How to Download NMR Data to Your Personal Computer

Bruker AVIII-400: Download the zip file with your NMR data from this website:

http://aviii400.chem.arizona.edu/

Click on your username. For a course, use the course name (e.g., chem243b). You may have to click on a range of section numbers as well. The files displayed should have your filename with the ".zip" extension. Drag this file to your desktop (you may get a security question, answer "yes"). Double-click on the zip file icon on your desktop and select "Open". This opens a window with your NMR data folder. This is a temporary internet file and cannot be dragged into MestReNova. You must first drag this folder into another folder (named "AVIII400_NMR_Data" or named for a particular project) or onto the desktop. Open this folder and you will see your NMR experiments: 1, 2, 3, etc. If you only did a proton, you should only see a folder named "1". Drag and Drop the NMR experiment number folder into the MestReNova open pages thumbnail or the open pane of the document; the NMR spectrum should appear.

Varian Unity-300, Bruker DRX-500, Bruker DRX-600 or Varian Inova-600: Use the file transfer program "WinSCP" to transfer your data from the NMR server "**uanmr**" to your computer. Please note that all NMR data is remotely mounted on uanmr, so there is no need to transfer data directly from the NMR instruments. Using the central server protects the NMR instruments from disruption. Please note that **you must be on the CHEMISTRY network** to access uanmr. The University network is not good enough. We have computers in room 121 and 122 Old Chemistry that are on the Chemistry network: you can use them to download data, dropping the folders into your own data stick.

If you don't have WinSCP, download it from UITS:

https://sitelicense.arizona.edu/ssh/

Click on "Download the WinSCP FTP Client" and install the software.

Double-click on the WinSCP icon on your desktop to get the Login window. Click on "New" (top right) and enter the Host name:

uanmr.chem.arizona.edu

Enter your NMR login and password. If you are using a course NMR account, your login on the instrument will end in the course number (e.g. smi446), but for WinSCP you will use the full login (e.g., smithr) that you use for the NMR reservation system. Click on "Login".

The WinSCP graphical user interface shows the remote computer (uanmr) files on the right and the local computer (your personal computer) files on the left. Focus on the right side. Above this frame on the right, near the center of the space above the frame, is an icon showing an open folder. Hover over this icon and you will see "Open Directory / Bookmark". Click on this icon to set the **path** to your NMR data. The "Location profiles" frame will open and in the "Remote Directory" field you need to enter the path:

Varian Unity-300: /unity300/<group>/<login>/vnmrsys/data
or /unity300/<group>/<login>

Bruker DRX-500: /drx500/u/data/<login>/nmr

Bruker DRX-600: /drx600/u/data/<login>/nmr

Varian Inova-600: /inova600/<login>/vnmrsys/data
or /inova600/<login>

All slashes are forward slashes, with no spaces. <login> is your NMR login (on the NMR instrument) and <group> is your NMR group in lower case, for example "njardarson" or "chem446". For the Varian instruments, your NMR data should be in your vnmrsys/data directory, but some people fail to do this right and it ends up in the home directory. Check both locations if you are missing data.

From the remote computer side of the WinSCP frame you can click and drag your dataset directly to your desktop or to a folder on your computer. You don't need to use the left side (local computer) of the WinSCP frame.

Varian NMR data (*.fid) folders can be directly dropped into the MestReNova frame. Bruker NMR data folders must be opened first to reveal the experiment numbers (1, 2, 3, etc.). These numbers can then be dragged and dropped into the MestReNova frame.

When you are finished with WinSCP, close the software (X in upper right corner) and confirm. Leaving it open leaves the uanmr server and your NMR data vulnerable to anyone who walks up to the computer.