Instructions for Processing DEPT Spectra Using MNova

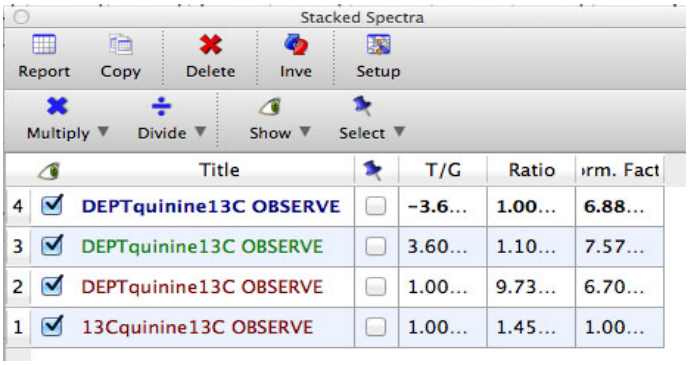
(Revised 2-3-2016)

1. Open the MNova program and connect to the NMR computer to get at your NMR data folder.

2. If you used IconNMR to collect your data, the ^{13}C spectrum and the three DEPT spectra are probably all contained in the same dataset folder. If so, simply drag this folder to the open MNova window and the 4 spectra will appear in the **Pages** side bar (keep in mind you may have acquired other spectra – like a ^{1}H-NMR spectrum – that may appear, too). The spectra appear in the **Pages** side bar from top to bottom in the order that they were acquired (likely: ^{13}C, DEPT45, DEPT90, DEPT135.

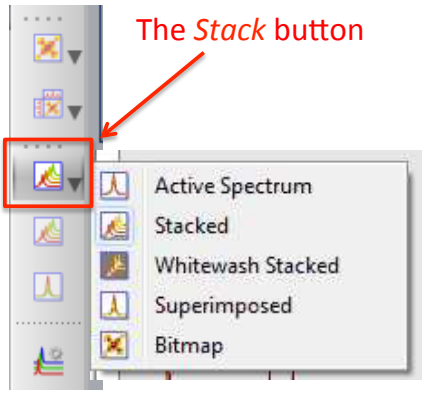
3. Stacking the spectra: In the **Pages** side bar, select all 4 spectra (leave out any other spectra that may be open), then go to the **Stack** menu and select **Stack Spectra**. The ^{13}C spectrum and the three DEPT spectra will appear in a new page. It is customary to display the spectra stacked from bottom to top: 13C, DEPT45, DEPT90, DEPT135. It is likely that the spectra will appear in this order.

   Note: you can always change the order of the spectra in the stacked plot, as follows: Go to the **Stack** menu and select **Stacked Spectra Table (Stack → Stack Spectra Table)**. The dialog box shown to the right will appear. The order can be changed by dragging the spectrum number, at the far left of the table, up or down to the desired position.

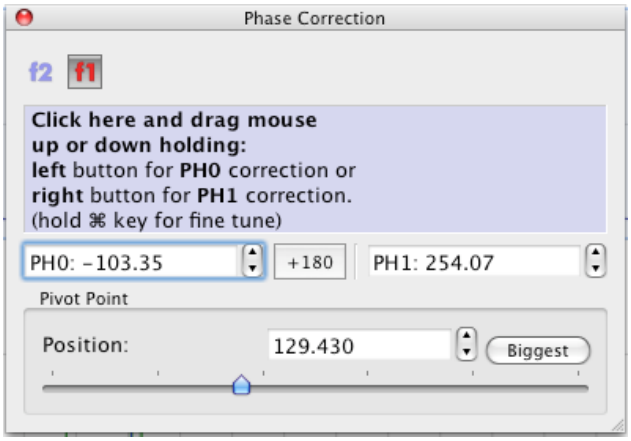


4. The spectra likely will need to be manually phased. Remember that for the ^{13}C spectrum, the DEPT 45, and DEPT 90, peaks should all have positive phase, while for DEPT 135, C and CH_3 peaks are positive and CH_2 are negative. From the stacked plot you can phase the ^{13}C spectrum at the bottom of the stack, and then all others will be phased correctly, based on the ^{13}C spectrum's phase parameters.

   Phasing the stacked spectra: Activate (click on) the bottom ^{13}C spectrum in the stacked plot, and manually phase this one with all peaks positive. When you quit the phase routine after phasing the ^{13}C spectrum, the phase of all DEPT spectra will be adjusted based on the phase parameters you set on the ^{13}C spectrum.* Manual phasing requires two phasing adjustments: the so-called *zero order* and *first order* phase parameters. To manually phase, click on the *phase* icon on the toolbar (shown to the right) and select **Manual Correction**. You can also get to the phase routine using the menu: **Processing → Phase Correction → Manual Correction**.



* Optional Tip: To make it easier to phase, you can display (temporarily) only the "active" spectrum in a stacked plot using the *Stack* button on the vertical tool bar on the left side of the window. Select "Active Spectrum" and the currently active spectrum will be displayed alone. After you are done phasing or otherwise manipulating this spectrum, you can use the Stack button again to return to the full stacked plot.



The *Phase Correction* dialog box appears and a blue cursor line (Pivot) appears on the largest peak in the spectrum. You get best results if you move the Pivot (use the slide bar in the dialog box) to a reasonably large peak at one end of the spectrum or the other. As noted in the dialog box, apply the zero order correction by **left** clicking (hold click) in the blue portion of the dialog box and drag up or down to flatten the baseline about the peak that has the Pivot on it. When that peak looks good, then identify a poorly phased peak at the opposite end of the spectrum from the Pivot (don't move the Pivot!) and click (and hold) the **right** mouse button in the dialog box, again, dragging up or down to flatten the baseline around this peak. Once you are happy with your phasing of the ^{13}C spectrum, close the phase dialog box. The program will automatically phase the DEPT spectra to match. You may find that the ^{13}C spectrum is not really in need of phasing. Nonetheless, going through the phasing routine on this spectrum (even if you don't really need to change much) will phase all spectra in the stack based on these phase parameters.

Look at all the spectra to make sure the phasing in each is correct! The ^{13}C spectrum and the DEPT 45 and 90 should have all **positive** peaks. Very occasionally, phasing all spectra based on the ^{13}C spectrum will result in the DEPT 135 spectrum to be 180° out of phase (and possibly the other DEPT spectra, too). The tip off to a phasing problem in the DEPT 135 is to find the TMS peak (CH_3), or other peak you know to be a CH or CH_3 carbon: the CH and CH_3 peaks **should be positive**. If any of the DEPT spectra are not phased properly, then you need to go back to the individual spectra and phase each one properly. *Then* stack these already-phased spectra.

5. The middle mouse wheel, controls the vertical scale of all spectra together, but the vertical scale of the 4 spectra may not be comparable. To fix this problem, you can first try to normalize the scale of the 4 spectra by going to the **Stack** menu and selecting **Auto Scale**. If using the **Auto Scale** does not give the desired results, the vertical scale for individual spectra can be adjusted with the × and ÷ buttons on the vertical tool bar. To use these tools, activate the spectrum of interest (click on it) and click the × or ÷ button to increase or decrease the vertical scale of just the activated spectrum. The little triangles to the right of each button activates pulldown menus that allow you to increase or decrease the scaling factor of a button click.

6. You can expand and manipulate the spectra in the same way you do regular proton and carbon spectra. You will see that when you expand a region, all spectra expand together.

7. Save your work as a *.mnova* document so you don't have to re-download and process all the data files again, in case you want to look at your spectra again.