

# Spinsolve Multi X<sup>n</sup>

The next Generation of fully automated multi-nuclear NMR

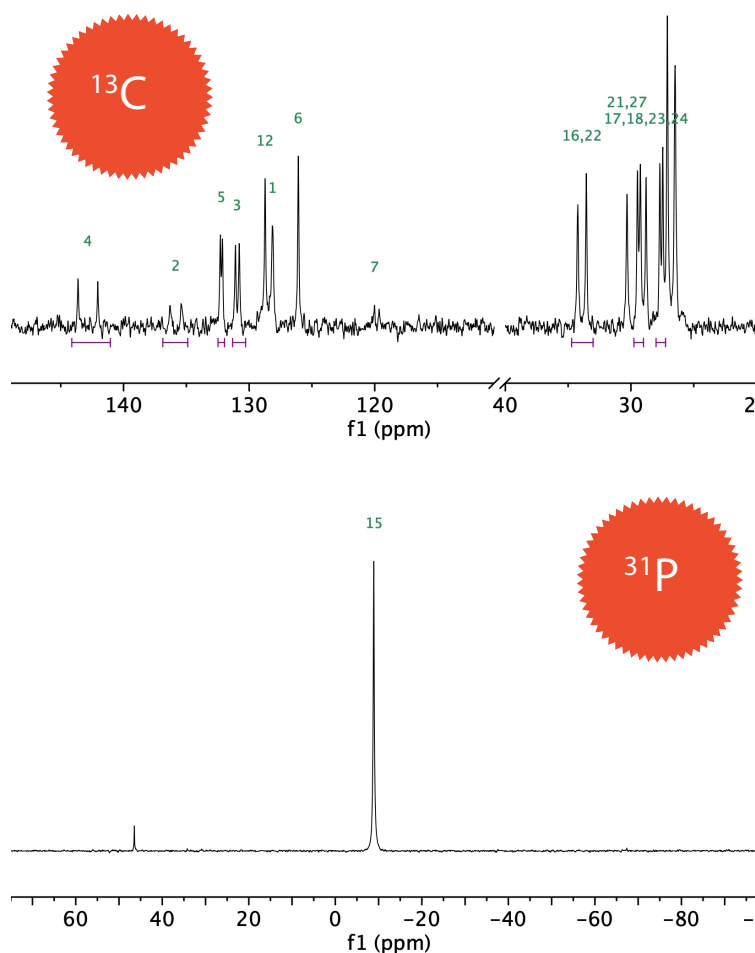
Measure all the nuclei you need with one NMR spectrometer in a fully automatic way



## Benefits of the Multi X<sup>n</sup> Probe

- Configure the system with unlimited number of nuclei
- Instant switching between nuclei without any loss in sensitivity
- No manual intervention required for switching nuclei
- Works with optional autosampler so all available nuclei can be acquired unattended
- Interleave multinuclear experiments for online reaction monitoring
- 1D and 2D experiments calibrated at factory, switch back and forth without recalibration
- No training requirement for operator

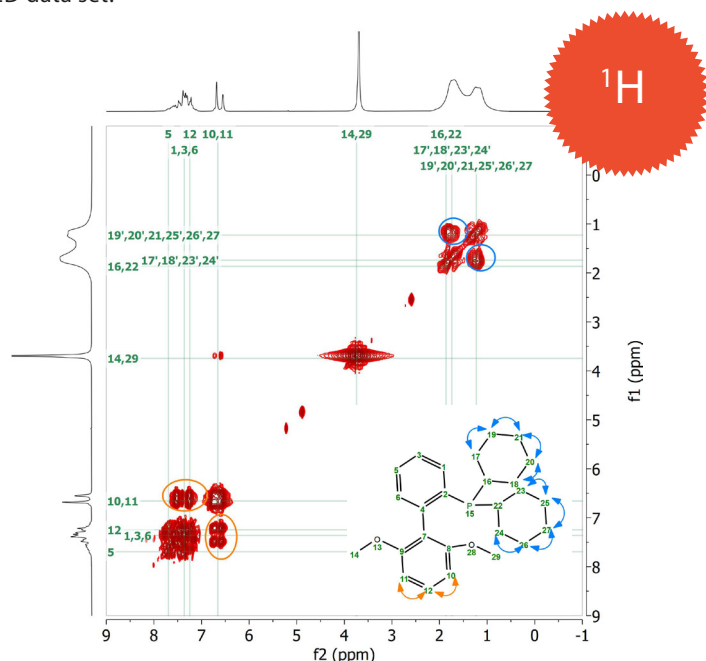
## <sup>13</sup>C and <sup>31</sup>P measured in a Spinsolve Multi X<sup>n</sup>



