

FTMS Interest Group Workshop Report

ASMS 2025, Baltimore

Title: FTMS Community Resources: Access, Education, and Data Analysis

Presiders: Yury Tsybin and Martha Chacon-Patino

Date: Tuesday, June 3, 2025

Attendance: ~60

Overview

The 2025 FTMS Interest Group Workshop brought together researchers, educators, and industry partners to strengthen the growing Fourier Transform Mass Spectrometry (FTMS) community. The session emphasized collaboration, accessibility, education, and data analysis, all of which are critical for advancing the field.

At the opening, the presiders introduced a new social platform for community interaction: the professional LinkedIn group “Fourier Transform Mass Spectrometry – ASMS Interest Group”. Members are encouraged to join and actively participate in sharing knowledge and opportunities.

The workshop was structured around **three focus areas**:

1. **Access to FTMS Instruments:** The discussion highlighted the importance of broadening global access to FTMS instrumentation, both ICR and Orbitrap platforms, through user facilities, institutional initiatives, and international networks. Overall, the presentations provided a comprehensive overview of the current options for FTMS data generation and processing at user facilities in the US and in Europe.

First, the available access options were briefly presented for the main FTMS manufacturers, Bruker and Thermo. The presiders acknowledged and thanked Alexander Makarov from Thermo Fisher Scientific and Paul Spier from Bruker for providing information on the FTMS resources covering Orbitrap and MRMS (FT-ICR MS) technologies (access and education) from the corresponding manufacturers.

Secondly, the two major user programs were covered in detail: the NHMFL/MagLab ICR Program (presented by ICR Program Director, **Kristina Hakansson**) and the EMSL/PNNL ICR & Orbitrap program (presented by Lab Fellow, **Ljiljana Pasa-Tolic**). The **Maglab** user program is detailed here: <https://nationalmaglab.org/user-facilities/icr/>. The **EMSL** user program is described here: www.emsl.pnnl.gov/user-program, and proposals are welcome for submission here: www.emsl.pnnl.gov/proposals.

Thirdly, **Carlos Afonso** presented **Infranalytics**, the only European network currently providing access to FT-ICR MS instruments in France. For more details and submission of a scientific project proposal, please visit <https://infranalytics.fr>. He also showcased early results from the newly installed 18 T TIMS FT-ICR MS (Bruker Daltonics), which is already accessible through the program.



Figure 1: Impressions from the 2025 ASMS FTMS IG Workshop: presidents, Yury and Martha, in front of the great audience listening to the informative presentation by Ljiljana Pasa-Tolic (PNNL).

2. **Teaching FTMS Principles:** Education remains central to sustaining and growing the FTMS community. This year's session emphasized the creation of shared educational resources, including animations, tutorials, and simulations, with the long-term goal of building an open-access repository for educators and learners.

David Kilgour (Vibration Ltd., UK) presented his view on how FTMS is currently taught, outlined key challenges, and shared thoughts on future improvements to enhance teaching effectiveness. As an enthusiastic teacher of FTMS, David shares multiple related tools and materials on the web. These can be accessed here <https://tinyurl.com/mr489aud> and here <https://kilgourlab.com/teaching-resources/>.

Konstantin Nagornov (Spectroswiss Sarl, Switzerland) introduced a new open access tool that allows simulation of FTMS data via time-domain (transient) data generation: <https://www.peakbypeak.com/>. The tool is a hybrid web-app with many capabilities implemented using browser-based calculations. This novel tool should be of an interest and importance to someone learning and practicing FTMS. The stand-alone desktop version of this web-app is the FTMS Simulator from Spectroswiss. The former, in its present state, is suited for simulation of individual isotopic envelopes, whereas the latter can be employed to generate highly complex mass spectra and large datasets.

3. **Data Analysis Challenges & Solutions:** The final focus area addressed the complexity of FTMS data processing and the need for robust, accessible workflows. Several software tools were highlighted:
 - **Ryan Rodgers** of MagLab presented the mass difference analysis (MDA) method for complex mixtures, a fully automated approach for recalibrating FT-ICR MS data without internal calibrants and for assigning molecular formulas by leveraging repeated, theoretically defined mass differences. This method will be released

through the PyC2MC pipeline. Currently, only the viewer is available at <https://github.com/iC2MC/PyC2MC>, and the repository will be updated periodically to include the MDA tools. He emphasized the need for accessible workflows capable of handling large, time-resolved datasets with high confidence.

- **Boniek Gontijo Vaz** from the Federal University of Goiás in Brazil described their new tool for isotopic ratio analysis for FTMS, **IsotoPy**; the tool is accessible as a web application via www.isotopy.com.br.
- **Robert Chalkley** from UCSF updated the community on the existing and more recently updated functionalities of one of the (FT)MS data analysis cornerstone software tools – **Protein Prospector**. This famous tool is available as a web application since 1996 (!!) at the same address: www.prospector.ucsf.edu.



Figure 2: Presiders and presenters of the 2025 ASMS FTMS IG Workshop: (left to right) Konstantin Nagornov, Ljiljana Pasa-Tolic, Ryan Rodgers, Kristina Hakansson, Robert Chalkley, Martha Chacon-Patino, Yury Tsybin, and Boniek Gontijo Vaz. Missing presenters: David Kilgour and Carlos Afonso.

Closing

The presiders expressed gratitude to all presenters and participants for contributing to a lively, collaborative, and forward-looking workshop. The session concluded with open discussion, inviting suggestions for future topics and volunteers for presider roles in upcoming meetings.

See you at the LinkedIn group page! <https://www.linkedin.com/groups/13187570/>