

Instructions for Download, License and Use of MestReNova Software (8/30/16)

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 (Windows 7). 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:

www.cbc.arizona.edu/mnova

You will be prompted for your University of Arizona NetID and password.

Under the heading "License", Right-click on "Mnova NMR" and select "Save Link As". Put it on your desktop. Mac Users: instead of Right-Click, hold down the Ctrl key and click the mouse button. You may have to change your security settings.

The icon for the file "TheUniversityofArizona_2015ULTD_NMR.lic" will appear on your desktop.

2. Download MestReNova 10.0 software from MestReLab site.

Go to the MestReLab download website:

www.mestrelab.com/software/mnova/download/older-versions/

Click on the tab labeled "10" and **Select Version 10.0.2** under your operating system (e.g., for Windows click on Win: **msi**). If the download doesn't start, it may be blocked by your security settings. When the download is complete, double-click on the MestReNova-10.0.2-15....msi icon to start the installation. You may get a Security Warning (Do you want to run this file?), click on Run. If you have an earlier version of MestReNova, you will have to uninstall it first.

In the Custom Setup window, click on the drop-down menu and click on the red X ("Entire Feature will be unavailable") for every feature **except** the NMR Plugin (unwanted features: NMR Predictor Plugin, DB Plugin, Mass Plugin, Verify Plugin). You won't have a license for these other features so, if you install them, you will be hassled regularly about not having the license. **The only things you want are the MestReNova Framework and the NMR Plug-In; disable all other items with the red X.** Click Next, and then click Install in the next window. Click Finish when the installation is complete.

3. Double-click on the MestReNova icon on your desktop to start the software. You will get a window with the heading “License Validation Errors”, saying “you are not entitled to run this version...”. Don’t panic, just click the box (“I’ve read the above information) and click OK. Next you get a window with the heading “Registration Wizard” saying “You will need one or several license files ...”. Click on Install, navigate to your desktop, and select the file “TheUniversityofArizona_2015ULTD_NMR.lic”. This is the license file you downloaded in step 1 above. Click on Open.

You may get a window with heading “License File Installation” that says “A license file for NMR already exists. Do you want to replace it?”. In this case click on Yes.

Now you should see a window with heading “License File Installation” that says “The following licenses were successfully installed: NMR”. Click on OK. Exit the MestReNova software by clicking on File / Exit (upper left). Re-start MestReNova by double-clicking on the MestReNova icon. In the lower right corner of the MestReNova window you should see after “Licenses:” a yellow circle with a yellow exclamation point (!) inside it. This means you are ready to use the software. You can also check the license using the Help drop-down menu and selecting License Manager. You should see the yellow circle with an exclamation point next to “NMR”. Click OK to exit this window.

License Problems. If you see a red circle with a red “X” in it in the lower right corner of the MestReNova window, or next to NMR in the License Manager window, you do not have a valid license and the software will not accept NMR data. Possible causes for this problem include:

- 1) You downloaded a version **more recent than 10.0** (the current version is 11.0). Uninstall the version 11 and go back to step 2, making sure that you download version 10.0. We don’t have a campus license for version 11.
- 2) You are **not connected** to the University of Arizona network. for a laptop, this means UAWiFi, not UAGuest. Your computer has to connect to the license server on campus to validate the license – this is how it knows you are a member of the U of A community. When the license is validated you get 90 days to use it anywhere – including at home. If your license suddenly stops working, it’s probably because you haven’t connected your computer to the University network for 90 days. Just connect to the network and start MestReNova; it should reset your valid days to 90 days.

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.

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 (for course samples submitted in lab: LastName.FirstName.Section...) with the “.zip” extension. Right-click on the zip file and select "Save Link As", select the location, and Save. You can save it to the Desktop, or create an NMR Data folder or course folder.