## Extensive software library of pre-calibrated protocols for all available nuclei

### 2D COSY

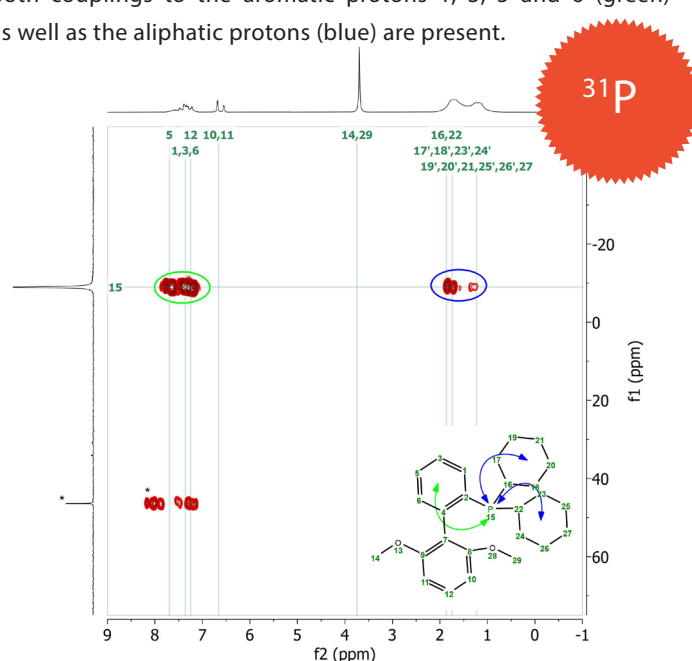
The 2D COSY experiment allows one to identify coupled  $^1\text{H}$  nuclei as they generate cross peaks out of the diagonal of the 2D data set.



$^1\text{H}$  2D COSY experiment of a 800 mM SPHOS sample in  $\text{CDCl}_3$  acquired on a Spinsolve Multi X 60 MHz system.

### 2D $^{31}\text{P}$ -HMBC

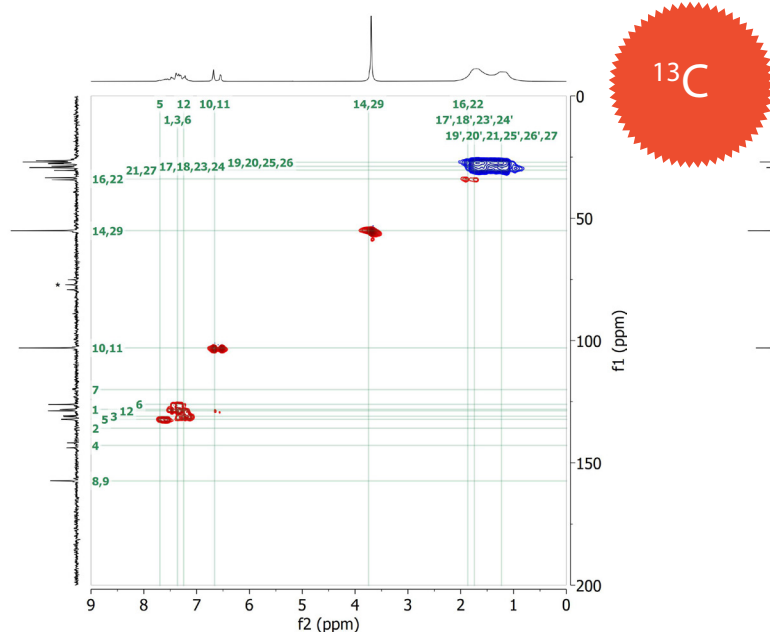
The long-range  $^1\text{H}$ - $^{31}\text{P}$  correlations can be observed for the phosphorus atom at position 15. It can clearly be seen that both couplings to the aromatic protons 1, 3, 5 and 6 (green) as well as the aliphatic protons (blue) are present.



$^{31}\text{P}$ -HMBC NMR spectrum of a 800 mM SPHOS sample in  $\text{CDCl}_3$  showing the long-range couplings between  $^1\text{H}$  and  $^{31}\text{P}$  nuclei.

