
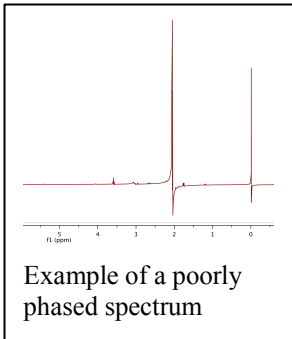


Guide To NMR Data File Access and MestReNova (MNova) Data Processing


IMPORTANT NOTE: MNova has two interfaces (or “Themes”) that can be used, the “Classic” and the “Modern”. **This handout is based on the Classic theme**, which is currently the default interface when using MNova on Carleton Mac computers. Go to Preferences to switch between the Classic and Modern themes .

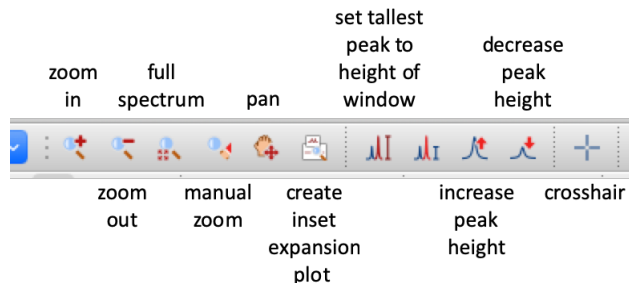
1. Start up MNova from the **Applications Folder**. In Windows, go to the start menu and under **programs** open **MNova**.
2. Access your NMR data:
 - On a Mac, from the Finder, select **Go > Connect to server**.
Type the following address, or select from the list of servers:
smb://and31167131.chem.carleton.edu/data
When prompted, enter your regular Carleton username and password.
Click **Connect**.
 - In Windows, right-click *My Computer*, and select *Map network drive...*
select **Go > Connect to server**.
Select any letter for the network drive.
In the *Folder* field, type: **\\and31167131.chem.carleton.edu\data**
Click Finish.
You will be prompted for a username and password
Username: ads.carleton.edu*<username>*, e.g. *ads.carleton.edu\dalberg*
Password: *<carleton password>*.
Click OK.
3. Once you are connected to the NMR computer, navigate to the appropriate directory (e.g. Chem233 or Chem234). Find your NMR data “file” – it’s really a folder. Drag and drop your folder onto the open MNova program window. Your spectrum should appear (or multiple spectra, if your dataset file contains more than one NMR experiment).
4. The program automatically *phases* the spectrum (flattens the baseline at the base of the peaks), and it almost always does a good job. But if the bases of your peaks don’t look flat (see figure to the right), try an automatic phase correction: Click on the **Phase Correction** icon on the toolbar, and select **Automatic**. If the phasing is still poor (very rare) you should manually phase the spectrum. Go to the instructions at the end of this document, if you need to manually phase.





Example of a poorly phased spectrum
5. To get good integral values you should apply a baseline correction. Click on the **Baseline Correction** icon on the toolbar and select the **Full Auto (Bernstein Polynomials)** option.

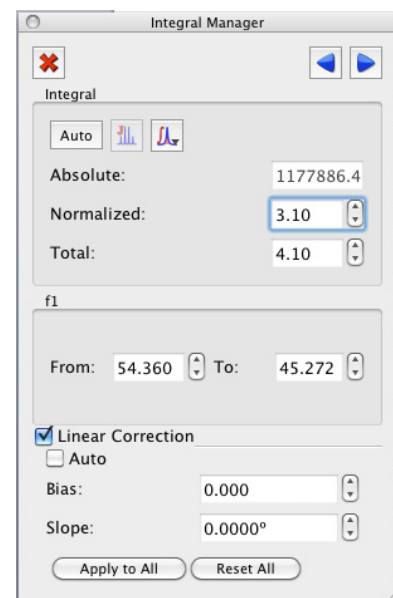

6. (Optional) If you don’t like the grid lines on the spectrum, they can be removed: **Right Click** → **Properties** → select **Grid**; then, unclick the **Show Horizontal** and **Show Vertical** boxes; finally, click **Apply** and then **OK**. You can also change other features of the spectrum in the Properties dialog box, like font sizes, *etc.*
7. The following toolbar buttons will be useful for zooming in or out on the spectrum, panning across it, etc. You can also adjust the vertical scale of the peaks with the scroll wheel on the mouse.



