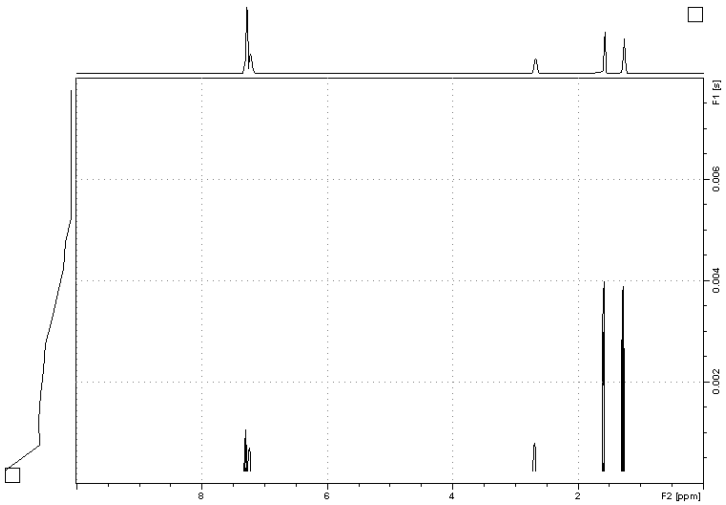
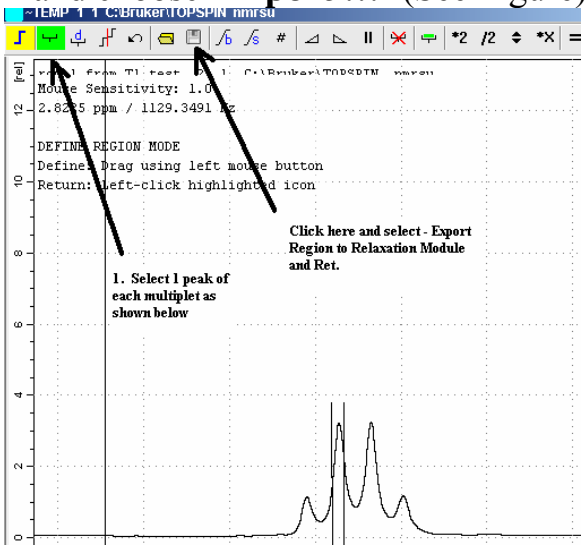
T2 Analysis - Quick Reference

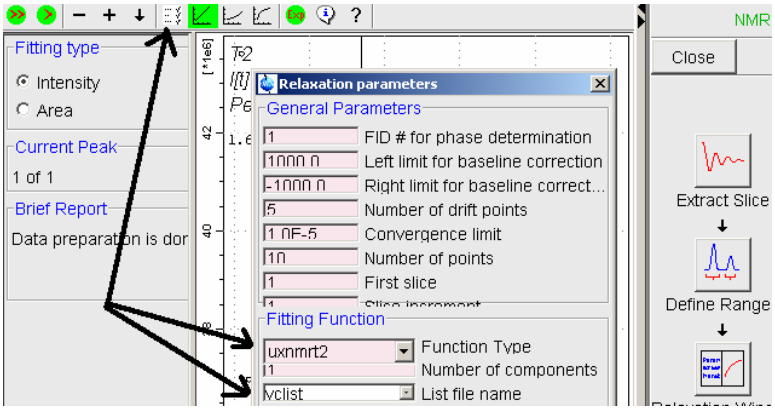
1. Setup and obtain a 1-D proton spectrum. Optimize your SW and o1p according to the directions on the COSY Guide. Rerun your experiment with the new values. Record the values.
2. NOTE: T2* values can be estimated from the linewidth at half-max of the resonance in question. To do this, perform peak picking on the expanded area of your peak of interest (select the option to only do peak picking on the expanded area). After it labels your peak, type hwcal in the command window the peak width at ½ max should be displayed in Hz =1/s). T2* = 1/π*width in seconds.
3. Type **edc** [enter] and change the experiment number to **2 (**or type **iexpno** [enter]). Type **rpar** [enter] and select **T2_Proton, copy all**. Type '**eda**' [enter] and change the values of **sw** and **o1p** to those you recorded from **exp 1**. Select the proper solvent and click the little blue test tube 'prosol' button. This is not a 2-D experiment, but it is set up in 2-D mode as it is an array of 10 different experiments. Each experiment uses a different variable delay, read from the default **vc list**, **t2delay**. To view the default values, type '**edlist**' [enter] and select **vc** and then **t2delay**. You may need to generate your own vdlist if the default list does not afford you a reasonable fit when calculating T1. To generate your own vclist, type **edlist**, select **vc**, a list of vc files will pop up, type in a new filename in the window in the bottom, and an editor window will pop up. Click in the bottom section of the window and type in your vclist. Be sure to put an **s** for seconds after each number, or ms, us. Be sure to write down how many entries are in your list, as well as the name of your list. In the eda window, you will need to put your filename in the vdlist window, and the number of entries in your vclist is the value that goes in the td box of F1. Type **rga** [enter] and then **zg** [enter] when rga is finished.
2. When the acquisition is finished, type **'xf2'** [enter]. Increase the intensity until you see intensity form at the bottom of the screen at the chemical shifts of your spectrum (see figure). Click the phase button  . Right mouse click on one of the signals in your spectrum and select '**add**'. Next click on the  horizontal arrow with the R over it. Your spectrum should appear. Phase it and save it. Type '**abs2**' [enter]. Select '**T1/T2 Relaxation**' from the '**Analysis**' pull down menu at the top of the screen. Select '**Extract Slice**' [enter], '**Spectrum**' [enter], '**Slice #1**' [OK]. Your spectrum should appear and it should be phased. Select '**Define Ranges**' in the relaxation module and click [OK] to the pop-up box. Use the normal expansion tool to expand around each of the peaks you wish to analyze. Next, click the little bracket tool to select a region in each of your resonances of interest. NOTE: For multiplets,



