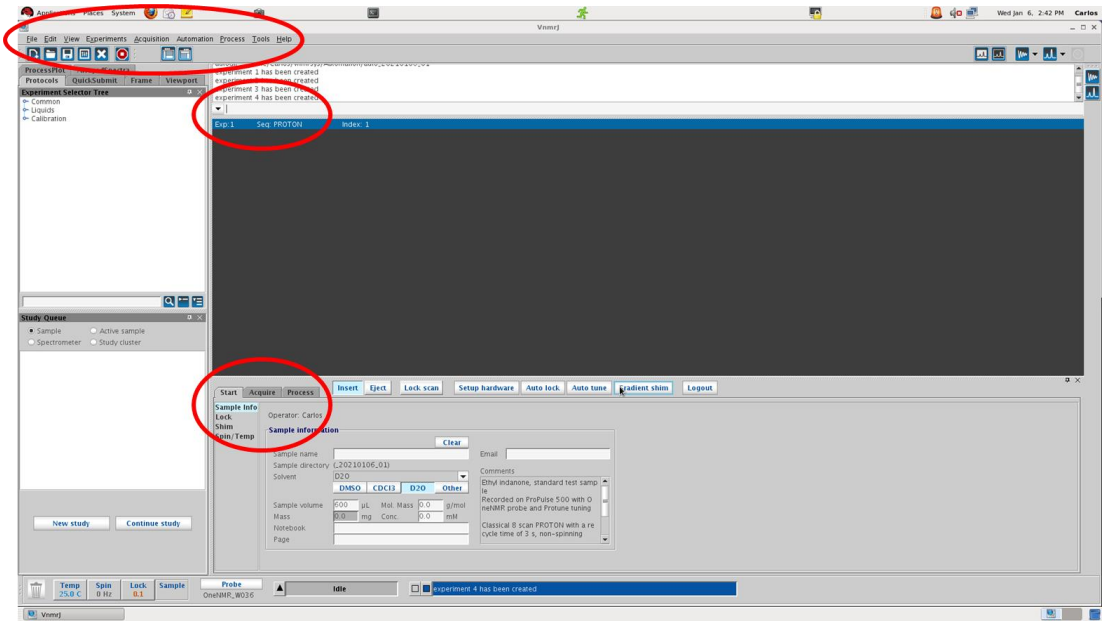
Department of Chemistry NMR Facilities

Varian 600 Tutorial. Acquisition of 1D ^{1}H and ^{13}C spectra

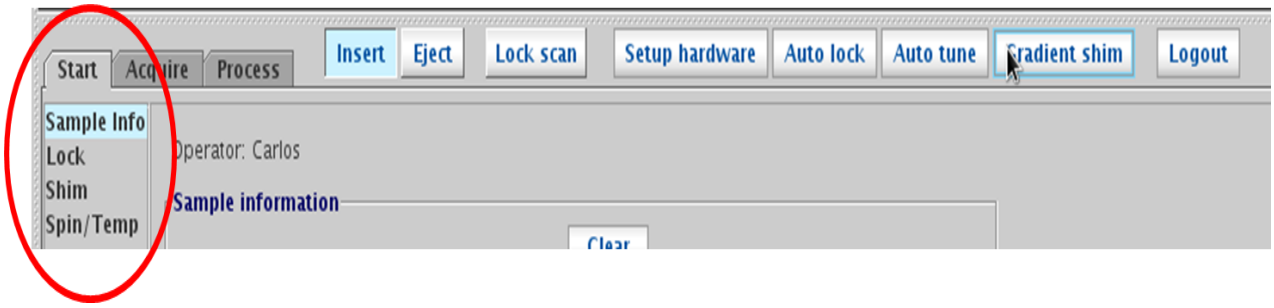
The VNMRJ layout.

VNMRJ window. Main menus, command line and tabs are highlighted.

