Account Set-Up Suggestions for the New NMR Computer

General Notes

- Note that commands and filenames are case-sensitive in Linux.
- Some of the Linux software will cut/paste using the usual Windows keystrokes (`ctrl-c`/`ctrl-v`), but other software uses the following method:

  to cut: highlight the text you wish to copy
  to paste: middle click (with the scroll-wheel)
- If a blue screen with the time is up, press the enter key to get to the login screen.

Transferring Data from the Old Computer

Note that this would be an ideal time to archive old data to a CD.

1. Open the WinSCP software on the old computer, and double-click New Computer. *Do not close TopSpin on the Windows computer — it takes forever to reload.*
2. Sign on with your new username/login
3. Browse to your old data in the left window (`C:\Bruker\TOPSPIN\smith`), and to your folder on the new computer in the right window (`/spectra/smith`).
4. Drag your directory on the old computer in the left panel, to the new computer in the right panel
5. Close the SCP window. OK to terminate the SCP session.
6. Log onto the new computer, click the NMR_Directory icon, and thin out any data you don't wish to retain.

New Account Set-Up

Desktop Environment

- On a first login, the system will ask for a new password. It wants a minimum of seven characters which must not form a dictionary word. You can always put in a dummy "strong" password and change it to something weaker through the System Settings panel ("Start Menu" → Computer → System Settings → Account Details).

TopSpin

- Create an entry for your own data in the Browser sidebar:
  1. Right-click in the sidebar and Add a New Data Dir. Browse to your directory,
     `/spectra/`*login-name*`/`*user-name* (*eg,* `/spectra/advisorname/studentname`)
     or `/spectra/`*login-name* ,
     and set it as the DIR.
  2. Right-click the Exam Data folder and remove it from the list.
- First Spectrum:
  - If you have old data, open one of your old spectra to set the path for new data in the edc menu.
  - If you do not, set the directory to `/spectra/`*login-name*`/`*user-name* .
- Useful Preferences:

  I have not yet figured out how to set default TopSpin preferences for new accounts, but here are some additions to the standard set that I find a useful starting place as you tweak to your taste. Most are click-boxes within TopSpin's Manage → Preferences tab.

- Administration: auto-open last, automatic command-spooling
- Acquisition: automatic getprosol
- Display: peak labels, peaks/integrals → 2 digits (*ie.* decimals) for integration, 3 for peak positions (may need to click "+/–" button to get these).
- Browser Font: 11 pt
- Status Bar: autoopen, spooler, time, sample temp, aqn status, aqn indicator, lock signal
- Lock: autoopen lock display, 9×5 grid
- BSMS: external window

In addition, I find it convenient to have the second row of manipulation buttons shown (icon).

TopSpin Notes

- If the sidebar spectrum-browser gets stuck maximized, type `ctrl-d` to shrink it.
- The path to your datafiles is one of

  `/spectra/`*username*`/data/`*filename*`/1o`

  or `/spectra/`*username*`/`*filename*`/1o` .

  If you use operator names (eg, research students), the path is

  `/spectra/`*advisorname*`/`*studentname*`/`*filename*`/1o` ,

  but the sidebar browser doesn't always seem to pick these up. Also, the sidebar browser is not happy if the operator-directories are included directly — it wants only the top (advisorname) directory.
- The second-row buttons behave differently if one clicks, holds, or drags on them:
  - Hover to get information
  - Click to activate or get a sub-menu (depending on the button)
  - Click-Hold to get a sub-menu
  - Click the triangle to see the submenu of buttons that activate on clicking
  - Drag to enter a sub-menu .

Accessing Data for iNMR

One convenient aspect of the Linux environment is that it accepts ssh connections, allowing the use of SSHFS, which is installed on the ChemClub computers. Thus, if you wish to use iNMR, you can process your data on the hard-drive just as you processed the data on the NMR drive in Organic.

(0. If this is the first time you are connecting from a given computer, you must use SSH first. In the Terminal program (/Applications/Utilities), type `ssh username@nmr400 true` .)

1. Click the SSHFS icon on the dock, SSH, and enter the following:

Server:	nmr400
Directory:	/spectra/*username*
Password:	password for your account

2. A folder should appear on the desktop, within which you can navigate to your data just like you did in Organic. If it does not, verify that "Connected Servers" is checked in the Finder preferences.