### 2D HSQC-ME

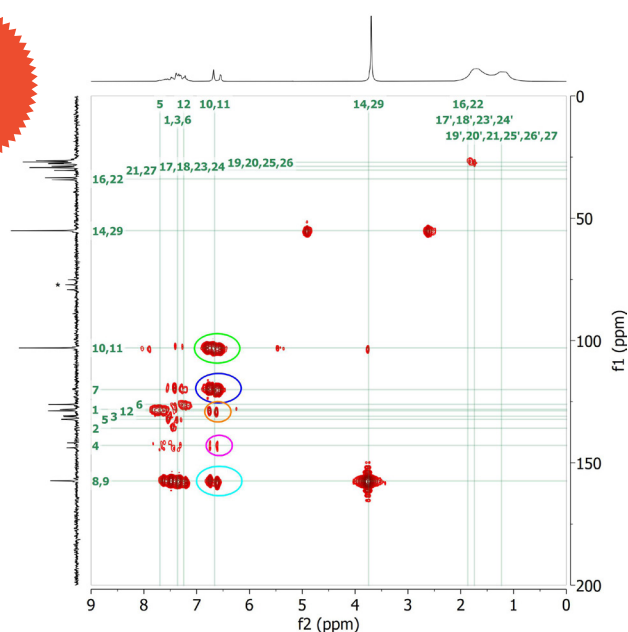
The HSQC is a powerful sequence widely used to correlate the  $^1\text{H}$  with the one-bond coupled  $^{13}\text{C}$  nuclei.



HSQC-ME spectrum of a 800 mM SPHOS sample in  $\text{CDCl}_3$  showing the correlation between the  $^1\text{H}$  (horizontal) and  $^{13}\text{C}$  (vertical) signals.

### 2D HMBC

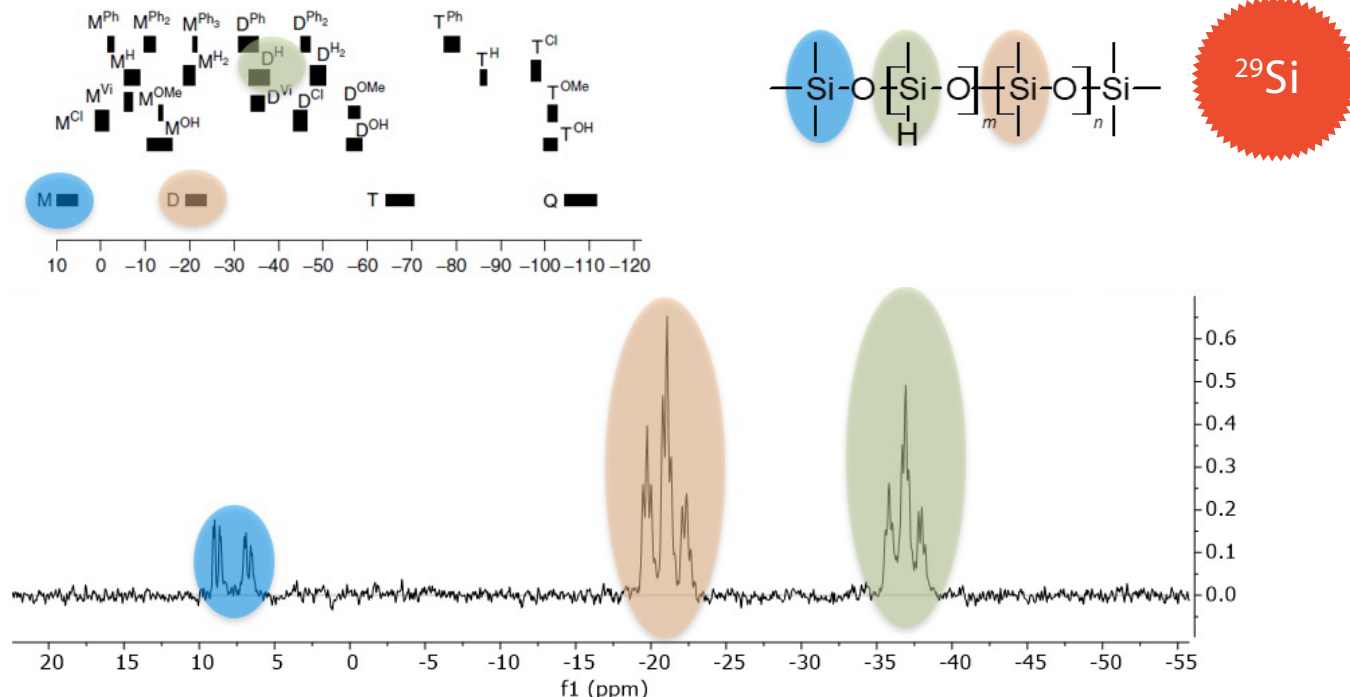
The Heteronuclear Multiple Bond Correlation (HMBC) experiment shows the long-range correlation of protons 10 and 11 with carbons 4, 7, 8, 9 and 12 (the sequence shows the correlation with quaternary carbons, too).



