COSY processing in ssNake

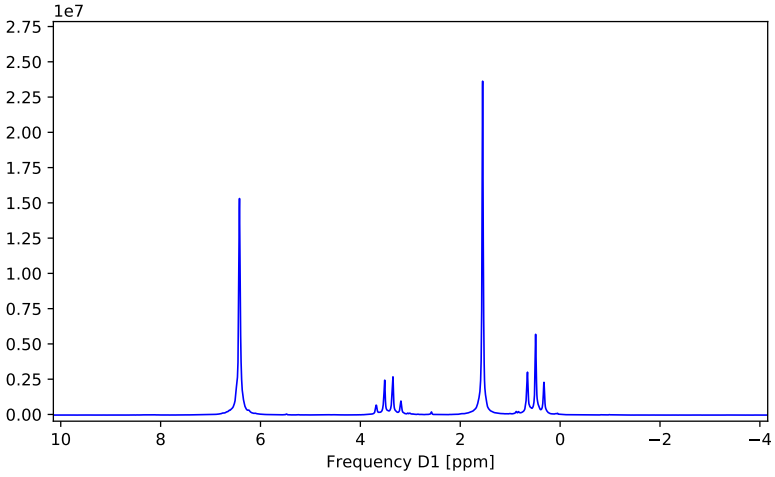
13th December 2018

1 Introduction

A correlation spectroscopy (COSY) experiment is one of the most common 2D NMR experiments. It is used to visualise through-bond connections in molecules (via J-couplings). In the 2D spectrum, cross-peaks appear between lines which are J-coupled. As J-couplings are hard to observe in the solid state, COSY experiments are usually only recorded for liquid state samples. In this tutorial, we will show how to process magnitude COSY data (a phase sensitive COSY should be processed differently).

2 Data

The data for this tutorial is a magnitude type ^{1}H–^{1}H COSY spectrum of a mixture of toluene and ethyl pyruvate (1:1) recorded on a 1 T (43 MHz) Magritek device. In this case, we expect to see cross-peaks between the two lines of toluene, and between the CH_3 and CH_2 resonances of ethyl pyruvate (the base methyl group of ethyl pyruvate overlaps with the methyl group of toluene). The 1D ^{1}H spectrum of this sample is shown below.

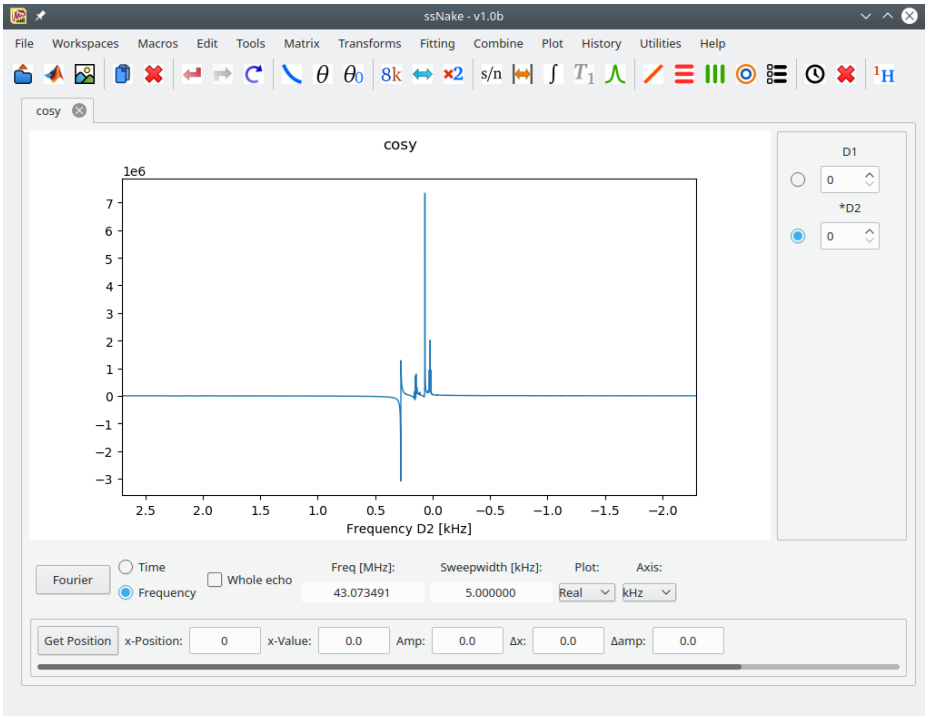


3 Processing the data

In principle, processing a magnitude type COSY spectrum is no big deal. All that is required is a Fourier transform along both axes.

