# Catalysis Hub – Swiss Cat+

2021 – 2023 Activity Report

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# Executive summary.

The Catalysis Hub - Swiss Cat+ project is a research infrastructure funded by the ETH-domain, aimed at facilitating data-driven, high-throughput, and automated discovery and optimization of homogeneous and heterogeneous catalysts. It is an open-access platform offering experimental services and expertise to the academic and industrial scientific community. The project is split between the two Swiss federal institutes, with the East hub at ETH Zurich focusing on heterogeneous catalyst technology, and the West hub at EPFL targeting homogeneous catalysis.

This activity report describes the project's current status and milestones from its initiation in 2019 by Prof. Dr. Christophe Copéret (ETHZ) and Prof. Dr. Nicolai Cramer (EPFL) until mid-2023. A general introduction presents the project governance, the Steering and Advisory Boards and the synergies shared by the two hubs. Then a paragraph dedicated to each hub describes in detail the respective teams, the initial hardware acquisitions, scientific and data management strategies, as well as the main challenges and collaborations. Finally, the document lists the communications done through scientific publications, patents and attendance at conferences and workshops before presenting the 2021/2022 financial statement of the project.

As of May 2023, the East Hub at ETHZ counted three scientific collaborators and an administrative assistant. The first laboratory unit in Honggerberg HCI G120 is operational from January 2023 offering a complete data-driven, closed loop, automated and high-throughput heterogeneous catalysts synthesis and testing capabilities. The hub has already performed experiments for several users from ETHZ, PSI and EMPA testifying of the high interest of the scientific community for such services. Two additional labs are being prepared to complete the range of proposed applications and will be operational early 2024.

The West Hub at EPFL includes two scientific staff, a robotics engineer, and an IT developer, as well as a chemical technician and an administrative assistant. The automated analytical part of the infrastructure is complete and operational and has already started to produce data for algorithm development. The robotic synthesis section is being completed. In addition, full IT integration and laboratory orchestration is well advanced in combination with a locally developed global sample transfer system. A first level of high throughput operation including partially automated sample preparation, synthesis, analysis and characterization, data processing and analysis coupled with optimization algorithms for homogeneous catalysis is expected to be achieved by the end of 2023. The open access service should start in early 2024 in parallel with the ongoing development of infrastructure, robotics, and algorithms.

The two Hubs have also initiated several academic and industrial collaborations to develop new tools, experimental methods, and machine learning algorithms.

Dr. Paco Laveille
Managing Director East Hub - ETHZ

Dr Pascal Miéville
Operational Director West Hub - EPFL

# ETHZ Foreword.

As one of the world's leading universities, ETH Zurich's mission in a complex world is to pave the way for future research discoveries through the education of the next generation of critical and creative thinkers, whose job will be to generate new knowledge and technologies as well as to find answers to the important questions of our time. In doing so, we advance our society, strengthen the economy, and protect nature and the environment.

With automation and artificial intelligence, scientific research has entered a new area. The way we conceive and perform experiments in laboratories, and in which we generate and analyze data, has experienced a dramatic shift in recent years. The conventional, and century-old, one at a time experiment, performed by a researcher standing in a laboratory taking notes manually, is slowly disappearing. Modern computational methods are used to design experiments, and automation supports complex tasks in a highly reproducible manner. The combination of these technologies greatly accelerates the generation of data while improving their data quality and therefore the acquisition of scientific knowledge, which is the source of new discoveries. The Swiss Cat+ project, approved by ETH Board in 2020, with the mission to set up such an automated infrastructure in the field of catalysis, combines several of these aspects thus making it a strategic development for ETH Domain.

- It creates the laboratory of tomorrow, combining robotic tools and machine learning supported analysis and decision methods. Considering those developments are still rare in academia, it places the ETH Domain a step ahead of other leading research institutes. It also provides an incredible opportunity for the students in chemistry, chemical engineering, computer science and robotics to be exposed and trained in such technologies.
- As a technology platform, the Swiss Cat+ aims at offering high-end tools and expertise to the scientific community, maximizing the scientific output from the investments. This is the most cost-efficient and effective way to invest in such advanced and expensive equipment.
- Co-headed by ETH Zurich and EPFL, Swiss Cat+ is a perfect example of creating synergies between the two institutions. Specialized in two distinct chemical areas of expertise, the two hubs benefit from the support of both universities, recognized talents, and facilities. By sharing best practices, they develop and operate more efficiently.
- Catalysis, the core topic of the Swiss Cat+ project, is at the heart of all processes needed to produce tomorrow's sustainable and renewable chemicals, fuels, and pharmaceutical compounds. By supporting this field of science, Swiss Cat+ will help many researchers to make discoveries impacting our society.

ETH Zurich will continue to support the development of the Swiss Cat+ project.

We wish the Swiss Cat+ teams at ETH Zurich and EPFL a successful development, and their users to benefit from this unique facility.

With best regards,

Prof. Dr. Joël Mesot
President of ETH Zurich

Prof. Dr. Christian Wolfrum
Vice President of Research, ETH Zurich

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# EPFL Foreword.

Catalysis is recognized as a key technology. It has been awarded a Nobel Prize in 2021 and is clearly the future of the chemical industry. It is a key component of the sustainable energy production and storage strategy that is essential to reduce global warming and ensure long-term energy availability. Catalysis is also fundamental to reducing the amount of solvents used in industry and reducing waste by significantly increasing the efficiency and selectivity of chemical processes. Nature has provided efficient catalysis for millions of years, and mankind must now learn to master it.

To develop new efficient catalysts, chemists need to explore a vast number of molecules, known as chemical space. Calculations show that the total number of different molecules that could be explored is far greater than the number of stars in the galaxy. Exploring such a space, which means synthesising, analysing and testing the molecules with different substrates under different conditions, is a complex and lengthy process. Such a process also generates a huge amount of rich, multidimensional data. To explore this chemical space on a reasonable scale and with a high degree of reproducibility, and to exploit the content of the data generated, chemists need to work closely with engineers and data specialists to develop a new generation of data-driven automated laboratories.

The Catalysis hub - Swiss Cat+ project, carried out in collaboration between EPFL and ETHZ and officially launched in January 2021 thanks to the support of the ETH Domain, aims to develop such a pioneering data-driven research infrastructure for automated catalyst discovery. This research infrastructure will soon become an open-access platform supporting high-frequency catalysis research, open to academia and industry. It will also be the basis for long-term methodological development in open research data applied to chemistry, algorithms and robotic chemistry through multiple internal and external collaborations. We are proud that after only two years of the project, we already have two unique automated platforms at both institutions, which are already internationally recognized as highly innovative and paving the way for a new way of doing chemistry.

After all, EPFL and ETHZ are schools, and digital chemistry is now an essential skill. The Swiss Cat+ project is also a great opportunity to provide our students and young researchers with a wide range of new theoretical and practical competences directly related to digital and robotic chemistry.

With best regards,

Prof. Dr. Martin Vetterli
President of EPFL

Prof. Dr. Jan S. Hesthaven
Vice President of Academic Affairs, EPFL

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# Founders' Foreword.

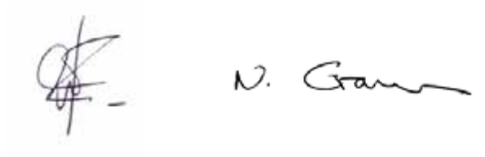
Nutrition, health, environment and the sustainable manufacture of goods and products are central to our future. A sustainable future will require to shift many of our current chemical processes from the use of products derived from fossil resources to biomass derivatives, and in particular to develop new chemistry and catalytic processes, bringing with it several unmet challenges. In parallel, chemistry itself is undergoing a transformative change by the arrival of data-science and robotics speeding up discoveries and developments, opening new opportunities, but also leading to novel challenges, e.g. the need of reproducible high quality robust data. Furthermore, chemical laboratories are witnessing the transformation of its very science, from research projects that were carried out by one single person in front of a bench to the need of teams of experts and the use of advanced technologies at each step, from the synthesis to the characterization and the evaluation of the desired properties.[1]

Swiss Cat+ has been conceived and launched by the ETH Domain to take a leading role in this chemistry revolution in order to tackle these challenges and to support both academia as well as the Swiss chemical industry to develop sustainable chemical processes, by providing beyond the state-of-the-art tools and expertise in data-science and high-throughput experimentations, approaches that would be impossible at a single PI or university/research center levels.

A national infrastructure, located at EPFL and ETHZ, has now emerged and offers an array of integrated top-notch equipment and instruments along with leading expertise thanks to a dynamic team. Swiss Cat+ is now able to tackle the challenges discussed above, from the parallel and robust synthesis and testing of catalyst libraries to the automated analysis, collection of clean data and guidance through machine learning.[2]

With best regards,

Profs. Christophe Copéret and Nicolai Cramer



[1] Link to the Swiss Chemistry Roadmap: https://scnat.ch/en/for_a_solid_science/networks_and_infrastructures/research_infrastructures | [2] Swiss Cat+, a Data-driven Infrastructure for Accelerated Catalysts Discovery and Optimization. P. Laveille, P. Miéville, S. Chatterjee, E. Clerc, J.-C. Cousty, F. de Nanteuil, E. Lam, E. Mariano, A. Ramirez, U. Randrianarisoa, K. Villat, C. Copéret, N. Cramer, Chimia 2023, 77, 154. DOI:10.2533/chimia.2023.154

# The Catalysis Hub – Swiss Cat+ project.

# a. Project history & foundation.

Initiated by Prof. Dr. Christophe Copéret (ETHZ) and Prof. Dr. Nicolai Cramer (EPFL) in 2019, the Catalysis Hub project - Swiss Cat+ aims to establish a national infrastructure, open to the entire scientific community, devoted to data-driven, high-throughput and automated chemical experimentation. In particular, the Swiss Cat+ will support the discovery and optimization of sustainable catalytic processes.

In 2020, the project was approved by the ETH-domain and received a four-year start-up fund of 25 MCHF with the mission to establish a technology platform, co headed by both federal institutes, and hosting state-of-the-art robotic and parallelized tools for the synthesis, characterization and performance evaluation of libraries of solid and molecular compounds[1,2]. For an efficient dissemination within Switzerland, the Catalysis Hub - Swiss Cat+ is divided between the two institutes according to their specific expertise: the East Hub at ETH Zurich focuses on heterogeneous catalyst technology, while the West Hub at EPFL focuses on homogeneous catalysis.

Automated high-throughput machines can generate a large amount of reproducible data in a short time. This helps in screening vast and complex parameter spaces and accelerating the identification of highly performant compounds among thousands of potential candidates. This approach also makes it possible to digitize the complete experimental workflows by eliminating manual activities and capturing all process and analytical parameters into databases. It is therefore a perfect environment to implement advanced computational data analysis using Artificial Intelligence (AI) tools, such as Machine Learning (ML) methods, for both closed-loop optimization of experimental conditions and scientific knowledge extraction from large datasets, such as hidden chemical descriptors that lead to specific performance[3,4].


**Figure 1 :** Scheme representing the Catalysis Hub – Swiss Cat+ data-driven automated and high-throughput experimentation approach.

[1] R. Buller, C. Copéret, L. Emsley, K. Gademann, Y. Hari, L. Merz, 'Chemistry Roadmap for Research Infrastructures 2025–2028 by the Swiss Chemistry Community', 2021, https://doi.org/10.5281/ | [2] P. Laveille, P. Miéville, S. Chatterjee, E. Clerc, J.-C. Cousty, F. de Nanteuil, E. Lam, E. Mariano, A. Ramirez, U. Randrianarisoa, K. Villat, C. Copéret, N. Cramer, Chimia 2023, 77, 154, DOI: 10.2533/chimia.2023.154. | [3] S. Borman, Chem. Eng. News Arch. 1998, 76, 47, https://doi.org/10.1021/cen-v076n014.p047. | [4] W. F. Maier, ACS Comb. Sci. 2019, 21, 437, https://doi.org/10.1021/acscombsci.8b00189.

# b. Governing structures.

Catalysis Hub - Swiss Cat+ is a key project of the ETH Domain. It is therefore directly subordinated to the ETH Domain through local administrations at both federal institutes. Defined as a technology platform, the Hubs are directly below the authority of the Vice President of Research at ETHZ and the Vice President of Academic Affairs at EPFL. The two Hubs operate under a unified governance document, jointly built, and approved by both local authorities in March 2022.

Two directors have been appointed to oversee the day-to-day development and operation of the respective hubs at ETHZ and EPFL. Dr. Pascal Miéville to head the West Hub at EPFL and Dr. Paco Laveille for the East hub at ETHZ. Inspired by the same vision of the project, both directors have regular discussions to share respective knowledge and best-practices. Following the approved project master plan, the two directors independently develop their infrastructure and adapt it to the inherent differences between the two areas of chemistry, homogeneous at EPFL and heterogeneous at ETHZ.

A Steering Committee, including the two founding PIs and both Hubs' directors, is in charge of proposing and validating the project strategy and reporting to the school and ETH Domain managements. The Steering Committee also coordinates the Advisory Board built in 2022 and composed of recognized experts from academia and industry, covering the entire catalysis field. A User Assembly meeting will also be organized annually once the Hubs are operational in 2024 to gather feedback from the key users and take them into account for future improvement and developments. The governing structure is depicted in Figure 2.

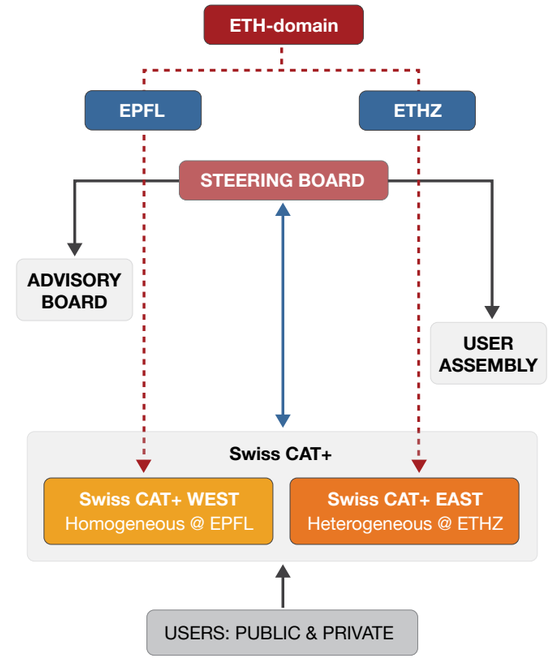



**Figure 2 :** Governing structure of Catalysis Hub - Swiss Cat+ as signed by the two institutions in 2022

# c. Project schedule and funding.

The Swiss Cat+ was approved by the ETH Domain in 2020 with an initial budget of 25 MCHF for the first four years (Phase I: 2021-2024). In addition, the respective institutes agreed to provide the project with adequate infrastructure and specialized platform support. According to the 202-2024 master plan (Figure 3), teams of experts have been assembled since 2021 to prepare the laboratories to host state-of-the-art equipment. In 2022, the Hubs began to receive and install the first equipment. Machines and experimental workflows are being validated since the beginning of 2023, with the aim of an open-access operation in 2024. The activity for each Hub is presented in detail in their respective section.

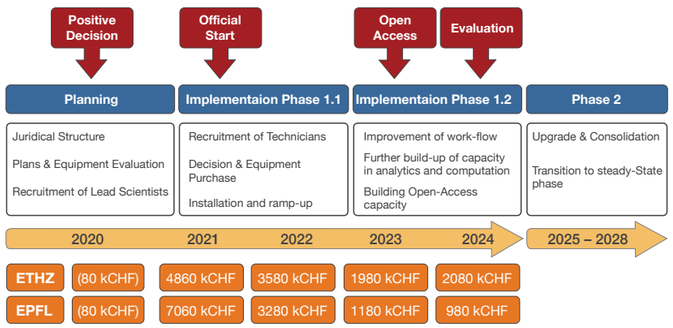



**Figure 3 :** Phase I implementation plan (2020-2024)

A second round of funding is currently being sought for Phase II (2025-2028, Figure 4). During the second phase, in parallel with the operational exploitation of the current equipment, the Hubs will increase their capacity, install new equipment, develop full automation capabilities as well as data-driven tools (optimization algorithms, automated data analysis, chemical space exploration, closed-loop experimentation). Swiss Cat+ is a research infrastructure project with a long-term goal; its future evolution will depend on the needs of the community and the rapid evolution of the field, with the ultimate aim of providing beyond state-of-the-art tools and expertise for the data-driven discovery and optimization of catalysts libraries. The detailed development plans are presented for each hub in their respective section.

