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1. Logging onto the new Bruker 400 workstation:

Computer name = **ucsf400.ucsf.edu**

Username = contact the curator for this Password = contact the curator for this

2. How to change your password:

1) Open a new terminal from the main Linux window and type "passwd" at the prompt.

2) You will be asked to enter your old password, then your new password (twice).

3. How to Setup a Basic New Experiment:

- 1) Go to the Start tab.
- 2) Left-Click on the "Create Dataset" Icon.

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 USERS ∴ /home/data/jtgrp/Adolfo ∴ /home/data/jtgrp/Geoff 	Spectrum ProcPars AcquPars Title PulseProg Peaks Integrals Sample Structure Plot Fid Acqu Image: Structure New X Prepare for a new experiment by creating a new data set and initializing its NMR parameters according to the selected experiment type. For multi-receiver experiments several datasets are created. X Place define the number of receivers in the Options. NAME MY_SAMPLE Place EXPNO 1 PROCNO 1 PROCNO 1 PROCNO 1 Outrent parameters Experiment PROTON Select Select Select Select Select Select Dill New New			
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This creates a "**New**" experiment window.

3) Fill in slots 1 through 8, then click **OK** when done.

NOTES:

- A) Slot #1 (Experiment Name): Please do not include spaces.
- B) Slot #2 (Experiment Number): Iterate numbers to store multiple experiments under same folder. See the example in Section 4.1 below. Enter numbers only. No characters or symbols allowed.

C) Slot #7 (Data Directory) should be set to: /home/data/OWNER/operator

D) Slot #8 (Title/annotations): Annotate your expt. here - this is good for bookkeeping purposes.

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4. Accessing your data:

• You can transfer your data to your local network using the secure ftp program of your choice (e.g. WinSCP for PCs or Cyberduck for Macs). Computer name = ucsf400.ucsf.edu

NOTES:

A) Access must be done through a <u>secured</u> protocol such as **sftp** or **scp** (port 22).

B) Use your linux account username and password.

• The root directories are located here:

/home/users/OWNER

• The main data directories are located here:

/home/data/OWNER

• A suggested account structure in Bruker Topspin 3.5 is as follows:

Owner

→ Operator
 → Experiment name
 → Experiment #
 → pdata/Process #

(linux account) (individual user) (name of your experiment queue) (experiment #) (processed experiment #)

The **Operator**, **Experiment name**, **Experiment #**, and **Process#** are automatically created when you launch a **Create Dataset** job.

Owner = user name, linux account.

Operator = individual user or project name.

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4.1 An example:

Owner = my_lab Operator = john-doe Experiment name = my_sample						
Experiment # 1 (example = 1-D PROTON) Experiment # 2 (example = 1-D CARBON)						
→ The resulting data will be located in:						
/home/data/ my_lab/john-doe/my_sample/1/fid (PROTON) /home/data/ my_lab/john-doe/my_sample/2/fid (CARBON)						
The number after my_sample corresponds to the Experiment #.						
2-D experiments will be named " ser ".						
If you have processed your data using TopSpin on the workstation:						
/home/data/ my_lab/john-doe/my_sample/1/pdata (PROTON) /home/data/ my_lab/john-doe/my_sample/2/pdata (CARBON)						
Under the pdata directory:						
…/pdata/1/1r …/pdata/1/title	(Your processed data) (Text file containing your annotations, if any)					
The number after pdata corresponds to the Process #.						
Processed 2D experiments will be named "2rr".						