

De novo design of functional peptides with non-natural chemistry

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Peptides are a promising therapeutic modality, but their de novo design is fundamentally limited by small binding interfaces. Incorporating non-canonical amino acids (ncAAs) expands this chemical space, yet modelling non-natural chemistry remains a major computational hurdle. In this talk, I will introduce RareFold, a deep learning framework for predicting and designing ncAA-containing peptides. I will demonstrate how diverse functional peptides can be designed; including inhibitors, agonists, and molecular glues. Finally, using GLP-1R as an example, I will show how non-natural chemistry enables precise signalling tuning, paving the way for a new era of functional molecular design.

Agentic Verification of Chemical Makeability and Synthesis with Chemputation

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Recent advancements in automation and digitization of chemistry have opened new avenues for exploring chemical complexity, but the proliferation of robotic architectures in chemistry mean that no standard is being adopted and hence there are real issues associated with reproducibility and safety. These issues have been compounded with the explosion of 'AI-for-science' endeavors that promise discovery with no framework to quantify any such discoveries. In this talk I will present a new ontology for chemical synthesis called chemputation[1-2], which defines a new standard for digital chemical synthesis and allows the development of digital twins, safe control of reactive chemistry[3], and allows us to make new potential drugs[4] by allowing us to determine which molecules are really 'makeable' using known chemical reactions[5]. I will also present a new approach to understanding chemical complexity using Assembly Theory[6-7] which provides a framework for quantifying molecular complexity and understanding the emergence of complex chemical systems. Chemputation, on the other hand, offers a standardized method for digitizing and automating chemical synthesis through modular robotic platforms and a chemical programming language (χDL).

By combining these approaches, researchers can systematically explore vast chemical spaces, optimize reaction conditions, and potentially discover novel molecules and materials. The integration of these two methodologies enables a new approach to explore chemical space with autonomous experimentation and discovery. As these technologies continue to evolve, they promise to accelerate chemical research, improve reproducibility, provide new insights into the fundamental nature of chemical complexity, as well as an entirely new language to describe chemical synthesis.

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Enabling chemical synthesis via machine learning

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Machine learning (ML) methods have driven key developments in the natural sciences: virtual screening of drug-like molecules for medical applications, rapid prediction of physical data, and computer-aided synthesis planning have all been facilitated by ML. The development of ML tools for synthetic methodology development and catalysis could enable chemists to make data-efficient choices and learn from that data in the course of reaction prediction, reaction condition optimization, and mechanistic interrogation. This lecture will describe my group's efforts to develop and apply open-source data science tools to numerous aspects of synthetic methodology development, including substrate scope design, ligand discovery, reaction optimization and mechanistic elucidation.

From Molecular Transformers to Quantum-Enabled Chemical Discovery AI, quantum computing, and the next digital layer for chemistry

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Over the last six years, AI has changed how we work with chemical information. We started by treating reactions as a language problem: molecules and reactions could be written, translated, predicted, and searched. This led to Molecular Transformers, at the core of the forward and procedure prediction models, as well as retrosynthesis workflows all combined in a platform named RXN for Chemistry. The same architecture was at the core of the first integration of AI-controlled laboratory automation (RoboRXN).

But chemistry is not only text. It is also spectra, structures, simulations, procedures, and experimental results. In this talk, I will show how our work moved from reaction prediction to models that connect molecules with measurements, especially IR and NMR spectra, and how this is now evolving toward multimodal models for chemistry.

I will also discuss the Swiss AI Initiative and the effort we made to build models that combine different types of chemical evidence in a reliable and reproducible way.

Finally, I will explain where quantum computing fits into this picture, not as a magic shortcut, but as part of the next digital layer for chemistry. The goal is simple: help chemists make better decisions, faster.

Probing biology using computational binder design

Prof. Martin Pačesa

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Proteins that bind a chosen target with high affinity and specificity are among the most versatile tools in biology, underpinning therapeutics, diagnostics, biosensors, and a growing range of applications across health and agriculture. Generating them has traditionally required slow, resource-intensive experimental campaigns. Our previously developed software BindCraft made protein binder design broadly accessible to biologists. Now, we introduce BindCraft2, which makes the process substantially faster, fully open, and far more general. Its central advance is breadth. From a single settings file, BindCraft2 can design against essentially any protein target, structured or disordered, a single target or several at once, and can be deliberately steered to avoid off-targets. Across all of these, it produces the full range of protein-based binder modalities, from de novo miniproteins to antibodies and nanobodies, oligomers, and cyclic peptides. In doing so, BindCraft2 brings the entire breadth of protein-based binder design into one open, easy-to-use framework, putting the design of a binder for any target, in any format, within routine reach for biology.

Chemistry in the age of foundation models

Prof. Philippe Schwaller

EPFL Lausanne, CH

Chemistry faces a fundamental challenge: the space of possible molecules and materials is nearly infinite, yet discovering useful new ones requires navigating costly cycles of design, synthesis, and testing. In this talk, I will show how language models — the same technology behind modern AI assistants — can be adapted to "speak" the language of chemistry and dramatically accelerate this discovery process. We explore how small, specialized models can learn to propose novel molecules atom by atom, while respecting real-world constraints like available building blocks and preferred chemical reactions. We then turn to large language models and show how they can reason about chemistry and even assess whether a proposed synthesis is practically feasible. Finally, we present a general framework that uses language model representations to efficiently guide experimental optimization across diverse scientific domains — from drug discovery to materials science — with minimal data. Together, these advances illustrate how AI and chemistry are converging to help scientists explore chemical space faster and more creatively than ever before.