Table 2: End-to-End Automation: Sample Prep to Data Analysis for MS Workflows

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Key Words: Automation, End-to-end, Integration

Table Scope:

The automation of end-to-end mass spectrometry has encountered several formidable challenges. The seamless integration of components into a cohesive system has proven intricate due to the complex amalgamation of various devices, often needing more standardized application programming interfaces (APIs). Furthermore, the diverse landscape of data processing software, often tailored to specific types of molecules under analysis, still heavily relies on manual scrutiny and adjustments of data outputs. However, these hurdles have not halted progress, as recent strides in automation technology have unlocked the capability to automate intricate, multi-step mass spectrometry processes.

In this context, automation has emerged as a pivotal breakthrough in mass spectrometry, particularly in the nuanced characterization of biologics. The synergistic integration of advanced robotics, cutting-edge software, and automated data processing has paved the way for the inception of end-to-end automated mass spectrometry characterization pipelines. This revolutionary development significantly heightens laboratory efficiency, curtails hands-on involvement, and curbs the inconsistencies that stem from manual sample preparation. As a result, these advancements substantiate the onward progression of biopharmaceutical research and development.

We will discuss recent advances and accomplishments in this evolving field and foster an open dialogue on enhancing automation efficiency and potential.

Discussion Notes:

Attendees:

- Software vendors
- Scientists currently using or planning to use automation

Summary:

- Automation was observed at all levels, including sample preparation, data analysis, and documentation.
- Hamilton, Beckman Coulter, and Tecan automated systems were specifically mentioned for peptide mapping during sample preparation.
- Advantages of end-to-end automation include reproducibility, accuracy, and high throughput.
- The need for scientists knowledgeable in script writing to automate various processes for drug development activities was emphasized
- Protein Metrics, Genedata, and Chromeleon software were predominantly mentioned for automated data processing and reporting.
- Developing scoring algorithms to minimize manual data review and utilizing artificial intelligence (AI) for training processing and scoring algorithms were discussed.

- Developing better data viewing dashboards and improving raw data storage were topics of discussion.
- The development of protein modeling software to predict protein hotspots under stress conditions was mentioned as a potential aid in the development of stable therapeutics.
- System suitability to monitor instrument performance and sample prep during the automated workflow was discussed, with many using in-house proteins/peptides for tracking performance