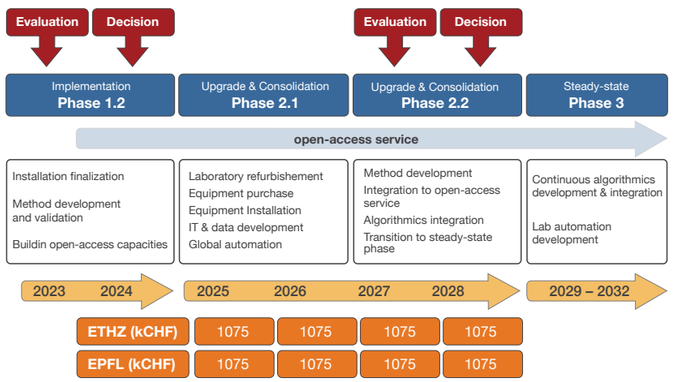



**Figure 4 :** Phase II implementation plan (2025-2028)

# d. Advisory Board.

The Swiss Cat+ Advisory Board has the role to maintain a close contact between academic and industrial stakeholders, improve networking and gather feedback about the project status and the state-of-the-art in this fast-moving research area. As of March 2022, it is composed of twelve members, presented below in alphabetical order.

**Prof. Dr. Matthias Beller – Director of the "Leibniz-Institut für Katalyse" – LIKAT (Germany).**
Matthias Beller research focuses mainly on functionalization of aryl halides, enantioselective oxidation reactions, metal-catalyzed hydroformylations, catalytic aminations and carbonylation. He completed his PhD thesis in 1989 in the group of L.-F. Tietze, at the University of Göttingen (Germany). He then spent a year with K. B. Sharpless at MIT, USA. From 1991 to 1995, he worked in industry before moving to the Technical University of München as Professor for Inorganic Chemistry. In 1998, he relocated to Rostock to head the Institute for Organic Catalysis, which became in 2006 the Leibniz-Institute for Catalysis. The work of his group has been published in >1075 original articles, reviews and >150 patent applications (H-index: 142). He has received a number of awards including the Otto-Roelen Medal, the Leibniz-Price of the DFG, the German Federal Cross of Merit, the "Paul-Rylander Award" of the Organic Reaction Catalysis Society of the USA, the Gay-Lussac-Alexander-von-Humboldt-Prize of the French Academy of Sciences, the Emil Fischer Medal of the German Chemical Society, the Wöhler price for Sustainable Chemistry from the German Chemical Society and the Karl Ziegler Prize from the German Chemical Society and the Karl Ziegler Foundation. Matthias Beller is also Vice President of the Leibniz Society, a member of the German National Academia of Science "Leopoldina" and three other Academies of Sciences.

**Dr. Mikael Berthod – Head of the Competence Center Process Technology & Chemistry at Borealis (Austria).**
Dr. Berthod has obtained his PhD from Claude Bernard University (Lyon, France). After a post-doctoral fellowship at the prestigious Montreal University (Canada), he worked as senior research engineer at IFPEN supervising multiple national and international research projects involving several PhD holders, laboratory chemists and post-doctoral personnel. With a portfolio of more than 15 years of experience in homogeneous and heterogeneous catalysis and considerable expertise in pilot plant and industrial projects in the downstream sector, he joined the Abu Dhabi National Oil Company (ADNOC) in 2012 as the Research Centre manager. Dr. Berthod played a pivotal role in managing the sole refining applied research center in the country, bearing in mind ADNOC's vision to couple research and technology to evolve the national refining industry. From 2015, In his capacity of Research Centre Vice President, he led a team of 90 multidisciplinary scientists, technicians and operators to set a solid expertise for the refining R&D activities of ADNOC. Since 2022, Dr. Berthod has been leading the Process Technology & Chemistry Competence Centre of Borealis Innovation & Technology Division. In this new role, he is supporting the company's transformation towards a circular and a carbon-neutral polyolefins activity. He is the author of over 20 scientific articles and 13 patents and has participated in several national and international conferences, seminars, symposia.

**Prof. Abigail Doyle – Professor of Chemistry at the University of California, Los Angeles (United States of America).**

Abigail Doyle received her A.B. and A.M. summa cum laude in Chemistry and Chemical Biology from Harvard University in 2002 and her PhD from the same department in 2008. Professor Doyle began her independent academic career in the Department of Chemistry at Princeton University in 2008. In 2021, she moved to UCLA as the Saul Winstein Chair in Organic Chemistry. The Doyle lab conducts research at the interface of organic, organometallic, physical organic, and computational chemistry to address unsolved problems in organic synthesis through the development of catalysts, catalytic reactions, and synthetic methods. She applies mechanistic and computer-assisted techniques to the analysis of these reactions to uncover general principles that can guide the design of improved catalysts and the discovery of new reactions.

**Prof. Dr. David Farrusseng – Research Professor at CNRS – Lyon 1 Univ. (France).**

David Farrusseng research work deals with the design of materials for original catalytic & separation processes. He was among the pioneers in the design, synthesis up-scaling and application of MOF to catalysis. He completed his PhD thesis in 1999 at the Institut Européen des Membranes de Montpellier (France) under the supervision of C. Guizard, A. Julbe, and his post-doc at MPI für Kohlenforschung in the group of F. Schüth. In 2001, he was appointed CNRS researcher at IRCELYON in the group of Dr. C. Mirodatos for the development of high-throughput approaches and Artificial Intelligence in Catalysis. He is currently group leader at IRCELYON which consists of 10 full time researchers and engineers and approximatively 20 students. He has published more than 200 papers and 17 patents cited >10000 times. He received many prestigious prices, among them, the Silver medal of CNRS in 2020, the IACS award in 2016 and the Power and & Energy Society (PES) award in 2010 and 2015. He also holds the position of CTO at MOFapps, Board member of the French Zeolite Association (GFZ), and Member of the editorial committee of ChemCatChem (Wiley).


**Dr. Edouard Godineau**

**Syngenta Fellow - Head of Green and Sustainable Chemistry at Syngenta Crop Protection AG (Switzerland).**

Edouard Godineau received his PhD from the University of Bordeaux in 2007, with Prof. Yannick Landais. After a post-doctoral stay with Prof. A. Fürstner at the Max-Planck-IstitutInstitute für Kohlenforschung in Mühlhein a.d.R, he joined Syngenta Crop Protection in 2009 as a process chemist. Since 2014, he ishas been leading the process chemistry group at Syngenta where is he is responsible to identify and design most cost-effective possible synthetic routes to new active ingredients. Edouard was appointed Syngenta Fellow in December 2019.

**Dr. Thomas Heinz – Global Head of Chemical R&D in Chemical & Analytical Development at Novartis (Switzerland).**

Thomas Heinz studied chemistry at the University of Basel and completed his PhD at the University of Basel and the Max-Planck-Institut für Kohlenforschung, Mülheim-Ruhr, Germany, under the supervision of Prof. A. Paltz in 1997. After his postdoctoral studies at the Scripps Research Institute, San Diego, Thomas joined Novartis as Laboratory Head within Chemical & Analytical Development (CHAD) Switzerland in 1998. He held different positions with growing responsibility and since January 1st, 2016, Thomas is the Global Head of Chemical R&D in CHAD. Thomas is an active member in the Swiss Chemical Society. From 2014 to 2023, he was a Board Member of the Division 'Industrial & Applied Chemistry' (DIAC) of the Swiss Chemical Society. In addition, he was a founding member of the Swiss Industrial Chemistry Symposium (SICS).

**Dr. Till Kuehn – Vice President – Head of global R&D within Bruker Biospin (Switzerland).**

Dr Till Kuehn studied Chemistry between 1993 and 1997 at the University of Tübingen, Germany and University of Missouri, Columbia, MO, USA, got his Diploma in Chemistry in 1997 then between 1997 and 2000 made his PhD work at University of Frankfurt, Germany and MIT, Cambridge, MA, USA with Harald Schwalbe on time resolved NMR to study protein folding processes. Between 2000 and 2003 he became applications Scientist at Bruker BioSpin in Fällanden, Switzerland, then from 2003 to 2007 Product Manager for Automation at Bruker BioSpin. In 2008 he was promoted Team leader for NMR application software development at Bruker BioSpin, in 2014 he became Head of global Applications Development for the MRS division for Bruker BioSpin and since 2018 VP and head of global R&D at Bruker BioSpin

**Dr. Luc Nougier – Director Catalysis, Biocatalysis and Separation at IFP Energies Nouvelles (France).**

Luc Nougier, graduated from CPE Lyon, joined IFPEN in 1989, to work on the development of high temperature chemical processes. He develops multidisciplinary research and combines experimentation and reactor modeling. He has taken responsibility for various research projects involving industrial partners (Technip, Nova Chemicals…) covering a wide range of developments from laboratory facilities to demonstration units. In 2005, Luc Nougier was appointed as Head of Department of Chemical Engineering and since 2016, he has been in charge of the Catalysis, Biocatalysis and Separation Division. The division provides IFP group and its industrial partners with the scientific and technical skills in Catalysis and Biocatalysis necessary for the development of innovative catalytic processes serving the energy transition. Research areas cover bio-products, alternative fuels and recycling, leading to approximately 60 patents and 40 publications per year. Luc Nougier is also IHEST (Institute of High Studies for Science and Technology) auditor.

**Dr. Kurt Püntener – Head of Roche's Catalysis & Flow Reaction section (Switzerland).**

Dr. Kurt Püntener obtained his diploma in chemistry (1990) and his PhD (1994) in the group of Prof P. Pregosin (ETHZ). After postdoctoral stays at Colorado State University (USA) and Philipps

University Marburg (Germany) in the research groups of Prof L.S. Hegedus and Prof. P. Knochel, Kurt joined the catalysis group of Process Research & Synthesis at F. Hoffmann-La Roche Ltd in 1996. After his promotion to group leader (2011), he was nominated in 2013 for the position of Head of Process Research at the Roche Innovation Center in Basel where he is responsible for preclinical process research for small molecules, peptides, and oligonucleotide drug substances. In 2019, Kurt became Head of Roche's Catalysis & Flow Reaction section, which focuses on the design of enzymatic, microbial, and metal-catalyzed transformations as well as continuous processes for the development of robust and cost-efficient drug substances.

**Dr. Maud Reiter – Vice President of Discovery Chemistry & Development at Corporate R&D Division of Firmenich S.A (Switzerland).**

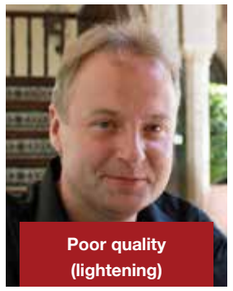
Dr. Maud Reiter is the Vice President of Discovery Chemistry & Development at Corporate R&D Division of Firmenich S.A. in Geneva (Switzerland). Maud received her undergraduate degree from Imperial College, London in 2002, followed by a PhD under the supervision of Professor Véronique Gouverneur at the University of Oxford. After postdoctoral work with Professor David MacMillan at Caltech/Princeton University, Maud joined Merck & Co. in 2008 in Rahway, NJ, USA as a medicinal chemist. In 2011, Maud moved to Firmenich in Switzerland as Director of Ingredients Discovery and got promoted into her current position in April 2022, in which she is responsible for the introduction of new palette ingredients & conversion of existing ingredients into renewable versions. Dr Reiter is an executive Board member of the Swiss Chemical Society, a co-founder of Swiss Women in Chemistry, member of the NCCR catalysis industry panel and Swiss Cat+ Advisory board.

**Dr. Stephan Schunk – Vice President – Executive Expert within BASF SE and hte GmbH (Germany).**

Stephan Schunk research work focuses mainly on industrial inorganic catalysis, high-throughput technology and digital chemistry. He completed his PhD in 1998 at the Johann Wolfgang Goethe-University of Frankfurt in the group of Prof. Ferdi Schüth and his post-doc in 1999 within BASF under the supervision of Dr. Ekkehard Schwab. He then worked as a scientist for HTE and BASF before being appointed Vice President and executive expert in the "Process Research and Chemical Engineering" division. Since 2021 he is also Honorary Professor for Digitalization in Catalysis and Materials Sciences at University Leipzig. He is the author of more than 100 scientific papers and patents and has been honored with multiple awards and prices. Among others, he received the best Process Innovation Award for Linde´s "DryRef Process" and BASF´s "Synspire Catalyst" in 2019, the Science Price of the "Stifterverbandes für die Deutsche Wissenschaft" in 2001 and the Jochen-Block-Price of the Section of Catalysis of the DECHEMA in 2000. He is also a member of the Expert Commission of GECATS since 2014, of the "Physical and Computational Sciences Directorate Advisory Committee '' of Pacific Norwest National Laboratory since 2022, and of the Board of NFDI4cat since 2019.

**Dr. Normen Szesni – Head of Future Technologies, BU Catalysts at Clariant ( Switzerland).**

Normen Szesni received his PhD in Chemistry from University of Konstanz, Germany (2005) before working as a lab manager at M-Cat, where he was responsible for custom catalyst synthesis (2005). In 2006 he joined Süd-Chemie (now Clariant), where he held various research positions in the Catalysts Business Unit related to hydrogenation and homogeneous catalysis. Since 2012 he is heading the strategic R&D department "Future Technologies", responsible for early scouting, incubation and implementation of pioneering catalyst technologies.



# ETHZ – East Hub.

# a. Strategic approaches.

Swiss Cat+ East focuses on data-driven high-throughput and automated heterogeneous catalyst synthesis, characterization and performance evaluation. However, the inherent flexibility of the tools allows for accommodating studies beyond heterogeneous catalysis, including the synthesis of functional materials and the evaluation of catalysts in homogeneous phases.

Three laboratory units, for a total of 170 $m^2$, hosted by the Department of Chemistry and Applied Biosciences (D-CHAB) in the HCI building of ETHZ Hönggerberg campus, have been secured for the first phase of the project. A first lab of 70 $m^2$ (HCI G120) has been equipped in 2022 and is fully operational since January 2023 offering a complete experimental workflow combining ML-supported design of experiment with heterogeneous catalysts synthesis and testing. Two other labs units (HCI H241 and G226/228) are in preparation to broaden the capabilities of Swiss Cat+ East. Additional laboratory space is being identified to plan for the foreseen extension in 2025.

Automating heterogeneous catalyst synthesis, characterization and evaluation has been a challenge since the 90s, mostly due to the specific conditions required along the experimental workflow which are very different from homogeneous or biological chemistry (solution phase). Those challenges include the dispensing of powders having different properties, the possible high-temperature and pressure needed for the synthesis and/or testing of the catalysts, the sieving/crushing/pelletizing of solid materials and their transfer to specific vessels for thermal treatment, the broad range of sample preparation for characterization and/or testing activities. Even though several research groups and companies propose solutions to overcome some of those problems, building a fully automated experimental workflow for heterogeneous catalyst discovery and optimization is still not yet achieved and typically requires making automation compromises[5, 6, 7].

For the first phase of the ETHZ Catalysis Hub, the laboratory is designed as “islands” of automated tasks, with manual transfer of sample plates between each equipment. A strong effort is placed to digitize the whole experimental workflow and remove any manual activity directly impacting the experiment. As depicted in Figure 5, the typical experimental workflow consists of:

- Computer-assisted experimental design.
- Compounds library synthesis by robotic platform.
- Thermal treatment of the libraries in automated furnaces.
- Primary screening of the library microplates in batch mode.
- Basic surface characterization of a subset of candidates.
- Secondary screening of sub-set of candidates in fixed-bed reactors.
- Computer-assisted data analysis and visualization.

