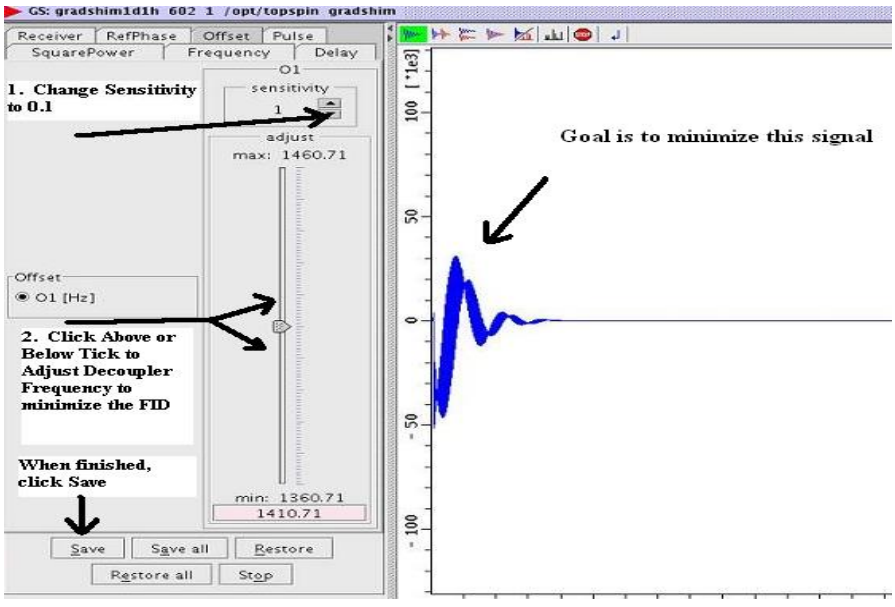
Solvent Suppression - Presaturation

(NOTE: There are many types of solvent suppression – this is presaturation and all exchangeable protons will be attenuated-instructions for other types follow)

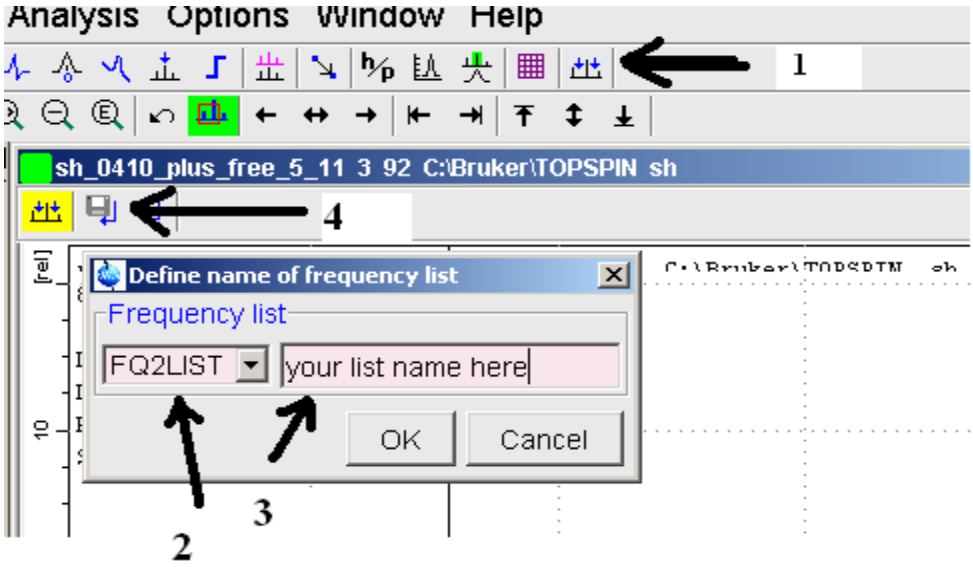
1. Turn off the spinning. Lock and shim on your sample like normal and acquire a normal proton experiment to ensure good shimming. Be sure to do ATMA on Zeus or Cronus, and wobb on Artemis.
2. Type 'iexpno' [enter] to create experiment #2. Type 'rpar' [enter] and select SOLVENT_SUPPRESSION (on Artemis add suffix _BROWN). Type 'eda' and check to ensure your solvent is selected. If you are suppressing water, skip to step 3. Type 'o1p' [enter], and enter the ppm value of the solvent peak you wish to saturate (you can get this from experiment #1). You may need to change SW to view all the peaks in your spectrum (ie. If you are decoupling DMSO-d6 @ ~2.5ppm and the default SW is 12, your spectrum will end at 8.5ppm). The default values of SW and o1p are 12 and 4.69 respectively. Change SW by typing 'SW' [enter] and typing a value in the box that pops up. If you change SW, please type 'AQ' [enter] and enter 1.5.
3. Click the 'getprosol' button . DO NOT TYPE 'RGA'. The receiver gain needs to be at least 128 for this experiment to work properly. Type 'gs' [enter]. A new screen will appear. Change the sensitivity setting to 0.1 as shown in picture and adjust the offset frequency by left mouse clicking above or below the tick. The goal is to minimize the FID area. You should be very close already so it really only requires minor adjusting. Click 'Save' and Stop' when you are done. Type 'zz' [enter]. You may get a better result if you optimize the lock settings (see Lock Optimization Instructions).



