# *VNMR 6.1C 1D NMR Quick Guide (Nightmare/NMR500)*

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## 1. To Begin:

- Logon to computer with your username and password
- VNMR Software should launch automatically, if not, Right Click (**RC**) on desktop, if you don't see xterm, **RC** on Program, then Left Click (**LC**) on shell tool. Then type *vnmr* on the UNIX prompt.
- Type *e* <rtn>. Place sample in the spinner. Gauge properly. Place on top of magnet. Type *i* <rtn>.
- Type *reshim* <rtn>. Enter solvent name, for e.g. *CDCl3* <rtn>.
- Click Acqi button. A new window will pop up. If you don't see the Acqi button, you can type *acqi* <rtn>.

## 2. Lock and Shimming:

- Check spinning, it should be off (set to 0).
- Click on LOCK panel, Click LOCK off.
- Increase lockpower and gain.
- **Lockphase** Nightmare=144; NMR500=310
- Move Z0 slider slowly until one 'beat' is visible. Reduce the lockpower and gain if lock level went over 100. Keep adjusting Z0, lockpower, and gain until the lock level maximized at around 70.
- Click LOCK on. Then click SHIM.
- Adjust Z1 with ± 16 button to maximize lock level. Repeat on Z2 (Z2C for NMR500 and using ±4 button). Adjust X1 follow by adjustment on Y1. Continue to alternate Z1, Z2, X1, and Y1 until no improvement.

## 3. Shimming:

- Click CLOSE to exit the lock/shimming window.
- Type *proton* <rtn> to load a proton experiment. Also enter the appropriate solvent name: *CDCl3* <rtn>.
- Type *nt=1 ss=0 ga* <rtn>
- When complete, type *f full aph* <rtn>, expand around solvent peak or suitable well-resolved singlet. Type *vsadj* <rtn>.
- Is this peak well shimmed (is it narrow or symmetric)? If yes, proceed to acquistion. If not, click Acqi then SHIM.
- Adjust appropriate shim (e.g. Z1 for symmetric broadening or Z2 for asymmetric peak shape).

## 4. Acquiring a Spectrum:

- Type *proton* for 1D 1H experiment and type *carbon* for 1D carbon. Also enter the appropriate solvent name.
- For $^{1}$H, type *ss=8 nt=16* <rtn>
- Type *ga* <rtn> to start the experiment. If the concentration of the sample is low, you may want to increase nt.
- For $^{13}$C, use *nt=1e6 bs=8* <rtn>
- Type *ga* <rtn>. For 13C, after a few data blocks are complete (message: BS # completed), type *wft* to process. When sufficient S/N is obtained or your experiment time slot is finish, type *aa* to stop the experiment.
- To save, type *svf('Desire_name')* <rtn>

## 5. Reference Your Spectrum:

- Type *dscale* for to display ppm scale and find your solvent peak.
- With left mouse button (**LC**) click to the left of solvent peak. With right mouse (**RC**) button click to the right of solvent peak.
- Click Expand. Place cursor on top of solvent peak with **LC**.
- Type *nl rl(7.26p)* <rtn> for CDCl3.c

| | $^{1}$H ppm | $^{13}$C ppm | HOD ppm | Mel/Boil °C |
|---|---|---|---|---|
| $CDCl_3$ | 7.24 (1) | 77.23 (3) | 1.5 | -63.5/61 |
| Acetone-$d_6$ | 2.05 (5) | 29.8 (7) | 2.8* | -94/56.5 |
| Benzene-$d_6$ | 7.16 (1) | 128.39 (3) | 0.4 | 5.5/80.1 |
| DMSO-$d_6$ | 2.50 (5) | 39.51 (7) | 3.3* | 3.81/101.42 |
| $CD_3CN$ | 1.94 (5) | 1.3 (7) | 2.1* | -45/81.6 |
| $D_2O$ | 4.80 (1) | | 4.8 (1) | 3.81/101.42 |
| $CD_3OD$ | 3.31 (5) | 49.15 (7) | | -97.8/64.7 |
| $CD_2Cl_2$ | 5.32 (3) | 54.00 (5) | 1.5 | -95/39.75 |
| DMF-$d_7$ | 2.92 (5) | 34.89 (7) | | -61/153 |
| | 2.75 (5) | 29.76 (7) | | |

## 6. Common VNMR Commands:

aa – abort acquisition
aph – auto-phase correction
cexp(2) – create experiment
dscale – display scale
f – display full spectrum
full – display spectrum in full
ga – acquire and process
go – acquire spectrum
jexp1 – join experiment 1
nl – nearest line
nt – number of transients
page – send to plotter
pap – plot all parameters
pl – plot spectrum
pscale – plot scale
res – resolution of peak
rl – reference line: rl(7.24p)
ss – steady state scans
su – setup hardware param
svf – save FID
svs – save shims only
unlock(2) – unlock experiment 2
vsadj – vertical scale adjust
wft – weighted Fourier transform

| | |
|---|---|
| pl pap pscale page | print plot with parameters |
| plloo | print plot with peak pick |
| pl1d | print plot with integration |
| stackplot | stack two plots together |