NMR Processing on PCs outside the NMR laboratory

There is now a server that stores the NMR data from all spectrometers and can be accessed from PCs anywhere. For processing, we have a campus license for 200 users for MestreNova software which runs on Mac, Windows, and Linux.

Downloading Data from the NMR server

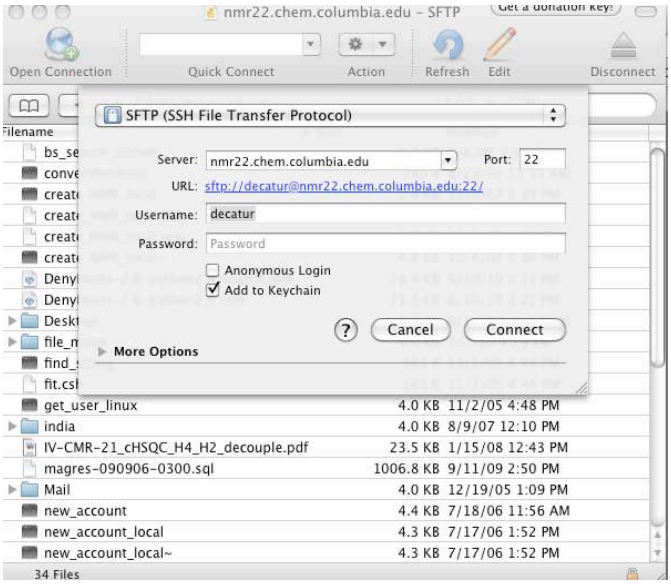
To download your data (and MestreNova license) from the NMR server onto your mac or PC, you need a client scp program. On Windows, the free SCP client program is WinSCP. On the mac, it is Cyberduck or Fetch. Cyberduck is free for all. Or, you may download a licensed copy of Fetch from the data server using Mac's terminal.

WINDOWS

Download WinSCP from http://winscp.net/eng/index/php. Choose the latest version and the "installation package" type of download. During the install, select all components and the Norton Commander type interface. Launch WinSCP and enter the following: hostname is nmr22.chem.columbia.edu (or 128.59.112.134), port is 22, enter your username and password that works for the NMR computers, and select SCP type of transfer. Leave blank the space for private key file. Click login. Once the program logs in, your home directory on the server will be displayed on the right, and your windows directories will be on the left. Navigate both sides to reach your desired source and destination directories. For the server, navigate to the root directory (/), and then choose the disk you want: 300nb, 300wb, 400L, 400SL 500, or 500asc and then your name, and then data set. To download, press F5, or right-click the mouse and select copy (F5).

MAC

Download and install Cyberduck from http://cyberduck.ch/
After it downloads, click on cyberduck.zip to decompress it and then move it to your application folder. After Cyberduck is launched, choose connect using SFTP and enter info for hostname, which is nmr22.chem.columbia.edu (or 128.59.112.134), and YOUR username, as show in the graphic below. Make the initial folder / . Then, once you log in you will be in the root directory. Choose the disk you want: 300nb, 300wb, 400L, 400SL 500, or 500asc and then your name, and then nmr and then the data set. Download the entire dataset and not just the fid file.



The NMR server is completely updated every night between 1 AM and 5 AM. Thus, data collected today will be always available tomorrow. If you need access to recently acquired data you can manually update the server for only your data. On one of the NMR linux computers, type **update** and follow the directions. You will be prompted for your password, which is the same as on the NMR computers. The update may take a few seconds or minutes depending on how much data you have. Do not logout of the computer until it is finished. Only one disk (400L, 300wb, etc..) is updated at a time. From a spectrometer computer you may only update data from that particular spectrometer.

Only NMR data directories are transferred to the server, not your home directories. If you wish to have access to pdf or other graphic files created by Xwinplot on the linux NMR computers, then you must store them in the corresponding data directory, and not in your home directory.

Obtaining and Using MestreNova

We now have a campus license (up to 200 users) for MestreNova NMR processing software, which runs on Mac, Windows, and Linux. We also have ONE shared license for its Spectral Prediction module. Only one user at a time may use the program. The license is becomes available again shortly after another person stops makes predictions.

1. You can download the MestreNova software here:
http://www.mestrelab.com/Products/Mnova/Product-download.html
Only install the NMRPrediction Desktop plug-in if you intend to run NMR spectral predictions.

2. You need to download with an scp client (see above) one or more of the license files listed below, which are available on the NMR data server, nmr22.chem.columbia.edu, in the root (/) directory. The first file is for the main program and that is all you need unless you intend on doing spectral predictions.

ColumbiaUniversity125Extension.lic
Columbia University_Conc1_USunltd_NPL.lic

On a Mac you can use Fetch or Cyberduck or, use the terminal program and type, for example:

scp username@nmr22.chem.columbia.edu:/ColumbiaUniversity125Extension.lic .

Where username is YOUR username and there is a space between the lic and final .

3. To install the software and activate the license, follow the procedure in this guide:
http://mestrelab.com/resources/mnova-suite/installing/how-to-install-mnova
I've summarized the steps: Within MestreNova, under Help, choose evaluate/buy, click yes, click Activate…, then find the license files you downloaded above and choose open. Exit and restart MestreNova. The license server works as follows: up to 75 users, based on computer host id, can obtain a license to MestreNova. If a user doesn't open the program and connect to the license server for three months, he is dropped from the server list and that license becomes available again. If you experience an error connecting to the server, you may be behind a firewall.

Quick Guide to Data Processing with MestreNova

The following are quick start guides for 1D and 2D NMR processing using MestreNova.
http://www.mestrelab.com/a-quick-start-guide-to-mnova-nmr-1d.html
http://www.mestrelab.com/a-quick-start-guide-to-mnova-nmr-2d.html
Full manuals can be found on the MestreLab website: http://mestrelab.com/resources/

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

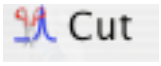
 Phase correction, select manual if desired, but automatic works.

 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. To get a journal-ready printout of the shifts and couplings, select Analysis, Multiplets Analysis, Report Multiplets.

 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 mulitplet) 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 use dual display mode, open two spectra so that there are two pages on the left. Highlight both spectra pages and then select Stack, stack spectra. This creates another page containing both spectra. Click this icon  , located on the left, to adjust the stacked plot.

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, 

Brief 2D Processing Notes:

Automatic phasing usually works. Under Processing, phase correction, select "automatic along F2" and then "automatic along F1". For the HMBCEA experiment, you must select "magnitude along F2" that is found under Processing, Phase Correction.

Spectral Prediction with MNova

MestreNova includes a plug-in for Modgraph's prediction software. 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. Or, http://mestrelab.com/Products/Mnova-NMRPredict-Desktop/Features.html 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. Using a drawing program, draw a structure. To show stereochemistry, simply use the UP/DOWN bonds in the structure. (ChemDraw seems to work fine but in the past only versions pre ChemDraw 10 worked. You may have to save as file type MDL .mol file.)
2. Start MestreNova,  .
3. Bring a structure into MestreNova. Files can be drag-and-dropped or brought in via the open dialogue, or copy and pasted.
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, or best.
5. Highlight the structure by clicking on it. Under Molecule, select either Predict 1H spectrum or 13C spectrum. The calculated spectrum will be displayed, 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 Desktop. Click on Predictor Properties:
The default parameter values are fine but can be changed, if desired. For 1H, algorithm can be either increment or (CHARGE)conformer, or best, which is a combination.