

## InsightXpress™

### ● Very Fast Reaction Monitoring and Optimization

Process understanding and optimization either with DoE or kinetic modelling, QbD assessments of API reaction conditions, kinetic repeatability studies... Have you thought about using NMR? Due to its quantitative nature and the unparalleled structural information that it provides, solves your problem quicker and with higher confidence.

Bruker's new InsightXpress is a stopped-flow solution for monitoring reactions by NMR. It enables the screening of many reaction conditions in a short period of time, dramatically increasing your productivity. Even laborious and time consuming kinetic studies that once were conducted by standard NMR tube procedure are now rapidly screened.

... and what about understanding fast reactions? InsightXpress is again the solution! InsightXpress combines very fast sample/reaction delivery with the analytical power of NMR. Insights into the mechanism and kinetics of fast chemical reactions, not understood so far, is now at your fingertips!

#### Your Benefits

- Reaction understanding - unique insights into the mechanisms of chemical reactions
- Direct quantitative and detailed structural information from only one single analytical technique
- Unprecedented speed to monitoring the fast depletion of reagents with half-life of less than 1 s!
- Rapid screening of reaction conditions
- Automatic experiment set-up even in fully protonated solvents

## Key Features

- Used when needed, seats on SampleXpress base (compatible with open access system)
- Rapid and easy set-up
- Low sample volumes (600  $\mu$ L/shot)
- Unlimited shots
- Variable ratios of reagents to explore different reaction conditions
- Accurate temperature control (allows detailed kinetics studies)
- Pre-magnetization volume for 3 different reagents (precise quantitative information)
- Precise timing using a trigger pulse
- Reproducible with stable measured volume
- Dead-time less than 150 ms, enabling the monitoring of fast reactions
- Fast flow-rate injection (0.2 – 2 ml/s)
- In-situ cleaning using dedicated solvent flush line
- Compatible with all Bruker 5 mm Probes
- Easy automatic optimization of NMR parameter
- Intuitive software for data acquisition and analysis



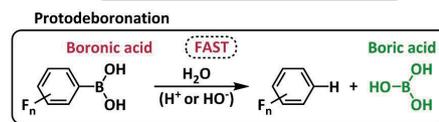
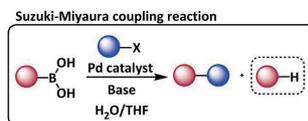
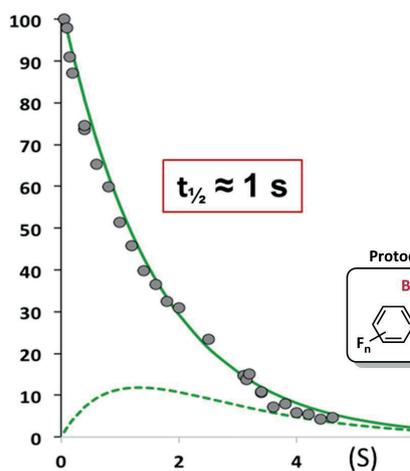
InsightXpress is a stopped-flow solution consisting of a pumping unit, a temperature controlled transfer line, a flow tube and software. The system is designed for seamless set-up in Bruker high-resolution NMR spectrometers with shielded magnets (300-700 MHz). Bruker's InsignMR™ software makes acquisition and analysis straightforward. It now has new functionality to enable the monitoring of very fast reactions.

### Optimizing the Suzuki-Miyaura Coupling

Suzuki-Miyaura couplings are among the most utilized reactions in organic chemistry, particularly in the pharmaceutical industry. However the reaction and side reactions are not yet well understood.

InsightXpress allowed Professor Lloyd-Jones and co-workers to gather insights into the reaction mechanism of very fast protodeboronation, Suzuki-Miyaura side reaction. (1,2).

Using InsightXpress they were able to monitor the decay of a reagent with half-life time of about one second. They monitor the reaction at different conditions of concentration, pH and temperature (0-70°C).



1) Cox PA, Reid M, Leach AG, Campbell AD, King EJ, Lloyd-Jones GC, *J Am Chem Soc*, in Press, DOI: 10.1021/jacs.7b07444

2) Cox PA, Reid M, Leach AG, Campbell AD, Lloyd-Jones GC, *J Am Chem Soc*, 138, 9145-57 (2016)