2018 ASMS Workshop Report – FTMS Interest Group
Deconvolution of FT-**MS Spectra: How it Works and What's Available**
Tuesday June 5, 2018: 5:45-7:00 pm
Melinda McFarland and Matt Renfrow, Presiding

Estimated Attendance: 175+

Summary of Program and Discussion

Mass spectrometry has been called on to deal with increasingly complex samples, ranging from complex mixtures of intact proteins and large protein complexes to non-targeted screening for contaminants. The result is a heightened need for software for accurate determination of masses from overlapping or poorly resolved charge state species. This year's FT-MS workshop focused on challenges and solutions for spectral deconvolution.

The workshop began with an overview of common approaches to deconvolution presented by Marshall Bern (Protein Metrics). The aim of the tutorial was to provide a general understanding of the logic behind classical deconvolution algorithms before delving into targeted data challenges and software solutions presented by subsequent speakers.

Following the introductory talk, four volunteers from the FTMS interest group gave talks that presented data analysis challenges that require novel deconvolution solutions. Impressively, three speakers presented publicly available software developed in their labs. Links to publicly available software solutions can be found next to the speaker's name. Thank you to everyone who volunteered but, due to time constraints, only 4 could be presented:

- Michael Marty (University of Arizona) – UniDec software. Universal Deconvolution software. Provides quantitative extraction of mass and intensities, can deconvolve ion mobility data in 3D, and more. Freely available at https://github.com/michaelmarty/UniDec

- Jim Prell (University of Oregon) – iFAMS software. Interactive Fourier-Transform Algorithm for Mass Spectrometry. Advantageous for systems with repeating subunits or adducts, such as nanodiscs and lipids. Calculates charge states, subunit mass, and stoichiometry with no smoothing. Freely available at https://github.com/seanpatcleary/iFAMS

- Lissa Anderson (National High Magnetic Field Laboratory) – Challenges of using averagine based software for automatic assignment of fragment ions in highly complex 21T top-down spectra was presented. A Most Abundant Isotopes Search (MAIS) is presented as a solution. Isotopic distributions of candidate fragment ions are matched to the 3 most abundant isotope peaks. poster ThP736

- Michael Knierman and Tony Major (Eli Lilly) – DeCharger software. Leverages high resolution, high mass accuracy MS1 and MS2 spectra for decharging, de novo sequence tags, protein ID, and quantification. MS2 de novo tags can be used to query a database for potential proteins and candidates are ranked based on how well they explain the spectrum. Soon to be freely available at github.com

Extra thanks to Michael Marty and Jim Prell who came straight from winning the Thermo and Waters research awards to give their talks. It was quite beneficial to have so many software developers in the same room with FTMS users in search of solutions. Many compliments regarding the presentations were given in the days following the workshop. There were many more excellent volunteers than we had time for. We would encourage future FTMS workshop coordinators to re-visit the topic of deconvolution in the near future.

Requests have been made for access to the presentation slides given at the workshop. Those for which we have received permission to make available can be downloaded from: http://www.kilgourlab.com/asms-ftms-interest-group-2018/

An announcement was given reminding FTMS Interest Group members to double check their ASMS interest group preferences due to recent technical difficulties and the meeting was adjourned. Thank you to the ASMS organizing committee for putting the FTMS workshop on a different night than the Top-Down workshop. An increase in attendance was noted.