

**This Document contains information for a new NMR user. Carefully read and accomplish each section before moving to the next. If you can't finish a section please request help**

**You must be a ThinkPad and on campus on VPN. A "loaner" computer will not work. Using a wired connection will make downloading the MNova program much faster.**

#### **Download and install the MNova license file**

- 1) Open the Lab's Sakai site and navigate to the "MNova installation and Instructions" folder.
2. Click the "Mestrelab.reg" to download the license file.
3. Run this file and answer **yes** to any questions concerning modifications to your registry.

#### **Download and install MNova**

- 1) Go to the following web site, download and install the software. (latest version is 9.0.0)  
<http://mestrelab.com/software/mnova/download/thank-you?url=%2Fdownloads%2Fmnova%2Fwin%2Fmsi%2FMestReNova-9.0.0-12821.msi>
- 2) Run the installation file to install the software. On Windows 8 you may need to run as "administrator". Right click on the file and choose "run as administrator".

#### **Using MNova**

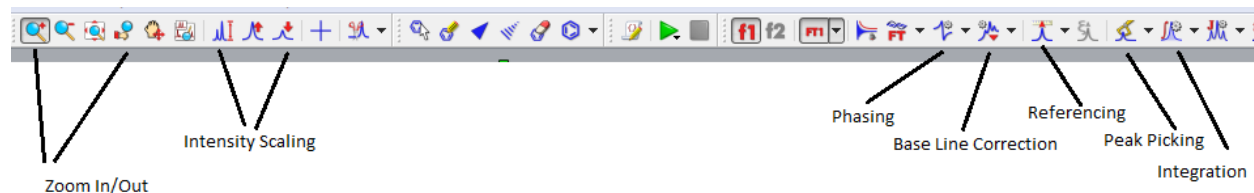
This version of the software works much like the previous version. Hover your mouse on an icon to see its description. There are several new features that will be discussed in classes or as you need. Please see the Help→Contents menu for specifics.

#### **Short Set of Directions:**

Download your data from the Saki site, usually in the resources folder.

You can only open NMR (fid file) or GC-MS (Data.ms file) from inside MNova. Use the File→Open menu.

Frequently used icons:

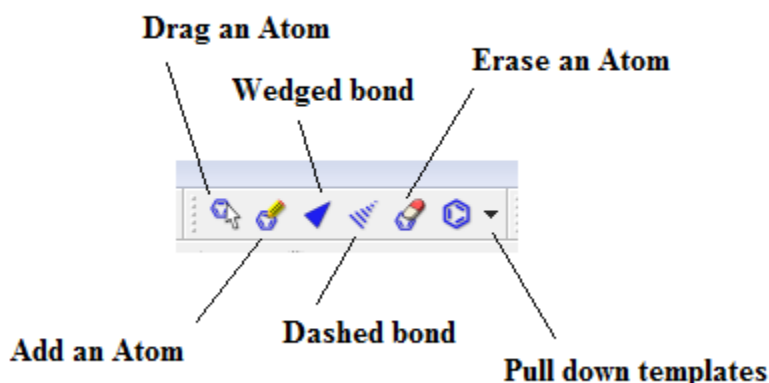


- 1) If needed perform a Base Line Correction using the Auto or Whittaker Smoother method.
- 2) Perform an Auto Phase Correction or Manual correction by choosing the icon and manual option. Left click and push the mouse forward and backwards to flatten the baseline

around the red pivot line and right clicking and pushing/pulling the mouse flattens the baseline away from the pivot.

- 3) Zoom (pick icon and left click drag) region around your Internal Reference (TMS or Solvent) and using the Reference icon set its chemical shift.
- 4) With the Peak Pick icon you can perform an Auto or Manual Peak Pick. Manual mode: left click on the left side of spectrum and drag the threshold line to encompass your peaks. The top threshold line should be below the top of the peaks to be selected and displayed.
- 5) Perform a the Auto or Manual Integration. Manual mode: choose icon and manual option then left click and drag on either side of peak, giving some room before and after each peak to establish a flat baseline if possible. Right click on the integral trace (sigmoidal line) above a known peak and set the Normalized value to a known integer and press enter.
- 6) Print or copy spectrum for presentation.

