

NMR Processing on Windows 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. The freeware program SpinWorks can be used for NMR data processing on Windows PCs. For the Mac, there is Mestrelab's MNova, but this costs \$370 (but you can ask for a discount!) MNova is also a good choice for the PC.

Downloading Data from the NMR server

To download your data from the NMR server onto your PC, you need the free SCP client program, WinSCP, on your PC. Download 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 nmr14.chem.columbia.edu (or 128.59.74.141), 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, 400, 500a, or 500b, and then your name, and then data set. To download, press F5, or right-click the mouse and select copy (F5).

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 (400, 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 the freeware program SpinWorks for NMR processing

Download SpinWorks from

<http://www.umanitoba.ca/chemistry/nmr/spinworks/index.html>

The following is a quick, abbreviated guide to 1D processing. See the Spinworks manual, which is available at the above web site, for more details on 1D processing and a 2D guide.

1. To open data, click on **Open** under the **File** menu, and navigate to your desired data set and find the file *fid*. Although the *fid* file is the only file loaded, other parameter files must be present for SpinWorks to correctly recognize the data. (This means you must download the entire directory and not just the file *fid* to your PC.)
2. To perform the FT including exponential multiplication, click on the yellow proc button  on the toolbar and then click **process**.
3. To enter phasing mode, click on the yellow phase button  on the toolbar. A green line on the spectrum indicates the reference point. Adjust the zero order phase sliders to a properly phased peak at the reference point. Adjust the first order sliders to phase the remaining peaks. Click **Apply and Exit**.
4. For baseline correction, click on the yellow bpt button  on the toolbar. This may be necessary to accurately integrate your spectrum. Use the cursor to define at least 6 baseline points in the spectrum. Click Return and then select **Automatic baseline correction (least squares)** in the processing menu.
5. To calibrate the chemical shift, click the left mouse on the reference peak. A cursor will remain at the chosen position. Then click the **Cal** button on the toolbar.
6. To integrate, click  on the toolbar. Use the cursor and left mouse button and to define the starting and ending points. To select an integral, place the cursor over an integral and click the left mouse button once. Nothing appears to have changed but it is selected. A selected integral may be deleted or calibrated. To calibrate, enter a value and click **calibrate**.
7. To peak pick, select **Pick Peaks and Append to List** in the Peak Pick menu. The minimum height for picking is defined by the horizontal line, which can be moved by its handle on the left end of the line. Pick peaking is cumulative so to re-pick with a higher threshold, first select **Clear Peaks in Region** under the Peak Pick menu and then repeat **Pick Peaks and Append to List**. This cumulative feature allows you to customize your peak pick list; one can expand the spectrum and pick region by region, each with a different threshold.
8. To add a title, select **Plot Title** under the Edit menu.
9. To print, select **Print** under File.
10. To transfer spectra to Word, PowerPoint or other applications, under the Edit menu select **Copy Metafile to Clipboard**. In Word, select paste or paste special. To increase the resolution of the metafile, in SpinWorks select **Plot Options and Parameters** under the Edit menu. The MetaFile Resolution parameter, which is a multiple of the screen resolution, can be increased (2 is default).

Other methods to transfer data from the NMR computers:

Email

Email is no longer supported. If you know how to configure it, please feel free to use kmail.

USB memory sticks and ZIP disks (substitute ZIP for USB memory sticks below)

1. Lift FRONT cover and insert USB memory stick.
2. Open a file tool. Click home icon, located at bottom. Enter the location of your data directory, which has the form `file:/disk_unit/data/username/nmr`
3. Click `USB_memory_disk` icon to open a second file tool. Drag data to the USB memory stick.
4. To prevent confusion, only copy complete data sets, that is, from the directory level `/root/disk_unit/data/username/nmr` AND return complete data sets to this directory. All other possibilities are the user's responsibility! When data is restored from storage device to hard disk, it must be restored to the exact original directory level or else the NMR program will not recognize it!
5. When finished, right click mouse over USB memory stick icon and select `umount`. Then remove USB memory stick.

CD and DVD

1. Insert blank CD and open K3b CD burning program. At the bottom, left menu, under the Red Hat icon, select `Sound & Video, CD & DVD Burning (K3b)`. DVD burning is possible on the data station in 208 Havemeyer (nmr10).
2. Select `File-New Project-New Data CD Project`, or click on its icon.
3. Choose data to back up. In upper left corner window of the program, the `directories` window, select `root`, then `disk unit`, then `username`, `nmr`, then choose your data sets. Drag selected data sets into project window below.
4. Select `burn` (icon located in lower right). Set options. Under `Filesystem`, check 'preserve file permissions'. Under `Advanced`, check 'allow untranslated filenames'.
5. Click `burn`. CD will now be burned and will eject when finished.