Title

Optimization of Chemical Reactions on a Robotic-Flow Platform Guided by Artificial Intelligence

Biosketch

François-Xavier Felpin was born in France. After earning his Ph.D. at the University of Nantes (France), he pursued postdoctoral studies at The Ohio State University (USA). He began his academic career at the University of Bordeaux as an Assistant Professor. In fall 2011 he moved to the University of Nantes where he was promoted full Professor. Prof. Felpin was a junior member of the Institut Universitaire de France (2012-2017). His research interests include catalysis, material chemistry and automated flow chemistry.

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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, we recently developed a simple and comprehensive optimization strategy for self-optimizing flow reactors. Our approach, which includes automated sampling, statistical analysis, and black box optimization, is coupled with an automated micromole scale flow platform to perform complex optimizations with limited chemical expense and minimal human intervention. The efficiency of our strategy was demonstrated with the development of ultra-fast, sustainable and mild formal cycloadditions [3 + 3] that usually require in batch prolonged reaction times and/or high temperatures. Successful scaling experiments demonstrated the transferability from the micromole scale flow platform to a standard flow chemistry reactor.

Recent references

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