

## SpinsolveExpert release notes

**Note:** items in **red** may require modifications to your own sequences. All personal sequences should be recompiled after each software update.

### Version 2.02.09 (24-March-2025)

#### *New experiment*

- Added a new X-nucleus PGSTE sequence in the X menu.

#### *Modified experiments*

- QuickShim now supports short samples and has different parameters for the reference and 'other' samples.

#### *Bug fixes*

- Fixed a bug in some of the Proton diffusion sequences which was causing an error when the dwellTime or nrPnts parameter was modified.
- Fixed a bug when post processing non-Proton diffusion sequence.
- Corrected a calibration error in the q-axis for non-proton PGSTE sequences.
- Arrayed experiment can now communicate automatically with the Viewer allowing updates to be displayed as they become available.
- A bug in PGSTE-Si fixed which was returning the power level instead of the pulse length for Silicon.
- The stacked plot view dialog now keeps the trace name after the Apply button is pressed.
- Post processing of PGSTE data in the 1D Data Analyser now uses the correct experiment parameters.
- QuickShim parabolic class modified arbitrary shim lists that needs optimising (the order is no longer important).

#### *Miscellaneous new features*

- The protocol editor now supports syntax highlighting for the default parameter tab.
- Support is now provided for up to 7 X nuclei + tuned Fluorine.
- Support provided for magnets with extra temperature sensors.
- Program checks for duplicate experiments on startup (with locations)

### Version 2.02.06 (11-March-2025)

#### *New experiments/scripts*

- HOESY-HF has been divided into two versions, decoupled and not decoupled. The latter may be more sensitive in some situations.
- COSY-TPPI-HF experiment added as an example of how to collect and process a TPPI experiment

#### *Modified experiments*

- PGSTEstandardCdec has been renamed PGSTECdec. Note that experiments collected using the old name will **need to be renamed** (see 'Rename Experiment Folders' option in the File menu).
- PGSTE\* experiments modified to reduce phasing errors as the gradient is changed.
- PGSTE\* experiment now have a logarithmic q-axis sampling mode – this requires adding an estimated diffusion coefficient and required attenuation range.

- QuickShim slow modes modified to just one. You can now also change the repTime and dwellTime/nrPnts from the parameter list if you require more control.
- All Fluorine experiments simplified as the getXChannelParameter("19F") function now takes into account whether the Spinsolve has tuned 19F or not.
- Check shim includes SNR and ppm/Hz post processing.
- T1-X now supports MNova and ROSY analysis.

#### *Bug fixes*

- A bug in QuickShim (fast mode) on Multi-X Spinsolves cause zero Proton signal to be detected. This has been fixed.
- Scripts which displayed common parameters would not have these overwritten by the latest common parameter. This could cause unexpected peak shifts (e.g. in arrayExperiment).
- Fixed an issue in the compiler which prevented modified files from being saved unless the importer tab was selected in the preferences.
- Presat and T1IRT2 weren't working correctly in the arrayedExperiment script because of a bug in saveProcPar.
- In batch processing, only modified experiments selected from the batch list will now cause the check mark to go red.
- Receiver phases can now be set with more precision than 1 degree.
- Locking should now work more reliably even if the Spinsolve 19F frequency is not very accurate.
- The gLock->uBPar structure is no longer critical which means that switching between two Spinsolves should not cause the lock to be refound.
- In some parts of the code expNr was used in others exptNr. Support for both variants is now included.

#### *New features: main interface*

- Modifying the batch interface from the viewer interface while a batch is running now limits where you can move the modified experiments to below the currently running experiment.
- The maximum number of plots/images has been increased from 6/4 to 10/10.

#### *Miscellaneous new features*

- Further improvements and simplifications to experiments which involve the lock (LockWobble and setting the lock receiver gain).
- The script editor now supports procedure sorting and general text sorting from the edit menu.

#### *Documentation updates*

- The script ArrayedExperiment now has help.

### **Version 2.02.04 (5-February-2025)**

#### *New experiments/scripts*

- A heteronuclear NOESY (HOESY) between proton and fluorine has been added.
- PGSTESHims added – this allows diffusion experiment to be performed on some samples without special hardware.
- A new experiment folder called SelectivePulses added which gives examples of using selective pulses.
- Carbon T1Bulk, CarbonT2Bulk and T2Bulk-N added.

#### *New features: main interface*

- A viewer button added to open a second instance of Expert for viewing data while the main program is running.
- The batch list can now be modified using the Viewer interface while it is running.
- The button to restore the UI after a crash has been enlarged and made more obvious.

#### *Miscellaneous new features*

- New debug commands added to Prospa: callstack and showerrors (see help for details)
- 1Pulse1H has a disable processing check box added to allow smaller repetition times.
- QuickShim now works in fast mode without applying a lock and calibrate step at the end. This means it can be used to shim on sample.
- The locking processes now uses the same code for FX3 and DSP Spinsolves.
- The expected duration for a selected group of batch experiment can be found by holding down the shift-key when selecting this option in the experiment menu.
- If the command gDebug->showLevel = 1 is set in the CLI then the transmit and receive frequencies will be reported when running experiments. Useful when designing new sequences.
- A command to sort procedures alphabetically has been added to the text-editor edit menu.
- The current shims are now stored in the structure gData->shims.

#### *Bug fixes*

- HMBC-B and HSQC-B now correctly calculate the frequency axes.
- CarbonHFDdec updated and tested.

#### *Documentation updates*

- Help added for experiments PGSTE, T2Bulk, ProtonAmpSweep, ProtonCDec the User Manual and two new Prospa commands (callstack and showerrors).

### **Version 2.02.00 (10-January-2025)**

#### *New experiments/scripts*

- Addition of two Boron experiments, HMBC and HSQC.
- 19F 2D PGSTE experiment added.
- New arrayed experiment script added, allowing experiment parameters to be systematically modified and displayed in a stacked plot. This also replaces the repeated experiment script.
- ReactionMonitoring script improved to work with any 1D experiment.
- A Proton/T2Bulk script added showing how to use the output of one experiment to modify another.
- A ROSYT1Simulation script has been added to generate a simulated T1IR experiment. This can then be processing with the new ROSY interface.
- A fast power-shim added in the scripts menu.
- New improved Carbon HSQC experiments added.
- New single shot Proton T1 experiment added (T1Bulk).

#### *New features: main interface*

- Addition of a multi-line pulse sequence visualization tool in the Experiment menu.
- Added option in the history list to view the acquisition parameters for an experiment.
- Information item in some menus giving a brief description of the scripts present.
- New option in Files menu to save all (not 'fid') plots and the current layout.
- Option to display parameter help in the CLI included in Preferences->General page.
- New option in View menu to manually modify plot layout.

