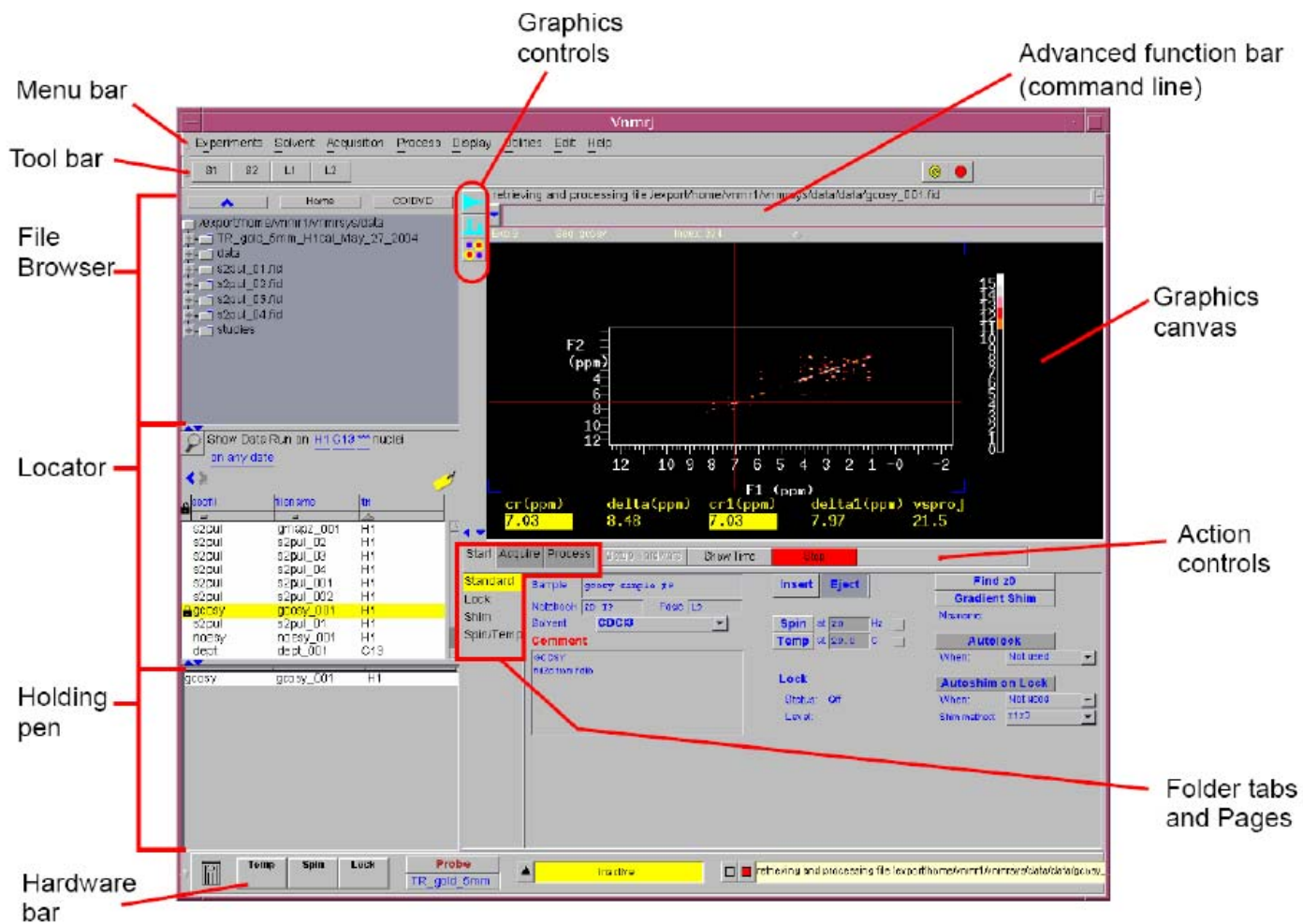