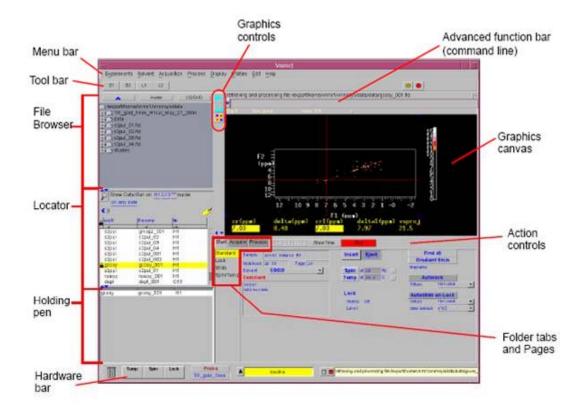# NMR VNMRJ Training Sheet (*ver 1.1.2*)

**Note: Many of the commands used in the old software should work on the new version. (e = eject; i = insert, etc.)

Recommendation: Before you log in click **sessions** at the bottom right of the screen and select **KDE**. The KDE mode is more user friendly than GNOME.
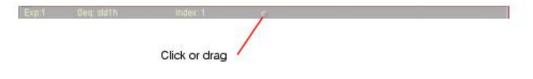
Log In

Double Click on VNMRJ icon

VnmrJ Experimental Liquids Interface

Command Line:

To display the keyboard entry line click on the button on the "Advanced function bar". Or drag the button to display the keyboard entry line and a few lines of the message window. Clicking on the arrow of the keyboard entry line displays a command history.

<u>Setting Experiment:</u>
Choose your desired experiment under **Experiments** in the menu bar (Proton, Carbon, etc…). This will load the standard parameters. Alternatively, double click on the desired experiment in the **locator** window (see picture above).

Everything else will be done using the command line or the options in the **Folder tabs and Pages section.

<u>Sample Insertion:</u>
Click on the **Start** tab then click **Standard**
To insert or eject click on the corresponding (insert/eject) button
*(or type **e** or **i** in the command line)

While on the **Start** tab/**Standard** page you can also:
1. Choose appropriate solvent from pull-down solvent menu
2. Set spin by typing number then clicking **spin** button (i.e. 20 hz)
3. **Optional- Change sample name/ notebook number/ comment to your desired text

<u>To Lock:</u>
Under the **Start** tab/**Lock** page
Click the Lock Scan button to bring up visual lock signal
Find Lock by using Z0 / Lock Power, Lock Gain
Click the ON button to turn lock on
(To change Z0 value click the Z0 button: the left mouse button subtracts the increment, the right mouse button adds the increment, and the middle mouse button (clicking the wheel) will change the increment value.)

<u>To Shim:</u>
Under the **Start** tab/**Shim** page
You should see a dial (like a clock face) representing the current lock level. The circular dial has replaced the horizontal bar system used in the previous software. Using the mouse buttons adjust the appropriate shims (i.e. Z1, Z2, Z1C, Z2C (Z3 on Inova500) to increase the lock level.
***(Left button = subtract; Right button = add; Middle button = change increment)
***Note: on left side of the shim panel you have the buttons to adjust Lock Power / Lock Gain (ie. If the shim value goes off-scale)

<u>Acquisition:</u>
In the **Acquire** tab/**Default H1** page you will see the basic parameters which you can adjust as needed.

To start the acquisition type **ga** <Return> in the command line.

After you have acquired your spectrum type **f aph vsadj** <return> in the command line
f = full spectrum, **aph** = auto phase, **vsadj** = vertical scale adjust
This will display the spectrum in the graphics canvas
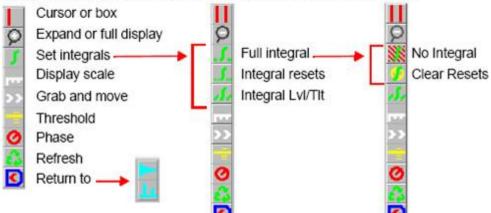
To Save File:
Type either **svf('filename')** <return> or type **svf** <return> and you will be prompted for a filename

Phasing, integrating, threshold, dscale, cursor/box mode, expand:
These operations work the same as they did in the old software. In the new software the operations are represented by icons to the left of the graphics canvas.

To the left of the display is the spectral display graphics control buttons (note that the labels change on some of the buttons according to the mode the program is in):

Chemical shift referencing:
Under the **Process** tab / **Default** page, or **Display** page
Put cursor on solvent / reference peak (type **nl** <return> in command line)
Under Reference / Underthe **Set cursor to** button highligt the current value / type new value for peak / hit <return>

Reference Integrals:
Under the **Process** tab / **Default** page, or "**Cursors/Integration**" page
Put cursor on desired reference integral
Default page: Under Integration / To the right of **Set norm to** type desired integral value then click **Set Norm to** button
or **Cursors/Integration** page: Under Integration / To the right of **Normalization Value** type desired integral value, then click **Set Integral Value** button

Printing:
The plotting commands will work on this version of the software in the command line (for example **pl pir pscale ppf page** <return>)

Loading files on workstation:
Click **home** in the **file browser** window. The spectrometers are seen as folders Mercury.300, Inova.400 and Inova.500. Double click on the spectrometer folder to list the spectra collected on that instrument. The spectra folders have an fid extension. Double click on the spectrum folder and your spectrum will be loaded in the graphics canvas.