#### *New features: 1/2D post-processing*

- The 2D post processing dialog now supports exponential apodization (exp:xx) and the updating of the other functions using the filter dialog.

- Added Experiment menu option to check for duplicate experiments.
- Disable2DProc flag added to most 2D experiments to allow data acquisition without real time processing and display. This provides a reduction in repetition time in some cases. These experiments use the Processing2D\_Std pulse sequence parameter group.
- 2D processing has been updated in many experiments to reduce memory usage and make the f1/f2 order more logical.
- The 1D and 2D post processing dialogs have improved phasing tools added.
- Added check boxes in the 2D FT postprocessing interface to allow halving of the first data point.

#### New features: compiling

- Tabs in the compiler interface are now active while an experiment is running, allowing viewing of the different files.
- The ASM file tab in the compiler interface is now hidden on FX3 systems (not needed here)
- Option to view standard software importer files now available in preferences and compiler editor.
- Option in the pulse program compiler and editor to change multiple strings in all pulse program files. Can be used to change the nucleus.
- Option in the pulse program compiler and editor to compile all pulse programs in the user menus.
- Sort selection option added to edit menu in text-editors.
- Making a copy of an experiment with a new name now also copies the MNova folder. (**Some post-editing in MNova folder may be required!**)

#### New features: batch mode

- The same parameter can now be modified in all selected batch experiments.

#### Miscellaneous new features

- Basic support for 1D and 2D JCAMP export to MNova and TopSpin added – [needs more work for calibration](#)
- Improvements to the 2D inverse Laplace interface.
- Improvements to the 1D analysis interface.
- Reduced quick shim time significantly in fast mode.
- **Parameter controls which require callback procedures should now using the “proc” flag. See 1Pulse-X for examples. (This improves UI performance).**
- MNova export added and checked for most experiments. (Some experiments such as T1 and T2 required the addition of a second dimension ‘delay’ list).
- Access to Spinsolve parameters simplified in all experiments minimizing reads from the spectrometer.
- ROSY post processing added to T1 and T2 experiments
- DOSY post processing added to 2D PGSTE experiments
- COSY anti-diagonal artefacts reduced by increasing the spoiler gradient amplitude.
- More standard software experiments can now be imported into Expert.
- T1Analysis macro in 1D menu; maximum points increased from 200 to 1000
- Added linear prediction to the Fluorine experiment.
- CheckShim and StandbyShim now generate reference FIDs for use with 1D deconvolution (see FT postprocessing).
- Rather than having a different preferences file for each Spinsolve there is now only one: ucsPreferences.par.

#### Bug fixes

- Modified the experiment search paths to minimise incorrect macros from being run or viewed.

Note old experiments should be recompiled to take advantage of this.

- Unused 'progress' group removed from pulse program group lists.
- Fixed a bug which was causing older DSP Spinsolves to show they had lost the lock when in fact they hadn't.
- Copying from the compiler path name textbox now works reliably
- A bug in slider interactions fixed. Sometimes it would not release the slider when the mouse button was released.
- Can now load, modify and compile experiments more reliably in a second instance of Expert while experiments are running in the first.
- Removed template option from compiler file menu as this is not currently working.
- To avoid confusion, only one instance of the 1D and 2D processing dialog is now possible.
- It was possible to still have multiple instances of the compiler for the same experiment. This should now be fixed.
- More consistent variable names in the returned results from experiments (this is needed for some of the new script based experiments).
- More robust locking.
- Fixed location on macro runBatch.mac.
- Fixed the Wobble macros which might have been causing relay clicks on old DSP based spectrometers.

#### *Documentation updates*

- User manual and programming guide updated.
- Some pulse programming commands updated.
- All main-menu help files updated.
- Help added for Pulse program compiler and editor user interface.
- Help added for 1D/2D FT and 2D display.
- Help added for INEPT, T1Bulk, T1IRT2, and TOCSY experiment.
- Help added for ROSYT1/T2 analysis.
- Help added for Presat and ProtonDurationSweep and APT experiments.

#### **Version 2.01.19 (9-October-2024)**

- Modified Search history macro to speed up searches.
- Inverse Laplace based DOSY processing added to PGSE experiments.
- All PGSE experiment now save the q-space axis not gradient list.
- 2D Nitrogen experiments added.
- New global 2D processing class added (gFFT)
- New post processing interface added (2DPostProcessing.mac) – replacement for apodizeNTransform2D.mac
- Fixed startup problem when there is no connection to a Spinsolve.
- The parameterCallBack procedure can now also be added to the Experiment control macro.
- A TriggerOut script added to UserScripts folder to work with the TTL box.

#### **Version 2.01.18 (30-September-2024)**

- Addition of 3 experiments which use inter-experiment timing: T1iet (1H), Carbon-T1iet (13C), T1iet-F (19F). These experiments run in a shorter time and give more accurate results than their repetition time counterparts.
- Corrected a bug which prevented inter-experiment time experiments from being added to a batch list.
- The sequence visualizer can now hide table index control commands to simplify the view.
- The procedure ucsRun:getData can now be replaced with two separate commands ucsRun:runExperiment and ucsRun:readData if more control is required. (See experiment

- ProtonLPShowDetails).
- Fixed a bug which was preventing the manual phasing dialog from saving the phasing limits.
- A new version of the Spinsolve parameter updater (V1.54).

#### **Version 2.01.17 (26-September-2024)**

- If the shift key is held down when starting a batch just the selected lines will be run.
- Fixed a bug in ProtonCDec which was preventing it working on DSP Spinsolves.
- Added power of 2 scaling option when collecting data with ProtonFDec. Also added linear prediction.
- Added the ramprfpulse command to sequence visualisation.
- Added WaitForTrigger script for use with the TTL box and batch processing.
- Restored the phasecorrect command in the linearprediction DLL.

#### **Version 2.01.16 (19-September-2024)**

- Fixed a bug on DSP systems with lock offsets which was preventing the lock from being disabled during experiments (since V2.01.14).

#### **Version 2.01.15 (18-September-2024)**

- Fixed a bug in the FX3 transceiver firmware which caused the lock and saturate command to be unreliable. New version V122.
- Increased lock-gain for single receiver-gain stage Spinsolves from 20 to 35 dB.
- Added html help for new shaped RF pulse commands (shapedrf1, shaperf2, dualshapedrf1, dualshapedrf2).
- Lock repetition time on FX3 reduced from 25 to 20 ms to make it the same as on DSP systems.

