

Imaging Mass Spectrometry Interest Group Workshop Report 2022

Workshop held Tuesday, June 4th 5:45-7:00 pm at the ASMS Annual Conference in Minneapolis, MN.

Topic:

Imaging MS: Opportunities for Artificial Intelligence and Machine Learning

In-Person Moderators:

Alison Scott – University of Maryland Baltimore; Maryland, United States
Ingela Lanekoff – Uppsala Universitet; Uppsala, Sweden

Session Description and Goals:

Background: Artificial Intelligence (AI) and Machine Learning (ML) methods are maturing in parallel with spatially resolved, 'omics-scale mass spectrometry applications. A growing number of computational experts are working with imaging mass spectrometry data, and through this work, experimental conclusions and new information embedded in a dataset can be explored and unlocked. Impressive strides are made in this area each year. Yet, few tools exist to apply AI and ML to imaging mass spectrometry that function at an accessible level for a non-computational scientist. This workshop aims to discuss the current state of the field, identify accessible tools and software, best practices and pinpoint hurdles to the broad uptake of AI and ML tools for imaging mass spectrometry analysis.

Organization: This workshop will be presented in two parts. First, an invited speaker will briefly present current background, tools, and hurdles in AI and ML applied to imaging mass spectrometry followed by Q&A. Second, an organized panel discussion will explore the pros and cons of these techniques and address participant questions and challenges. Please come with questions, comments, and discussion topics for the panel and audience.

Speakers:

Wout Bittremieux (University of California San Diego): An introduction to AI & ML – terminology and general strategies

Olga Vitek (Northeastern University): Applications of AI & ML techniques within imaging MS – tools and strategies

Panelists:**Wanqiu Zhang (KU Leuven)****Nathan Heath Patterson (Vanderbilt University)****Theodore Alexandrov (EMBL)****Raf van de Plas (TU Delft)****Aivett Bilbao (Pacific Northwest National Laboratory)****Debangshu Mukherjee (Oak Ridge National Laboratory)****Discussion:**

The two introductory presentations from Wout Bittremieux and Olga Vitek were informative and well received. First, Wout explored the basics of ML and AI, specifically, what machine learning is at its core. Some elements of modeling were introduced, and thought-provoking situations where ML fails were presented. Next, Olga gave a thorough explanation of how the Cardinal team approaches complex problems in imaging MS. Data analysis vignettes were shown to illustrate several workflows available for imaging datasets. Finally, freely available and GUI-supported tools were shown.

Following the introductions, we transitioned to a panel discussion led by audience questions. The panelists were teamed up into 'pro' and 'con' teams to provide a point-counterpoint perspective for each question. The audience responded positively to this format and stayed engaged throughout the discussion. Some highlights of the discussion included topics such as:

- Incorporating new analysis methods into old data analysis workflows – identifying barriers to just getting started.
- Panel recommendations to work early and often with your data analysis team – that vocabulary and common language about the problem are often the missing links to getting started
- How many replicates are enough replicates to validate a model?
- Who is responsible for negative outcomes when the AI/ML model fails?

Overall, the audience was engaged with the material and enjoyed the format. The introductory material was helpful to get all participants on the same page with vocabulary, and that helped propel the discussion panel forward. This is an active area for research in imaging MS and may be a good topic for a focused mini-symposium in the near future.

Participants:

Room attendance estimated at ~100.