NUS processing in ssNake

22nd June 2019

1 Introduction

Is this tutorial, we will process some data that was recorded using non-uniform sampling. In non-uniform sampling, the indirect dimension of a 2D data set (or high dimensions) is not recorded using a standard linear array ($t = 0, x, 2x, 3x, \cdots$), but only has selected data points on this grid measured. The rational behind this, is that a higher information density is possible when we only measure the spectra that have relevant information.

The tricky thing with data recorded using NUS, is that the processing is more involved, and requires choices to be made. The problems in processing NUS data is that a regular Fourier transform can only be performed for data that is recorded on a linear grid. In the case of NUS, this is not the case, and alternative methods are needed to go from time-domain data to a spectrum[1].

2 Data

The data for this tutorial is a 2D ^{1}H–^{13}C HETCOR that was recorded at 850 MHz on a Varian spectrometer. The sample was solid state adamantane. Magic angle spinning and ^{1}H-decoupling were used. 50% of the points in teh indirect dimension was recored (NUS 50%).

3 Processing NUS data

Start by loading the data:

- Load the 'fid' file that was delivered with this tutorial
- Zerofill to 2048 data points using 'Matrix ⟶ Sizing'
- Fourier transform

[1]Note the careful choice of words. I call it "a spectrum", and not "the spectrum". For regular data, the Fourier transform is unique, and a data set can be viewed in both the time and frequency domain by using Fourier transforms. For NUS data, there is no unique way to do this. Therefore a single time-domain data set can lead to multiple different spectra, depending on the choices that we make in processing.

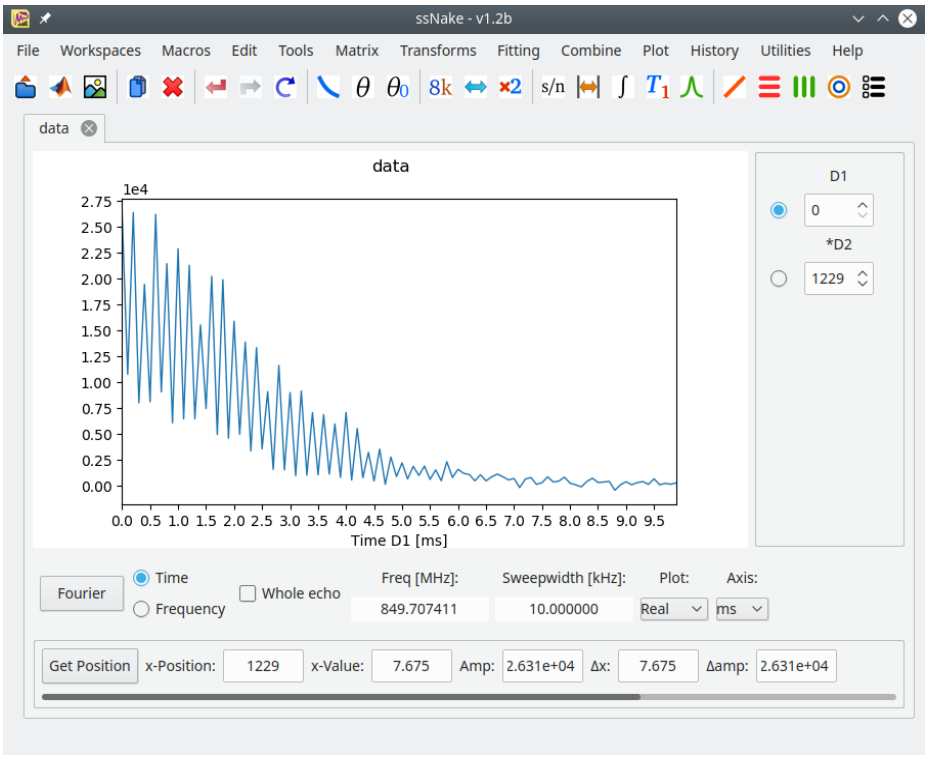
- Phase using 24.74 degree zero order, and −42.14 degree first order (or phase yourself)

Now, we have processed the direct dimension. This dimension is the one that is recorded normally, so regular processing can be used.