#### **Version 2.01.14 (12-September-2024)**

- Fixed a bug in the stats2d macro.
- Improved timing estimate in T1 experiment.
- Support for inter-experiment repetition times returned.
- Added a new T1 experiment which uses interexperiment timing (T1ieTime)
- Renamed T2BulkScale T2Bulk replacing old version.
- Expert is now ignoring a DSP Kea spectrometer which is connected.
- Moved example proton sequences to a new folder ProtonExamples.
- Removed 'Find Lock' option from Setup menu –use 'Lock and Calibrate' instead.
- Now decaching sequences when removing a folder from the experiment menu in preferences.
- Provided fast linear prediction as an option (fastlinearpredict) for high SNR samples.
- New FX3 transceiver firmware added, V121 which modifies the stoplockandsat command so the sequence will abort if the trigger signal from the lock is not detected in the duration of the command.
- Fixed stacked plot range bug in ProtonAmplitudeSweep and ProtonDurationSweep.
- Added linear prediction to ProtonBW experiment.

#### **Version 2.01.13 (4-September-2024)**

- The experiment base path field now has a drop-down menu and will remember previous locations.
- The addition of a single channel receiver gain introduced a bug when trying to load a sequence when the spectrometer was not connected. This has been fixed.
- Reverted to more complex Linear Prediction as there were some cases where the simpler version failed.

#### **Version 2.01.12 (15-August-2024)**

- Fixed a bug on DSP systems which caused long delays on lock experiments after running a long non-lock experiment.
- Simplified the Linear Prediction DLL.
- Included preliminary support for Spinsolves with a single receiver amplifier channel.

#### **Version 2.01.11 (10-July 2024)**

- Increased maximum size of acquire("sum") array to 4096 points for FX3 systems (this includes a shift factor). This requires a transceiver firmware update to V120.
- Added a "hex" data type for textboxes. In this case any number written to a textbox with the setctrlvalues command will be converted to the closest hex integer.

#### **Version 2.01.10 (24-June 2024)**

- Support added for the new FX3 hardware trigger input and output. This requires a transceiver firmware update to V120.

#### **Version 2.01.09 (19-June 2024)**

- Support for post processing of diffusion spectra in the 1D analysis window.
- Importing of various PGSTE standard experiments supported.
- Fixed naming check in the pulse program editor which prevented two editors being display when the protocol names were similar.
- Additional post processing of stacked plots introduced (apodization and PPM/Hz)
- Support for up to 5-X nuclei and tuned 19F in the parameter updater.

#### **Version 2.01.08 (28-May 2024)**

- Support for 14N added.

#### **Version 2.01.07 (21-May 2024)**

- Fixed an error in FindLock which would cause the stoplockandsat command to fail (Using in the Fluorine experiment).

#### **Version 2.01.06 (16-May 2024)**

- Linear prediction added to Fluorine experiment.
- FX3 support added for: T2-Li, T2-P, T2-Na, T2Bulk-Li, T2Bulk-P, T2Bulk-Na.
- A 4th step added to Powershim.
- 3<sup>rd</sup> order shimming added to StandbyShim.
- Access to pulse programming guide from pulse program editor fixed.
- Removal of relay checks in Spinsolve parameter updater.
- Real time modification of 2D plots during experiments disabled to prevent occasional crashes.

#### **Version 2.01.05 (24-April 2024)**

- For the FX3 the following commands now more fully support tables: delay, gradon, pulse and shim16. The delay command now supports delays up to 42 seconds while wait supports delays much longer than 42 s.

- The program now supports 2H and 3H nuclei.
- A new option in the file menu added to rename the protocol in experiment folders
- QuickShimTest -> QuickShim
- A bug in updating the project path fixed if a flat folder hierarchy is chosen.
- A bug in the DSP version of checkTemps fixed.
- Relay delay to switch to the X-nucleus increased from 1.5 to 2.0 ms.
- 0.5 us removed from dwelltime dropdown as this causes a crash on DSP Spinsolves.

#### **Version 2.01.04** (28-February 2024)

- Removed some duplicate code in all interface macros.
- Restricted the dwelltime to 1 us in the experiment UI for compatibility with the DSP Spinsolves.
- Restricted the minimum number of data points to 4.
- Fixed a bug in ProtonTTL which would result in phase shifts between scans.
- Increased the delay at the start of FX3 sequences from 1.5 to 2 ms to give slow receiver relays time to switch.

#### **Version 2.01.03** (16-February 2024)

- Rebuilt Prospa using only Visual Studio 2022.
- Improved the find-lock stability.
- Improved the phase stability of the FluorineHDec experiment.

#### **Version 2.01.02** (2-February 2024)

- Missing preferences parameter caused problems with common parameter list. (Also default common parameter list includes too many parameters).

#### **Version 2.01.01** (28-January 2024)

- Extra repetition time at the beginning of each batch experiment removed.
- Bug when adding waits before all batch experiments fixed.
- Pulse program information now added to each batch experiment file.
- Removed TTL trigger code from Proton experiment and added two new example experiments ProtonTTL and ProtonTTLFast
- Added code to allow the TTL output to be switched on before an experiment starts (for fast mode).
- Additional documentation for the pulse programming on FX3 Spinsolves.

#### **Version 2.01.00** (16-January 2024)

- Pulse programming documentation updated for DSP and FX3
- The 'Phase cycle' checkbox now works as expected.
- Fixed a bug in Prospa command execandwait which was preventing the TTLControllerTest scripts from working.
- Support added for 90 MHz spectrometer when accessing recommended dwellTime and rxGain.
- Ensured that double precision is used with the time command throughout Expert.
- Made repTime visible in the T2Bulk experiment.

#### **Version 2.00.29 - alpha** (30 November 2023)

- First step when locking now uses FFT to find peak fixing an occasional bug.
- Addition of new script to check system temperatures between batch experiments.



- Fixed a bug which was preventing the rampdrfpulse sequence command from working.
- Allowed for more than one shift point in the FluorineHDec experiment.
- Fixed issue with MNOVA exporting from NOESY experiments.
- Made switching between spectrometers without restarting Expert more robust.
- Fixed p1 phasing error in manualPhase1D macro (out by a factor of 2)
- Added 90 MHz magnet option to procedure getModelBasedParameters.

#### **Version 2.00.28 - alpha (23 November 2023)**

- CarbonNoP1 replaces Carbon
- DeptNoP1Short replaces DEPT
- DEPTX removed (same functionality in DEPT)
- FluorineHDecWaltz renamed FluorineHDec
- Fluorine now has no-P1 functionality.
- New offline development flag in preferences to allow saved preferences to be used or not.
- Bug in WobbleLock fixed (showed corrupted data sometimes).
- No-p1 delays for many experiment improved.
- Fixed a bug if loading save spectrometer parameters in off-line mode which was showing halved frequencies for 80/90 spectrometers.
- Parameter updater now shows connected spectrometer name.

