Ion Mobility Spectrometry-Mass Spectrometry Workshop Report:

Ion Mobility MS Data Analysis Tools: What's There and What Isn't

Wednesday, Nov. 3, 2021

Pennsylvania Convention Center

Presiding: Kelly Hines, UGA, Ian Webb, IUPUI, and Xueyun Zheng, PNNL

Panelists:

Chae Jeon (CUI-Suite, Ruotolo Lab, University of Michigan)

Matt Willets (Proteomics, Bruker)

Sarah Stow (IM Data processing, Agilent)

Hannes Röst (Lipidomics/TIMS-TOF, University of Toronto)

Attendance: In person, ~60; more online (77 responded to survey)

At this year's IMS/MS workshop, we invited panelists to discuss software tools they were actively developing or using in support of IM/MS datasets. First, Chae Jeon spoke about the CIU-Suite Software that is being developed by the Ruotolo Laboratory for enabling the analysis of collision induced unfolding experiments performed on various ion mobility mass spectrometry platforms. Next, Matt Willets discussed the software workflows at Bruker for analyzing proteomics data generated by trapped ion mobility spectrometry instruments. Sarah Stow discussed analysis workflows at Agilent for processing ion mobility data on the Agilent platform including collision cross section measurements. Finally, Hannes Röst spoke about an open source workflow for analyzing trapped ion mobility lipidomics data currently under develop.

The panel sparked a lively discussion. One of the major points of discussion was the ability to analyze and represent data on open-source libraries and file formats. While there are tools for some applications that can use these formats (such as Skyline), there was a divided perspective on whether current open-source libraries and file formats are suitable for big IMS/MS data set analysis. Several questions were asked about the suitability of different tools for different projects. Discussion closed with mentioning specific features that community members need in software tools in order to help support their experiments.

Below is the feedback that we received for the workshop:

Comments:

Some vendors were not represented in this workshop: Waters Corporation

Same topic as 4 years ago.

I think this session needed a broader overview of the available tools before the mini talks highlighting particular software. That overview could have replaced one of the other talks. The panel discussion format works best when the presenters are knowledgeable about the field as a whole, not just their own work, and that aspect could have been better. That said, there was some good discussion about open source and related issues.

Overall favorable, One presenter, Sarah Stow, give very good general information. The others where more niche, but also useful.

This workshop had brief presentations and a discussion - so it was suitable for virtual attendees (although they did seem a bit shocked/baffled when I asked a question via the app.!). This was, by far, the best workshop I attended this year - although it was nowhere near as good as IM workshops in previous years.

Watched

There's a challenge in presenting all vendor software options

I would have wished for a longer discussion round.

More of a panel discussion than a workshop, but quite informative. Many talks walked through basic concepts and introduced analysis software currently in the field and in development
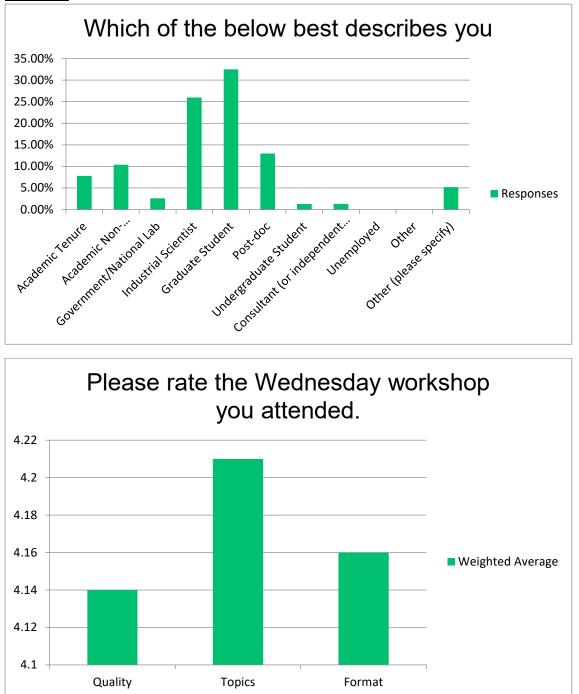
This would have benefitted from a more guided discussion. The audience may have been a bit too broad to facilitate a cohesive discussion. Ion mobility may be becoming too broad of a field to have a general interest workshop.

I think this workshop may have started a few minutes early (or perhaps started on time, but the plenary session ran over time). Thus, I missed the beginning of the workshop, so I am not sure if there was a general introduction. I think this workshop would benefit from splitting up those who are interested in ion mobility of small molecules and using it as an orthogonal separation technique vs. those who are interested in using ion mobility in native MS to learn something about biomolecular complex size/shape/structure.

Good discussion. (No consensus as always)!

I presented at this workshop so I probably shouldn't be rating it

As a remote attendee I was disappointed that we can't be part of the live discussion.

Surveys of Attendees: 77 total responses were received, 59 in-person attendee, 18 online attendees

Which of the below best describes you

Please rate the Wednesday workshop you attended.