Processing 2D Data Sets

This document describes the interface used to reprocess 2D data which has been collected with SpinsolveExpert. This can displayed by pressing on the FT post-processing button for 2D experiments. This displays an interface with 3 tabs. One for processing the f2 (horizontal) axis of a 2D FID, another for processing the f1 (vertical) axis after f2 has been processing and then any further processing which should be applied to the spectrum (the Other tab – currently only used for the JRES experiment).

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Description automatically generated

Both the f2 and f1 axes tab have identical processing possibilities. We can apply apodization, zero fill, Fourier transform and then post-phase. 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.

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. See section xx for details on how to add items to the apodization menu.

The apodization function will be multiplied by the current row (f2) or column (f1). This can be used to improve the spectral SNR or reduce artefacts.

In the Fourier transform section is a Zero fill field (zf). This will increase the length of each row (f2) or each column of the f2 transformed data set 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 fill smooths the spectrum by interpolating between points and may give a small resolution improvement.

Once apodization and zero filling have been applied a one dimensional fast Fourier transform is applied to the resultant row or column. Note that the number of points in the raw data must be a power of 2, Prospa does not support arbitrarily sized FIDs. There are several type of transform provide. In f2 the most common one is Complex which generates a spectrum with the same number of points as the zerofilled FID with frequencies ranging from -0.5/dwellTime to 0.5/dwellTime with a resolution of 1/(nrPnts\*zf\*dwellTime). This is the same as the transform applied to most 1D experiment.

The Real option performs a real fast Fourier transform which just generates real data with half the number of data points as the original data set with frequencies ranging from 0-0.5/dwellTime and a resolution of 2/(nrPnts\*zf\*dwellTime). This option is included for completeness but would only be used if the second dimension did not need to be transformed.

The Origin option can be Start or Center. This reflects whether the f2 data is FID or Echo like. The vast majority of 2D experiments in Expert should use the Start option.

If checked the halve first point option will hlave the value in the first row or column of the data before transforming it. This accounts for the asymmetry of data collected in NMR – negative time is not present. The result of not doing this can be a small offset in the spectrum. If an apodization is applied which is zero at the start (such as sinebell or sinebellsquared) then this option is not required.

Once the f2 transform has been applied a second transform along f1 is then performed. This can be more complex depending on the experiment. Experiments which will be displayed in magnitude mode (such as gCOSY or gTOCSY) will have a Complex transform applied in f1 followed by a magnitude calculation (this option is selected in the phasing section) or in the case of TPPI collected data a real transform in f1. Phase sensitive experiments require two FIDs to be recorded per evolution time which the phase of the data modified such as to give complex data in both dimensions. Two variants are supported by Expert – the echo-anti echo transform and the hypercomplex transform. Examples of both of these transforms can be found in the HSQC experiments provided.

The last step for most experiments to phasing. For magnitude mode experiments this simply means taking the magnitude of the final spectrum. This is selected using the f1 phasing method. For phase sensitive experiments the data should be phasing using the fixed phasing options. The phase values (p0 and p1) can then be optimized using the phasing updown controls:

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Here the range of the updown control defaults to +- 1 degree per click but can be adjusted by holding down the shift (+-10 degrees) or Alt key (+-0.1 degrees)

More rapid adjustments can be made using the phase sliders which become visible when the Phase button on the right of the interface is selected.

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The phase range of each slider can be controlled by entering the desired range to in the text-box to the right of the slider and pressing enter.

Note that the correct phase adjustment will depend on the type of experiment being performed.

Once a 2D FID has been reprocessed the result can be saved using the post processing save button on the right of the main interface or more conveniently using the Ctrl+S short cut defined in the main File menu. This will also save the plot layout.

Note that it is possible to just process the data in f2 and do nothing in f1. In this case choose the type *None* for the f1 transform, *None* for Phasing and Apodization and remove the PPM display check.

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| You may you need to adjust the 2D display controls (color-scale) to see the resultant data. This option, shown here, is available in the default 2D post processing button list. |  |

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Please refer to the help in this interface for more details. This also allows you to change the number of contours plotted and the color scale used.