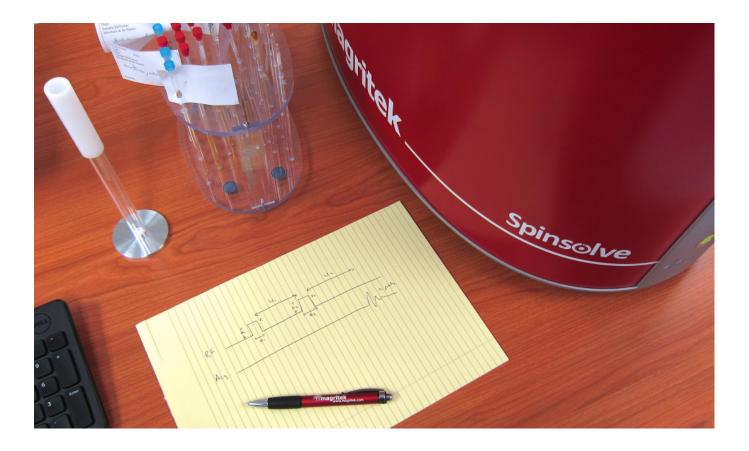


# Spinsolve Expert

## **Spinsolve Expert**

Advanced control of Spinsolve for the expert NMR user



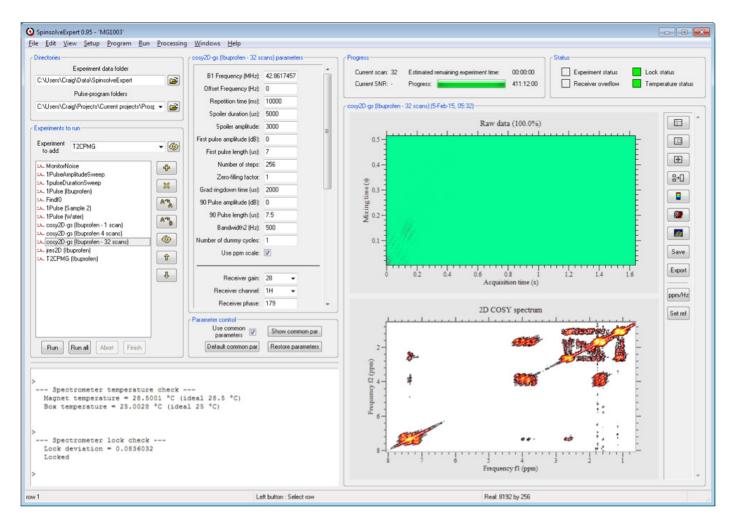
# Spinsolve software with pulse programming capabilities

- Adjust any acquisition or processing parameter
- Modify and write new pulse sequences
- Create new data processing and control algorithms
- · Write scripts to control a series of experiments plus processing
- Modify the display

The Spinsolve Expert interface is designed to optimize the running and display of experiments.

Experiments are grouped together into projects with all experiments in the current project visible in the user interface.

Clicking on each experiment will display any previously collected data along with all the parameters used.



The Spinsolve Expert interface showing a COSY spectrum of Ibuprofen

Pulse programs can be entered along with higher-level experiment control scripts, default parameters and parameters from the user interface.

The expert user can **configure the display interface** and **post processing** controls as well as have **detailed control** over the experiment.

New experiments are easily added using the pulse program editor and compiler.

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The pulse program editor and compiler showing the jres2D sequence

## **Spinsolve Expert Features**

### Setup and monitoring

- · Manual and automatic shimming
- Automatic lock-find
- Temperature monitor
- Proton and Lock probe matching check

### Data display

- Each experiment has an optimized plot layout (user controlled)
- 1D and 2D plots can be displayed together in the main interface
- · 3D plots can be displayed in separate windows

### **Experiment control**

- All experiment parameters are visible and can be modified
- Multiple versions of the same experiment can be run in the same project
- Experiments can be controlled using the scripting language
- Includes looping and user defined processing
- Experiments can be batched
- Data is saved to the file system and can be easily exported

### Pulse program generation

New pulse programs can be written allowing full control of the spectrometer

### Post processing

Specific post-processing can be defined for each experiment. Available commands include

- A variety of predefined and user definable apodization filters
- · Fourier transform
- · Manual and automatic phase correction
- · Baseline correction
- 1D and 2D inverse Laplace (a special license is required for 2D inversion)

# Spinsolve Expert

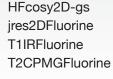
### Supplied pulse programs

#### Proton (1H)

1Pulse 1PulseAmplitudeSweep 1pulseDurationSweep cosy2D-gs Findf0 jres2D MonitorNoise T1IR T1IRT2 T2CPMG T2CPMG\_bulk Watergate

### Fluorine (19F)

1PulseDispFluorine 1pulseDurationSweepFluorine Fcosy2D-gs FHcosy2D-gs Fjres2D



### Phosphorus (31P)

1PulsePhosphorus 1PulsePhosphorusMLEV 1PulsePhosphorusWALTZ HMBC\_Phosphorus T1IR\_Phosphorus\_WALTZ T2CPMG\_Phosphorus\_WALTZ

### Carbon (13C)

1PulseDispCarbon 1PulseDispCarbonMLEV4 1PulseDispCarbonMLEV4\_CA 1PulseDispCarbonMLEV4\_HF 1PulseDispCarbonWALTZ16\_CA 1PulseDispCarbonWALTZ16\_HF 1PulseDispProtonMLEV4 1PulseDispProtonMLEV4\_CA 1PulseDispProtonWALTZ16\_CA DeptMLEV4 DeptMLEV4\_CA DeptQMLEV4 DeptWALTZ16 CA HetcorMLEV4 HetcorWALTZ16\_CA HMBC-gs HMBC-gs-CA HMBC-gs-CA-P HMBC-gs-F HMQC-gs HMQC-gs-CA HSQC-gs HSQC-gs-CA HSQC-qs-F MonitorNoiseCarbon

### Spinsolve Carbon

All Spinsolve Experiments PLUS

- <sup>13</sup>C capability
- Spectral editing with DEPT
- 2D heteronuclear correlation
- experiments HETCOR, HMQC, HMBC
- (Phosporus <sup>31</sup>P capable system (available)

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**SpinsOlve** 

<sup>1</sup>H and <sup>19</sup>F nuclei

2D COSY and JRES

Reaction monitoring

Relaxation time experiments

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