#### **Version 2.00.27 - alpha (14 November 2023)**

- Fixed timing for rampdrfpulse on FX3 to match DSP version
- APT working more reliably.
- Fluorine pulse and collect with decoupling improved
- ProtonRepeat added – demonstrates how to write and reaction monitoring experiment.
- USB lights on Spinsolve now operate more sensibly.
- Jitter parameter for lock should now be chosen correctly on both FX3 and DSP systems.
- Lock mode reset if escape button pressed during find lock.
- Fixed a small delay error for FX3 version in MLEV and WALTZ pulse sequence blocks.
- Bug fix in ucsFiles relating to MNOVA export for X-channel nuclei.
- Version 3.20 of MSP430 software supporting improved USB LED management.
- Negative relay codes possible in spectrometer parameter block
- RepeatedExperiments expanded in script menu to make it more useful

#### **Version 2.00.24 - alpha (18 October 2023)**

- Missing DLL added for FTDI controller.
- Support for fast triggering using the FTDI controller for DSP Spinsolves
- Select Spinsolve works more reliably between FX3 and DSP Spinsolves
- Better support for multi-X DSP Spinsolves
- Modification to the find lock code to make it more reliable on some Spinsolves.
- Support for legacy 'enhanced Fluorine' systems added.

#### **Version 2.00.23 - alpha (4 October 2023)**

- All proton and carbon sequences updated and checked.
- Suppression sequences (WET) returned.
- MLEV4 sequence added for older Spinsolves.

#### **Version 2.00.21 - alpha (19 September 2023)**

- First version to support FX3 as well as DSP based processors.
- Allows interacting with multiple spectrometers simultaneously by using several Expert instances. This is done via a File menu option 'Select Spinsolve'.
- Better support for dual monitors.
- Dark mode slowly being introduced.
- 1D analysis tool added. Ability to compare multiple data sets.
- Current trace in 1D plots is indicated by a small coloured square in top left corner.
- For reference all experiments save a copy of the pulse program in the experiment data folder.
- Improved support for Multi-X spectrometers.
- Support for fast triggering using the FTDI TTL controller supplied by Magritek
- Note – not all experiments have been checked and the programming manual needs updating – hence the alpha tag.

#### **Version 1.41.20 (6 July 2022)**

- Support for Enhanced-Tritium added to the Spectrometer parameter reader/writer.
- New pulse program commands for generating isolated ramped RF pulses (rampedrfxx)
- Fixed bug in waltzend command: not switching off RF.
- All sequences recompiled.
- Delay on starting a sequence increased by 1.5 ms to allow for slow receiver relays.

#### **Version 1.41.19 (8 June 2022)**

- Fixed a bug in Prosopa which was causing a crash with large explicit arrays.
- Fixed bug introduced in 1.41.18 which caused an error if parameters changed using dropdown menus after selection from the history list.
- Removal of legacy sequences some of which were not working (Please contact Magritek if you need sequences which are not in the default menus).
- Improved support in SpinsolveParameterUpdater for 80 and 90 MHz Spinsolves.

#### **Version 1.41.18 (20 May 2022)**

- Removed the WET sequences (please contact Magritek if you need the flexibility of the Expert interface with these sequences.)
- Fixed a positioning bug in the variable temperature option in the Spinsolve Parameter Updater interface.
- Addition of INEPT and INEPT-Refocus experiments
- Addition of parameter callback possibility in pulse program file.
- xNuclei and allNuclei types added to pulse sequence UI
- Fixed a timing error in the T1IRT2 experiment.

#### **Version 1.41.16 (3 March 2022)**

- Addition of minimum magnet temperature parameter.
- Addition of CarbonDurationSweep experiment

#### **Version 1.41.15 (18 February 2022)**

- Addition of NOAH and NUS experiments. (Note that processing should be carried out in MNova).
- Removal of unnecessary lock delays at start of each sequence (Proton and Carbon).
- Replacement of settxfreqs command in some sequences with explicit channel 1 and 2 frequencies in relationships table.

- Use of the improved waltzdec command compared to WALTZ16 (uses ramped RF pulses to minimise cross channel interference on some Spinsolves).
- Replacement of ucsPlot:getPlotRegions command with the simpler ucsPlot:getPlotReferences in the experiment macros.
- A delay has been added between switching to the X channel and starting a sequence which fixes occasional first scan problems when changing nuclei. (This also helps with item 2).
- Better support for multi-X systems (explicit setting of channel relay for those experiments which need it e.g. HMQC)
- WETSuppression sequence added back after some modification.
- Powershim and Quickshim protocols now restore the shims on abort.
- Quickshim performance should now match standard software.
- Exporting shims and calibration to standard software should now be more reliable.
- Menu drag and drop working again in standard Prospa interface.
- Support for Sulphur 33 and Tin 119 added.
- New Sodium 23 menu added (see preferences).

#### **Version 1.41.13** (22 November 2021)

- New silicon menu with several experiments.
- Fixed bug in 'List parameters' option (Experiment menu).
- Experiment help now also displays the comment in the pulse program file in the CLI.
- Fixed bug in the PGSE post processing interface.
- Major tidy up of the DSP parameter read/writer macro.
- Addition of WETSuppression sequence as an option to the DSP parameter reader/writer.

#### **Version 1.41.12** (3 November 2021)

- New pulse program FluorineEnhanced for systems with Fluorine relays.
- New pulse sequence command skiponzero for jumping over code in certain cases. Used this new command in the FluorineEnhanced experiment.
- New pulse sequence command stoplockandsat to reduce the effect of the lock hump in Fluorine spectra (requires new firmware). Used in the FluorineEnhanced experiment.
- New pulse sequence acquire mode (integrateandscale) to prevent overflow during echo integration. Used in the pulse programs FluorineHDecScaled and ProtonFDecScaled.
- Fixed plot copy bug which prevented the correct range or text from being displayed.
- New pulse program FluorinePhDec.
- New lithium menu with several experiments.
- New preferences option to save the temperatures and lock history continuously. Still needs some debugging so use with caution!
- Option to specify a fixed pulse phase value instead of using the phase cycling table values p1, p2 .... Just use pName.
- New option to add a note to an experiment – see File menu.
- Removal of lock check after each experiment – should produce fewer false red lock indicators.
- Fixed bug which was causing the temperature setpoints to be invalid after writing the DSP parameters.
- The controllInfo dialog now has a button to copy the control parameter name to the clipboard. Useful when writing new pulse programs.
- Additional checks that the lock is running.
- More reliable monitoring of temperatures and lock status.

#### **Version 1.41.11** (10 September 2021)

- Addition of new Waltz command for decoupling which introduces less interference (waltzdec). Currently not included in sequences.
- Removal of a lot of redundant code.

