

Table 7: MS Data Analysis - Feedback and Suggestions to Improve Software Tools

Facilitator: Olivier Mozziconacci, *Merck & Co., Inc., Rahway, NJ USA*

Scribe: Haichuan Liu, *SCIEX, Redwood City, CA, USA*

Scope:

Liquid chromatography-mass spectrometry (LC-MS) is an essential tool for identification, and structure elucidation for a wide array of molecules from small organic molecule, to large biotherapeutics. The multi-dimensional data matrix obtained from LC-MS/MS (or MS/MS) analyses makes the data interpretation complex. The roundtable discussion is intended to establish better guidance with regard to using data analysis software, and application of LC-MS. A better understanding of current practices to handle LC-MS (and MS/MS) data will be achieved, and experience in the field will be exchanged.

Questions for Discussion:

1. Could mass spectrometer manufacturers provide a better guidance to the different software available to the end users? Could trainings on these software depending on the applications be provided earlier in the process of the acquisition of a mass spectrometer?
2. How to analyze the LC-MS/MS data: software or manual interpretation? Raw data pre-process: noise removal, peak detection, etc., list of software, manual analysis tools.
3. Could the following tools be integrated in current software: i) integration of HTML format to generate live data, with the possibility to zoom into the details of a mass spectrum or an LC trace after data were processed, ii) Integration of tools to generate publishable high-quality figures.
4. What kinds of information can be achieved from LC-MS/MS analysis and how to achieve? Sequence coverage, identification, structure elucidation, quantitation. What is currently available to analyze automatically small organic molecules?
5. LC-MS/MS and Machine Learning integration.
6. What are critical areas of improvement for MS data analysis software?
7. How to deal with false positives and false negatives?

Discussion Notes:

This table did not have attendees.