

OPTIMIZATION OF CHEMICAL REACTIONS ON A ROBOTIC-FLOW PLATFORM GUIDED BY ARTIFICIAL INTELLIGENCE

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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 Chemistry 4.0. 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, our research aims at transforming the efficiency of AI-assisted chemical reaction optimization by i/ requiring fewer experiments, ii/ delivering faster results and iii/ acquiring better-quality data. In this frame our guiding principle is: Fewer, Faster and Better".

Our methods will make AI-assisted optimisation (of yield, productivity, cost...) more broadly accessible and applicable for synthetic and process chemists of all backgrounds.



Reference(s)

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