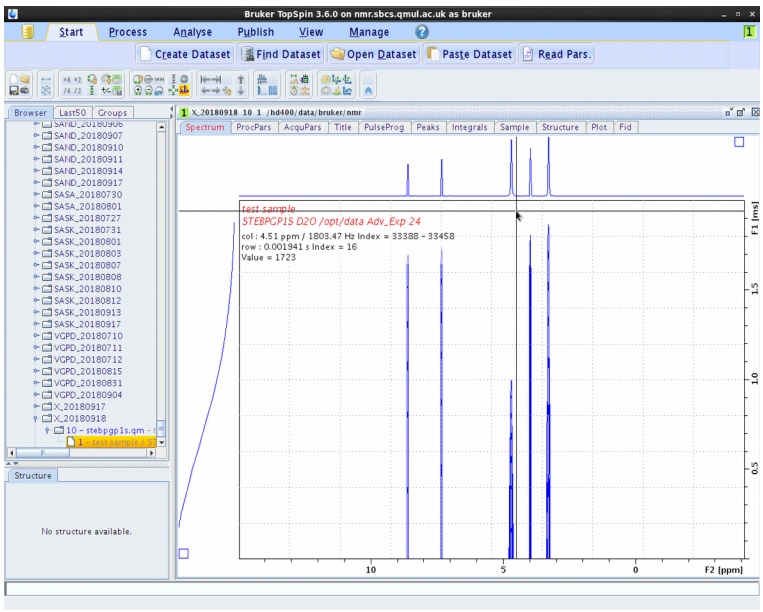
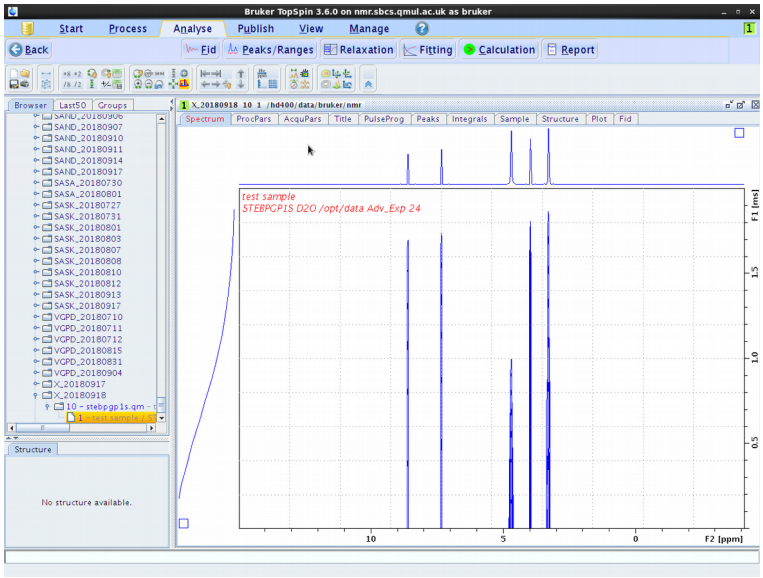
Processing 400 MHz Diffusion data

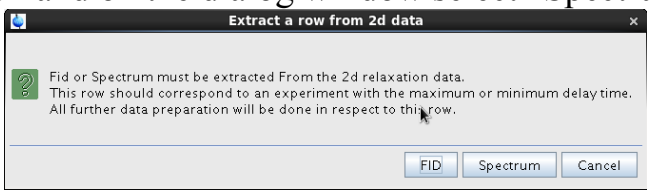
Open your diffusion dataset. It will be called something like X_20180918 and will be under either hd400->bruker or av3400->bruker in the TopSpin data browser (depending on which spectrometer was used). Once opened it should look something like:



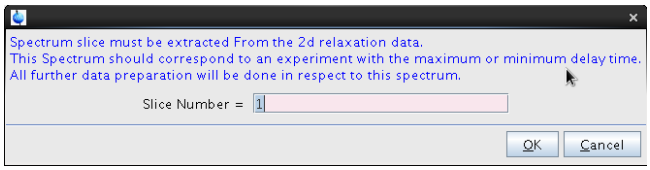
Select “Analyse” and then “T1T2(t1t2)” from under the “Dynamics” menu and the display should change to:



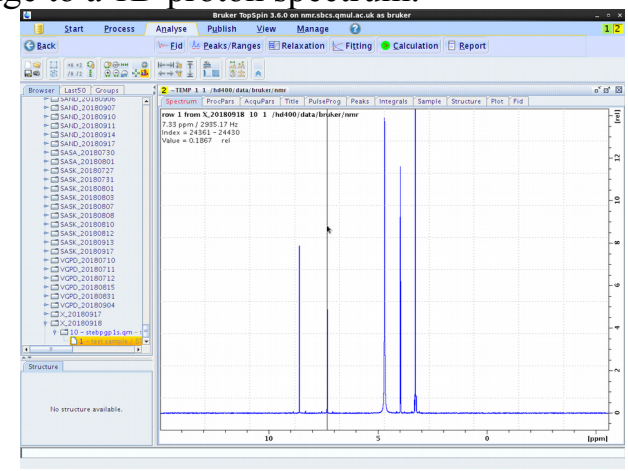
Select the “Fid” button and on the dialog window select “Spectrum”:



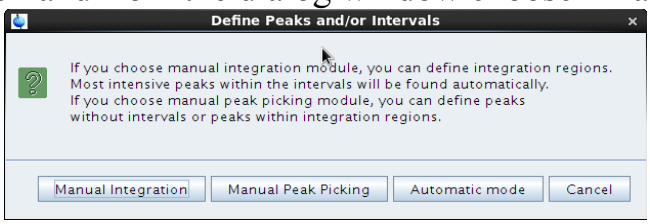
Then slice number “1”:



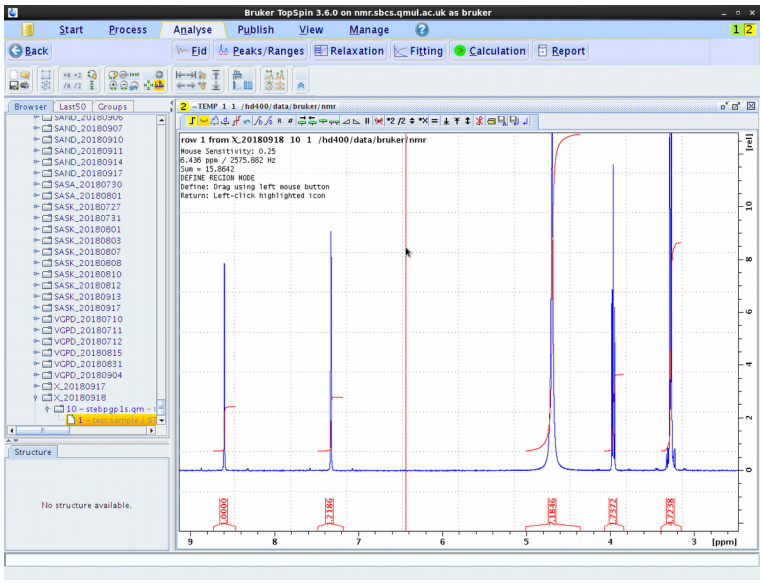
The display will change to a 1D proton spectrum:



Expand to the region containing the peaks of interest by dragging the mouse over the spectrum from left to right while holding down the left button, then select the “Peaks/Ranges” button and from the dialog window choose “Manual Integration”:

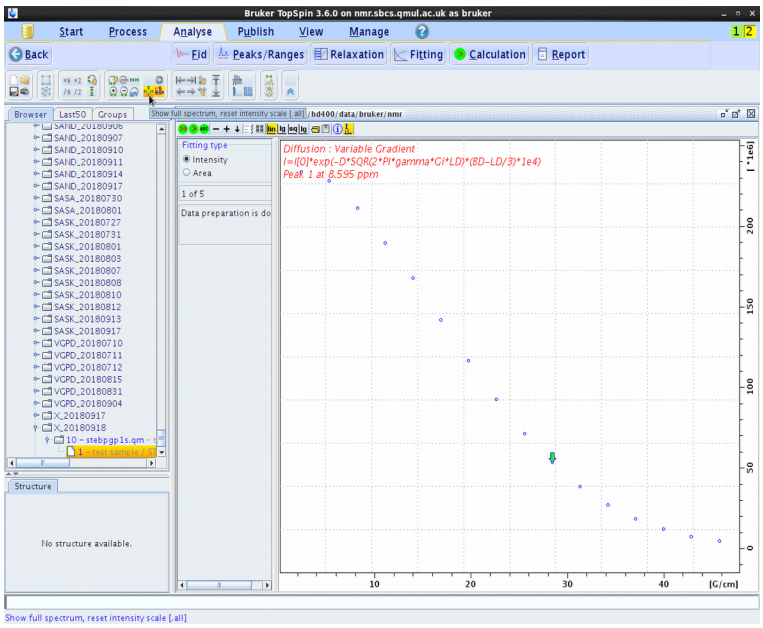


Select the “Define region” icon (next to the yellow integration symbol). Integrate the peaks by dragging the mouse from right to left while holding down the left mouse button:

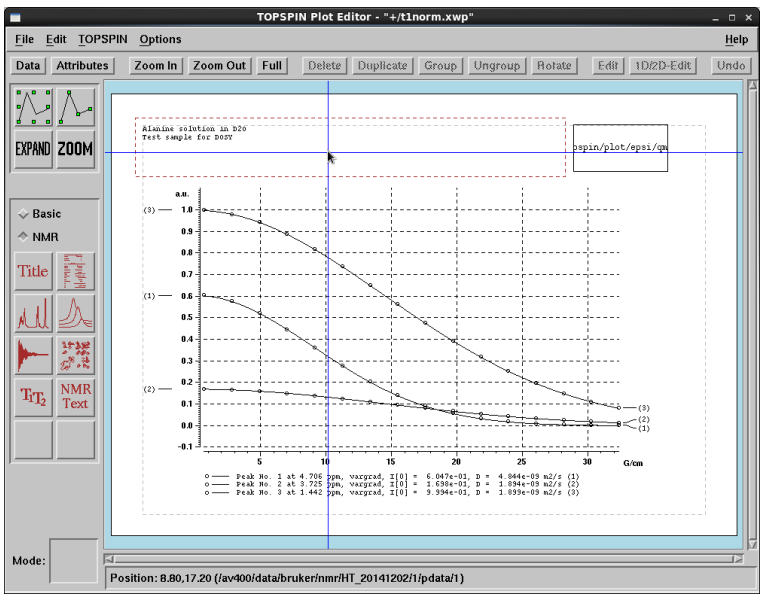


Save the results by clicking the third icon from the right in the integration window (the one that looks like a floppy disk with the letter “A”). Select the option “Export Regions To Relaxation Module and .ret.”

Select the “Relaxation” button and the display should now show the data points for the first peak in the spectrum. Click the reset icon (where the mouse is in the image below) and select fitting type “Area”.



Click on the (>>) icon in the left corner and the curve for all the peaks will be automatically fitted. Then choose the “Report” button to obtain a text report of the results which may be printed via the “File” dialog. Finally, close the fitting window by clicking on the [x] just above the graph (not the one in the top left corner!) which will return you to the 2D display of the data. A graphical representation of the data may be obtained by typing the command “plot0” in the command box at the bottom of the window:



A set of tools for re-scaling axes etc... is obtained by right-clicking on the plot (this only works if the [NUMLOCK] is off). The plot can either be printed, or saved to a file e.g. on a USB key via the “File” dialog. The computer to plug your USB into is below the desk on the left.