Selective Decoupling

Homonuclear Selective Decoupling

To selectively decouple peaks in a spectrum, you will need to adjust the decoupler frequency and power. The frequency should be centered on the peak you want to irradiate, and the power should be sufficient to saturate the peak irradiated, yet not spill onto adjacent peaks. You will obtain the frequency values for the decoupler from a standard (coupled) spectrum. In this case, you will perform homonuclear decoupling of a proton spectrum ($^1H\{^1H\}$), so F2 (the decoupled nucleus, ^1H) and F1 (the observed nucleus, ^1H) will be the same.

Reference Spectrum

1. Insert a sample, lock, shim, and record a normal ^1H spectrum.
2. Note the position (in Hz or ppm) of the peak you wish to decouple.
   This is easiest done by entering peak-pick mode ( ), placing the cursor on the peak, and recording the peak position at the left of the screen.

Decoupled Spectrum

3. Create a new dataset in a new window.
   The easiest method seems to be reopening the reference spectrum from step 1 in a new window, then typing "iexpno" to increment the experiment number.
4. Recall the proton homonuclear decoupling parameters: "rpar PROHOMODEC all". "getprosol" as usual. Take a look at the pulse program (button under Pulse Program tab), noting the timing of the decoupling.
5. Set the decoupler frequency offset, O2, to the value you obtained in step 2 above. (O2P if your value was in PPM).
6. Check the decoupler power level, PLdb24: it should be around 30 dB.
7. Acquire the spectrum as usual (RGA; ZG; EFP).
8. If necessary, tweak the decoupler power and repeat from step 7.

   IMPORTANT: *the PLDBxx settings are attenuation settings*. Higher numbers give lower power.
   Although there should be safety-checks in the software, be careful to never send too much power through the coils — high power decoupling (small settings) can fry them. ($$$$)

Multiple Display and Difference Spectra

Note that increasing the LB setting will help peaks to cancel out when you subtract, rather than generating dispersion-like peaks.

9. From the Reference Spectrum, enter multiple display mode. ("mdisp" or button in top row).
   It is important that the reference be the first spectrum in the stack: the order of the others can be changed, but the first one in cannot be moved.
10. Open the other spectra you wish to display by left-dragging them from the Browser window (on the left of the screen) into the main window.

    If necessary, you can toggle between stacked and superimposed spectra with the button.

11. Obtain the difference spectrum.
    Select a spectrum by clicking the box at the right of the screen.
    The △-button will generate the difference between the selected spectrum and (the sum of all ?) the other(s). (The ∑-button will similarly display the sum of the spectra.) You may need to adjust the vertical scale (⬍S) of one spectrum or shift it (⟷S) to get peaks to cancel reasonably.

    Lastly, the distance tool (↘) will let you measure coupling constants by dragging on the spectrum.