



FONDAZIONE
EDMUND MACH
dal 1874

25/03/2026

h. 09:30 - 10:30

Room 6302 - PRC

Fondazione Edmund Mach

SEMINAR

Foundation models in mass spectrometry: from general tabular data to targeted models



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Mass spectrometry generates complex, high-dimensional data across a wide range of scientific and industrial applications. Making sense of these data requires powerful and flexible machine learning approaches, capable of handling small sample sizes, high noise levels, and diverse analytical contexts. In this talk, we explore the use of foundation models for tabular data — large-scale models trained on broad data distributions that can be applied across domains without task-specific training. As a concrete application, we focus on the analysis of volatile organic compounds (VOCs) profiled by PTR-ToF-MS and GC-MS, showing how TabPFN achieves state-of-the-art performance in both classification and regression tasks. We also discuss strategies to further enhance performance, including ensembling and fine-tuning, and outline future directions towards foundation models specifically designed to handle raw mass spectrometry data.