#### **Version 1.41.10 (9 August 2021)**

- Added new experiment in Proton menu: ProtonFDec. Proton with Fluorine decoupling.
- Added new experiments in Fluorine menu: T1-F and T2-F. T1-IR and T2 experiments with Fluorine.
- Added new experiment in Carbon menu: T1-C. T1-IR experiment with Proton decoupling.
- Added new experiment in Phosphorus menu: T1-P. T1-IR experiment with Proton decoupling.
- When an error occurs while running an experiment the user interface is automatically reset. (No longer need to do this manually)
- If an error occurs during compilation when the temporary files generated are automatically removed.
- MNova call bug fixed for 2D data sets.
- gradpulse command added to pulse program blocks.
- WALTZ16 pulse programming block modified so it can run with RF gating switched off.
- Fixed out of range ppm axis error when plotting. (e.g. if central display frequency is outside display range limits).
- Added option to provide a ppm range number rather than explicit limits.
- Fixed bug where user menus with 'escaped' characters (t,n,r) at the start of directories were causing problems.
- Fixed a bug in QuickShim which caused it to incorrectly calibrate at the last step if the system had drifted too far from the factory default.

#### **Version 1.41.09 (15 July 2021)**

- Channel 2 frequency now added to the pulse program header along with option to explicitly set the channel 1 and 2 transmit frequencies and receive frequency in the pulse program relationship table (see Carbon experiment for an example).
- Parameters of selected experiments in the history list are now merged with the defaults for that experiment in case new parameters have been added since the experiment has been run.
- The number of scans performed in an experiment is now displayed when reselected from the history list.
- The display range in PPM can now be a 1D parameters (dispRangePPM) as opposed to explicit limits. This supported by the parameter group display\_PPM\_Range.
- Exit option added to the editor window file menu.
- ASM code in compiler window not loaded until the ASM tab is selected. This improves load time performance for some sequences.
- The 'Check X Wobble' option in the Monitor menu now supports multi-X systems.
- Spinsolve parameter updater now correctly displays basic Proton systems as P\$freq\$ rather than just \$freq\$.
- Spinsolve parameter updater now supports up to 5 X channels.
- QuickShimTest added which shows the parabolic fit for each shim step (only available in test mode).
- The sample changer interface now shows a progress bar.
- Corrected an error in the Nitrogen gyromagnetic ratio.
- The parameter updater has been modified to handle certain parameters used by the basic Proton spectrometer which are stored in the X-channel section.
- When the spectrometer is connected to the PC the SetLockShim code is automatically

copied to the spectrometer.

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#### **Version 1.41.08** (21 June 2021)

- Bug in QuickShim and StandbyShim corrected. They were adjusting the shims in the wrong order.
  - Pulse sequence DLL now includes dual channel shaped RF pulse that was removed from V1.41.00.
  - New composite pulse and spoiler pulse sequence blocks added.
  - Deuterium added as a possible nucleus in the Spinsolve parameter updater.
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#### **Version 1.41.07** (7 June 2021)

- Class documentation updated.
- acquireon/off commands documentation updated.
- Findf0 experiment updated to include spoiler at the end of the sequence. This improves the Lock and Calibrate script.
- Plot order corrected in the T1IR-H experiment
- Negative data in a log mode PGS(T)E plot was causing a fault.
- Delays in suspendLock and resumeLock modified to minimise distortions.
- Spinsolve parameter dialog now correctly updates the user interface for variable temperature systems.
- Functions which generate numerical table values in the pulse program relationships table are no longer copied to the guipar variable. This should speed up pulse programs in which these functions are slow.

#### **Version 1.41.06** (24 May 2021)

- External control of Expert now possible from Python.
- The acquireon/off commands have been extended to allow appending data.
- New experiments HMBCCOSY and HSQC\_HMBC demonstrate super-sequence pulse programming (CarbonLegacy)
- selmaging experiment demonstrates simple spin-echo imaging using shims. (ProtonLegacy)

#### **Version 1.41.03** (6 May 2021)

##### *Known bugs:*

- Some older legacy experiments will still not work without some modification.

##### *User interface*

- The SpinsolveExpert preferences dialog has been rewritten and now includes the interactive menu designer which previously was in the edit menu. Unnecessary items have been removed.
- The Program menu has been replaced with an Experiment menu. This contains some items which were in the edit and view menus but are more related to experiments.
- A new Scripts menu has been added with some example scripts including

ReactionMonitoring.

- Access given to some of the post-processing scripts - hold down the shift key and click to see the code (but see item 6 below).
- A Window-7 style button mode is available for use in Windows 10. See General page in the new SpinsolveExpert Preferences dialog.
- Various permissions now restrict accidental access to various parts of the program. See General page in the new SpinsolveExpert Preferences dialog.
- The history controls now skip empty days.

### *History mode*

- In addition to the year/month/day way of storing and viewing data you can also now view data stored in a single folder.
- A folder with data in it can be dragged and dropped onto the history list. This changes the experiment basepath.
- Expert experiments stored outside the date hierarchy can now be copied into it.
- Multiple history items can now be selected for comment renaming or trashing. (Depending on permissions settings – see preferences general button)

### *Batch mode*

- Batch mode now uses numbered folders which means comments no longer have to be unique for identical parameters.
- new/load/save/rename interfaces have been added to simplify handling of batches.
- Selecting a sample now gives a dropdown menu in the parameter area. This choice is reflected in the comment.
- A batch loop can control the sample selection. The sample comment can be a number, a loop index or using the 'samples' array and loop index, a name.
- Groups of batch entries can be copied, pasted, renamed, or deleted.
- Warnings have been added if batch parameter entries have not been saved.
- Array loops can now be added, allowing only certain samples to be selected.
- When running a batch, it is now possible to complete and halt the complete batch by holding down the shift key on the complete button.
- The total duration of a batch is now calculated and displayed with a second progress bar. This value can also be determined without running the batch by selecting the option from the Experiment menu (Ctrl-Alt-T)

### *Experiment handling*

- A new tool in the Experiment menu is provided to display the sequence in a graphical form.
- The code in each experiment can now be simplified by hiding some of the unnecessary details in a new procedure call runSequence (see Proton)
- Timing and progress commands have been removed from the execpp procedure (although old versions will still work).
- Timing an experiment has been significantly simplified with an expectedDuration procedure.
- The progress bar is continuously updated during an experiment (not just at each scan).
- The total duration of an experiment can be determined without running it, by selecting the option from the Experiment menu (Ctrl-Alt-T)
- A parameter list can now be saved for later use (option in the Experiment menu)
- Better MNOVA support using Javascript and MNOVA templates taken from the standard software.

### *Protocols*

- The experiments T1, T2, PGSE and PGSTE now support real time integration selection.
- T1T2 and DT2 experiment have been tidied up and moved from the legacy to Proton and Diffusion folders.
- A reaction monitoring experiment has been added to the Scripts menu which supports real time integration selection.
- A bug in calibration has been fixed. Before there was an issue if lock and calibration was done on a non-water sample and then the calibration was imported from the standard software.
- Expert shim and calibration data can now be exported back to the standard software.
- The COSY experiment has been improved - it now supports the FAD modification and multiple scans.

