UNIVERSITÀ DI PAVIA

PhD School in Chemical, Pharmaceutical Sciences and Industrial Innovation

PhD CHEM PHARM
UNIVERSITY OF PAVIA

INAUGURAL LECTURE 2026

A Fourth Force in the Laboratory

Generative models alongside intuition, theory, and measurement

Chemical research has long been a craft built on three pillars: intuition, theory, and experiment. In the last few years, a new set of tools has started to sit at the same bench with us, statistical and generative models that can learn from large collections of data and help us connect things we often treat separately: reactions, IR/NMR spectra, and biological readouts.

Used well, these models do not replace chemical reasoning. They make it more effective: they help us focus our hypotheses, decide what to test first, and design experiments that give clearer answers.

In this lecture I will show its potential in everyday work: predicting and interpreting IR and NMR spectra; relating signals to structure, properties, and reactivity; supporting choices in synthesis and molecular design; and bringing chemical evidence together with biological data. I will also discuss what determines whether these methods hold up in the real world, such as data quality and traceability, uncertainty we can quantify, and a frank view of model limits.

To the PhD students of the University of Pavia, whether you work in synthesis or materials, biological chemistry or pharmaceutical technology, I would like to leave one message. These approaches are not just a specialist topic in the doctoral curriculum, nor a black box to trust on autopilot. They are quickly becoming part of the basic toolkit, alongside reading a spectrum or thinking through a mechanism. The goal is not simply to move faster, but to decide better: to turn data into knowledge more reliably, while keeping our curiosity, not the model, in the driver's seat

Dr. Teodoro Laino, Ph.D.
IBM Research Center
Zurich

March 11th, 3.00 pm

ROOM CO1, Dept. of Chemistry