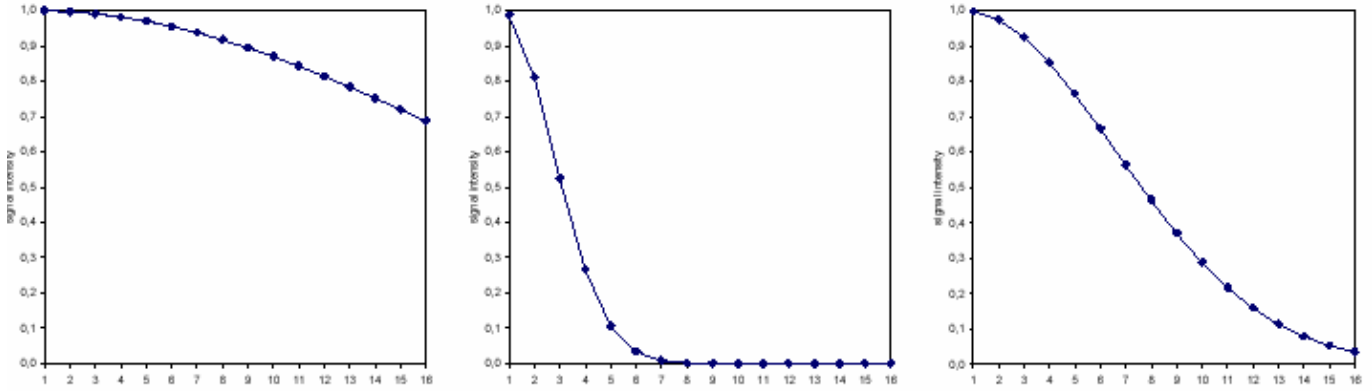
just select one peak as shown in the figure. This process avoids baseline artifacts. When all of your resonances are selected, click the disc button and choose '**Export** …' (See Figure).

3. Click the Relaxation window icon. The relaxation parameters screen may pop up. If so, make sure that under 'Fitting Function' that the type is **uxnmrt2**, and that the list name is **vclist**. If you notice it says T1 data instead of T2, click the little white icon with the check marks (see figure) to launch the parameters and change the values aforementioned. Click 'OK'. Click the  icon to calculate the T2 of all the resonances you selected. The default mode is '**area**'. You can try '**intensity**' as well. The data should be close either way. Click the + or – to scroll through the different curves. You want the curves to look like a smooth decay. Click the 'Display Report' icon and you will see a tabulated data table for each of your resonances that you can print if you wish. Obviously if your curves look bad, you will need to run the experiment again with an edited vdlist.





Examples of good curves and bad curves.



A **B** **C**

A – Delays would not be long enough
B – Delays would be too long.
C – Delays would ideal.