- Open the Magritek file using `File` ⟶ `Open` and navigate to the 'cosy' folder. Opening one of the files here opens the data
- Fourier transform via the 'Fourier' button

This should give:



Note that the line we see here have a very bad phase. This is not important, as the final view of this data only means something in absolute mode (we will do this later on). We also need a Fourier transform in the indirect dimension:

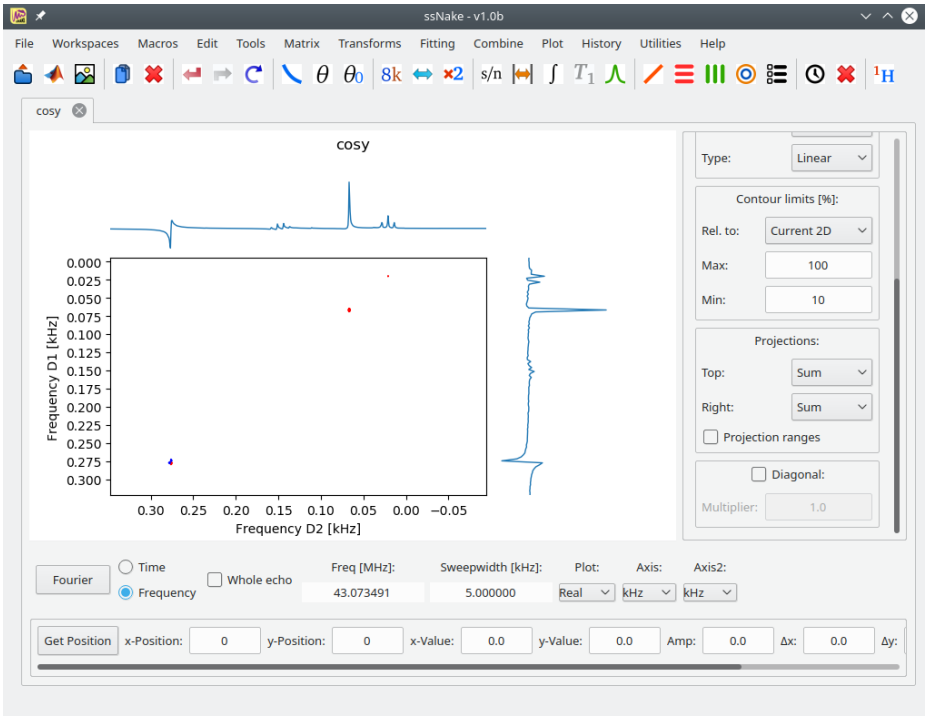
- Switch to viewing D1 by clicking on its radio button in the sideframe
- Do a complex conjugate via `Tools` ⟶ `Complex Conjugate` [1]
- Fourier transform via the 'Fourier' button
- Switch back to viewing D2 by clicking on its radio button in the sideframe

[1] Doing a complex conjugate flips the resulting spectrum. This is needed in ssNake, as Magritek uses a different definition for the rotation direction of the magnetization. For the direct dimension, this is always necessary, and is done by ssNake upon loading the data. If the indirect dimension is also a spectral axis, you need to do this manually for this axis. If you do not do this, the resulting spectrum will be mirrored.

