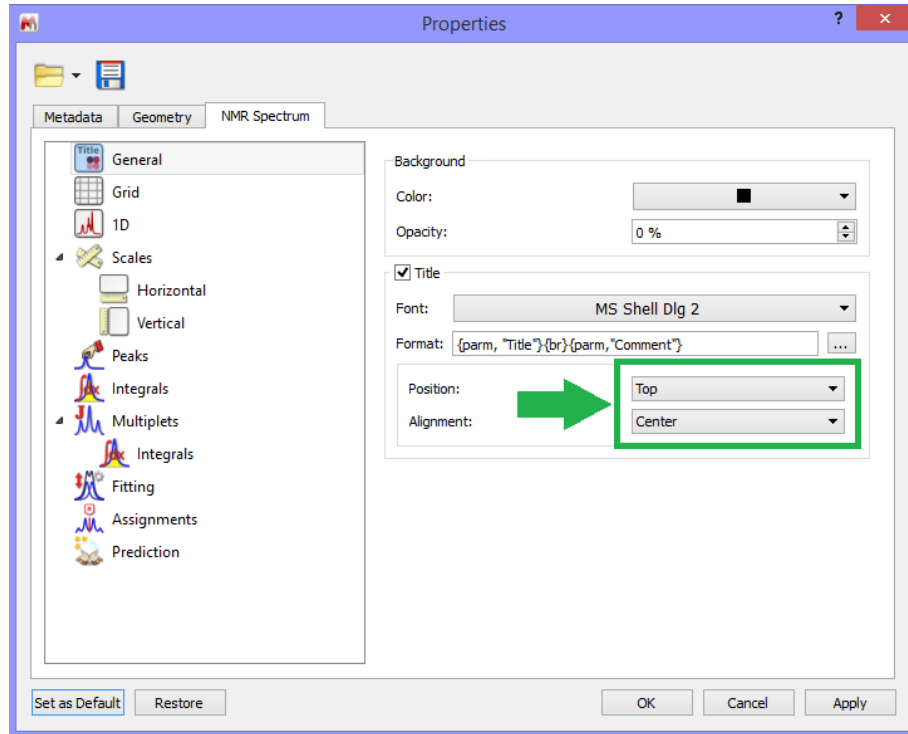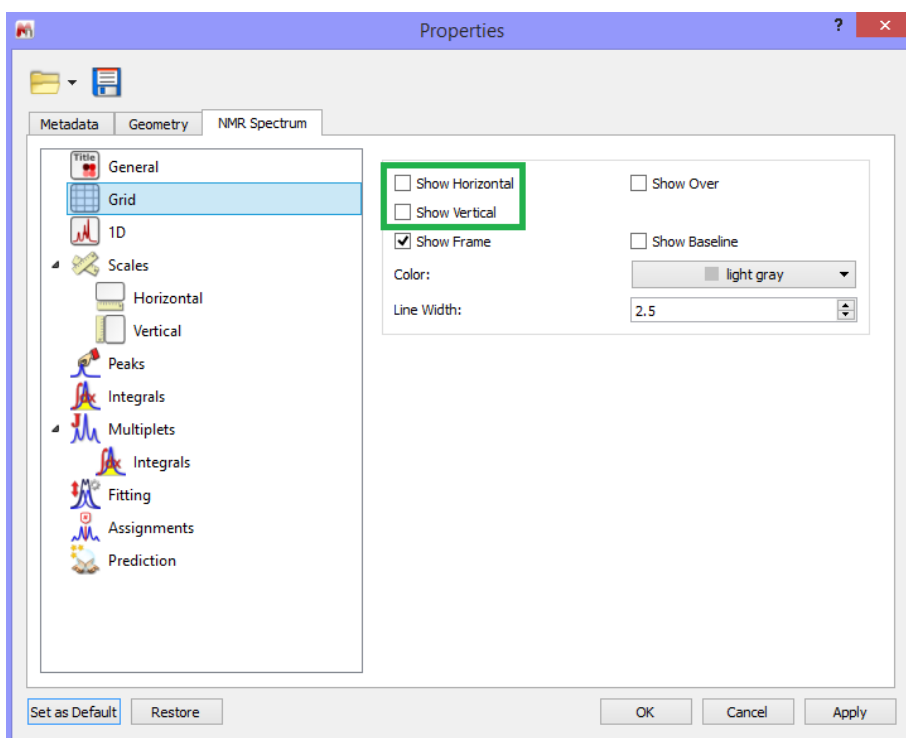**MestReNova Suggested Setup**
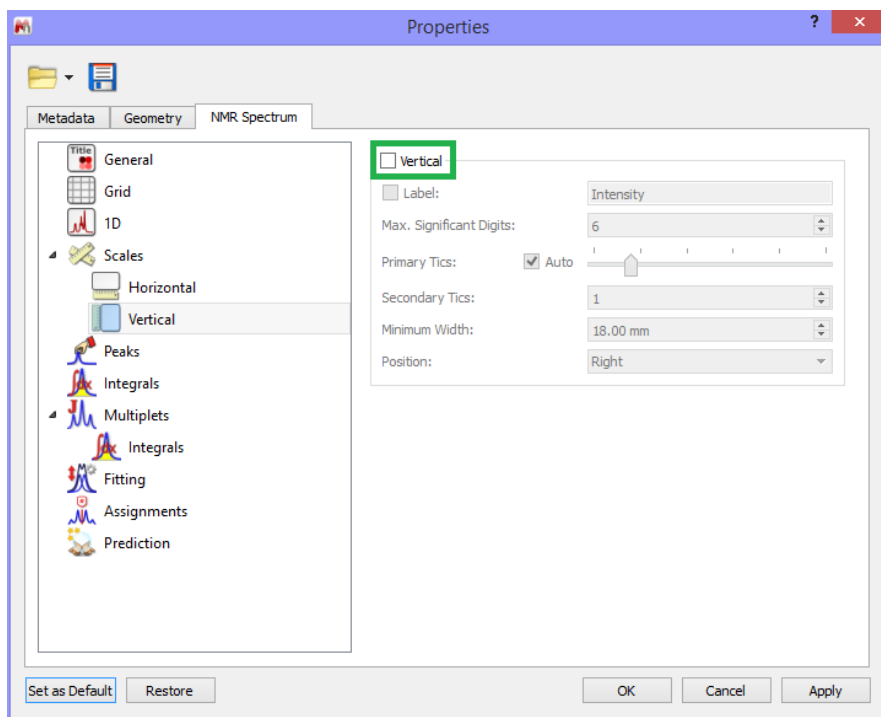
1. Import any spectrum into MestReNova. Right-click on the spectrum and select "Properties" from the menu that appears.