We will process the indirect dimension while viewing the top of the leftmost peak in the direct dimension (i.e. the carbon-13 dimension).

- View point 1229 in D2 (fill it in in the box in the sideframe, and press enter).

This should show:

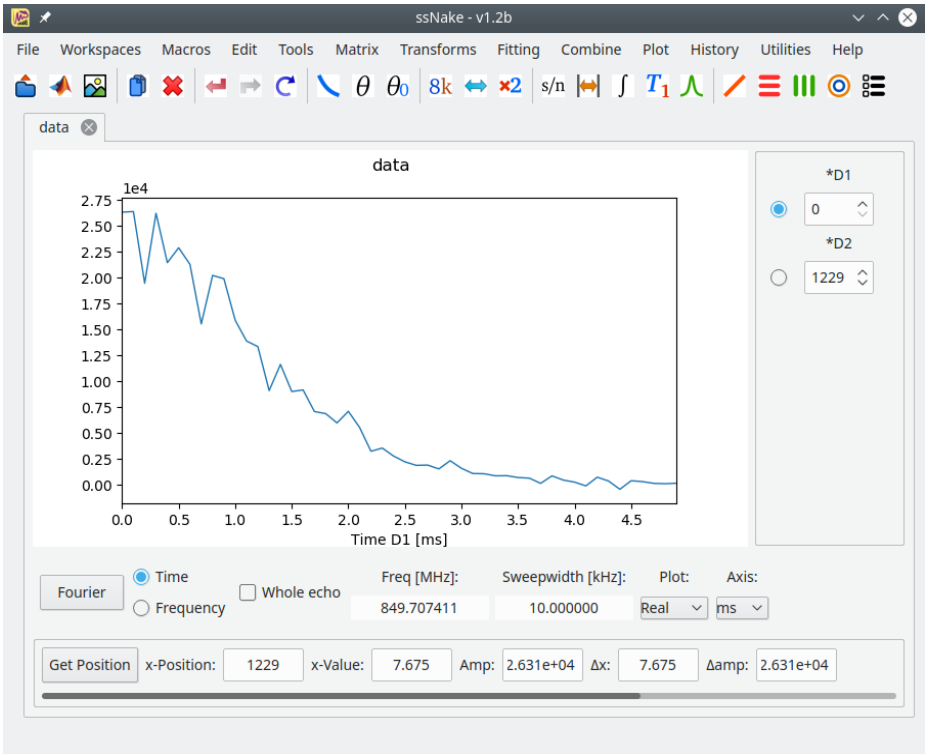


The rapid oscillations we see here are due to the phase-sensitive recording of the data (i.e. states). We must transforms this data to the hypercomplex definition:

- Convert the States data via 'Transforms ⟶ Hypercomplex ⟶ States'
- Take the complex conjugate via 'Tools ⟶ Complex Conjugate'[2]

This should show:

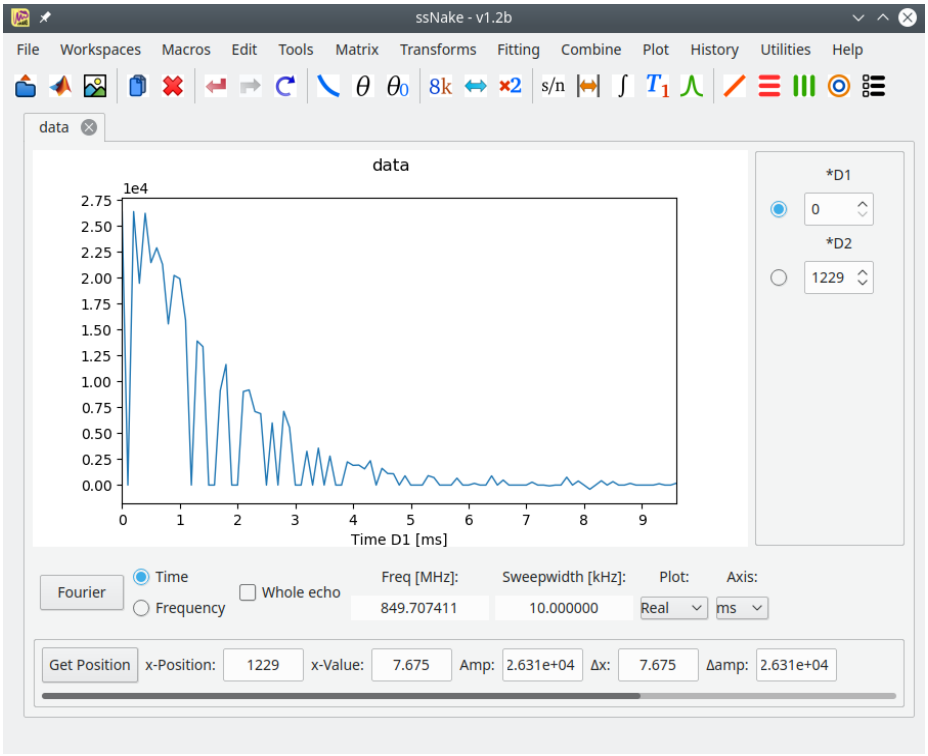
[2]This is required to mirror the spectrum. This is because Varian data uses a different definition for the sign of the imaginary part than ssNake.



This looks OK, but actually the time axis is not correct. The current figure shows the data in the order which they were recorded, not taking the missing point into account. To correct for this, we must reorder the data, using the information saved with the experimental data (in 'sampling.sch').

- Reorder the dating using 'Matrix ⟶ Reorder', browse for the 'sampling.sch' delivered in the data directory of this tutorial, and apply.

This should show:



Here, it can be clearly seen that we have many points which are not recorded: they are zero. This is essentially what non-uniform sampling entails.

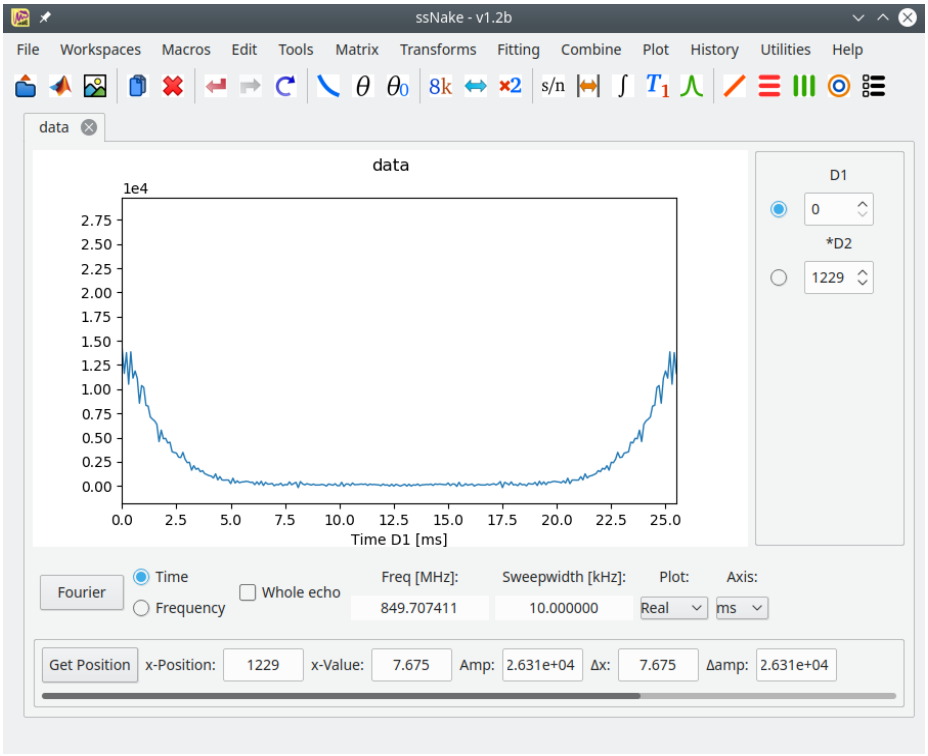
Now that we have our non-uniform 'FID', we can start to reconstruct a spectrum based on this. First, we must phase the data. This is because most reconstruction algorithms can only accurately reconstruct in-phase data. We will phase in the spectrum, which will look really bad due to all the zero's in our FID (we have not yet reconstructed the data).

