggi Angel
Medical University of
South Carolina



Madeline Colley
Vanderbilt
University



Christina Ferreira
Purdue University



David Muddiman
North Carolina
State University

TARGET AUDIENCE / LEVEL

This course is designed for individuals who are new to MALDI/DESI in mass spectrometry. It is ideal for:

- **Graduate Students** in fields such as chemistry, biology, biochemistry, pharmacy, materials science, and related disciplines who want to gain a foundational understanding of MALDI and DESI.
- **Early-Career Researchers** looking to incorporate MSI into their research for the first time. This includes those working in academic, clinical, or industrial settings where MALDI or DESI applications are relevant.
- **Scientists** from pharmaceutical, biotechnology, or environmental sectors who are interested in learning about the practical applications of MALDI and DESI for research, product development, or quality control.
- **Scientists new to Mass Spectrometry** who have little to no prior experience with mass spectrometry and wish to learn about ionization techniques like MALDI and DESI, as well as their potential uses in various scientific and industrial contexts.

No prior experience with mass spectrometry is required for this course, making it suitable for anyone seeking a comprehensive introduction to these powerful analytical techniques.

DESCRIPTION

This two-day introductory course is designed for those interested in learning about Matrix- Assisted Laser Desorption/Ionization (MALDI) and Desorption Electrospray Ionization (DESI) in mass spectrometry. The first day, the participants will gain a theoretical understanding of the fundamental principles of these ionization methods and insights in the sample preparation, and applications. The second day will be dedicated to data analysis, giving an overview of all the available software. The course will focus on key concepts in data acquisition, processing, and interpretation, while exploring the use of specialized software tools for analyzing complex data sets. Participants will leave with practical knowledge of how to analyze imaging data and be able to draw meaningful conclusions from their experiments. The course will include lectures, examples, and interactive discussions.

Data analysis

There are several platforms to analyze MSI data and an overview of all the available options will be provided at the start of the second day of the course. For hands-on data analysis and live demonstration, this part of the workshop will utilize MSiReader as the platform, which is vendor neutral. All attendees will receive a free 3-month license to the program. This aspect of mass spectrometry imaging takes on many different aspects typically starting with the following key functions: importing data, visualization, normalization and analysis. The functions will be illustrated in a live demonstration using shared datasets. This will be followed by more deep analysis and characterization of the data using a variety of tools including statistical methods, machine learning and AI approaches. This module will conclude with a section on data annotation, multi-modal integration (e.g., LC-MS/MS based proteomics data with MSI data), and how to turn these data into a biological interpretation. Attendees can bring their own laptop to actively participate during the live demonstration; however, this is not necessary. If you chose to follow the live demonstration, please have MSiReader downloaded prior to Day 2

(assistance will be available via zoom before the short course and on Day 1 of the short course).

Preliminary Agenda Day 1

9:00 a.m. **Introduction to mass spectrometry imaging: Overview and roots of MSI** (GC)
10:15 a.m. Coffee break
10:45 a.m. **Advancements in Instrumentation** (MC)
12:00 p.m. Lunch (provided by ASMS)
1:00 p.m. **Sample Considerations and Sample Preparation Protocols for MALDI and DESI part I (small molecules, lipids)** (GC, CF)
2:15p.m. Coffee break
2:45p.m. **Sample Considerations and Sample Preparation Protocols for MALDI and DESI part II (proteins, glycans)** (PA, CF)
4:00p.m. **Multimodal analysis** (PA, MC)
5:00 p.m. **Discussion, Q&A, wrap up** (All)

Preliminary Agenda Day 2

9:00 a.m. **Software overview of MS imaging data analysis** (GC and MC)
10:15 a.m. Coffee break
10:45 a.m. **Processing MS imaging data (data import, analysis and visualization): theory and live demonstration of a vendor neutral software** (DM)
12:00 p.m. Lunch (provided by ASMS)
1:00 p.m. **Statistical methods, machine learning and AI approaches for MS imaging data: theory and live demonstration** (DM)
2:15p.m. Coffee break
2:45p.m. **Data annotation, multimodal integration, and biological interpretation** (DM)
4:30p.m. **Discussion on future developments and needs in the field** (All)
5:00 p.m. **Q&A, wrap up**

Abbreviations for Instructors

Georgia Charkoftaki (GC)
Peggi Angel (PA)
Madeleine Colley (MC)
Christina Ferreira (CF)
David Muddiman (DM)