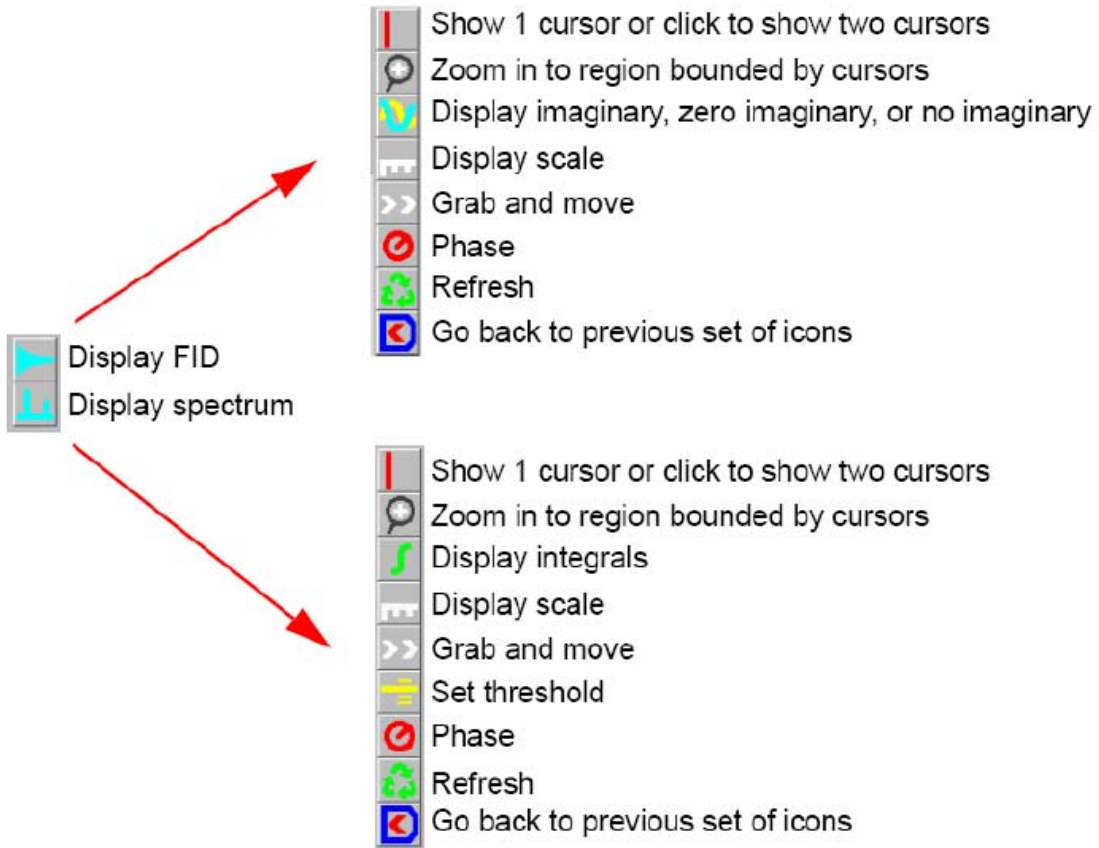# VnmrJ Manual