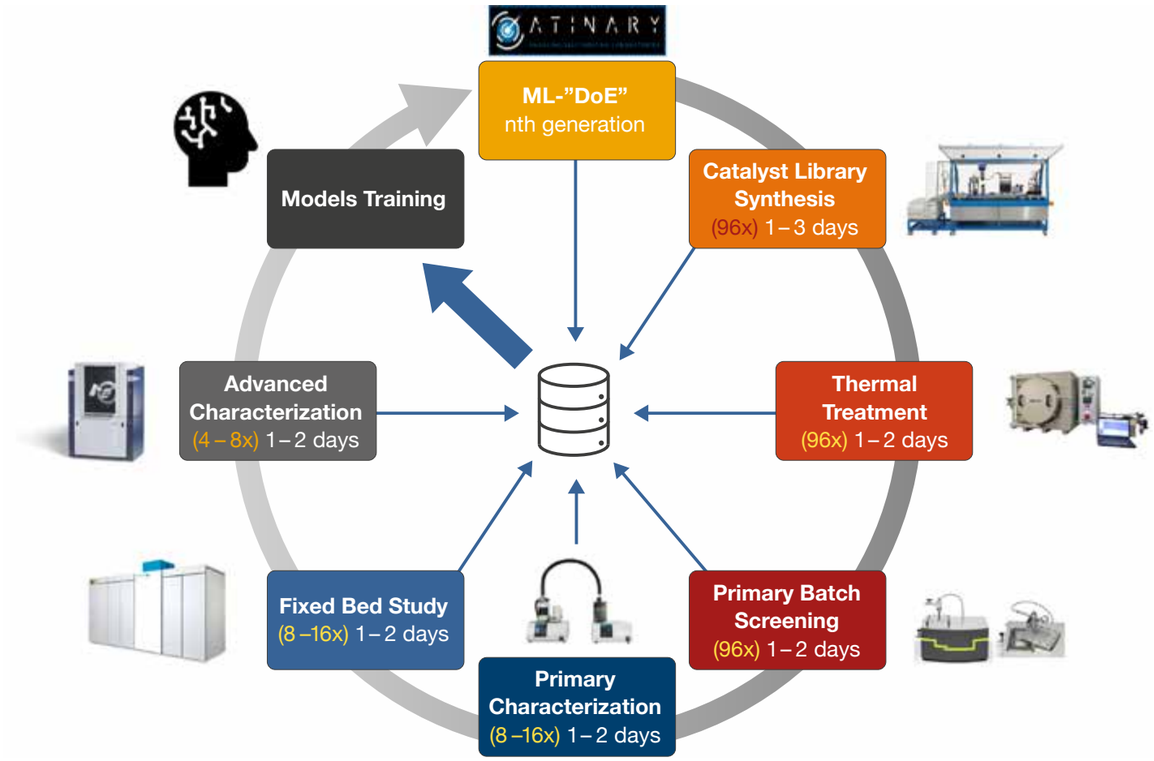



**Figure 5 :** Scheme depicting the Swiss Cat+ East closed-loop workflow for data-driven automated and high-throughput heterogeneous catalyst discovery and optimization, available from January 2023.

[5] A. Holzwarth, H.-W. Schmidt, W. F. Maier, Angew. Chem. Int. Ed Engl. 1998, 37, 2644, https://doi.org/10.1002/ | [6] B. Jandeleit, D. Schaefer, T. Powers, H. Turner, W. Weinberg, Angew. Chem. Int. Ed Engl. 1999, 38, 2494. | [5] D. E. Akporiaye, I. M. Dahl, A. Karlsson, R. Wendelbo, Angew. Chem. Int. Ed Engl. 1998, 37, 609, https://doi.org/10.1002

# b. The team.

In 2023, the East Hub counted three scientific experts, and an administrative assistant among its staff. The platform plans to hire additional staff members as the activity ramps up.

**Dr. Paco Laveille – Managing Director.**
Paco Laveille holds a PhD in Materials Chemistry from ENSCM, France (2009). After a post-doc at the Institut Français du Pétrole – Energies Nouvelles (France), he worked as a Research Engineer at the KAUST Catalysis Center in Saudi Arabia, overseeing the high-throughput experimentation platform and participating in the design of various heterogeneous catalysts in the group of Prof. J-M Basset. In 2015, he joined the Abu Dhabi National Oil Company in the UAE as Senior Scientist and led projects related to hydroprocessing catalyst technology and sustainable fuels production. He was appointed Managing Director of the ETH Zurich Catalysis Hub – Swiss Cat+ East on January 2021.

**Dr. Erwin Lam – Scientist Data management & Analysis.**
Erwin Lam received his Bachelor's (2014) and Master's (2015) degree in chemistry at ETH Zürich and carried out his PhD at ETH Zürich (2015-2020), where he studied the understanding of heterogeneous catalysts by combining synthetic, spectroscopic and computational methods. In 2020, he joined the group of Prof. Erwin Reisner at the University of Cambridge UK, developing electro- and photocatalytic approaches for the valorization of waste chemicals. Since 2022, Erwin Lam joined Swiss Cat+ at ETH Zürich as a Scientist responsible for chemical data analysis and management strategy and developing automated high-throughput workflows in catalysis.

In the making

**Dr. Yuhui Hou – Senior Scientist Automation.**
Hou Yuhui received her PhD degree in Physical Chemistry from Xiamen University, China in 2015. After her PhD, she furthered her skills in heterogeneous catalysis at Hokkaido University, Japan. In 2017, she joined the research group of Prof. Peter Broekmann at the University of Bern and extended her research interests to electrocatalysis. In 2021, she joined Chemspeed Technologies AG in Switzerland as Automation Chemist. There, she leveraged her knowledge of automation to provide technical expertise and support the organization implement digital and automated chemistry. She was promoted Workflow Architect and Project Manager before joining Swiss Cat+ ETH Zurich in 2023. At Swiss Cat+ East, she is responsible for implementing high-throughput and automated experimentation for catalytic applications.

In the making

**Ms. Corinne Strässle – Administrative assistant.**
Corinne Strässle has extensive experience in marketing, sales, event organization and executive office administration. She worked several years for international companies such as Swissscom, supporting the marking and sales of major accounts before joining the Alpinias Institute for life sciences, as assistant manager of a pharmaceutical research group. In 2022, she joined ETHZ, as the administrative assistant of the Swiss Cat+ East and two other professorships, providing her with a profound knowledge of the university structure and processes. Corinne has a pivotal role within the hub taking care of all the aspects related to HR, purchasing, events and communication. During her spare time, Corinne loves to practice all kind of outdoor activities, accompanied by her family and dog.

In the making

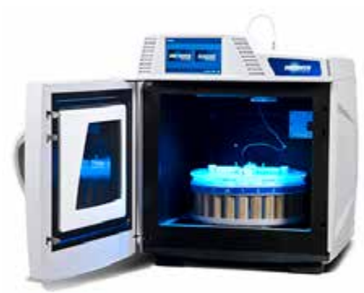
# c. Hardware infrastructure.

The initial investment (2021-2022) made to furnish the first lab unit (HCI-G120) includes the following capital equipment:

## Catalysts Synthesis Capabilities.

**Chemspeed Swing XL Catprep robot.**
The Chemspeed swing XL unit is configured to prepare heterogeneous catalysts (metal-supported on oxides, mixed oxides, zeolites, or metal organic framework) in a fully automated way, operating 24/7 according to established synthesis methods (impregnation, precipitation, hydrothermal synthesis) . In a typical workflow, the liquid and solid dispensing tools prepare stock reagent solutions from metal salts and solvents. Those solutions are combined in reaction vessels, with other chemicals and/or solid supports, typically 24x4mL to 24x20ml vials on standard microplates. The unit can control the temperature and the shaking of each microplate individually from -20 to 150 °C. Depending on the protocol, the pH can be automatically adjusted in each reaction vial. The solids can be centrifuged, washed, dried under vacuum and/or thermally treated up to 150 °C and 80 bars under various atmospheres, without manual intervention. All the experimental steps are recorded by the software and linked to the barcode of each reaction vial. Generally, each round of synthesis allows the preparation of 24 to 96 catalysts (0.1 to 1g each) in 2 to 5 days.

**CEM Mars 6 Multi-position microwave oven.**
In the case of synthesis requiring several days of hydrothermal step, a multi-position microwave oven (MO) can be used. The oven cavity can fit rotors with 40x20 mL or 12x100 mL reactors. The temperature is measured in each individual reactor. If needed, the reaction mixtures prepared with the Chemspeed Swing XL Catprep unit described above can be transferred to the MO vessel for thermal treatment under autogeneous pressure. Then mixtures containing the precipitates are transferred back to the barcoded vials and the washing/drying steps are continued on the Chemspeed Swing XL Catprep unit.

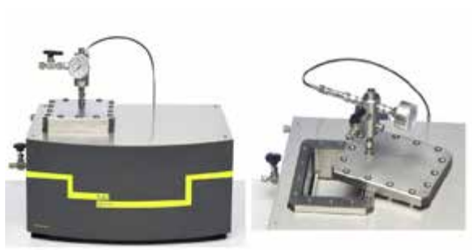


[8]X. Hai, S. Xi, S. Mitchell, K. Harrath, H. Xu, D. F. Akl, D. Kong, J. Li, Z. Li, T. Sun, H. Yang, Y. Cui, C. Su, X. Zhao, J. Li, J. Pérez-Ramírez, J. Lu, Nat. Nanotechnol. 2022, 17, 174, https://doi.org/10.1038/s41565-021-01022-y.

**Hobersal furnace.**
The Hobersal oven is a fully automated oven allowing to thermally treat materials up to 1100 °C either under vacuum, nitrogen, air, or hydrogen atmosphere. The furnace chamber can accommodate up to four standard microplates, giving a capacity to treat up to 96 catalysts simultaneously.

**Unchained Labs Junior.**
The Unchained Labs Junior (ULJ) is used as a central solid and liquid dispensing unit. After thermal treatment, the catalysts libraries are placed on the ULJ and are automatically dispensed in the milligram range to other reaction vessels for downstream activities (batch testing, fixed-bed testing, characterization). The unit is equipped with barcode readers to track and record the exact amount dispensed of a given catalyst.

## Catalysts Testing Capabilities.



**H.E.L CAT96 Batch Reactor**.
The H.E.L CAT96 batch reactor allow to perform batch reactions up to 250 °C and 100 bars under inert or reactive gas (e.g. $CO_2$, CO and/or H2). The unit is installed inside a glovebox offering the additional capability to test air sensitive catalysts. The reaction chamber fits standard microplates of 96x1mL or 24x4mL vials, with reaction mixtures (solid and liquid dispense) being prepared automatically by the ULJ described above. The reaction conditions (pressure, temperature, gas mixture, stirring) are controlled and recorded digitally. After the reaction, the microplates containing the reaction vials are transferred to the Chemspeed Swing XL CatPrep unit to prepare analytical samples for gas chromatography analysis.

**Avantium XR 16x fixed-bed unit.**
The Avantium XR is a 16-fold parallel fixed-bed reactor, allowing to evaluate the performance of heterogeneous catalysts under plug-flow conditions. It can be operated 24/7 unattended at up to 950 °C and 100 bars with various gases (up to 5 different reaction gases) and/or one liquid feed. The nanoflow technology allows performing reactions with 10 to 100 mg of catalyst. Two gas chromatographs connected on-line analyze continuously the gaseous products and reactants coming from the outlet of the reactors (permanent gases and up to C9 paraffins, olefins, aromatic and oxygenates). The process parameters and analytical data for each reactor are automatically aggregated into a dedicated database. It is currently configured and validated for $CO_2$/CO hydrogenation, methane dry reforming, propane dehydrogenation and methanol to olefins conversion[9, 10, 11].

**Avantium XD 4x fixed-bed units under glovebox.**
Two Avantium XD are connected to a glovebox to evaluate the performances of air-sensitive heterogeneous catalysts or retrieve catalysts after fixed bed testing without affecting the chemical state of their surfaces. Each unit has four fixed bed reactors in parallel and one GC continuously analyzing the gaseous products and reactants coming from the outlet of the reactors (permanent gases and up to C9 parafins, olefins, aromatic and oxygenates). It can be operated 24/7 unattended up to 950 °C and 100 bars with various gases (up to 5 different reaction gases) and/or one liquid feed. The process parameters and analytical data for each reactor are automatically aggregated into a dedicated database. It is currently configured and validated for $CO_2$/CO hydrogenation, methane dry reforming, propane dehydrogenation and methanol to olefins conversion..

[9] P. Laveille, K. Guillois, A. Tuel, C. Petit, J.-M. Basset, V. Caps, Chem. Commun. 2016, 52, 3179, https://doi.org/10.1039/C5CC09561A. | [10] A. Ramirez, X. Gong, M. Caglayan, S.-A. F. Nastase, E. Abou-Hamad, L. Gevers, L. Cavallo, A. Dutta Chowdhury, J. Gascon, Nat. Commun. 2021, 12, 5914, https://doi.org/10.1038/s41467-021-26090-5. | [11] P. Laveille, G. Biausque, H. Zhu, J.-M. B asset, V. Caps, Catal. Today 2013, 203, 3, https://doi.org/10.1016/j.cattod.2012.05.020.

# d. IT architecture and data-driven strategy.

## Catalysts and Reaction Characterization Capabilities.

**Agilent Gas Chromatography Mass Spectrometer (GCMS).**
The Agilent GCMS serves to analyze liquid samples collected during the evaluation of the catalysts with the HEL CAT96 and prepared with the Chemspeed Swing XL CatPrep, presented above. It is equipped with an non-polar column, two detectors (FID and MS), an autosampler and a barcode reader.

**Netzsch TGA/DSC-MS.**
The Netzsch TGA/DSC-MS (Thermal Gravimetric Analyzer/ Differential Scanning Calorimeter-Mass Spectrometer) is used as a primary catalyst characterization tool. The unit can perform thermogravimetric analysis such as coke quantification or temperature programmed reactions with gas quantification through the mass spectrometer. The unit is equipped with a 20-position autosampler allowing continuous analysis. Samples are prepared automatically through the ULJ unit presented above, automatically dispensing the targeted mass (up to 30 mg). By recording simultaneously, the mass variation, the heat transfer and the evolved gas during the thermal treatment under specific atmosphere, the TGA/DSC-MS provides a fingerprint of the catalysts surface properties, which can be linked to their performance behaviors measured under batch or fixed bed conditions[12, 13].

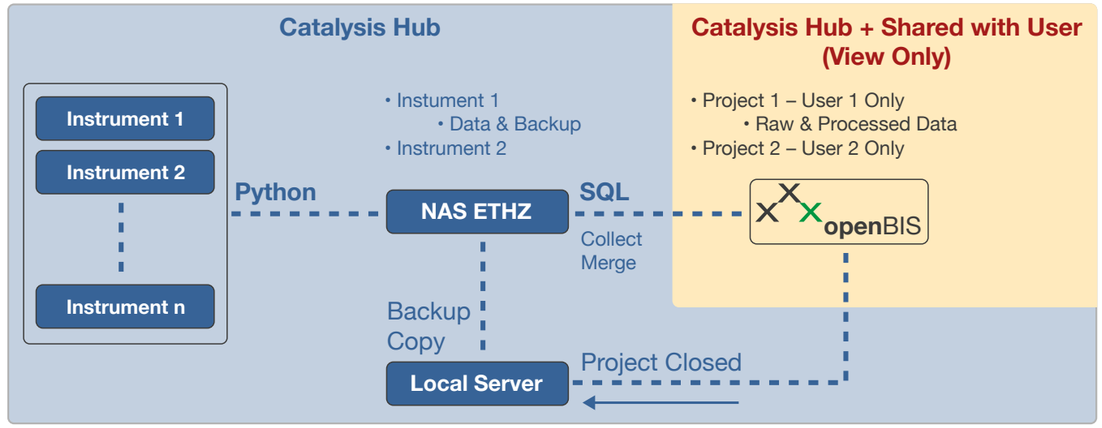



**Figure 6 :** Data processing, backup and sharing strategy within Swiss Cat+ East

One of the main objectives of the Swiss Cat+ project is to digitize all the input/output of the experiments and use advanced computational tools (AI/ML) to support closed-loop experimentation and identify chemical descriptors leading to a given catalytic activity/reaction mechanism. To this end, all outputs (experimental conditions and/or analytical results) from the instruments are monitored and recorded digitally. No manual activity is needed during the experiment, except for sample transfer between the instruments. The individual databases generated by each hardware described above are automatically copied and aggregated to a physical server and backed-up periodically for ease of manipulation and visualization (Figure 6). Furthermore, the raw and processed data corresponding to each individual project are then shared with the individual users.