### *Postprocessing*

- A simplified interface has been added for defining post processing controls (see Proton for example).
- A new integration tool has replaced the previous peak-picking and integration tools.

### *General*

- Now supports multiple X nuclei.

### **Version 1.40.9** (14 October 2020)

- Power and Quick shim now have options to support Spinsolve Ultra systems.
- Quick shim is now more efficient performing fewer measurements.
- The fraction of an experiment completed is now recorded and shown when an experiment is reloaded.
- The overflow light wasn't being reset when a new experiment was started.
- The Setup menu has been simplified and the documentation updated.
- The Script Template has been simplified to make file saving easier.
- Monitor experiments now show progress.

### **Version 1.40.8** (28 September 2020)

- Updated experiments modified to use a central ppm value rather than an offset.
- Updated experiments modified to show the detection bandwidth in ppm.
- Updated experiments now export the ppm scale correctly to MNova.
- Updated experiment now reprocess data correctly.
- New updated experiments for Phosphorus and Fluorine.
- Bug fix: acqu.par file was not being updated with correct common parameter values.
- More sensible 2D contour levels chosen.
- Help added for all fixed main menu items.

### **Version 1.40.7** (16 September 2020)

- Check marks added in some of the menus to show status.
- Simplification to the multiview options in the view menu.
- Dividers are more obviously draggable.
- History list is now sorted with most recent file at the top.

- Missing batch boundary entries in the history list restored.
- Changes to the batch list are immediately saved.
- Copy protocol gives the list of previous comments as an option.
- Batch commands which don't collect data now blank the graphs
- Batch commands without parameters now blank the parameter list.
- Can now load previous experiments even if not connected to a spectrometer.
- A new experiment can now save the defaults file even if one is not present.
- Options for different digital receiver N values added (experimental only)
- The temperature monitor has been extended to also show the lock offset.

#### **Version 1.40.6 (3-August-2020)**

- A data file search option added to the file menu.

#### **Version 1.40.5 (27-July-2020)**

- Titles added to all list boxes and columns can be resized.
- Bug in StartAtTime and WaitTime preventing batch abort. Fixed.
- Changing comment/sample name in batch list now has access to full sample name list.
- Some icons next to batch list changed to make their function more obvious (?)
- Clearing the batch list now removes all data folders to the trash.
- Making a change to the parameter list changes the batch parameter update icon (a check)
- Autophase option added to time domain data in Proton protocol.
- Data sets for Proton, Carbon and COSY acquired with the standard software can now be viewed using SpinsolveExpert.
- Bug in sample control in which blank entries can be entered preventing reloading. Fixed.
- Target linewidth added to Quickshim. (To prevent double shim).
- Short cuts for cut, copy and paste now working in textboxes.
- Addition of Prosopa Window Designer in Program menu.
- Additional parameters added to SpinsolveParameterUpdater to support lock shimming.

#### **Version 1.40.4 (24-June-2020)**

- Updated all Proton and Carbon pulse programs to use more descriptive variable names.
- Introduced pulse program blocks such as WALTZ16 and MLEV17 to simplify complex sequences.
- Checked that all Carbon sequences can export to MNova (Only HSQC-ME needs work). This required f1 bandwidths in kHz.
- Most Proton and Carbon sequences can now be post processed using the FT command button.
- Extended the batch loop command to allow an arbitrary list of numbers e.g. loop 1, lc1=[1,4,12,19] Good when the sample changer is only partially full.
- Selection of PGSE and PGSTE integrated peak curves for NNLS fitting improved.
- Selection of T1 and T2 integrated peak curves for NNLS fitting improved.
- Sample name (comment) now has a drop-down menu with all sample names entered visible.
- Quickshim has a target linewidth - if above this it will reshim.

#### **Version 1.40.3 (12-June-2020)**

- Updated the PGSE and PGSTE experiments and moved them from the DiffusionLegacy to the Diffusion folder.
- The maximum gradient for the PGSE experiments is now taken from the DSP parameter



- block not from the preferences file.
- A special version of the integrate macro added for PGSE experiments.
- Updated the AnalyseDiffusion macro to work better with the PGSE and PGSTE experiments.
- Fixed a bug which was preventing several Setup macros from being added to the batch list.
- "Load Expert Shim and Calibrate" option added to setup menu.
- Parameter ranges are now checked before running an experiment or adding to the batch list.
- Legend option added to 1D plot view along with axes menus in 1D and 2D plots.
- Drag and dropped pulse program folders are now added to the valid pulse program list immediately.
- Buttons added below the history list to allow stepping through dates.

#### **Version 1.40.2 (9-June-2020)**

- Addition of minimum visibility files to Carbon experiments.
- "Load Standard Shim and Calibrate" option added to setup menu.
- Import old data option added to files menu.
- Common parameters now readonly and coloured dark green in parameters list.
- Checks are made so that all delays and waits must be  $\geq 0.2$  us before a sequence can run.
- 'Open application folder' moved to files menu.
- Help added for File and Edit menus.
- Confirmation added when exiting SpinsolveExpert
- Removed restriction check on linewidth before saving shims to prevent batch blocking
- Updating common parameter file when saving selection in preference dialog.

#### **Version 1.40 (21 May 2020)**

- The standard mode of operation has been changed so that data is stored in a date and time stamped history list. All experiments recorded in a single day can be viewed.
- The experiment number option have been removed since there is now no possibility of overwriting previous data.
- A special batch mode has been added to replace the previous default experiment mode. This has been extended to include loops.
- All experiments are now accessible from the main menu. This menu can be modified to add new experiments.
- Most of the setup experiments now save their data and are added to the history list.
- By default, experiments are now displayed with a minimal list of parameters. This can be modified in the Edit and View menus.
- Experiments recorded with older versions of Expert will need to be modified before they can be opened with the new version (option to be added).
- The core macros of the program have been reorganised to make them class based (hence the version number jump).

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#### **Version 1.33 (11 March 2020)**

- The Proton experiments have been renamed and trimmed to match those in the standard software. All experiments have been tested to work 'out of the box' without changing sequence specific parameters.
- For improved data security previously run experiments are now write protected by

default. Parameters cannot be modified and the experiment cannot be rerun. Just copy the experiment if you want to rerun it or use sub-experiment numbers.

