Cloud-based AI-driven Autonomous Lab

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The process of synthesizing novel compounds involves multiple steps including 1) suggesting an adequate synthetic route, 2) specifying reaction conditions and parameters for each reaction step, and 3) executing the synthesis in the laboratory. Typically, these steps are guided by the knowledge and experience matured by chemists in decades of practice. Still, they remain complex and time-consuming.

Automation systems have helped to reduce this problem. While these technologies have demonstrated exceptional efficacy in a select fields, such as high-throughput chemistry, automating general-purpose jobs remains an extremely complex issue even today. It requires chemical operators to develop unique software for various operations, each of which codifies a distinct sort of chemistry. Meanwhile, Artificial Intelligence (AI) has established itself as a valuable complement to human knowledge and creativity in organic chemistry, performing tasks such as predicting chemical reactions [1-2], retrosynthetic routes [3], digitizing chemical literature [4], and predicting experimental procedures for previously unseen chemical reactions [5].

Our group has implemented the first cloud-based AI-powered autonomous laboratory. It is made accessible to chemists through the cloud [6] 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 for the synthesis execution. I will present the platform architecture and demonstrate it with the live synthesis of a compound.

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