

T2 Determination

T2: the spin-spin (transverse) relaxation time is a measure of the decay constant for the component of Magnetization (M_{xy}) perpendicular to the external field B_0 . After time T2, transverse magnetization has lost 63% of its original value (at time zero: $M_{xy}(0)$). In principal (a homogeneous system), T2 can be obtained by measuring the linewidth at half-high ($\frac{1}{2}$ line-width = $1/(\pi*T2)$). Normally T2 is determined accurately using Carr-Purcell-Meiboom-Gill pulse sequence by varying the delay time (big tau) between the spin-echo and the next 180 degree pulse, and by fitting the magnetization (signal intensities: peak heights or integral values) to a mono-exponential function: $M_{xy}(t) = M_{xy}(0)e^{-t/T2}$.

Procedure:

1. Collect a ^1H spectrum
2. Determine the pw90 for your sample by arraying pw value (see pw90 determination handout)
3. Collect another ^1H spectrum with optimized pw90
4. Move your ^1H 1D spectrum to experiment 2 by typing:
mf(1,2) jexp2
5. In experiment 2, type:
doT2 (This loads in the CPMG pulse sequence for T2 experiment)
then type:
T2setup
Follow the prompts:
ENTER MINIMUM T2 EXPECTED (sec): 0.1
ENTER MAXIMUM T2 EXPECTED (sec): 5
ENTER EXPERIMENT TIME (hrs): 0.5 (for example, normally 0.5-1 hr)
Depending on the experimental time entered, d1 and nt will automatically be set. You will also see an array of bt values (big tau). (Note: please check nt by typing nt? If the nt is less or more than the number of scans you're desired for your sample depending on the concentration, you can repeat T2setup, and use a shorter or longer time.)
6. Start the T2 measure, type:
ga
7. When experiment is finished, save data set by typing: svf('filename')
8. Process your data and calculate T2 by typing the following:
wft dssh (to view arrayed spectra)
dg (to view parameter page on bottom of screen)
da (to view arrayed parameters)
ds(1) (displays spectrum 1)
f full aph (view full spectrum and autophase. may need to adjust phase)
9. Set the threshold by clicking on the "Set Th" button and adjusting the height such that all peaks are selected.
10. Type:
dll (to display lines selected)
fpdc (to find peaks and do a dc offset correction)
t2 (calculates T2 values of peaks)
At this step, you'll see the T2 result and analyzed data on the dg (bottom window) for all the peak selected.
11. Type:
printon dll t2 printoff (prints T2 values)

T2 Processing using Mnova

1. Open T2 experiment in Mnova: this opens stacked spectra containing all arrayed time points of the T2 experiment
2. Perform Fourier Transform, phasing and baseline correction as needed on one spectrum, normally the first spectrum (shortest time point)
3. Click on Advance -> Data Analysis -> Create -> Integral Graph (or Peak Graph)
4. If you choose Integral graph, an integral icon shows up at the mouse pointer, you can integrate on the peaks you want to calculate T2. Meanwhile the "Data Analysis" window pops up
5. In the "Data Analysis" window, the first column X(I) contains the time points, the Y(X) column contains the integration values of the first peak at different time points, Y1(X) contains the integration values of the second peak at different time points....and so on.
6. Right after the Y(X) column, there is another column (before Y1(X)) labeled Y'(X), also Y1'(X) after Y1(X), and so on. At this moment, the cells in these columns have value of "o".
7. Click on the empty cell below Y'(X), a Y'-Column Model Function window pops up. choose (highlight) "Mono-exponential Fit", then click "Calculate". The bottom box in the window will show the fitted value. Click on "OK" to close this window. Now the Y'(X) is being populated with fitted values. B is the Magnetization at time 0, and F is the 1/T2 value of the Y(X) peak. Repeat this for Y1(X) and so on.
8. You can copy these data (X(I), Y(X), Y'(X), Y1(X), Y1'(X)...) to excel or word document.