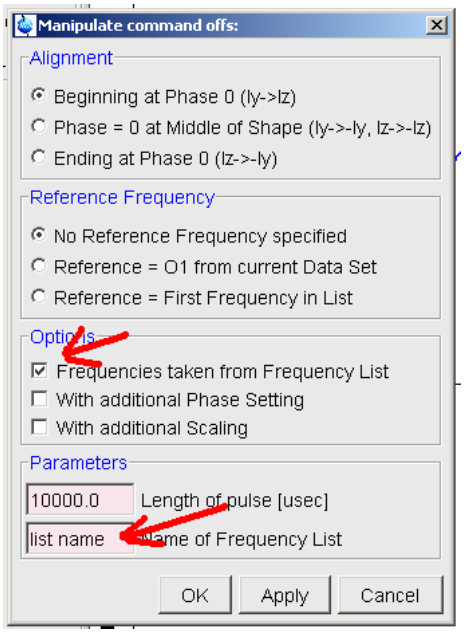
4. You can adjust pl9 down to 40dB if you are not getting a satisfactory saturation of your solvent resonance. Do this by typing 'pl9' [enter] and putting in the value (**On Artemis and Cronus, make sure you are adjusting the dB scale and not the watts**). NOTE: Peaks close to the solvent peak may exhibit a shift change and these as well as exchangeable protons may also be attenuated.

Solvent Suppression – WET

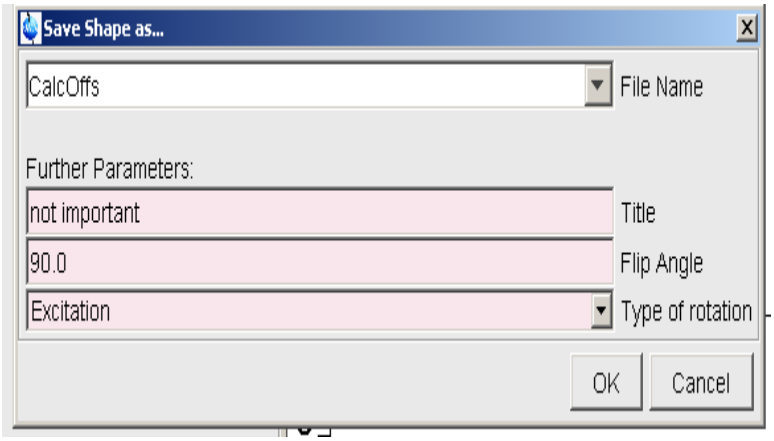
1. Rpar WET (or WET_BROWN on Artemis/Cronus). Copy all. If you only want to remove one peak, the tallest peak in the spectrum, you need only adjust your SW, o1p, and aq. Next, type xaua. The next thing you see should be your spectrum with the tallest peak showing significant attenuation. You may be prompted to override a spectrum that already exists. Just click ok as it is just the spectrum generated during the automatic optimization procedure.
2. If you are unhappy with the result, you can optimize removal of the peak by typing gs, and then click on the shape tab and adjust SP7 in 0.1db increments to optimize removal of the peak of interest (be sure to adjust the dB scale and not watts on Artemis/Cronus). Remember, it is a shaped pulse and so the power level governs the shape, so very small differences can result in better suppression.
3. You can irradiate more than one peak automatically as long as the peaks you are attempting to suppress are the tallest in the spectrum. Just type L30 and set it to the number of peaks you wish to suppress (I have successfully suppressed 3).
4. To irradiate more than one peak that is not the tallest, you will need to create a list. To do this, from the normal ^{1}H spectrum, click on the  tab as seen in the picture below. You will be prompted for a FQ1LIST name (don't worry that it says FQ2LIST in the figure below). Type in a name for your list. Next use the left mouse button to select the peaks you wish to suppress (up to 4-but it is not that effective above 2). When finished click the save/return icon  .



5. Next, move back to the WET experiment if you are still in the normal 1H spectrum and type stdisp to launch the shape tool. Click the  icon to open the Sinc.1.1000 shape. Click on the 'Manipulate' button at the top of the page and select the first option. A new box will open. Select 'Frequencies taken from Frequency List' under options as seen in figure below. Finally, type in your listname in the parameters box and click 'apply', then ok.