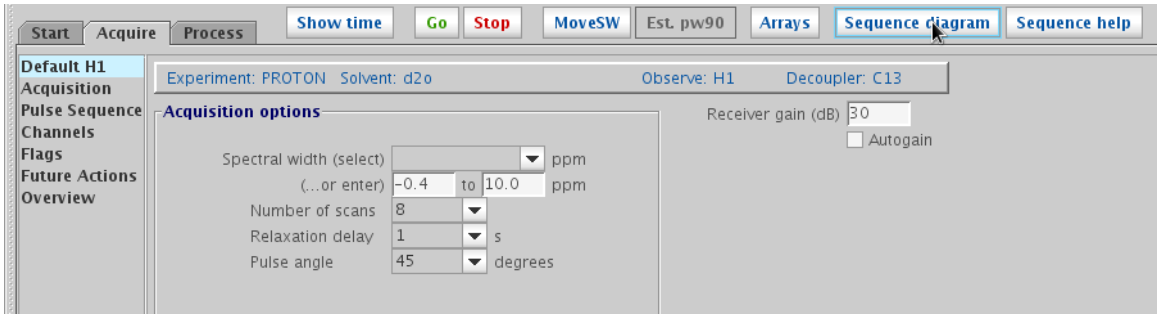


All the commands to operate the NMR spectrometer are within three tabs; **Start, Aquire and Process** and, the lines below each tab.

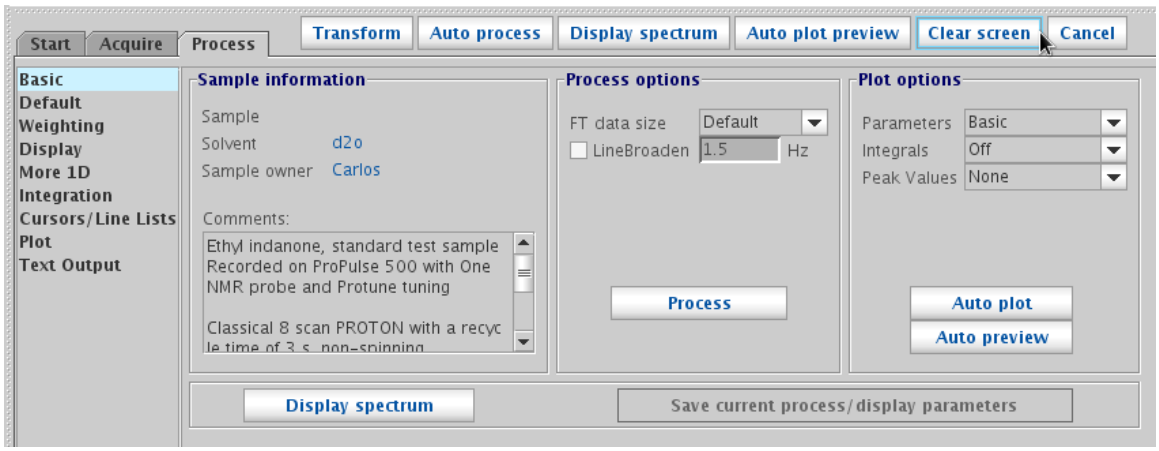
Start



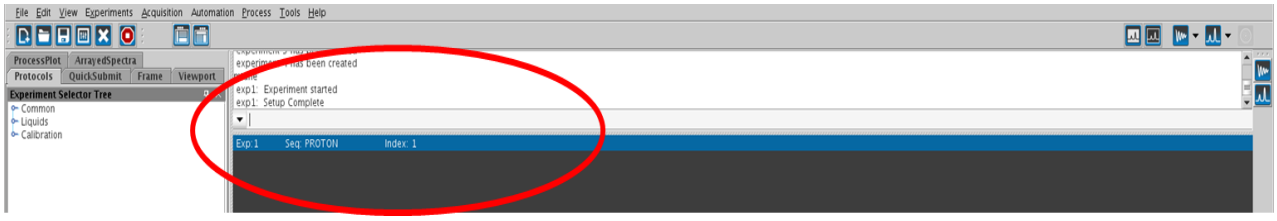
Aquire



Process



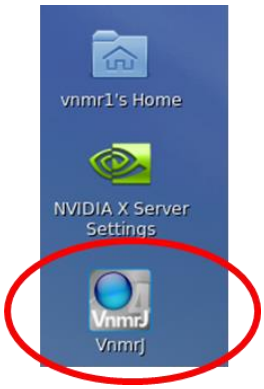
Commands can also be entered in the “command line”.



