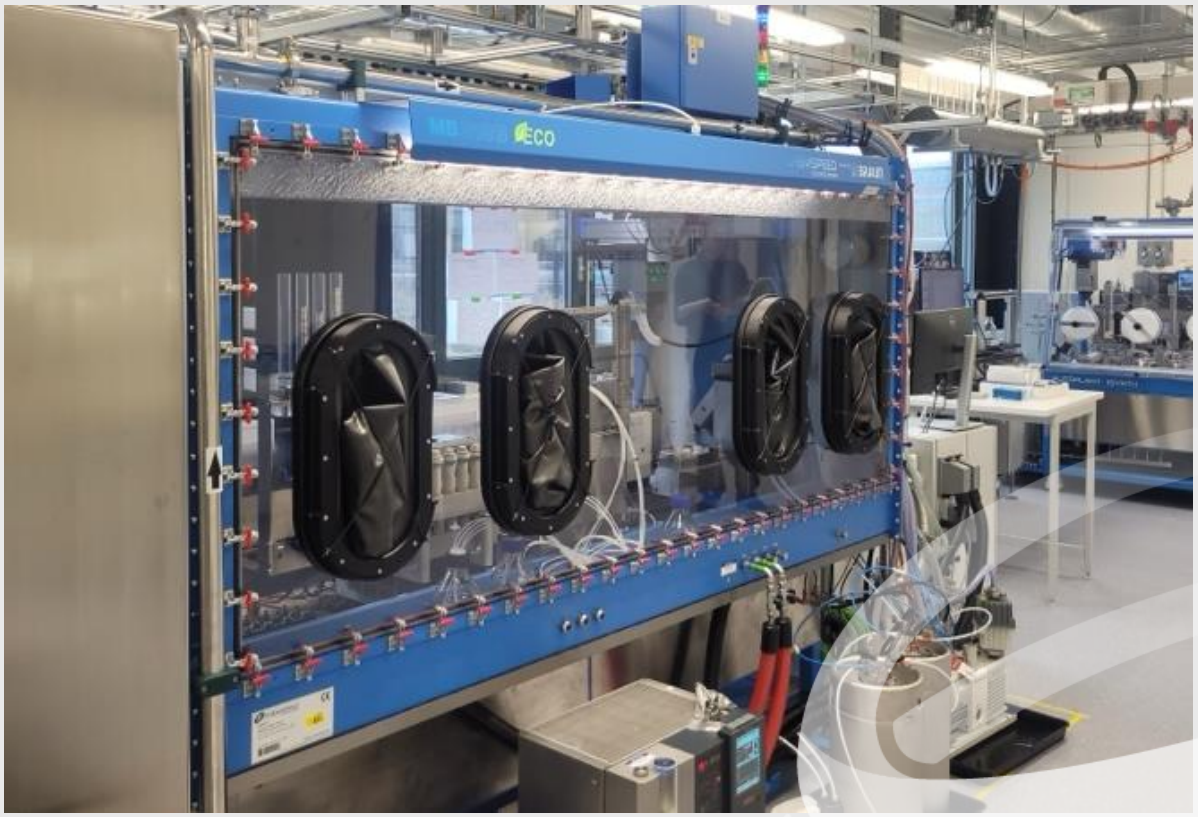
techvolver

Discovering new catalysts

The Swiss Cat+ project aims at developing a fully automated and digitized chemical laboratory dedicated to the discovery and optimization of new catalysts.



Interview with Pascal Miéville,
Executive Director Swiss Cat+ EPFL Lausanne

What is your role in the Swiss Cat+ project?

West hub executive director at EPFL Lausanne. The Swiss Cat+ West hub has a specific focus on homogeneous catalysis. The Swiss Cat+ project is a national research infrastructure shared with the East hub at ETHZ in Zürich. This second hub has a focus on heterogeneous.

The starting point is an automated, data-driven, and high-throughput infrastructure dedicated to discovering and optimizing new catalysts for chemistry. To cover a sufficient chemical space to identify interesting new molecules, you need a robotized system, that is fast and reliable. This last point is essential to generate high quality data, that can then be used to train the algorithms and to improve the input inside the system.

Having this combination of automation and algorithmics allows us target closed-loop optimization strategies. Indeed, the automated systems on the platform are used to feed the algorithms better and then generate predictions that are reinjected into the system at every iteration.

Where did the idea for the project come from?

Back in 2016 two catalytic scientists, Professor Cramer from EPFL and professor Copéret from ETHZ, they are still on board in the steering committee. The idea was to improve the domain of catalysis using automation and optimization algorithms. When they got the funding from the Swiss government, they asked me to join as a specialist in automation of lab instrumentation. We formally started in 2021 – with a first round of 4 years. Now we are in the process of extending the project running from 2025 to 2028.

