Optimization of Chemical Reactions on a Robotic-Flow Platform Guided by decision-making algorithms

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Flow chemistry has attracted significant interest in recent years for the synthesis of small molecules. This technological tool is now highly regarded in R&D because it enhances operator safety, facilitates scale-up, and allows access to chemistry that is impossible using conventional approaches. Additionally, flow chemistry is particularly well-suited for the automation and digitalization of processes according to the principles of digital Chemistry. The integration of advanced analytical tools with flow reactors enables the rapid, and even real-time, acquisition of analytical data. This data can subsequently be used by AI-based algorithms for process optimization, accelerating processes, and achieving a better understanding of chemical phenomena (such as the observation of intermediates and the measurement of kinetics).

In this frame, we recently developed several optimization strategies for self-optimizing flow reactors. Our approaches, which includes automated sampling, statistical analysis, and black box optimization, are coupled with an automated micromole scale flow platform to perform complex optimizations with limited chemical expense and minimal human intervention. The efficiency of our strategies was demonstrated in both in-silico and real-world examples. Successful scaling experiments demonstrated the transferability from the micromole scale flow platform to a standard flow chemistry reactor.

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