1 Getting Started:
- Log on using your Username and Password.
- Click on the VnmrJ Desktop Icon.
- **Click Eject**, remove sample. Place your sample in spinner, check height. Place on top of magnet. Click **Insert**
- **Click Experiments**=>**Proton**
- Type sos <rtn>. Wait for beep.
- In the bottom Parameter Panel, select the Start tab and the Standard page.
- Choose your solvent from the Solvent drop-down 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.
- Adjust **Power** and **Gain** slider until you see a lock signal.
- Adjust Z0 slowly until no ‘beat’ is visible.
- Click **Lock On**.
- Reduce **Power**: D₂O, acetone=15-20; C₆D₆ =10-15; CDCl₃ =25-35.
- You can use findz0 to lock automatically
- Select the **Shim** page.

3 Shimming:
**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 until maximum. Repeat with Z2.
- Readjust Z1 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).
- You can use gradient autoshim for auto shimming

4 Acquiring Your Spectrum: **Choose appropriate Experiment**
- 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 ¹³C, use nt=1e6 bs=8.
- Click on the green Acquire & Transform button.
- For ¹³C, 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>.

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 rhl(<your solvent ppm>) <rtn>. For example, for CDCl₃ you would type nl rhl(7.24p) <rtn>.

### Common Deuterated Solvents:
- CDCl₃ 7.24p(¹H) 77p(¹³C)
- Acetone-d₆ 2.04p(¹H) 29.8p(¹³C)
- Benzene-d₆ 7.15p(¹H) 128.0p(¹³C)
- DMSO-d₆ 2.49p(¹H) 39.5p(¹³C)
- CD₃CN 1.93p(¹H) 1.3p(¹³C)
- D₂O 4.63p(¹H)
- CD₃OD 3.30p(¹H) 49.0p(¹³C)
- CD₃Cl 5.32p(¹H) 53.8p(¹³C)
- DMF-d₇ 2.91p(¹H) 35.2p(¹³C)
- 2.74p(¹H) 30.1p(¹³C)
Integrating Your Spectrum (Not for 13C 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. 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.

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 df dpir <rtn> to display your integrals.

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

Saving Your Data:
- Type svf <rtn>.
- Type your filename with no spaces.

Logging Off of a Session:
- Click eject to eject sample.
- Place standard in spinner. Gauge properly. Place on top of magnet.
- Click Insert.
- Type exit <rtn>.
- Click the System button on screen top, click Log out… and Log Out....

For questions/Comments contact
Dinesh Sukumaran (dks@buffalo.edu)

Icon Guide:
- Full Spectrum
- Magnifying Glass (Zoom)
- Hand Icon (Pan & Scan)
- Integral Resets
- Cursor
- Phasing
- Threshold
- Display Scale

Adapted from MSU handout: http://www2.chemistry.msu.edu/facilities/nmr/QuickGuide_VnmrJ.pdf
### VNMR Basic Commands

<table>
<thead>
<tr>
<th>Command</th>
<th>Description</th>
<th>Typed Example</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>nt</strong></td>
<td><strong>number of transients</strong>: 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.</td>
<td><em>nt=16</em> : default setting for 1H,CDCl3</td>
</tr>
<tr>
<td><strong>bs</strong></td>
<td><strong>block size</strong>: Directs the acquisition computer, as data are acquired, to periodically store a block of data on the disk.</td>
<td><em>bs=8</em> : sets the block size to 8 scans.</td>
</tr>
<tr>
<td><strong>ga</strong></td>
<td><strong>submit experiment to acquisition and FT the result</strong>: Performs the experiment described by the current acquisition parameters and Fourier transforms (<em>wft</em>) the result.</td>
<td><em>ga</em></td>
</tr>
<tr>
<td><strong>wft</strong></td>
<td><strong>weight and Fourier transform 1D data</strong>: Performs a Fourier transform on one or more 1D FIDs with weighting applied to the FID.</td>
<td><em>wft</em> : used if you stop the acquisition prior to completion or when loading a saved FID.</td>
</tr>
<tr>
<td><strong>aph</strong></td>
<td><strong>automatic phase of rp and lp</strong>: Automatically calculates the phase parameters <em>lp</em> and <em>rp</em> required to produce an absorption mode spectrum and applies them to the current spectrum.</td>
<td><em>aph</em> usually gives well phased spectra</td>
</tr>
<tr>
<td><strong>f, full</strong></td>
<td><strong>full</strong>: Sets the horizontal and vertical control parameters to produce a display on the entire screen.</td>
<td><em>f or full</em></td>
</tr>
<tr>
<td><strong>vsadj</strong></td>
<td><strong>Automatic vertical adjustment</strong>: Automatically sets the vertical scale, <em>vs</em>, in the absolute intensity mode so that the largest peak is at the requested height.</td>
<td><em>Vsadj</em> : resets the vertical scale to fit on the screen</td>
</tr>
<tr>
<td><strong>dscale</strong></td>
<td><strong>Display scale below spectrum or FID</strong>.</td>
<td><em>dscale</em></td>
</tr>
<tr>
<td><strong>aa</strong></td>
<td><strong>abort acquisition</strong>: immediately aborts the acquisition.</td>
<td><em>aa</em></td>
</tr>
<tr>
<td><strong>sa</strong></td>
<td><strong>stop acquisition</strong>: stops acquisition after acquiring current transient.</td>
<td><em>sa</em></td>
</tr>
<tr>
<td><strong>su</strong></td>
<td><strong>submit a setup experiment to acquisition</strong>: Sets up the system hardware to match the current parameters but does not initiate data acquisition.</td>
<td><em>su</em></td>
</tr>
<tr>
<td><strong>svf</strong></td>
<td><strong>Save FIDs in current experiment</strong>: Saves parameters, text, and FID data in the current experiment to a file.</td>
<td><em>svf('H1_070703')</em> : saves the FID as a file named H1_070703</td>
</tr>
</tbody>
</table>