

Table 9: Software Analysis of MS Data - Emerging Approaches and Best Practices

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Scope:

Mass spectrometry provides essential biomolecular characterization information but the increasing volume and complexity of the data demands specialized analysts and sophisticated software tools. Furthermore, technological advances and shifting analytical needs make it difficult for any single solution to be comprehensive. In this roundtable, we will discuss both the landscape of public and commercial software tools as well as the “best practice” considerations for implementing an analysis pipeline. Attention will be given to the balance between speed, power, flexibility, accessibility, and cost of the available options.

Questions for Discussion:

1. What MS data analysis tools are in use by your organization?
2. What standards/practices are in place to ensure high quality data interpretation?
3. What is the level of automation in your data analysis pipeline?
4. What are the major unmet needs of current software tools/suites?

Discussion Questions:

Attendees: half are MS users, another half are from instrument/software vendors

What MS data analysis tools are in use by your organization?

Most used software by attendees were ProteinMetrics, Skyline, and MS vendor’s software (BioPharma Finder, Xcalibur, MassLynx, Mass hunter, BioPharmaView, etc).

What standards/practices are in place to ensure high quality data interpretation?

Ensuring high quality data interpretation is important when users choose software for high throughput data processing. It is of particular valuable for new users with less experience and overwhelmingly challenged by MS data analysis. How can quality standards be enforced through data quality software? To meet the needs of users, some software vendors introduced “validators” that annotate/comment peaks automatically to help users identify/filter true or false positives. They also introduced various “workflows” with optimized parameters for users to quickly set up consistent workflows for their analyses. Training users is high priority for vendors to ensure the software is used properly and effectively.

What is the level of automation in your data analysis pipeline?

- Data integrity: storage & retrieve raw data, IT involvement across company sites for data
- e.g., Automatic file transfer to data server after acquisition;
automatic data process of standards to generate pass/fail notification to users
- Automatized & efficient data analysis and reporting in QC environment
- Different companies are in different stages of automation

What are the major unmet needs of current software tools/suites?

- Be able to put data (Figure labelling/reporting) in a generic format, or to customize into desired format (e.g., IND filing format)
- Glycan or oligo- fragmentation interpretation
- DIA library
- To develop automated processes in the future to manage data and/or analytics across vendors