

## Spinsolve 80

## Unparalleled performance with unique flexibility



### The benchtop NMR spectrometer with the most powerful features



### Unique resolution

The high homogeneity of the Spinsolve magnets delivers the highest resolution available today. The superior line-shape is not only specified at 50% and 0.55% but also at 0.11% of the peak height.

#### Solvent suppression

The ULTRA narrow line widths of this model make it possible to strongly attenuate the solvent peaks to confine them to a region narrower than 0.2 ppm.



The new Multi-X family of probes can measure multiple nuclei with a single instrument in a fully automatic way. Switching between nuclei is instantaneous and no manual retuning is needed.







### **On-line monitoring**

The flow kit developed for the Spinsolve can be easily mounted to pump chemicals through the Spinsolve for real time monitoring of reactions.

### Autosampler

The compact sample changer designed for the Spinsolve sits directly on top of the system conserving precious bench space. It is controlled by the software to offer full automation.

### **DOSY Gradient**

The Spinsolve 80 can be equipped with the strongest pulsed field gradients (0.5 T/m) for diffusion or DOSY experiments.





# Spinsolve 80

The ULTRA high magnetic field homogeneity of the Spinsolve magnets guarantees you the highest possible spectral resolution for your data.



### Resolve the finest structures

Resolve up to <sup>5</sup>J couplings as small as 0.07 Hz better than any other benchtop NMR spectrometer.



### Improve quantification accuracy

The ULTRA resolution makes it possible to integrate acetic acid without suffering from overlapping with larger adjacent signals. When the standard resolution of 0.4 Hz is used, the overlapping is more pronounced and the integrals are affected.



### Superior solvent suppression performance

Resolving metabolites in urine at milli-molar concentrations in a few minutes



Urine contains a large number of metabolites dissolved in water at very low concentrations. The figure above shows the comparison of two spectra acquired with (red) and without (black) solvent suppression. The suppression sequence strongly attenuates the water signal (marked in blue) with impressive efficiency.

### Reference for evaluating the performance of the solvent suppression method

To quantify the efficiency of the solvent suppression method, the attenuation and the linewidth of the residual solvent peak need to be measured. While the attenuation factor can be easily determined by comparing the residual peak with the amplitude of the full solvent peak, the linewidth of the residual signal needs to be measured at an absolute height in the spectrum. This absolute height is typically defined by a reference compound added to the sample at a given concentration. In the figure below we measured the residual width at the height of the alpha anomeric protons of glucose dissolved at 20 mMolar in pure water.



## Spinsolve Multi X

## The new generation of fully automatic multinuclear probes

The Spinsolve spectrometers can be equipped with the new Multi-X probes to automatically measure multiple nuclei with the one instrument. These probes are equipped with a set of electronic switches that eliminate the need for any user intervention to switch from nucleus to nucleus. Electronic re-tuning ensures that calibrations of the system for the different nuclei remain unaffected when nuclei are switched back and forth. This feature is essential when using an autosampler to run multinuclear experiments on a set of samples.



### Advanced multinuclear experiments automatically acquired for a SPHOS sample



## The most advanced multi-nuclear methods with one click!

Collect the full set of homo- and hetero-nuclear multidimensional experiments providing decisive information for structure confirmation **in less than one hour**.



## **On-line Reaction Monitoring kit**

All Spinsolve models can be equipped with the RM flow kit developed to pump samples through the system for on-line analysis directly inside the fume hood. This kit includes a glass flow cell that minimizes the dead volume of the flow setup by using thin capillary tubes that go from the inlets to the center of the cell and maximizes the NMR sensitivity by expanding the tubing in the center, where the NMR coil is positioned. Thanks to the optimized design of the flow cell, the SNR in flow mode is identical to using standard 5 mm tubes. The kit includes also a peristaltic pump that is controlled by the Spinsolve software to run in continuous or stop flow mode. The flow cell can easily be inserted in the Spinsolve and is connected to the pump by means of thin PTFE or peek tubing. The Spinsolve software includes a powerful monitoring module that has been developed to follow reactions in real time. It synchronizes the pump with the measurements of the different protocols that are included in the loop and offers advanced data processing tools to display the conversion curves.



## **Full Automation**

Increase your sample measurement throughput by integrating the new fully automated autosampler carousel with your Spinsolve. The autosampler fits directly on the top of the Spinsolve and can easily be added or removed for transportation. The queue of protocols to be run for each sample can be entered in just a few seconds and it can be edited by the user at any time, even while data is being collected.

