

PINMRF

Bruker NMR Spectrometers - Data Transfer between Bruker Spectrometer and User PC

Version 11-13-2007, IH.

Overview

These notes cover the steps involved in moving an NMR dataset from a Bruker spectrometer or offline data station to a personal computer for archiving or manipulation by a third party processing program. These notes are designed to be used in conjunction with the PINMRF Bruker 1D Training Guide.

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 (<http://www.purdue.edu/securepurdue/download/>). 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.

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: 22
 - c. Hostname: *spectrometer_name*.pinmrf.purdue.edu (where *spectrometer_name* could be arx300, dpx300, arx400, drx500-1, drx500-2, av800, galileo or pathfinder)

- d. Username: your NMR User ID
 - e. Password: your NMR password for that machine
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 saved data. This is typically located in: */u/data/userID/nmr/datasetname*, where *userID* is your NMR username and *datasetname* is the name of the NMR data set.
 6. Locate the datasets of interest. Each dataset is a directory 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.

NOTE: Bruker NMR data will require a third-party NMR data processing program in order to view and manipulate your data on a PC or Mac. An excellent choice for this is MestreNova, a reasonably priced comprehensive package available at www.mestrec.com. Other packages such as NUTS or Perch should also suffice.