

# COSY processing in ssNake

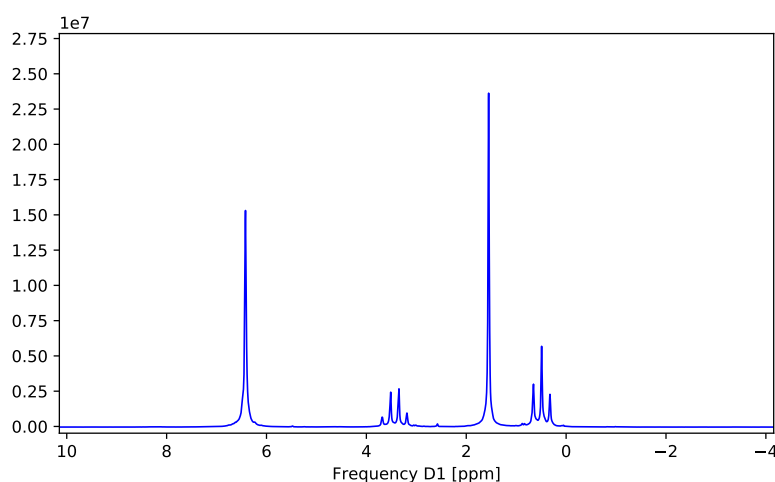
15th January 2019

## 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 resonances 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  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of a mixture of toluene and ethyl pyruvate (1:1) recorded on a 1 T (43 MHz) Magritek spectrometer. In this case, we expect to see cross-peaks between the two lines of toluene, and between the  $\text{CH}_3$  and  $\text{CH}_2$  resonances of ethyl pyruvate (the base methyl resonance of ethyl pyruvate overlaps with the methyl resonance of toluene). The 1D  $^1\text{H}$  spectrum of this sample is shown below.

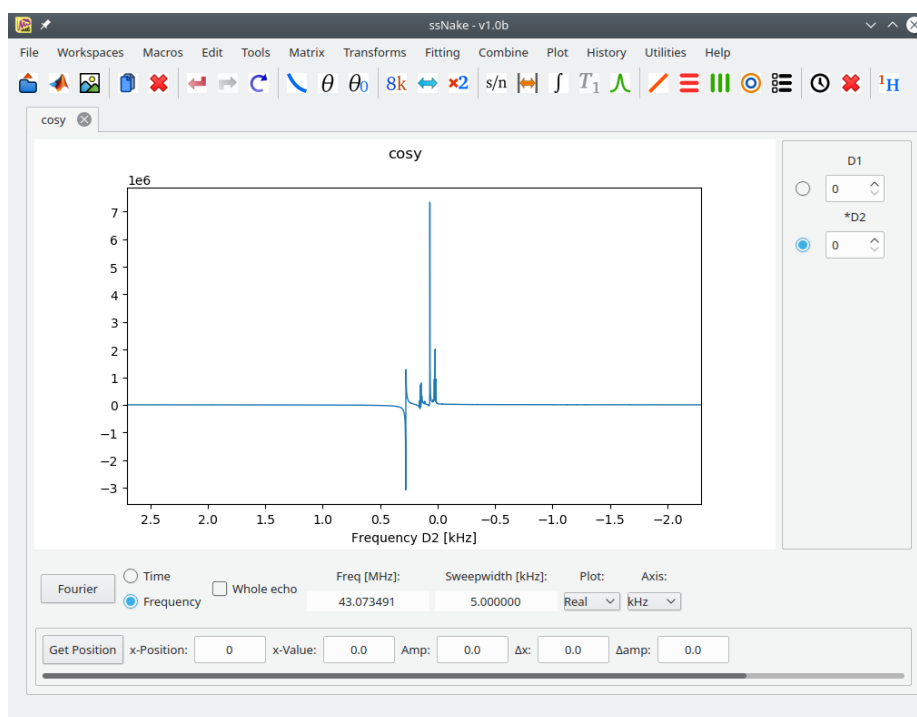


### 3 Processing the data

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:

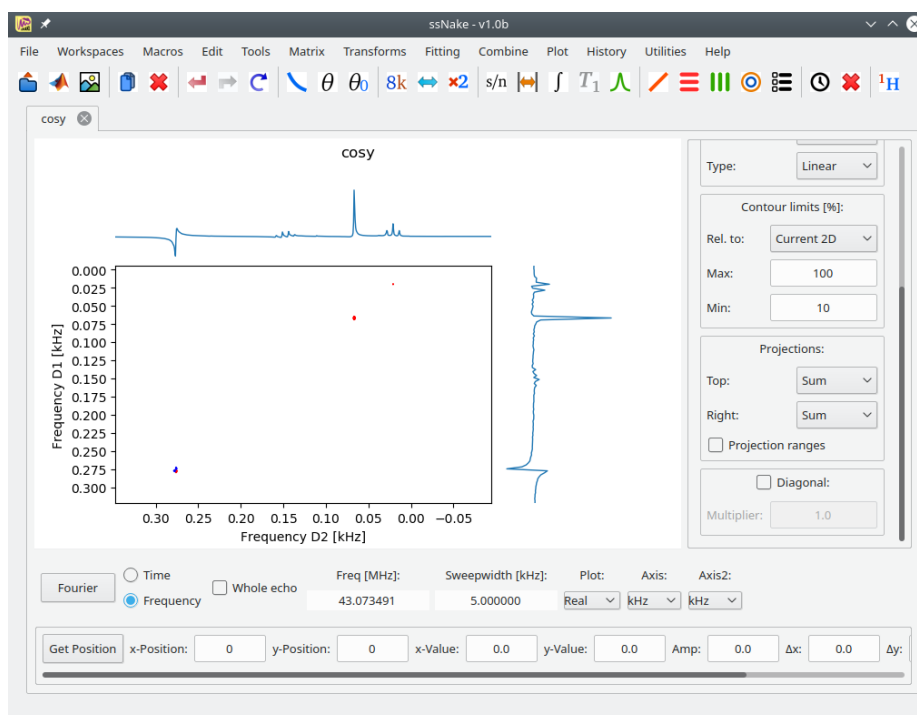
- Switch to a view along D1 by clicking on its radio button in the sideframe
- Perform a complex conjugate via Tools → Complex Conjugate<sup>1</sup>
- Fourier transform via the ‘Fourier’ button
- Switch back to viewing D2 by clicking on its radio button in the sideframe

<sup>1</sup>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 spectrum should look similar to:

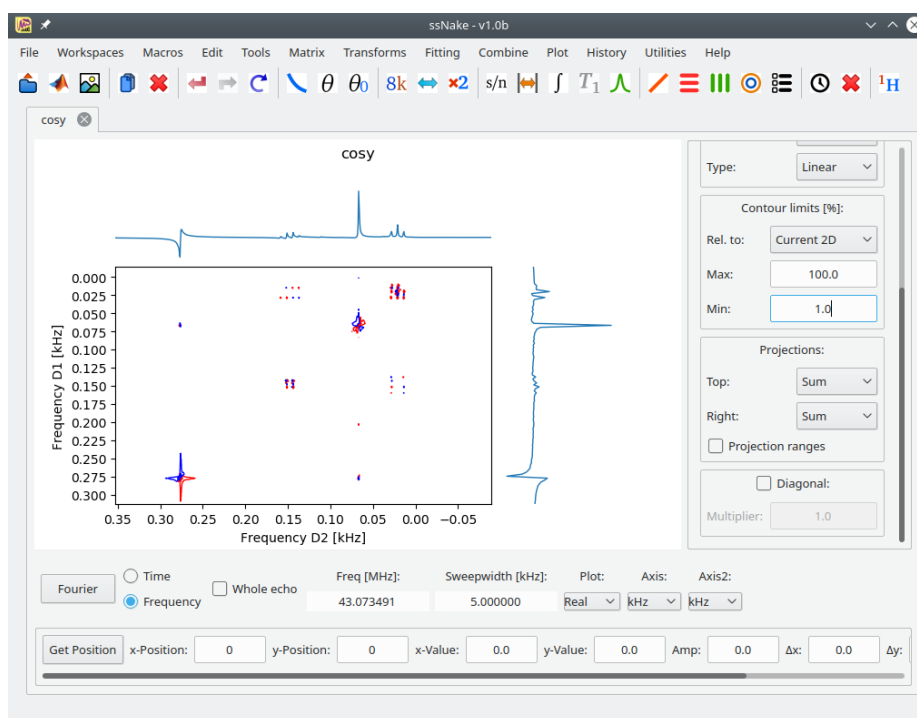


The cross-peaks are not visible since the lower contour cutoff is at 10%, so we should lower this to make them visible:

- Set the minimum contour limit to 1% (in the sideframe, under 'Contour limits')<sup>2</sup>

The spectrum will no look like this:

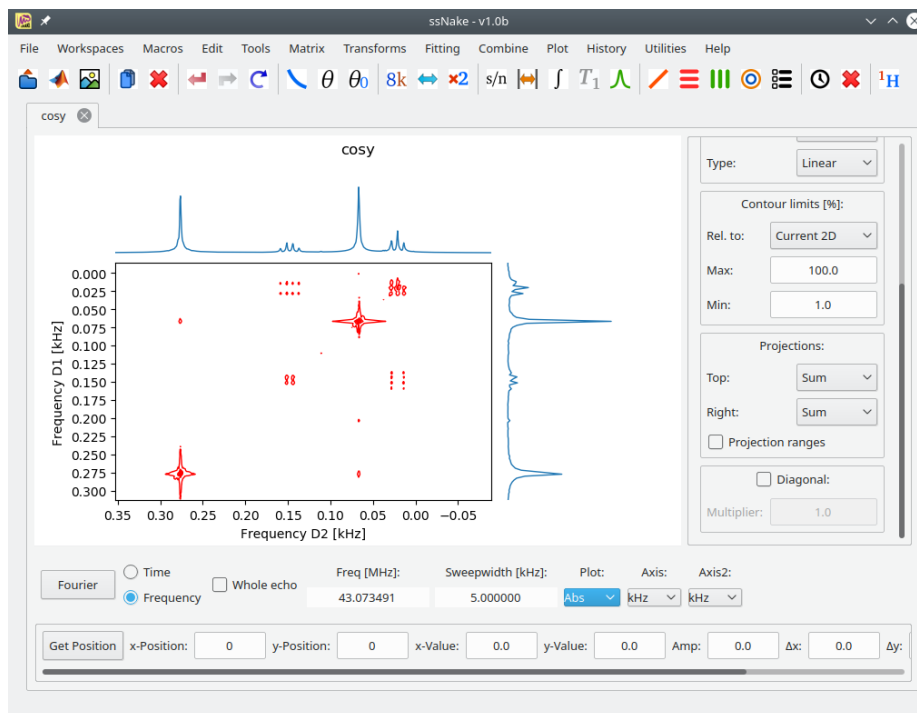
<sup>2</sup>You can also 'zoom' the contours by scrolling the mouse button while holding the 'shift' button



As you can see, the phase of the peaks is distorted in magnitude mode COSY experiment. So we should view this data in absolute mode:

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

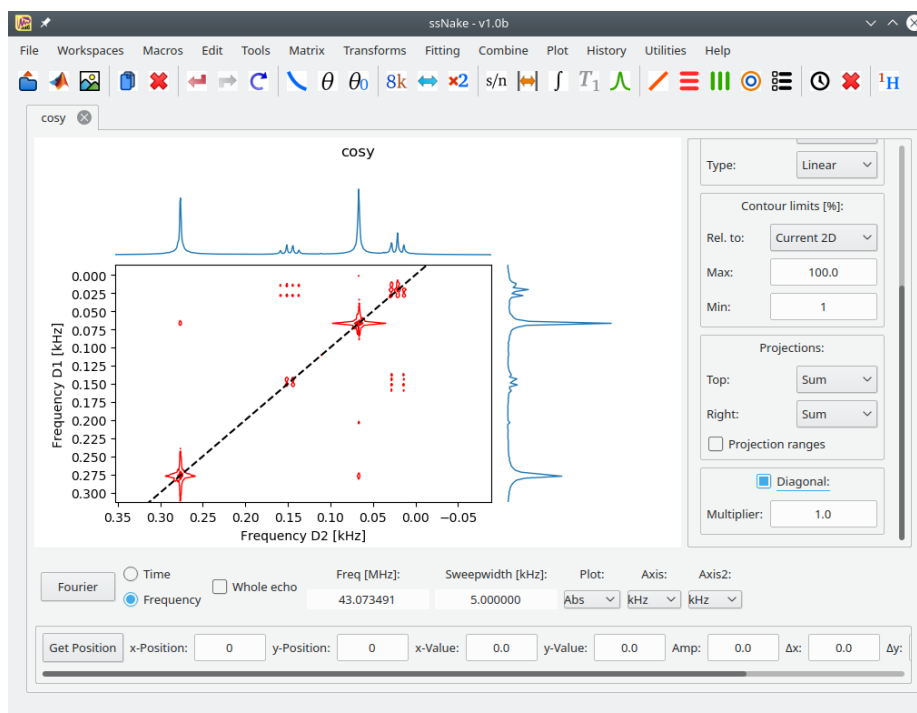
This results in a spectrum like:



This now 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 will now show:



