

# Spinsolve<sup>Multi X</sup>

# The world's only broadband autotunable probe

Measure multiple nuclei in one NMR spectrometer in a fully automatic way



# Benefits of the Multi X Probe

- 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



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

#### 2D COSY

The 2D COSY experiment allows one to identify coupled <sup>1</sup>H nuclei as they generate cross peaks out of the diagonal of the 2D data set.



<sup>1</sup>H 2D COSY experiment of a 800 mM SPHOS sample in CDCl<sub>3</sub> acquired on a Spinsolve Multi X 60 MHz system.

# 2D HSQC-ME

14,29

10,11

1 53<sup>12<sup>6</sup></sup>

à

8 7 6

12 10,11

16,22 21,27 17,18,23,24 19,20,25,26

1.3.6

The HSQC is a powerful sequence widely used to correlate the <sup>1</sup>H with the one-bond coupled <sup>13</sup>C nuclei.

14,29

16,22

17'.18'.23'.24'

19',20',21,25',26',27



The long-range <sup>1</sup>H-<sup>31</sup>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.



<sup>31</sup>P-HMBC NMR spectrum of a 800 mM SPHOS sample in CDCl, showing the long-range couplings between <sup>1</sup>H and <sup>31</sup>P nuclei.

#### 2D HMBC

-n

50

150

200

ń

1

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).





5

f2 (ppm)

3 2

> HMBC spectrum of a 800 mM SPHOS sample in CDCl<sub>3</sub> showing the long-range couplings between <sup>1</sup>H and <sup>13</sup>C nuclei.

## Spinsolve Multi X with <sup>29</sup>Si for structural characterization

The strong dependency of <sup>29</sup>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 with optional PFG 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 <sup>1</sup>H, <sup>19</sup>F and <sup>7</sup>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 <sup>11</sup>B NMR

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



# Spinsolve Multi X

- Nuclei: All models can measure <sup>1</sup>H and <sup>19</sup>F in the first channel and multiple X nuclei, like <sup>13</sup>C, <sup>15</sup>N, <sup>29</sup>Si, <sup>31</sup>P, <sup>7</sup>Li, <sup>11</sup>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

The high homogeneity of the Spinsolve ULTRA Multi X models is possible thanks to the patented shimming technology used in the Magritek High Homogeneity Halbach Magnets\*

\*Patent US 8,148,988 and EP 2,144,076

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

 Email:
 sales@magritek.com

 Website:
 www.magritek.com/contact-us

 GERMANY
 +49 241 9278 7270
 UNITED STATES
 +1 855 667 6835

 UNITED KINGDOM
 +44 7468 529 615
 NEW ZEALAND
 +64 4 477 7096

For a complete listing of our global offices and distributors visit: www.magritek.com/about-us/distributors/