

# MestReNova Quick Start Guide

(Updated May 14<sup>th</sup>, 2008)

*This quick summary of the MestReNova Manual is designed for new MestReNova users at the UC Davis Chemistry Department. It covers software installation, getting data obtained using the departmental instruments, and getting started processing 1D spectra. For further information, please download the full MestReNova Manual available online from Mestrelab Research:*

[http://www.mestrec.com/mnova/MestReNova-5.0.3-2367\\_Manual.pdf](http://www.mestrec.com/mnova/MestReNova-5.0.3-2367_Manual.pdf)

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## Installing MestReNova

### *Getting the Software*

1. Go to the Mestrelab Research website:  
<http://www.mestrec.com/descargas.php?idp=1&i18n=1>
2. Under the “**Version**” pull down menu, select the most recent version (currently 5.2.1).
3. Under the “**Operating System**” pull down menu, select your system.
4. Click on the “**Download Now**” button.
5. A new page will load (you can ignore these instructions), and again click on the “**Download Now**” button.
6. Read the terms and conditions, then click on the “**I AGREE, PROCEED TO DOWNLOAD**” button.
7. A new window will open asking if you would like to save the file. Click on the “**Save File**” button.
8. Save the file to the desktop.
9. Once the file has finished downloading, run the Setup Wizard by double-clicking on the file you just downloaded.
10. Follow the instructions in the Setup Wizard to install the software.

### *Activating the License*

1. You will need two license files (UCDavis\_Campus150\_NMR.lic and UCDavis\_EvNPL.lic) which can be obtained by emailing Professor Jared Shaw at [shaw@chem.ucdavis.edu](mailto:shaw@chem.ucdavis.edu).
2. Download both license files to your computer and note where you save them.
3. Run MestReNova.
4. The Registration Wizard will ask if you already have a license file. Click on the “**Yes**” button.
5. A new window will pop up saying you must activate the license. Click on the “**Activate:**” button.
6. Use the browser to find and select UCDavis\_Campus150\_NMR.lic, then click on the “**Open**” button.
7. Click on the “**OK**” button in the new window that appears.
8. Now you're back to the window saying you must activate the license. Click on the “**Activate:**” button.

9. Use the browser to find and select UCDavis\_EvNPL.lic, then click on the **“Open”** button.
10. Click on the **“OK”** button in the new window that appears.
11. Now you're back to the window saying you must activate the license. This time click on the **“Finish”** button.
12. You will be asked if you want to register another product. Click on the **“No”** button.
13. MestReNova will then open. You will see a red X in the lower right hand corner of the screen.



14. Exit MestReNova.
15. Next time you open MestReNova, the red X should be replaced with a green check mark.



## Retrieving Data Obtained Using the Departmental Instruments

*This method works best for retrieving a single file. For multiple files, it is recommended to use another method (i.e. FTP).*

1. Save your NMR file, noting where you saved it.

2. Send an email to yourself containing the “fid” and “propar” files (these will be located in the folder called your\_filename.fid).
3. Save these files to the same folder on a computer with MestReNova installed.
4. Run MestReNova.
5. Click the “**Open**” icon located on the toolbar.



6. Locate the folder containing your files, then click on the “fid” file.
7. Click on the “**Open**” button.
8. The spectrum will automatically open already processed.

## Getting Started Processing 1D Spectra

### *Referencing your spectrum*

1. Click the “**Reference**” icon located on the toolbar.



2. Click on the peak you wish to reference.
3. In the “**New Shift:**” box, enter the desired value.
4. Click on the “**OK**” button.

