

1D NMR VnmrJ Quick Guide

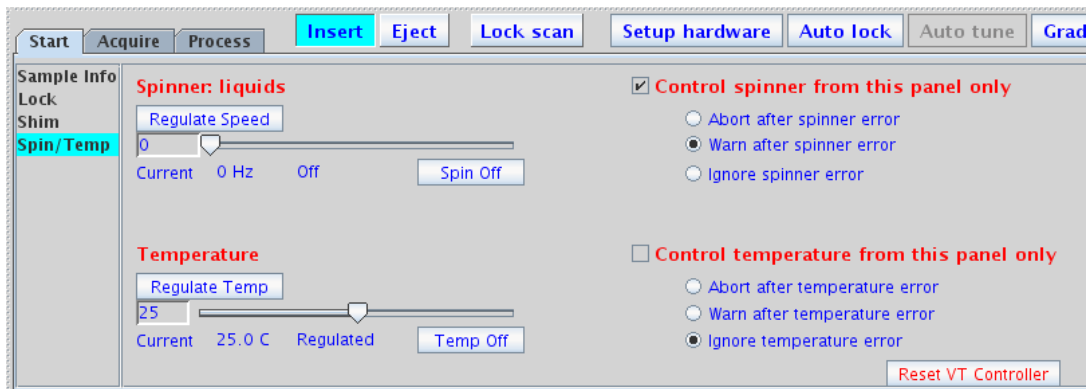
Rosha Teymoori

1) Getting started

- Log on using your Username and Password.
- Click on the VnmrJ Desktop Icon.
- Type *e* <Ent>. Place sample in spinner. Gauge properly. Place on top of magnet. Type *i* <Ent>.
- Click **Experiments**=>**Proton** (or desired expt.) type *su* <Ent>.
- In the bottom Parameter Panel, select the **Start** tab and the **Standard or sample info** page.

The screenshot shows the VnmrJ software interface. At the top, there are several tabs: 'Start', 'Acquire', 'Process', 'Insert', 'Eject', 'Lock scan', 'Setup hardware', 'Auto lock', and 'Auto'. The 'Start' tab is selected. On the left side, there is a vertical menu with 'Sample Info', 'Lock', 'Shim', and 'Spin/Temp'. 'Sample Info' is selected. The main area displays 'Operator: vnmr1' and 'Sample information' in red. Below this, there are input fields for 'Sample name', 'Sample directory' (with a dropdown menu showing '_20150731_01'), 'Solvent' (with a dropdown menu showing 'DMSO', 'CDCl3', 'D2O', and 'Other'), 'Concentration' (with a value of '0' and 'mM'), 'Notebook', and 'Page'. There is also an 'Email' field and a 'Comments' field containing the text 'STANDARD FLUORINE PARAMETERS'. A 'Clear' button is located next to the 'Sample name' field.

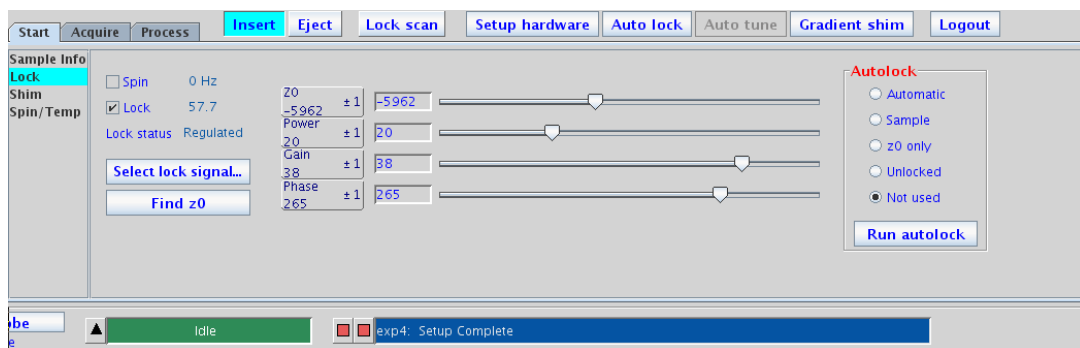
- Choose your solvent from the **Solvent** dropdown menu.
- Add your text to the **Comment** field.
- Check spinning. If you want to spin the sample. Go to start menu, left side Spin/Temp section to regulate spinning speed