HMBC spectrum of a 800 mM SPHOS sample in  $\text{CDCl}_3$  showing the long-range couplings between  $^1\text{H}$  and  $^{13}\text{C}$  nuclei.

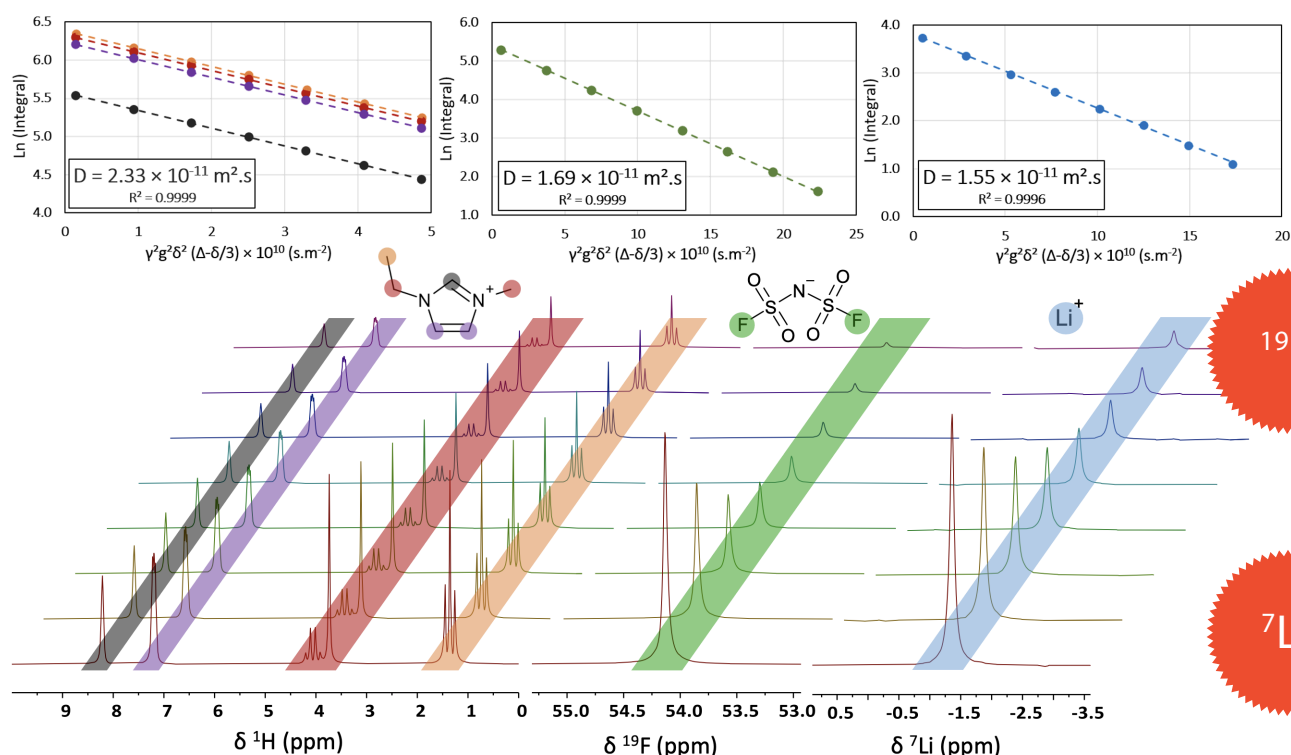
## Spinsolve Multi $X^n$ with $^{29}\text{Si}$ for structural characterization

The strong dependency of  $^{29}\text{Si}$  chemical shift to the chemical environment makes silicon NMR a suitable tool to determine the composition of polysiloxanes. The figure below shows the DEPT spectrum of poly(dimethylsiloxane-co-methylhydrosiloxane), trimethylsilyl terminated, measured by setting the X channel of the Spinsolve to silicon. The result is in excellent agreement with the predicted chemical shifts of the single building blocks.



