

2017 ASMS Workshop Report

FTMS: Successes and Challenges of Achieving Routinely High Mass Accuracy

Monday June 5, 2017: 5:45-7:00 pm

David Kilgour and Melinda McFarland, Presiding

Estimated Attendance: 100

Summary of Program and Discussion

The aim of the workshop was to discuss the experiences of the community when trying to analyse samples, to a consistently high mass accuracy, by FTMS methods – based on what was identified as an area of key interest at the previous workshop. We were particularly interested in discussing which factors impact mass accuracy on FTMS instruments and when is mass uncertainty adversely affecting results or the confidence in results, in practice?

The workshop began with two excellent short tutorials, covering the underlying theoretical reasons that govern achievable mass accuracy for both ICR and Orbitrap type FTMS instruments, given by Prof Peter O'Connor (University of Warwick, UK) and Dr. Konstantin Aizikov (Thermo Fisher Scientific). The aim of these tutorials was to remind us, as a community, how our use of our instruments has a direct effect on their performance, and why.

The interest group had been contacted, prior to the ASMS meeting, in order to solicit short (5 min) presentations, summarizing occasions where mass accuracy for FTMS had been a key component of some recent research – either with a fundamental positive or negative impact. The aim of these short presentations was to catalyse discussion. A number of proposals were received but, owing to time constraints, only 5 could be given:

- Don Smith (NHMFL) – The National High Magnetic Field Lab’s approach to high mass accuracy in ICR: High magnetic field, harmonized ICR cell, conditional signal averaging/automatic gain control, absorption mode, and the walking mass calibration
- Benjamin Oyler (Institute of Marine & Environmental Technology, University of Maryland) – high confidence structural elucidation of dinoflagellate polyol toxins by ICR MS
- Konstantin Nagornov (Spectroswiss Sàrl) – an implementation of very high mass accuracy in petroleomics using internal calibration and a moving calibration function
- Pieter Kooijman (M4I, Maastricht University) – current fundamental mass (in)accuracy issues in DESI imaging by FT-ICR MS
- Arpad Somogyi (Ohio State University) – identifying organic materials in meteorites by high mass accuracy FTMS

After these very well presented talks, the floor was then opened for discussions that included consideration of the minimum number of peaks required to process absorption mode FTMS spectra by internal phase calibration, the underlying ion population variation issues that result in the well-known mass accuracy problems being encountered in the FTMS imaging community, and what might be done about them and individual examples of unexpectedly poor mass accuracy and what might be changed to improve the results (often related to ion population control). One key point that has been raised in many previous FTMS interest group sessions was raised again: how does the Orbitrap software calculate the noise level? That this question is asked so consistently at these workshops is an indication of the benefit that might derive if that information was to be published.

Members of the interest group requested that the presentation slides given at the workshop be made available. Those for which we have received permission to publish can be downloaded from: <http://www.kilgourlab.com/asms-ftms-interest-group-2017/>

An announcement was given regarding seeking a new co-chair of the interest group (with one application already received by email) and the meeting was adjourned.

The fact that the workshops for both the FTMS and Top-down proteomics interest groups were scheduled at the same time, for the second year in a row, was noted. This has been raised to ASMS and we hope efforts will be made to avoid this conflict in future meetings.