DATA-DRIVEN FRAGMENT SCREENING: COMBINING NMR SPECTROSCOPY AND ARTIFICIAL INTELLIGENCE

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Fragment-based drug discovery (FBDD) has become a cornerstone for identifying novel chemical starting points, with NMR spectroscopy serving as a highly sensitive tool for detecting weak fragment–protein interactions and guiding optimization. Recent advances have expanded the scope of NMR-based screening and improved throughput and sensitivity, reinforcing its role as a key technique in early drug discovery.

At the same time, artificial intelligence and machine learning are emerging as powerful complements to these experimental approaches. From automating spectrum interpretation to supporting fragment prioritization and optimization, data-driven methods are helping overcome long-standing bottlenecks in fragment screening.

This talk will explore how the integration of NMR spectroscopy with AI-driven analytics is reshaping fragment-based drug discovery, offering new opportunities to accelerate workflows, increase efficiency, and enhance the success rate of fragment-to-lead development.