How to Run a Simple Diffusion Experiment on the AVANCE 500

1. Run a reference proton spectrum in experiment 1. This will not be overwritten.

2. Type “dodiffusion”.

3. When asked, enter the total number of spectra you would like to include in your diffusion measurement.

4. When asked, enter how many scans you would like each spectrum to contain.

5. When asked, enter the time interval, Δ, in msec. If you are not sure of this, leave the default value of 10 msec.

6. When asked, enter the duration of the gradient pulse, δ, in msec. If you are not sure of this, leave the default value of 4 msec.

7. Your diffusion experiments will be set up in the experiments 2,3,4...etc. The gradient strength will be set to 0% for experiment 2 and be increased linearly to 100 % based on the number of spectra requested. Allow the experiment to run until completion. You can calculate the approximate total experiment time from the following:

   Total Time = (Number of spectra)*((NS)*(AQ+D1))
   (11 spectra each with 8 scans will take approximately 8 minutes)

8. Fourier transform the first spectrum in experiment 2 (using 0% gradient strength) and integrate the peaks of interest. Save the integrals in the usual way.

9. Enter the command “wmisc”.

10. Click “intrng”.

11. In the “Type New Name” field enter “diff”. If “diff” is already present in the list then just click on it. If asked to override, click “OK”.

12. Enter the command “procdiffusion”.

13. When asked to use EXPNOs (0) or PROCNOs (1), enter “0".

14. When asked to enter the first experiment number, enter “2".

15. When asked to enter the number of experiments, enter the number of diffusion spectra collected.

16. When asked to enter the name of the intrng file, enter “diff”.

17. Allow all the calculations to finish. All the spectra will be integrated automatically and a summary of the data, easily imported into a spreadsheet, will be stored with your data in the file (/datasetname/2/1/datasetname_int_txt). The first column of the file contains the gradient strength for each spectrum and the subsequent columns contain the integrals for each spectrum.

18. Plot ln (I/Io) vs G^2 Where Io is the intensity of the line at 0% gradient strength and G^2 is the square of the gradient strength in $(T/m)^2$. Use the following calibrated values of G^2 for each gradient strength.

Grad strength %	G^2 $(T/m)^2$
0	7.24395E-07
10	0.002821537
20	0.011106035
30	0.024854217
40	0.044066085
50	0.068741637
60	0.098880874
70	0.134483796
80	0.175550403
90	0.222080694
100	0.274074671

The slope of this plot is given by:

$$\text{Slope} = -(\gamma\delta)^2(\Delta - \tfrac{1}{3}\delta)D$$

where γ is the gyromagnetic ratio for the nucleus ($\gamma = 2.67519 \cdot 10^8$ rad $T^{-1}s^{-1}$ for protons) and D is the diffusion constant in m^2/s. The diffusion constant is easily calculated from the slope:

$$D = \text{Slope} / [\, -(\gamma\delta)^2(\Delta - \tfrac{1}{3}\delta)]$$