Varian NMR machines (R2D2-V300 and Amidalah-V400) training note:

You need book nmr time first from SUMS and then can open OpenVnmrJ software in your account, next:

1. Put the sample NMR tube in the sample spinner nicely; and use the sample gauge to find the proper depth.

2. (Always)**eject** sample first and then **insert** the sample tube into the magnet. (use the eject and insert buttons, or type **e** or **i** in command line)

3. **Lock** Deuterium signal by click **find Z0** button. (Watch: Lock scan; lock level; lock power; lock gain; lock phase values, etc., adjust lock gain if needed.)

4. V300-R2D2 and V400-Amidala have been **TUENED** well when installed the probes, you don't need do tuning here.

5. Manually do **shimming** by clicking **Z1C** and **Z2C** button, (patiently clicking buttons for increasing or decreasing lock value. If shimming getting even worse, type **rts('cdcl3') su**)

6. Check the "**auto gain**" button; click "**time**" button to see the total nmr experiment time; and then click "**Go**" to start acquiring. Just use the default parameters to run first spectrum, you can adjust: **sw** – sweep width; **nt** – number of scans; receiver **gain**, etc. if needed. (H1 90° pulse value, etc. has been calibrated.)

7. Save your spectrum by clicking "**File**" and go to "save as", give your file name.

8. Use Google Chrome to log into your GT email account, upload your spectra folders into your Onedrive.

Notes:

- Mostly you just use room Temp. (If you want to do variable temp. expt., go to **Temp** tab to adjust the temperature. But let me know first!)
- If you want to run 90%H2O/10%D2O samples, it needs water suppression pulse sequences, suggest running on Bruker machines.

The basic operation commands:

su	setup hardware parameters ready
go	Start acquiring data
ga	acquire data and then wft
aa	abort acquisition
e	eject sample
i	insert sample

Common basic spectra parameters:

nt	number of transients
ss	number of dummy scans
bs	block size
d1	relaxation delay, also called recycle delay
sw	spectral width; sw1, sw2,
tof	transmitter offset; be the center of spectrum
solvent	for adjusting referencing; D_2O in most case here
pw	pulse width in us
tpwr	transmitter power level; dpwr --- decoupler power level
pw90	changing pw90 has no effect; some macros use pw90 to determine other pulse widths to be used in the experiment
gain	receive gain
at	acquisition time
np	number of total points in direct detect dimension; not complex points
tn	transmitter nucleus; dn --- decoupler nucleus
sfrq	spectrometer frequency of the nucleus being detected in MHz; dfrq --- decoupler frequency in MHz
dm	decoupler mode; e.g. dm = nny
dmm	decoupler modulation mode; e.g. dmm = ccg
dmf	decoupler modulation frequency; the frequency range that needs to be decoupled in Hz; 1/dmf = 90° pulse at decoupling power level (e.g. 41dB)

Common spectra display and manipulate commands:

jexp1	jump to exp1
explib	list all created exp.
wft	Weighted FT
time	show total exp. time
movetof	move tof to where the current cursor is; follow by tof?
movesw	set spectral width as the range between both current cursors on the spectrum
centersw	put cursor in center of spectrum
aph	autophase spectrum
ft, wft	Fourier transform, or weighted Fourier transform
f, full	display full spectrum in current range or in full graphic area
vs	vertical scale; press middle mouse button to adjust or type vs? vs = 34567
vsadj	auto-adjust vertical scale
df	display fid
ds	display spectrum
nl	nearest line; puts cursor on the nearest peak top
th	threshold; in millimeters
dpf	display frequency values for all peaks above certain threshold
dscale	display scale
rl	reference line, put cursor on the resonance peak, rl(4.772p)
dps	display pulse sequence
res	resolution; displays the line-width at 50%, 55%, and 10% of peak intensity; for checking shims and the base of the resonance
dres	display resolution; displays the line-width at 50% of intensity for analyzing quality of shims and the digital resolution
array	setup a series of values for a parameter
dssh	display stacked spectra horizontally
dssl	display stacked spectra with number
svf	save fid as a directory (filename.fid) including (binary) fid, (parameters file) procpar, (note) text, and log file in /home/username/vnmrsys/data
svs	save current shim settings to a file stored in /home/username/vnmrsys/shims
rts	Load shimming file
mp	move parameters, mp(10,12) move parameters of exp10 to exp12
rp	right phase correct
lp	left phase correct