

NMR Spectral Prediction + Processing using MestreNova

Mestrelab's updated version of MestreC, called MestreNova, can do processing and spectral prediction on several platforms (currently Windows and Mac. Linux is coming). MestreNova is installed on the Windows PC next to the 500; use the account NMR users.









Data Processing with MestreNova

Data needs to be transferred from the NMR data server (nmr14.chem.columbia.edu) prior to processing. On the PC, use WinSCP3 as the sftp or scp client. On the Mac, use Fetch (its free for education). See the separate handout for details.

Here are the basics to using MestreNova  for 1D NMR.

The common tools are shown below. Be aware that many of the tools function such that once selected, they continue to work until deselected (ESC works to deselect). Many are automatic and selecting the adjacent down arrow gives options including manual adjustment. The spectrum must be selected before choosing a tool.



-  Open a file. Navigate to your data and select the fid file. FT and phasing will automatically be done and you will see a spectrum immediately.
-  Expansion. Turns left mouse button into expander. Drag to choose region.
-  Resets to full spectral width
-  Phase correction, select manual if desired
-  Set reference
-  Peak picking. Automatic works well. Then one can add or delete picks manually.
-  Integration. After integrating, one can select an integral by pointing at it. Then doubling clicking allows one to set its value and adjust its bias and slope.
-  Multiplet analysis. Assigns multiplets first-order names such as doublet-doublet.



used to remove “empty” regions of the spectrum. Very useful!

To create an inset or expanded multiplet plot on the same page as the full spectrum, follow this procedure: expand around the multiplet, select edit, copy which copies the multiplet to the clipboard. Now, paste the spectrum and resize it. Both objects (full spectrum, and multiplet) are present on a single page. You can remove the grid on the insert by double-clicking on it and then adjusting its preferences.


To display lists such as peaks or multiplets, highlight the spectrum and select View, Tables. At the bottom of the table, select the type of list. To create the list as an object on your spectrum, click the report icon, .

To print in 208 Havemeyer, select the HP LaserJet 5000 printer.

Spectral Prediction

MestreNova includes a portal to Modgraph’s prediction engine. Modgraph in turn uses several academic programs for its prediction and is superior to ACD labs or Chemdraw. See www.modgraph.co.uk for a full overview. For C13 shift prediction, the traditional reference database approach is combined with neural networks to give accurate values. Stereochemistry is explicitly considered. For 1H shift prediction, either the traditional approach (called increments) or a conformer approach (CHARGE program) is an option. CHARGE considers partial atomic charges and steric interactions. To read about CHARGE, see www.modgraph.co.uk/product_nmr_proton.htm.

1. If necessary, draw a structure. ChemDraw 8.0 is installed on this PC. To show stereochemistry, simply use the UP/DOWN bonds in the structure. Save as file type MDL .mol file. Currently only MDL .mol files work. (Currently ChemDraw 10 does NOT work with MestreNova)
2. Start MestreNova, .
3. Bring a structure into MestreNova. A .mol file can be drag-and-dropped or brought in via the open dialogue.
4. To adjust preferences, Under Molecule, Prediction Options, Click on Predictor options. The default parameter values are fine but can be changed, if desired. For 1H, the algorithm can be either increment or conformer.
5. Highlight the structure by clicking on it. Under Molecule, select either Predict 1H spectrum or 13C spectrum. The software logs into a server and when finished will be display the spectrum, which can be treated as an ordinary spectrum (can be integrated, etc...)
6. When you pass the cursor over the atoms of the molecule, the corresponding peaks in the spectrum are highlighted in blue.
7. To display the assigned calculated peak list, highlight the spectrum and select View, Tables. At the bottom of the table, select the 13C Prediction or 1H

prediction list. To create the list as an object on your spectrum, click the report icon, 

Configuration Information for MestreNova Prediction

Under Molecule, Prediction Options, make sure Predictor is set to Modgraph NMRPredict. Click on Predictor options:

Server is

Port is 9055 when behind the chemistry firewall as we are in 208 Havemeyer. Port is 9212 when NOT behind a firewall.

username is `jdd13@columbiaedu`

Don't change the password.

The default parameter values are fine but can be changed, if desired. For ¹H, algorithm can be either increment or conformer.