2. In the *General* properties, set the title position to "Top" and alignment to "Center".

3. In the *Grid* properties, un-check "show vertical" and "show horizontal".


4. In the Properties → Vertical (Scales), un-check the "Vertical" option to remove the vertical scale.


5. Most of the spectra you will examine will be ^{1}H-NMR spectra, where you will typically use peak picking to measure coupling constants in Hz. Thus, it may be convenient to have the default

peak picking unit in Hz, but this means you will need to go into the Properties → Peaks window and change it any time you desire peaks in ppm (such as for ^{13}C-NMR).
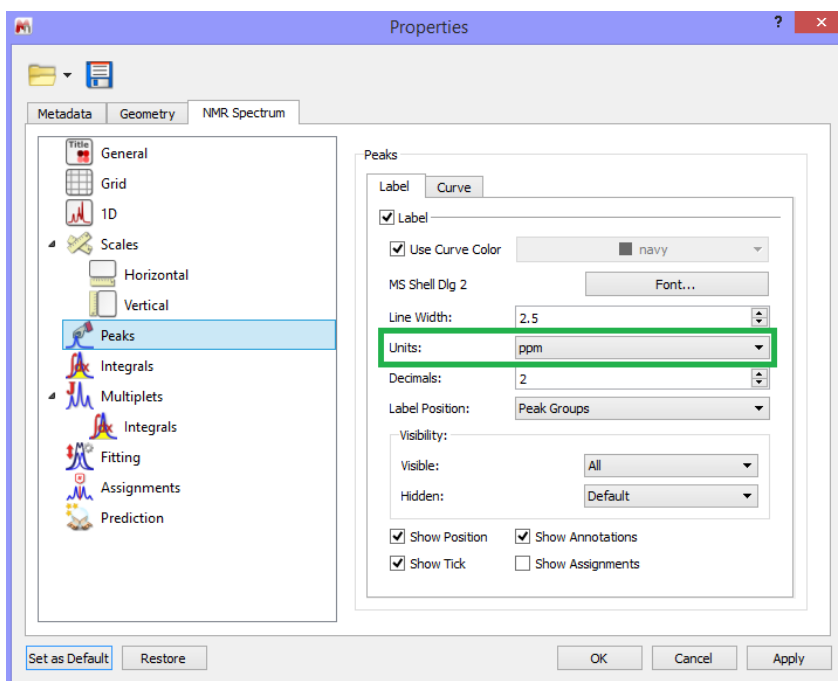
You may also wish to set the "Label Position" to "Peak Groups" to make peak picked labels appear near the tops of the corresponding peaks.

6. Should you wish to change the font, size, or color of text marking peaks, you may do so by clicking the "Font…" button in the Properties → Peaks window.

