User's quick guide for walkup operation on Varian 500 NMR

This is the first version and far from completed. Any comment and suggestion are welcome.

NMR is a very expensive instrument

Know what you are doing. Never do what you do not know how, don't even try it. Always ask if you are not sure.

Running NMR in Walkup mode is very friendly and easy. Each user in walkup mode is a NMR operator under a group account (untnmr), a NMR operator does not have his/her own computer account, but the operator has to log into vnmrj with a password in order to run the NMR.

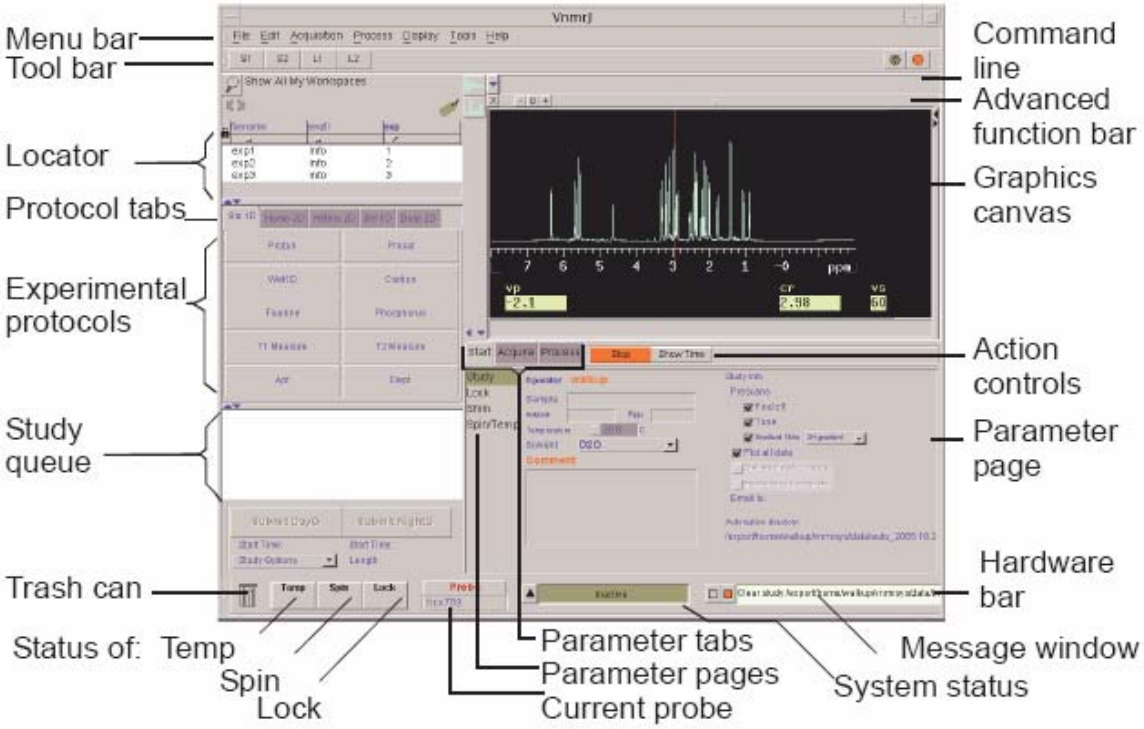
Remember, it is your responsibility to back up your data. NMR lab is not responsible for any data loss at any situation.

Log in the computer with group username and passwd.

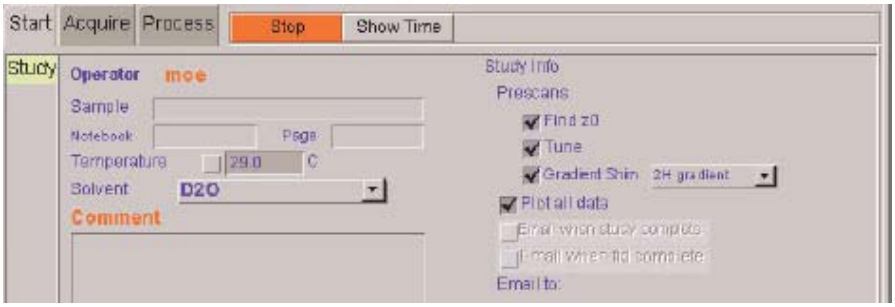
Click vnmrj icon on the top tool bar

You will see the vnmrj login window. Click "User Login" button, select your login name, enter the passwd.

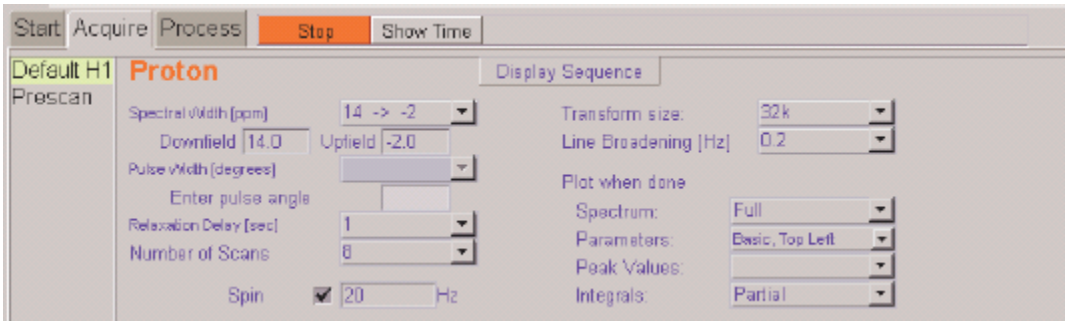
You will see the following window. Get familiar with this window with each button and its function.