- Set up the temperature if you are planning to run an experiment at higher temp (max Temp = 65C)

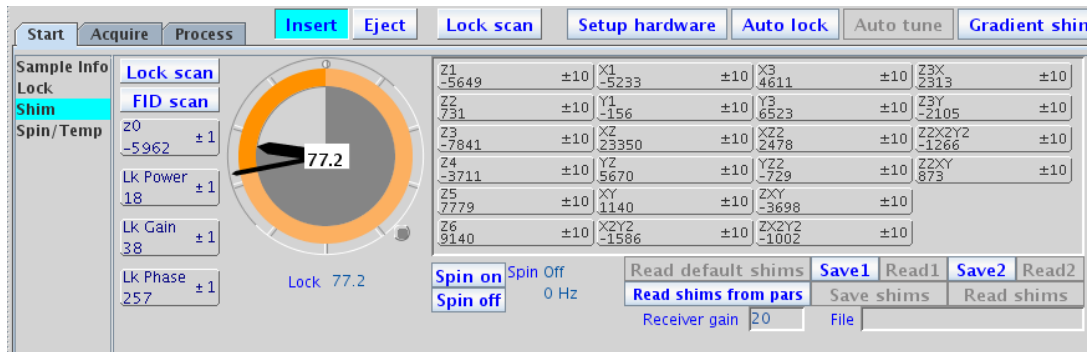
2) Lock

- Type **Lock**
- Wait for the message Idle in the message box at the bottom of the panel



3) Shimming

- Go to start shim
- Adjust Z1, and Z2 until the lock signal is max



4) Tuning

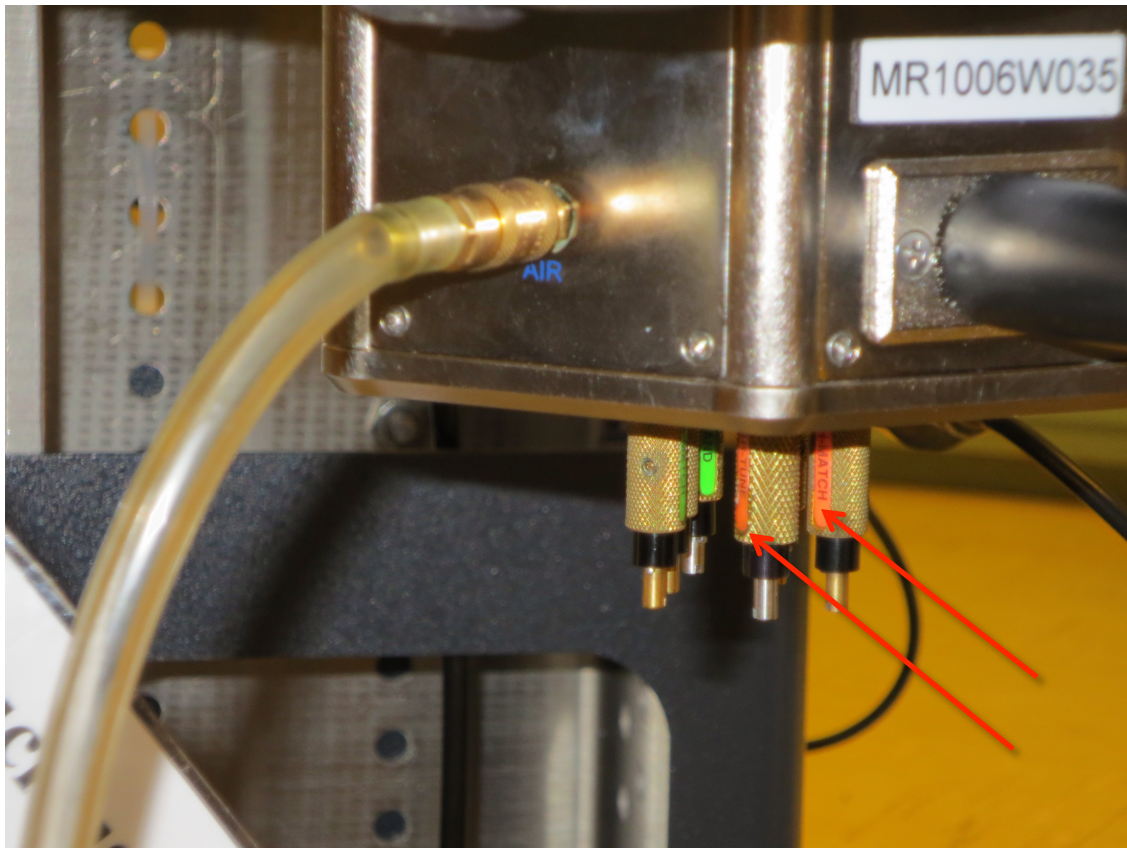
- Type *su* <Ent> tune via the pre amp, press the chan bottom