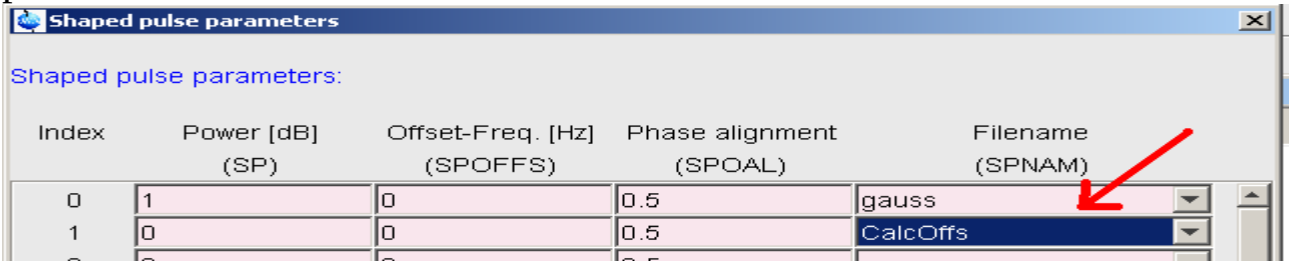


6. Click the  icon to save the shape. A new box will open. The default filename is CalcOffs and that is fine. Click OK.



Exit from the shape tool by clicking the  on the top far right of the shape tool box (careful not to close Topspin).

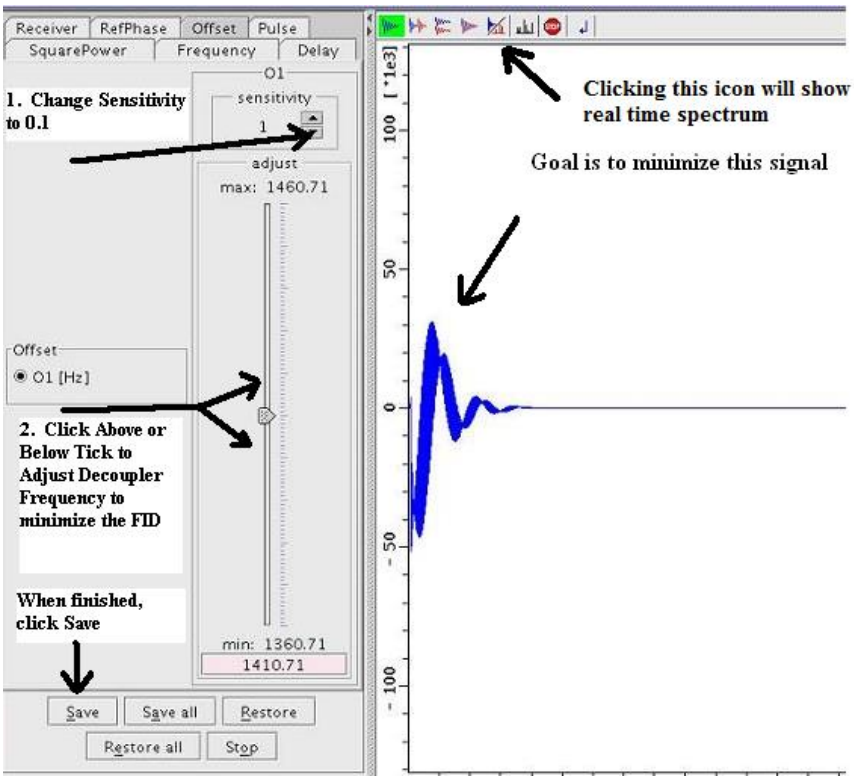
7. Type shape [enter] on the command line. Select CalcOffs from the pull down selector next to SPNAM1. Click the OK button. Finally, type lcwetset in the command line. Ensure the number of scans, ns is 8, and ds is 16. Perform RGA. When finished type xaua. When the experiment is over type 'efp' to process the data.



Solvent Suppression – Excitation Sculpting)

(WET and ES work best on Artemis, Cronus or Ares)

1. Turn off spinning. Lock and shim as normal (If you are using a 90:10 H2O:D2O, use the topshim 3d command on Artemis). Make sure you are tuned well, ATMA on Zeus/Cronus/Aress, wobb on Artemis.
2. RPAR Excitation_Sculpting (suffix _Brown on Artemis/Cronus). By default the parameter set is going to suppress H2O at 4.72ppm. If you need to suppress a different resonance, you can either move o1p, or measure the frequency difference in Hz from your desired o1p and put that value in the SPOFFS box in the ased window. Remember, if the peak you are trying to suppress is upfield of your o1p, you need a negative sign in front of your SPOFFS value.
3. The parameter set is also stored with reasonable starting values for this experiment to work. You can type gs [enter] in the command box and optimize the shaped pulse power (found by clicking the 'shape' tab and then selecting SPdB1 and then adjusting the slider – begin with increments of 1 and then fine tune with 0.1) and the offset (found by clicking the 'offset' tab as shown below. The goal here is to minimize the size of the fid or solvent peak if you choose to watch the real time spectrum (see figure). After you have optimized as best you can, click 'save all' and 'stop'. Perform rga and zz to begin experiment. Process as usual.


Receiver
RefPhase
Offset
Pulse
SquarePower
Frequency
Delay
O1
1. Change Sensitivity to 0.1
sensitivity
1
adjust
max: 1460.71
Offset
O1 [Hz]
2. Click Above or Below Tick to Adjust Decoupler Frequency to minimize the FID
When finished, click Save
min: 1360.71
1410.71
Save
Save all
Restore
Restore all
Stop
Clicking this icon will show real time spectrum
Goal is to minimize this signal
100 [*1e3]
50
0
- 50
- 100