- Fourier transform
- Phase with 18.180 degree zero order phasing
- Push the Fourier button again (do an inverse transform)
- Zerofill to 256 data points using 'Matrix ⟶ Sizing'

Now, we are ready to do a reconstruction. We will use IST (iterative soft thresholding) in this case. It requires as inputs the threshold ($0 < x < 1$, with closer to 1 slower, but more accurate), the maximum number of steps, and the stopping condition (percentage of the maximum). The stopping condition should be roughly the intensity of the noise (no useful information is add after this point).

- Do IST via 'Transforms ⟶ NUS ⟶ IST', put the Threshold at 0.95, and the Max. Iterations at 200. Also required is the sampling scheme again:browse for the 'sampling.sch'.

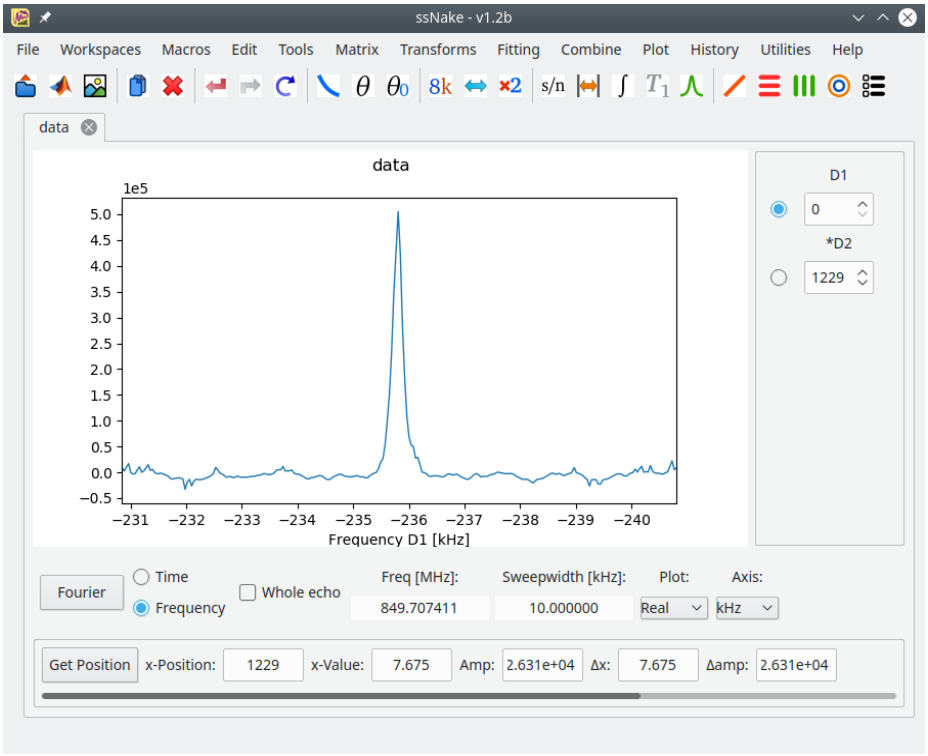
This shows:



