Universität Zürich[UZH]

Institut für Chemie

DSA Symposium:

Automation and Data Science in Action

Lecture room Y11-F-06

27 May 2026, 08:30 – 16:00

Agenda

Morning session: Automation and Accelerated Life Science Research

08:30 – 09:15	*Advancing hair and nail matrix analysis with automated workflow solutions* Tina Binz (Zurich Institute of Forensic Medicine)
09:15 – 10:00	*Biocatalysis as a Tool in Synthesis: Continuous-Flow Routes to Greener Chemistry* Glenn Bojanov (University of Bern)
10:00 – 10:30	*Coffee break*
10:30 – 11:15	*Tracking plant volatiles in real time: New tools for studying biotic interactions* Tristan Cofer (University of Bern)
11:15 – 12:00	*Optimising Chemical Process Development with Automation and Machine Learning: An Industrial Perspective* Joshua W. Sin (F. Hoffmann-La Roche Ltd)

Lunch break

12:00 – 13 :00	Lunch for speakers and registered participants (**Kitchen Y38 K-floor**)

Afternoon session: AI and ML in the Life Sciences

13:00 – 13:40	*Machine learning for predictive ecotoxicology.* Christoph Schuer (Eawag)
13:40 – 14:20	Virtual Lecture: *Generative machine learning for catalyst discovery* Sarina Kopf (EPFL)
14:20 – 15:00	*From automation to autonomy: the rise of Self-Driving Labs®* Loïc Roche (Atinary Technologies Inc.)

Apéro (Y38-G-32), Lab tours

15:00 – ~16:00	Apéro, lab tours on request

Symposium: Abstracts

PD Dr. Tina Binz
Head of the Center of Forensic Hair Analytics
Zurich Institute of Forensic Medicine
University of Zurich

Advancing hair and nail matrix analysis with automated workflow solutions

The keratinized matrices hair and nails are used in forensic toxicology for the long-term detection of drugs. The development of methods for quantitative determination of novel drugs and metabolites as well as endogenous compounds in keratinized matrices is challenging. Highly advanced methods are therefore needed for extraction and detection. In this presentation three different examples for the analysis of challenging compounds form keratinized matrices will be discussed that show methodological advancements using automated workflows.

Glenn Bojanov
PhD student in Paradisi Research Group,
Department of Chemistry, Biochemistry and Pharmaceutical Sciences
University of Bern

Biocatalysis as a Tool in Synthesis: Continuous-Flow Routes to Greener Chemistry

Enzymes are most useful not as a replacement for organic chemistry but as one tool alongside it. In the Paradisi group at the University of Bern we build on this idea, combining biocatalysis with classical synthesis in continuous flow to produce chiral, high-value chemicals at preparative scale.[1]

With industry partners we have shown that enzymatic and classical organic steps can be combined into a single continuous process. By pairing an immobilized enzyme with downstream organic transformations, multi-step syntheses can run continuously at liter scale with high enantioselectivity and improved productivity compared to batch.[2]

We also explore what enzymes can do that classical chemistry cannot easily achieve. Using iron-dependent halogenases,[3] we perform selective chlorination of unactivated C-H bonds under mild aqueous conditions, delivering halogenated chiral building blocks through a two-enzyme cascade in flow.

Central to all of this is enzyme immobilization, which is what makes flow biocatalysis practical at scale. Conventional immobilization ties enzyme and support together, so when one is spent, both are discarded. Our recent work on reversible boronate ester immobilization decouples the two, allowing enzyme and resin to be reused independently.[4] We are now extending this to a fully in-flow loading and regeneration cycle, a step toward self-monitoring, continuously regenerable flow reactors.

References

[1] A. I. Benítez-Mateos, F. Paradisi, *ChemSusChem* **2022**, *15*, e202102030. [2] P. Díaz-Kruik, D. Roura Padrosa, E. Hegarty, H. Lehmann, R. Snajdrova, F. Paradisi, *Org. Process Res. Dev.* **2024**, *28*, 2683–2691. [3] M. E. Neugebauer, K. H. Sumida, J. G. Pelton, J. L. McMurry, J. A. Marchand, M. C. Y. Chang, *Nat Chem Biol* **2019**, *15*, 1009–1016. [4] G. Bojanov, J. Swit, F. Paradisi, *Chem. Sci.* **2026**, DOI 10.1039/D5SC08585C.

