PINMRF

Bruker AV-III / Avance DRX NMR Spectrometers running TopSpin
Data Transfer between Spectrometer and Linux Workstation

Overview

These notes cover the steps involved in copying an NMR dataset from a PINMRF Bruker TopSpin spectrometer to a PINMRF Linux offline workstation.

Bruker TopSpin / Linux data transfer

1. **On the TopSpin spectrometer** open a Linux terminal window.
2. Type:

cd /opt/topspin/data/*login-ID*/nmr

where

login-ID is your One-Purdue login ID. Be sure to include all the slashes exactly as shown.

(cd = change directory.)

3. Type ls -l to get a listing of all the experiment names in your NMR data directory.

(ls -l = long (detailed) file listing.)

4. Type:

scp -r *experiment_name login-ID@offline_workstation*:/opt/topspin/data/login-ID/nmr

where

1) *experiment_name* is the experiment name of the dataset you want to copy,

2) *login-ID* is your One-Purdue login ID (as above) and,

3) *offline_workstation* is the name of the PINMRF Linux workstation you want to copy your data to, either Atlantis (G43 RHPH) or Freedom (369 WTHR).

(scp -r = secure copy of a directory and all its contents.)

5. You will need to enter your One-Purdue password at the prompt to complete the secure copy process.

6. Please note that this process leaves the original dataset on the spectrometer. Please do not keep too much NMR data on the spectrometer's disk drives – we ask that you remove unneeded

data to keep disk space usage to a minimum. You can use the del command in TopSpin to bring up a list of datasets and then select specific ones for deletion.

Notes on file system trees on a Bruker TopSpin spectrometer

The Bruker TopSpin spectrometer has two separate file system trees. The user's login home directory is completely different from the TopSpin software tree. When a user creates a dataset, or saves a parameter set, an AU program or a shim set, the saved directories and files are all saved within the TopSpin filesystem tree, but with the user's ownership. Thus, the user who saved e.g. a shim set can change or delete it, but another user can only read it. The only files which get saved to the user's home directory by default are printer output files (e.g. PS or PDF files).

Here are the trees:

/home/*login-ID* (user *login-ID*'s home directory)

/opt/topspin/data/*login-ID* /nmr (user *login-ID*'s NMR data directory)
/opt/topspin/exp/stan/nmr/par (parameter sets)
/opt/topspin/exp/stan/nmr/au/src (AU programs)
/opt/topspin/exp/stan/nmr/lists/bsms (shim files)
/opt/topspin/exp/stan/nmr/lists/pp (pulse programs)
/opt/topspin/exp/stan/nmr/lists/f1 (f1 frequency lists)
/opt/topspin/exp/stan/nmr/lists/wave (pulse and gradient waveform shape files)

Note that on PINMRF Bruker TopSpin spectrometers the directory /opt/topspin is symbolically linked to another location.

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