

Spinsolve Expert

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Advanced control of Spinsolve for the expert NMR user



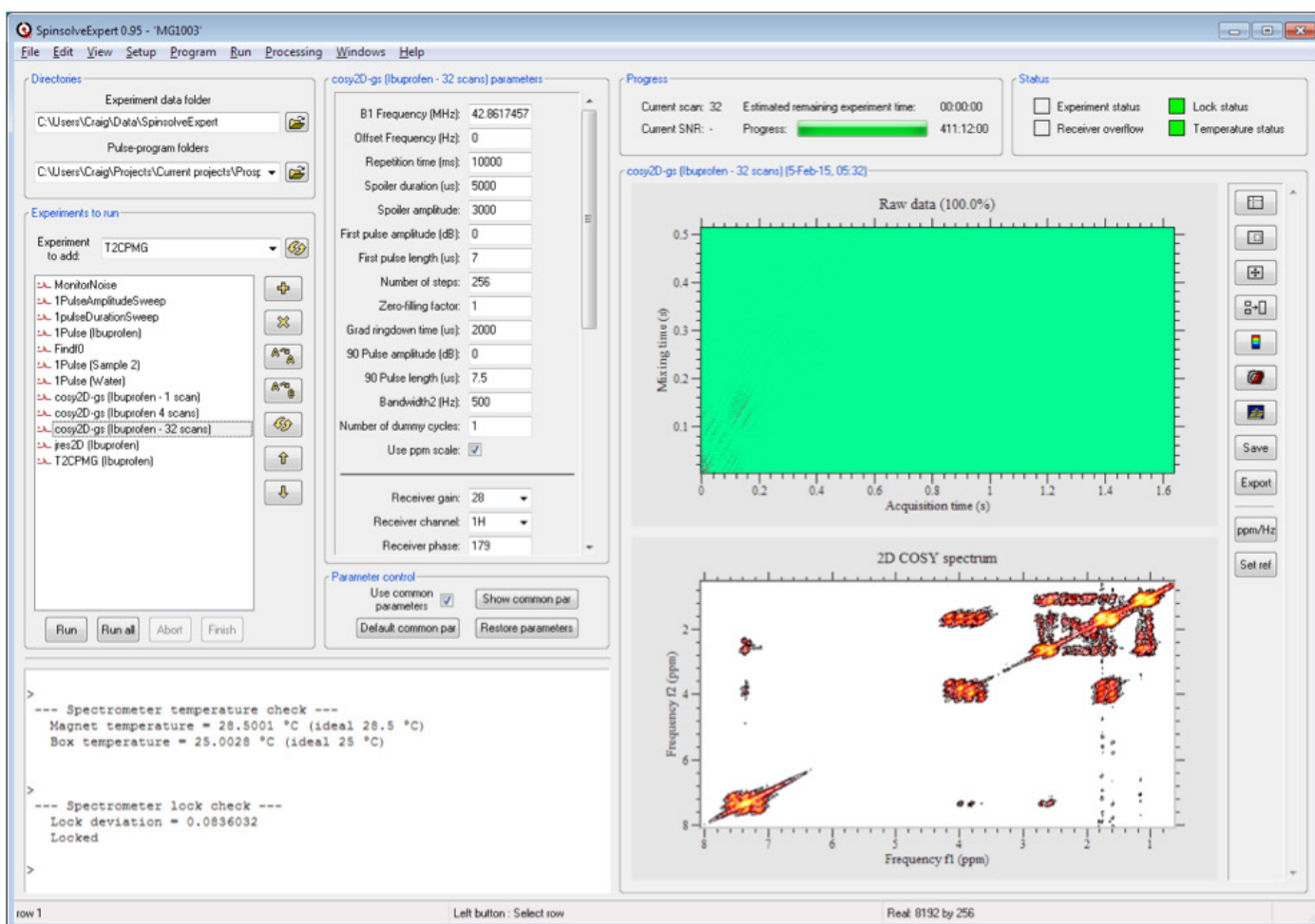
Spinsolve software with pulse programming capabilities

- 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.

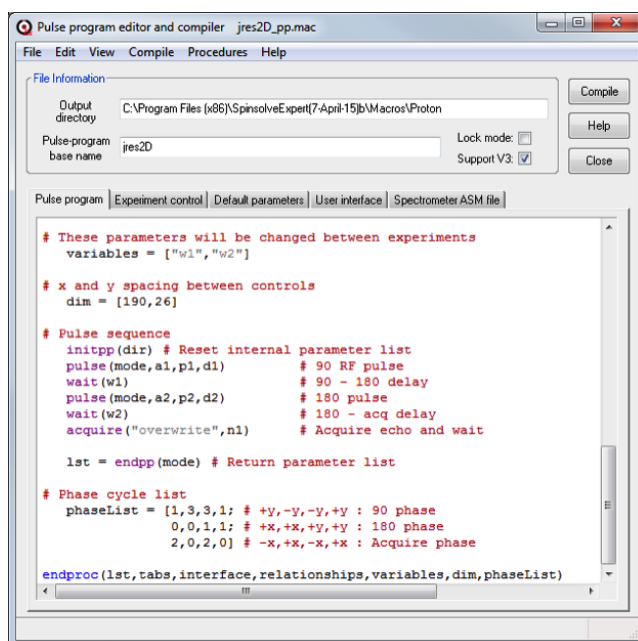


The *Spinsolve Expert* interface showing a COSY spectrum of Ibuprofen

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.



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

HFcosy2D-gs
jres2DFluorine
T1IRFluorine
T2CPMGFluorine

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-gs-F
MonitorNoiseCarbon



Spinsolve

- ^1H and ^{19}F nuclei
- Relaxation time experiments
- 2D COSY and JRES
- Reaction monitoring



Spinsolve Carbon

All Spinsolve Experiments PLUS

- ^{13}C capability
- Spectral editing with DEPT
- 2D heteronuclear correlation experiments HETCOR, HMQC, HMBC
- (Phosphorus ^{31}P capable system (available))

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