- Simple Quickshim and Powershim options have been added to the Setup menu.
  - The scripting interface has been rewritten to make it more reliable. If used, user interfaces for scripts are now displayed in the main window rather than in a pop-up dialog (see reactionMonitoring or autoSamplerTest scripts).
  - A new Setup pulse program folder has been added with experiments to shim and lock.
  - A new experiment type has been added called a Protocol. This allows multiple experiments to be run from a single experiment name in the 'Experiments to run' list using the scripting commands (e.g. loadStandardShimLockAndCalibrate in the Scripts folder) or more traditional backdoor techniques (e.g. PowerShim in the Setup folder).
  - Zooming can now be performed in most 1D plots while acquiring data. Some limitations still.
  - The main menus have been reorganised to allow easier access to the experiments (Proton and Carbon for now).
  - Basic Autosampler control has been added with the SelectSample option in the 'Experiment to add' drop-down menu and also autoSamplerTest in the Scripts menu.
  - A new procedure called getFactoryBasedParameters can be added to the Experiment control macro to automatically update special parameters which are dependent on the Spinsolve factory (DSP) parameters. See the PresatMulti experiment for an example.
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#### **Version 1.31 (18 September 2019)**

- Support added for experiments which use bandwidth (variable bandwidthPPM and acquisition time (variable acqTime) rather than dwellTime and nrPnts. See 1PulseBW-H for an example.
- Support added for additional nuclei 7Li, 11B, 15N, 29Si.
- Improvements to the locking algorithm.
- Monitor lock now scrolls after 100 time steps.
- Improvements in the initial shim algorithm (faster and QuickShim option).
- Nops added to several pulse program commands to improve stability on some electronics frames.
- disableLock and enableLock commands added to ucsUtilities.mac
- Correct jitter parameter used for Lock.
- Default frequency unit is now Hz, not kHz.
- jRes processing tab added.
- Bug when saving MNova parameters fixed.
- Generate1D/2DFrequency axis procedures added to simplify macros.
- Linear predication code added to ucsRun.mac
- Macros included in Spinsolve-Expert folder to batch compile all experiments (CompileAll.mac and CompilerBackDoor.mac).
- Fixed a bug which was preventing some common parameters from being updated.
- Multispectrometer support.
- More standard DSP parameter files added.
- Improved performance of 2D display macro.
- 2D display viewer supports ctrl-drag zooming.
- Fixed phasing included for 2D processing.
- Bug fixed in calibrateXAxis.mac
- Bug fixed in calibrateXYAxis.mac
- Receiver phase is now taken from user interface and not from common parameter file.
- Commands added to support alternative board to DSP (test only)

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**Version 1.28** (17 July 2018)

- Support for Spinsolve Ultra and 80 added.
- New DSP firmware included to initialise shims at startup.
- New DSP parameters added.
- Easier zoom mode in plots (ctrl-z).
- Simplification in experiment macros with introduction of generate1DFrequencyAxis procedure.
- Array type added to pulse programs.
- Linear prediction prototype added for p1 free spectra.
- MNova data parameters improved.
- New experiments added.
- Numerous bug fixes.

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**Version 1.24** (18 March 2017)

- Six X-nucleus experiments and support added.
- Documentation for Proton and X nucleus added.
- 1 Proton, 16 Carbon, 4 Diffusion and 3 new Phosphorous experiments added.
- All Proton and X nucleus experiments can now export to MNova.
- Experiment names can be modified from the user interface if necessary.
- The pulse program list is reset when a new install occurs.
- Fully interactive help can be displayed in a separate window while an experiment running.
- TTL external trigger option provided for those Spinsolves which support it.
- Improved line drawing in plots.
- Improved zooming display added in plots.
- Hypercomplex option added in 2D FT dialog along with several display bugs fixed.
- Improved Spinsolve DSP parameter dialog added.
- Support for 60 MHz Spinsolve added.
- Spinsolve-Expert preferences dialog updated to include spectrometer controlled timing, trigger activation, spectral ppm offsets and gyromagnetic ratios.
- New DSP firmware added to support spectrometer controlled timing.
- New transceiver firmware included to provide improved dynamic range.

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**Version 1.20** (26 January 2016)

- The Hz/ppm post processing button does not flip the spectrum (proton experiments only as yet)
- Combined peak picking and integration post processing interface with automatic peak picking and integration options. (Post processing button 'Peak')
- Use of stacked plots within many Proton experiments rather than 2D plots.
- Fixed bugs in movement of stacked plots.
- Addition of tilted and hidden line removal in stacked plots (see post processing button 'View')

- Curve fitting post processing button interface for stacked plot experiments. ('Integ.')
- Enlarging/reducing the plot view does not reset the display.
- PPM integration range parameter entry now possible (e.g. see 1PulseDurationSweep) in proton experiments.
- Lorentzian or Gaussian line-broadening possibilities following reference deconvolution in 1D post processing interface ('FT' button)
- Ability to hide certain rarely changed parameters using 'Toggle parameter visibility' in View menu.
- Ability to apply common parameters to all experiments in a project list ('Apply common par' button functionality extended)
- The processed FID following reference deconvolution is saved to a .1d file suitable for MNova import (see 1D post processing interface - 'FT' button)

Notes:

- A new 1D plot file format is introduced to support features 1 and 5. This means older versions cannot read this data.
- New peak picking and integration file formats. This means the new version can no longer read old peak lists.

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### Version 1.11 (11 December 2015)

Parameter handling made less confusing:

- Common parameters are only applied when a new experiment is added. Changing between experiments does not update common parameters.
- A new experiment takes the default parameters and merges them with common parameters. The last experimental parameters or other experiments of the same type in the experiment list are no longer used (although the latter are still used in scripts).
- Common parameters must be entered manually apart from B1 frequencies which are updated by the Findf0 experiment. Previously this was done automatically when changing experiments which could cause confusion.
- Experiments can be set up so they automatically generate subexperiments when run. In this way new experiments will not overwrite old ones.
- By default overwriting existing experiments now displays a warning.

Access to MNova is now easier:

- Previously the 'd' used at the end of B1 frequencies stored in the acqu.par file was a problem for MNova. This has been removed and the numbers are now longer to reflect their double precision value. This change has only been applied to the acqu.par file to minimise possible bugs this change might other introduce.
- A special command to save data in MNova compatible format can be added to the experiment file.
- Because of these two changes SpinsolveExpert data can now be loaded into MNova by opening the file or by dragging and dropping. Some experiments also have an MNova button which allows this to be done directly from SpinsolveExpert.

- A modification to the experiment icon in the experiment list shows when MNova compatible files are available.
- More than 30 new experiments have been added.

#### Some minor new features added

- Different common parameters are stored for each spectrometer which might be connected to the software. This includes the built in simulator.
- The name of the spectrometer used to acquire the data is stored with the recorded data and also displayed in the plots when loaded.
- The FT button for 2D data sets now support hypercomplex transforms.