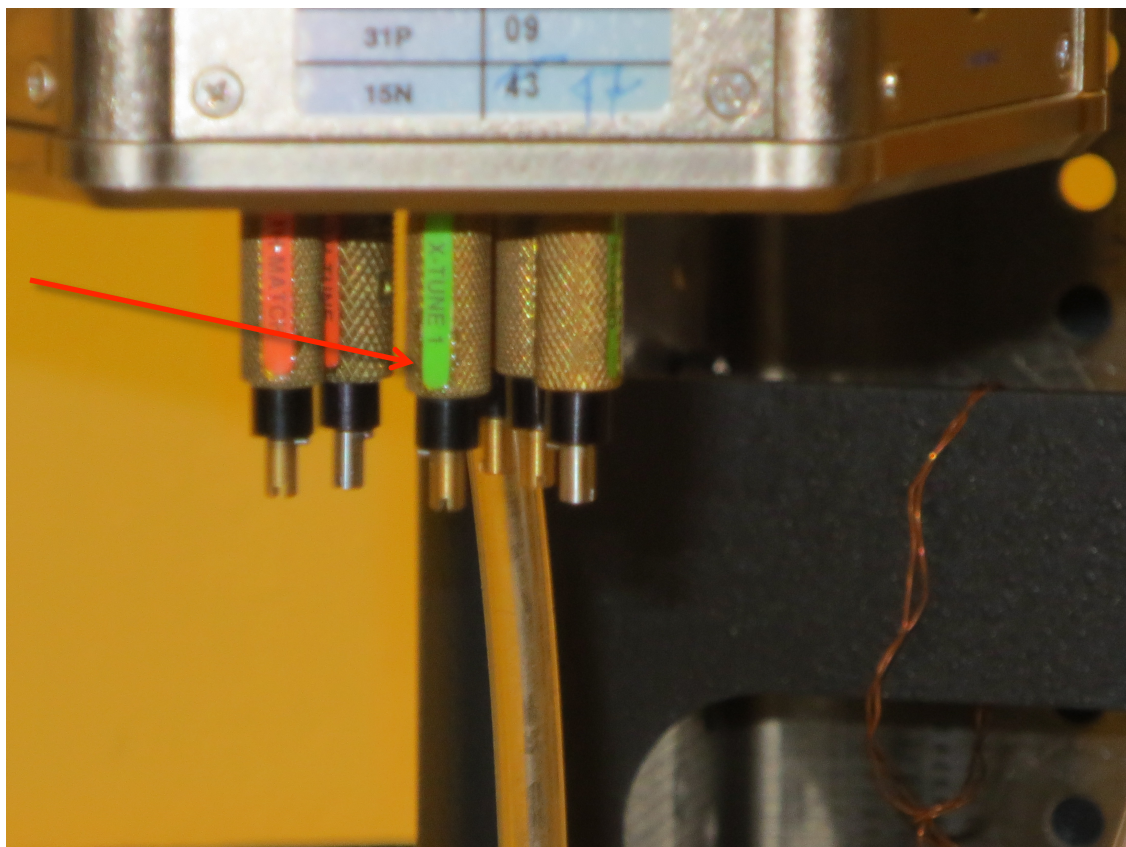
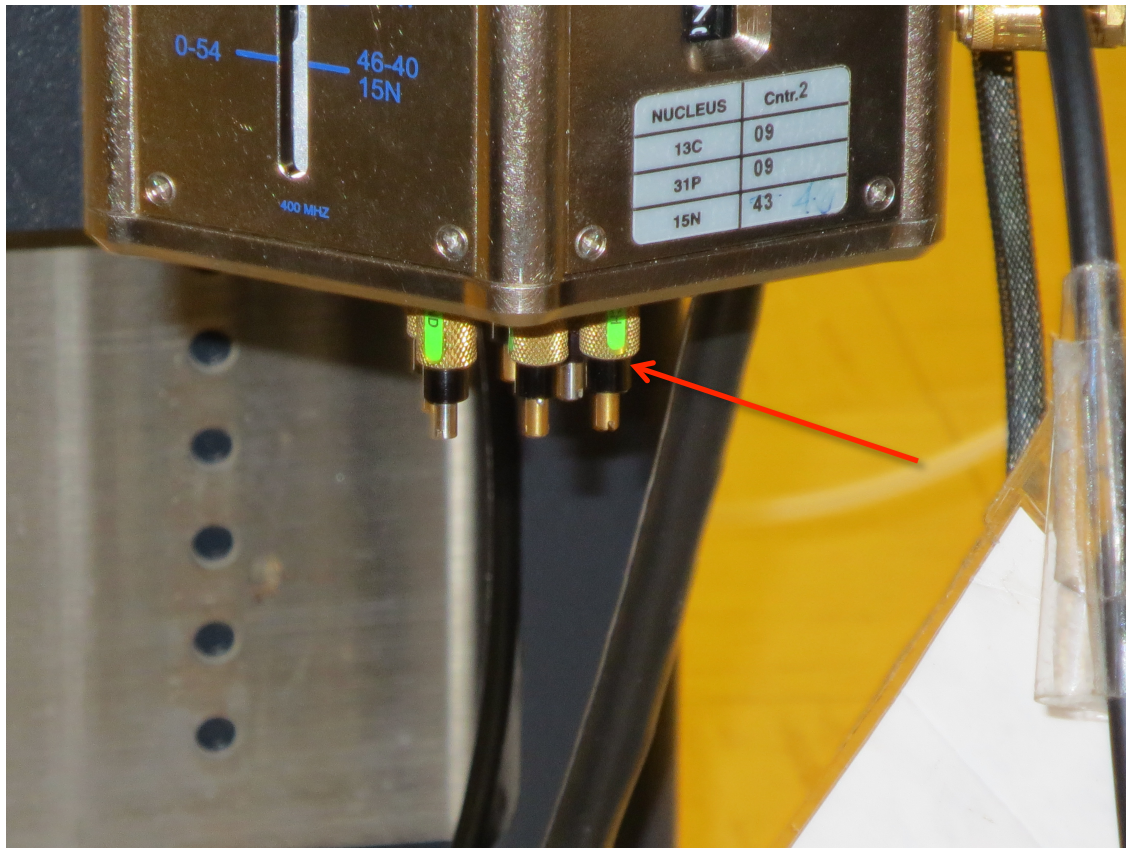
- Take the probe cable from pre amp (right side) and attach it to probe in ‘tune interface’



