MNova Version 12.0.0 Installation Instructions.

*Note: 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***.**

General Operating Procedures: Requesting an Account

1) Request an account and training from the NMR lab manager.
2) Read the following information and install the PC processing program prior to training.

Know These User Policies

1) Walk up access is from 8am to 8pm.

2) Time quotas: Experiments requiring more than 15 minutes must be run at night or approved by Dr. Wright. See next step for making reservations.

3) Nighttime Reservations (8pm to 8am) are made on a Google Calendar. New users in the Chem department need to ask their advisor for the lab's google calendar login information. For outside users send the email address you wish to use for the Google Calendar account.

You can take up to 15 minutes of spectrometer time at one login session. Locking and shimming requires about 5 min per sample and 2 min. to acquire an average 1D data set. Here are some possible combinations you could run:

1H NMR spectra on 3 different samples
1H and 13C128scan on 1 sample
1H and 19F, 31P and 13C 256scan on 1 sample

You can always setup more experiments but you must mark the excess experiment time as *delayed *(change the sun to the moon). Or you can wait 15 min, log back in and submit another 15 min without delaying anything. The advantage of delaying experiments is you don't have be there to start and you can submit as many as you want. The experiments will run when the instrument is idle.

If an experiment's *acquisition* time is over 15 min and its marked delayed, then it runs after 8pm and you must have the instrument reserved on the Google calendar.

3) Orphaned samples are removed and placed in the beaker near the computer.

4) ***NO heterogeneous samples.*** Instrument may fail to lock. Filter or centrifuge toi remove solids.. *To filter an NMR sample:* Tightly pack a small piece of cotton into a glass pipette using a long glass pipette. Add about 2-3 mm of celite to the top of the cotton plug. Tap pipette on it's tip to compact celite filter bed. Add NMR sample to top of filter bed and force through (if needed) into NMR tube.

5) Use 0.6 mL of your solvent, too high or too low solvent level effects shimming times and quality. Use about 1 to 10 mg for 1H, 19F and 31P samples. 13C on low concentrations samples my require 4K to 10K scans (1K = 1024)

6) ***SET THE SAMPLE HEIGHT.*** Sample will not spin if too low and **can/will** break the probe. Too high can fail to lock and shim.

7) Put your sample in the lowest available (green) position holder avoids your experiment being skipped.

Step 1. Mapping your hard drive to the NMR(ThinkPad)

You must be on campus or use VPN.

Access to Bruker 400:
1. Right click on the "My Computer" icon on your desktop
2. Choose "Map Network Drive"
3. In the "Folder" field of the window that pops up, type:

\\wfuarchives\Chemistry\NMRData\bruker400

4. Click on "Reconnect at log on"
5. Use you Wake login and password.
7. Click on "OK" then click "Finished". If login fails try using deacnet\"user name" and password.

Step 1. Mapping your hard drive to the NMR(Apple)

Procedure to connect to data folder on a Mac:

1. Pull up Finder
2. Under "Go" on the top bar, click "Connect to Server"
3. Connect to "smb://wfuarchives/Chemistry/NMRData/bruker400"
4. Finder should pop up with "data."
5. Under "data," find your file and drag it into your "document" folder.
6. Pull up MestReNova, then open your NMR file from documents.

Step 2. Download and install the MNova with license licenses files (Windows only)

1. Click on the Window's key and press R at the same time. Enter and run the command: \\Mestrelab\wake\MestreLab

2. A new window will open double click on the MestReNova_12.0.0-20080_Mestrelab.exe file.
3. Finish the installation process. MNove should now be ready to use.

Step 2. Download and install the MNova license file(Apple Only)

1. Download version 12.0.0. Try here: http://mestrelab.com/downloads/mnova/mac/MestReNova-12.0.0-20080.dmg

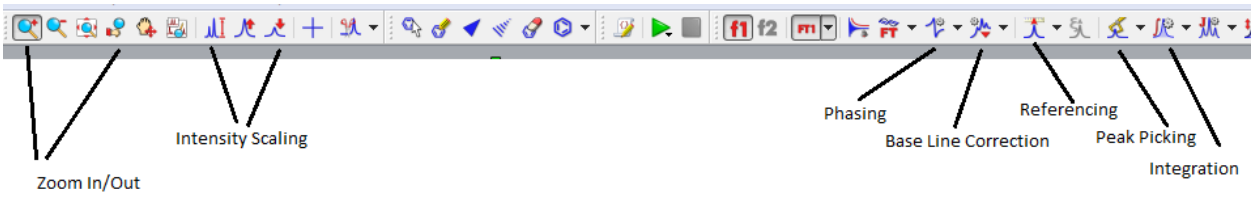
2. If possible, navigate to \\Mestrelab\wake\MestreLab and download all the license files and install from within MNova when prompted. If you can't navigate to the folder then send a request to wright for the license files and then install.