7. If you wish to change the font, size, or color of text marking integrals, you may do so using the analgous button in the Properties → Integrals window.
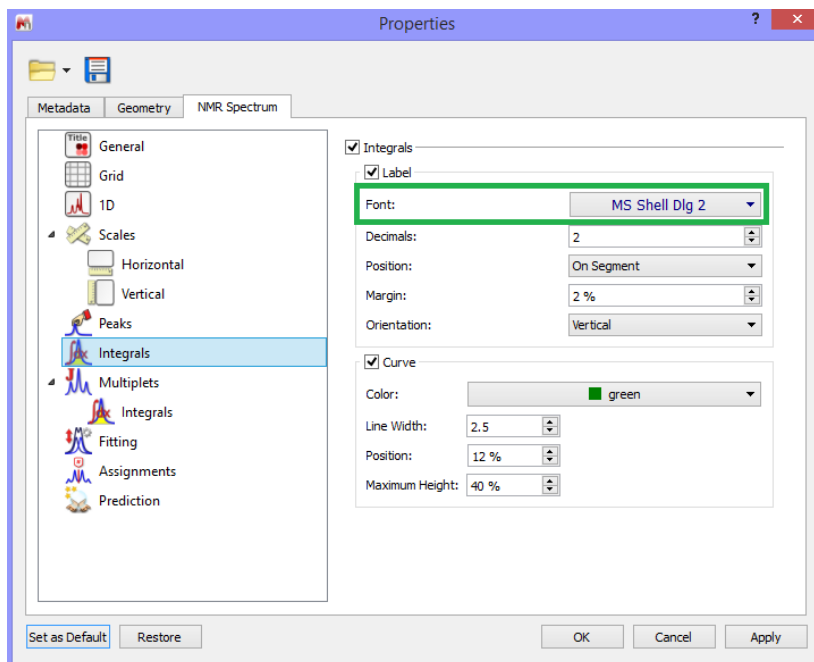
8. Once you have made the style changes you would like standard your spectra, click the "Set as Default" button in the lower left-hand corner of the Properties window.

Quick Guide to Useful Buttons

– Zoom in/ zoom out, respectively

– View full spectrum

– Set view to specific ppm range

– Expansion tool creates inset spectrum

– Scale spectrum to max/min intensity, respectively

– Increase/decrease spectrum intensity, respectively (you can also scroll on a mouse)

– Phase Correction

– Baseline correction

– Reference button (for referencing chemical shift)

– Absolute Reference button

– Peak picking tool

– Integration tool

Standard ^{1}H-NMR Spectral Workup

1. Download and extract your NMR file as necessary. Open MestReNova, then drag and drop the FID file or folder containing the FID file into MestReNova.

2. Adjust phasing on your spectrum. The phasing is typically good to begin with and the automatic phase tool will works well. Shown below, however, is an example of a poorly-phased spectrum. Note the asymmetry of the aromatic ^{1}H-atom signals and the poorly shaped TMS peak where one side of the peak is actually negative.
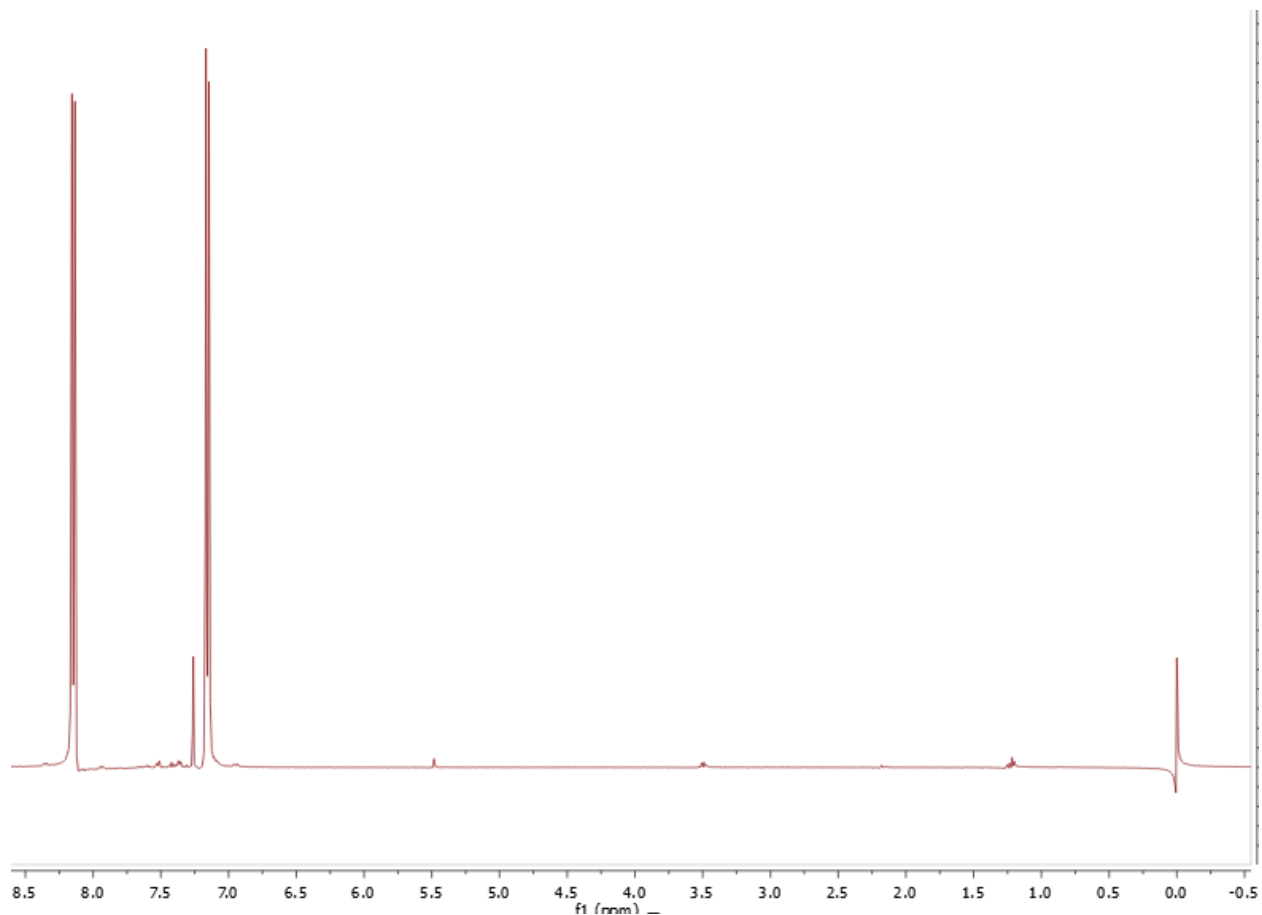

