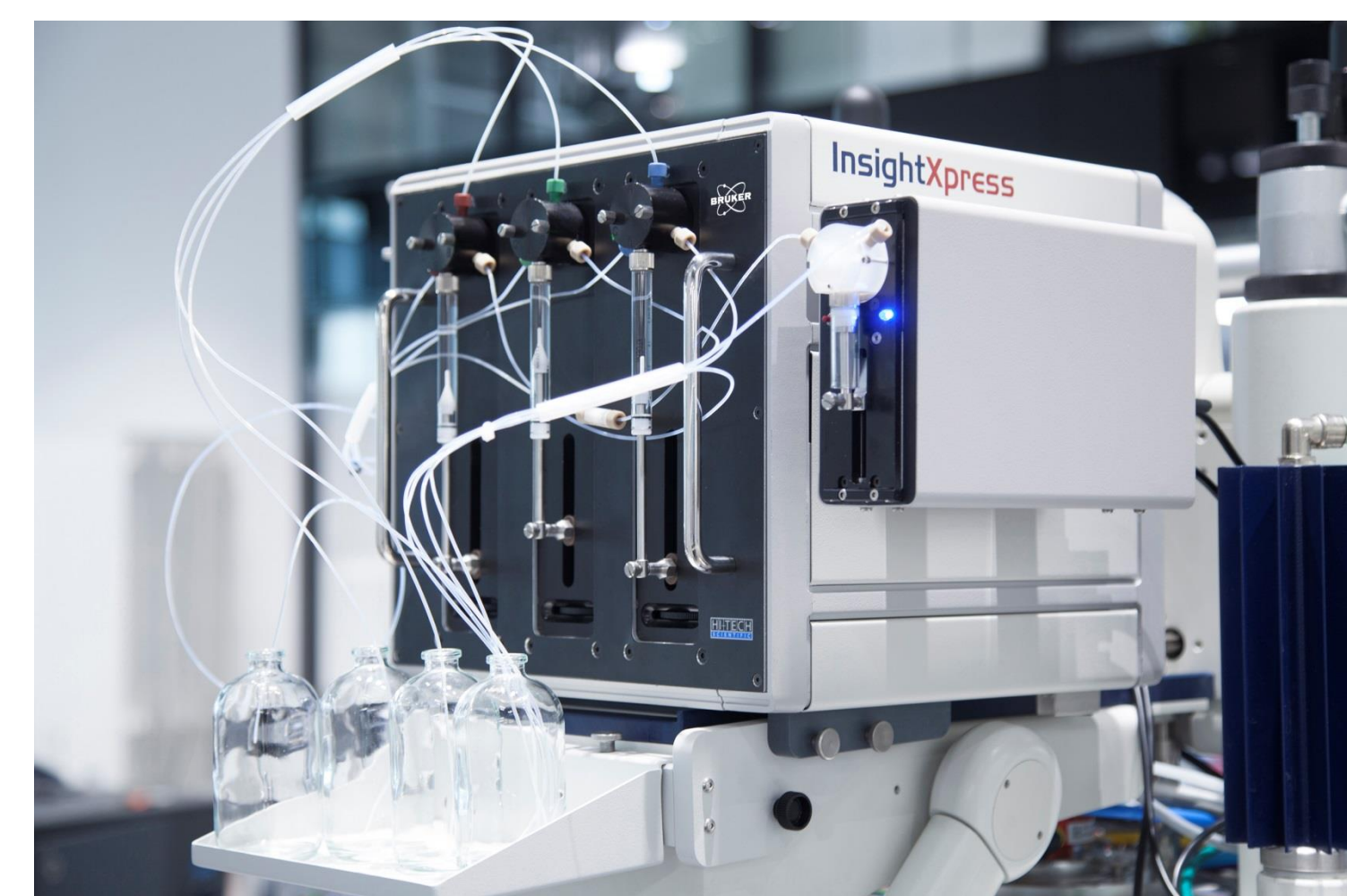


Easy monitoring of fast reactions and rapid exploration of different reaction conditions

InsightXpress™ is a stop-flow solution with rapid mixing to monitor very fast reactions by NMR. Another application of InsightXpress™ is reaction optimization. Monitoring different reaction conditions can be labor intensive and time consuming. InsightXpress™ with the use of small reagent volumes, fast injection and easy direct customization of settings (e.g. changing concentration, stoichiometry and/or temperature) provides a simple and time efficient solution.



