Bio-NMR facility training protocol

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

2. eject and insert the sample tube into the magnet.

3. Adjust the temperature.

4. Lock Deuterium signal. Lock scan; lock level; lock power; lock gain; lock phase; Z0;

5. mtune, matching and tuning for the 1st channel (H^1), check tuning for the 2nd (C^{13}) and the 3rd (N^{15}) channels,

6. Z gradient shimming, use the proper shimming map file and number of shim iteration,

7. H^1 90° pulse calibration using "water" pulse sequence: make sure to check "presaturation" off, nt = 1, ss = 0, gain = 0, array pw, increment = 0.4, do 360° pulse calibration; and then find tof, (also can find H_0 in this step if you use DSS as the internal reference, zoom DSS peak, put curser on it, nl, movetof, spcfrq, go to the text area and writer down the H_0 value.)

8. N^{15} 90° pulse calibration using "gNhsqc" pulse sequence: update the parameters: H^1 pw, tof, tpwr, gain, ni = 1, ss = 4, calN = 2; array pwN,

9. C^{13} 90° pulse calibration using "gChsqc" pulse sequence: update the parameters: H^1 pw, tof, tpwr, gain, ni = 1, ss = 4, calC = 2; array pwC,

The basic operation commands:

su	setup exp.; setup parameters, and communicates with console
go	acquire data
ga	acquire data and then wft
sss	input the filename first and save it automatically after acquisition is finished
ssq	input the filename first and save it, and then quit VNMRJ and log your account out automatically after acquisition is finished
aa	abort acquisition
e	eject sample
i	insert sample

underscore – customized commands

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)
ni,ni2	number of complex points in indirect detect 2^{nd} or 3^{rd} dimension
dof,dof2	decoupler offset; equivalent to tof for decoupler nucleus

dmf2, dpwr2, dmm2, dm2 are equivalent for 3rd channel decoupler nucleus

Common spectra display and manipulate commands:

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
jexp1	jump to exp1
explib	List all created exp.
mp	move parameters, mp(10,12) move parameters of exp10 to exp12
wft	
wft2da	weighted Fourier transform 2D for phase sensitive spectra (phase = 1,2)
rp	right phase correct
lp	left phase correct
time	show total exp. time