Welcome to the latest edition of the Magritek Messenger newsletter.

Our **Spinsolve family of benchtop NMR spectrometers** continues to develop and help chemists around the world with their daily research. In this issue, we are pleased to share with you the latest information about our:

The new Spinsolve Multi X

Benefits of the Spinsolve Multi X

• All models measure **^{1}H** and **^{19}F** and one or more optional nuclei, like **^{7}Li, ^{11}B, ^{13}C, ^{15}N, ^{29}Si, ^{31}P** can be added according to your needs

• Automatic 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 measured unattended

• Acquires interleaved multinuclear experiments for online reaction monitoring

• 1D and 2D experiments calibrated at the factory, switch back and forth without recalibration

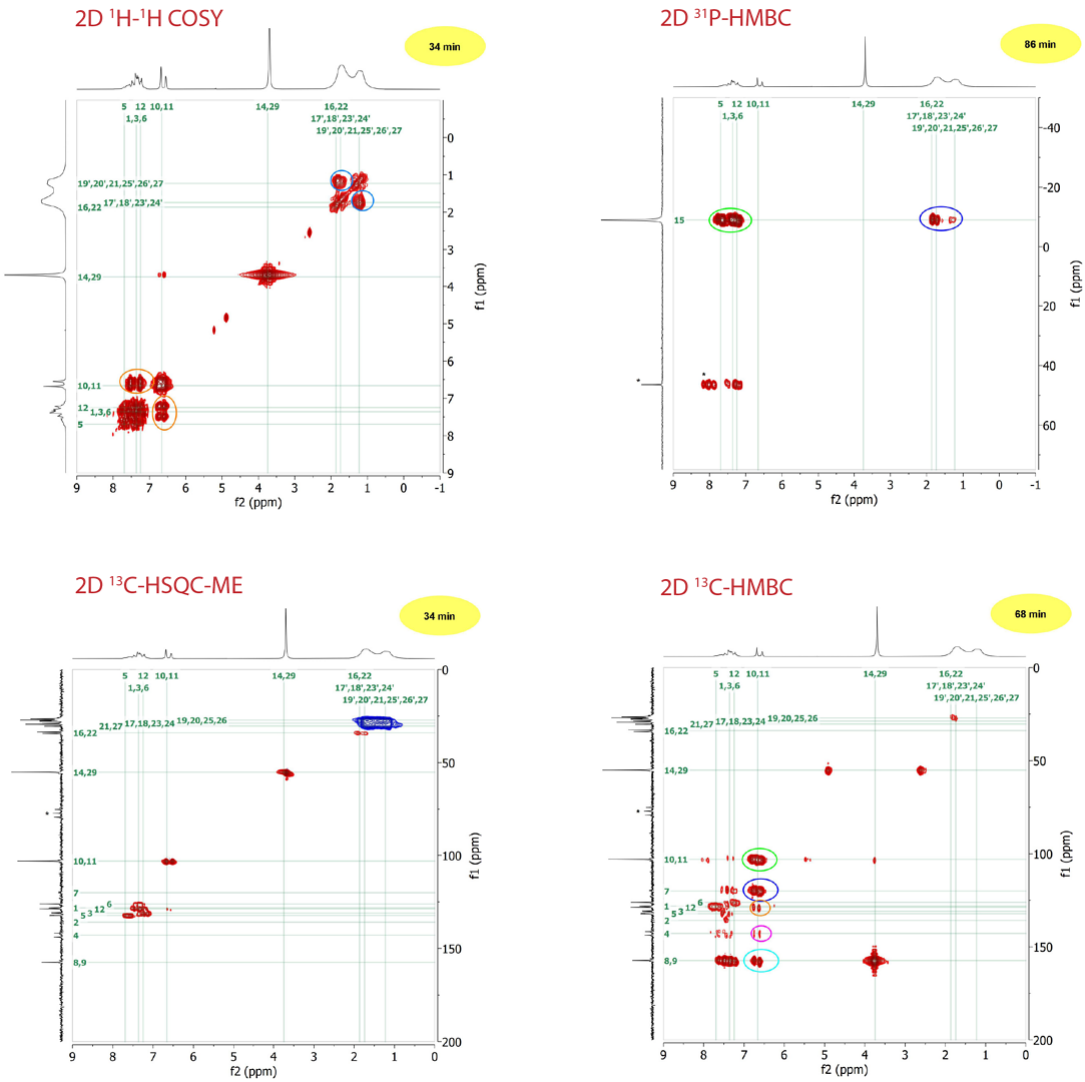
• Includes powerful multi-line solvent suppression