This brief manual can be used for running the Varian 600 MHz instrument in NMR facility.

1. Login your account, click the "**VnmrJ**" icon on the desktop to start VnmrJ.

2. Insert the spinner into the top of the sample depth Gauge and insert your NMR tube in to the spinner. Gently push your sample tube down until it touches the movable bottom of the sample depth gauge.

3. Go to "**folder tabs and pages**" (on the right side of VnmrJ interface). Click "**Eject Sample**" button, wait for a loud sound of a rushing air and then put your sample into the top of upper barrel of the magnet. Then click "**Insert Sample**" to let the sample descend into the probe.

4. Go to **Setup->Lock** subpanel, enter your sample name in the "**Name Sample"** field.

5. Go to, **Setup->Spin & Temp** sub-panel, enter the desired temperature and click "**Regulate Temperature at this Value**". The default temperature is room temperature and spin rate is zero.

6. Go to **Setup->Lock** and click "**Find Lock**" to set the lock frequency for the solvent chose. Click "**Lock Scan**" to see lock trace. If it has sinusoidal character, adjust **Z0** to make it flat. If it is necessary, adjust "**Lock power**" and "**Lock gain**" to change the lock level. Then, click "**Activate Lock**". Click "**Lock Scan**" again to remove lock display.

7. On **Setup->Lock** subpanel, adjust lock power and gain (keep them roughly equal) so display shows lock level between 80 and 95. Then click on "**Gradient Autoshim on Z**" do the automatic shim, or do it manually. Go to **Setup-> Shim**, adjust Z1 to increase lock level. If the lock level goes above 100, reduce lock gain. Continue until you can no longer increase the lock level. Switch to Z2 and do the same. Return to Z1, and repeat. Stop when no increase in lock level is observed with either Z1 or Z2. You also can adjust Z3, Z4, Z5, X or Y etc if it is necessary.

8. Type "**jexp1**" at the VnmrJ command line (at the top of the right side of VnmrJ interface). Then double click "**Proton"** in the locator protocol list (left side of interface) to load the standard proton protocol and the appropriate parameters and their values into the workspace exp1.

9. Go to **Setup->Acquisition** and **Setup->Pulse Sequence** to check the parameters. You can change **nt** (number of transients) based on your sample's concentration. Click "**Sampl**e" and enter the solvent in solvent box.

10. Click the "**Acquisition Action**" button and select "**Acquire then process**" to acquire NMR data. Or Type "**go**" or "**ga**" at the VnmrJ command line to start acquisition.

11. After acquisition, type "**wft**" or "**ft**" at the VnmrJ command line to do Fourier transform with or without a weighting function. In "**Process**" tab, you also can change weighting function. Type "**aph**" to do automatic phase correction. If spectrum is not well phased using autophase, you also can do manually phase. Click on phasing tool icon. Click left mouse button on a peak on right of spectrum. Sliding mouse while holding left or right button will adjust phase on the selected peak. This is the zero-order phase (rp). Move mouse to peaks at left of spectrum and click left button. Sliding mouse while holding left or right button will adjust phase in this region of the spectrum while leaving the initial peak as before. This is the first order phase correction (lp).

12. Place a cursor on your reference signal (TMS or solvent), type "**nl**" and press enter, then go to **Display->More** and input the reference frequency and click on "**Reference Now"** or type "**rl**" to set the reference chemical shift.

13. Go to **Display-Line list**, click the "**Set threshold**" button, you will see a horizontal cursor appear on the screen. Drag it with the left mouse button to an appropriate threshold level.

14. Go to **Display->Curors/Integration**, click "**AutoRegion**" to select integrals. For selecting integral regions manually, click on integral tool, which will spawn additional integral icons. Click "**2nd integral icon**", the left mouse button will choose integral reset points. Click left mouse button at the left end of a peak to be integrated then click the left mouse button just to the right of the peak. This defines the integral region for that peak. Do the same for all peaks or regions of interest. Type "**setint(int, value**) to normalize the integration. Int is the integral.

15. Type "**pl pscale pap ppf pir page**" to print your spectrum. Based on your requirement, you can delete any options. "**pscale**": plot scale, "**pap**": plot parameters, "**ppf**" plot peak picking, "**pir**": plot integration.

16. Type "**pwd**" to print the current working directory. Change to your own directory using "**cd('/your directory/')**" command, then type "**svf('filename')** " to save the data.

17. Click "**eject**" button, move your sample, put standard sample at the top of the magnet, then, click "**insert**" button to let the sample descend into the probe.

18. Type "**exit**" on the command line to logout VNMR, then logout your account.

VnmrJ Experimental Liquid Interface

Display FID
Display spectrum

Show 1 cursor or click to show two cursors
Zoom in to region bounded by cursors
Display imaginary, zero imaginary, or no imaginary
Display scale
Grab and move
Phase
Refresh
Go back to previous set of icons

Show 1 cursor or click to show two cursors
Zoom in to region bounded by cursors
Display integrals
Display scale
Grab and move
Set threshold
Phase
Refresh
Go back to previous set of icons

Graphics Control icons