# Quick Guide for Taking NMR Spectra with VnmrJ

1) Login using your IU username and passphrase (when you do this the standard shims will automatically be loaded). Wait until "**Idle**" appears in the status window.
2) Click "**Start**" tab then click on "**Standard**" page if you're not already on this page.
3) Click "**Eject**" button (or type "**e**" in command line) to eject the standard sample, replace it with your sample then click "**Insert**" (or type "**i**") to insert the sample.
4) Click on "**Experiments**" in the menu bar, then click on whatever **nucleus** you want to run.
5) Click and select a **solvent** on the "**Standard**" page.
6) Click "**Setlock**" button (or type "**iusetlk**") to load optimum lock parameters.
7) If the sample is spinning, turn it OFF by clicking "**Spin off**" button on the "**Spin/Temp**" page.
8) Click "**Gradient Autoshim**" button on the "**Standard**" page. You should see "Gradient autoshimming on Z done!" in the message window in 30-45 seconds.
9) If you prefer to run experiments with sample spinning (it's not necessary), you could turn ON sample spinning now: on the "**Spin/Temp**" page, enter **18** in the spin rate box , then click the "**Regulate speed**" button.
10) Click "**Autolock**" to activate lock. You should see "**LOCK: Regulated**" displayed in "**Sample Status**" section in 10 seconds. If not, do the followings:
    a. Click on "**Lock**" page.
    b. Click **Lock** "**Off**" button to turn lock off.
    c. Click "**Lock Scan**" button to display lock signal.
    d. Adjust Z0 until lock signal is on resonance. You might need to adjust **lock power** and **gain** to get a better lock signal.
    e. Click **Lock** "**On**" button to activate lock.
    f. If lock still cannot be established, something is not quite right. It could be that your sample is very concentrated, very low volume, poorly positioned in the spinner, or a non-deuterated solvent is used.
11) If for some reason "**Gradient Autoshimming**" doesn't work at step 8), you need to do manual shimming:
    a. Click on "**Shim**" page.
    b. Adjust "**Z1C**" and "**Z2C**" (or "**Z1**" and "**Z2**") by clicking the left (-) and right (+) mouse button on them to get the highest lock level.
    c. You may have to decrease **lock gain** if your lock level goes above 100%. After you are finished shimming, adjust the **lock gain** to obtain an 50-80% lock level.
12) Click "**Acquire**" tab.
    a. If you need to change number of scans and/or spectral width, go to the "**Acquisition**" page and enter your numbers there.
    b. Click "**Acquire**" button (or type "**au**") to start acquisition. With default parameters, it will automatically set the receiver gain, acquire the spectrum, and perform fully automatic data processing after acquisition as described in 13a). If you're satisfied with the auto-processed spectrum, you may jump to 18) to make a plot.
    Alternatively, you may start acquisition by typing "**ga**", if you don't want the automatic data processing.
    c. During acquisition, you may see your spectrum after each "**bs**" number of scans. Type "**process**" or "**wft**" in command line.
    d. You may click "**Stop**" button (or type "**aa**" in command line) at any time to stop acquisition.
13) Click "**Process**" tab.
    a. Click "**Autoprocess**" button to automatically process your spectrum. This includes applying weighting function, doing FT ("**wft**"), autophase ("**aph**"), auto-reference ("**setref**"), auto-integration ("**integrate**"), autoscale ("**f**", "**vsadj**"), auto-peakpicking, etc. up to a point where the spectrum could be plotted.
    b. If autophase doesn't work well, you can manually phase it by clicking the graphic "phase" icon.
    c. You may need to click "**Display Spectrum**" button (or type "**ds**") to switch to interactive mode, so that you can use the mouse to interactively adjust spectral display (e.g. expand the spectral region between the two cursors, adjust vertical scale by dragging the spectrum with the middle mouse button, etc.).
14) To set your reference:
    a. You may expand your spectrum about the reference peak by clicking the left mouse button at the left edge and the right button at the right edge and click graphic "zoom in" icon.
    b. Click on "**Display**" page.

c. Mark the reference peak by clicking the left button.
d. Click "**Nearest Line**" button (or type "**nl**") to get the exact peak.
e. Enter the chemical shift value of the reference peak in the "**Reference cursor to**" field (7.24 for chloroform or other value for different solvent) and select "**ppm**" next to it, then click "**By Cursor**" button. Alternatively, you may type "**rl (7.24p)**" in command line.

15) To do a baseline correction, type "**abc**" in command line.
16) To integrate, click on "**Integration**" page.
    a. Click "**Clear Integrals**" button (or type "**cz**").
    b. Under "**Integral Display Mode**" click "**Partial**".
    c. Click "**Interactive Resets**" button.
    d. Chop your integral into pieces by clicking of your left button and erasing mistakes with right one.
    e. Click "**Scale display to fit**" button, then move cursor to the reference integral.
    f. Under "**Normalize Area to**" click "**Single Peak**".
    g. Enter "**Integral Area**" value (e.g. 3 for a CH3 peak), then click "**Set Integral Value**" button.
    h. Click "**Show Integral Values**" button to display normalized integrals under spectrum.
17) To pick peaks, on "**Default**" or "**Display**" page click "**Peak Threshold**" button followed by dragging of your left button on the popup yellow line, then click "**Find Peaks**" button.
18) To plot:
    a. Click on "**Basic**" page. Enter comments in "**Comments:**" field (or type "**text('Here is my comments')**").
    b. Click on "**Plot**" page.
    c. Select:
        - "**Basic (left)**" under "**Parameters**";
        - "**Scaled, Horiz**" under "**Integrals**";
        - "**On peaks, Var, ppm**" under "**Peak Frequencies**"
    d. Click "**Automatic Plot Page**" button to plot.
    e. You may also do manual plot: on "**Plot**" page, click to select whatever you want to plot, then click "**Plot Page**" button at end.
19) To save your FID and parameters, in the menu bar:
    a. Click on "**File**" then "**Save as…**"
    b. Enter filename such as "**jxh_C13_11-06-2003**" then click "**Save**".
    Note: file names should only use alphanumeric characters, underscores, and hyphens. The following characters are reserved in Linux/Unix therefore should never be used: / > < \ | : & ? * and space.
20) To load your spectrum back later, click on "**File**" then "**Open…**".
21) Make sure sample spinning is OFF – click "**Spin off**" button on the "**Spin/Temp**" page.
22) Please be sure to put back the standard sample before you log out.
23) Click on "**File**" then "**Exit VnmrJ and Logout**" (or type "**iuexit**") to log out.

**Other things you may want to know:**

To reset shims:

Click "**Getshim**" button on "**Stardard**" page under "**Start**" tab (or type "**getshim**").

To reset the spectrometer:

If the system does not respond to your actions, click "**Reset Console**" button on the "**Stardard**" page (or type "**reset**").