

## **Imaging Mass Spectrometry Interest Group Workshop Report 2021**

Workshop held Wednesday, November 3<sup>rd</sup> 5:45-7:00 pm at the ASMS Annual Conference in Philadelphia, PA.

### **Topic:**

Interpreting Imaging MS Data at 'Omics Level: Integration with Other 'Omics Platforms

Due to changing travel restrictions a group of people contributed to running the workshop. Everyone's contribution was acknowledged in the opening remarks.

### **In-Person Moderators:**

Alison Scott – University of Maryland Baltimore; Maryland  
Boone Prentice – University of Florida; Florida

### **Hybrid/Online Moderators:**

Jens Soltwisch – University of Münster; Germany  
Tiffany Porta Siegel – Boehringer-Ingelheim; Germany  
Gus Grey – University of Auckland; New Zealand

### **Session Description and Goals:**

Progress continues to be made in interpreting imaging mass spectrometry data at the omics level and validating imaging results with other omics techniques for comprehensive spatial omics. From these investigations, several new software tools and experimental strategies have emerged to more confidently interpret metabolomics and proteomics imaging MS data in biological and pathological contexts. In this workshop, we will discuss these tools, their strengths and how to address current limitations. Preliminary topics to be addressed include:

- 1) Current software solutions for omics level interpretation of imaging MS data
- 2) Pathway analysis integration with IMS
- 3) How to integrate imaging interpretation software with other omics software
- 4) Advanced analytical methods for validation of identities in imaging MS
- 5) Quantitation

A goal is to further disseminate information on challenges and solutions for integration of imaging MS with other omics platforms for confident biological interpretation.

### **Session Organization:**

The workshop session topic and a call for interested speakers was sent to the distribution lists of both the Imaging Mass Spectrometry Society (IMSS) and the Mass

Spectrometry Imaging Society (MSIS). A lineup of speakers was curated from the responses to highlight an array of the topics within the session description. The final format was similar to previous years with 5 speakers giving short and targeted presentations aimed at prompting discussion. The session was introduced by Alison Scott and Boone Prentice. All speakers gave their presentation and a group discussion followed with questions from the attendees (in person and online) and from a moderated list of discussion topics.

### **Speaker Lineup:**

**Evan Larson (Iowa State University):** “METASPACE enables metabolite annotation of on-tissue derivatized mass spectrometry imaging data”

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**Peggi Angel (Medical University of South Carolina):** “A strategy for determining tumor associated spatial variation in proline site modifications from collagen peptides”

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**Meng Xu (University of Wisconsin):** “Reconciling MALDI-TOF MS imaging and LC-orbitrap multiomics data”

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**Shannon Cornett (Bruker Daltonics):** “Using LCM to bridge imaging and omics”

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**Heath Patterson (Vanderbilt University):** “Linking and integrating omics data through the spatial domain”

### **Discussion:**

The speakers gave on-topic, intriguing presentations prompting a lively discussion to close out the workshop. Broadly, the multi-omics approach to imaging mass spectrometry is an expanding area and does still lack robust tools and pipelines for correlating *in situ* spatial data with spatially-extracted data. Several speakers highlighted attempts to fill this gap. One topic that prompted an active discussion was the consideration of universality of an ion association with a histological feature. How can the community begin to build consensus around this topic? Several solutions were proposed, all with clearly articulated hurdles and challenges. One of the first comments to this point was without standardized reporting, instrumentation, biological samples (including diverse species) and preparation building these consensus associations could prove difficult with a low level of confidence. On further consideration, it was noted, if the same ion (or sets of ions) is routinely associated to a biological or histological feature using diverse methods, ionization methods, detectors, and sample preparations the confidence could be much higher.

The active discussion could have continued on much longer as online questions and in person attendee questions were still coming in at the close of the session. To keep on timing the session was closed at 7:00 pm.

**Participants:**

Room attendance was estimated at 60+ with 46 in-person attendees responding to the survey that they attended the Imaging workshop. Online attendance was robust and remote participants were active in sending discussion questions.

**Survey Input:**

Overall, the workshop quality, topic, and format were well-received by the participants scoring between 4 and 5 (scale of 1-5) on average (each category). Survey comments indicated more discussion time would have been welcomed.