Technical Detail

InsightXpress™ sits on top of the NMR system*. The flow-tube, connected to its transfer line is inserted into the magnet until it reaches the probe.

The pumps can be prepared for delivery before the acquisition with a few mouse clicks.

InsightMR™ software is now

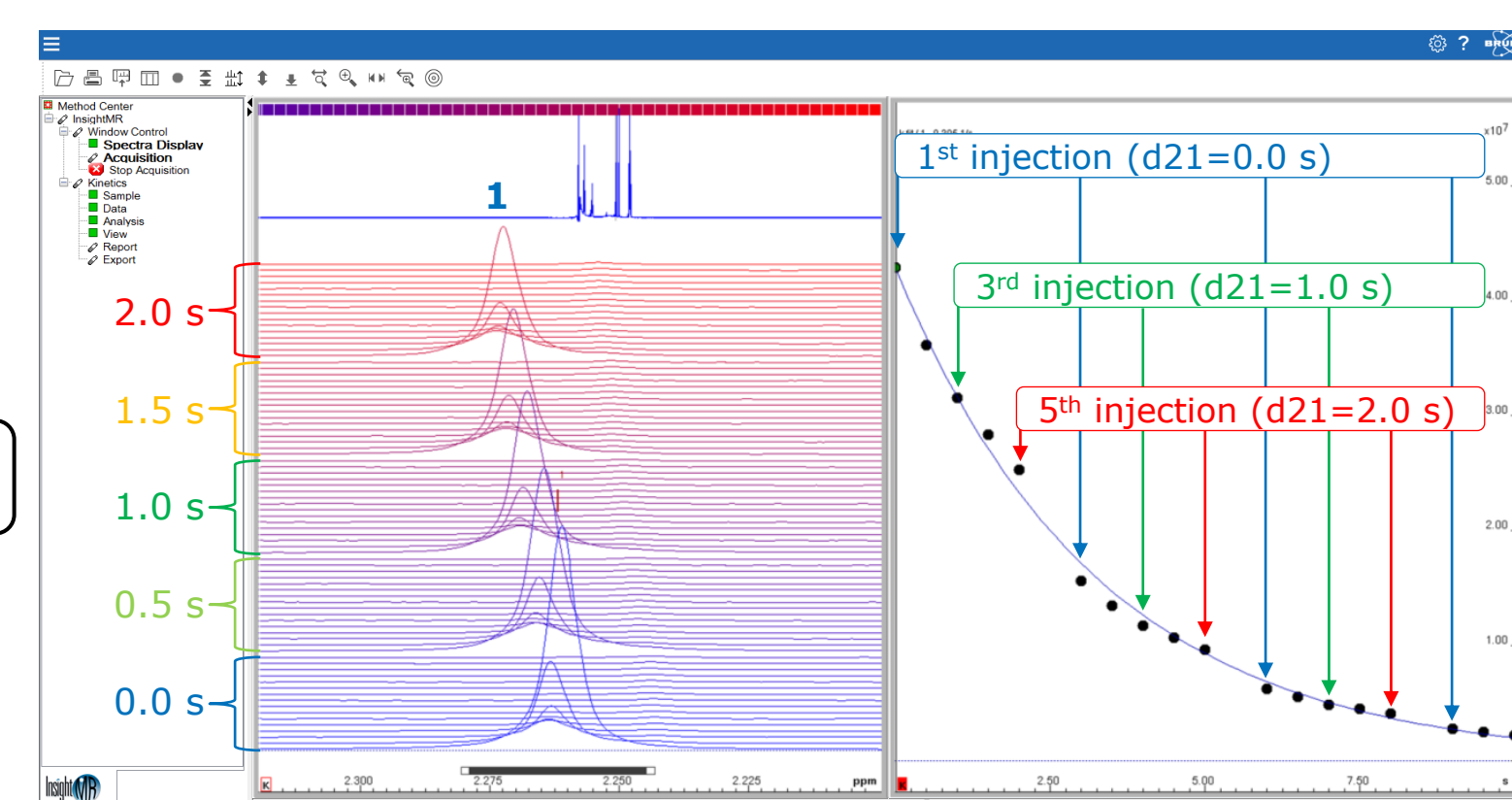
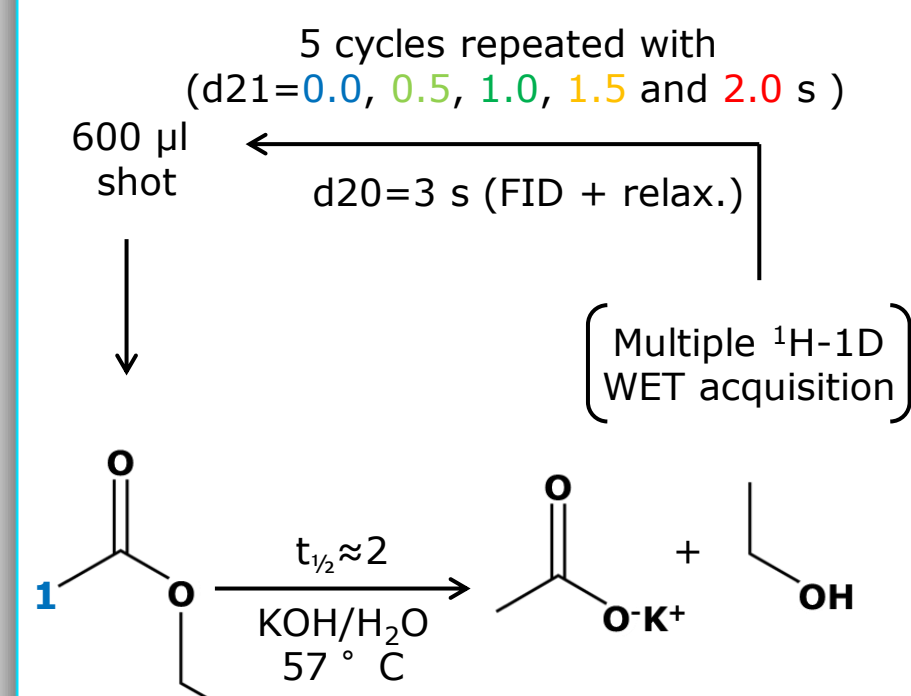
equipped with preparation experiments to automatically optimize NMR acquisition (e.g. solvent suppression and shimming). The injection of reagents and the start of the NMR acquisition is co-ordinated by a trigger pulse.