- channel 1 is proton, the matching and tuning rod has an orange labeling, tune and match until you see small number like 001 which is shown in the above picture.

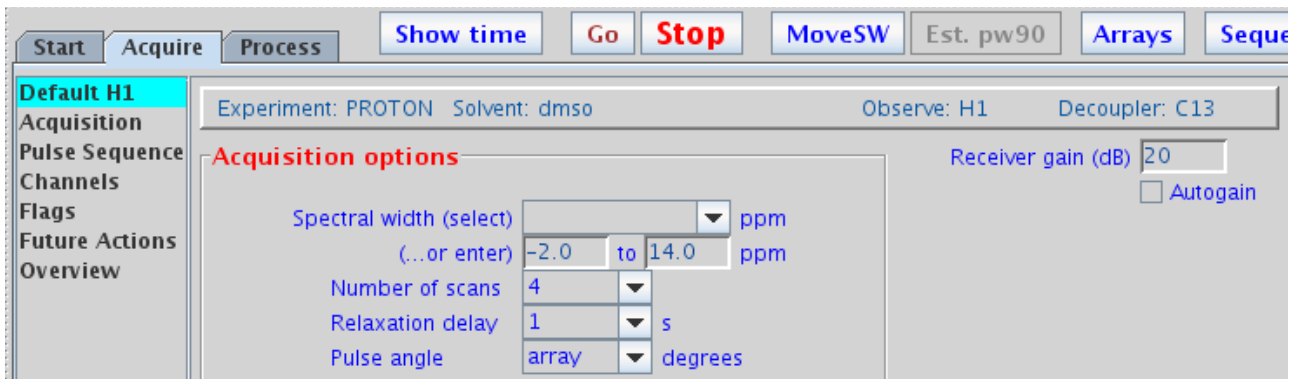


- For ^{13}C acquisition, channel 1 is ^{13}C and channel 2 is ^1H , ^{13}C rods are green. Turn match 4 and tune 1 rods



