May Institute on computation and statistics for mass spectrometry and proteomics

May 6, 9am - 5:00pm, 2024. Analysis of mass spectrometry images with Cardinal

#### Venue:

Northeastern University main campus, Shillman Hall, 3rd floor. Please see the annotated map.

#### Lead instructors:

Kylie Bemis, k.bemis@northeastern.edu

### **Speakers**

Sai Lakkimsetty, lakkimsetty.s@northeastern.edu

### **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 programming with R. We begin by introducing the fundamental ways of interacting with MS imaging datasets and experimental metadata using Cardinal and R, followed by tutorials on pre-processing and visualization of mass spectra and ion images. Finally, we will demonstrate the application and interpretation of statistical methods including segmentation, classification, and testing. 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. Examples will use datasets from public repositories such as PRIDE or MassIVE.

# **Target audience**

Biologists, chemists, bioinformaticians, computer scientists, data scientists, statisticians, engineers, who are comfortable with basics of R, and interested in working with Cardinal.

### **Tentative schedule**

#### Monday May 6, 2024

 $9:00\ a.m.$  Basics of MS imaging data import, manipulation, and visualization, Kylie Bemis

10:30 a.m. Refreshments

11:00 a.m. **Processing spectra and advanced manipulation of MS imaging data**, Kylie Bemis 12:30 p.m. Lunch on your own

1:30 p.m. Statistical methods and interpretation for MS imaging, Kylie Bemis

3:00 p.m. Refreshments

3:30 p.m. Future advances and Q&A roundtable, Kylie Bemis and Sai Lakkimsetty

5:00 p.m. Q&A

6:00 p.m. - 8:00 p.m. General course dinner in <u>Back Bay Social Club</u>. The dinner is free. All the participants and the instructors are invited.

# Requirements

The Beginner's R session is recommended for participants without prior R experience.

We will use the latest versions of R 4.4 with Bioconductor 3.19 and Cardinal 3.6. Please install or update to these versions if you wish to follow along with the examples.

# **Course materials:**

Course materials can be downloaded here.

# Link to participant lunch order pickup

If you would like us to pick up your pre-payed lunch order from Tatte or B.Good, <u>please fill this form</u>

# Course dinner signup

If you are joining the free dinner on May 6, 6:30pm at Back Bay Social, RSVP through this form

# **Course evaluation**

Please help us improve the program in the future by filling in this evaluation form