InsightXpress™ Case Studies

During the acquisition of the kinetic profile, the minimum delay between data points is limited to the NMR acquisition time + relaxation delay (d20). In order to monitor very fast reactions (e.g. $t_{1/2} \approx 2$ s) and reduce this limit, multiple injections with a variable incremented first point delays (d21) is possible.

Fast hydrolysis reaction



InsightMR™ software showed on the left the methyl peak region of the reagent. On the left side of spectra the incremented d21 delay used for each injection. On the right, the zoom of the first part of the proton kinetic profile.

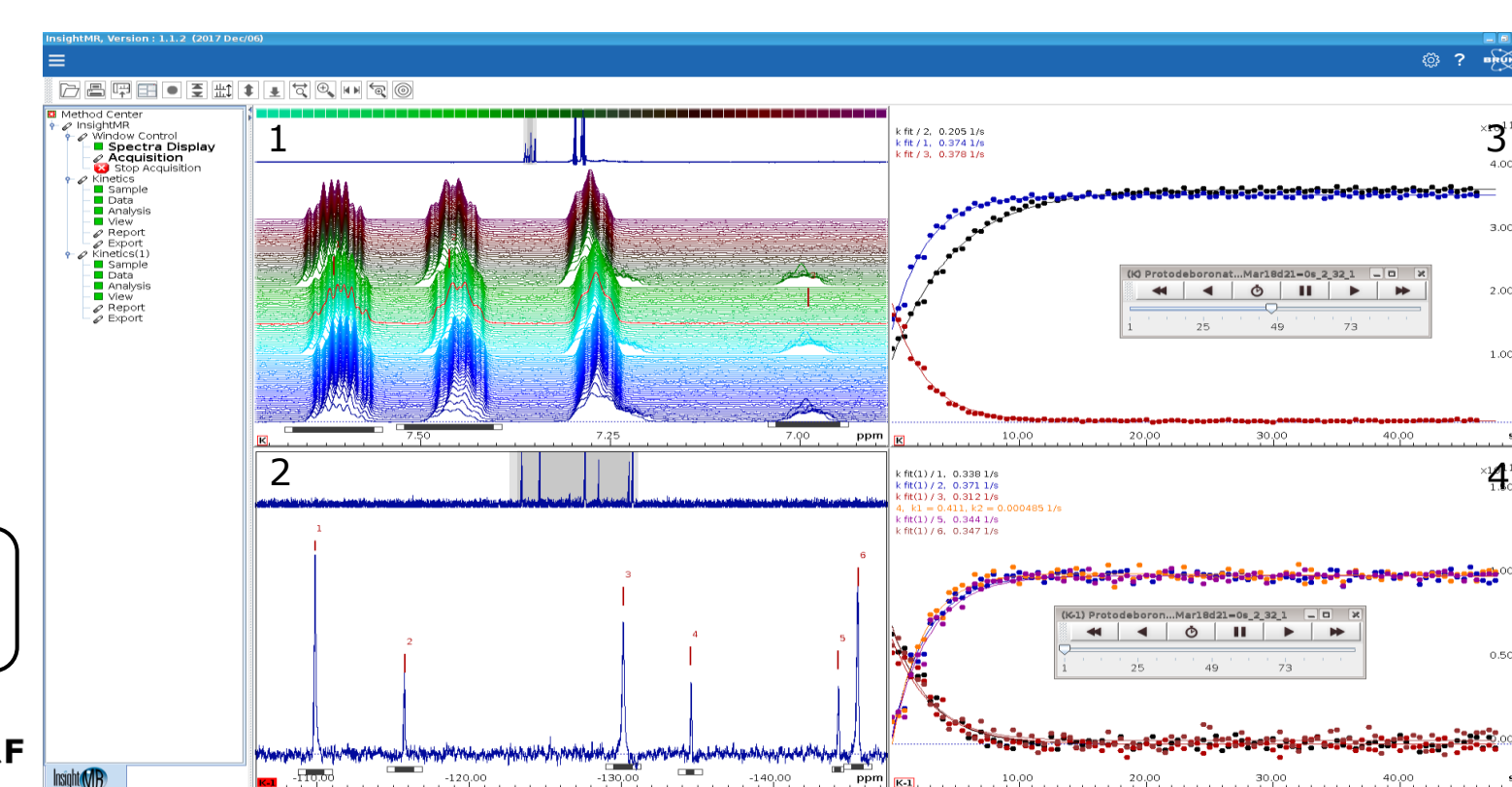
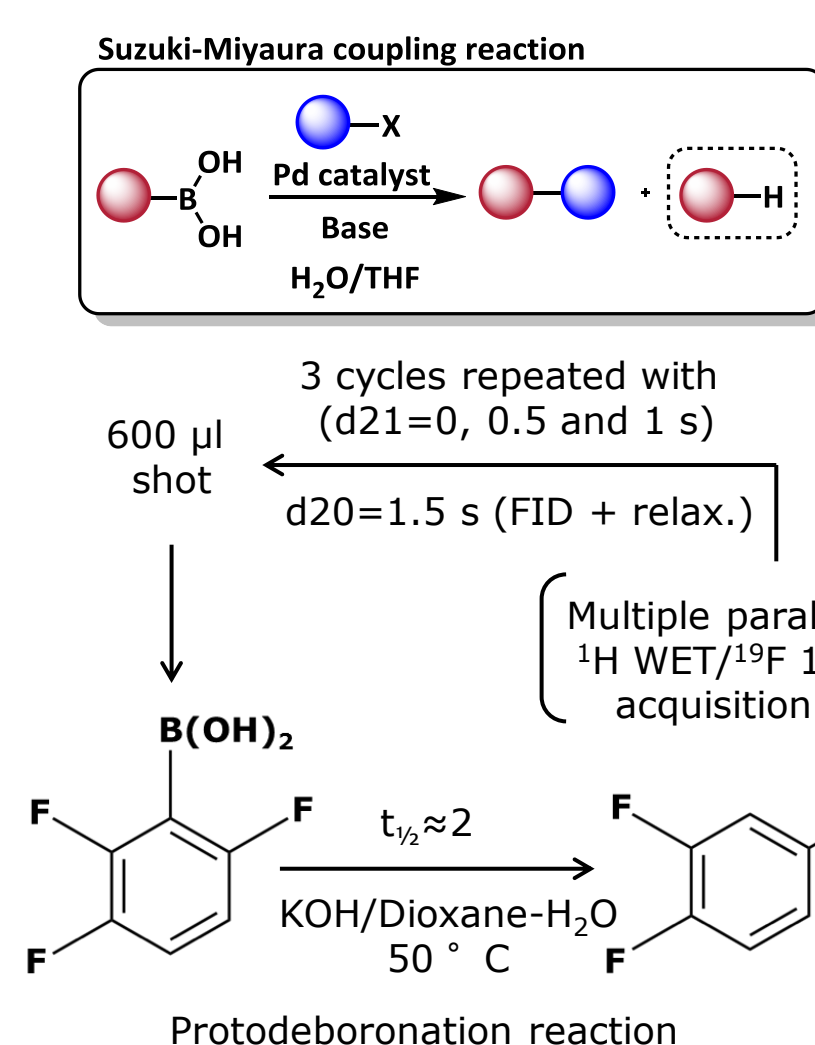
Features at a Glance