5) Acquiring your spectrum

- Select the **acquire** tab and the **default** page



- Chose your parameters, or type
- *nt* (number of scan) = desired number
- *dl* (delay between scans) = desired number
- *bs* (block size) = desired number
- Type *ga* or *go* or click on GO bottom
- Message :BS# completed
- Type *wft* to process
- When complete *f full aph vsadj* <Ent>

6) Referencing your spectrum:

- locate your solvent peak
- Click the **Cursor** icon and place red cursor line on top of solvent peak.
- Type *nl rl(<your solvent ppm>p)* <Ent>. For example, for CDCl₃ you would type *nl rl(7.24p)* <Ent>.

7) Integrating your spectrum (not for ¹³C NMR)

- Click the **Full spectrum** icon and click the **Integral** icon
- Type *cdc dc cz* <Ent>
- Expand around first desired integral region.
- Click **Resets** icon (it has scissors).
- Use a *left* mouse click for each integral reset point. If you make a mistake, use the *right* mouse button to undo last reset point. To restart, type *cz* <Ent>.
- Click the **Hand** icon and drag the spectrum to next region, click **Resets** icon, left click your next points, repeat for every region.
- When complete, click **Full spectrum** icon.

8) Plotting your spectra

- Typical example, *pl pscale ppf pir pltext page* <Ent>
- Type *ds* <Ent>, expand desired plot regions, and repeat plot command

Common Plotting Commands:

<i>pl</i>	plot spectrum
<i>pscale</i>	plot scale
<i>pir</i>	plot integral regions
<i>ppf</i>	plot peak frequencies
<i>pll</i>	plot line list with freqs in Hertz
<i>pltext</i>	plot text
<i>pltext(150,150)</i> parameters	plot text in top right (<i>use with pll</i>) <i>pap</i> plot all
<i>page</i>	send plot to printer

Icon Guide:



Full Spectrum



Magnifying Glass (Zoom)



Hand Icon (Pan & Scan)



Integral Resets



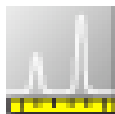
Cursor



Phasing



Threshold



Display Scale

VNMR Basic Commands

<i>Command</i>	<i>Description</i>	<i>Typed Example</i>
nt	number of transients: Sets the number of transients (scans) to be acquired. You should always select a multiple of 4 (e.g. 4, 8, 128). The larger the number of scans, the better the signal to noise.	<i>nt=16</i> : default setting for 1H,CDCI3
bs	block size: Directs the acquisition computer, as data are acquired, to periodically store a block of data on the disk.	<i>bs=8</i> : sets the block size to 8 scans.
ga	submit experiment to acquisition and FT the result: Performs the experiment described by the current acquisition parameters and Fourier transforms (<i>wft</i>) the result.	<i>ga</i>
wft	weight and Fourier transform 1D data: Performs a Fourier transform on one or more 1D FIDs with weighting applied to the FID.	<i>wft</i> : used if you stop the acquisition prior to completion or when loading a saved FID.
aph	automatic phase of rp and lp: Automatically calculates the phase parameters lp and rp required to produce an absorption mode spectrum and applies them to the current spectrum.	<i>aph</i> usually gives well phased spectra
f, full	full: Sets the horizontal and vertical control parameters to produce a display on the entire screen.	<i>f</i> or <i>full</i>
vsadj	Automatic vertical adjustment: Automatically sets the vertical scale, vs, in the absolute intensity mode so that the largest peak is at the requested height.	<i>Vsadj</i> : resets the vertical scale to fit on the screen
dscale	Display scale below spectrum or FID.	<i>dscale</i>
aa	abort acquisition: immediately aborts the acquisition.	<i>aa</i>
sa	stop acquisition: stops acquisition after acquiring current transient.	<i>sa</i>
su	submit a setup experiment to acquisition: Sets up the system hardware to match the current parameters but does not initiate data acquisition.	<i>su</i>
svf	Save FIDs in current experiment: Saves parameters, text, and FID data in the current experiment to a file.	<i>svf('H1_070703')</i> : saves the FID as a file named H1_070703