Running the MR-400 in the Davidson Building

Preliminary work (to be done by TA)

- Check the autosampler, make sure the status light is green. If it is not then restart the autosampler. To restart the autosampler turn key off then on and push green start button on side of autosampler.

- In Linux you'll be using the ochem user, there is no password.

- Launch VNMRJ from the desktop icon if VNMRJ is not running yet

- At the beginning of each day start a new automation run. Automation -> Automation Run (autodir) -> New Automation Run. In the Study Queue section of VNMRJ you'll see the current automation directory listed like auto_20100913_01, this example indicates a automation folder created on 09/13/2010 and it the first one of the day.

- If in the Study Queue section of VNMRJ the Sample location is blank you'll need to assign it a location. GO to **Tools** -> **Sample in Magnet**. Type in 96 in *Assign sample location (input as integer)*. Make sure position **H6** on the autosampler has no sample in it.

Running samples

- Put your samples in the correct position, record the positions that you put your samples in. To add samples to the autosampler trays you must first unlock the autosampler doors by pressing the **Access Request** button. Once the doors are unlocked put samples in autosampler tray. Then close the doors. The door should lock and the status light will go back to green.

- Click **New Study** in the Study Queue window- enter in sample info and choose the correct solvent in the parameter window. Note you must enter a sample name. Use alphanumeric, underscore, and dash only in sample names.

- Click on the desired experiments from the Protocol panel.

- Double click on one of the added experiments in the Study Queue to load its parameters.

- Modify the experiment on the Acquire tab in the Parameter window. Typically the only thing you'd modify is the Number of Scans and the Relaxation delay. Then click green **Save** button at the top of the parameters window to save the modifications.

- If the graphics window is not displaying the autosampler tray click the small **o** in the upper left hand corner of the graphics window to switch to autosampler view.

- Select the position that has your sample. Use only the letter/number combination along the sides, for example H1 instead of 43 to indicate the position.

- Click the **Submit** button. Click the **Done** button after you see *RetrieveSample* in the status bar at the bottom center of the VNMRJ window.

Processing

- If you want to see the results from past samples of the day using the dropdown **View** box in the Study Queue and select **Spectrometer**. Note: View -> Sample does not update until you make another selection and click off of it.

- Printing is done through **Process/Plot** tab of the parameters panel.

Notes:

- Do not let students play with the underlying Linux operation system. They are to be using the VNMRJ software only.

- Warn students this is a powerful magnet; no metal objects or electronics should be brought near the magnet.

To Reset the spectrometer (if the status goes inactive)

- Exit VNMRJ
- Open a terminal
- In the terminal type **su acqproc**
- In the NMR console press the black button on the master card.
- Wait for lights on cards to start cycling
- In the terminal type **su acqproc** again and close terminal
- Relaunch vnmrj
- When you re-launch vnmrj if when you exited vnmrj the software was doing something vnmrj may launch into experiment #0. You cannot do anything in experiment #0. To see if you're in experiment #0 look while in autosampler view in the upper left hand corner and it will give you the experiment number. To change back to experiment #1 type in the command line unlock(1) then press enter then type jexp1.
- Load the shims. **Tools** -> **Locator…** -> Left-click on the magnifying glass icon and choose by **probe and shim**. Click on the **time_saved** header first then double-click **5mmATB_lk_d2o_2010-08-16**. Close the window and type **su** in the command line.