The first requirement for a suitable data-driven approach is to apply statistical experimental design methods to reduce the number of experiments needed to screen a given parameter space (e.g., Design of Experiment, Genetic Algorithms, Bayesian Optimization)[14, 15, 16, 17]. The Swiss Cat+ East is currently developing proprietary ML algorithms but in an attempt to demonstrate the readiness of the first lab set-up and the efficiency of the proposed data-driven experimental workflow, we have also established a partnership with Atinary (https://atinary.com), a Swiss start-up active in the field of self-driven laboratory platforms offering a commercial ML-Bayesian-based experimental multiple-parameter and -objective optimizer including constraints[18, 19, 20]. Atinary provided us with a customized version of their optimizer that we have combined with the hub's automated catalyst synthesis and fixed bed testing equipment. We have implemented in a demo/proof-of-concept project a closed-loop data driven automated and high-throughput workflow (Figure 7) targeting the optimization of a metal-supported heterogeneous catalyst composition active for the conversion of $CO_2$ to methanol,which is currently a major research activity worldwide, in Switzerland and in the ETH domain in particular.

[12] F. Eigenmann, M. Maciejewski, A. Baiker, Thermochim. Acta 2000, 359, 131, https://doi.org/10.1016/S0040-6031(00)00516-5. | [13] M. Maciejewski, C. A. Müller, R. Tschan, W. D. Emmerich, A. Baiker, Thermochim. Acta 1997, 295, 167, https://doi.org/10.1016/S0040-6031(97)00105-6.

[14] D. B. Hibbert, Chemom. Intell. Lab. Syst. 1993, 19, 319, https://doi.org/10.1016/0169-7439(93)80031-C. | [15] S. Greenhill, S. Rana, S. Gupta, P. Vellanki, S. Venkatesh, IEEE Access 2020, 8, 13937, https://doi.org/10.1109/ACCESS.2020.2966228. | [16] D. Farrusseng, Surf. Sci. Rep. 2008, 63, 487, https://doi.org/10.1016/j.surfrep.2008.09.001. | [17] T. A. Beltrán-Oviedo, I. Batyrshin, J. M. Domínguez, Catal. Today 2009, 148, 28, https://doi.org/10.1016/j.cattod.2009.05.023. | [18] F. Häse, M. Aldeghi, R. J. Hickman, L. M. Roch, A. Aspuru-Guzik, Appl. Phys. Rev. 2021, 8, 031406, https://doi.org/10.1063/5.0048164. | [19] S. Langner, F. Häse, J. D. Perea, T. Stubhan, J. Hauch, L. M. Roch, T. Heumueller, A. Aspuru-Guzik, C. J. Brabec, Adv. Mater. 2020, 32, e1907801, https://doi.org/10.1002/adma.201907801. | [20] F. Häse, L. M. Roch, C. Kreisbeck, A. Aspuru-Guzik, ACS Cent. Sci. 2018, 4, 1134, https://doi.org/10.1021/acscentsci.8b00307.

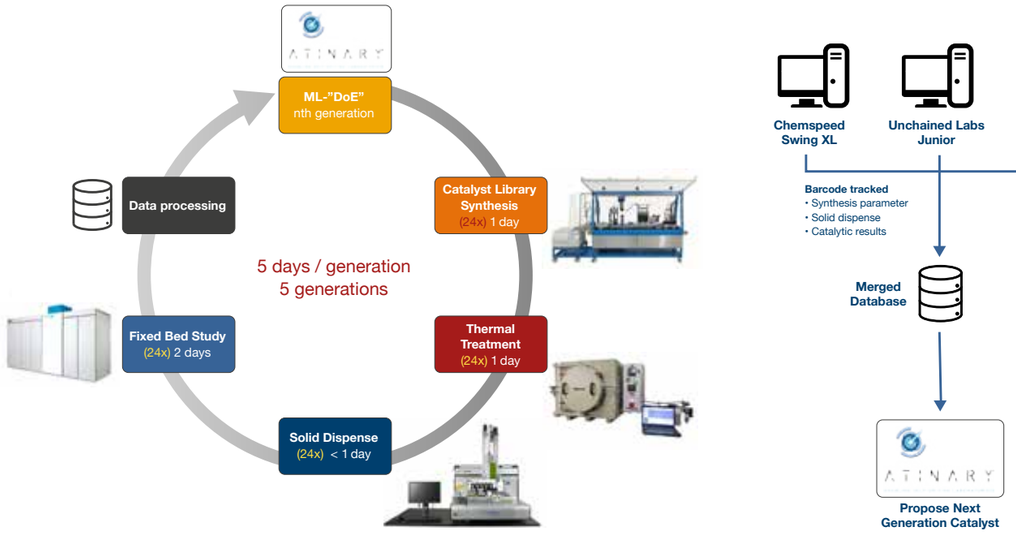



**Figure 7 :** Closed-loop ML-driven optimization approach for heterogeneous catalyst discovery in collaboration with Atinary.

The optimizer was fed with the chemical parameter space (1 categorical parameter (support) and 7 continuous parameters (7 metal source concentrations), synthesis constraints (up to 4 metal sources for a total metal loading not exceeding 6wt%), and multiple objectives (high CO2 conversion, high methanol selectivity, low methane selectivity and low catalyst cost).

Five generation of 24 catalysts have been synthesized successively by the Chemspeed Catprep unit by incipient wetness impregnation following the composition recommendations provided by the Atinary optimizer, calcined with the Hobersal oven and tested for CO2 hydrogenation with the Avantium XD and XR (5 days per generation) (Figure 7). The catalytic performance results of each generation were fed back to the optimizer to train the surrogate model and suggest the catalysts' composition for the next generation. Figure 8 show respectively the evolution of the catalyst composition and their performances. In 5 weeks, 120 catalysts have been prepared and tested with a significant improvement of the catalytic performances towards the objectives of the study. It shows how efficient this approach is to optimized catalyst composition from a large parameter space and toward multiple-objectives simultaneously in short time. It can obviously be applied to other chemical spaces, objectives and applications. It also demonstrates the Swiss Cat+ East capabilities, immediately available to the users, to perform ML-driven closed-loop heterogeneous catalyst optimization.

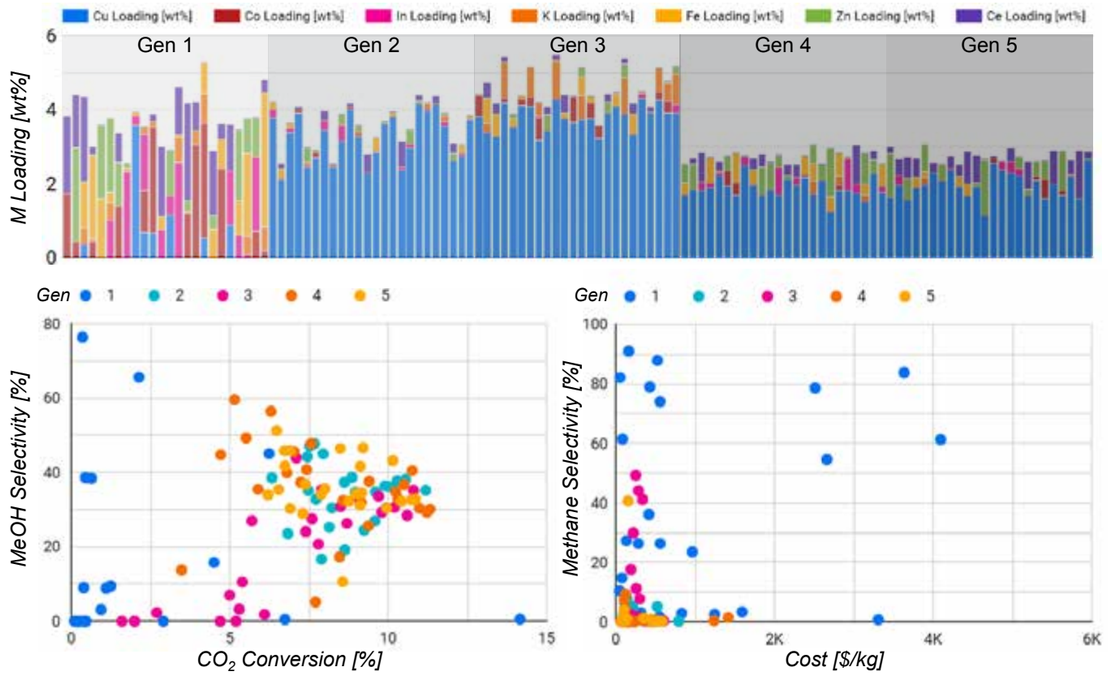



**Figure 8 :** Composition of the 120 catalysts prepared and tested following Atinary ML suggestions (top). Evolution of the four study objectives (Methanol selectivity, CO2 conversion, methane selectivity & metal cost) along the generations (bottom).

# e. Developments and challenges.

Since January 2023, a first lab unit of Swiss Cat+ East (HCI G120) is operational in a “beta-testing” phase. In four months, the team has already received more than 18 project requests from various research groups of ETHZ, PSI and EMPA. A first project request from an external university (university of Sevilla in Spain) is also under progress. The Swiss Cat+ East is also part of a large research project initiated by BASF, and including several German institutes (CARLA, Max-Planck-Institutes, KIT, BasCat, hte, Fritz-Haber-Institut) aiming to develop new catalysts and processes for the conversion of sugars to chemicals.

The high number of requests testifies of the scientific community strong interest for such a technology platform. The project requests are varied and consist of isolated synthesis, characterization, or performance evaluation of a catalyst library, to the complete experimental workflow combining ML-assisted design of experiment, synthesis, and testing of several generations of catalysts. In addition, Swiss Cat+ East is involved in several projects involving Master students at ETHZ, providing training and exposure for students to lab automation, high-throughput experimentation, and data science. The involved projects include the synthesis and testing of heterogeneous catalysts, as well as implementation of ML algorithms for accelerated catalyst discovery.

During this “beta-testing phase”, the users requests serve the Swiss Cat+ East to develop and validate the different methods, including the synthesis of catalysts according to various protocols (impregnation of metal-supported oxides, precipitation of mixed oxides, zeolites, MOF), and their testing under multiple conditions of interests, in both fixed-bed and batch mode (alcohols oxidation, CO2 reduction, propane dehydrogenation…). This phase is also critical to identify the existing weak points and provide leads to fix them. Some of the challenges identified so far include:

**Standardizing catalyst performance evaluation tests.**
Users from different research groups tend to ask for different testing conditions for the same application. Therefore, it makes the comparison between catalysts and the further use of the data by machine learning models more complicated than if they would be tested under the same conditions. Standardizing catalyst performance evaluation tests for a given application would allow for a more efficient testing of catalysts and utilization of the data. As part of this effort, Swiss Cat+ East plans to develop collaboration with major catalyst manufacturers to establish community-wise accepted catalyst testing conditions.

**Developing automated sample preparation for various analytical equipment.**
To identify the chemical descriptors leading to a given catalytic performance, the Hub should link catalytic performance data with catalyst characterization data obtained from several methods. However, up to now, heterogeneous catalyst characterization is poorly automated and rarely high-throughput, limiting the potential equipment that the Hub can acquire. In an ongoing effort to offer more advanced catalyst characterization services to its user, the Hub is working on developing automated sample preparation for various equipment such as X-ray diffraction, X-ray fluorescence, Raman, infrared, in close collaboration with analytical equipment suppliers, such as Bruker.

**Developing an automated and high-throughput electrocatalysts screening unit.**
Electrocatalysis is a topic of growing interest in the scientific community, in particular to convert green house gases and bio-feedstocks into sustainable chemical building blocks. However, the existing equipment are also not automated and high-throughput. Therefore, the Swiss Cat+ East is considering developing such a unit, either internally or in collaboration with an equipment supplier.

**Developing ML-algorithms predicting chemical descriptors of the catalysts.**
Despite the remarkable power of existing commercial machine learning models for closed loop statistical experimental optimization, they operate as a black box without taking into account the underlying chemistry. The Swiss Cat+ East has therefore initiated collaboration with Prof. Andreas Krause from ETH AI Center and Prof. Copéret from ETHZ Chemistry department to develop algorithms making use of the chemical descriptors of the catalysts, targeting the prediction of original catalysts compositions outside the trained parameter space.

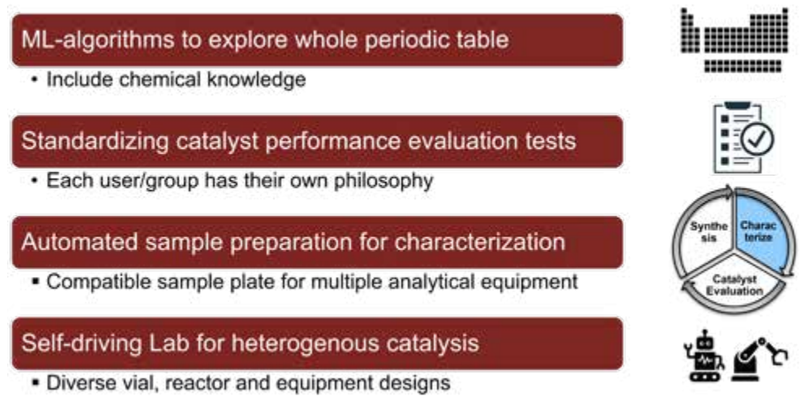



**Figure 9 :** Scheme presenting some of the main challenges for the Swiss Cat+ East.

**Improving our data management strategy**.
As a part of our ongoing development, we are continuously improving our data management strategy to fit the FAIR principles and the Open Research Data philosophy. As such, the hub serves as the perfect place to evaluate different solutions and provide feedback to the research groups before they consider implementing a specific approach locally. Recently we have started to implement OpenBis, an electronic laboratory notebooks and information management system, developed by ETHZ IT department.

**Broadening the capabilities of the Swiss Cat+ East.**
Broadening the capabilities of the Swiss Cat+ East is of paramount importance to accommodate all potential types of requests coming from diverse academic and industrial research groups, and to remain at the forefront of data-driven automated and high-throughput experimentation. In view of this objective, the Swiss Cat+ East continuously stretch the capabilities of the recently acquired tools by adapting or upgrading them to accommodate additional applications. To further expand the application range capabilities, and fulfill the approved 2021-2024 master plan, the Swiss Cat+ East has initiated purchases to furnish the two additional labs (HCI H241 and G226/228) in 2023 and 2024. The new tools will allow the following strategic developments:

# f. Partnerships and collaborations.

**Catalysts synthesis under controlled atmosphere.**
A second robotic catalyst preparation unit from unchained las will be installed in H241 existing custom-designed glovebox to provide air-sensitive catalysts synthesis capabilities. This unit will complement the Chemspeed Catprep unit acquired recently covering conventional (non-air sensitive) catalysts synthesis.

**Individual Batch testing of catalysts under controlled atmosphere.**
A set of 8 automated batch reactors from unchained labs will be installed in H241 existing custom-designed glovebox to evaluate the performance of air-sensitive catalysts individually up to 250 °C and 100 bars (e.g. hydrogenation, polymerization). It will complement the HEL CAT96 microplate batch testing unit already installed in a glovebox used for primary screening of up to 96 (conventional and air-sensitive) catalysts simultaneously.

**Fully automated ultra-high screening of catalytic performances in microplate batch mode**.
A fully automated microplate batch unit from Chemspeed is being purchased to evaluate the performance of conventional (non-air-sensitive) catalysts up to 250°C and 100 bars of reactive (or inert) gas. The unit will automate the tasks currently performed by three individual equipment (microplate preparation by ULJ, reaction study by HEL CAT96, and sample preparation by Chemspeed CatPrep), removing all the manual transport of the samples plates. It will also be fitted with 6x100 mL individual automated batch reactors to study more accurately the performance of a fewer number of promising candidates.

