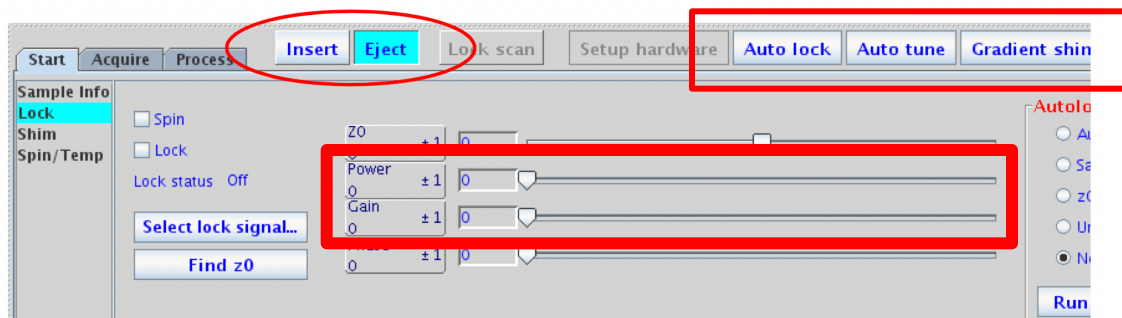# Running NMR Experiments on the CIC v400 NMR

1. Log in to VNMRJ by entering your username and password on the login screen.
2. Click the **Eject** button. Put your sample into the spinner using the sample depth gauge provided and sits next to the computer.

3. Remove the dummy sample and replace with your sample.
4. Click the **Insert** button.
5. In VNMRJ go to **Start>Shim** tab and click **Read1** or **Read2** to load a good set of shims.
6. Click the **gradient shim** button. Wait for gradient shimming to finish and notice the rms error in the message line during gradient shimming. When it is done rms error should be as close to zero as possible. Any **rms values below1 is good**. If rms error is still high (for example rms error of 6) click the **gradient shim** button again. <mark>Aim for a rms error of below 1</mark>.
7. After gradient shimming is done, in the *Start>Lock* tab, click the **find z0** or the **Auto lock** button. Wait for the sample to lock first. The sample is locked when the lock level is >20. A good lock level should be **40+**. Set the **lock power 30-35** and **lock gain to 40**.
8. Click **New Study** button (lower left corner), and in the *Start>Sample Info* tab, enter your **Sample Name**. Note: **Only use LETTERS, NUMBERS, HYPHEN AND UNDERSCORE. No PERIODS or SYMBOLS or PARANTHESIS and BRACKETS are allowed.**
9. Select the appropriate **Solvent** in the *Start>Sample Info* tab.
10. Select the experiments that you want to run from the **Experimental Panel** to the left of your VNMRJ screen and build your study queue. Double click on each experiment in the study queue to load it. In the *Acquire>Default* or *Acquire>Acquisition* tab, edit the number of scans, spectral width etc for your sample.
11. After you have customized your experiments, click the **Submit** button to run your experiments.
12. When done **eject** your sample from the magnet and replace it with a dummy sample.
13. Click the **Logout** button in the *Start>Sample Info* tab to log out of your account.

NOTE: If your peaks are broad or splitting, you can reload the shims by:
- Clicking **Read 1** or **Read 2** in the *Start>Shim* tab.
- Click the **gradient shim** button and wait till it finishes. **Make sure that the final rms error is as close to zero as possible. Repeat this step if necessary**.
- then click the **find z0** button and wait till the process is completed.
- rerun your experiment.

More…….tips

1. For 1H NMR: use **5 – 15 mg** of sample dissolved in **600-700 uL** of solvent.
2. For 13C NMR and all 2D NMR experiments use **20 mg** or more of sample dissolved in **600-700 uL** of solvent. **If you have less than 500uL of solvent the NMR won't be able to shim your sample properly resulting in broad peaks.**
3. To Optimize 2D experiments:
    a. gCOSY: use number of scans per increments >4
    b. gHMBC: use number of scans per increments >8
    c. gHMQC or gHSQC: use number of scans per increments >8
    d. NOESY: use number of scans per increments >8. For molecules of MW around 500, set mixing time to 500ms as a starting point. For weak NOEs, increase the mixing time to about 700-900ms.

Leave the number of increments as is. Also run the 2D experiments that have gradients (those with the G in front of the name) as this minimizes the T1 noise.

If you are running overnight experiments, make sure that the probe is properly tuned to proton and carbon before your start your experiments. See instructions next page on how to do this.

Note, these are just guidelines. The end result ultimately depends on sample preparations (**solvent amount**), paramagnetic components, NMR tubes and shims etc.

Making NMR time Reservations: Before you can use the NMRs you may need to reserve the instrument first.

1. Go to **http://cic.bu.edu/cgi-bin/Calcium40.pl?Op=UserLogin**
2. Click on the "NMR Reservation Calendar" link, log in to your account, and select the appropriate Calendar to reserve instrument time.
3. **Please read the reservation rules (LOCATERD ABOVE AND BELOW THE CALENDARS) for each Calendar before you make your reservations**.