

## **Combining HTE and Data Science to Optimize Chemical Processes**

**Prof Philippe Schwaller**, Raphael Bigler

**Laboratory of Artificial Chemical Intelligence** | LIAC - Institute of Chemical Sciences and Engineering -  
School of Basic Sciences - École Polytechnique Fédérale Lausanne EPFL

We present initial results from the collaboration between Roche's High-Throughput Experimentation (HTE) team in Process Chemistry and the Laboratory of Artificial Chemical Intelligence (LIAC) at EPFL. We will showcase the setup of our cutting-edge HTE facility and demonstrate how we improve traditional screening strategies using advanced data science tools. This synergy has led to the development of Minerva, an ML optimization workflow that effectively covers large chemical search spaces, resulting in more informative and enhanced screening designs.