Now that we have processed both dimension, we want to view the spectrum as a contour plot:

- Switch to view to a contour plot via `Plot` ⟶ `Contour`

This should show (zoomed in):

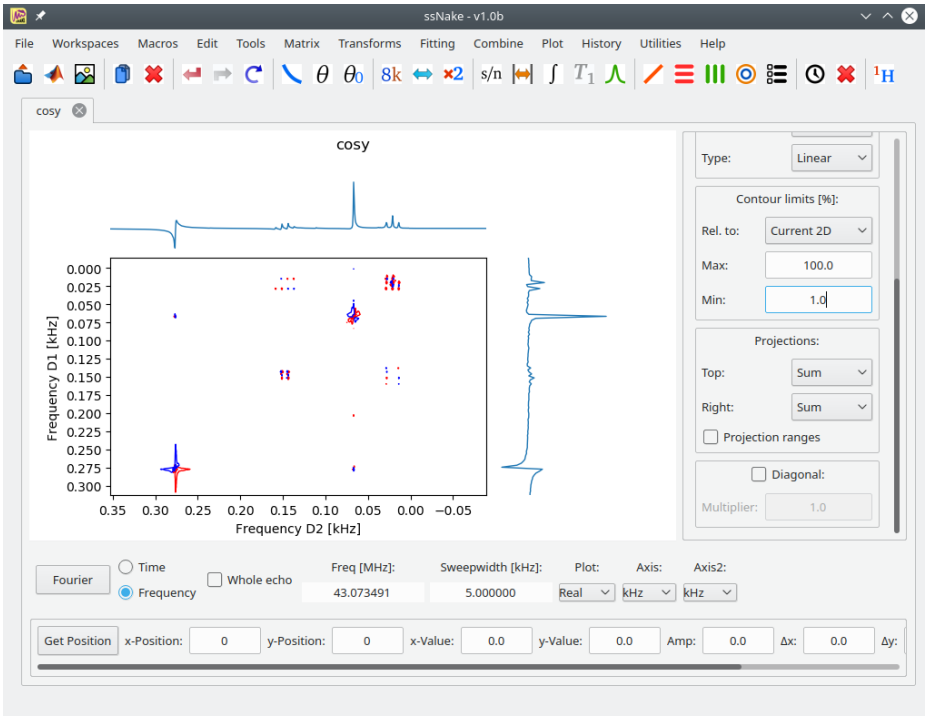


We are not seeing much, but the lower contour cutoff is at 10%, so we should lower this to see more:

- Set the minimum contour limit to 1% (in the sideframe, under 'Contour limits')[2]

This shows:

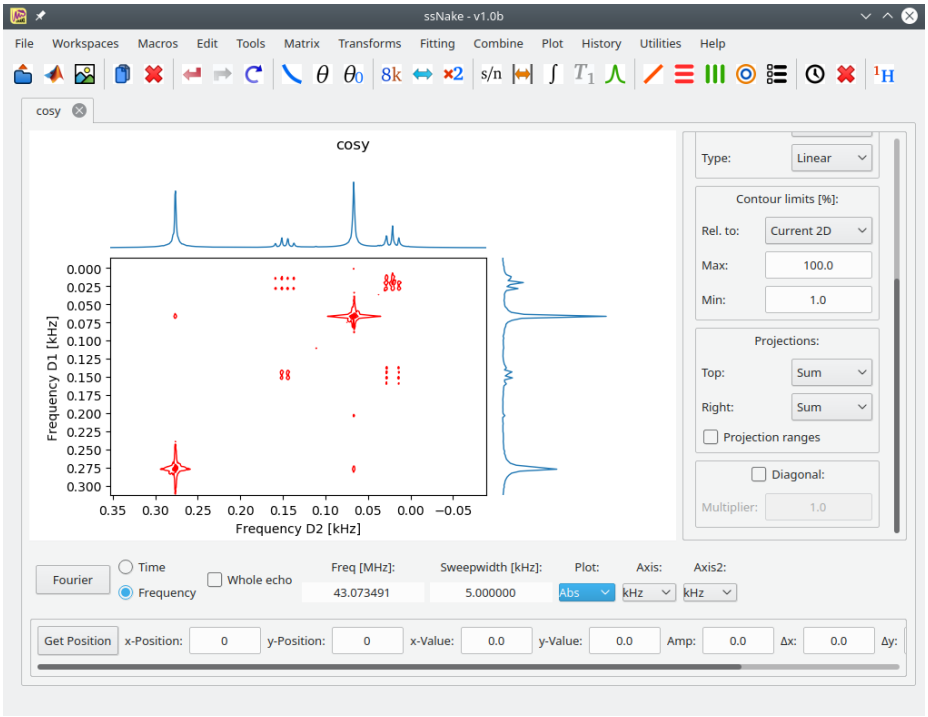
[2]Note that you can also 'zoom' the contours by scrolling the mouse button while holing the 'shift' button



