

PINMRF

Bruker Avance / ARX NMR Spectrometers - Data Transfer between Bruker Spectrometer and SGI Workstation

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Overview

These notes cover the steps involved in moving an NMR dataset from a Bruker spectrometer to an SGI offline workstation. These notes are designed to be used in conjunction with the PINMRF Bruker 1D Training Guide.

Bruker / SGI data transfer

1. **On the offline SGI workstation** (Galileo, Mariner or Pathfinder), enter your login ID in the login field.
2. Enter your password in the password field.
3. Wait for the window manager to start completely. Move the mouse pointer to the toolchest icon in the upper left corner of the desktop.
4. Right-click the DESKTOP button on the icon. Then, right-click the ACCESS FILES button, followed by the IN MY HOME DIRECTORY choice. This will open a “file manager” window.
5. In the pink area of the file manager window, you will see a string of text with slash characters (/) in it. Highlight this string of text and replace it with the following text string that you enter:

/u/data/userid/nmr

(example: /u/data/harwood/nmr)

where “userid” = your own login ID. Be sure to include the leading slash. This file manager window will be referred to from now on as the “target file manager window.”

6. Repeat step 4 to open a second file manager window. Move this window such that you can easily see all of both the file manager windows on the screen.
7. The second file manager window is the “source file manager window.”

8. In the pink text field of the source file manager window, replace the current string with the following string that you enter:

`/nfs/spectrometer/d2/data/userid/nmr` (example: `/nfs/drx500-1/d2/data/harwood/nmr`)

where “spectrometer” is the name of the Bruker spectrometer you want to get your data from and “userid” = your own login ID. Be sure to include the leading slash.

9. In the source file manager window, you should now see individual folders for each different dataset name you have on the spectrometer.

10. To move a folder from the spectrometer to the offline, first left-click the desired folder to highlight it. Next, right-click the folder followed by clicking the MAKE COPY menu item.

This will make a duplicate of the folder (dataset) on the spectrometer, with the name “copy-of-originaldatasetname.” A message window will appear while the duplication takes place. NOTE: this may take some time if the dataset is large.

11. Drag the “copy-of-...” folder from the source to the target file manager window. A message window will appear during the moving of the dataset. NOTE: this occurs over the network and may take some time if the dataset is large and/or the network is slowed for any reason.

12. When the folder has been moved to the target file manager window, left-click the folder to highlight. Then, left-click the name area of the folder and remove the “copy-of-” text from the beginning of the folder’s name.

13. When you are finished moving data, left-click the ACTIONS pull-down menu and go to CLOSE to close the file manager windows. Alternatively, you can leave them open, or iconify them, and open XWinNMR with them in the background.

14. 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. If you want to move a dataset without keeping a copy on the spectrometer, just skip step 10 and simply move the dataset as in step 11, above.

File system trees on a Bruker spectrometer

The Bruker spectrometer has two separate file system trees. The user's login home directory is completely different from the Bruker 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 Bruker 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 are printer output files (e.g. PS or PDF files).

Here are the trees:

/usr/people/userid (user "userid"'s home directory)

/u/data/userid/nmr (user "userid"'s NMR data directory)

/u/exp/stan/nmr/par (parameter sets)

/u/exp/stan/nmr/au/src (AU programs)

/u/exp/stan/nmr/lists/bsms (shim files)

/u/exp/stan/nmr/lists/pp (pulse programs)

/u/exp/stan/nmr/lists/fl (fl frequency lists)

/u/exp/stan/nmr/lists/wave (pulse and gradient waveform shape files)

Note that on PINRMF Bruker spectrometers the directory /u is symbolically linked to another location.