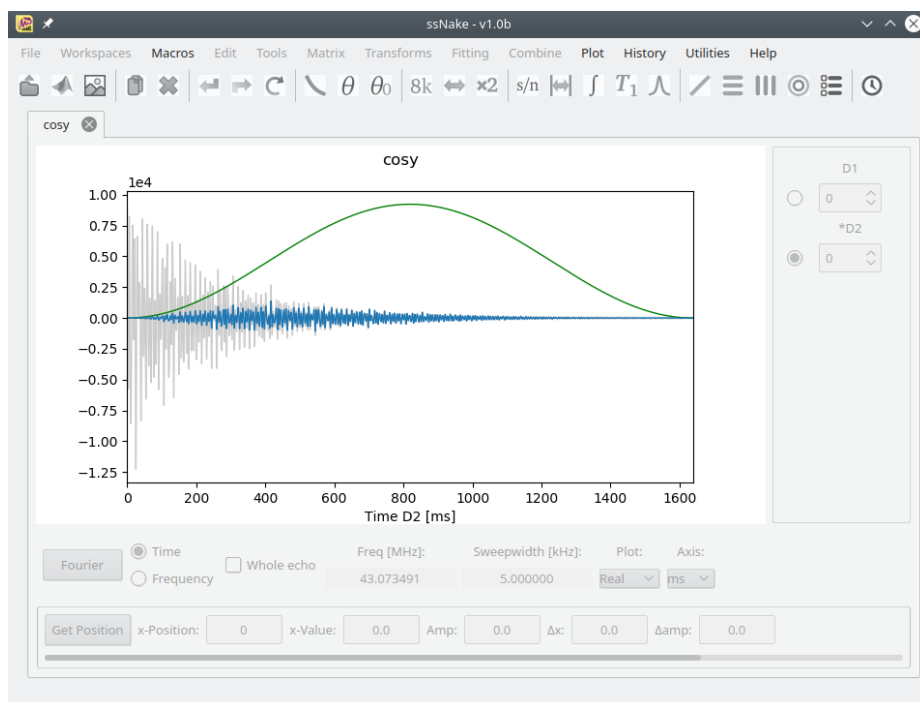
Which is our final spectrum. You can see some ‘star’ patterns in this spectrum, especially for the strong toluene lines. This come from the fact to we view the data in absolute mode (which is unavoidable for this experiment). The next section will describe how we can reduce these.

## 4 Sine square apodization

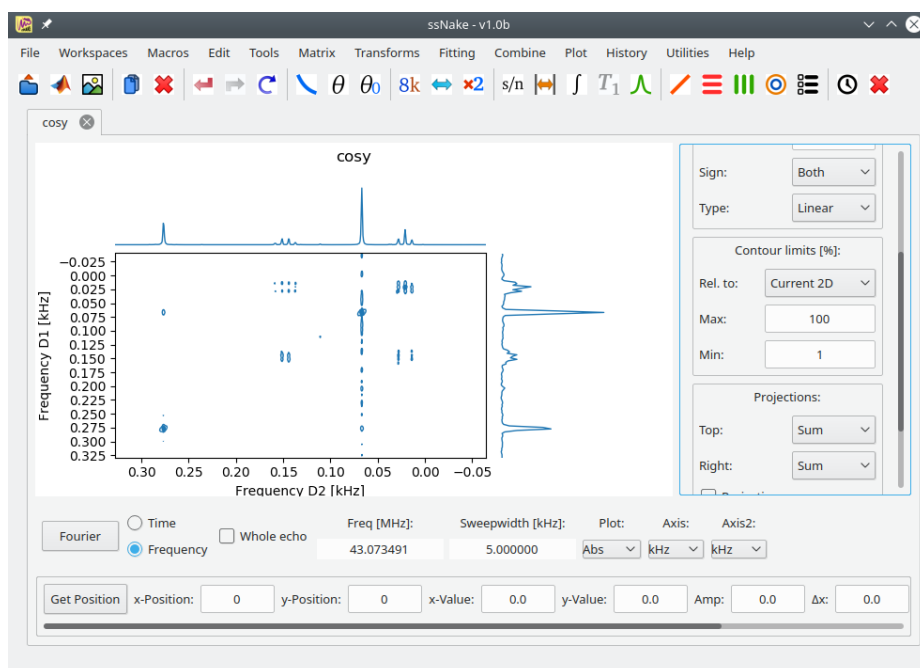
In order to reduce the ‘star’ artifacts in a COSY experiment, we can use some special apodization along both D2 and D1. For this, we perform the same processing as before, but before each Fourier transform we apply sine square apodization (which in ssNake is a 90° phase shifted cosine square apodization):

- Apodize with  $\text{Cos}^2$  with frequency 2, and phase 90 (Tools → Apodize)

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



Performing this along both dimensions leads (after performing all the steps described above) to the following 2D spectrum:



Which shows a strong reduction of the 'star' effect.