To use auto-phasing, click the arrow right of the phase tool button and select "Automatic".
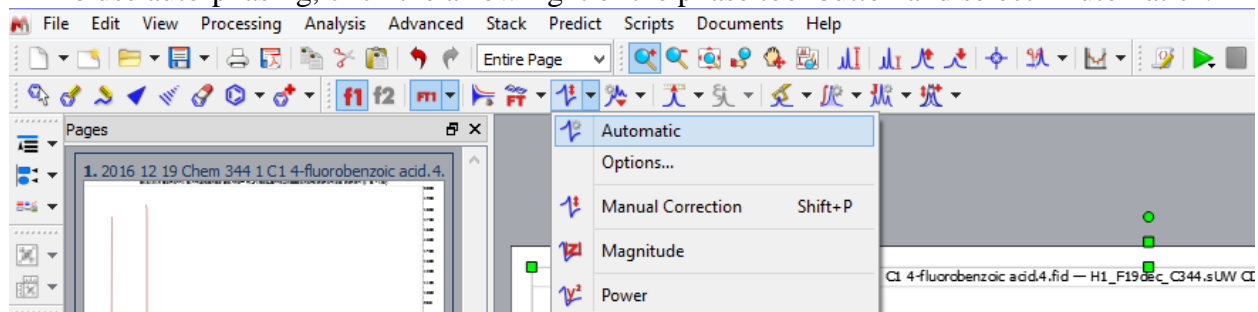
If it fails to correct phasing sufficiently, you may do a manual phase correction by selecting the "Manual Correction" option from the same menu.

- Increase the intensity of your spectrum to clearly see the asymmetry of signals.
- Scroll the blue bar to the left- or right-most signal in your spectrum.
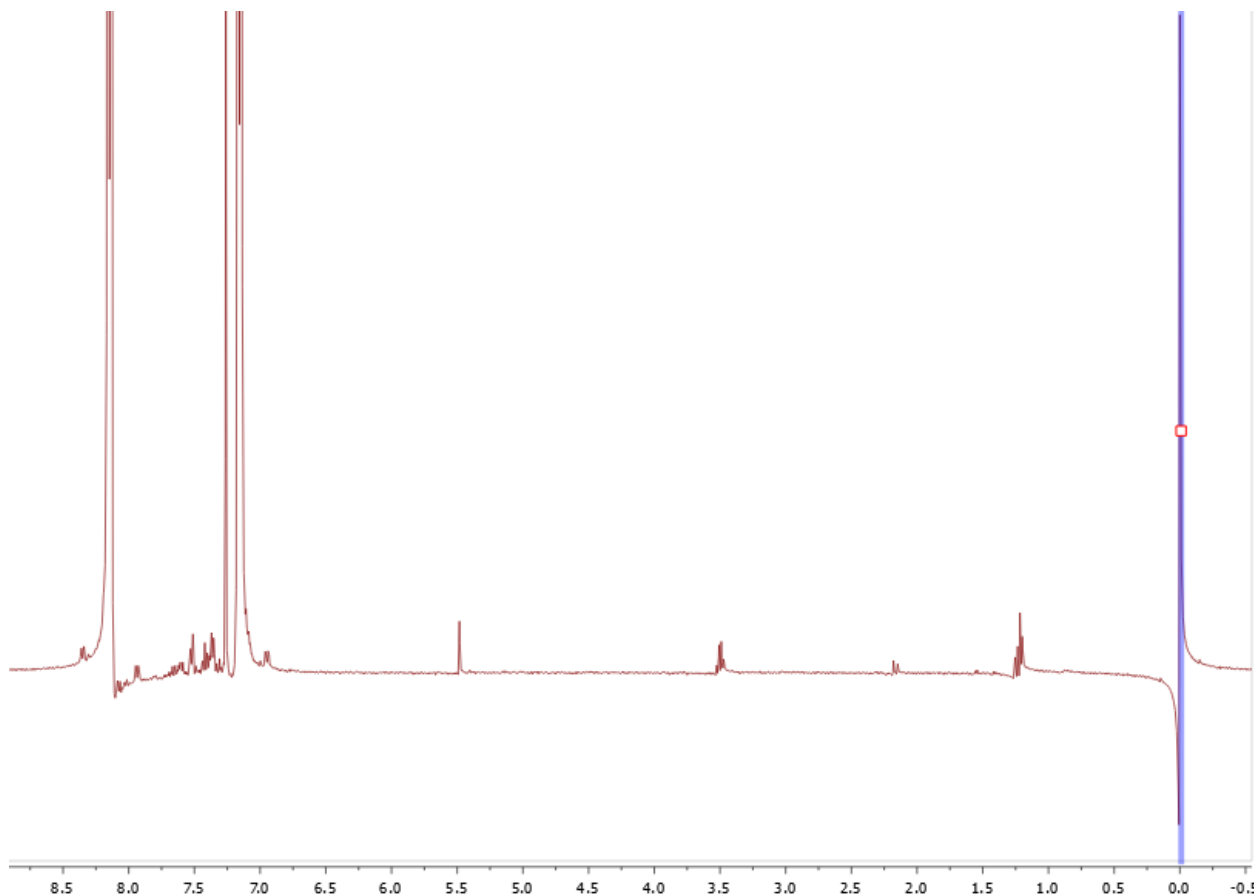
- Click and drag the left mouse button up/down in the Phase Correction Window to make the sides of the peak under the blue line symmetric. Press and hold CTRL while adjusting phase to make it change less dramatically. Note that this will likely put distant signals further out of phase – that's okay.

