

DOSY for Topspin

Experiment Setup

DOSY uses three parameters to define the duration of the diffusion: gradient length (**P30**, the total gradient defocusing time, **1ms**), the diffusion gradient level (**GPZ6**, maximum **95%**), and the diffusion delay (**D20**, **200ms**). In most case, **GPZ6** is the variable parameter to be arrayed for DOSY purpose.

- 1) To set up a DOSY experiment, start with recording a normal proton spectrum, followed by optimizing **P1**, **SWH**, and **O1**, if necessary.
- 2) Type "**rpar dstebpgp3s1d_nu all**" to retrieve 1D dosy parameters (or "**rpar**" to select "**dstebpgp3s1d_nu**"). Update solvent with yours (default is CdCl3)
- 3) Check to make sure the **P1**, **SWH**, and **O1** are same as your proton experiment. The recycle delay **D1** should be 1-2 T1 and dummy scan **DS** should be at least 8. Adjust **NS** accordingly to give sufficient S/N.
- 4) Change **GPZ6** to 2% and type "**zg**" to collect data.
- 5) Use "**edc**" to create another 1D experiment and change **GPZ6** to 75% and type "**zg**" to collect data
- 6) Click  (dual display) to compare the 1D data with **GPZ6** at 75% to the previous 1D of 2% to check if the nmr signals of interest are attenuated to less than 5-10% of the intensities obtained with **GPZ6** at 2%. If you don't get there or already past it, adjust **GPZ6** (to 95% or 50%) accordingly to make sure you get there. Write down the **GPZ6** value for 2D DOSY setup.
- 7) Type "**rpar dstebpgp3s_nu all**" to retrieve 2D dosy parameters (or "**rpar**" to select "**dstebpgp3s_nu**"). Update solvent, **P1**, **SWH**, and **O1** with the values from your proton experiment
- 8) Type "**dosy**" to create the gradient ramp function:
Enter first gradient amplitude: 2
Enter final gradient amplitude: 95 (or the value obtained from 1D DOSY)
Enter number of points: 32 (or the number you think appropriate for your sample)
ram type (l/q): l
and finally, **Do you want to start acquisition?** Select **OK** to collect 2D DOSY data.

DOSY Processing

- 1) Set the proper window function.
- 2) Type "**eddosy**"
- 3) Type "**setdiffparm**" (or click )
- 4) Type "**xf2**" (or click )
- 5) If you need phase the spectrum, type "**rser 1**" to read the 1st fid to a new prono and type "**efp**" and "**apk**" to get correct **PHC0** and **PHC1** numbers. Then go back to 2D DOSY dataset and correct the phase values. Remember the phase mode is "**pk**" for direct dimension (F2).
- 6) Type "**dosy2d setup**" (or click )
- 7) Type "**dosy2d**" (or click ) , you should see the 2D DOSY spectrum with chemical shift along the detected F2 axis and diffusion coefficient along F1 axis.