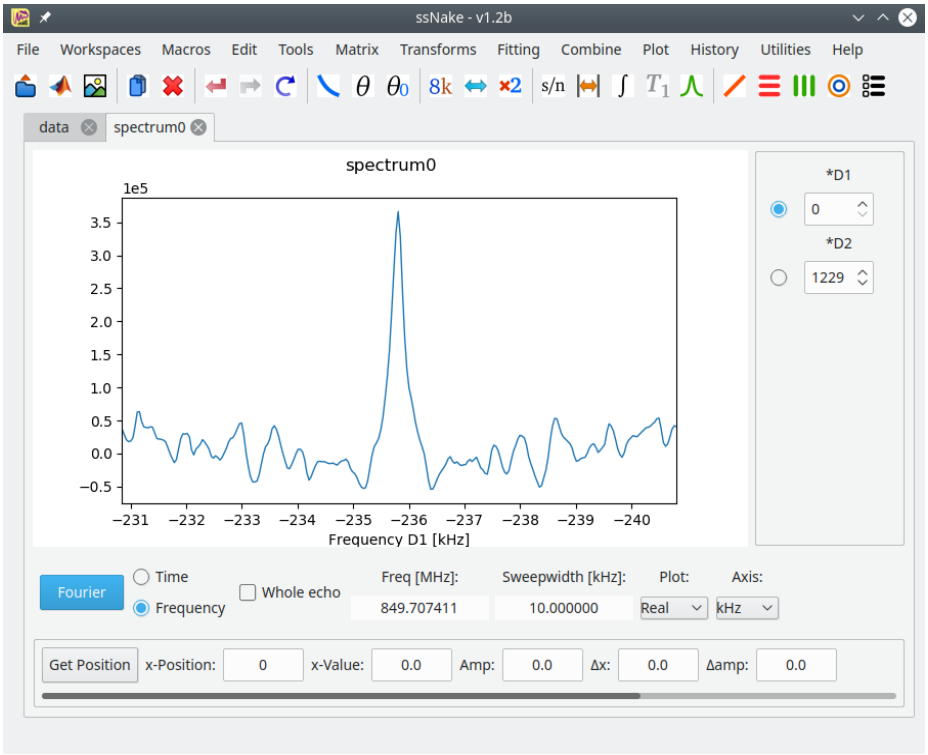
Which is our reconstructed FID. It looks a bit funny (why is the intensity going up at the end?). This is due to the fact the we have not reconstructed the imaginary part of the spectrum in this analysis. We can fix this later on. First we go to the spectrum:

- Push Fourier button

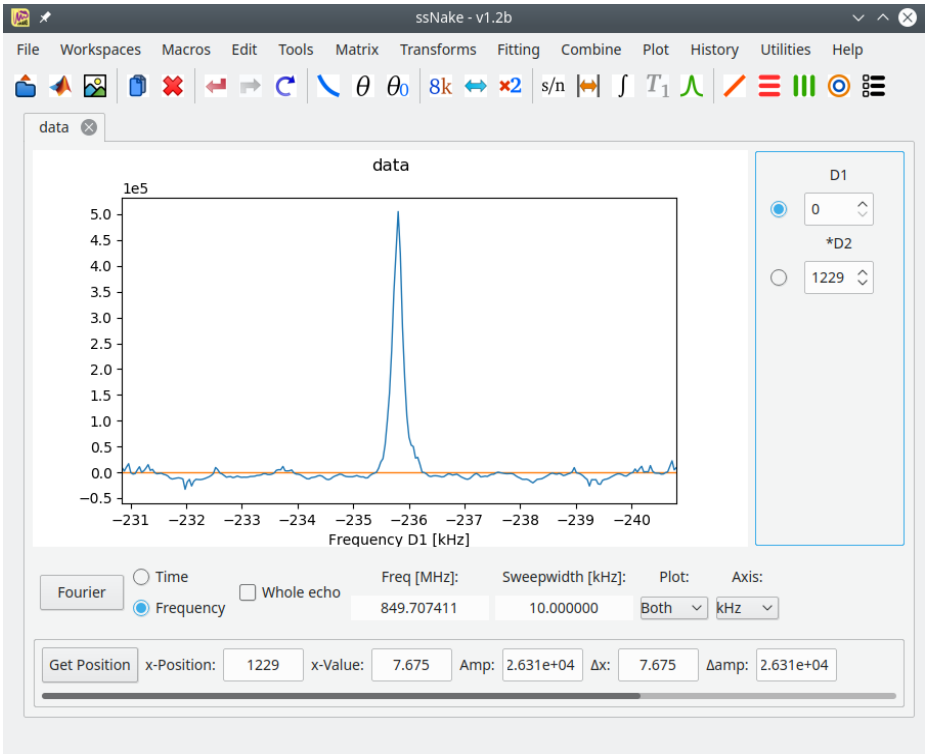
This shows:



which is our reconstructed spectrum. This is clearly much better than what we get without doing the IST:



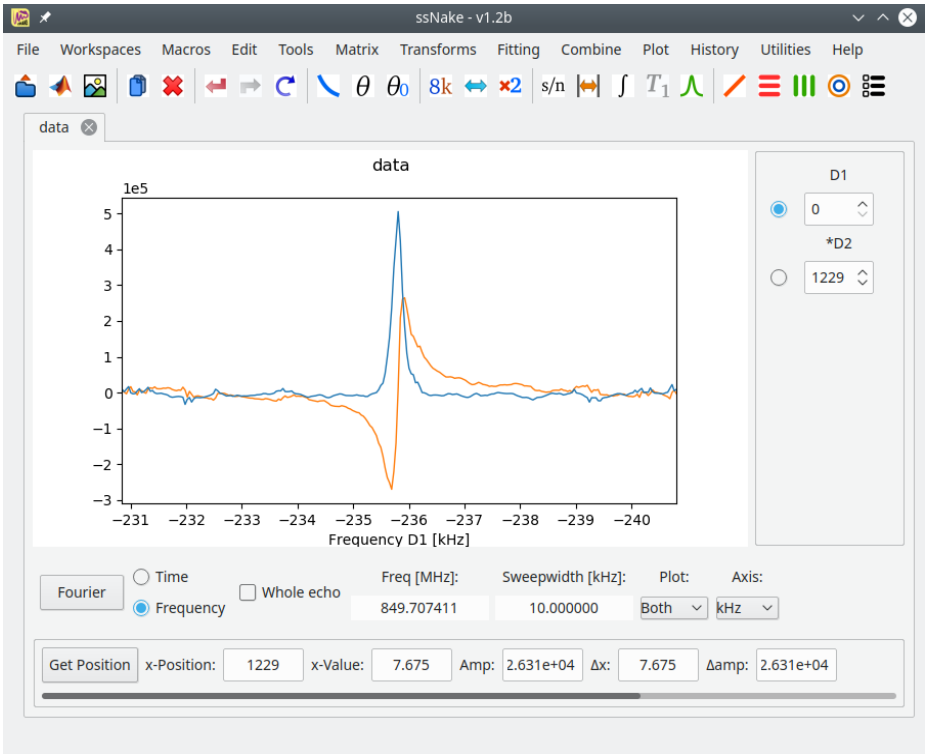
Plotting the imaginary data also, we see that it is zero:



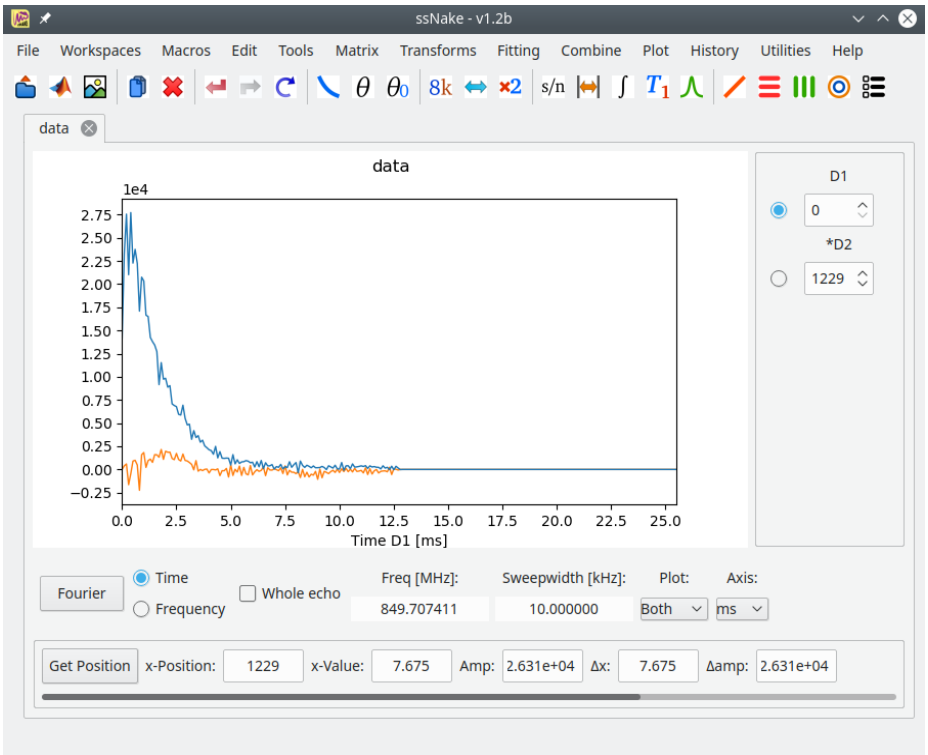
We decided to not reconstruct the imaginary data by default in ssNake. This is because imaginary data would allow for phasing, which is not allowed after IST: only in-phase data can be properly reconstructed. If desired, the imaginary data can be generated manually, by performing a Hilbert transform:

- Do a Hilbert transform via 'Transforms ⟶ Hilbert Transform'
- Take the complex conjugate via 'Tools ⟶ Complex Conjugate'

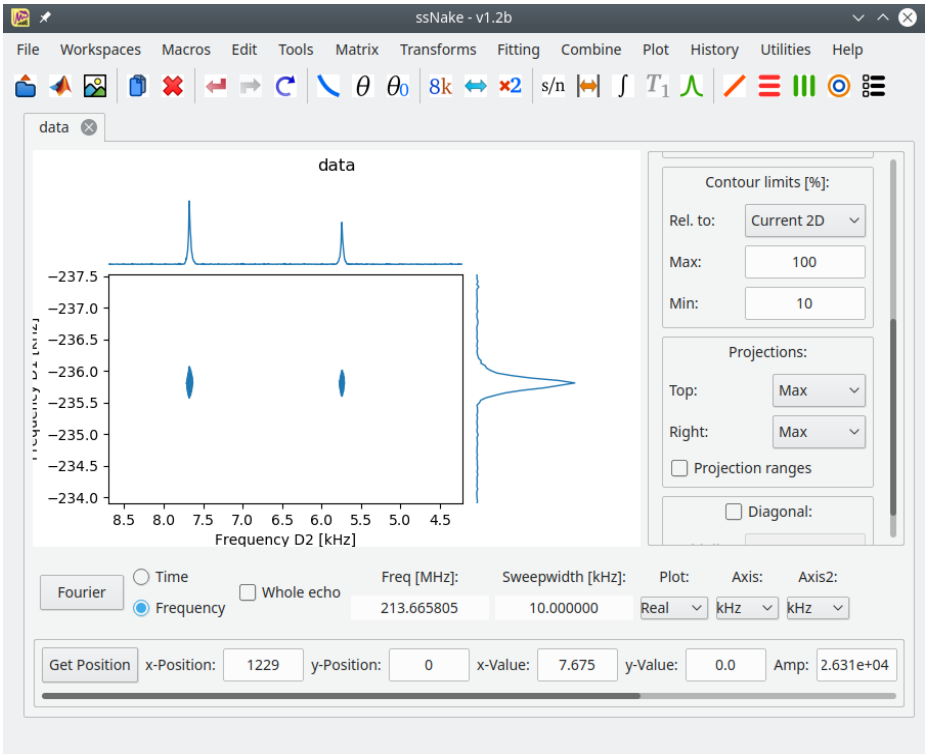
This shows:



Doing an inverse Fourier Transform shows an FID as we are used to:



Finally, we can also view our reconstructed spectrum as a 2D contour plot:



This concludes this tutorial on NUS processing.