**Fixed bed catalyst testing for gas to liquid and bio-feedstocks conversion applications**.
A second 16-fold fixed bed unit from Avantium dedicated to reactions using and/or producing difficult liquid compounds is planned (e.g Fischer-Tropsch and hydroprocessing of bio-feedstocks). It will be designed to operate up to 150 bars and 500°C, with an extremely accurate liquid mass balance, a system to collect several liquid samples from each reactor and a GC for analyzing the remaining gas phase. This equipment will complement the current Avantium units dedicated to gas/vapor phase reactions. It will bring the overall fixed bed testing capability of the Swiss Cat+ East to 40 reactors.

**Liquid phase products and polymers analysis.**
An Agilent UPLC-GPC will be added to analyze the products of polymerization studies and the liquid fraction in matrices not suitable for GC analysis (aqueous phase, sugar-based matrices).

**Catalysts surface and pore characterization.**
Two Microtrac Belsorb-Max X physi/chemisorption units (8 ports) will be acquired to perform specific surface area, and pore size/distribution analysis of mesoporous and microporous materials.

**Expanding further.**
To reach a critical size and offer capabilities covering the major applications in the field of heterogeneous catalysts R&D for sustainable fuels and chemicals production, the Swiss Cat+ East, in coordination with the West Hub, plans to apply for a second round of funding for 2025-2028. The budget will serve to purchase new tools, and/or upgrade existing ones, with features broadening the spectrum of high-throughput and automated experimentation to offer to its users. This includes additional automated catalysts' characterization units (XRD, XRF,), automated synthesis units dedicated to specific preparation routes (electrocatalysts) and new high-throughput fixed bed and batch units covering other application fields (electrocatalysis, photocatalysis, ammonia synthesis).

The Swiss Cat+ East has partnered with several private companies and research groups to develop original tools and methods.

**Automated sample preparation for spectroscopic analysis.**
Under the umbrella of an Non Disclosure Agreement, we are continuously discussing with Bruker since March 2021, to develop an innovative fully automated sample preparation method suitable for XRD, XRF, IR and Raman. Despite most of those equipment able to accept microplate format to perform several analyses consecutively, the sample preparation from powders remains very specific for each analyzer and is typically performed manually. The development and validation of such automated sample preparation methods would be a significant progress to accelerate and standardize the data acquisition by several analytical equipment for heterogeneous catalysts.

**Broader application range of automated microplate batch testing.**
A service agreement has been signed with Chemspeed in September 2022 targeting the improvement of one of their automated tools to better fit the Swiss Cat+ East applications range. Following several discussions and experiments performed by the Hub, Chemspeed has successfully increased the temperature range of their microplate pressure block reactor from 150 to 250°C. This tool which will be installed at the end of 2023 will provide the Swiss Cat+ East user a broader spectrum of application screening capabilities (hydrogenation, hydroformylation, bio-feedstock conversion).

**ML-supported Bayesian experimental optimization.**
End of 2022, the Swiss Cat+ East has partnered with Atinary, a start-up active in the field of lab automation and ML-based experimental optimization, to demonstrate the potential of their Bayesian algorithms with the hub's specific set-up and workflow, dedicated to heterogeneous catalysis. Using their closed loop experimental optimization approach, the hub has synthesized and tested about 150 catalysts in 5 weeks, with a significant improvement of the catalytic performances generation after generation. A scientific article describing the study is being prepared and should be published before the end of 2023.

**Best practices-methods in high-throughput fixed bed catalyst testing.**
Avantium is one of the three main suppliers of high-throughput fixed beds and batch units. The Swiss Cat+ East has selected their fixed bed technology because it combines a reduced equipment footprint, simplified operation, and high reactor-to-reactor reproducibility thanks to their proprietary microfluidic flow distribution. In view of a long term collaboration, the Swiss Cat+ East and Avantium agreed to share best-practices methods in this field of research.

**Automated high-throughput elemental analysis of heterogeneous catalysts.**
Performing precise elemental analysis of heterogeneous catalysts is critical, but not trivial in an automated fashion and on large libraries. Micro-XRF techniques are easy to implement, but the data analysis can be difficult when targeting precise quantification of elements not known prior to the analysis. ICP-MS is highly sensitive but the sample preparation for inorganic materials, requiring acid digestion, is time-consuming and complicated to automate safely. On the other hand, LA (laser-ablation)-ICP-MS does not require complex sample preparations and could be a suitable solution for the Swiss Cat+ East environment. To evaluate this technique, we have initiated a collaboration with Prof. Dr. Detlef Günther and his group, who are renown experts in this field. Initial results are very promising and could lead to the development of a new fully automated, high-throughput and highly sensitive elemental analysis of heterogeneous catalysts

**ML-supported prediction of optimal heterogeneous catalysts' chemical descriptors.**
The Swiss Cat+ East is part of a collaboration with Prof. Andreas Krause (ETHZ AI Center) and Prof. Christophe Copéret (ETHZ Laboratory of Inorganic Chemistry) to develop new machine learning algorithms making use of heterogeneous catalysts' chemical descriptors. By training the models with the right set of chemical descriptors related to the materials' composition, also associated to their performance toward a given reaction objective, it is expected to predict ideal sets of chemical descriptors leading to high catalytic performances. By reversing the association process, the model will suggest new elemental compositions matching the ideal set of chemical descriptors.

**Experimental Support for Switzerland largest Catalysis Community.**
Co-directed by Prof. Dr. Javier Perez-Ramirez (ETHZ) and Prof. Dr. Jérome Wasser (EPFL), the NCCR Catalysis is a national-wide network of research groups working in all areas of catalysis. It supports numerous research projects focusing on carbon-neutral catalytic processes to produce fuels and chemicals from renewable resources and aiming to transfer the fundamental discoveries into practical technologies. The Swiss Cat+ East and West will play a pivotal role in several of these projects seeking a data-driven high-throughput approach.

# EPFL – West Hub.

# a. Strategic approaches.

According to the project established in 2019, the aim of the project is to build and operate a world-class infrastructure for the data-driven discovery and optimization of new homogeneous catalysts. This will require the integrated design and development of a fully automated and integrated sampling, synthesis, and characterization line capable of performing high-frequency chemical experiments under inert conditions and generating highly controlled data. To reach the previous goal, we established a list of guidelines and principles used to keep a high coherence in the designs and developments.

| | |
|---|---|
| • generating highly controlled and validated data<br>• preserving chemical flexibility<br>• complete integration of sample and data transfer<br>• adopting machine point of view | • preserving data integrity (data processing, data storage)<br>• open-sourced and FAIR<br>• using the adequate data analysis tools<br>• AI/ML : Avoid Garbage In – Garbage Out |

**Chemical development strategy**

Automated laboratory synthesis and analysis are new and rapidly developing fields[21, 22, 23, 24, 25]. They are very different from automated chemical manufacturing. In the latter, the chemical reaction is selected from among thousands and optimized to be adaptable to a specific automation setup. In the Swiss Cat+ project, the goal is to preserve the strength of chemical flexibility as much as possible, similar to a classic in a "manual" organic laboratory. The new automated setup must be able to handle vastly different properties of used chemicals (solids, liquids, waxes) with different types of risks and characteristics (sensitivity to air, fire risks, stickiness...). The chemical workflows that have to be coded and operated in this infrastructure have to adapt to different types of catalytic reactions. The novelty of the field had two major consequences for the project: firstly, only part of the equipment required was available on the market at the start of the project. This means that we had to and still have to develop an important part from scratch. This is done either through massive collaborations with equipment companies (see sections dedicated to "developments" and "collaborations") or through completely local developments. The second consequence is that we have had to make strategic choices about the types of reactions we can handle in the setup. In order to be consistent with our main guidelines, we decided to focus on one-step batch mode reactions. In fact, we felt that focusing on batch mode one-step reactions would allow us to test a wide variety of homogeneous catalyst reactions while maintaining the best level of condition control.

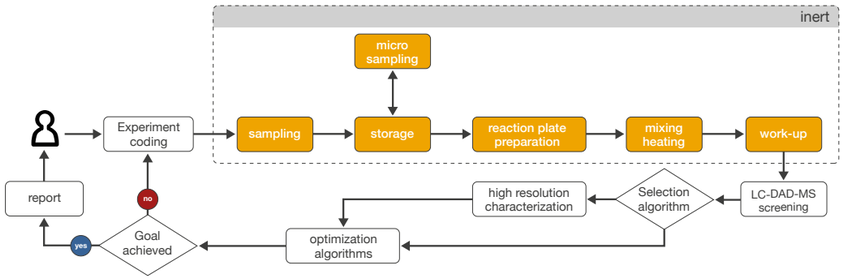



**Figure 10 :** Discovery workflow at the Swiss Cat+ West hub. All steps in pink are performed under inert conditions (nitrogen, argon) in Chemspeed CATSYNTH glove boxes. Steps in white are performed under normal atmosphere. All transfers (arrows) are fully automated in terms of both sample and data. The selection algorithm is used to define the unknown compounds to be fully characterized in the high-resolution analysis.

[21] Shi, Y.; Prieto, P. L.; Zepel, T.; Grunert, S.; Hein, J. E. Automated Experimentation Powers Data Science in Chemistry. Acc. Chem. Res. 2021, 54 (3), 546–555. | [22] Sanderson, K. Automation: Chemistry Shoots for the Moon. Nature 2019, 568 (7753), 577–579. https://doi.org/10.1038/d41586-019-01246-y | [23] Coley, C. W.; Eyke, N. S.; Jensen, K. F. Autonomous Discovery in the Chemical Sciences Part I: Progress. Angew. Chem. Int. Ed. 2020, 59 (51), 22858–22893 | [24] Coley, C. W.; Eyke, N. S.; Jensen, K. F. Autonomous Discovery in the Chemical Sciences Part II: Outlook. Angew. Chem. Int. Ed. 2020, 59 (52), 23414–23436 | [25] Krska, S. W.; DiRocco, D. A.; Dreher, S. D.; Shevlin, M. The Evolution of Chemical High-Throughput Experimentation To Address Challenging Problems in Pharmaceutical Synthesis. Acc. Chem. Res. 2017, 50 (12), 2976–2985

Based on this, we have defined four sub-families of reactions that we can run on the facility:

| Sub-family of reaction tasks | Substrates | Catalysts | Conditions | Expected results |
|---|---|---|---|---|
| 1. Hits research | Small series | Defined list | Limited variations | Interesting hits |
| 2. Conditions optimization | Fixed | Fixed | Variable | Best yield, ee |
| 3. Scope research | Libraries | Fixed | Limited variations | Interesting hits |
| 4. Catalyst optimization | Fixed | Cat, metal, ligand libraries | Fixed | Optimal ligands |

The sub-families of tasks can be viewed as steps in a global catalyst development process, where hits found in step 1 are optimized in step 2, extended in scope in step 3, and finally challenged with new competitive structures in step 4. Each step can also be performed independently, depending on the level of information already available about the catalyst under investigation. There are also several other approaches that we would like to explore in the future and make available to users of the infrastructure, such as batch-mode multistep reactions to synthesize de novo ligands and flow-mode reactions to test continuous variables.

**Chemical workflow .**

The strategy described above has been translated into two global chemical workflows described below. The first workflow (Figure 10) is dedicated to discovery. It is fully integrated and mainly covers steps 1, 3 and 4. Step 2 can also be performed on it, but with limited access to kinetic information due to the structure of the micro-reactors (100 x 1 ml) combined in globally controlled temperature plates. In fact, it is almost impossible to sample the solution or to insert a probe for simultaneous measurements. This workflow is designed for a capacity of 300 reactions per day, organized in batches and grouped into campaigns. The actual plans are to run 1 campaign per week with 3 to 4 batches, for a total of 900 to 1,200 reactions per week.

The second workflow (Figure 11) is dedicated to conditions optimization and reaction kinetic analysis (mainly step 2). In this case, the sample preparation is only partly automated due to the reactor configuration (3 x 250 ml).

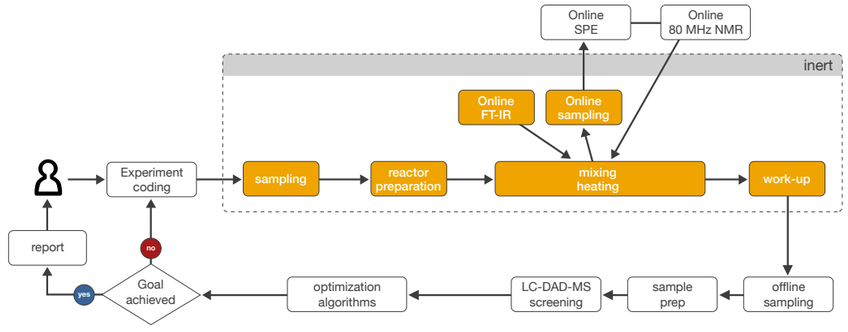



**Figure 11 :** Optimization workflow at the Swiss Cat+ West hub. All steps in pink are performed under partially inert conditions (nitrogen, argon) in a Chemspeed ISYNTH purge box. Steps in white are performed under normal atmosphere. All transfers (arrows) are fully automated in terms of both sample and data. FT-IR analysis is performed in-situ using a Bruker Matrix MF fiber-optic IR spectrometer and online NMR analysis is performed using a Bruker Fourier 80 bench-top NMR. The online sample line and the SPE module have been developed within the Swiss Cat+ project in collaboration with Advanced MicroFluidics.. The selection algorithm is used to define the unknown compounds to be fully characterized in high resolution analysis.

# b. The team.

Active members directly funded (April 2023)

**Dr. Pascal Miéville – Executive Director, chemist.**
Pascal Miéville started his career as technician in pharmaceutical development industry with a focus on MRI contrast agents, before completing his studies with a Bachelor's degree in Chemistry at the University of Geneva, a Master's degree in Physical Chemistry at EPFL and a PhD in Nuclear Magnetic Resonance hyperpolarisation (DNP) in the group of Prof. G. Bodenhausen at EPFL. In 2012, he took over the management of the NMR platform at EPFL, where he developed the automation, data management and piloted the acquisition and installation of the world's largest 900 MHz solid-state DNP NMR system. In September 2020, he was appointed Executive Director of the EPFL Catalysis Hub - Swiss Cat+ and in parallel obtained a Master in Public Administration from IDHEAP at the University of Lausanne.

In the making

**Dr. Florian de Nanteuil – Senior scientist, chemist.**
Florian de Nanteuil obtained his PhD in Organic Synthesis from EPFL and then moved to the University of California, Irvine for a two-year post-doctoral fellowship working on the total synthesis of antimalarial natural products. He then joined the perfumery discovery group at Firmenich as a laboratory manager. He joined Swiss Cat+ in 2021. Overall, he has contributed to innovation in pharmaceuticals and F&F by applying his knowledge of organic synthesis, data science and automation. He is an experienced public speaker, roundtable panelist and consultant for innovative chemistry projects. He has worked in the USA, Ireland, Switzerland and France. His current focus is on designing the labs of the future, integrating automation, robotics, data analytics and AI to accelerate the discovery of sustainable chemical processes.

In the making

**H. Francelet – Administrative assistant.**
Heidi Francelet is the Administrative Assistant of the Swiss Cat+ West Hub since the start of the project. She brings a profound knowledge of EPFL's administrative procedures, tools and structures after having worked in several departments since 2005. Before that time, she gathered a decade's experience in Swiss political asylum and integration programs for recognized refugees at the Swiss Refugee Council. In her spare time, Heidi likes to read, garden, visit museums and catch up with friends.

In the making

**J.-C. Cousty – IT Manager.**
Jean-Charles Cousty has an IT Engineering background from Central School in France. He is an experienced IT project manager who has managed and developed application projects (PHP, C#, Python, SQL). With four years experience at Eurofins and Swiss Cat+, he excels at working with laboratory equipment companies, IT teams and chemists. He understands their specific needs and requirements to propose efficient and reliable software, hardware and data management strategies. He aims to make a significant contribution to laboratory automation by using his expertise in both IT and laboratory operations to implement tailored automated solutions.

In the making

**E. Mariano – Robotics engineer.**
Edy Mariano holds a degree in microengineering from the University of Applied Sciences in Yverdon-les-Bains, Switzerland. He is currently in charge of hardware automation for the Swiss Cat+ project at EPFL. His journey began at an innovative 3D bioprinting start-up where he honed his skills as an automation engineer. In his role at Swiss Cat+, he is automating processes to gradually turn the lab into a fully autonomous entity. Edy's expertise is focused on laboratory automation, with particular emphasis on sample transfer, robotics and equipment scheduling.