*On the Main Library and Science Library computers, students will have to save the zip file in the Documents area, not on the Desktop. There is no MestReNova icon on the Desktop; you can find it in the **Class Software** or **Math, Science & Engr Software** folders.*

5. MestReNova 10 now allows you to drag and drop a zip file directly into the MestReNova window. Drag and Drop the zip file (Mnova 10 only) or the NMR experiment number folder (“1”, “2”, *etc.*, inside the NMR data folder) into the MestReNova open pages thumbnail or the open pane of the document; the NMR spectrum should appear.

6. Process data as follows (this is just a quick summary). Note that any action can be reversed by clicking on the red “back” arrow:

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 single-letter shortcuts (*e.g.* **i** for integration, **k** for peak picking, **l** for reference, **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 (^1H) 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).

Horizontal Expansion: Press **z** to get the zoom magnifying glass icon. Click anywhere and drag right or left to mark the desired region. Release the mouse button and the spectrum will expand. Press **f** (Full Spectrum) to return to the full horizontal display.

Vertical Scale: Use the mouse wheel to increase or decrease the vertical scale of the spectrum display. You can also use the “+” and “-“ (plus and minus) keys to increase and decrease the vertical scale. Press **h** to return to the Highest Intensity (tallest peak near the top of the display).

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. You can also click on the ppm scale at the bottom and drag left or right at any time.

Reference: Expand the region of the reference peak using the zoom (magnifying glass) icon (**z** on the keyboard). Press **l** (reference line) and move the cursor to the top of the desired peak (TMS, CHCl_3 , center line of CDCl_3 triplet, *etc.*). Click the left mouse button and enter the chemical shift in the “New Shift” window, then click OK.

Integration: Horizontally zoom (**z**) to the appropriate region. Manually integrate the peaks of interest by pressing **i** (toggles integral icon) and dragging the area of interest. Double click within the region of an integral. A horizontal line appears under the peak with the numerical value of the peak area. The first integral you create is always set to 1.00. To change an integral value, place the cursor on the horizontal line and right-click, selecting “Edit Integral”. Edit the number in the “Normalized:” field and then click on the small “x” in the upper right of the dialog box to exit. All other integrals will be changed by the same factor. To display the integral curves on the peaks, right click anywhere in the spectrum and select “Properties”, select Integrals at the left and then check the “Curve” box. Click OK to exit the “Properties” dialog box.

Peak picking: Peak picking is used to display the numerical chemical shift value (in ppm or Hz) above each line in the spectrum. Zoom to the desired region and press **k**, (cursor changes to a peak with plus and red arrow). Position the cursor above the peak and to the left, click and drag down and right to select the region (pink area) that will be picked. Any line whose top is within the pink area will be labelled. To delete a label, hover over it and right-click, selecting “Delete Peak”. Hit **Esc** to turn off the Peaks cursor. Use ppm units for ^{13}C spectra, and Hz units for ^1H spectra (so *J* values can be obtained by subtraction). Right-click on the spectrum and select “Properties” and click on “Peaks” at the left, then in the “Units” field use the drop-down menu to select Hz or ppm. Always use 2 in the “Decimals” field.

J coupling (manual): Horizontally zoom the peak of interest (**z**). 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 “Cursor Info” box in the [B-A] row under the “Hz” setting. 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 arrow 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: Highlight the spectrum, click on File and Export to PDF, navigate to the desired folder, enter a File Name and click Save. Select Current Page for Range and click OK. You might need to save more than one pdf to get the details of the coupling patterns.

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

SUMMARY OF ONE-LETTER SHORTCUTS:

z:	Zoom (click and drag to expand spectrum horizontally)
f:	Full Spectrum (return to full horizontal display)
p:	Pan (click and drag to move entire spectrum)
l:	Reference Line (select a reference line and enter correct ppm value)
h:	Highest Intensity (put highest peak near the top of display)
+ (plus):	Increase vertical scale (make all peaks taller)
- (minus):	Decrease vertical scale (make all peaks shorter)
i:	Integrate (measure Peak Areas)
k:	Peak Picking (put Hz or ppm values on peaks)
c:	Crosshairs (display precise chemical shift value or Hz separation)