More out of phase than before

Symmetric baseline
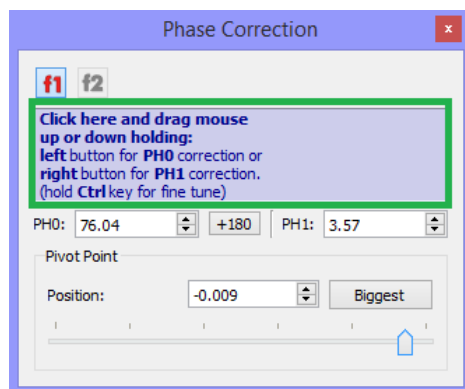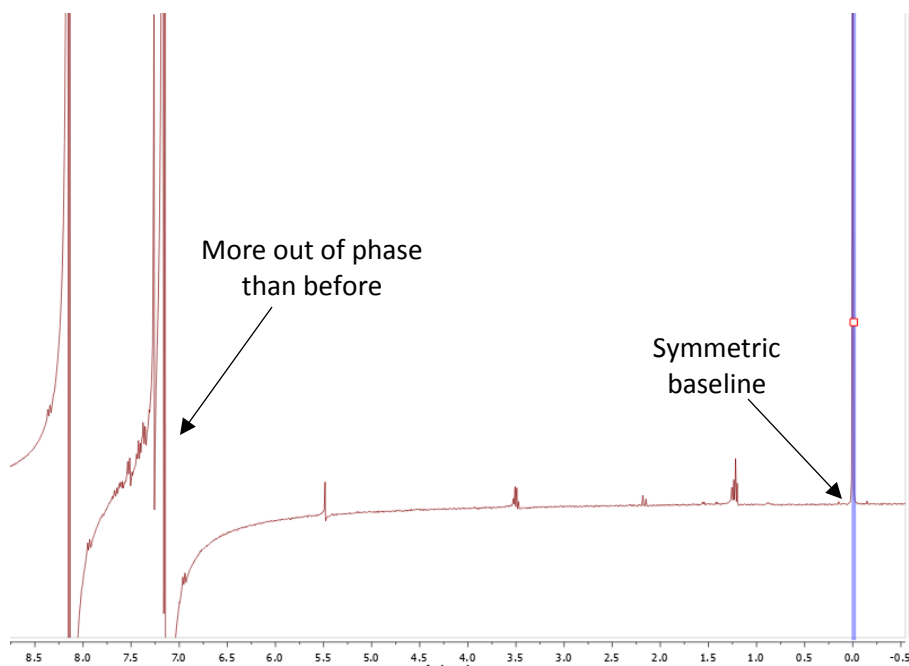
- Use the right mouse button in the same way to adjust the phasing of distant signals.