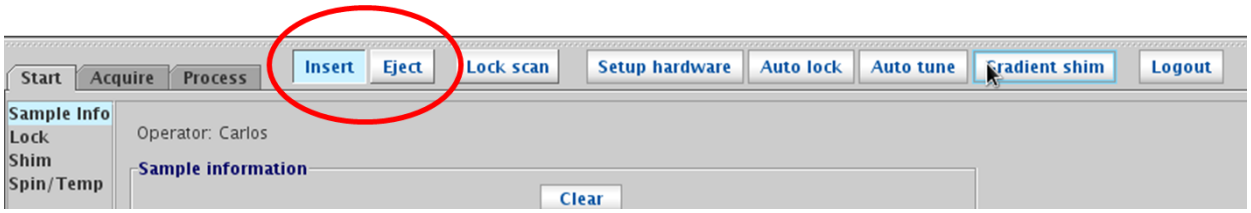
Starting the program and setting up the sample.
Tuning, locking and shimming the sample.

1) Log on into the linux account.

2) Click on the VNMRJ icon to open the program.



3) On the tab Start, click on <**Eject**> to eject the sample from the magnet.

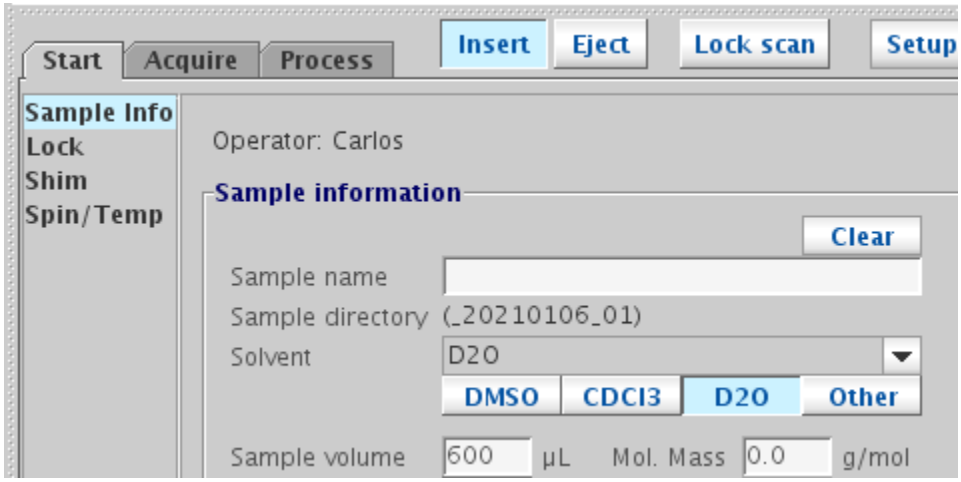


4) Clean the sample.

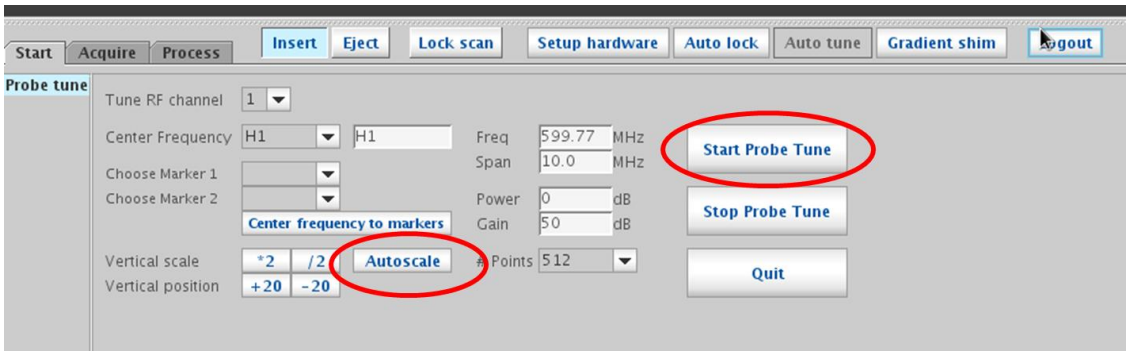
5) Insert the tube in the spinner. Use the gauge to measure the depth.