In the making

**P. Gaumann – Chemistry technician.**
Philippe Gäumann is a laboratory technician with over 33 years of experience in analytical chemistry within the pharmaceutical and perfumery sectors. His expertise lies in utilizing advanced instruments like GC-MS and LC-MS for chemical compound analysis and developing innovative analytical methods. Recently, he joined EPFL's Swiss Cat+ project to specialize in the exciting field of robotic synthesis. Philippe is enthusiastic about merging his video production skills with his new role, leveraging visual storytelling to support his group's endeavors.

In the making

**Active members funded through external grants**

**K. Villat 30%** (Microtechnics engineer)
**E. Clerc** (Apprentice chemistry laboratory technician)
**C. Cheyrouse** (Apprentice chemistry laboratory technician)
**M. Lowenberg** (Apprentice automation technician)
**Y. El Goumi** (EPFL robotics master student)
**A. Duranceau** (EPFL robotics master student)

**Former members**

**U. Randrianarisoa** (Chemist)
**A. Gauthier** (EPFL chemist master student)
**E. Correia** (Laboratory technician from Vaud state admin)
**J. Geissmann** (HEIG-VD automation bachelor student)
**Y. Jacquat** (HEIG-VD automation bachelor student)

# c. Hardware infrastructure.

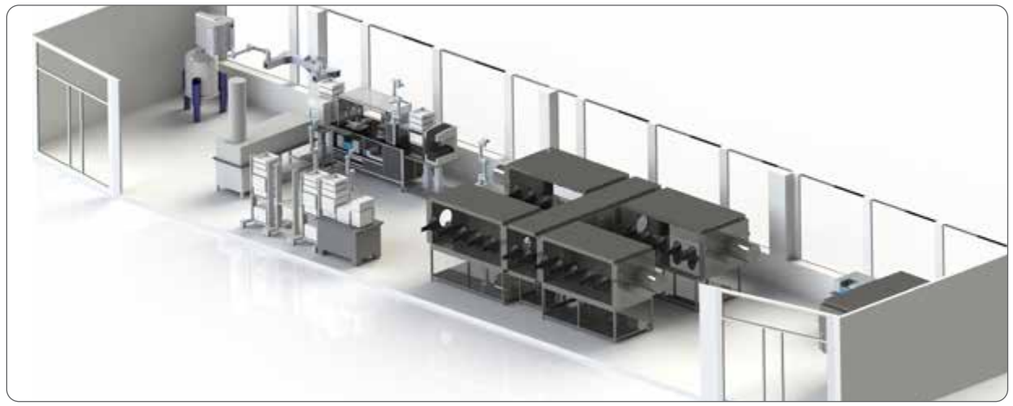


**Figure 12 :** CAD rendering of the main structure of the laboratory. Its dimensions are 27 m long by 7 m wide at the largest point, giving a total surface area of 190 m2. The laboratory faces north-east (open side in the picture) to limit solar radiation and all windows are covered with IR/UV reflective film. The temperature inside the laboratory is maintained at 21 +/- 0.5 °C and the ventilation rate is set at 8 times/h. The floor is continuous and flat, allowing free positioning of all equipment. The sample pathway runs from left (sampling and synthesis glove boxes) to center (LC-MS for screening) to right for high resolution MS and NMR. The robotic track for sample transfer is visible at the top of the instrument.

**Laboratory environment**

In order to respect the guidelines described in the strategy section, we designed and built a specific and optimal laboratory environment. We transformed a 300 $m^2$ sector of the chemistry building (CH-A2) of the EPFL, with 190 $m^2$ dedicated to the main automated laboratory (Figures 12 and 13) and 110 $m^2$ to the support. The main laboratory was designed with the following requirements: a global flat slab allowing any configuration of equipment and free paths for mobile robots, an absolute temperature control of +/- 1°C, all energies (electricity, network, gas, cooling water, exhaust air) coming from the ceiling and concentrated in standardized connection platforms, and the highest level of safety for both chemistry and robotics. To meet these requirements, the EPFL-DII completely renovated and equipped the 300 $m^2$ for a total work budget of 1.5 MCHF taken from the EPFL budget.

**Preparative sample preparation (complete delivery expected by end of 2023)**

- DEC solid sampling and storage projects in inert conditions (see developments)

**Synthesis**

- Chemspeed CATSYNTH 1 in glove box for discovery (300 x 1 mL reaction plates, Mai 2023)
- Chemspeed CATSYNTH 2 in glove box for discovery (work-up, August 2023)
- Chemspeed ISYNTH for optimization (3 x 250 mL automated reactors + sample prep, fig X5)

The DEC solid sampling and storage platform is directly and inertly connected to the two Chemspeed CATSYNTH glove boxes to form an automated ensemble visible at the center of the laboratory on Figure X.

**Figure 13 :** View of the analytical sector of the actual laboratory (March 2023)

**Analytical sample preparation (planed for 1st semester 2024)**

- 2 Agilent liquid handling Bravo stations
- 1 Agilent automated centrifuge
- 1 Agilent PlateLoc automated sealer

**Fast chromatographic screening**

- 2 Agilent LC-DAD-MS (Figure 15)
- 1 Agilent SFC-DAD-MS
- 1 Agilent GC-MS (autumn 2023)

**Reaction kinetic online analysis (see developments, section 3.e)**

- 1 Bruker Matrix MF optical fiber FT-IR spectrometer
- 1 Bruker Fourier benchtop 80 MHz NMR spectrometer
- 1 Advanced MicroFluidics (AMF) reactor multiplexer and online SPE

**Figure 14 :** Actual Chemspeed ISYNTH and CATSYNTH for reaction optimization and discovery

**Figure 15:** Actual Agilent LC-DAD-MS for fast sample screening

**Figure 16 :** Agilent SFC-IM-Q-TOF for ion mobility (CCS) determination and high-resolution mass spectrometry.IT architecture and data-driven strategy

**High-resolution characterization**

- 1 Bruker Auto-400-NMR (see developments, section 3.e)
- 1 Agilent SFC-IM-Q-TOF (Figure 16)
- 1 Bruker high-resolution Invenio FT-IR
- 1 Agilent high-resolution Cary 60 HR-UV-VIS
- 1 Modified Agilent RapidFire for automated NMR sample preparation and optical spectroscopy (see developments, section 3.e)

A pivotal part of the development is related to the IT architecture of the project. The IT architecture includes the data structure (what data to store in what format and where, see Data Structure section), the programming or coding strategy for the operations (see HCI section), the scheduling and orchestration of the operations (see Scheduler section), the data pre- and post-processing (see Data Processor section), and finally the strategies for directly interfacing all the scientific equipment with the scheduler and further with the coding strategy (see API section). In this section we will also discuss the optimization strategies (see Digital Chemistry Algorithms section) that will be used in the project. At the beginning of the project we considered using existing Electronic Lab Notebook (ELN) and Laboratory Information Management Systems (LIMS). After analysis, we found that these tools appear to be generally well adapted to biological or pharmaceutical workflows, but are less suited for the needs of inorganic chemistry. In addition, they were mainly oriented towards an industrial set-up with limited flexibility in terms of the workflows required in an academic/early and highly adaptive discovery environment. Finally, although ELN and SLIMS capture information electronically, the data are not sufficiently systematic in terms of metadata, workflow descriptions, experimental coding and data formats. For this reason, we decided to create our own specific architecture, which is described below.

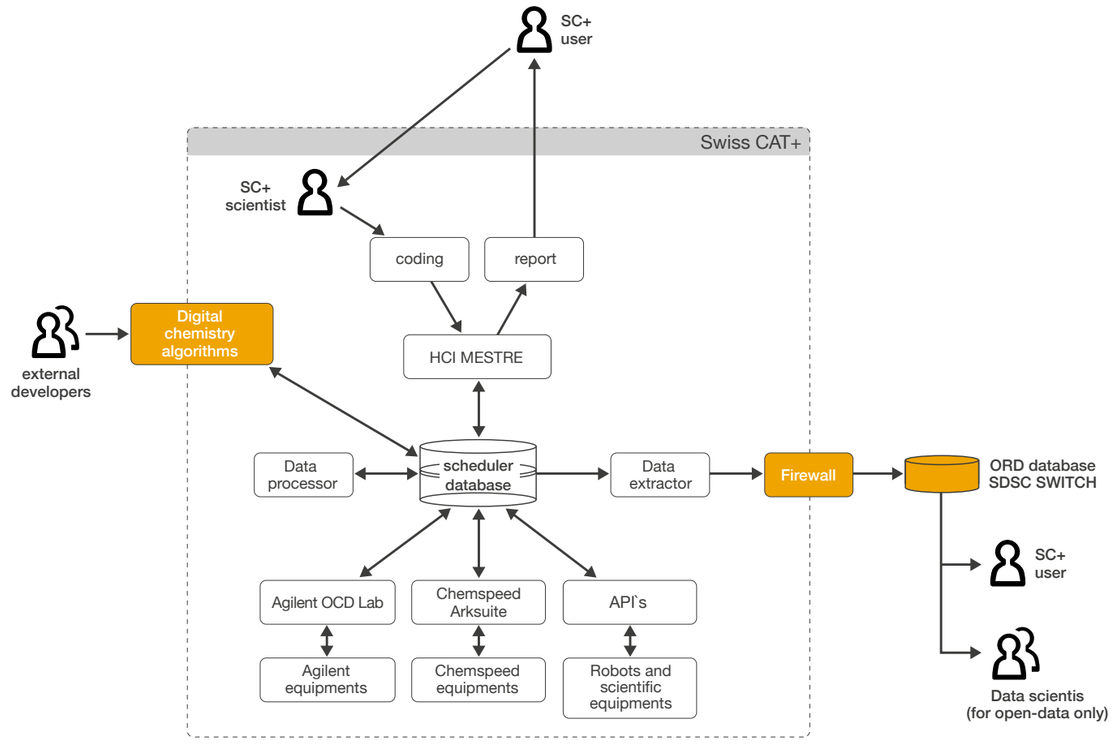



**Figure 17 :** Simplified global IT architecture of the Swiss Cat+ West Hub. Elements in pink are accessible to external users according to IP policy. Most of the elements visible in this figure are described in more detail in the following subsections. The IT architecture, with the exception of the ORD database, is integrally stored and managed on-premises at EPFL with a multi-site backup strategy. The ORD database will be stored in the Switch environment and access to it will be developed in collaboration with SDSC as part of a joint ORD project.

The global IT architecture is constantly evolving and represents a large part of the workforce involved. It also relies on essential collaborations with academia (Swiss Data Science Center – SDSC), institutions (Switch Foundation) and key industry leaders (MestreLab, Agilent, Bruker, Chemspeed). Figure 17 below shows a simplified vision of the IT architecture of the Swiss Cat+ West Hub.

The data structure consists of two main elements: first, the local database organization, which is directly related to the laboratory hardware configuration and workflows. Second, the data structure or ontology, which is related to the information content to be stored.

**Local database**

On the first point, we have developed a complete relational database architecture (SQL) based on the specific hardware of the Swiss Cat+. Much work was done to systematize and minimize the number of tables. The aim was to ensure that the database could be used systematically for all experiments, without evolving with each experiment and with conservative table names and definitions. This requirement is essential to comply with the FAIR principles[26]. The Swiss Cat+ West Hub database is directly connected to the laboratory scheduler (REST API) and to the various instrument interfaces (APIs) in order to be directly fed with metadata from the Human Computer Interface (HCI) and with experimental results from the scientific instruments.

**Data ontology**

Regarding the second element, i.e. how to store the information, we have established an important collaboration with the Swiss Data Science Center (SDSC, https://datascience.ch) of the ETH Board. As part of this collaboration, we are developing a comprehensive Swiss Cat+ data ontology[27] based on FAIR principles. To the best of our knowledge, there is no standard data ontology that is able to cover the entire chemical workflow, from chemical sampling through synthesis steps to analysis and characterization. One of the risks was to develop another "pseudo" standard data format that would only add to existing formats (e.g. JCAMP-DX for spectroscopy , AniML for analytical workflows ) and might only be suitable within the Swiss Cat+ infrastructure. Another important issue was how to convert the proprietary format data generated by scientific instruments. Some equipment companies are now part of a consortium called Allotrope (https://www.allotrope.org/), which aims to provide systematically structured and partially open data to users . Not all equipment companies are part of this consortium, and even within the Allotrope project there is virtually nothing for sample preparation and synthesis. Therefore, in order to avoid the pitfalls of pseudo-standards, to be tolerant of a maximum of proprietary data formats, to take into account all the steps of the Swiss Cat+ chemical workflow, and finally to respect the FAIR principles, we have created a systematic data ontology based on simple cross-cutting rules called the "Matryoshka file".

The matryoshka file (mat.file, Figure 18) is a composite file based on the .ZARR file architecture (https://zarr.dev/) that groups and links all metadata and data aggregated along chemical workflows. The mat.file name comes from the fact that data is progressively added within the previous layer of information, progressively forming a typical matryoshka figure. All the information is concentrated around the LC peak (DAD spectrum and low-resolution mass) collected in the LC-DAD-MS screening step (see Figures 1 and 2). Considering that several sample preparations and syntheses can lead to the same LC peak and that for each LC peak we will aggregate different high resolution analyses, a mat.file combining all these data for each LC peak (synthesized compound) can be seen as a complete data set representing all tested pathways and analyses for a specific molecule.

The rules we have established for the generation of mat.files are as follows:

- Data must be human readable,
- aggregated data files must be in standard computer formats (.txt, .csv, .json, .xml,..)
- a complete and systematic description of the content and structure of the file must be provided at the beginning of all data files,
- Data must be separated by unique and described tags,
- contain all necessary metadata and data to repeat the experiment on any other setup,
- data are classified into metadata containing contextual data and chemical method data independent of instrumentation and experimental data dependent on instrumentation.

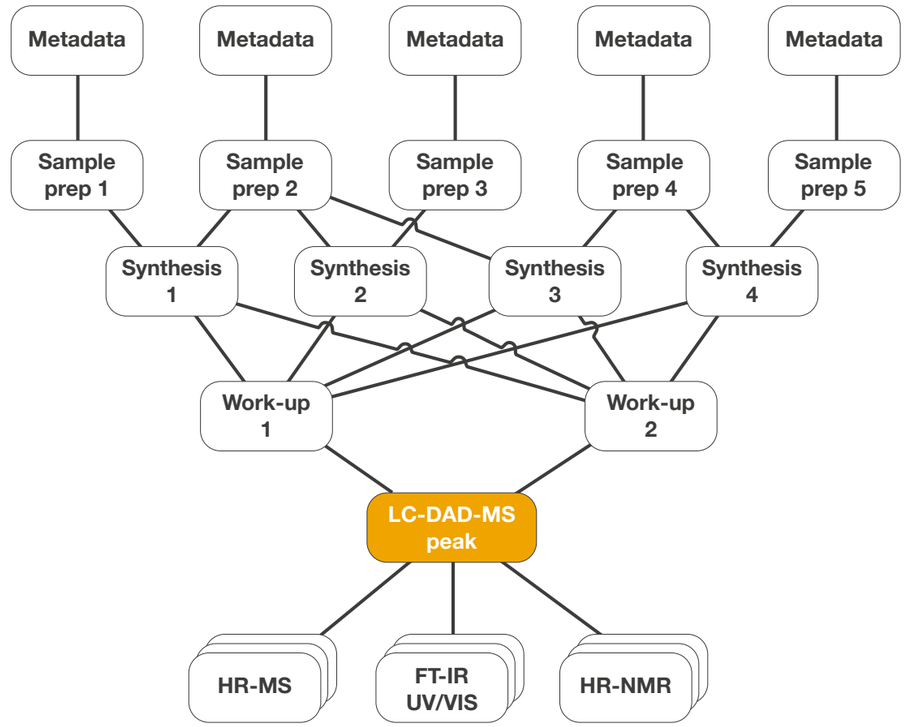



**Figure 18 :** A mat.file for a single LC-DAD-MS peak schematic description gathering all synthetic experimental data and analytical data.