• Allows for X nuclei decoupled proton acquisition (nuclei included on the X channel)

Spinsolve Multi X with Autosampler: All nuclei can be acquired unattended

The software has a library of pre-calibrated protocols for all available nuclei

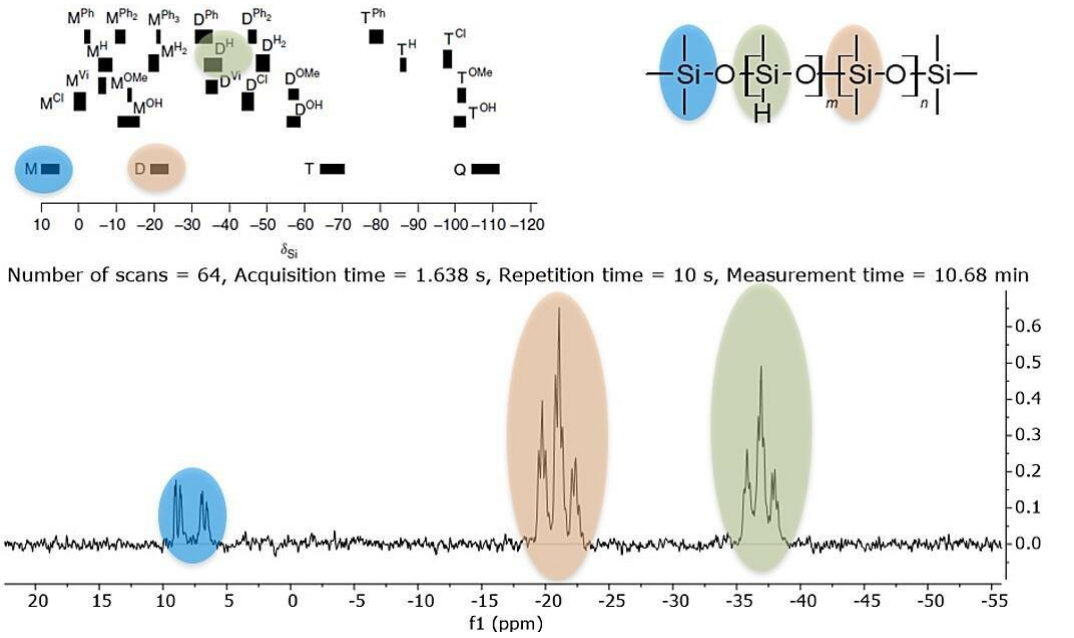
Below you see a collection of homo- and heteronuclear 2D spectra of the phoshine ligand SPHOS dissolved in CDCl3. The data set which was acquired on Spinsolve MultiX system in a fully automated way can be used for structure elucidation and confirmation studies.



For example, in the 2D ^{31}P-HMBC the long-range ^{1}H-^{31}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.