6) Place the new sample on top of the magnet. Click on <**Insert**> to insert the sample into the magnet.

7) Select the **solvent** on tab "**Start/Sample Info**"



8) Type "mtune" on the command line and then press <enter>. The window shown below pops up.



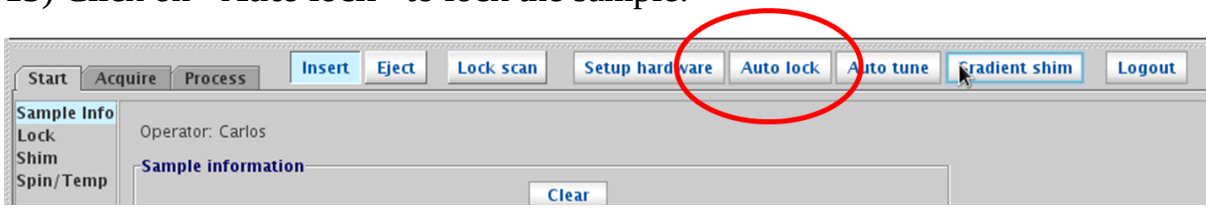
9) Only the tuning of the ^{1}H channel is needed on the Varian 600. Click on <Start Probe Tune>.

10) Click on <Autoscale>.

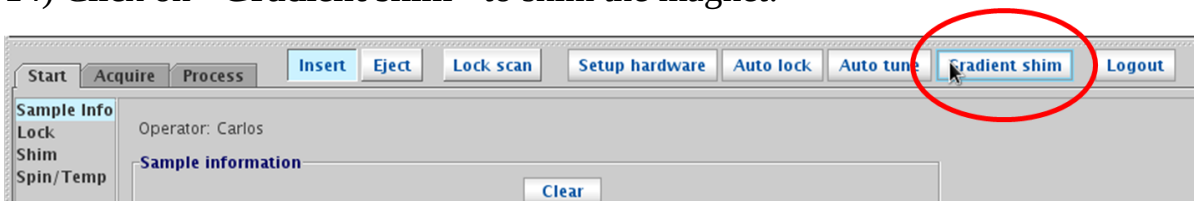
11) Manually tune the probe.

12) After tuning ^{1}H, click on <Stop Probe Tune> and then on <Quit>.

13) Click on <**Auto lock**> to lock the sample.



14) Click on **<Gradient shim>** to shim the magnet.

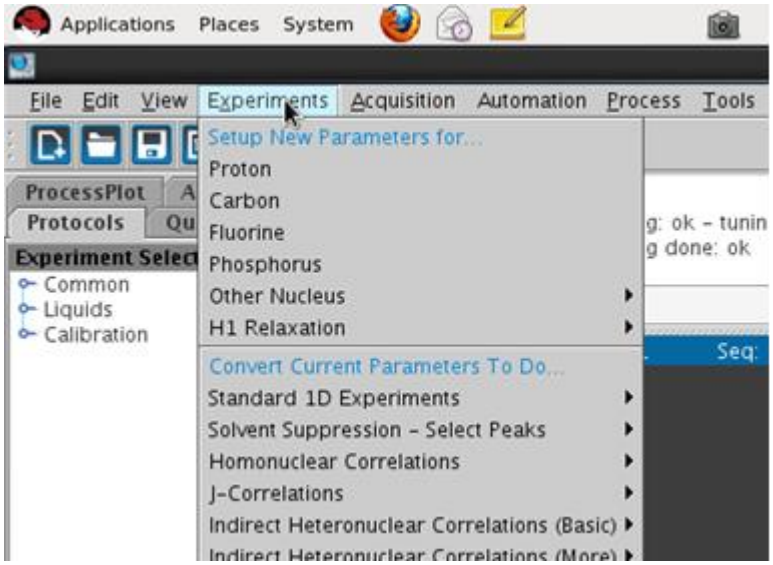


When doing Gradient shim and Auto lock, the solvent will temporarily switch to D_2O and spinning will turn off.

