Homonuclear $^1$H-$^1$H Decoupling on the QE-300

There are several ways a homonuclear decoupled spectrum can be obtained on the QE-300. The following procedure seems to be the most readily understandable and useful way for most people.

1. Acquire a normal proton spectrum in the usual way.

2. Enter command mode, if not already there, and do a `<control> F` to make certain the entire spectrum is visible on the screen.

3. Reference the spectrum via the `O` subcommand of >PP (i.e. TMS = 0)

4. Set the decoupler power level with L1 (i.e., >L1=nnnn3035 <return>). Currently 3035 is a typical value but it may vary from sample to sample. A larger number results in less power and changes in increments of 50 are noticeable. (Also keep in mind that typing >L1 at any time will turn the decoupler off.)

5. Turn the decoupler on with >DN. The letter D will appear on the top line of the screen to the right of the lock level. (The decoupler must always be turned on again after changing L1.)

6. Type >EF to enter the decoupler frequency offset(s) via the cursor. A cursor will appear at the left edge of the spectrum.

7. Type `<control> R` to clear any previously used offset(s) from the CD (decoupler offset) list. The CD list must be cleared, otherwise the entry will be added to the current list.

8. Using the knob, move the cursor to the peak(s) to be irradiated and type D. This enters a value into the CD list. Type <return> to exit the EF subroutine.

9. Type >CD and answer the question appropriately (Y or N) to be certain the CD list is on and that the value just entered in step #8 is correct. This first value should be followed by a 0 value (type <return>) to terminate the list. Typing <return> again will exit the CD list.

10. Acquire and process the decoupled spectrum as you would a regular spectrum.

11. One must type >DF to turn the decoupler off after the acquisition has finished.

Either a single frequency or a list of frequencies (up to 32) can be entered into the CD list with the cursor and D subcommand in step #8 above. If more than one frequency is entered, a >GS should be used in step #10 and set equal to the number of frequency values entered into the CD list. Better results are obtained if >NA is set to at least 4. An FID will be collected and stored for each of these values. Filenames for successive FIDs are automatically incremented by >GS (i.e., if the initial filename is KMC.001, then the second FID will automatically be called KMC.002, etc.). This series or array of FIDs can be automatically called up, transformed, and the spectra stored by using the linked list as follows:
>LI = XXXX GABCEMFTPSSB <return>
>AU = \textit{N}, where \textit{N} is the same number used for the >GS. Answer \textbf{Y} to the question "increment names?"
The FIDs will now exist as (for example) KMC.ØØ1, KMC.ØØ2, etc..., and the spectra will exist as (for example) KMC.5Ø1, KMC.5Ø2, etc..., (note the 5). Spectra may be quickly viewed with >VW, giving it the filename of the first spectrum, and then using \textbf{N} and \textbf{R} to view the next or previous spectrum in the array. Type <return> to exit >VW.

To enter a list of frequencies directly (as from a peak printout) into the CD list, do the following:

1. \textbf{F2} = nØ <return>. The values entered into the CD list are offsets from F2, therefore it should be set to Ø.

2. >CD, answer so as to turn it on.

3. >CD list values may now be entered directly, in Hz, from a >PP printout. Start with the highest frequency first, type <return> after entering each new value, and use a Ø and <return> to terminate the list.

4. >DN and >GS equal to the number of offsets in the CD list, not counting the Ø.

It is relatively easy to decouple peaks which are more than 2Ø Hz from each other. To decouple peaks which are less than 2Ø Hz apart, the decoupler frequency must coincide exactly with the geometric center, which may not necessarily be the tallest resonance of a multiplet. To find the center, use the CD list and increment the values by 2 Hz through the region being irradiated. Then, use the value that gives the best decoupling. L1 values will have a similar range as that used for $^{13}$C; 26ØØ (max. power) - 31ØØ (min. power), in increments of 5Ø units.