Table of contents:

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:

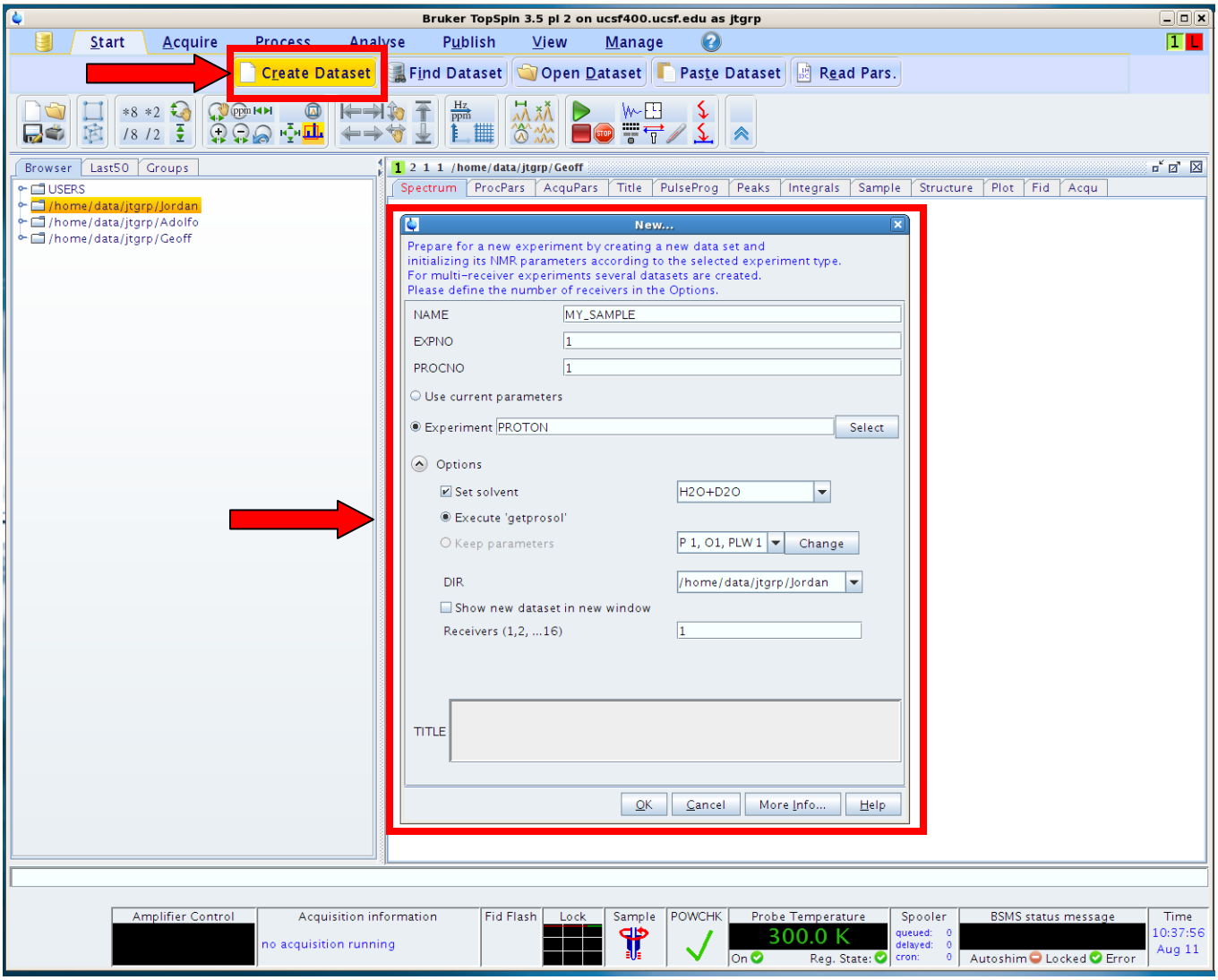
1) Open a new terminal from the main Linux window and type "**passwd**" at the prompt.

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.



This creates a "**New**" experiment window.