All in phase!
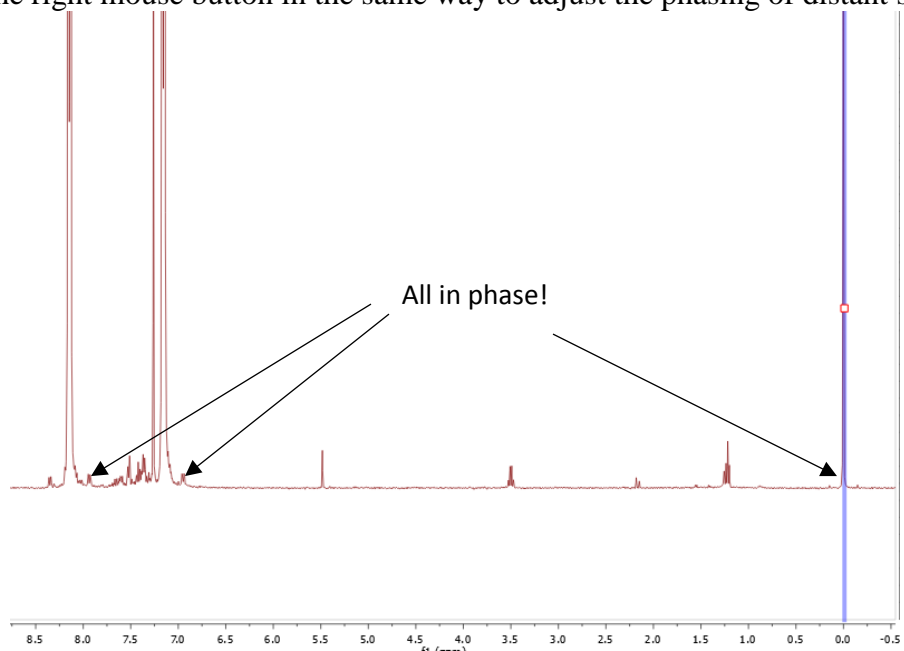
3. Correct the baseline of the spectrum by clicking the Baseline Correction button ( ). Again, the automatic baseline correction will usually do the job, but if necessary, a polynomial manual baseline correction is suggested.

4. Use the "Scale to Max Intensity" button ( ) to return your spectrum to a reasonable scale.

5. Click the "Reference" button (), then select the TMS peak and set the "New" chemical shift to 0 ppm to properly reference your spectrum.
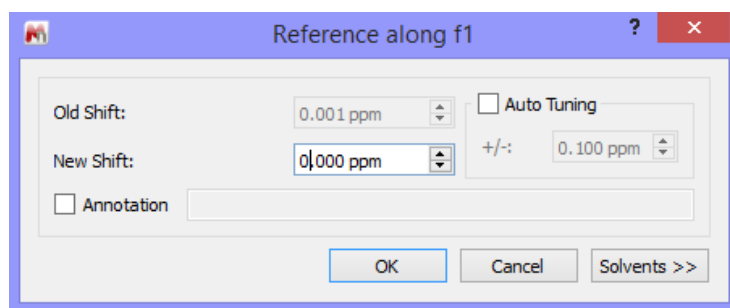

6. Press "I" or select the Manual option from the "Integration" button menu. Click and drag from baseline to baseline on individual signals to integrate them. Do not integrate the TMS or $CHCl_3$. For aesthetics, click on the green integral symbol that appears above peaks you have integrated and drag it down so that all integral symbols rest on the spectral peak.
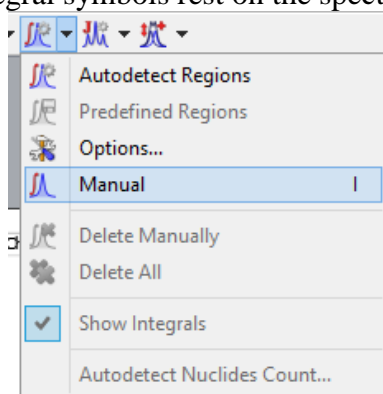