	MEN	J 14 13C 43 MHz	"C	ne ne		IPTS QUEUE	CONNECTED TO SPA1029	LOAD		
							SAMPLE CHANGE DELAY 00:05:00 AUTOSAMPLER INSERT STOP	EMER		
							NEW PROTOCOL DELAY 00:00:30 QUEUE RUNNING			
and the second s	1	2 3	4	5	6 7 8	9	) 10 11 12 13 14 15 16 17 18	19		
	Slot	Protocol	StartTime	EndTime		ſ		1		
	1	SHIM++	12:53:27	12:55:54	Snincol		Spectrum Scan [3163/8192]			
	7	1D CARBON+ WALTZ	13:01:05	22:07:13		Shinsone				
5 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 -		SHIM++	13:01:24	13:01:24	^					
	7	DEPT WALTZ	13:06:54	15:57:34	1D CARBON+ WALT	1D CARBON+ WALTZ				
	1	SHIM++	16:03:04	16:03:04	CONTRACT		4			
	7	HSQC-ME-WALTZ	16:08:34	18:26:20	SAMPLE \$7					
	1	SHIM++	18:31:50	18:31:50	CCANE 010					
		COSY 2D 18:37:20	18:37:20	19:15:40	SCANS 8192					
	7	1D EXTENDED+	19:16:10	19:16:25	REPETITION TIME 4 s	~	2- 			
		1D EXTENDED+	19:16:55	19:20:55	PULSE ANGLE 45	PULSE ANALE 45 2 2 BANDWOTH 333 Ppm 2 NOE EINAACEMENT 10 Ppm 2 NOE EINAACEMENT 20 0-4554 North Andrea Markada and Andre				
		1D EXTENDED+	19:21:25	19:29:25	BANDWIDTH 333		ΨΨ · · · · · · · · · · · · · · · · · ·			
	1	SHIM++	19:34:55	19:34:55	CENTER FREQUENCY 110					
		1D EXTENDED+	19:40:25	19:41:05	NOE ENHANCEMENT		o - Nurshi mundaana jima kukakaa awaayaa Mansahira kasadaa , waxaana waya kasada waxaa iyo waxaa iyo waxaa kasa			
	8	1D CARRONI, WALTZ	19:41:35	20:16:01	1H DECOUPLE	$\checkmark$				
m		SHIM++	02:03:21	02:03:21						
uidgritek	-	HSOC-ME-WAITZ	02:03:21	06:42:37	PROGRESS: 38% THE REMAINING: 5	PROGRESS: 38% TIME REMAINING: 5 HOUR, 35 MIN, 13 SEC	-2			
	1	SHIM++	06:48:07	06:48:07						
Williti X <sup>13</sup> C - <sup>31</sup> P - <sup>7</sup> Li Diffusion		HMBC WAITZ	06:53:37	11:27:13						
	1	SHIM++	11:32:43	11:32:43			150 100 50 0			
	1						ppm			

## The strongest diffusion gradients for DOSY experiments

- Separate the spectra of different components in a mixture by molecular size (DOSY-type experiments)
- · Measure self-diffusion coefficients to understand molecular mobility (PFG diffusion measurements)



Diffusion Ordered Spectroscopy (DOSY) creates a two-dimensional plot by acquiring a set of spectra as a function of the amplitude of the gradient. The chemical shift is measured along the horizontal axis, and along the vertical axis the self-diffusion coefficient is shown. In this 2D spectrum the peaks are aligned along horizontal lines. Each of these lines corresponds to a different self-diffusion coefficient, and therefore a different component of the mixture. We can immediately separate the solvent peak, as well as the other two components, although their diffusion coefficients differ only by a little more than 10%. This makes DOSY a very powerful tool for mixture analysis in NMR spectroscopy when the components have different diffusion coefficients.

### Measurement of self-diffusion coefficients for different nuclei

As the Spinsolve can measure several nuclei on one instrument, the diffusion constants of the species containing the different nuclei can be measured automatically without any retuning. Below we show an example where we measure a mixture of 1-butyl-3-methylimidazolium tetrafluoroborate ( $BMIM-BF_4$ ) and lithium tetrafluoroborate ( $LiBF_4$ ). The diffusion coefficients were measured with a stimulated – echo sequence run for each particular nuclei. From left to right we can see the PGSTE experiments of 50 mg/mL LiBF4 in BMIM-BF<sub>4</sub> for proton, fluorine and lithium.



# Spinsolve 80



### **Specifications**

- Nuclei: <sup>1</sup>H, <sup>19</sup>F, <sup>13</sup>C, <sup>31</sup>P, <sup>29</sup>Si, <sup>7</sup>Li, <sup>15</sup>N, <sup>11</sup>B, <sup>23</sup>Na (more available)
- Operating frequency: 80 MHz (<sup>1</sup>H)
- <sup>1</sup>H Linewidth:
  - Classic 50 / 0.55 / 0.11% < 0.4 / 15 / 30 Hz
  - ULTRA 50 / 0.55 / 0.11% < 0.2 / 8 / 16 Hz NEW
- <sup>1</sup>H Sensitivity:
  - Single channel: > 280:1 for 1% Ethyl Benzene
  - Dual channel: > 200:1 for 1% Ethyl Benzene
- External hardware Lock system / no need for deuterated solvents
- Available with automatic sample changer
- · 3D PFG gradients optimized for gradient-assisted sequences
- Diffusion pulsed field gradients of 0.5 T/m NEW
- Standard 5 mm OD NMR sample tubes, 7" long
- Minimum sample volume: 250 ul
- Operating Temperature Range: 18° C to 28° C (65° F to 82° F)
- Dimensions: 58 x 43 x 40 cm (23" x 17" x 16") (D x W x H)
- Weight: 72.5 kg (160 lb)
- Stray Field: < 2 G all around system

#### Pulse sequences available on the Spinsolve 80 Carbon spectrometer

Proton	Fluorine	Carbon
1D with <sup>19</sup> F and <sup>13</sup> C decoupling	1D Fluorine with <sup>1</sup> H decoupling	1D Carbon with <sup>1</sup> H and <sup>19</sup> F decoupling
1D paramagnetic	2D F - COSY	DEPT
2D gs-COSY*, gs-JRES	2D F - JRES	APT
2D gs-TOCSY, and gs-ROESY	2D FH - COSY	HETCOR
1D solvent suppression (Presat and WET)	T <sub>1</sub> , T <sub>2</sub>	gs-HSQC
1D solvent suppression with $\mathrm{T_2}$ filter	PFG-DOSY	gs-HSQC-ME*
2D gs-COSY with solvent suppression	Reaction Monitoring	gs-HMQC
T <sub>1</sub> , T <sub>2</sub>		gs-HMBC*
PFG-DOSY		gs-NOAH*
Reaction Monitoring		*Non-Uniform Sampling (NUS) available

Other sequences available, contact us!

### 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 KI	NGDOM +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/