### *Phasing your spectrum*

1. Click the “**Phase Correction**” icon located on the toolbar.



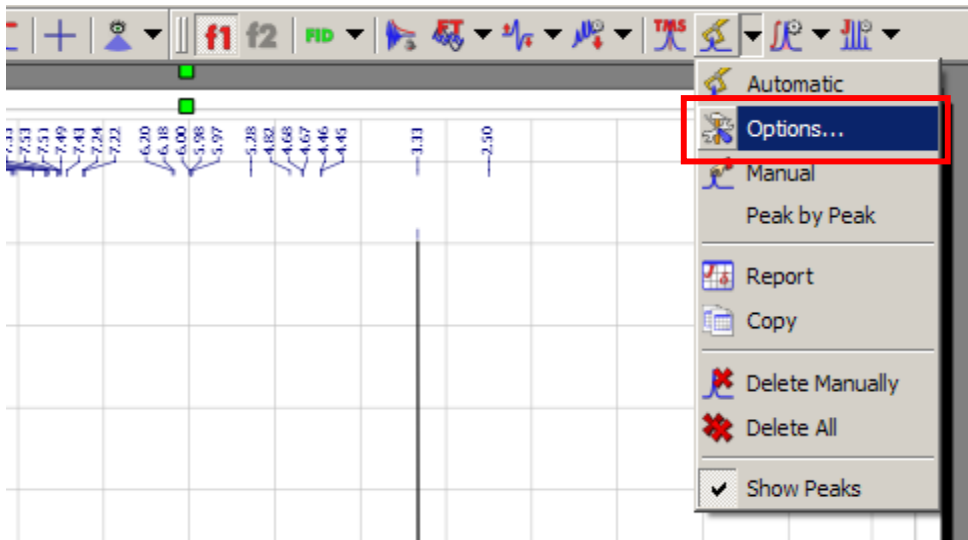
2. Click and hold the left or right mouse button inside the blue box.
3. Move the mouse up and down to phase your spectrum.
4. Click on the “**OK**” button.

## Peak Picking

1. Click the “**Peak Picking**” icon located on the toolbar.



2. Peaks will be automatically selected.
3. To adjust peak picking sensitivity, select “**Options...**” from the pull down menu located to the right of the “**Peak Picking**” icon.



4. In the “**Sensitivity:**” box, increase or decrease the sensitivity as needed.
5. Click on the “**OK**” button.

## Integrating Peaks

1. Click the “**Integration**” icon located on the toolbar.



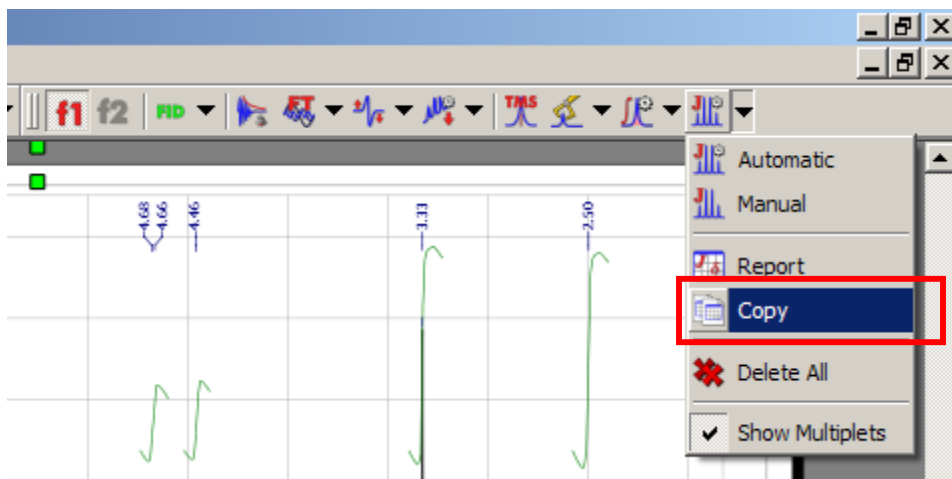
2. The spectrum will be integrated automatically.
3. To adjust integral values, run the mouse over an integral until it is highlighted pink.
4. Right click and then select “**Edit Integral...**”
5. Adjust the value in the “**Normalized:**” box as needed.
6. Click on the “**OK**” button.

## Generating a report

1. Click the “**Multiplets Analysis**” icon located on the toolbar.



2. Multiplets will automatically be analyzed.
3. To generate a report that can be pasted into a Microsoft Word document, select “**Copy**” from the pull down menu located to the right of the “**Multiplets Analysis**” icon.



4. Select the desired report format (JACS, RSC, or Angewandte).
5. Click on the “**OK**” button.
6. Follow the directions below specific to your operating system:

### Windows

Paste the report directly into your document (**Ctrl+V**).

### Mac

- a. Paste the report into the MestReNova pane (**⌘+V**).
- b. Copy the report from MestReNova pane (**⌘+C**).
- c. Paste the report into your document (**⌘+V**).