Using MNova (Classic View, Modern View in process)

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.

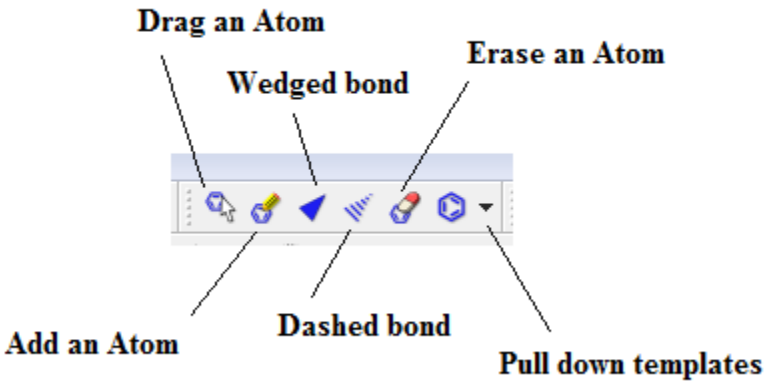
Short Set of Directions:

1) You can only open NMR data from MNova. Open the "fid" file in 4v00current\data\"user"\"file name"\"exp number" folder.
2) Frequently used icons:



3) If needed perform a Base Line Correction using the Auto or Whittaker Smoother method.
4) 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.
5) Zoom (pick icon and left click drag) region around your Internal Reference (TMS or Solvent) and using the Reference icon set its chemical shift.
6) With the Peak Pick ion 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.
7) 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.
8) 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.

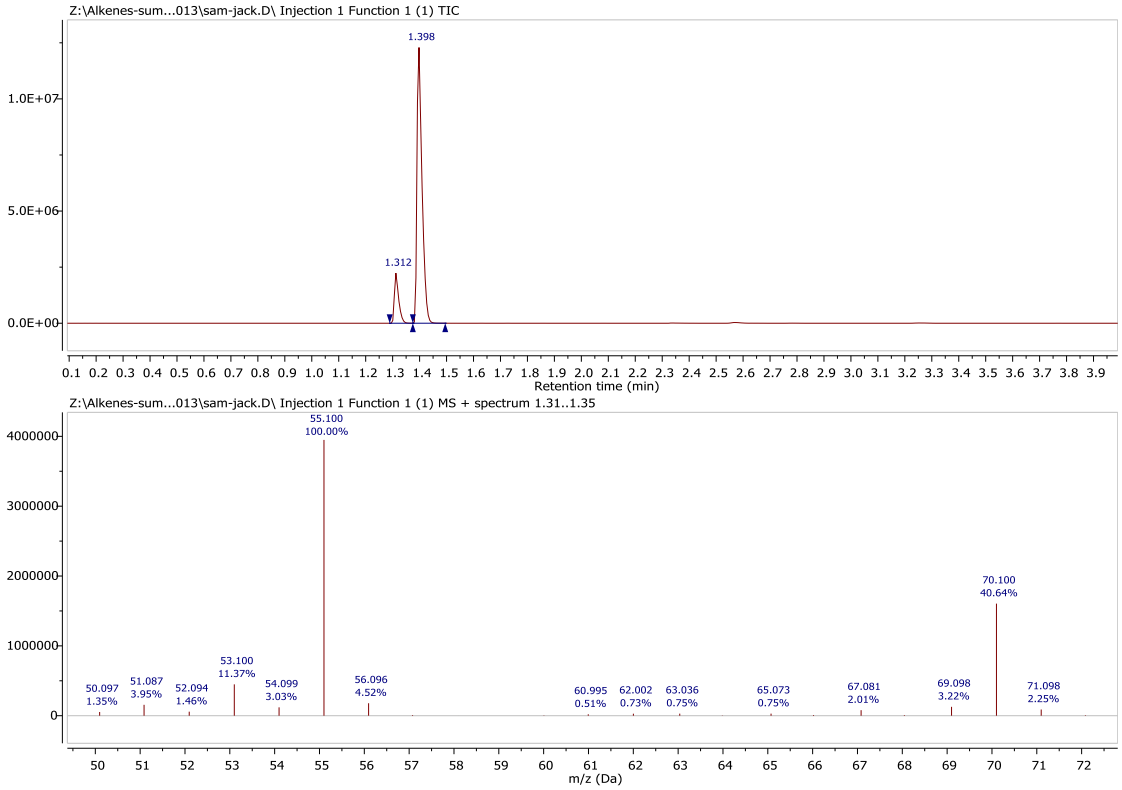
3. Once drawn go to the top menu and choose Predict→ 1H spectrum.

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.

