

Table 4: End to End Automation: Sample Prep to Data Analysis for MS Workflows

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Scope:

In biologics therapeutic discovery and development, mass-spectrometry is a pervasive technique with applications ranging from target discovery (proteomics) to protein characterization (peptide map, intact mass) to monitoring of critical quality attributes for release testing. However, typically executing MS assays are time-consuming, involving sample preparation, data acquisition and complex data analysis. Recently, advancements in automation technology have enabled hands-free execution of multi-step protocols. Furthermore, sophisticated software platforms are making fully automated data analysis a more likely reality. This round table we will discuss how teams are implementing both robotic and software automation to streamline their MS workflows. What are the challenges or limitation to achieving true E2E automation and what are the opportunities for the future?

Questions for Discussion:

1. To what degree are teams using automation in the laboratory? What processes are being automated (e.g. purification, digests, etc)? What advantages and limitations have been realized?
2. To what extent are teams implementing E2E processes? What are the current challenges (robotic automation, data analysis and data management)? What is the future of MS automation?
3. Is metadata currently implemented in automation? What information are included in metadata?
4. Peptide mapping: Is automated data analysis routine for confirming peptide identity and modifications? How often is MSMS data being evaluated for manual confirmation? What kinds of attributes are being screened (e.g. PTM, seq variants) and are certain modifications a bigger challenge?
5. Is Qualification performed on the automation system? If so, is the qualification performed by vendor, contracted to a company or done internally, or combination?
6. When automating sample prep and data analysis how is system suitability monitored? Is method and instrument performance being tracked? What metrics are being monitored, and can this be automated?

Discussion Notes:

The round table attendees include vendors and scientists who use automation or planning to use it in the future. It was very encouraging to see automation used at all levels, including sample preparation, data analysis, and documentation.

While discussing automated sample preparation, Hamilton, Beckman Coulter, and Tecan automated systems were brought up, especially for peptide mapping and ProA purification. There was also talk about using a barcode scanner in documenting reagents during sample preparation.

There was a discussion about End to end automation, its advantages, and limitations. The benefits are reproducibility, accuracy, and high throughput. Limitations are the availability of SMEs to write scripts to suit the assay's specific needs, the time required to validate the process, and the cost involved.

Attendees predominantly talked about using Genedata and Chromeleon software for automated data processing and reporting into LIMS. The discussion also included data presentation software Spotfire.

Attendees discussed the system suitability to monitor instrument performance and sample prep during the automated workflow. Most scientists used in-house proteins/peptides to track system and sample prep performance.