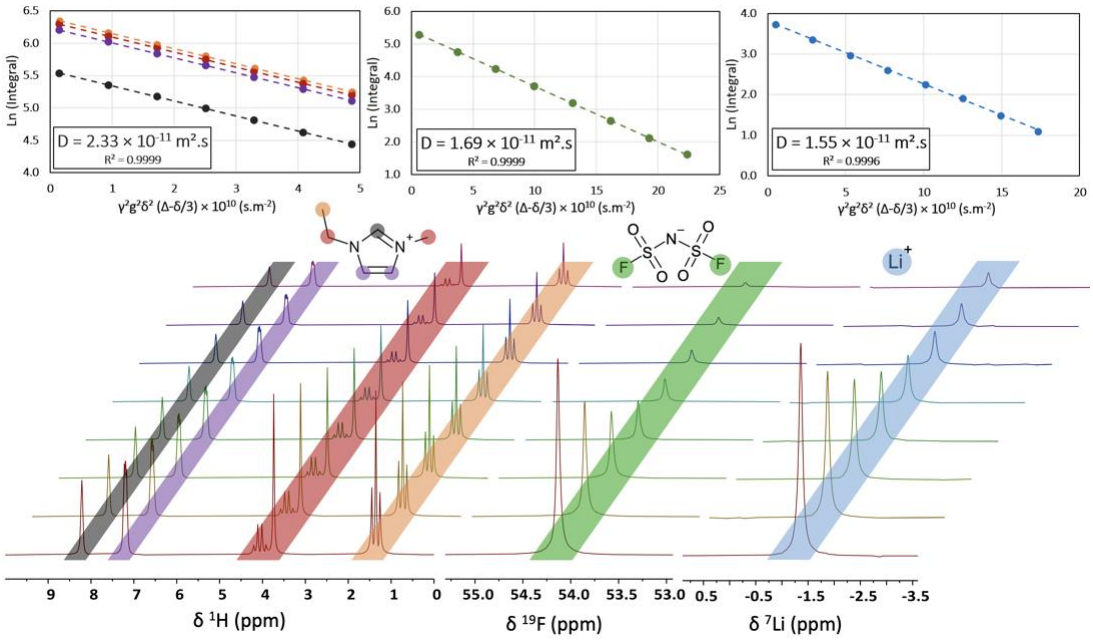
Include silicon on a Spinsolve Multi X for structural characterization

The strong dependency of **^{29}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.



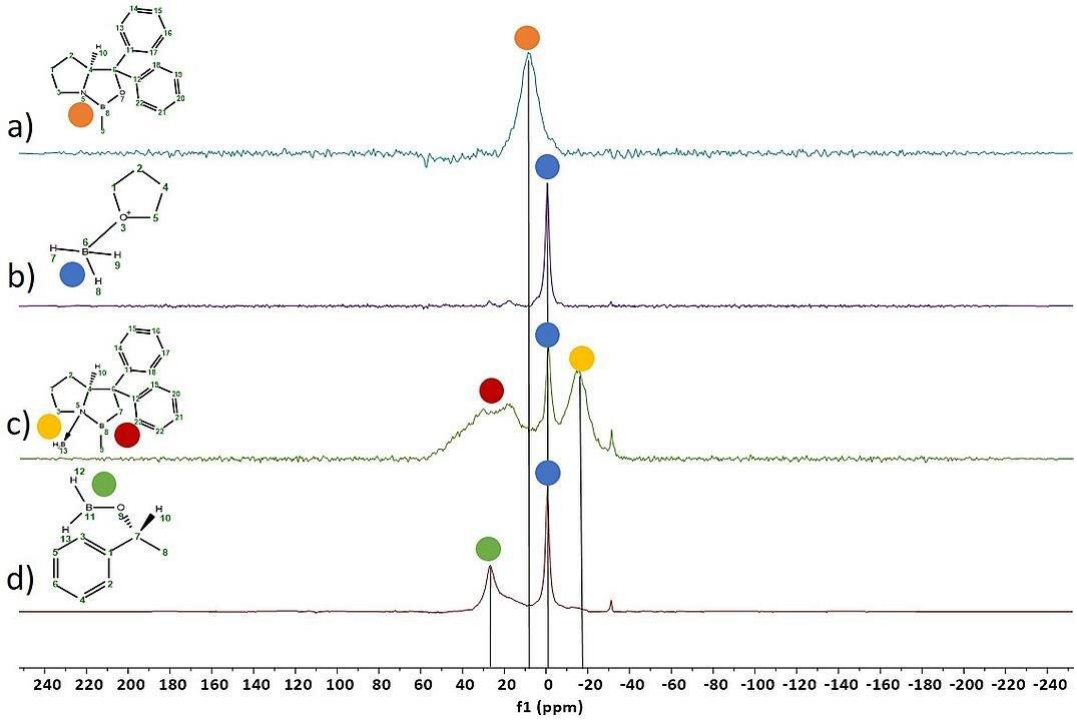
Add PFG to a Spinsolve Multi X system to measure molecular mobility

