NEW SOFTWARE: Use on Isis, Ra, and Anubis

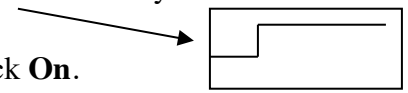
1D NMR VnmrJ Quick Guide

1 Getting Started:

- Log on using your Username and Password.
- Click on the VnmrJ Desktop Icon.
- Type *e* <rtn>. Place sample in spinner. Gauge properly. Place on top of magnet. Type *i* <rtn>.
- Click **Experiments**=>**Proton** (*or desired expt.*).
- Type *fixshims* <rtn>. Wait for beep.
- In the bottom Parameter Panel, select the **Start** tab and the **Standard** page.
- Choose your solvent from the **Solvent** dropdown menu.
- Add your text to the **Comment** field.

2 Establishing Lock and Shimming:

- Select the **Lock** page and click Lock **Off**.
- Click **Lock Scan** to display lock trace.
- Move **Power** and **Gain** slider until you see a lock signal. ***NOTE***:(The slider can be dragged or you can click on the button with the right mouse to increase or left mouse to decrease.)
- Move **Z0** slider slowly until no 'beat' is visible.



- Click Lock **On**.
- Reduce **Power** until correct value: D_2O, acetone=5-10; C_6D_6 =10-15; $CDCl_3$ =20-32.
- Adjust **Phase** in units of ±10 to maximize height of lock level.
- Select the **Shim** page.

3 Shimming (*continued*):

Tip: Right or left click the Z shim buttons to adjust shims. Middle mouse click to change the scale (i.e. from ±1 to ±10 to ±100).

- Adjust **Z1** ±100 until maximum. Repeat with **Z2**.
- Adjust **Z1** ± 10 until maximum. Repeat with **Z2**.
- Type *nt=1 ga* <rtn>. (Use with ^1H spectra only.)
- When complete, type *f full aph* <rtn>, expand around solvent peak or suitable well-resolved singlet. Type *vsadj* <rtn>.
- If not shimmed, adjust **Phase** and readjust appropriate shim (e.g. **Z1** for symmetric broadening or **Z2** for asymmetric peak shape).
- Repeat single scan acquisition. Reshim, if necessary.

4 Acquiring Your Spectrum:

- Select the **Acquire** Tab and the **Default** page.
- Choose your spectral window, relaxation delay, and number of scans from the appropriate dropdown menus. ***Tip***: If you want accurate integration, increase Relaxation Delay to 10 or more.
- For **^{13}C**, use *nt=1e6 bs=8*.
- Click on the green **Acquire & Transform** button.
- For ^{13}C, after a few data blocks are complete (message: BS # completed), type *wft* to process. When sufficient S/N is obtained, stop with *sa('bs')*.
- When complete, type *f full aph vsadj* <rtn>.

Manual Phasing (*Optional*):

- If autophasing did not work, type *lp=0 rp=0* <rtn>.
- Click on **Phasing** button to the right of the spectrum. Using the ***left*** mouse button, click and hold on the ***Rightmost*** peak. Drag the mouse up or down to phase that peak.
- Using the ***right*** mouse button, click and hold on the ***Leftmost*** peak. Drag the mouse up or down to phase.

5 Referencing Your Spectrum:

- Type *dscale* <rtn> and locate your solvent peak (use the reference chart below or one near the instrument).
- Click on the **Magnifying Glass** icon to the right of the spectrum.

Note: It does ***not*** have the **+** symbol next to it.

- Click the **Cursor** icon and place red cursor line on top of solvent peak.
- Type *nl rl(<your solvent ppm>p)* <rtn>. For example, for $CDCl_3$ you would *type nl rl(7.24p) <rtn>*.

Common Deuterated Solvents:

$CDCl_3$	**7.24p(^{1}H) 77p(^{13}C)**	**D_2O**	**4.63p(^{1}H)**
Acetone-d_6	**2.04p(^{1}H) 29.8p(^{13}C)**	**CD_3OD**	**3.30p(^{1}H) 49.0p(^{13}C)**
Benzene-d_6	**7.15p(^{1}H) 128.0p(^{13}C)**	**CD_2Cl_2**	**5.32p(^{1}H) 53.8p(^{13}C)**
DMSO-d_6	**2.49p(^{1}H) 39.5p(^{13}C)**	**DMF-d_7**	**2.91p(^{1}H) 35.2p(^{13}C)**
CD_3CN	**1.93p(^{1}H) 1.3p(^{13}C)**		**2.74p(^{1}H) 30.1p(^{13}C)**

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6 Integrating Your Spectrum (Not for ^{13}C NMR):

- Click the **Full Spectrum** icon and click the **Integral** icon.
- Type *cdc dc cz* <rtn>.
- 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* <rtn>.
- Click the **Hand** icon and drag the spectrum to next region, click **Resets** icon, left click your reset points, repeat for every region.
- When complete, click **Full Spectrum** icon.

7 Referencing Your Integrals:

- Expand around Integral to be referenced.
- Place cursor on an integral region. The red vertical cursor must be on an integral trace.
- Select **Process** Tab, input integral value in Integral area field, and click **Set Integral Value** button.
- Type *ds f dpir* <rtn> to display your integrals.

7a Saving Your Data:

- Type *svf* <rtn>.
- Type your filename with no spaces.

8 Peak Picking:

- Click **Full Spectrum** icon. Click **Threshold** icon and place yellow threshold line below top of smallest desired peak.
- Type *dpf* <rtn>. If too many peaks, click **Threshold** icon and move threshold up. Type *dpf* <rtn> to recheck.

9 Plotting Your Spectrum:

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

Common Plotting Commands:

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

10 Logging Off of a Session:

- Type *e* to eject sample.
- Place standard in spinner. Gauge properly. Place on top of magnet.
- Type *i* <rtn>.
- Type *exit* <rtn>.
- Click the **System** button on screen top, click **Log out…** and **Log Out....**

Icon Guide:


Full Spectrum


Magnifying Glass (Zoom)


Hand Icon (Pan & Scan)


Integral Resets



Cursor


Phasing


Threshold


Display Scale

1D NMR Acquisition Quick Guide

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VNMR Basic Commands		
Command	***Description***	***Typed Example***
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.	*nt=16* : default setting for 1H,CDCl3
bs	**block size**: Directs the acquisition computer, as data are acquired, to periodically store a block of data on the disk.	*bs=8* : 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 (*wft*) the result.	*ga*
wft	**weight and Fourier transform 1D data**: Performs a Fourier transform on one or more 1D FIDs with weighting applied to the FID.	*wft* : 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.	*aph* usually gives well phased spectra
f, full	**full**: Sets the horizontal and vertical control parameters to produce a display on the entire screen.	*f* or *full*
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.	*Vsadj* : resets the vertical scale to fit on the screen
dscale	**Display scale below spectrum or FID**.	*dscale*
aa	**abort acquisition**: immediately aborts the acquisition.	*aa*
sa	**stop acquisition**: stops acquisition after acquiring current transient.	*sa*
su	**submit a setup experiment to acquisition**: Sets up the system hardware to match the current parameters but does not initiate data acquisition.	*su*
svf	**Save FIDs in current experiment**: Saves parameters, text, and FID data in the current experiment to a file.	*svf('H1_070703')* : saves the FID as a file named H1_070703