2021 ASMS Workshop Report — FTMS Interest Group **Protips and Life Hacks for FTMS** Wednesday November 3, 2021 Philadelphia, Pennsylvania Lissa Anderson (NHMFL) and Chad Weisbrod (NHMFL), Presiding

Estimated in-person attendance: ~50

Summary of Program and Discussion

Did you know that mass measurement accuracy can be significantly improved by employing calibrants that have charge distributions like those of the analytes of interest? Ever wonder what the difference between reduced and full profile modes was? Users of FTMS cannot all be instrumentation experts! Most have no idea what a Hanning apodization is, let alone its effect on peak shape. The goal of the 2021 FTMS workshop was to outline important considerations for FTMS and distill relevant information in the simplest way possible for end users. Speakers were recruited from academia and industry to provide expert advice tailored to those of us who don't know how to use SIMION.

To open the workshop, Lissa Anderson demonstrated how the selection of proper (external) calibrants improves mass measurement accuracy (MMA) for intact proteins on instruments that utilize automatic gain control (Thermo). Common calibrants like those found in "calmix" are much smaller and carry far less charge relative to the analytes of interest. The gain of an electron multiplier (the ratio of output electron current to the input ion current) as a function of analyte charge is an important consideration for accurate ion counting, which is crucial for appropriate selection of calibration parameters and therefore, MMA. Use of abundant isotopologue peaks of intact proteins as calibrants improves MMA by a factor of ~2-3. Since the signal-to-noise ratios of protein monoisotopic peaks are often too low to allow them to be used as calibrants, calculators like the web-based UCSF MS-Isotope must be employed to model the isotope distributions and calculate accurate isotopologue masses for proteins used as calibrants.

Additional speakers were recruiting from the laboratories of FTMS interest group members. The majority (5/6) were graduate students:

Dennys Leyva — DOM Analysis and Current Validation Tools (Fernandez-Lima Lab, Florida International University)

David Roberts — Characterization of Large Proteins by Native Top-Down Mass Spectrometry on FT-ICR MS (Ying Ge Lab, University of Wisconsin)

Carter Lantz — Absorption Mode Processing Enhances Native Protein and Top-Down Mass Spectra (Joe Loo Lab, UCLA)

Carson Szot — Bruker FTMS Tuning and Data Processing (Kicki Hakansson Lab, University of Michigan)

Yuri Tsybin — Time-Domain Isotopic Beats of mAbs in FTMS (Spectroswiss)

Robert Williams — Tips for glycan mapping (Jon Amster Lab, University of Georgia)

Due to the number of speakers, there was not much time for questions, so questions from the audience were invited after half the speakers presented, and at the end of the workshop. After the workshop was adjourned several participants remained to ask questions of speakers and terrific discussion was had by all that participated.

Speaker presentations received by the FTMS interest group coordinators will be made available for download from the Open Science Framework (DOI 10.17605/OSF.IO/CF2QD). Tremendous thanks go to the student speakers (and Yuri) that volunteered to participate and to the folks who attended.