- Used when needed
 - Simple install
 - Low sample volume
 - Time efficiency
 - Variable ratios
 - Temperature control
 - Pre-magnetisation
 - Precise timing
 - Reproducible
 - fast reactions
 - In-situ clean
- seats on SampleXpress base
 - 10-15 minutes
 - $a+b+c \leq 600$ μ L / shot
 - unlimited shots
 - explore kinetics
 - detailed kinetics
 - quantitative data
 - triggered pulse trains
 - stable measured volume
 - <150 ms dead-time
 - solvent flush line

*Independent stand for InsightXpress™ is in development for compatibility with all sample changers.

Understanding the Suzuki-Miyaura coupling reaction using parallel acquisition and InsightXpress™

This reaction is one of the most popular in pharmaceutical industry. Using InsightXpress™ it was possible to study the very fast protodeboronation side reaction.



InsightMR™ software was used to monitor the protodeboronation reaction. Parallel receivers (default with Avance NEO technology) allow the acquisition of simultaneous ^1H and ^{19}F NMR experiments. Screenshot of the software showing a waterfall plot with all the ^1H spectra (1), a single ^{19}F spectrum (2) and ^1H and ^{19}F NMR kinetic profiles (3 and 4 respectively).

Summary

- Stop-flow monitoring of very fast reactions
- Rapid screening of different reaction conditions (e.g. temperature, concentration and stoichiometry)
- Compatible with all Bruker 5 mm RT- and CryoProbes and shielded magnets
- Straightforward data acquisition and analysis with InsightMR™ software