PINMRF

Bruker AV-III / Avance DRX NMR Spectrometers running TopSpin

Data Transfer between Spectrometer and User PC

Overview

These notes cover the steps involved in moving an NMR dataset from a PINMRF Bruker TopSpin spectrometer or Linux offline data station to a personal computer for archiving or manipulation either by TopSpin or a third party software package.

NOTE: You will be able to move NMR data from a spectrometer host computer ONLY if you are connecting from the Purdue domain. If you want to move data to a computer off the Purdue domain you will need to first initiate a VPN connection to the Purdue domain from your off-domain computer.

Secure File Transfer

1. **On your personal PC/Mac** download and install a Secure File Transfer Protocol (SFTP) client if you do not already have one set up.

Purdue has made available a program called *SecureFX* through the security resources section of the ITAP website (https://communityhub.purdue.edu/storefront/browse/securitysoftware/). After authenticating as an authorized Purdue user you will be allowed to download SecureFX and be sent a license code via e-mail. Install on your PC following all standard options. PC users also may use PuTTY (https://www.chiark.greenend.org.uk/~sgtatham/putty/latest.html).

Mac users may use any free option, such as *Fugu* (http://rsug.itd.umich.edu/software/fugu/) or *CyberDuck* (http://cyberduck.ch/) which provide the same functionality. Mac or Linux users may also use the scp -r (secure copy) command from a terminal window within Mac OSX if they are comfortable with Unix command-line input. The scp command does not have a GUI so directory locations must be entered manually.

2. Launch the SFTP client and open a new connection.
3. Enter or select the following parameters for that connection:
    a. Connection Type/Protocol: SFTP

b. Port: 2200 (if 2200 does not work, try 22 or leaving the port field blank)

c. Hostname: *spectrometer_name*.pinmrf.purdue.edu (where *spectrometer_name* could be e.g. av400, drx500-2, av800, atlantis, freedom)

d. Username: your One-Purdue user ID

e. Password: your One-Purdue password

4. Click CONNECT and wait for the client to connect. A file management window should open showing your home directory.

5. Use the navigation buttons to get to your NMR data directory. The standard location is:

/opt/topspin/data/*userID*/nmr/*datasetname*

where *userID* is your username and *datasetname* is the experiment name of the NMR data set.

6. Locate the datasets of interest. Each dataset is a directory, and within this directory are the experiment number directories, each in turn containing several files and subdirectories. Typically you will want to move the whole dataset directory.* In most cases you may copy them by clicking on them to highlight, and then dragging the data directory directly to the desired location on your computer. Otherwise, click the data set name to highlight, and select DOWNLOAD in the client. You should then be prompted to choose a save location. Click SAVE to save the file to your PC.

7. Repeat step 5 until all desired files have been transferred.

8. Disconnect from the host spectrometer and quit your SFTP client.

NOTES ON DATA PROCESSING

Bruker TopSpin NMR data will require NMR data processing software in order to view and manipulate your data on a PC or Mac. Bruker offers a free student version of TopSpin that will run under Windows, Linux or MacOS. Go to http://www.bruker-biospin.com/topspin-edu.html for more details. Another choice for this is MestreNovaNMR, a third-party data processing package available at http://mestrelab.com/software/mnova-nmr/. Purdue has a license for the MestreNova package, details on this can be obtained from the Chemistry Library.

*NOTE: you may transfer individual experiment number directories but you must ensure that the destination location is correct and unambiguous.

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