8. Calibrate your spectrum so that your TMS peak is at 0ppm by clicking on the **Reference** toolbar button and then selecting the peak you want to be the reference. Finally, type in 0 (or other relevant value) in the **New Shift** box in the dialog box that appears.



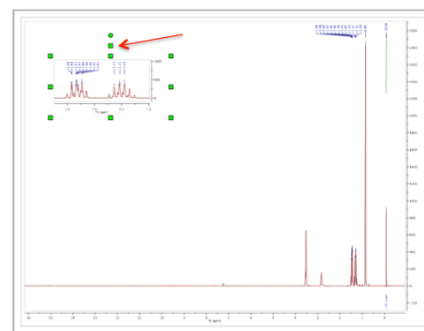
9. **Integration:** You can have MNova select the peaks for integration automatically, but it is almost always preferable to select the peaks yourself. To manually integrate, click on the **Integration** icon on the toolbar and select **Manual**. Then you will be able to integrate each peak individually by dragging your mouse (left click and hold while dragging) from left to right across the region you would like to integrate. You can normalize the integral values to any peak of your choosing. In order to normalize the integral values, scroll over the peak of your choosing until it is **red**, and then **Right Click** → **Edit Integral**. In the dialog box that appears, type the number you would like to set that peak to in the **Normalized** box. To see the numerical value of the integrals look below each integral. To display a list of the integral values and the regions integrated go to **View** → **Tables** → **Integrals**.



10. (Optional) To identify desired peaks, click on the **Peak Picking** icon to obtain an automatic peak picking analysis. Better: if you would like to choose only certain peaks, choose the **Manual** option and drag your mouse from the left side of the desired peak to the right side in order to mark the peak. Repeat this process for all the peaks you would like to identify.



11. (Optional) You can create inset expansion plots on your spectrum (as shown to the right), using the **Expansion** tool. Click the **Expansion** icon, then drag across the portion of the spectrum you want to expand while holding down the left mouse button. When you release the mouse button, the inset will appear. Left click on the inset and you can **Resize** the inset spectrum using the boxes in the corner of the image. Finally, in order to move the spectrum, grab the green box above the middle of the inset spectrum (red arrow).



12. (Optional) To add **annotations** to your spectrum, use the toolbar at the bottom of the screen to add shapes or text. To choose which type of annotation you would like, *click* on the triangle next to the first icon.



click on the triangle and select the "T" (Text Tool)

13. To **Print** or **Save** your spectrum choose **File** → **Print/Save**. You can also convert the spectrum to a PDF: choose **File** → **Export to PDF**. It is strongly recommended that you save your processed spectrum as an MNova file, so you don't have start completely over if you want to print again later, or make any changes.

Manual Phasing: if required, in the rare case that the automatic phasing routine (step 4) does a poor job.

Manual phasing requires two phasing adjustments – the so-called *zero order* and *first order* phase corrections. To manually phase, click on the *phase* icon on the toolbar and select **Manual Correction**. A Phase Correction dialog box appears (below) and a cursor line (pivot point) appears on the largest peak in the spectrum. If the pivot point is on a peak near the middle of the spectrum, it is usually best to move the pivot point to a peak on one side of the spectrum or the other using the **Position** slide bar in the dialog box.



As noted in the dialog box, apply the zero order correction (PH0) by **left** clicking (hold click) in the dialog box and drag up or down to flatten the baseline about the peak that has the pivot point on it. When that peak looks good, you are ready to apply the first order correction (PH1). To do so, look to a peak at the other end of the spectrum from the pivot point (do **not** move the pivot point) and **right** click (and hold) the mouse, again, dragging up or down to flatten the baseline around this peak. Once you are happy with your phasing, click **OK** in the dialog box.