### To Predict NMR spectra and Stack the results

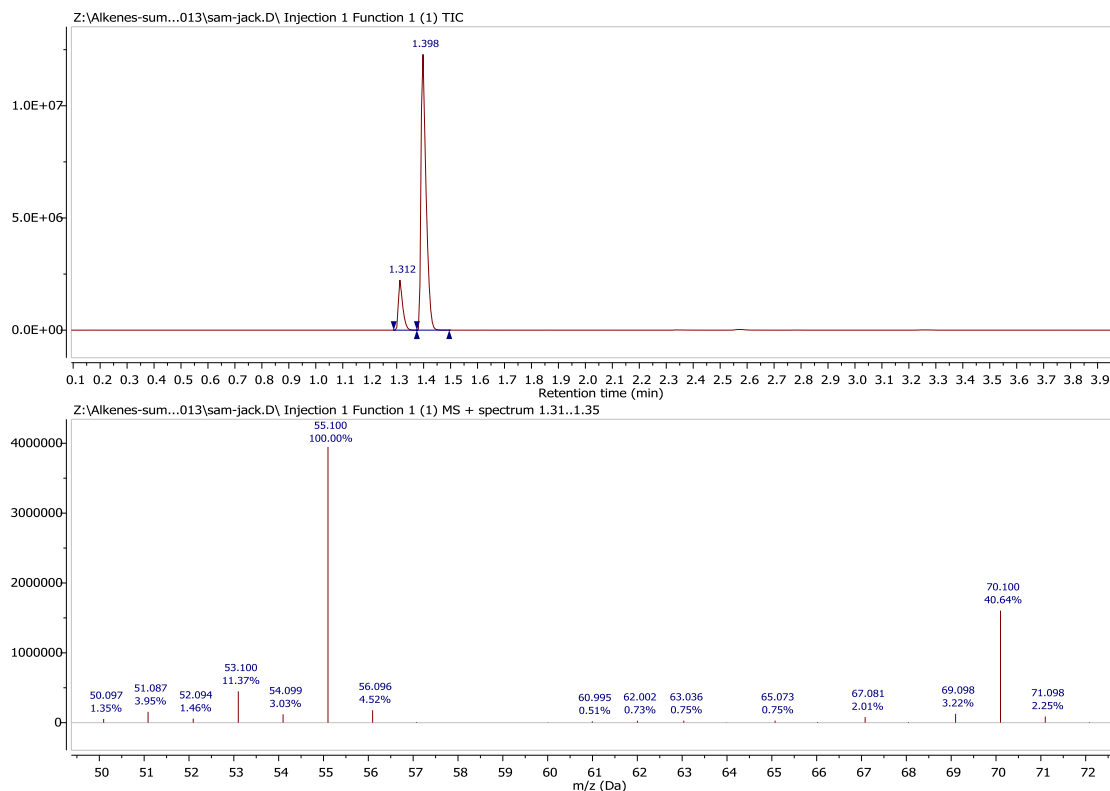


1. Starting with a new page draw the molecule you wish to simulate.
2. Use the tool pallet to make rings and chains. To change a carbon to another atom deselect the current tool and then click on the carbon to change and enter the lower case element symbol.
3. Once drawn go to the top menu and choose Predict → <sup>1</sup>H spectrum.
4. To make another prediction right click the left navigation window and choose **Create New page**. Repeat drawing and predicting.
5. Once all of the same spectra are drawn you can **superimpose or stack** the spectra by first left clicking on one of the small navigation windows on the very left then holding shift and click on

the other spectra to stack. Next, go to the top menu and choose **Stack** and choose your desired option. You can also choose **Auto Scale** form the **Stack** menu as well.

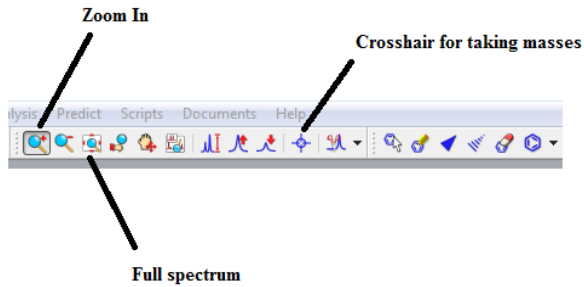
### Processing MS Data:

Go to File→Open and navigate to your data folder. Double click on the DATA.MS file and you should see the total ion chromatogram (TIC) in the top window and a mass spectrum in the lower window.