#### A number of minor bugs have been fixed:

- A correction was not being applied to some of the measured Spinsolve temperatures.
- A correction has been made to the pulse program compiler to make Wobble pulse sequences compatible with the new PIN diode based duplexers.
- Optimize shims would not run unless Initial Shim had been run first. Also Optimize shim now uses a longer acquisition time to improve resolutions.
- Subexperiments cannot have a parent (toplevel) experiment and vice-versa.

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#### Version 1.01 (20 August 2015)

- Support for numbered sub-experiments added to the main interface and recompiled experiments.
- A new scripting menu added. Scripts are now more general and can be run from menus or user generated dialogs.
- A windows designer has been added to the Script menu to allow user generation of dialog based scripts.
- A new 1D stacked plot display mode added (new pulse sequence T1IRSP-H added to demonstrate this).
- A peak integration and curve fitting example script added to post process data from T1IRSP-H.
- Spinsolve-Expert can now be started from external programs.
- Less control flicker when running experiments, especially scripts.
- Faster processing.
- Help viewer can be opened while running an experiment.
- Fixed a scrolling bug in the parameters panel.
- Holding down the shift and control keys when starting SpinsolveExpert resets parameters.
- A reaction monitoring example script added.
- The 1Pulse experiment modified to return the complete parameter list. This is used in the reaction monitoring script.
- Small errors in gyromagnetic ratios and B1 frequencies fixed in the FindF0-H experiment.
- Initial shim takes longer but should give narrower linewidths.

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**Version 1.00** (24 July 2015)

- 1D post processing macro expanded to include segmented baseline correction and deconvolution.
- Expanded 2D post processing macro with separate f1 and f2 tabs with baseline correction and deconvolution.
- proc.par file added to some experiments to store processing parameters.
- Better multinuclear support.
- New carbon experiments added.
- Standard Spinsolve data set importer added.
- New viewing controls allow plot enlargement while running experiments.
- A ppm display range added to many experiments.
- The initial shim function is now easier to use.
- Proton presaturation experiment added.

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**Version 0.98** (4 June 2015)

- Peak picking added
- Peak integration added
- 2D plot viewer added which includes row/column and projection display.
- Waterfall display moved to 2D plot viewer
- New autophase algorithm added based on maximising the baseline extent.
- First order phase correction now tied to experiment rather than fixed
- Separate application included to allow extraction of shim settings from standard Spinsolve software.
- A simulator menu option added which allows 1Pulse experiments to be performed without a spectrometer.
- Interactive help provided for special commands in Script Editor.

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**Version 0.97** (14 April 2014)

- WaitUntilTime command added to script editor.
- ppm offsets can be applied to 1D spectra
- Autophase and zerofill options added to Transform post processing interface.
- Ability to load factory defaults for shim settings added.
- New script example added which emulates the 1PulseAmplitudeSweep expt.

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**Version 0.96** (10 March 2014)

- New Proton experiments added: T1IRT2
  - Major internal reorganisation of macros.
  - Actual probe parameters used in setup experiments rather than defaults.
  - T1 and T2 relaxation spectra inversion options added.
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#### **Version 0.95 (15 February 2014)**

- Splash screen added on startup.
  - Lock and temperature checked before and after experiments.
  - Lock starts searching using correct resonant frequency.
  - Layout lists can now be 2D simplifying code.
  - Data file names removed from load layout list (only in experiment macro now).
  - Experiment specific post processing buttons and macros added.
  - 2D apodization, zerofill and FT macro added.
  - MNova button added (limited functionality as yet)
  - New 2D display control macro added.
  - Restore common parameters to default setting button added.
  - Previous project folders can be recalled.
  - Added option to view experiment help (although no help added yet!)
  - Progress bar updates added to autoshim.
  - Tooltips added to autoshim controls.
  - Linewidth reported to CLI when checking shims
  - Improved autophase option based on minimising rms value added to T2CPMG\_Bulk.
  - Definition of apodization sinebellsquared filter modified to match MNova's
  - A new pulse program can now be saved in a different location than the default.
  - Plot margins can be correctly set and remembered.
  - Uncertainty option added to T2Analysis macro.
  - All experiments now load and save data in V3 as well as V4 format.
  - 2D images can now be displayed in log mode to give better peak visibility.
  - Script editor interface now disabled during experiments.
  - To open compiler from experiments to run list press enter now don't double click.
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#### **Version 0.94 (4 December 2014)**

- Layout and Windows menu combined.
  - Searchable Help added.
  - Faster 2D inverse Laplace added (license required)
  - Additional error checking added
  - Pulse programs moved from subfolder of Spinsolve-Expert to subfolder of Macros
  - Both version 4 and older version 3 pulse programs can be compiled and executed.
  - Version 3 of the interface can be opened from the File menu.
  - Script editor checks for modified files before exiting.
  - Image, GetCommon, GetPrefs and SetCommon and UseCommon commands added to script editor.
  - Various NMR experiments upgraded to work with SpinsolveExpert.
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#### **Version 0.92 (19 August 2014)**

- Fixed bugs in File menu options: Save project parameters, Load and Save default parameter file.
- Hz/PPM post processing button now checks to see if the current plot is a spectrum or not so as to display the correct label.
- The Restore parameters button now works with numbered sub-experiments.
- "Display release notes" added to Help menu.
- Spinsolve DSP parameters accessible from all edit menus.

- Export post processing button added. Can export in Prospa binary or csv format.
  - Manual phase doesn't reset the zoom setting when closed.
  - 1Pulse default parameters corrected.
  - Common parameters set correctly in Spinsolve preferences dialog.
  - 2D data sets will now save in .csv or .2d format if selected from preferences dialog.
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#### **Version 0.91** (15 August 2014)

- Program now keeps track of plot changes. Several of the processing macros now flag that a change has occurred. If these have not been saved you will be prompted to save them on closing the program.
  - The experiment list folder now displays icons. A dot to show there is an acqu.par file, a spectrum to show data (pt1/pt2) is present. These are combined when both are present.
  - Pulse programs can be stored in multiple folders (typically outside the install folder). The folders are accessible via the pulse-program folder text menu. There is also a reset in the menu. This information is stored between shutdown and startup.
  - Calibrate2D initialises the ppm values to 0.
  - Pulse Program Compiler
  - Commented out template option in Files menu – this is not ready yet.
  - The Files-Copy option allows user to copy pulse programs to other folders in addition to the default.
  - The Files-Copy option Interface file is also copied (so plot layouts are kept)
  - Script Editor
  - Updating experiment list icons before and after each experiment and when data is saved.
  - Can work with pulse programs from multiple folders.
  - Modifications to parameter files for lock, shim and wobble to ensure no data is saved and acquisition files are saved to a temporary directory rather than to random locations on the C drive.
  - Can't run lock or wobble experiments in shim mode.
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#### **Initial release Version 0.90** (13 August 2014)