

## Acquiring 1D spectra on VNMRJ using automated locking and shimming

First time you use a spectrometer you must do the following:

In VnmrJ enable the command line (View→Command line) and type **newuser** and hit enter.

Obtaining 1H/13C spectra:

1. Log in with your username and Linux password (**NOT** the scheduler password)
2. Start VnmrJ by double clicking the desktop icon
3. Click Start tab → Standard group
4. Click [Eject]
5. Remove the standard and place/position your sample in the spinner (see handout)
6. Put the spinner with the sample into the magnet
7. Click [Insert]
8. Click Experiments menu → Proton
9. Select solvent (**very important!**)
10. Enter description if desired (what you enter here will be imported by MNova)
11. Click [FindZ0]
12. Click [Gradient Autoshim]
13. Check to make sure Lock is regulated, and level is between 30 and 99. If not, go back to step 11.
14. Click Acquisition tab → Default group (or Acquire group) and set number of transients, spectral width, relaxation delay and pulse angle as desired. Use 1s relaxation delay and 45 deg pulse for standard spectra. Use 25s relaxation delay and 90 deg pulse for quantitative spectra.
15. Click the [Acquire] button
16. Click File menu → Save as...
17. Confirm that folder is */data/your\_username* (You may create and use sub-folders but keep them inside */data/your\_username*.)
18. Confirm that "File type" is ".fid"
19. If you want a 13C as well, select Experiments menu → Carbon
20. Adjust parameters in Acquisition tab → Default or Acquire group
21. Click [Acquire]
22. When done, save the data as before.
23. Click Start tab → Sample group
24. Click [Eject]
25. Put the standard back in the spinner and put the spinner back in the magnet.
26. Exit VnmrJ and log out from the computer