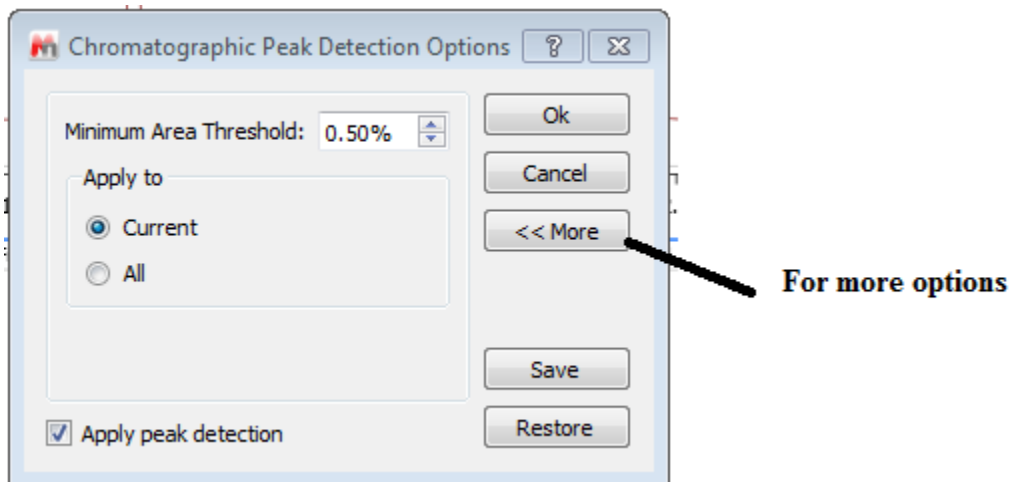


You can zoom in and out of each window by clicking on a window and using the zoom or full spectrum tool.

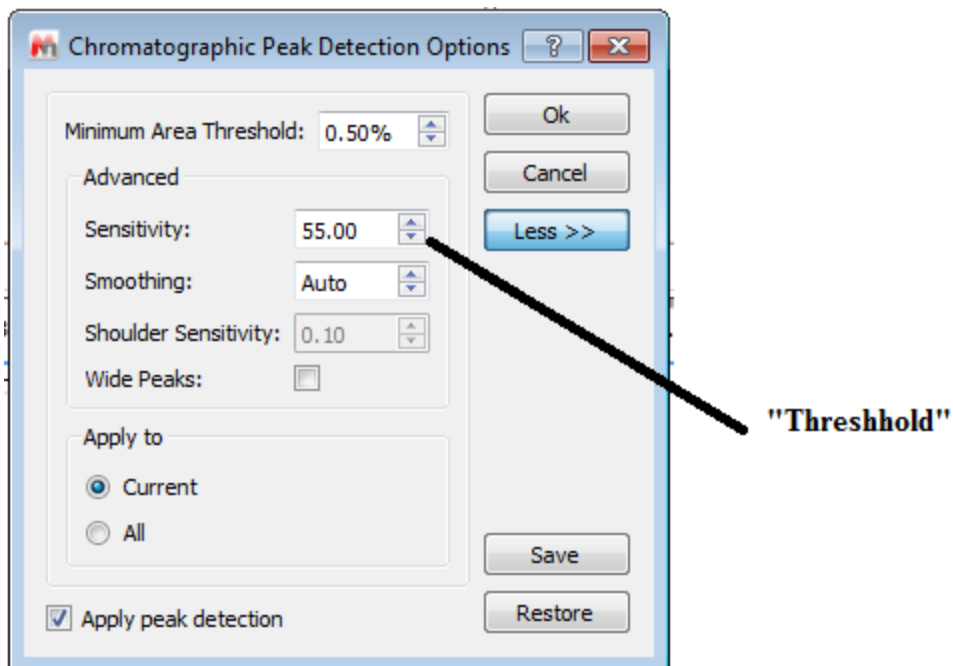
If the TIC is selected by clicking on it the crosshair tool will display the mass spectrum at a point by simply clicking on the TIC or left click drag on the TIC for an average mass of that region. So to display the MS for a well resolved peak grab the crosshair tool and left click and drag the peak.



Most of the time peaks in the TIC are correctly selected. But if you need to integrate peaks in the TIC manually right click on the TIC and choose Add Peak. Then left click and drag on the peak. You can also let the program detect peaks as well. To change the way peaks are detected right click and choose Detect Peak Options



Clicking More gives you the chance to change the Sensitivity or “Threshold” to include or exclude peaks.



To display a table of the relative areas of the selected peaks in the TIC go to View→Tables→Mass Peaks. Then choose Paste to put on the data. You can select and drag the table where you want.

To display a table of the fragments in the mass spectrum just select the ms window and then go to View→Tables→Mass Peaks. Paste and move to where you like.