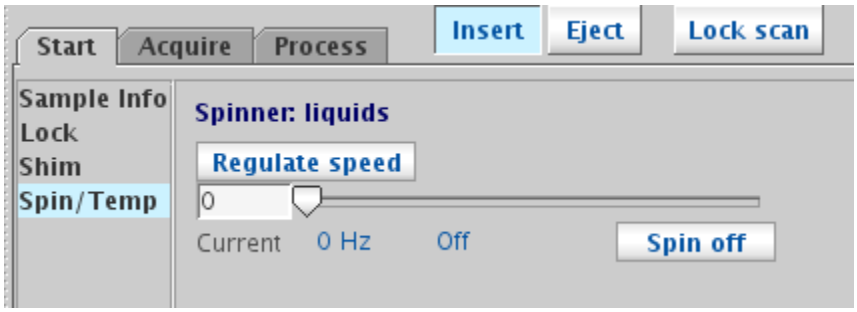
Tuning, locking and shimming must be done only once for each sample, right before running any NMR experiment.

Running a proton (^1H) experiment

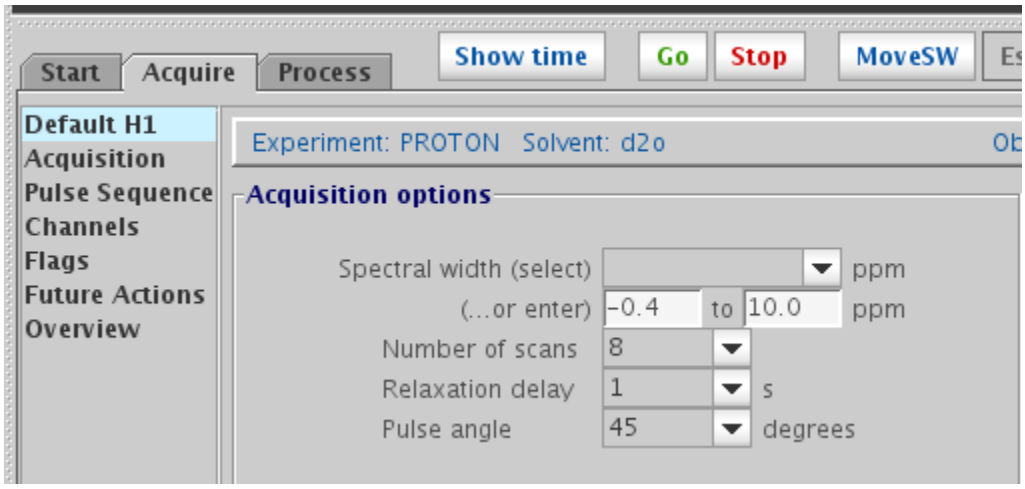
1) Select an experiment. Click on the menu "**Experiments"** and then click on "**Proton**", as shown below.



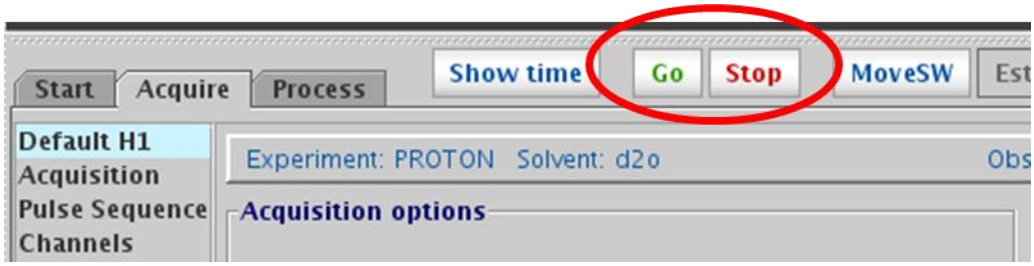
2) Regulate the spinning or enter “spin=0” in the command line.



