Reminder Sheet for UNITY-300 NMR Operation

1. With the mouse, select **Options/Session/Open Windows Desktop**
   
   Login with Username and Password

2. **[Acq]** 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,CDCl3] or [C13,CDCl3] or [Nucleus,Solvent]  
   
   Nuclei: H1, C13, N15, P31, or F19  
   
   Solvents: CDC13, 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;  
   
   **dpf** - 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]