How does the delivery from Techvolver tap into this global project?

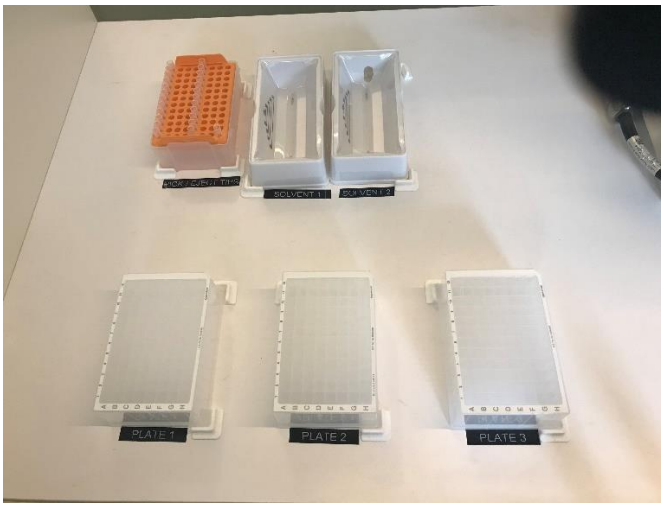
What exists to today in automated chemistry are ‘automated stations’, so in analytical and synthetic chemistry, you can buy equipment that have an internal automation that makes very systematized series of operations – for instance: injection of some samples into a HPLC to measure its content. This is very well developed.

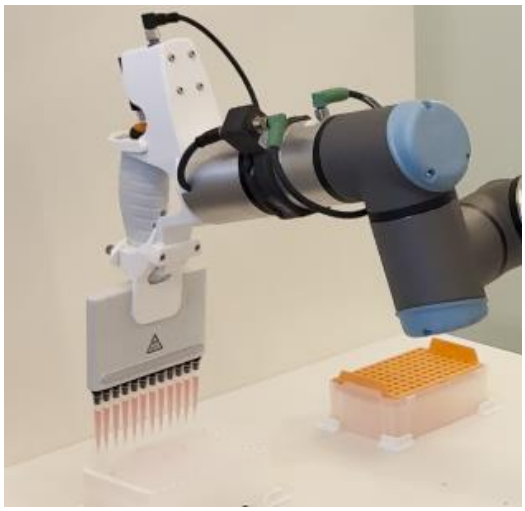
To the opposite to these locally automated stations strategy, is the Cooper Robot-Chemist model that was developed in the UK: he programmed a mobile platform with arms on it, mimicking what human operators are doing over a complete laboratory.

What is presently not well developed – or only very primitively - in terms of general lab automation, is the long-distance sample transfer between stations in a combination of a long range transfer system with local versatile tools allowing both for local sample transfer and sample processing. Tools that are not only designed for specific operations, but that can be easily reprogrammed for variable operations and different types of samples.

So, what the Techvolver solution brings using the UR robots is this kind of flexibility that we are looking for. Considering this, we will add your system to existing locally robotized stations to multiply the capability by introducing this expected flexibility.

With this, a single Universal Robot six-arm can, depending on the gripper, either transfer sample plates or pipet directly liquids into the plate. Thanks to your tool, we can adapt to many kinds of plates and solvents and design flexible workflows that can easily be encoded as CSV files.





To summarize, a lot of flexibility and adaptability to our robotics workflows, that is for me really a large PLUS and it is quite new.

How will the project be launched?

After now three years of development, the plan is to open service operations in autumn 2024 in parallel with a continuous development of our automation and algorithmic capabilities. The second funding round that is currently in discussion, will enable us to push automation much further and also to push the development of some complementary elements and we would like to discuss with you later on this.

Also, internally at EPFL, we are supporting other automation projects and teach lab automation to Master chemistry students. We become progressively a lab automation general resource and support different types of lab automation projects.

Who will benefit from the project in the short and long term?

Let us split the answer in two parts. First, we should consider the catalysis aspect. 35% of the global GDP is based on catalytical processes. Catalysis is the base for new energies. With the global warming, we need to find ways to generate hydrogen at a lower cost, to transform CO_2 into fuels or to feed chemical industry with non-petrobased starting materials.

On the more specific aspect of homogeneous catalysis, we must mention the active domain of asymmetrical catalysis, initiated by the 2021 Nobel Chemistry prize winner Mc Milan, where specific conformations of molecules are generated. This is used for ex. to develop more effective drugs with less side effects. Generally speaking, homogenous catalysis is largely used by pharma companies and fine chemicals companies as they are used to perform specific chemical transformations that are not possible without catalysts.

For the second part, the lab automation that we develop, is also interesting for both academies to increase the throughput of laboratories, generate higher quality data, and for companies that are working on optimizing lab workflows. Several solutions based on our work are already being implemented in the industry today.