Instructions for Download, License and Use of MestReNova Software

Note: MestReNova is now loaded on all of the public access computers in the science library.

Note: These instructions are for the Windows operating system. Mac and Linux operating systems are also supported. If you have problems with Mac or Linux, please contact Dr. Neil Jacobsen (neil@email.arizona.edu, 119 Old Chemistry).

1. Download UA Site license onto desktop

Go to the following website:

http://128.196.201.2/mnova/mnova.htm

Note You must be in the U of A network, either by using UA wifi (not UA public) or a hard-wired network connection on campus. UA wifi requires a netID login.

Under the heading "Licenses", Right-click on "Mnova NMR" and select "Save As Target". Put it on your desktop. You will get the message "Download Complete".

The icon for the file "The University of Arizona_CampusUnltd_NMR.lic" will appear on your desktop.

2. Download MestReNova 7.1 software from MestReLabs site.

Go to the MestReLabs download website (DO NOT DOWNLOAD Mnova 8 or 9!!!!):

http://www.mestrelab.com/Products/Mnova/Product-download.html

Scroll Down to the bottom of the page and click on the link “See older MestReNova versions for every OS available” (under the magnifying glass: Looking for an older version?)

Select Version 7.1.1 under your operating system (e.g., Windows). Our license only covers up to and including version 7.1.1. If the download doesn't start, it may be blocked by your security settings. Click on the link indicated if this happens. You will get the question "Save or Run"? Click on "Save". The icon for the MestReNova installation program will appear on your desktop. Double-click on this icon to start the installation. When it shows the Plug-Ins it will install, de-select the NMRPredict and Mass plugins. You won't be using these; you only need the NMR plug-in. When the installation is complete, you will get the question:

Do you already have a license file?

Answer yes and select the license file you just downloaded to your desktop.

If you have a Mac operating system, the license file will have the file extension ".txt" added to the ".lic" extension when it is downloaded. When you select the license file, you won't see it because MestReNova is looking for files of type "license file", ending in ".lic". You need to change the file filter from "license file" (.lic) to "all files". Then you will see the license file and you can select it.

3. Restart MestReNova and click that you have seen the error messages, also click to not show errors again. If the license is not accepted, you will find that when you try to open (or drag and drop) an NMR dataset into MestReNova you will get an error message like "data not in correct format" or "data format not recognized". To check the license, click on Help / License Manager. You should see a green circle with a check mark in it next to the NMR Plug-in line. You won't be using any other plug-ins (e.g., NMR Predict, Mass, etc.). Note that the first time you start MestReNova and load the license, you have to be connected to the University network so that MestReNova can connect with the license server. Your license lasts for 90 days, but the start date is reset each time you start MestReNova and are in the University network (UA wifi with netID or plugged into the network on campus).

Troubleshooting license problems. If you have an old license file (before Feb. 2012) it will not work on any version of MestReNova. You need to download and activate a new license file. When you re-start MestReNova, click on "Help" and "License Manager". You should see the NMR Plug-in with a green circle with a check mark in it. If you instead see a red circle with an "X" in it, you don't have a valid license. If you get the green circle, you are ready to use MestReNova.

If you download a new license file, you need to activate it. In the MestReNova window, click on "Help" and then "Evaluate / Buy". Click on "Yes" to the question: Do you already have a license file? Click on "Activate..." and navigate to the Desktop and select the license file you downloaded. If you have a Mac operating system, you will have to change the filter (bottom right) from "License Files (*.lic *.zip)" to "All Files (*.*) in order to see the license file. Select the license file (The University of Arizona_CampusUnltd_NMR.lic) and Click "Open". If you get the question "License file for the same product already exists. Do you want to replace it?" respond "Yes". Then click on "OK" and "Finish". You will need to Exit the software and restart it.

4. Download the zip file with your NMR data from this website:

http://aviii400.chem.arizona.edu/

This is the Bruker AV-III-400 NMR spectrometer. Click on your username. For course, use the course name (e.g., chem243b). You may have to click on a range of section numbers as well. The files displayed should have your filename with the ".zip" extension. Drag this file to your desktop (you may get a security question, answer "yes"). Double-click on the zip file icon on your desktop and select "Open". This opens

a window with your NMR data folder. This is a temporary internet file and cannot be dragged into MestReNova. You must first drag this folder into another folder (named "AVIII400_NMR_Data" or named for a particular project) or onto the desktop. Open this folder and you will see your NMR experiments: 1, 2, 3, etc. If you only did a proton, you should only see a folder named "1".

5. Drag and Drop the NMR experiment number folder into the MestReNova open pages thumbnail or the open pane of the document; the NMR spectrum should appear. The standard data processing involves a resolution enhancement. So your NMR lines will look amazingly sharp. You can do the same thing on the Bruker 500 or 600 by processing the data with SSB set to 4 and using the commands SINM and FT instead of the usual EF.

