

1D-TOCSY on Topspin (Katarina Only)

1. Turn off the spinning. Lock and shim on your sample like normal and acquire a normal proton experiment to ensure good shimming. You may want to optimize your SW and o1p. Expand your spectrum fully and put the cursor on o1p (the exact middle of the spectrum). Now, while depressing the left mouse button, slide down to the middle of the peak you wish to irradiate. Record the displayed frequency difference (Hz). If it is upfield of o1p, place a negative sign in front of it. Also, use this same procedure to measure the width in Hz of the peak you wish to irradiate.
2. Type 'iexpno' [enter] to create experiment #2. Type 'rpar' [enter] and select TOCSY_1D. Change SW and o1p, and td to the values used in step 1. Check to ensure your solvent is selected. Type 'ased' [enter] and scroll down till you see the box SPOFFS2. This is where you will put the offset value from o1p to define which resonance you wish to irradiate. NOTE: Resonances upfield of o1p need to have a negative sign in front of them.
3. Type 'stdisp' and new window will pop up. If you have multiple data sets open you will be prompted to select which data set you wish your changes to apply to....select the one you are in. Under 'analysis', select 'calculate bandwidth for refocusing' option. Put the width in Hz you determined for the peak you wish to irradiate into the Delta Omega box (see Figure) and hit the enter key. A new value should appear in the Delta T box. Record this value. The maximum allowed value of Delta T is 80000us for this experiment. Click the X in the top right hand corner to quit the shape tool. Type **p12** [enter] and record the number you just calculated.
4. The default mixing time is 300ms. This is a good place to start. Type 'rga' [enter] followed by 'zz' [enter] when rga is finished. The spectrum should show positive peaks for the peak you irradiated, the solvent peaks, and any peaks in the same spin system as your irradiated peak. You can try running the experiment with various mixing times. Just 'iexpno' and type 'd8' [enter] and change the value, however, d8 should be less than T1.