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



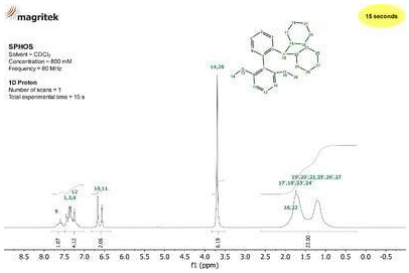
CBS reduction of acetophenone to its alcohol form by using a ^{11}B catalyst

To demonstrate the power of **^{11}B** NMR we followed a typical CBS (Corey, Bakshi, Shibata) reduction reaction of acetophenone to its corresponding alcohol by using both **^{11}B** and **^{13}C** measurements on a Spinsolve Multi X 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}B** NMR. The final asymmetric alcohol is obtained after an acidic work up employing HCl in MeOH. These steps have been confirmed by **^{13}C** NMR performed on the same spectrometer.

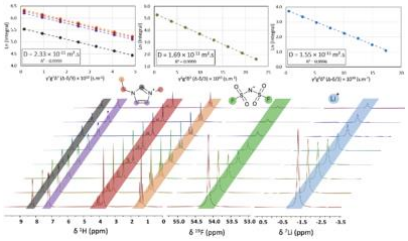


Check out our recent posts

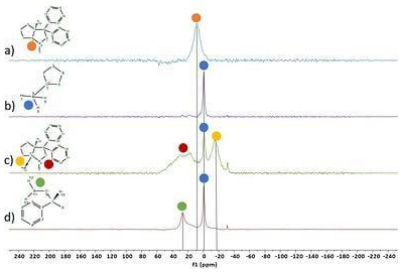
- Characterizing SPHOS by 1H, 13C and 31P NMR



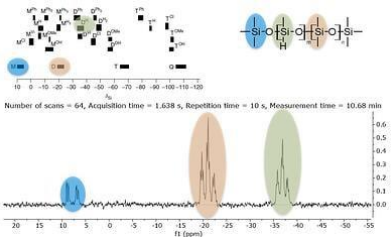
- [Self-diffusion coefficients of ionic liquids measured by multinuclear benchtop NMR]



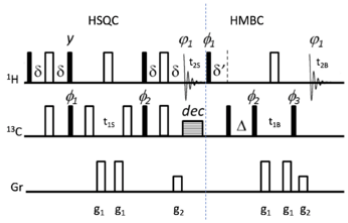
- [CBS reduction of acetophenone followed by 11B NMR]



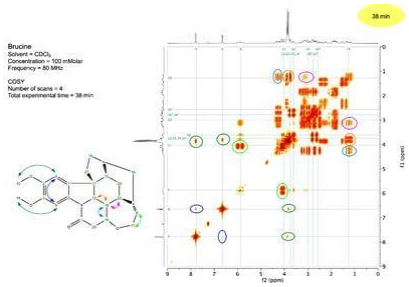
- [Silicon NMR on Spinsolve benchtop NMR spectrometers]



- [NOAH sequences for fast Small Molecule Analysis implemented on a Spinsolve benchtop NMR spectrometer]



- **Structure verification of Brucine by advanced homo and heteronuclear NMR**



- **How simultaneous decoupling of 1H and 19F can help to simplify crowded 13C spectra – A Multi-nuclei case study on 5-Bromo-1,2,3-trifluorobenzene without the need of user invention**