NMR Training VNMRJ 4.2A/VNMRS 400

The VNMRS/new 400 MHz NMR uses VNMRJ 4.2A. Although VNMRJ is different than VNMR-almost ALL typed commands that you know from VNMR should work.

LOGIN:
Your username is the same, you can set your password the same as well.

OPEN VNMR:
Double Click on this icon which should be on the side of the screen:

The program VNMRJ will open. If you do not see the icon for some reason, open Unix terminal-right mouse button, Open Terminal; then type:
vnmrj

Insert Sample
Type:
e
then
i
as on all other instruments

The Insert/Eject buttons are located in the menu buttons just below the spectrum in the middle of the screen.

If you do not see where to type commands in VNMRJ, it is in the upper middle, above the spectrum; if there is no command line visible, drag spectrum window down.

Lock your sample:
You can use Auto Lock button in the middle of the screen below the spectrum. This usually works.

The manual Lock is accessed through Start menu in lower center of the screen, then Lock menu on the left side of the lower panel. You can change Z0 to values in table on computer [right mouse button is increasing Z0, left button decreases, middle button changes the units that right and left change Z0 by]. You can also use scroll bar or type the number followed by <return>.

Note that Z0 changes at a rate of ~2 units/day on the VNMRS 400.

To find correct Z0, as on other instruments, turn Lock Off, click off the check mark on the Lock button. To see Lock Sweep, click on button that says Lock Scan, located in the middle of the window adjacent to the Eject/Insert buttons. Maximize the intensity (height) of the red sweep, ignore the blue sweep (blue is correlated to Lock Phase, but does not work well on this type of instrument). When you have reached maximum, click on the Lock box to turn in on.

Set Lock Power/Gain/Phase appropriately.

Spinning of sample:
Spinning at 20 Hz is normal in standard 1D experiments. When the spin is blue, that means it is regulating, red means it is not regulating and yellow means that the spin is turned off.

Control of the spin can be done in Spin/Temp menu under the Start menu (also spin can be turned on and off in Shim and Lock menu).

Shim sample:
Manual Shimming:
Click on Shim menu button under Start menu in lower center of screen.

Shim as on other systems, right mouse button increases shim, left decreases, center button changes the units to increase or decrease by.

The shims X1, Y1, XZ, YZ, XY, X2Y2, X3 and Y3 should not normally need to be adjusted, and if you do adjust them, the Spin must be turned off.

Gradient Autoshimming:
As on other instruments type:
gmapsys

Under Acquire Menu in lower middle of screen (next to Start menu), click on Gradient Shim menu.

Set nt and d1 appropriately for your solvent; see table posted on computer.

Then, click on large button that says Gradient Autoshim on Z (right side of screen).

You will likely need to turn the spin back on under Spin/Temp menu after gradient shimming. It is possible that you will need to reset the Lock parameters- Z0, Lock Power, Lock Gain as well.

Alternatively you could click on Gradient Shim button adjacent to Auto Lock.

Setup parameters for acquisition:
Click on button for Proton, Carbon, etc. on menu labeled Experiments in top left corner of screen or double on Proton in Experiment Selector to the left of the spectrum. Under Start menu below the spectrum, choose the side menu Sample Info, then select the appropriate Solvent. [or simply type solvent = 'cdcl3' etc.]

To change any acquisition parameter, type in the parameter name and the appropriate value as on other instruments.

To view the parameters in the experiment, click on the Process menu button below the spectrum, then the side menu button, Text Output and the button Basic on the right of the lower screen.

Acquire Data
Type:
go
(or ga)
as on other instruments

Process data:
Type:

wft f aph

(as on other instruments; all typed commands should work as they do on other instruments)

Zoom and Full spectrum.
The icon for Cursor mode (one cursor) is:

The icon for Box mode (two cursors) is:

To zoom, use Box as on other instruments and click on icon for zoom:

To get back to full spectrum, either type f or click on full icon:

Manual Phasing:
To start manual phasing click this icon, which should be to the right of the spectrum:

The mouse controls work as on other instruments- the right mouse button is coarse adjust, the left is fine adjust and the middle is vertical scale; the first click adjusts right phase only (rp) which is the frequency independent phase correct, the second click changes both rp and the left phase correct (lp), which is the frequency dependent phase correct.

Display Scale
Type:

dscale

or click on this icon:

Integration:

Integration is done in the same way as on other instruments with the following icons:

For lvl/tlt (level and tilt), the icon is:

For Part Integral, the icon is:

For Full Integral, the icon is:

For No Integral, the icon is:

For Resets, the icon is:

To reference an integral it is accessed under the menu button Process which is just below where the spectrum is. Then, under the Process menu choose the menu on the side labeled Integration. Put the cursor on the integral that you want to reference, type the number of protons that you want to reference that integral to in the box labeled Integral Area (lower right of screen), and click on the button that says Set Integral Value.

Reference the spectrum:

Pick a peak with cursor and the command for nearest line:
nl
then type:
rl(7.00p)
for 7.00 ppm, or
rl(0p)
for 0 ppm …

To reference the spectrum through menu buttons. The button is accessed through the Process menu (as with set integral), then, Display on the side menu, then put the cursor where you want to references either manually or with nl (nearest line) command or the Nearest Line button, type the value to reference to in space below Reference cursor to, and be sure that the choice selected next to the value is in ppm.

Peak Picking:

The Threshold is accessed through this icon:

Move threshold line as on other instruments, to display line list, use the commands dll or dpf, to print use pll pr ppf.

PRINT:

Printing can be done with same commands as on other instruments,
pl pscale pir ppf pltext ppf page
or
plot

SAVE FILE:
Type svf('filename') as on other instruments.

Other useful icons in 1D spectra:
Interactive menu button used to get back to normal menus is:

To return to the previous menu:

To return to full ppm and full screen:

When you are finished, reinsert standard CDCl3 sample, exit out of software by
typing exit, then logout by choosing Log Out under System menu in top left of
screen or Quit under your login name in top right of screen.
Then click on Log Out button
Do not choose Switch User.

If someone else is still logged in, then you can choose Switch User to login, but
please note this in logbook.

2D NMR

All 2D commands should work as on other instruments. Below are meanings of the icons that you will see.

One cursor:

Two Cursors (Box):

Contour Plot:

Stacked Plot (not useful)

Switch axes (F2 with F1):

Decrease Vertical Scale Displayed:

Increase Vertical Scale Displayed:

2D Phase Menu:

Phase x-axis:

Show Trace with Cursor:

Show 2D Vertical and Horizontal Projections:

Show 2D Vertical Projections:

Show 2D Horizontal Projections:

Peak Pick Menu:

Find Peaks and Measure Volumes:

Measure Peak Volumes:

Find Peaks