This ontology, combined with the rules we have established, has the advantage of not relying on interpreted data such as a chemical structure or SMILE. It is based only on experimentally verified data and should allow any other automated setup to repeat the entire experiment from sampling to characterization.

**Swiss Cat+/SDSC/Switch ORD database**

In order to make the results for Swiss Cat+ available in a simple and efficient way, and to support the chemistry community in storing chemical information in a structured way, we are developing a project for an open database capable of storing mat. files and providing data analysis tools for their exploration (see fig.X8). This development will be done in collaboration with the SDSC (Dr O. Grognuz) and the SWITCH Foundation (Dr C. Wittzig) in the context of an ORD fund call. The aim is for this experimental database to be gradually opened up to the community, both to store experimental results in a structured way,

[26] Wilkinson, M. D.et al.. The FAIR Guiding Principles for Scientific Data Management and Stewardship. Sci. Data 2016, 3, 160018 | [27] Strömert, P.; Hunold, J.; Castro, A.; Neumann, S.; Koepler, O. Ontologies4Chem: The Landscape of Ontologies in Chemistry. Pure Appl. Chem. 2022, 94 (6), 605–622. | [28] Baumbach, J. I.; Davies, A. N.; Lampen, P.; Schmidt, H. JCAMP-DX. A Standard Format for the Exchange of Ion Mobility Spectrometry Data (IUPAC Recommendations 2001). Pure Appl. Chem. 2001, 73 (11), 1765–1782

[29] Schäfer, B. A.; Poetz, D.; Kramer, G. W. Documenting Laboratory Workflows Using the Analytical Information Markup Language. JALA J. Assoc. Lab. Autom. 2004, 9 (6), 375–381 | [30] E. Vanderwall, D.; M.Vergis, J. Standardizing Data Management. Pharm. Technol. 2014, 2014 eBook (3) | [31] Moore, J.et al.. OME-Zarr: A Cloud-Optimized Bioimaging File Format with International Community Support. bioRxiv February 25, 2023, p 2023.02.17.528834

and to developers to provide them with high quality experimental datasets. There will be several ways to explore this database:

- Swiss Cat+ users will receive a URL that allows them to extract the ensemble of mat.files corresponding to a campaign. They can either use this URL to retrieve the files for exploration and individual processing, or simply provide the URL as supporting information when publishing.
- Data scientists can use metadata to filter the open access data contained in the database and extract specific experimental data sets for the development of new chemical algorithms.
- Swiss Cat+ users and non-specialist chemists will have access to tools to plot their results across batches and campaigns, while respecting good practice in statistics and data presentation.

We have already started the preparatory work in terms of file structure (see Developments) and also in terms of dataset selection tools. The ORD fund is targeted for spring 2024 and should be active for at least two years. Swiss Cat+ will provide the experimental data, SDSC the data analysis architecture and SWITCH the server infrastructure and security aspects.

**Laboratory scheduler**

The scheduler is an essential part of an automated laboratory. There are several options available on the market (Atinary, Optimal SyntQ, Perkin Elmer...). It converts the chemical workflows and experiments coded by the chemist (in our case in the HCI - see next section) into sequences of machine operations and corresponding database entries. It also receives all system feedback and informs the supervisor of any malfunction. Finally, it collects all the experimental results and stores them in the correct place in the database. As shown in Figure 17, it is the central node of the entire IT architecture. The Swiss Cat+ West Hub scheduler is a locally coded REST API based on C-DATA, compatible with our SQL database and with the post generated by the HCI. It is also configured to communicate with the scientific equipment via dedicated APIs.

**Human Computer Interface - HCI**

Another important development and part of the global IT architecture is the Human Computer Interface (HCI), which we are currently developing in collaboration with MestreLab (Dr Santiago Domingez, Dr Santiago Fraga). MestreLab is a leading company in the world of spectroscopy data analysis and automation. We are already using their MestreNOVA software at EPFL for NMR analysis. The HCI is a sophisticated ELN that incorporates some of the ideas of the Cronin Chemputer [32] and has the following functions: to systematically collect all the necessary metadata, to define the chemical workflow according to the methods available in the laboratory and to perform all the combinatorial calculations in terms of chemicals and consumables. Once the chemist has validated the sequence, the HCI generates POSTS, which are sent to the scheduler and converted into database entries and machine operations. A complete mock-up already exists and the entire program definition is now complete. MestreLab has started coding the software based on their existing MBook and MDrive tools. A first test version is expected in 2023.

**Data processor**

In order to populate the Mat.files with systematic and readable experimental data and selected metadata, the proprietary formats generated by the scientific instruments have to be processed by a data processor Figure 19). This data processor, developed in collaboration with MestreLab (Dr. Santiago Domingez, Dr. Santiago Fraga), can extract already processed data (e.g. LC peak list, areas, m/z) from proprietary formats (Agilent, Bruker...), on the one hand, and compile the information contained in the Allotrope files or analyze the XY data

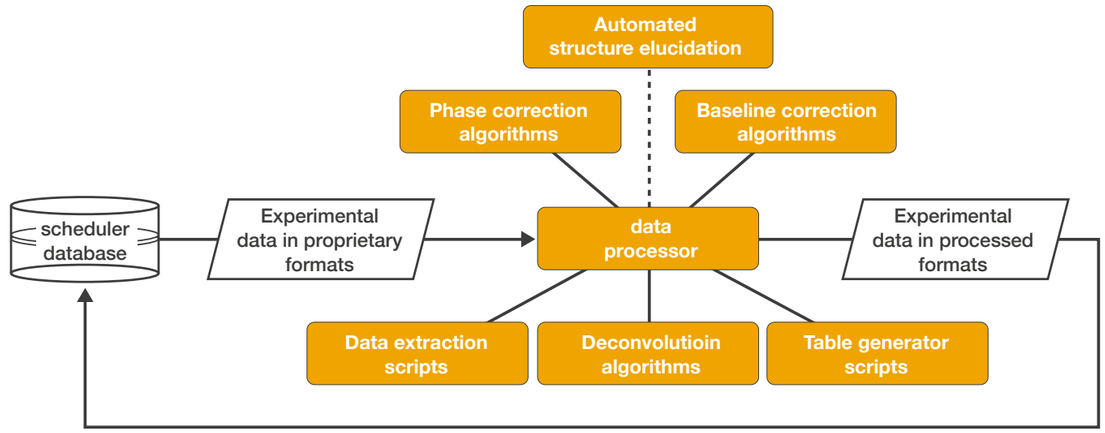



**Figure 19 :** Schematic description of the data processor (in pink). The dotted line indicates a possible integration of the automated structure elucidation algorithms currently under development (Bruker, Merstre, ACD). All other algorithms and scripts are planned to be integrated from the beginning.

lists, on the other. In the latter case, dedicated deconvolution algorithms are used to process the chromatograms and spectra. Chromatograms and spectra are converted into a numerical array containing all the necessary peak characteristics (rt, frequency, intensity, area, width, skewness, overlap, j-coupling...). Some recent ML algorithms developed by Cobas and Paruzo could also be implemented to extract more sophisticated information such as systematic molecular regions from NMR spectra. Finally, we plan to integrate increasingly automated structure elucidation algorithms to propose molecular structures and SMILES. These elucidation algorithms would build on ongoing developments at companies such as Bruker, Mestre or ACDLabs. We expect a first test version in 2023.

**API & Middlewares**

Communication between the scheduler, i.e. the database, and the scientific instruments must take place via interfaces called APIs. These APIs have three main functions: 1) converting the scheduler's instructions into appropriate commands for the instrument, 2) obtaining operational feedback from the instrument and informing the scheduler of its status, and 3) collecting experimental data. Almost all instruments require a specific API. This is a major problem when attempting to automate a chemical laboratory. There is no standard communication language such as EtherCAT or OPC-UA for scientific instruments. To limit the burden of developing an API per instrument and to have a more rational management, we have adopted a focus strategy based on working with the major instrument companies and using their middleware as an intermediate layer between the programmer and the instrument, i.e. all LC, SFC, MS are provided by Agilent and all controlled by OCD Lab Server. For all Chemspeed synthesis equipment we will be using a new middleware called Chemspeed Arksuite and for Bruker (NMR and IR) we are currently developing a local programming tool using Optimal SyntQ software. With Bruker we have also developed a command library to coordinate

[32] Shi, Y.; Prieto, P. L.; Zepel, T.; Grunert, S.; Hein, J. E. Automated Experimentation Powers Data Science in Chemistry. Acc. Chem. Res. 2021, 54 (3), 546–555

# d. Developments and challenges.

the operation of a six-axis Universal Robot UR5e arm with a 400 MHz high-resolution NMR spectrometer equipped with a SampleJet autosampler. For laboratory robotics (mobile robot for sample transfer and six-axis arm, see section 3.e) we use the ROS environment (https://www.ros.org). This is an open source robotics middleware suite. Finally, we had to develop some local APIs for some isolated equipment. In this context, collaboration with companies was essential, as the codes for these interfaces require access to a relatively low level of the machine control software.

**Digital chemistry algorithms**

As shown in Figure 17, a module directly linked to the local scheduler is dedicated to digital chemistry algorithms. This module is open to external collaborations and will allow specialized researchers and groups to test their own developments in "real" applications with experimental data. As described on Figure 21, we plan to rapidly integrate existing optimization algorithms such as Bayesian non-linear optimization[37, 38, 39] and in parallel, in collaboration with Prof. P. Schwaller (EPFL) and Dr. T. Laino (IBM Research GmbH), we already explore the potential of interaction between the data generation capabilities of Swiss Cat+ and the predictive tools for automated synthesis[40, 41].

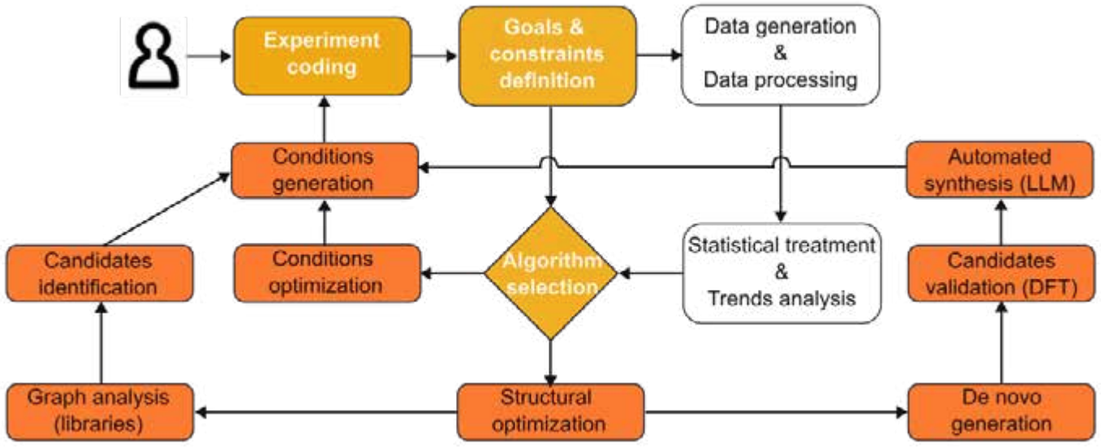



**Figure 20 :** Workflow of chemical conditions and structural optimization algorithms as currently developed and implemented in the Swiss Cat+ West Hub data architecture.

[37] Häse, F.; Roch, L. M.; Kreisbeck, C.; Aspuru-Guzik, A. Phoenics: A Bayesian Optimizer for Chemistry. ACS Cent. Sci. 2018. https://doi.org/10.1021/acscentsci.8b00307 | [38] Christensen, M.; Yunker, L. P. E.; Adedeji, F.; Häse, F.; Roch, L. M.; Gensch, T.; dos Passos Gomes, G.; Zepel, T.; Sigman, M. S.; Aspuru-Guzik, A.; Hein, J. E. Data-Science Driven Autonomous Process Optimization. Commun. Chem. 2021, 4 (1), 112 | [39] Ahneman, D. T.; Estrada, J. G.; Lin, S.; Dreher, S. D.; Doyle, A. G. Predicting Reaction Performance in C–N Cross-Coupling Using Machine Learning. Science 2018, 360 (6385), 186–190 | [40] Vaucher, A. C.; Schwaller, P.; Geluykens, J.; Nair, V. H.; Iuliano, A.; Laino, T. Inferring Experimental Procedures from Text-Based Representations of Chemical Reactions. Nat. Commun. 2021, 12 (1), 2573 | [41] Schwaller, P.; Vaucher, A. C.; Laplaza, R.; Bunne, C.; Krause, A.; Corminboeuf, C.; Laino, T. Machine Intelligence for Chemical Reaction Space. WIREs Comput. Mol. Sci. 2022, 12 (5)

To achieve the goal of a fully data-driven, autonomous laboratory, we first need to develop a fully automated laboratory. This presents several challenges, as the technology is not currently available on the scientific equipment market. In addition to the IT structure (see section 3.d), the several key hardware challenges we had to address were: 1. efficient solid sampling, 2. a global strategy for automated high-resolution NMR and optical spectrometry, and 3. automated sample handling and laboratory transfer.

**Efficient solid sampling - StoRMS**

Unlike automated sampling of liquids, which is well controlled, automated sampling of solids is complex. Solids can have many different shapes and characteristics (fluffy, sticky, waxy, electrostatic...). This makes it difficult to develop a universal sampling tool. The situation is even worse when it comes to micro sampling in the mg range. Here there is a major problem with the residual dead volume inside the sampling tool, which can easily be in the range of 10-20 mg. For rare catalysts, such a loss is simply unacceptable. Several of the existing tools also suffer from potential cross-contamination risks and all are slow (> 2 min/sample). This can be a serious limitation in terms of throughput, since in our case 300 reactors times 2-3 solids times 2 minutes results in up to 30 hours of plate preparation. For these reasons, we have started to develop an autonomous solid sampler that can be run in parallel with the synthesis to save time and that tries to overcome most of the drawbacks mentioned above.

In collaboration with Prof. M. Kunze of the HEIG-VD (Haute Ecole d'Ingénieur d'Yverdon, VD, Switzerland), we have developed and patented a new concept of stochastic robotic sampling called StoRMS (European Patent 2022 - F. de Nanteuil, E. Mariano, M. Kunz, P. Miéville, EPFL-HEIG-VD - Substance preparation method and system, 22215745.5EP). The central idea, which comes from the old days of chemistry when only mechanical balances were available, is not to aim for a specific mass but to use the natural variability of the robots to generate a precisely known distribution of masses and then to use the computer to recalculate the liquids to be added in the reactor. This makes sampling much faster as there is no need to target a specific mass. The solids sampling itself is carried out using a vacuum strategy developed and patented by the DEC Group SA (Ecublens, VD, Switzerland), which offers a high degree of versatility with regard to different types and shapes of solids and avoids cross-contamination, since the tubes used are disposable. Finally, the microsample is sealed in the glass tube using a laser, thanks to another patented development by Chemspeed Technology AG (SMOLE). The sealed microtubes containing the mass distribution are stored inertly until they are used in the synthesis. The compounds are released into the reactors by pressure burst or pin crushing. In autumn 2022, HEIG-VD,


**Figure 21 :** A robotized Bruker 400 MHz NEO NMR spectrometer equipped with a SampleJet autosampler. The six-axis robotic arm is a Universal Robot UR5e piloted through the laboratory scheduler and connected to the NMR with dedicated libraries.

**Figure 22 :** From left to right, the commercially available Agilent OmniFire. Then in the center we can see the CAD rendering (SolidWork) for the enhanced version of the original RapidFire from Agilent locally called OmniFire. It is designed to combine the initially existing high-throughput sample preparation and solvent management capabilities from the RapidFire with new NMR sample preparation and on-line optical spectroscopy. On the right, we can see the actual version of the OmniFire currently being finalized.

DEC, Chemspeed and Swiss Cat+ obtained an engineering Innosuisse grant (102.153 IP-ENG, 2023 - 2026, CHF 786,450) for the complete development of a functional and commercial version of the StoRMS solid sampling tool.

