

Diffusion analysis in ssNake (under construction)

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1 Introduction

In this tutorial, we will analyse a diffusion measurement of a liquid state sample in ssNake. Diffusion is a powerful tool to distinguish multiple molecules in complicated spectra, especially when other 2D methods cannot readily identify the different components. The diffusion experiment consists of a spin-echo experiment, with gradients present during the echo time. In case of no diffusion, each nucleus experiences the same B_0 field during the first part of the echo as during the last, and perfect echo refocussing occurs. In case of displacements in this time (i.e. diffusion), the B_0 field are different during part 1 and part 2 of the echo, and attenuation of the signal occurs. If the strength and durations of the gradients are known, the diffusion constant can be extracted from such a measurement.

2 Data

The data for this tutorial was recorded at 600 MHz. The sample was a mixture of 2-ethylpyridine and 2,3,3-trimethylpyrazine in DMSO (with TMS). The maximum gradient strength was 0.535 T/m. The relevant times were: $\delta = 1$ ms, and $\Delta = 100$ ms.

3 Fitting a diffusion curve

Start by loading the Bruker type data:

- Load the 'ser' file that was delivered with this tutorial

Now, we want to zero-fill the data, as well as correct for the Bruker time delay (i.e. digital filter). It is best to do the zero-filling first:

- Use 'Matrix \rightarrow Sizing', and set the size to 32768
- Correct the digital filter by using 'Tools \rightarrow Correct digital filter'
- Fourier transform

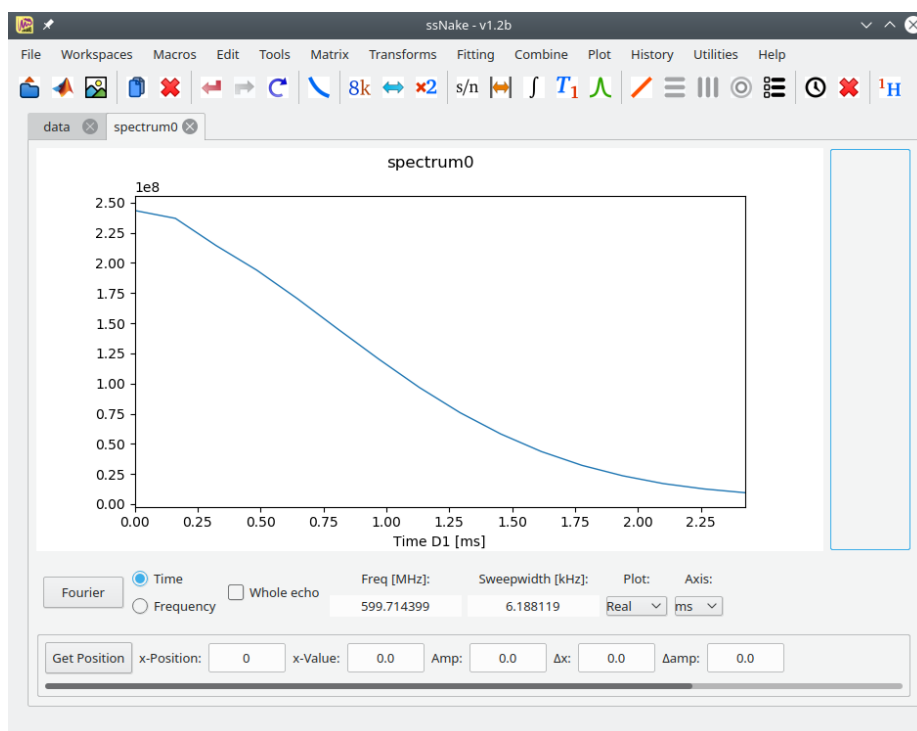
Correct for the phasing:

- Phase using ‘Tools → Phasing’ with 173.724 zero order, and -33.86 first order

Now, we will analyse the intensity variation of, say, the leftmost peak (highest ppm value). In order to do this, we will integrate this region, and send this data to a new workspace (to not remove the rest of the data).

- Use ‘Matrix → Region →’, and integrate between point 28482 and 28570. (or left click on the left and right side of the relevant peak in the spectrum. Remember to tick the box that says ‘Results in new workspace’).

This should show:



which shows a nice Gaussian decay due to the diffusion.

Now, we want to fit this decay, which means that we must supply ssNake with the relevant x-axis. In this case, we have measured multiple spectra with a different gradient strengths. The strengths were approximately linear, with real values: 2.408, 5.296, 8.186, 11.075, 13.963, 16.852, 19.741, 22.630, 25.520, 28.409, 31.298, 34.187, 37.076, 39.965, 42.854 and 45.742%. We must recalculate these values using the maximum gradient strength of the setup (0.535 T/m). With these values, we must change the x-axis in ssNake:

- Use ‘Plot → User x-axis’ and fill in: $\text{array}([2.408, 5.296, 8.186, 11.075, 13.963, 16.852, 19.741, 22.630, 25.520, 28.409, 31.298, 34.187, 37.076, 39.965, 42.854, 45.742]) \times 0.535/100$
- Set the Axis unit to ‘s’

Here, we make use of ssNake’s calculation capability to multiply the array by some values. Note that the axis still shows ‘Time D1 [s]’, while actually it is a gradient strength (you need to remember this for yourself!).