Putting NMR spectral data into reports

There are several options for inserting spectral data into presentations and reports. All require at some point the transferring of either your raw data or a prepared file from the NMR server onto your computer.

Transferring Files via FTP (File Transfer Protocol)

1. From a networked computer, open an FTP program. The PC in the NMR lab has a program called WS-FTP which can be used for this. Or download Filezilla from filezilla.sourceforge.net for the PC. For Macs, use the terminal in the applications folder or download the free cyberduck program from cyberduck.ch and use normal FTP. Files can then be saved on your personal flash drive.

2. FTP to the host: echo.chem.umn.edu and login with your NMR account and password.

3. Find the appropriate data direcotry.
Current data collected on the hands-on instruments is in your /data directory.
Current data on the VAC-300 is in your /v3data directory.
Current data from the VAC-200 is in your /v2data directory.
Old data is in the other directories (a1-w9, etc).

4. Select the appropriate files and transfer them to your flash drive.

Creating Postscript Files

Spectra, both 1D and 2D, can be saved as postscript files which can then be opened with a graphics program. We recommend the use of Adobe Illustrator, then saving your file as an .eps document for opening in Microsoft Office products such as Word or Powerpoint. Alternatively, Adobe Distiller will convert these files to .pdf files.

1. Log in to any workstation in the NMR lab.

2. Choose a PS-AR plotter (for landscape plots) using the **[Change Plotter]** button.

3. Process your spectrum. Display it the way you want it for the figure.

4. Make sure you are in your data directory. **[Main Menu] - [File] - [Data]** or by typing:

cd('/data/*6-lettercode*')

5. Type in all the commands necessary for plotting the spectrum, but give page a filename, e.g.:

For 1D spectra: **pl pscale pirn ppa ppf('top') page('*filename*.ps')**
For 2D spectra: **pcon(10,1.2) pap page('*filename*.ps')**

6. Transfer your files (see above).

Creating ASCII Files

In some cases, you may want to save your spectra as an ASCII file. This is a file consisting of 2 columns, the first is the ppm value and the second is the intensity. These can be graphed with any graphing program, e.g., Excel.

1. Log in to any workstation in the NMR lab.

2. Recall your FID.

3. Change the zerofill number (**fn**) to something more reasonable, e.g. **fn=16000**. This method creates a new entry for each datapoint; this is the reason for reducing the fn number.

4. Reprocess (**wft**) and make sure you do not lose too much resolution.

5. Make sure you are in your data directory. **[Main Menu] - [File] - [Data]** or by typing:
   cd('/data/*6-lettercode*')

6. Type **writespec('*filename*')** in the command line. *Use a different filename than that of your original fid.* Otherwise you will not be able to read the original fid later on.

7. Transfer your files (see above).

Using Third-party Software to Process NMR data

There are several programs that can be used to process and display NMR data.

These include: iNMR (for Macs), MestreNova and Spinworks for PC, and Know-It-All from BioRad. Links to some of these can be found on the NMR webpage: http://nmr.chem.umn.edu

Once you have one of these programs, you need to transfer the entire .fid directory (which consists of at least 4 files) to your computer, and you will open the fid file within that folder. Tell the program you are working with Varian files.