

## **Advancing MS/MS Structure Elucidation with Transformer Models: from Test-Time Tuning to Multimodal IR Integration**

Laura Mismetti

IBM Research Zurich

Determining the molecular structure of unknown compounds from spectroscopic data remains a central challenge in analytical chemistry, with broad implications for drug discovery, metabolomics, natural product research, and environmental monitoring. In this talk, I will show how machine learning can push the boundaries of this task removing intermediate steps and learning from multimodal signals. End-to-end encoder-decoder transformers can directly elucidate molecular structures starting from either tandem mass spectra (MS/MS) only or from a mix of MS/MS and infrared (IR) spectroscopy. The information is complementary: IR captures the three-dimensional structural information that fragmentation systematically destroys. Finally, to scale these models to new, unseen compounds, a missing block needs to be addressed, namely the distributional mismatch between previously seen and completely unknown compounds. Test-time tuning can dynamically address this challenge, achieving state-of-the-art performance on MS/MS benchmarks and suggesting chemically meaningful compounds even when an exact match is not found.