Dr. Tristan M. Cofer
Postdoctoral Researcher
Biotic Interactions Group
Institute of Plant Sciences
University of Bern

Tracking plant volatiles in real time: New tools for studying biotic interactions

Plant volatile organic compounds mediate interactions with herbivores, natural enemies, and neighboring plants, but their spatial and temporal dynamics are difficult to capture with conventional analytical methods. To overcome these limitations, new tools are needed that can monitor volatile emissions in real time, across many samples, and under more realistic conditions. We developed two PTR-ToF-MS-based sampling systems to meet that need. The first combines PTR-ToF-MS with an automated high-throughput autosampler for near-simultaneous monitoring of volatile emissions from large numbers of individual plants. The second couples PTR-ToF-MS to a robotic sampling arm for automated, spatially resolved measurements in open headspace environments. Together, these platforms make it possible to resolve volatile patterns from individual plants to the field. First results reveal that, in maize, plants exposed to volatiles from attacked neighbors can activate their own induced volatile release and begin emitting earlier than the attacked plants themselves, highlighting how stomatal regulation and rapid wound-derived cues shape defense responses. Work with the field-deployable system shows that plant volatile emissions are highly dynamic in time and space and provide direct evidence that volatile plant-plant interactions shape of canopy-level volatile patterns. Together, these technologies reveal previously hidden dimensions of plant chemical signaling and open new opportunities to reveal the scales at which plant volatiles mediate ecological interactions. The developed systems can be used to track volatiles with high throughput and spatiotemporal resolution in any biological system in the future.

Dr. Joshua W. Sin
Synthetic Molecules Technical Development
Process Chemistry & Catalysis
F. Hoffmann-La Roche Ltd

Optimising Chemical Process Development with Automation and Machine Learning: An Industrial Perspective

In this talk, I will introduce the process chemistry high-throughput experimentation (HTE) facility at Roche, an automated platform supporting reaction screening and optimisation from phase 0 through to phase 3 of clinical development. I will share insights into the infrastructure and workflows of our laboratory, from centralised data management to experiment orchestration. Through case studies spanning metal-catalysed and biocatalysed reactions, I will demonstrate how HTE and machine learning are being combined to accelerate process development, and how Roche is increasingly embedding these data-driven approaches into its broader digital strategy.

Dr. Christoph Schür
Postdoctoral Researcher
Department Environmental Toxicology and Systems Analysis, Integrated Assessment and Management
Eawag

Machine learning for predictive ecotoxicology.

Conventional chemical toxicity testing is outmatched by the growing number of chemicals and mixtures currently on the market. Here, machine learning has the potential to supplement, if not, ultimately, replace, animal testing. To achieve this, the elements of a lab experiment need to be translated into data that can be presented to a machine learning model. After integration of different data sources and types we assess model performance and try to understand which features contribute most to a good performance. Like its experimental counterpart, machine-learning-based research faces transparency and reproducibility issues. Additionally, this kind of research should be aimed to be translational, and not just stop at “applying a model to data” – it should strive to be informative for legislation and the public.

Sarina M. Kopf
PhD student in Schwaller Research Group
Laboratory of Artificial Chemical Intelligence (LIAC)
Institute of Chemistry and Chemical Engineering
Ecole Polytechnique Fédérale de Lausanne (EPFL)

Generative machine learning for catalyst discovery (virtual lecture)

Catalyst discovery remains a central challenge in organic chemistry. Computational approaches to this problem typically rely on a predictive model or simulation to estimate catalyst performance and then apply this figure of merit to screen libraries of candidate molecules. However, such workflows face fundamental limitations: the predefined library may not contain high-performing candidates, and the figure of merit itself is often calibrated against a narrow set of known catalysts, restricting its predictive power across broader regions of chemical space. In this work, we employ generative machine learning to propose new catalyst structures. Accurate assessment of freely generated candidates requires fitness predictors that can generalize across chemical space. We highlight the tendency of generative models to exploit predictors to produce high-scoring but chemically implausible candidates. After several rounds of experimental feedback to identify and overcome oracle hacking, we discover a promising new family of organocatalysts for the Morita-Baylis-Hillman reaction that are currently undergoing experimental validation.

Dr. Loïc Roch
Co-Founder and CTO
Atinary Technologies Inc.