As you can see, we have some issues with the phase. This is because we should view this data in absolute mode:

- Set the plot to absolute (bottom frame under 'Plot' set to 'Abs')

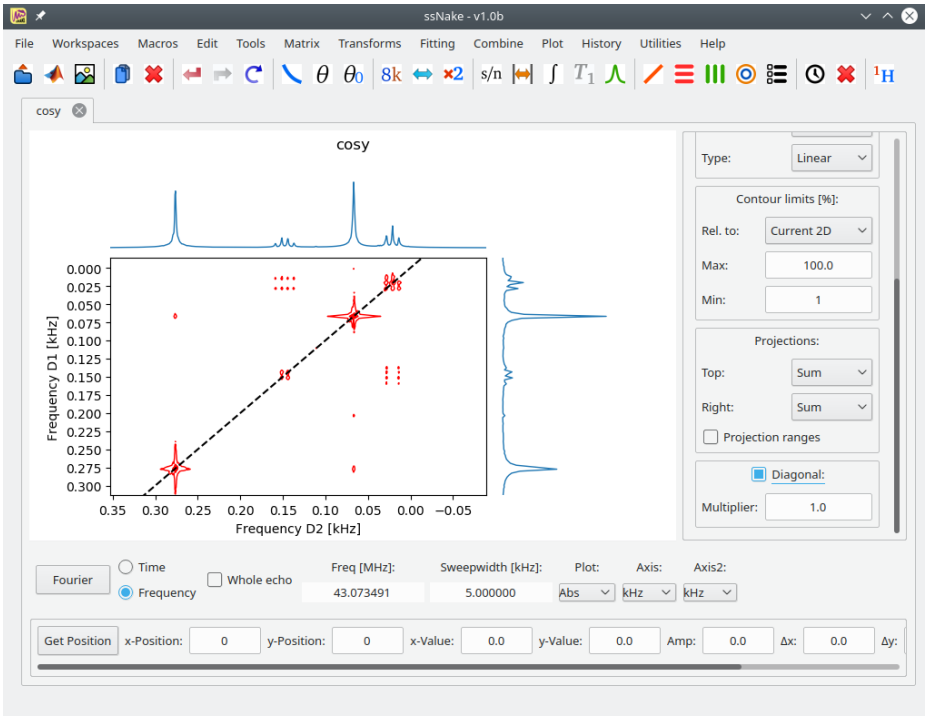
This gives:



which starts to look like a COSY! To better see what are cross peaks, and which lines are on the diagonal, we can ask ssNake to plot a line on the diagonal:

- Turn on the diagonal by ticking the box in the sideframe

This shows:



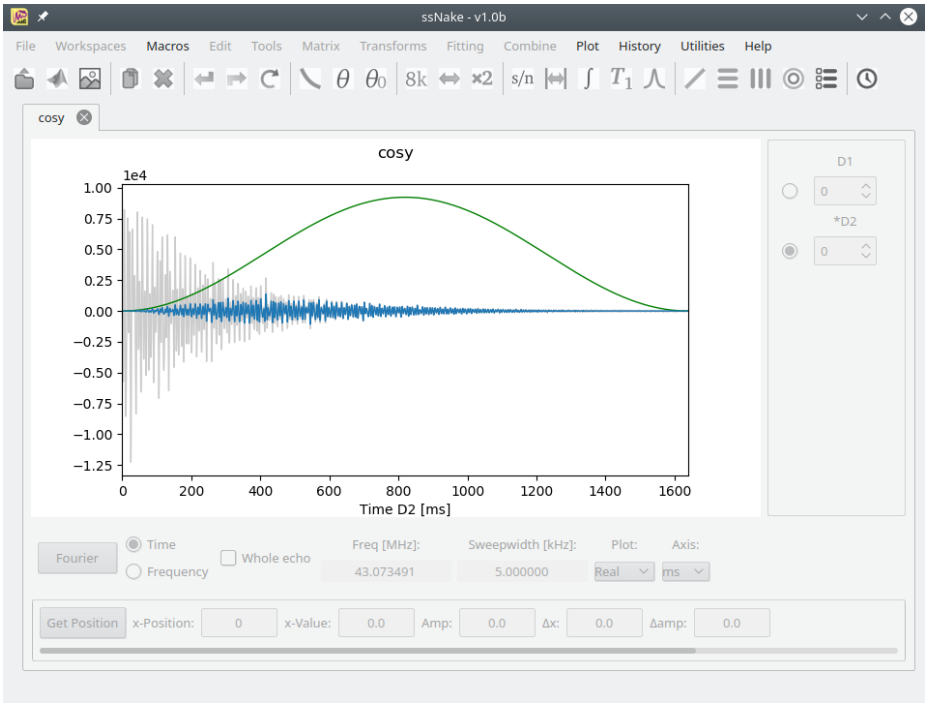
Which is our final spectrum. You can see some 'star' patterns in this spectrum, especially for the strong toluene lines. This come from the fact to we view the data in absolute mode (which is unavoidable for this experiment). The next section will describe how we can reduce these.

4 Sine square apodization

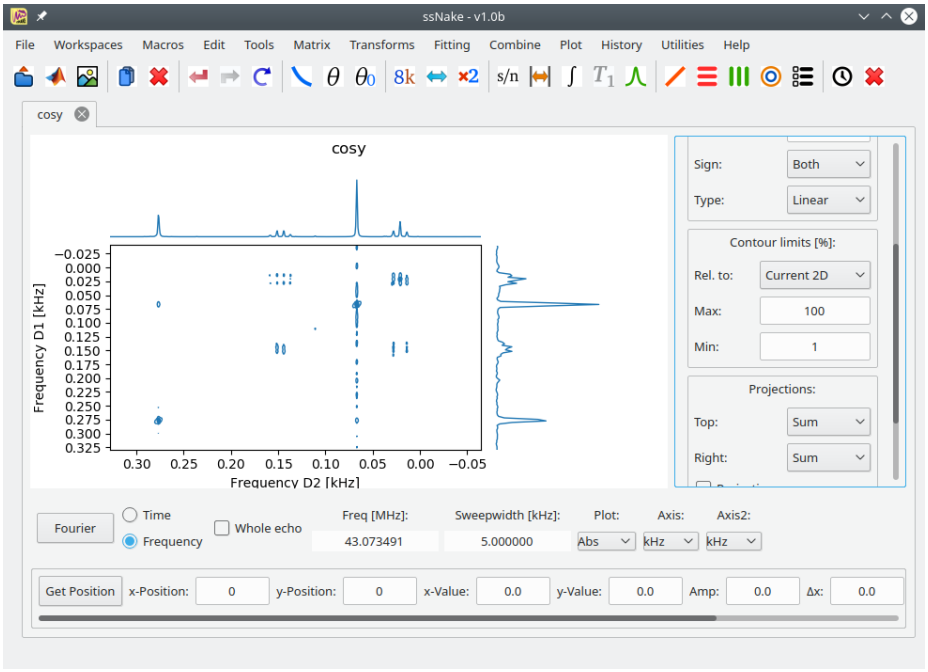
In order to reduce the 'star' artifacts in a COSY experiment, we can use some special apodization along both D2 and D1. For this, we do the same processing as before, but before each Fourier transform we do a sine square apodization (which we do in ssNake with a 90∘ phase shifted cosine square apodization):

- Apodize with Cos^2 with frequency 2, and phase 90 (`Tools` ⟶ `Apodize`)

If we do this along D2, we should see something like this:



Doing this along both D2 and D1 leads (after performing all the steps described above) to the following 2D spectrum:



Which shows a strong reduction of the ‘star’ effect.