Note that the very first signal you integrate is set to an integration value of 1.00 by default. The integral value is the area under the curve, so all other integral values will be relative to that set value. You may change the reference integral value by hovering over the green integral bar below a desired signal and right-clicking the red box that appears. Select "Edit integral" from the menu that appears.
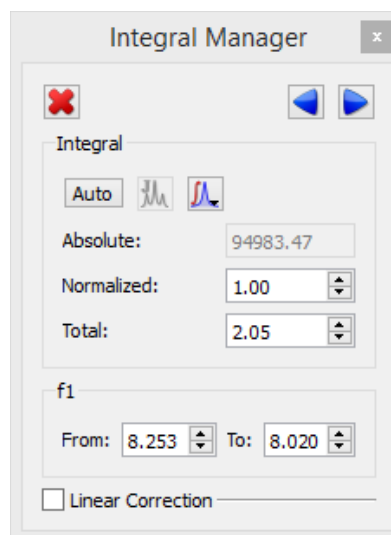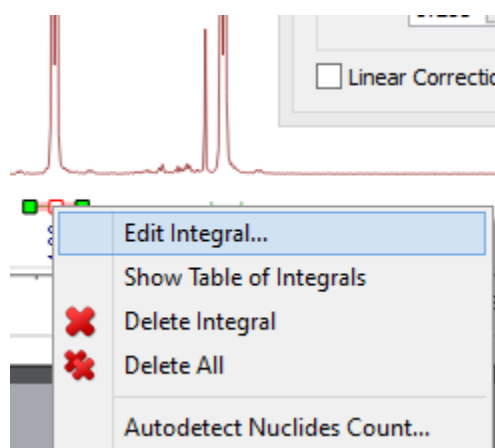
Set the "Normalized" value to the desired integral value. All other integral values will now be relative to this newly-set value.
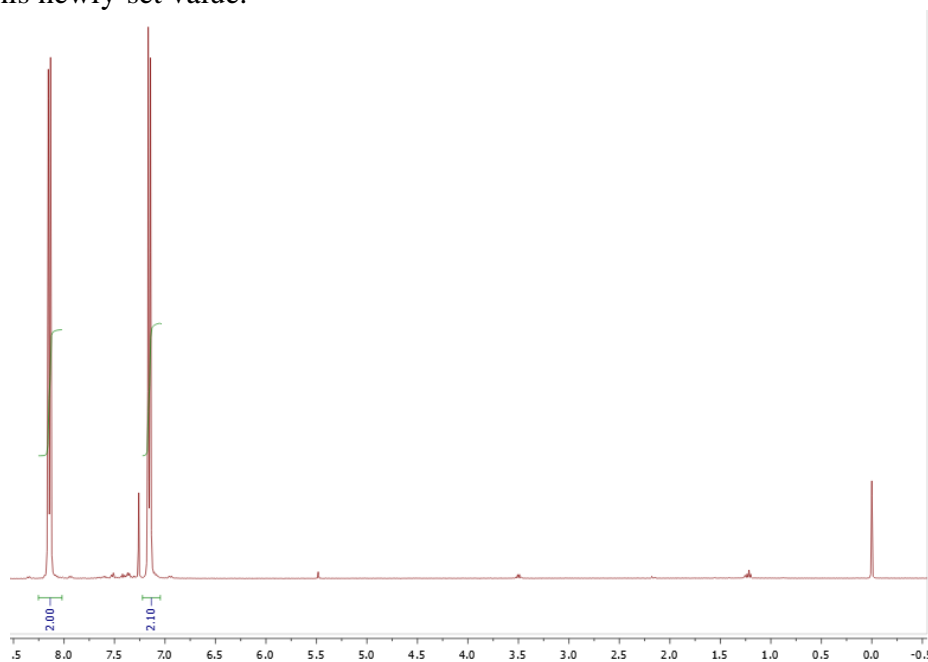

7. Use the "Zoom In" tool (🔍) to adjust the range from ~ -0.5 ppm to slightly downfield of your most downfield signal.

8. If there is visible coupling that is difficult to discern, create a spectral inset using the "Expansion" tool (▣). After selecting the tool, click and drag on your spectrum to encompass the range you want to see more closely. Position your inset in a convenient manner.

9. In the inset generated, use the "Manual Threshold" or "Peak by peak" tools from the menu of peak picking button (⚡▾) to peak pick your signals. You may need to adjust the intensity to make all peak pick labels visible. *Do not choose the automatic peak picking option.*

   a. To use the manual threshold, click and drag across your peak(s) at a level slightly below the peaks you wish to peak pick.

   b. To use the peak by peak tool, hover over each peak that you would like to pick and click to select it.
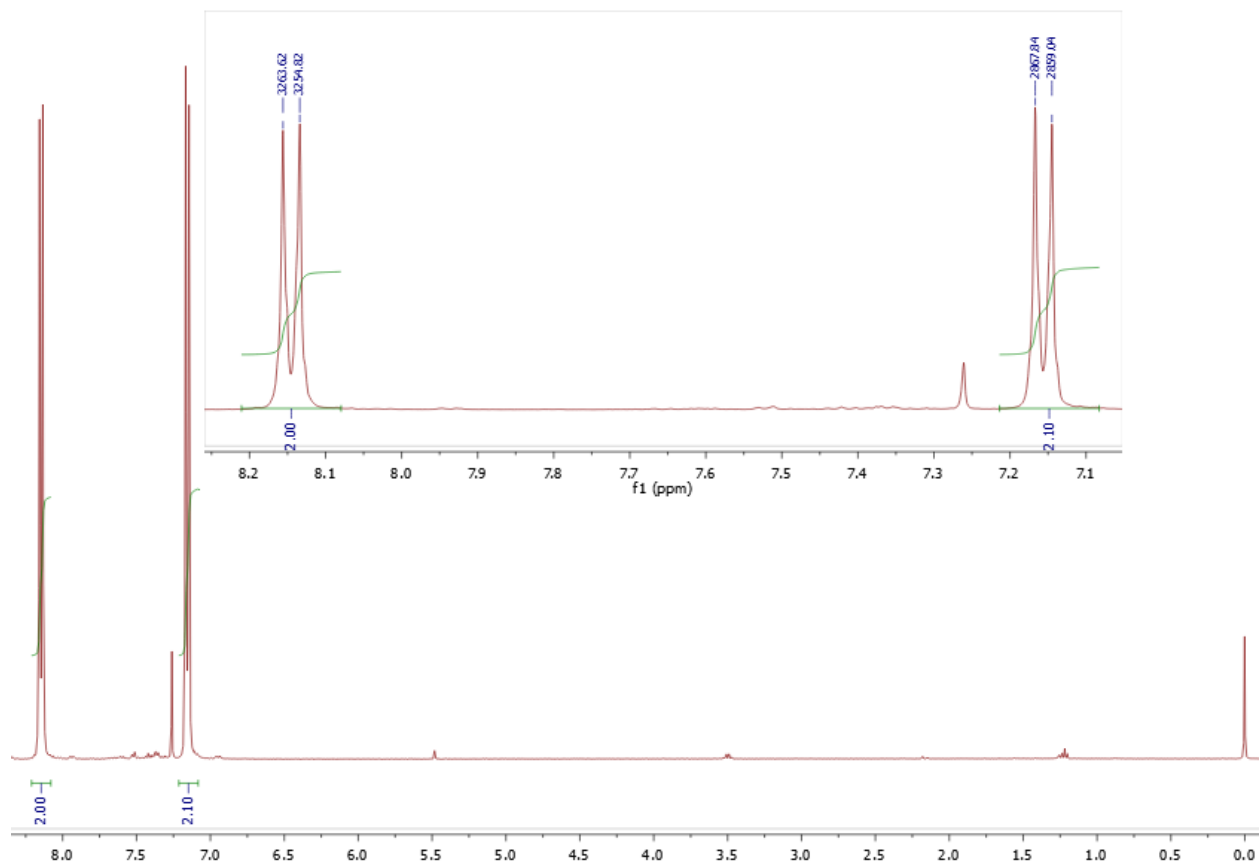
10. Export the spectrum to PDF before printing.