1. Click **Start** tab.
2. Click **Eject** button and remove the current sample.
3. Place your sample in the spinner and adjust the position of the sample in the spinner.
4. Place the new sample on the top of the upper barrel (top of magnet). Make sure that there is air flowing up. **Never place a sample on the top of magnet without air flow up, or serious damage will occur.**
5. Click the **Insert** button. Place checks on the **Find z0, Gradient Shim** and **Tune** for auto lock auto shim and auto tuning.
6. If you want to plot the spectra, check the **Plot all data**. Type in the sample's name, select a solvent and type in the comments. If you want to control temperature, check the Temperature and type in the temperature to be regulated (**for temperature control, your need additional training**).

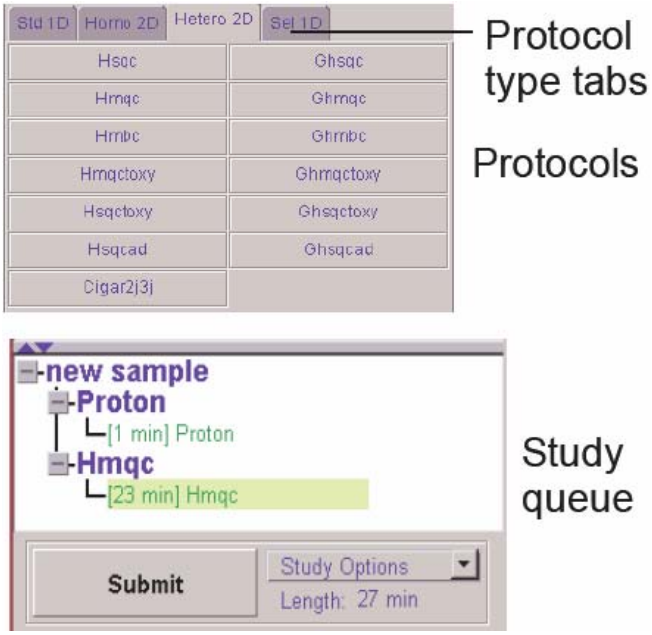


7. Click **File, New automation run**. A data directory /home/untnmr /vnmrsys/data/username_yyyy_mm_dd is created for your data. Use one automation for all your samples at this time. If you do not make new automation, your data will be stored in previous operator's automation directory.
8. Select an experimental protocol you want to run. Say, you want to run 1D proton NMR, click **Std 1D** tab, click **Proton**, the Proton protocol is loaded to Study Queue window. If you want to modify some of the acquisition parameter, such as the number of scans, spectral width, relaxation delay, you can double click the selected protocol in the study queue to load the protocol into canvas, pulse sequence is displayed. Click **Acquire**, you will the see following

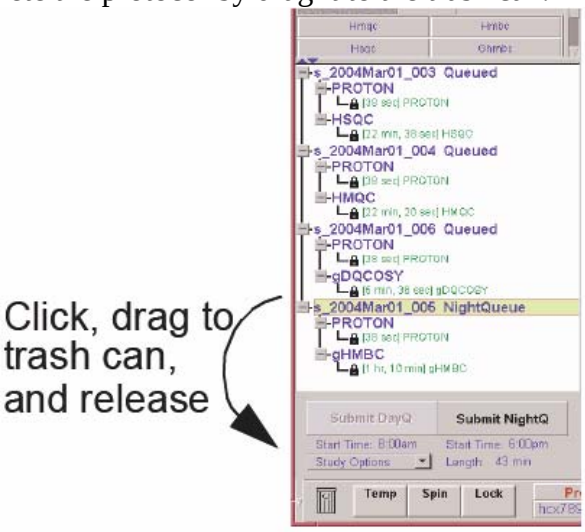


You can change any parameter you want.

9. At the left bottom you should see the current probe temperature, spin rate and lock level. If the sample does not spin but you want it to spin, click Spin/Temp button, at the **Spinner: Liquids** area, type in the rate (normally, 20) and click **Regulate Speed**. The sample should spin now. Remember that for 2D NMR, do not spin the sample.
10. If you want to run 2D HMQC experiment, click Hetero 2D tab, click **Hmqc**. The Hmqc is loaded into the study queue,



11. Select as many protocols as want you want and make adjustment on any parameters. **Always select a gradient version of the 2D protocol if it is available.** In the example above, you should select the Ghmqc protocol.
12. You may delete the protocol by drag it to the trash can.



Removing a Sample from the Study Queue

After finishing protocol selection and parameter adjustment, click "**Submit**" to start run all those experiments. At this point, all protocols are locked, no change can be made. But you can stop the run by clicking the red stop button. When all experiments are completed, all data are automatically processed, plotted and saved. Your data is in the directory

/home/untnmr/vnmrsys/data/username_yyyy_mm_dd/samplename/.

The data filenames will be **Proton.fid** and **Hmqc.fid**.

13. Take out the sample and put a standard sample into the magnet. Close the vnmrj program (you logout the vnmrj).

You may reprocess your data at the workstation when it is available.
If you want to reprocess the data, follow the instructions on the web.

File transfer:

It is your responsibility to back up your data files. NMR lab is not responsible for any data loss at any situation.

1. Download winscp 4.0 free software and install it on your window PC.
2. Run the program, type in the host name of the Varian 500 NMR computer (nmr500.ddns.unt.edu), and the groupname/password. At the Winscp window, the left side is your local directory and the right side is the remote computer directory. Change the directory to locate your sample-name directory, all your fid files for this sample are stored in this directory, drag the sample-name directory to you're a local PC directory.