

How to Run a Homo-nuclear Decoupling (HOMODEC) Experiment:

This guide will demonstrate a quick and simple means for determining if two resonances are coupled. The *HOMODEC* experiment is most effective for relatively simple spectra where the couplings are, at least, somewhat resolved (i.e. there is a minimal amount of spectral congestion). The experiment consists of irradiating a *single* selected resonance with a low power decoupler pulse. This pulse should eliminate any couplings to that resonance. By comparing the resulting spectrum to that without decoupling, it is easily determined which resonance(s) are coupled to the irradiated peak. The *HOMODEC* experiment will work on all Varian NMR instruments.

1. Acquire a typical ^1H spectrum in the usual fashion. Process and save the spectrum, as you may need it for comparison. If you're having problems already it would probably be best if you stop now. If you would like a Mercury or Unity 300 training sheet, they are available on our website. Click [here](#).
2. Convert the standard ^1H to homo-nuclear decoupling parameters. Type **HOMODEC** in the Input Window. This enables homo-nuclear decoupling by setting **dn='H1'**, **dmm='ccc'**, **dm='nny'**, **homo='y'**, **dpwr=0**.
3. Click the [**Cursor**] button and place the cursor on a 'clean' portion of the spectrum (i.e. contains no peaks within ~ 1 ppm). This will serve as a reference spectrum.
4. Type **sd** (*set decoupler*). This resets the decoupler offset (*dof*) to the cursor location.
5. Expand the spectrum around the spectral feature you would like to irradiate (i.e. the one that you want to determine coupling).
6. Expand the spectrum and place cursor on your desired peak to be decoupled. Type **sda** (*set decoupler array*). Repeat using **sda** for all peaks you wish to decouple.
7. When finished, set **nt** (*number of transients*) then type **ga**.
8. Process the 1st fid. Type **wft ds(1) aph vsadj** If necessary, manually phase. Ignore the irradiated peak, as it will not phase correctly.

Note!

If the irradiated peak is still positive and contains splittings, you may need to increase the decoupler power. Type **dpwr=4** (default is 0) and repeat the experiment. **Do not increase dpwr above 20!**

9. When 'zooming in' on spectral regions, you might want to familiarize yourself with the *s* (*save display parameters*) and *r* (*recall display parameters*) macros. For example, imagine that your full spectral region is quite congested due to a large number of resonances. During these experiments you are continually expanding and

moving between three regions of interest (say 8 to 6ppm, 5.5 to 4ppm, and 3.5 to 2.5ppm). To make this easier do the following:

- 1) Use the cursors to define the 8 to 6ppm region. Click [**Expand**] then type **s1**.
- 2) Similarly define and expand the 5.5 to 4ppm and the 3.5 to 2.5ppm regions. Define these expansions as **s2** and **s3** respectively.
- 3) Each of these expansions can now easily be recalled by typing **r1**, **r2**, or **r3**.
- 4) Now type **r1 ↵**, (or **r2**, or **r3**) to view the results.

10. Prepare to setup a stacked plot Type **vs=vs/#**, where # is the number of spectra in the array.

Example: if you did one reference and 2 decoupled spectra, type **vs=vs/3**.

11. Type **f full dssa**. This displays the spectra full screen in a *vertically stacked plot*. If you prefer, type **f full dssh** and this will display the spectra *stacked horizontally*.

12. Expanding regions is the same as with 1D spectra, but you must type **ds** (*display spectrum*) first. If you are interested in the closely examining the regions defined above (for example r2) type **r2 wft dssh**.

13. To plot all stacked spectra, type **pl('all') pscale pltext page**.

14. To plot selected spectra, type **pl(1, #) pscale pltext page**, where # is the number of the spectrum.

Example: if you want to print the reference and the third spectrum, type **pl(1,3) pscale pltext page**.