

Reminder Sheet for UNITY-300 NMR Operation

1. With the mouse, select **Options/Session/Open Windows Desktop**
Login with Username and Password
2. **[Acqi] Unity-300 ACQUISITION:** **[eject]** - eject standard; **[insert]** - insert sample; **[LOCK]** - interactive lock:
SPIN: **[on]**; **LOCK:** **[Off]**; Set **Z0**, **lockgain**, **lockpower** and **lockphase** to card values for your solvent. Adjust **Z0** to get zero frequency (flat line) display; **LOCK:** **[on]** ;
Adjust **lockphase** for maximum lock level.
[SHIM] - interactive shim: adjust **Z1C**, **Z2C**, using +4, -4, then +1, -1.
[Close] - leave interactive acquisition.
3. **[Main Menu] [Setup] ; [H1,CDCI3] or [C13,CDCI3] or [Nucleus,Solvent]** Nuclei: **H1**, **C13**, **N15**, **P31**, or **F19** Solvents: **CDCI3**, **CD2Cl2**, **D2O**, **CD3OD**, **ACETONE**, **BENZENE**, or **DMSO**.
4. Check **nt**; **go** - starts data collection; **df** - display FID; **lb=0.2** (¹H) or **lb=1.0** (¹³C); **wft** - Weighted Fourier Transform. **f** - display full spectrum; **vsadj** - vertical scale
aph - apply automatic phasing; Manual phasing (if needed): **rp=0 lp=0 [Phase]**
Click on a resolved upfield peak. Press and hold left mouse button, drag mouse up or down to correct phase.
Click on a resolved downfield peak. Press and hold the left mouse button, drag mouse up or down.
ds - exit the manual phasing mode to correct phase.
5. Expand the region of reference peak: using the left mouse button place the vertical cursor line to the left of a region to be expanded, then click with the right mouse button to the right of the region; click on **[Expand]**.
6. Place cursor on reference peak; **nl** - centers cursor on nearest line; **rl(#p)** - sets line to # ppm reference.
7. Peak Picking: **[Th]** - displays a horizontal threshold cursor; adjust using the left mouse button; **dpl** - display ppm values on screen; **dll** - display peak list
8. Integration: **cz** - clears integration markers; **[Part Integral]** - displays integrals; middle mouse button changes the integral scale; **[Resets]** and use left mouse button to mark integral regions; enter **vp=12 dpirn**; enter **ins=ins*a/b** where a = number of protons; b = integral area displayed; **ds dpirn**; repeat **ins=ins*a/b** if necessary.
9. Title: **text('title')** where title is a short text phrase; **ds** to re-display spectrum.
10. Define: **plotter='hp7550a'** (Pen plotter) or **plotter='hplj1200'** (LaserJet printer)
printer='hplj1200t' (for text printout on the LaserJet printer)
pl ... page - plots spectrum and integrals, with a ppm scale, and loads a fresh sheet of paper. Insert additional commands at "... " (see **plot options** below)
11. Eject the sample, insert the standard, lock and shim (see step 2 above).
12. Exit the VNMR program (**VERY IMPORTANT**): type **exit** in the text entry window
13. Log Out: Right mouse on wallpaper, drag down to **[Exit]**, confirm **[Exit]**.

Plot Options (Insert between **pl** and **page**, separated by spaces):

pscale – print a ppm scale under the spectrum
ppf - plot ppm values on spectrum above each peak;
pirn - plots the normalized integral areas under each peak;
pltext – prints a title on the spectrum;
pap – prints title *and* a list of parameters on plot.

Other options:

Retrieve Shims: **rts('current') su** (“current” is the latest good shim file)

Abort Acquisition: **aa**

Save FID Data to Hard Drive: **svf('filename')**

Retrieving FID Data: **rt('filename')** or [Main Menu] [Data]; select file; [Load]