Because there are some rules governing file download from the internet on Science Library computers, students using these computers will have to use a slightly different procedure:

1. Start Internet Explorer
2. Enter web address: http://aviii400.chem.arizona.edu
3. Navigate to your class or group of sections
4. Left-Click once on your zip file (e.g. Smith.John.243b.zip)
5. In response to the Open or Save? question, click Save.
6. Click Save.
7. Double-click on the Libraries / Documents folder icon.
8. Double-click on the Downloads folder icon.
   (NOT the Favorites / Downloads folder)
9. Right-click on your zip file, select Extract All
10. Double click on your filename (e.g., Smith.John.243b)
11. Drag the experiment folder ("1") into the MestReNova window.

6. Process data as follows (this is just a quick summary):

Icons and Shortcut Keys: Selecting an icon activates a feature (e.g., integration, peak picking) and changes the cursor from the simple arrow to a specific symbol (e.g., an integral symbol with a + sign to indicate "add an integral"). You can also use shortcuts (e.g. **i** for integration, **k** for peak picking, **c** for crosshair). Hit the Escape (**Esc**) key to go back to the simple arrow cursor.

Settings: Right-click on the spectrum and select "Properties". For **Scales**, select a Font size of 12 and uncheck the vertical scale. **Peaks** should be **Units** of **Hz** for proton, **ppm** for ^{13}C, **2 Decimals** in both cases. Click on the **Set as Default** icon and save these settings so you will have them each time you run MestReNova.

Parameters: Data processing parameters affect the quality and appearance of your spectrum. Click on **Processing** and **Processing Template** each time you put NMR data into MestReNova.

Proton (^{1}H) data: **Apodization** (click on the **…** icon) should be **Sine Bell** set to 45.00 degrees. **Spectrum Size** should be 128k (131072).

Carbon (^{13}C) and DEPT data: **Apodization** should be **Exponential** set to 1.0 Hz. **Spectrum Size** should be 128k (131072).

Pan: Press **p** to get a hand icon. Click and drag with this icon to move the entire spectrum up and down or left and right.

Reference: Zoom to the reference by clicking on the magnifying glass icon with a plus sign in it, then just click, drag and release on the spectrum. To return to the full spectrum display, click on the magnifying glass in a box icon. You can also undo a zoom by selecting Edit/Undo. After zooming, chose to select reference by clicking TMS icon at top (6th from the right side). A vertical line on the spectrum will appear, move line to desired peak, click and enter the ppm value.

Adjust Vertical Scale: Use the "+" and "-" key shortcuts, or click on the peak(+) icon or the peak(-) icon (center of the icon bar). To the left of these is a "Fit to Height" icon which you click once to fit the tallest peak to near the top of the vertical space.

Integration: Horizontally Zoom to the appropriate region. Manually integrate peaks of interest by pressing **i** (toggles integral icon) and dragging area of interest. Double click within the region of an integral. This brings up the properties box. Select integrals at left and check the "Curve" box. Save these settings again with the Save icon. Now you should see the integral curves at the top of the spectrum. Click and hold on any integral curve and you can drag them up or down. Double-click one of the curves and you get the integral manager. Here you can enter a value for the integral and exit by clicking the red "x" in the upper right corner of the box. All the other integrals will change by same factor. Exit the manager by clicking the x in the upper right. When finished with integration, hit i again or Esc to turn the integral cursor off.

Peak picking: Zoom to desired region. Manually select region and height by pressing **k**, changes cursor to peak with plus and red arrow. Drag and release to select region and peak threshold (horizontal line) across spectrum at desired minimum peak height. Hit **k** again or **Esc** to turn off the cursor. Use Hz units for 1H spectra so J values can be obtained by subtraction. Chemical shifts (ppm) are obtained by averaging the Hz values of two symmetrical lines and dividing by the spectrometer frequency (e.g., 400.13 MHz).

***J* coupling (manual)**: Press c to get a crosshair cursor. Click and drag the crosshair icon from one line to another in the multiplet and you will get a continuous readout of the Hz separation between the two vertical lines. This information appears in the "Info View" window in the upper left. Click the green "Hz" icon to use Hz units and read the difference as |B-A|: on the lower left. Hit c again or Esc to turn off the cursor.

Expanded Region in Box: Press **e** to get a magnifying glass with a **+** in it. Click and drag across any region and this region is put in an insert box. Get the regular cursor back

(**Esc**) and click on the box. It will be marked out with green squares and a "handle" at the top. You can click and drag on the handle to move the box, or click and drag corners or sides to re-size it. With the box highlighted, you can process it like the main spectrum: Expand, adjust peak height, integrate, peak pick, or remove peaks and integrals.

Save Current Spectrum Display as a pdf File: Select File and Save as pdf, navigate to the desired folder and enter a File Name. Select Current Page for Range and click OK. You might need more than one pdf to get the details of the coupling patterns.

Exit: Just select File/Exit. You can save the spectrum (all processed spectra are saved together in a single MestReNova file: *.mnova) if you want to, or just keep the raw data.