Standard ¹³C-NMR Spectral Workup

1. Open your spectrum in MestReNova.

2. Correct the phasing, as described for ¹H-NMR.

3. Correct the baseline, as described for ¹H-NMR.

4. Scale the spectrum to max intensity.

5. With the corresponding, correctly-referenced ¹H-NMR spectrum open in the same file, click the "Absolute Reference" button ( ). In the window that appears, check that the corresponding ¹H-NMR is selected in the "Use as Reference" line and that the ¹³C-NMR of spectrum of interest is checked. Click "OK".
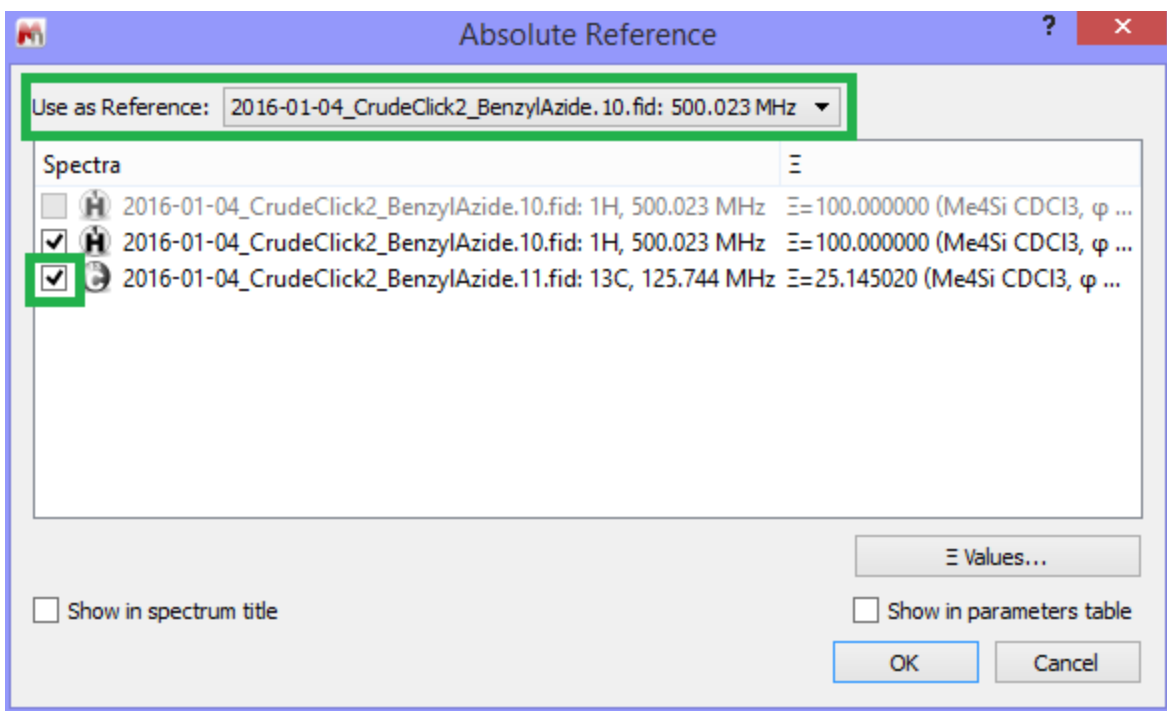
6. Adjust the spectral window to an appropriate range (~ -0.5 ppm to slightly downfield of your most downfield signal).

7. Peak pick the signals of interest. Make sure that the peak picking unit is ppm.

8. Export to PDF before printing.