QUICK GUIDE to USING the VARIAN 300 NMR SPECTROMETERS (vnmr 6.1c)

To change sample & set ^{2}H lock: **Acqi** button opens ACQUISITION menu. **Eject** the $CDCl_3$ standard. Carefully adjust tube position in sample holder (spinner) with depth gauge. Center short samples (< 5 cm) relative to the detection coil. **Insert** sample in magnet. Open the **LOCK** menu on the **Acqi** panel. Turn on SPIN (20 Hz; no spin for J-Young tubes). Turn *Lock* **off** to while adjusting **Z0** to match the deuterium resonance of the solvent.

$CDCl_3$	***INOVA-300:***	**Z0= +39**, **lockpower=30, lockgain=45** *(max 48)*	lock level ~68%
	***MERCURY-300*:**	**Z0=+387**, **lockpower=25**, **lockgain=26** *(max 38)*	lock level ~68%
	GEMINI-300:	**Z0=+232**, **lockpower=30, lockgain=20** *(max 30)*	lock level ~53%

These parameters differ on each spectrometer and for each deuterated solvent. Note that **Z0** drifts over a period of several months; When adjusting **Z0** it is helpful to temporarily increase the **lockpower** (be sure to turn it back down!). Engage the lock by clicking *Lock* **on**. *Autolock is not recommended*.
On the 300-NMR systems **lockphase** is only slightly sample dependent, but generally can be left alone. If necessary, tweak **lockphase** by +/-4 units at a time to optimize lock level. It may change after a power failure.

To shim: **Acqi** => **SHIM** (ACQUISITION menu)
Choose **manual** shimming. Open the **shim** menu with *RIGHT* mouse button and select "*fine Z*".
Alternately adjust **Z1** and **Z2** to maximize the lock level indicated by the color bars in the shim window.
Start with increments of +/-64, then +/-16. For more critical shimming use increments of +/-4 and also adjust **Z3**.
Repeat the cycle of adjusting **Z1**/**Z2**/**Z3** to achieve a maximum lock level, usually about *55-65%* for $CDCl_3$.
Exit the ACQUISITION menu by clicking the **CLOSE** button.
Note: shim and lock settings are shared from one user to the next.
If necessary, reload a fresh copy of the standard shim values by typing: **rts('std5') su**

To choose nucleus/solvent and modify/load parameters: **Main Menu** => **Setup** => **H1,CDCl3**
To list parameters, type **dg**, **dg1**, or **dgs** for *Acquisition Display*, or S*him* parameter groups, respectively.
Change parameters values by typing on the command line, e.g.: **nt=16** to collect 16 scans, *or* **sw=10000** to set the spectral width to 10,000 Hz. To check a parameter value, type the parameter name followed by a "?", e.g., **sw?**

To acquire & process spectrum:
Type **ga** (*get acquisition*) in the command line to start acquisition. Upon completion, spectrum is processed and displayed automatically. Type **dscale** to view the ppm scale. Auto-phase spectrum with **aph0** or phase interactively with the **Phase** menu button. To change the line-broadening and re-process, type: **lb=1 wft**

To expand the spectrum **Main Menu** => **Display** => **Interactive**
Set cursors on left and right of the spectrum with left/right mouse buttons and click on **Expand**.
To scale to the biggest peak type **vsadj**. Change the vertical expansion by dragging a peak up/down with the middle mouse button or with **vs** parameter; e.g., **vs=vs*10** increases the vertical expansion by tenfold.
To show the full spectrum, type **f full** or click the **Full** button. **Resize** increases/decreases the window size.

To display partial (segmented) integrals: **Main Menu** => **Display** => **Interactive** => **Part Integral**
Type the command **cz** to clear old partial integral marks. Click **Lvl/tlt** to adjust baseline tilt/offset.
Click on **Resets** and set new marks w/left mouse button. Use **isadj** to scale and **Set Int** to normalize integrals.

To pick peaks: **Main Menu** => **Display** => **Interactive** => **Th**
Set vertical threshold to desired level (yellow horizontal line) with mouse.
Type **dpf** in command line to view chemical shifts of the picked peaks.

To print:
For a basic plot, enter: **pl pscale page**. Plots are built up by a series of commands, terminated by **page**.
Optional commands: **pap** (*all parameters*), **ppa** (*parameters in "English"*), **pir** (*integrals*) and **ppf** (*picked peaks*).

To save data as a disk file:
To store a spectrum (including parameters, shims, text, etc) on the file server, type **svf('vnmrdata/*filename*')**.
To retrieve a spectrum file, type **rt('vnmrdata/*filename*')** or use the **File** => **Load** menu buttons.