Roundtable Session 2 – Table 12 – Use of Artificial Intelligence for Process and Analytical Method Development

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Abstract:

Artificial Intelligence (AI) is no longer a futuristic concept—it is actively reshaping biopharmaceutical development. From predictive modeling and process optimization to accelerating analytical method development, AI offers unprecedented opportunities to enhance efficiency and quality. This roundtable will explore practical applications, regulatory considerations, and strategies for integrating AI into development workflows. AI-driven solutions can significantly shorten development timelines and improve decision-making, but adoption requires overcoming technical, cultural, and regulatory hurdles.

Discussion Questions:

1. Which AI applications are delivering the most impact in process and analytical development today?

2. How do you ensure data integrity and robustness for AI-driven models?

3. What are regulators' current expectations for AI-based tools? Are formal guidelines emerging?

4. How do you validate and maintain AI models across the product lifecycle?

5. What barriers—technical, organizational, or regulatory—must be addressed for broader AI adoption?

Notes:

Question 1:

Participants highlighted several high-impact use cases:

- AI is being used to integrate and analyze chromatographic data, including automated comparison of chromatograms and identification of trends across large datasets.
- AI-enabled tools support screening of columns and reagents, significantly reducing experimental time while maintaining high-quality outcomes.
- AI assists with method troubleshooting, especially for scientists new to a technique, by suggesting relevant parameters and comparison conditions.
- In late-stage or commercial settings, AI is being applied to leverage existing datasets (e.g., historical chromatograms, PQA data) to generate integrated views and comparisons.

- AI tools, including copilots and internal bots, are increasingly used for productivity tasks, such as email management, document comparison, meeting preparation, and formatting.
- AI is also used to connect data across sources (e.g., plasma, urine, clinical datasets) to enable more comprehensive modeling, although this remains complex and evolving.

Question 2:

- The quality, format, and relevance of training data are critical; “right data in the right format” was emphasized repeatedly.
- Participants noted challenges with large volumes of historical data, particularly determining which data should be included or excluded from AI training.
- Clear instructions to AI tools (e.g., explicitly telling the system not to fabricate information) are essential.
- Human scientific judgment remains necessary to ensure scientific rationale, assess outputs critically, and avoid overreliance on AI-generated results.
- Internal controls, IT governance, and browser-level safeguards were noted as important enablers of responsible AI use.

Question 3:

Regulatory perspectives discussed included:

- Participants were not aware of formal FDA requirements or detailed guidance specific to AI use in development at this time.
- AI is generally viewed as acceptable for drafting documents, formatting, and data organization, but not for autonomous decision-making.
- There is interest in whether AI could eventually support regulatory review efficiency, though not replace human judgment.
- Some participants noted that regulatory agencies themselves are exploring AI tools internally, with appropriate firewalls, to assist with day-to-day workflows.
- For complex AI-driven bioinformatics or modeling decisions, early engagement with regulatory agencies and review divisions was recommended.

Question 4:

- Model validation and lifecycle management remain open and evolving challenges.
- Participants emphasized the importance of clearly defined training approaches, validation strategies, and expectations for AI outputs.
- Comparisons between AI-generated results and traditional human analysis were viewed as valuable for building confidence.

- AI was considered helpful for method comparison and data analysis, but less efficient for generating complete regulatory-ready documents.
- Ongoing monitoring, retraining, and documentation of AI performance were recognized as necessary but resource-intensive.

Question 5:

Several barriers and enablers were identified:

- Cultural adoption remains a challenge; mindset change and user confidence are critical.
- Structured training programs (e.g., multi-hour, in-person AI training) and sharing real case studies were viewed as highly effective in encouraging adoption.
- Users need clear expectations for AI outputs and guidance on which decisions must remain human-led.
- Gaps between internal AI tools and external/commercial tools were noted, particularly regarding access to training references and data completeness.
- Participants emphasized that AI adoption is a long-term journey, especially for complex, integrated modeling across diverse datasets.