3) On the tab “**Acquire/Default H1**” the experimental parameters can be modified, Spectra Width, Number of scans and Relaxation delay.



4) To run the experiment, click on <**Go**> on the Acquire tab.



5) To display the spectrum, type “wft” on the command line and then press <enter>.

6) Usefull commands: wft: to refresh the spectrum, aph0: automatic phasing, vsadj : adjust the high of the spectrum, f: brings back the full spectrum after it was zoomed.

7) Saving files: select “save as” in the “File” menu (top left side of the window).

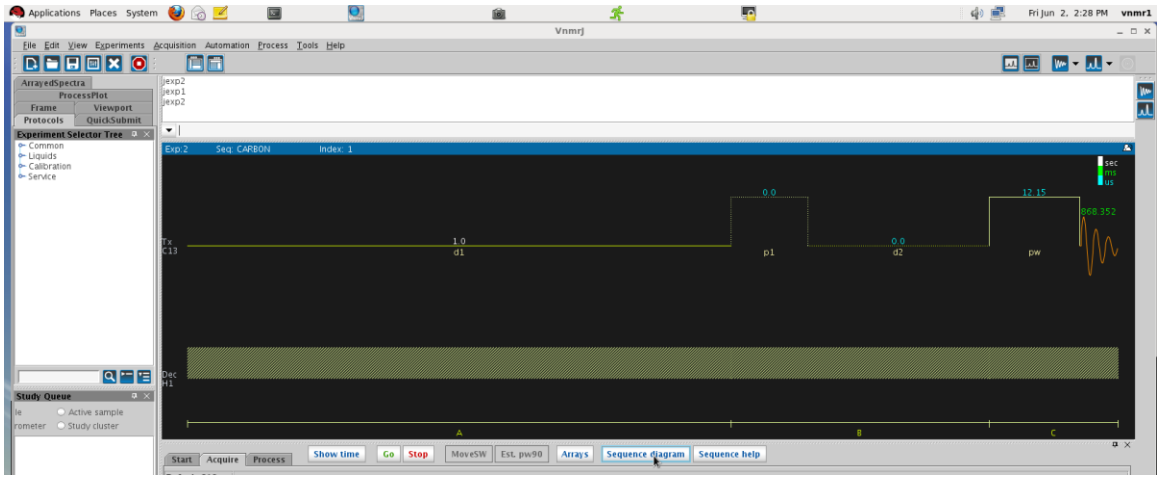
Running a carbon (^{13}C) experiment.

1) Switch to experiment 2; type “**jexp2**” on the command line and then press <enter>.

2) Select the **solvent** on tab “**Start/Sample Info**”. **Solvent must be set for each jexp.**

3) Open the file with the ^{1}H spectrum saved in the previous experiment.

4) Select the experiment “**Carbon**” from the “Experiments” menu.



5) Type “bs=8” in the command line and press <Enter>.

6) Regulate the spinning or enter “spin=0” in the command line.

7) Click on <**Go**>.

8) After the acquisition is done, save the file.

Once you are done;

1) Insert the dummy sample back in the magnet.

2) Close VNMRJ; select “Exit Vnmrj” from the menu “File”.

3) Log out from your account.

4) Log in the log book.

Retreiving data from the spectrometer computer using WinSCP

0) Open WinSCP program.

1) Click on <NEW>.

2) Fill in the window that pops up: host name: macbeth.chem.utk.edu, user name: …. , and password:…..

3) Click on <save>.

4) Click <OK> on next window.

5) When trying to connect for the first time, a window pops up. Just click on <yes>.

6) The right panel is the host computer, change the directory to vnmrsys/data.

7) Download the data.

8) Once you are done. Click on <Quit> to disconnect from the host computer.