A Cloud-based AI-driven Autonomous Lab

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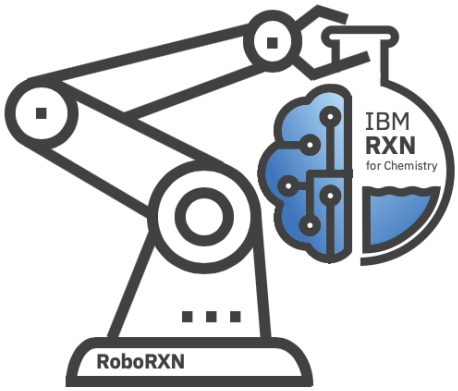
Designing and making new molecules is one of the most impactful outcomes of chemistry. The use of domain knowledge accumulated over multiple decades of laboratory experience, has been a crucial element for the synthesis of many new molecular structures. Still, most synthetic success stories are accompanied by long hours of unsuccessful exploration. No more than 20 years ago, automation systems were designed to support chemists in repetitive laboratory tasks. While this proved very effective in a few areas, such as high-throughput chemistry, the use of automation for general purpose tasks remains an incredible challenge even today. It requires chemistry operators to write different software for different tasks, each codifying a specific and different type of chemistry. Meanwhile, Artificial Intelligence (AI) has emerged as a valuable complement to human knowledge and creativity in organic chemistry - for tasks like predicting chemical reactions [1-2], retrosynthetic routes [3] or for digitizing chemical literature [4]. Here, we present the first implementation of a cloud-based AI-driven autonomous laboratory.



The remote laboratory is made accessible to chemists through the cloud and is equipped with automation technologies. The AI assists remote chemists with several tasks: designing retrosynthetic trees and suggesting the correct sequence of operational actions (reaction conditions and procedures), or ingesting literature on synthetic procedures to convert them into an executable program. Following supervision by synthetic chemists, the AI self-programs the automation layer and makes decisions on the synthesis execution using feedback loops from analytical chemistry instruments. I will present the platform architecture and its performance across various classes of synthetic tasks.

[1] IBM Research Europe, ***Chem. Sci.***, 2018, **9**, 6091-6098
[2] IBM Research Europe, ***ACS Cent. Sci.*** 2019, 5, **9**, 1572-1583
[3] IBM Research Europe, ***Chem. Sci.***, 2020, **11**, 3316-3325
[4] IBM Research Europe, ***Nat. Comm.***, accepted (https://doi.org/10.26434/chemrxiv.11448177)
[5] https://rxn.res.ibm.com