Processing 1D Data Sets

This document describes the interface used to reprocess 1D data which has been collected with SpinsolveExpert. This can be displayed by pressing on the FT post-processing button for 1D experiments. This displays the following interface.

A screenshot of a computer

Description automatically generated

Using this dialog we can reprocess the FID data setting the zero fill, phasing, and apodization as well as applying a reference deconvolution and a baseline correction. Then the axes can be displayed in PPM or Hz.

When the interface is first opened the various parameters are populated from the file proc.par which is generated when the experiment is run. (Using the procedure saveProcPar)

This ensures that, by default, pressing the Transform button should reproduce the saved spectrum. Any changes to the processing done using the above interface will modify this file.

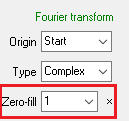
A variety of apodization functions are provided and more can be generated using the filter interface accessible from the Filters button or via the small button labelled ‘…’ in the Apodization section. Perhaps more usefully, there is an option called exp:1.

A screenshot of a computer

Description automatically generated

This will apply an exponential broadening with a linewidth of 1 Hz. This latter value can be modified by changing the ‘1’ to some other number.

In the Fourier transform section is a Zero fill field (zf).



This will modify the FID by a adding a number of zeroes at the end of the FID to increase the data set size by the factor in this field. A zero-fill of 1 does nothing, a zero fill of 2 will double the size of the data by adding zeroes at the end, 3 will triple it and so on. Zero-filling smooths the spectrum by interpolating between points and may give a small resolution improvement. Be careful when applying this without apodization as it may result in ‘sinc wiggles’ in the spectrum if the FID data is not close to zero at the end of the fid.

Another way to improve the resolution is reference deconvolution.

A screenshot of a computer

Description automatically generated

This is done by collecting a high-resolution spectrum of the reference sample using the CheckShim experiment in the Setup menu. Note that the dwellTime used here (which defaults to 200 us) should be the same as the one used for the FID you are trying to deconvolve. This is because the deconvolution process divides the sample FID by the reference FID, and so the times should match. You should always collect a reference FID soon after locking and calibrating to ensure you are working on resonance. (Otherwise a divide by zero may occur).

Because of the division process, noise at the end of the deconvolved FID will be enhanced. To preserve SNR you will need to add some additional line-broadening. You can select the resultant line-shape to be Lorentzian or the slightly narrower Gaussian. Note the improvement in resolution comes at the cost of a reduction in SNR.

Another way to collect a reference FID it to performing a StandbyShim with the Collect reference option selected.

A screenshot of a computer

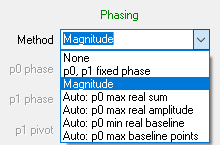
Description automatically generated

Note that the reference FID is stored in computer memory and so is lost if Expert is closed. If you wish to use a saved spectrum then you can choose the ‘From file’ method. In this case use the ‘Select reference FID’ button and navigate to a CheckShim experiment folder and select the fid.1d file.

A screenshot of a computer

Description automatically generated

The last step for most experiments is phasing. For magnitude mode experiments this simply means taking the magnitude of the final spectrum. This is selected using the Phasing method.



There are a number of autophasing options – select the one which works best – note that these only apply a p0 correction and are applied immediately when selected – you don’t need to press the Transform button.

Alternatively, you can select the fixed phase option.

A screenshot of a computer program

Description automatically generated

In this case you have phasing values you can enter manually and adjust using the up-down controls (steps are +- 1 degree but with shift held down +- 10 degrees and alt +- 0.1 degrees. Or perhaps more conveniently use the phase sliders which are displayed when the Phase button is pressed.

A screenshot of a computer

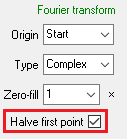
Description automatically generated

The final processing step might also include a baseline correction although if linear prediction has been used when collecting the data this should be minimal. There are two options; Offset and Segment.

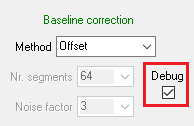
A screenshot of a computer

Description automatically generated

Offset just applies a vertical offset to the baseline so it is zeroed. This will also be affected by the ‘Halve first point option’ in the Fourier transform section. This should typically be selected.



If the debug checkbox is selected in the base-line correction section the spectral plot will display a line showing the calculated baseline but won’t apply the correction.



If the Segment option is chosen, then the algorithm will search for baseline points and in debug mode will mark these along with a trigonometric fit. The following data set was obtained with linear prediction turned off and a dwell-time of 1 ms. 64 segments were chosen with a noise factor of 2.

A graph of a graph showing a number of data

Description automatically generated with medium confidence

You can adjust the number of segments and noise factor to optimise these points. Once satisfied, remove the debug option to apply the correction. In the following plot this result is displayed in green, and compared with a data set (in red) obtained with linear prediction switched on.

A graph of a graph showing a number of different colored lines

Description automatically generated

The final option is to set the axis units. This can be in Hz or PPM – PPM is the default. Note for most experiments there is a post processing button with this option as well.