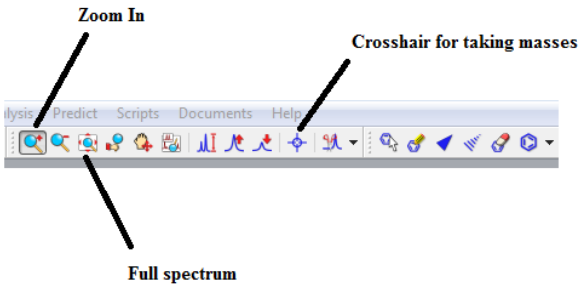
Processing MS Data from the SAMBA sever:

Open MNova and 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.

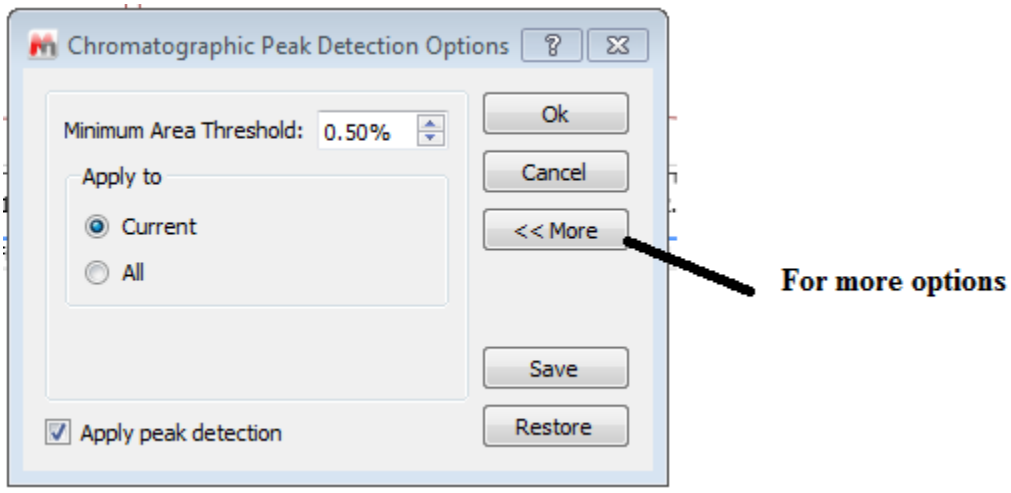


You can zoom in and out of each window by clicking on a window and using the zoom or full spectrum tool.

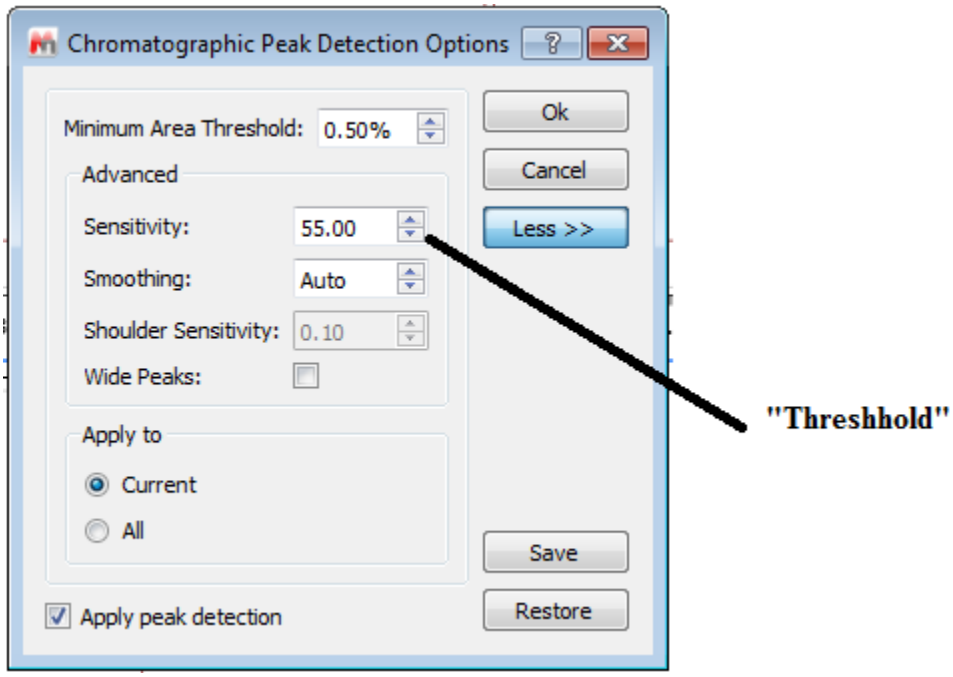
If the TIC is selected by clicking on it the crosshair tool will display the mass spectrum at a point by simply clicking on the TIC or left click drag on the TIC for and average mass of that region. So to display the MS for a well resolved peak grab the crosshair tool and left click and drag the peak.



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. The 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.