**A global strategy for automated high-resolution NMR and optical spectrometry**

We developed two different elements for this purpose. First, in collaboration with Bruker Swiss AG (Fällenden, ZH, Switzerland), we have robotized a 400 MHz NEO NMR spectrometer equipped with a SampleJet autosampler. The robotics is performed using Universal Robots (UR5e) connected via the Swiss Cat+ laboratory central scheduler and specially developed software libraries (Figure 21). A major challenge was to ensure the safety of the cryomagnet and not to interfere

Secondly, in collaboration with Agilent Technology (Santa Clara, CA, USA), we have transformed a high-throughput analytical sample preparation tool into a preparative LC collector combined with an NMR sample tube preparator (for use with robotic NMR) and a fully automated and on-line optical spectroscopy platform (FT-IR, UV-VIS) (Figure 22). In the context of this development, we have obtained a patent for the NMR tube sealing strategy using a 3D printer (2022 - K. Villat, P. Miéville, EPFL - Direct 3D printed seal for chemical containers 3D-CHEMSEAL, 0538B1001EP).

**Automated sample handling and laboratory transfer**

Whereas a certain degree of automation exists and is standard within the individual analytical instruments (autosamplers, auto-collectors, liquid handling) and preparative instruments (chemspeed platforms) , the options for sample transfer between instruments are extremely scarce. Conveyors are used in industry for this purpose. These are only optimal for long-term production workflows with very restricted flexibility. They also require significant ongoing maintenance to avoid jamming. Another option is the six-axis robotic platforms used by Cooper[42]. After an analysis, we concluded that this approach has serious and unacceptable safety issues, both for the human operators and for the scientific equipment. It is indeed complex to share the same space between humans and robots. Humans tend to generate trajectories that are difficult for robots to predict. Other major limitations of this approach are the large laboratory footprint, the cost (> 100 kCHF / robot) and the net

[42] Burger, B.; Maffettone, P. M.; Gusev, V. V.; Aitchison, C. M.; Bai, Y.; Wang, X.; Li, X.; Alston, B. M.; Li, B.; Clowes, R.; Rankin, N.; Harris, B.; Sprick, R. S.; Cooper, A. I. A Mobile Robotic Chemist. Nature 2020, 583 (7815), 237–241.

usable operational time considering the recharging time (up to 4h / day). To address these limitations, we have developed, in collaboration with Prof. J. Hugues (EPFL), a very efficient swarm of low-cost open-source (Arduino based, 3D printed) mini-robots designed around the samples to be transferred. These mini-robots move independently on a dedicated track on top of the instruments and are controlled by a drone-swarm algorithm (Figure 23). Samples are transferred from the mobile mini-robots (to the scientific instruments using static six-axis arms (Universal Robots, UR). The ensemble is controlled within the open-source ROS framework (https://www.ros.org) and directly linked to the Swiss Cat+ laboratory scheduler.

**Figure 23 :** Left, the dedicated track on top of the scientific equipment with the UR robots used to transfer the sample between the mini-robots and the equipment. On the right, an image of the actual 3D printed robot (25 cm diameter, 2 kg, < 1 kCHF / robot) with a standard 96 well SBS plate. The robot is located using an ultrasonic GPS (Marvelmind) and the robot is identified and precisely aligned using the QR code and a set of industrial cameras.

# e. Partnerships and collaborations.

As described in detail above, collaborations are of paramount importance in this project, as a significant part of the equipment and data structure has to be developed. Most of these collaborations are formalized by official agreements between Swiss Cat+, EPFL-TTO and the companies and institutions listed below. These collaborations are also the base for funding agreements (Innosuisse, ORD funds in preparation with SDSC, Bridge Discovery with IBM currently in evaluation). We will list below all the collaborations that have been established and are currently active.

## Swiss startups and SME industrial collaborations

**Microfluidics.**
Catalysis West Hub - Swiss Cat+ collaborates with Advanced Microfluidics SA (AMF) in the development of automated multiple fluidic and microfluidic applications. Notably, AMF is developing an automated low volume multiplexing fluidic system connecting online three reactors with a benchtop NMR, including online solid phase extraction (SPE) for deuterated solvent. This unique strategy allows the use of a single benchtop NMR spectrometer, in combination with an ATR-probe FT-IR spectrometer, to study the kinetic of up to six reactions in parallel in an automated manner.

**Automated synthesis and sample preparation platforms.**
Catalysis West Hub - Swiss Cat+ is collaborating with Chemspeed Technology AG in Füllinsdorf (Switzerland) on the development of an ensemble of automated synthesis platforms. In this context, Chemspeed is providing us with three adapted SWING XL modules, developing several new specialized tools and supporting us in the global IT integration of its platforms in the laboratory orchestration. Chemspeed is also helping us, in collaboration with HEIG-VD and the DEC Group, to develop a new micro-sampling system for solids as part of an Innosuisse project.

**Robotized microsampling and inert storage tools.**
Catalysis West Hub - Swiss Cat+ is collaborating with Dietrich Engineering Consultants SA (Dec group) in Ecublens (Switzerland) on the development of a complete solid micro-sampling system under inert conditions. In particular, DEC is developing an automated standardization platform to transfer commercial chemicals to gram scale standard flasks. DEC is also developing a unique solid micro-sampling system with HEIG-VD and Chemspeed as part of an Innosuisse project.

## Swiss based major industrial collaborations

**Robotized nuclear magnetic resonance, data analysis and laboratory scheduling .**
Catalysis West Hub – Swiss Cat+ collaborates closely with Bruker Switzerland AG, through an agreement signed with the support of our EPFL Tech Transfer Office (EPFL-TTO), The projects followed and executed in the context of this collaboration are, the development of an entirely automated high-resolution 400 MHz NMR setup using a Bruker SampleJetTM Autosampler for high sample throughput, the co-development of a strategy and adequate technology for a multiplexed benchtop NMR spectrometer setup allowing for the kinetic analysis of up to six parallel reactions and finally a concept definition for a centralized software control and rational data recovery for multiple instruments.

**ML - Foundation model development for automated structural elucidation.**
Catalysis West Hub - Swiss Cat+ is collaborating with IBM Research Europe GmbH in the development of a new generation of foundation model for automated structure elucidation. This development relies on both Swiss Cat+'s high-throughput analytical capabilities to generate a large controlled experimental dataset of spectroscopic information and IBM's extensive expertise in ML developments. This collaboration is currently the subject of a joint BRIDGE Discovery grant proposal.

## International industrial collaborations.

**Analytical instrument automation and central data management .**
Catalysis West Hub - Swiss Cat+ is collaborating with Agilent Technologies in the development of automated high-throughput analytical instruments (liquid and gas chromatography, mass spectrometers and liquid handlers) and in the development of a centralized data management strategy based on the Allotrope data format and prototypes of middlewares.

**Experiment encoding (HCI) and analytical data automated treatment.**
Catalysis West Hub – Swiss Cat+ collaborates strongly with Mestrelab Research in the development of a new way to support chemists to pilot our entirely automated laboratory. For this the two partners jointly develop the entry point of the Swiss Cat+ IT infrastructure through a new generation of chemistry software called Human-Computer-Interface (HCI). The HCI will become the interface between the chemist and the laboratory scheduler. In addition, the Mnova and Mgears software will be used as a base for the Data Processor needed to treat automatically the raw data and to export them into the open-access database.

## Swiss academic and institutional collaborations.

- **EPFL-SB-ISIC-LIAC:** Prof P. Schwaller – digital chemistry – generative algorithms
- **EPFL-STI-IGM-CREATE:** Prof J. Hugues – mobile robotics and sample transfer
- **HEIG-VD (CH):** Prof M. Kunze – laboratory automation (Innosuisse)
- **Swiss Data Science Center SDSC (ETH-Domain, CH):** IT and data structure, open research database ORD (see IT & data architecture)

# Publications and communications.

**Status on June 1st, 2023**

## Publications.

P. Laveille, P. Miéville, S. Chatterjee, E. Clerc, J.-C. Cousty, F. de Nanteuil, E. Lam, E. Mariano, A. Ramirez, U. Randrianarisoa, K. Villat, C. Copéret, N. Cramer, Chimia 2023, 77, 154, DOI: 10.2533/chimia.2023.154

A. Ramirez, Erwin Lam, Yuhui Hou, Loic Roch, Daniel Pacheco, Hermann Tribukait, Christophe Coperet, Paco Laveille, High-throughput and automated closed-loop AI-driven heterogeneous catalyst composition optimization for the conversion of $CO_2$ to methanol. in preparation

Edy Mariano, Jean-Charles Cousty, Florian de Nanteuil, Josie Hughes, Nicolai Cramer, Pascal Miéville, An open-source 2D drone-swarm for laboratory sample transfer, in preparation

Florian de Nanteuil, Jean-Charles Cousty, Edy Mariano, Nicolai Cramer, Pascal Miéville, A complete preparative chemistry laboratory automation concept, in preparation

## Patents

2022 - F. de Nanteuil, E. Mariano, M. Kunze, P.Miéville, EPFL-HEIG-VD, Substance preparation method and system, 22215745.5EP

2022 - K. Villat, P.Miéville, EPFL, Direct 3D printed seal for chemical containers 3D-CHEMSEAL, 0538B1001EP

## Conference and workshop participation

**2021:**

P. Miéville, Swiss Cat+ - An autonomous and automated platform for catalyst optimization and discovery, Idorsia, January 2021, online

P. Miéville, Swiss Cat+ - A new data-driven infrastructure for catalysis optimization and discovery, NCCR Marvel Industry sector Days , January 2021, online

P. Miéville, Swiss Cat+ - A new data-driven infrastructure for catalysis optimization and discovery, UNIBASEL - An Open Approach to Closed-Loop Experimentation workshop, June 2021, University of Basel, CH

P. Miéville, Swiss Cat+ , Une plateforme automatisée et pilotée par les données pour l'optimisation et la découverte de nouveaux catalyseurs, Journées scientifiques du CCCTA , Centre de compétence en chimie et toxicologie analytiques, September 2021, Les Diablerets

**2022:**

F. de Nanteuil, Swiss Cat+ An autonomous platform for the discovery of catalysis, Syngenta, February 2022, Basel, CH

F. de Nanteuil & P. Miéville, Swiss Cat+ @ EPFL Project status, Givaudan, June 2022, Geneva, CH

F. de Nanteuil & P. Miéville, Swiss Cat+ @ EPFL Project status, Roche, June 2022, Basel, CH

F. de Nanteuil, Swiss Cat+ @ EPFL Project status, Boehringer Ingelheim, July 2022, Mainz, D

P. Laveille, Swiss Cat+ East: ETHZ hub supporting data-driven automated and high-throughput catalytic materials R&D, Clariant Talent Program in Catalysis and Sustainable Chemistry, September 2022, Zurich, CH

P. Laveille, Swiss Cat+ East: ETHZ hub supporting data-driven automated and high-throughput catalytic materials R&D. Annual Digital Catalysis & Catalysis Related Sciences Conferences 2022 (ADRC22), September 2022, Frankfurt, D

P. Miéville, Swiss Cat+ @ EPFL Project status, Swiss Data Science Center SDSC, October 2022, Lausanne, CH

P. Miéville, Swiss Cat+ - A new data-driven infrastructure for catalysis optimization and discovery, Bristol University, talk and workshop animation about digital chemistry , November 2022, Bristol, UK

F. de Nanteuil, Swiss Cat+ - An Autonomous and Automated Platform for the Discovery and Optimization of Catalysis, HTE & lab automation conference - 20/15 Visioneers, November 2022, online

E. Mariano - A 2D-drone swarm system for sample transfer - EPFL Workshop on laboratory automation, December 2022 (poster and talk, best poster award), EPFL, CH

**2023:**

P. Miéville, F. de Nanteuil and J.-C. Cousty, Swiss Cat+ - A data-driven infrastructure for catalysis optimization and discovery, Agilent Research Center , January 2023, Waldbronn, D

P. Miéville, F. de Nanteuil and J.-C. Cousty, Swiss Cat+ - A data-driven infrastructure for catalysis optimization and discovery, IBM Research Center, January 2023, Zurich, CH

P. Miéville, Multidisciplinary challenges on the way to a fully autonomous chemistry laboratory at Swiss Cat+, Solvay Workshop - New ways to do chemistry - Emerging technologies for synthetic methodology, April 2023, Bruxelles, B

E. Mariano - A 2D-drone swarm system for sample transfer - Oxford Workshop Robot in Pharmaceutical Industry, April 2023, London, UK

P. Miéville and P. Laveile, Swiss Cat+, a Data-driven Autonomous Research Infrastructure for New Catalyst Discovery and Optimization, Swiss Chemical Society - Freiburger Symposium in Chemistry, April 2023, Freiburg, CH

Lam, E., Catalysis Hub - Swiss Cat+: A hub to support data-driven, automated and high-throughput catalysis R&D. Conference of Applied Surface Technology 2023 (COAST 2023), May 2023, Vienna, AT

P.Miéville, Storms and drones in a lab, Bristol Automated Synthesis Facility launching event, May 2023, Bristol, UK

Edy Mariano, A 2D-drone swarm system for sample transfer, Robotics-4-Labautomation Symposium, May 2023, Konstanz, D

Lam, E., Swiss Cat+ Case Study: ML driven high throughput optimization in heterogeneous catalysis. Future Labs Live 2023, June 2023, Basel, CH

P. Miéville, Swiss Cat+ A new generation of entirely automated and data-driven labs, Future Labs Live 2023, June 2023, Basel, CH

P. Laveille, ETHZ Catalysis Hub: A platform offering data-driven high-throughput experimentation, Inter-departmental Science Retreat "Life Science@ETH", June 2023, Zurich, CH

P. Miévile, What can we optimize in an automated lab ? Automatic Synthetic Forum, 27-28 November 2023, Novartis, Basel, CH

# Concluding remarks.


The ETH Domain Swiss Cat+ project is well on its way to establishing a state-of-the-art automated, high-throughput technology platform in the field of catalysis R&D. Combined with advanced computational data analysis, it aims to support users from academia and industry in accelerating catalyst discovery and understanding the chemistry that governs material performances.

Since 2021, both Hubs have built teams of scientific experts, prepared the laboratory infrastructure and acquired tools that allow the synthesis, characterization and performance evaluation of catalysts libraries in an automated ways. Several collaborations have been initiated with major suppliers of high-throughput/automated equipment, and also with academic research groups active in these fields. The positive feedbacks received so far from all stakeholders confirms the importance and potential of the project.

Furthermore, considering the ongoing research activities in catalysis and sustainable chemistry in Switzerland, there are many opportunities for the Swiss Cat+ to support the research landscape by providing such advanced tools and services. In particular, the Swiss Cat+ foresees a strong collaboration with the NCCR Catalysis, which funds research projects aiming at developing sustainable (catalytic) technologies and promoting the emergence of digital chemistry and data-driven discovery approach.

# Financial summary.

# Funding & Expenses 2021-2022.

| | in kCHF |
|---|---|
| **Funding** | |
| Funds granted by ETH Board | 18’900 |
| Funds by third party | 1’616 |
| **Total funding** | **20’516** |
| | |
| **Expenses by nature** | |
| Personnel expenses | 1’795 |
| Material expenses (excl. invest) | 201 |
| Matrix costs | 2’418 |
| Capital expenditures | 9’414 |
| Miscellaneous | 166 |
| **Total expenses by nature** | **13’994** |
| | |
| **Expenses by institution** | |
| East Hub ETHZ | 7’241 |
| West Hub EPFL | 6’753 |
| **Total expenses by institution** | **13’994** |



# Funding & Expenses forecast 31.12.2024.

| | | in kCHF |
|---|---|---|
| **Funding** | **Forecast** | **Budget** |
| Funds granted by ETH Board | 25’030 | 25’030 |
| Funds by third party | 3’848 | 7’650 |
| **Total funding** | **28’878** | **32’680** |
| | | |
| **Expenses by nature** | | |
| Personnel expenses | 4’815 | 3’040 |
| Material expenses (excl. invest) | 1’320 | 3’680 |
| Matrix costs (other costs) | 3’299 | 5’760 |
| Capital expenditures | 19’100 | 20’200 |
| Miscellaneous | 344 | |
| **Total expenses by nature** | **28’878** | **32’680** |
| | | |
| **Expenses by institution** | | |
| East Hub ETHZ | 14’100 | 16’340 |
| West Hub EPFL | 14’778 | 16’340 |
| **Total expenses by institution** | **28’878** | **32’680** |