From automation to autonomy: the rise of Self-Driving Labs®

High-throughput experimentation (HTE) has revolutionized chemical discovery, but the next frontier lies in the seamless integration of hardware, data, human expertise, and artificial intelligence. This requires a fundamental shift from traditional automation to autonomous discovery. For decades, the industry has relied on a trial-and-error paradigm and rigid Design of Experiments (DoE) which, while systematic, often struggle to navigate the exponential complexity of modern chemical spaces.

In this talk, I will share insights from our work at Atinary Technologies, where we have pioneered a modular, no-code AI orchestration platform to create a truly Self-Driving Lab®. By integrating the precision of ABB robotics and Chemspeed automated synthesis with high-performance analytical tools from Bruker, Agilent, and Mettler-Toledo, we have closed the loop between experimental design and execution.

Replacing linear, pre-programmed workflows with real-time, data-driven optimization allows researchers to discover and optimize new molecules at unprecedented speed. We will explore how AI agents transform the laboratory from a collection of isolated tools into an intelligent, collaborative ecosystem—shifting the chemist's role from manual operator to high-level orchestrator of scientific breakthroughs.

Apéro:

Location: **Y38-G-32** (Kitchen area on G floor of Y38)

Interact with our guest speakers, representatives of Chemspeed Technology or the members of the UZH HTEL.

Lab tours:

Want to find out more about the UZH labs, e.g. the High-Throughput Experimentation Lab (HTEL) or the MS lab?

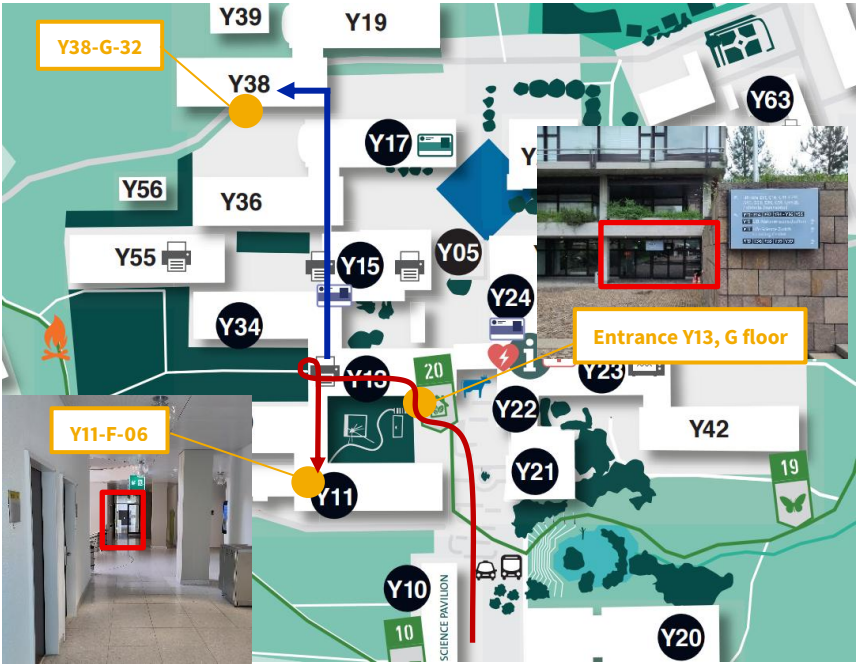
Simply let us know, we gladly open the doors for you and show you around.

Core facilities of the UZH Department of Chemistry are located close to the apéro location.

Just don’t bring any food or drinks to the labs!

Venue

Irchel Campus, University of Zurich
Winterthurerstrasse 190, 8057 Zürich
Lecture Room Y11-F-06



Heading up the campus, enter building Y13 on G-floor to the left of the UZH flags (red arrow in the picture above). After passing the two entrance doors, turn left and head towards the spiral staircase on the left of the cafeteria. Walk down one floor to reach the F-level. Turn right - you can already see the door to Y11-F-06 at the end of the corridor - just walk straight ahead.

To go to the apéro, take a staircase one floor up and follow the corridor on G floor straight ahead until you reach building Y38 (where the red floor starts. Enter the wing Y38 on your left when you reach the spiral staircase (blue arrow in the map above).

Financial support

We are very thankful to the UZH Alumni for the financial support of this event!