Coupling of a benchtop NMR spectrometer to a flow reactor for a fast optimization of hydrogenation reactions

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The synergy between continuous flow reactors and benchtop Nuclear Magnetic Resonance (NMR) spectroscopy has attracted significant attention in recent years due to its transformative impact on chemical synthesis and analysis. Continuous flow reactors offer distinct advantages, including precise control over reaction parameters, enhanced safety, and improved reaction efficiency. Conversely, benchtop NMR spectroscopy provides non-destructive, quantitative insights into reaction kinetics, intermediates, and final products. This integration enables real-time monitoring of the conversion as a function of the reactor parameters, facilitating rapid and even automated reaction optimization. The benefits of this hybrid approach are evident in the accelerated processes of reaction discovery and optimization. Researchers can utilize real-time NMR data to make on-the-fly adjustments to reaction conditions, resulting in enhanced yields and selectivity. Furthermore, in-line analysis reduces the need for laborious sample preparation and offline analysis, thus streamlining workflows and minimizing waste.

In this presentation, we will discuss the significance of effective solvent suppression, which, when combined with an external hardware lock, allows for measurements without the necessity of deuterated solvents. Additionally, we will explore typical setups for reaction monitoring and how solvent suppression techniques can be implemented online, using the example of coupling an H-Cube flow reactor with a Spinsolve benchtop NMR for the rapid optimization of hydrogenation reactions.