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

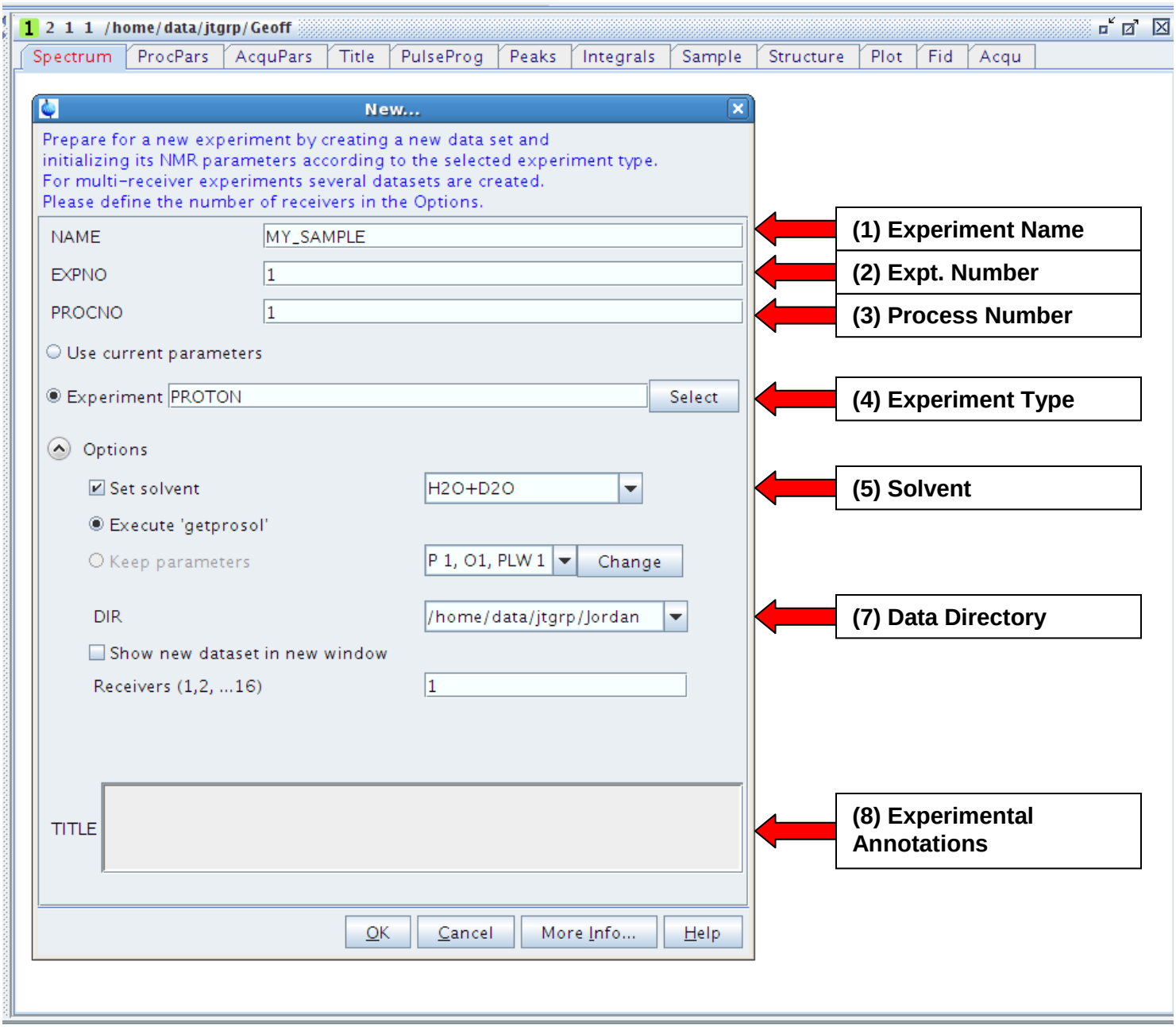
NOTES:

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.



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 secured 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	**(linux account)**
→ **Operator**	**(individual user)**
→ **Experiment name**	**(name of your experiment queue)**
→ **Experiment #**	**(experiment #)**
→ **pdata/Process #**	**(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.

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 **(Your processed data)**
…/pdata/1/title **(Text file containing your annotations, if any)**

The number after **pdata** corresponds to the Process #.

Processed 2D experiments will be named "**2rr**".