# ONE-DAY COURSE, Sunday

# Statistical Analysis of MS Imaging Experiments with Cardinal and R

### Instructors



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#### Description

The course will discuss the basics of data manipulation, visualization, and statistical analysis of mass spectrometry (MS) imaging experiments using Cardinal and R. The course is intended for scientists who are familiar with MS imaging (including DESI, MALDI, etc.), but who have limited exposure to statistics, machine learning, and programming with R. The course examples will focus on the open source Cardinal R package, but will also cover statistical practices that are useful for design and analysis of MS imaging experiments more generally.

We will begin by introducing the fundamentals of MS imaging data from a computational perspective. We will describe the open data format imzML used by open source tools for storage, import, and exchange of MS imaging data. We will use case studies with datasets from public repositories such as PRIDE and MassIVE to demonstrate pre-processing, visualization, and statistical analysis of MS imaging experiments. We will discuss selection of appropriate methods for different analytic goals including (1) segmentation, (2) classification, and (3) class comparison in the context of MS imaging, and we will demonstrate how to apply these methods using Cardinal. The day will end with a discussion of computational needs and future directions in MS imaging, a Q&A session, and limited hands-on help with participant datasets. Each topic will include a mixture of lecture and hands-on demonstration with live coding.

### **Target audience**

- 1. Biologists, chemists, and bioinformaticians who have familiarity with MS imaging experiments and want to learn how to apply pre-processing, visualization, statistical analysis, and machine learning methods for MS imaging using Cardinal and R.
- 2. Computer scientists, data scientists, statisticians, and engineers who are familiar with programming and mass spectrometry but are new to imaging and want to learn about existing computational tools and methodologies for MS imaging.

# Agenda

9:00 a.m. Basics of MS imaging data import, manipulation, and visualization
10:15 a.m. Coffee break
10:45 a.m. Processing spectra and advanced manipulation of MS imaging data
12:00 p.m. Lunch (provided by ASMS)
1:00 p.m. Statistical methods and machine learning for MS imaging experiments
2:15p.m. Coffee break
2:45p.m. Statistical interpretation for MS imaging models
4:30p.m. Future developments and Q&A
5:00 p.m. Wrap-up

## Requirements

We will use the latest versions of  $\underline{R}$  with <u>Bioconductor</u> and <u>Cardinal</u>. Please install or update to the current versions if you wish to follow along with the examples.