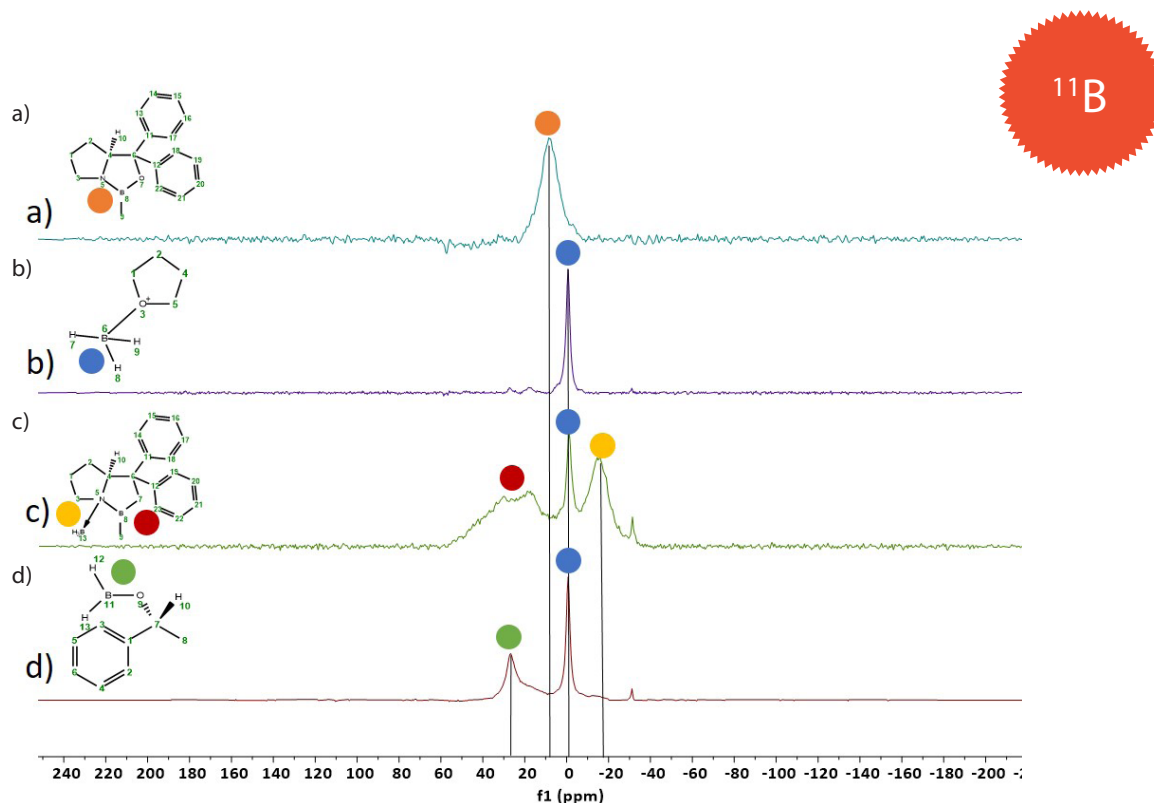
## Spinsolve Multi $X^n$ with optional PFG to measure molecular mobility

Pulsed field gradient (PFG) experiments are useful to assess the molecular mobility of different molecules dissolved in a mixture. By adding a gradient coil to the Spinsolve Multi  $X^n$  you can measure the diffusion coefficient of molecules containing any of the nuclei available on the spectrometer. The example below shows the  $^1\text{H}$ ,  $^{19}\text{F}$  and  $^7\text{Li}$  PFG experiments measured on a LiFSI:EmimFSI ionic liquid sample dissolved at a molar concentration of 2:3.



## CBS reduction of acetophenone studied by $^{11}\text{B}$ NMR

To demonstrate the power of  $^{11}\text{B}$  NMR we followed a typical CBS (Corey, Bakshi, Shibata) reduction reaction of acetophenone to its corresponding alcohol by using both  $^{11}\text{B}$  and  $^{13}\text{C}$  measurements on a Spinsolve Multi X<sup>n</sup> system. The CBS reduction employs a boron containing catalyst (a), which is first activated with a borane solution in THF (b). The activated species (c) serves as the catalyst in the reduction of acetophenone. The final product (d) can nicely be observed in  $^{11}\text{B}$  NMR. The final asymmetric alcohol is obtained after an acidic work up employing HCl in MeOH. These steps have been confirmed by  $^{13}\text{C}$  NMR performed on the same spectrometer.



## Spinsolve Multi X<sup>n</sup>

- Nuclei: All models can measure  $^1\text{H}$  and  $^{19}\text{F}$  in the first channel and all the X nuclei you need, like  $^{13}\text{C}$ ,  $^{15}\text{N}$ ,  $^{29}\text{Si}$ ,  $^{31}\text{P}$ ,  $^7\text{Li}$ ,  $^{11}\text{B}$ , and more, on the second channel
- Includes a powerful multi-line solvent suppression method
- Includes X-decoupled proton acquisition for all available X nuclei
- Available for ULTRA models with exceptional linewidth specifications
- Compatible with Spinsolve Temperature Control system
- Compatible with 0.5 T/m Pulsed Field Gradients for multi-nuclei diffusion studies

Contact us now for a quote, to request a demo, or to measure your samples

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