Basic Topspin commands for NMR at the BNSP Mar-1-2018

Action	Command‡	Comment
	Samples	
display **lock** window	`lockdisp`	adjust lock gain so lock is 80%
eject sample	`ej`	
edit **te**mperature	`edte`	enter target temperature
in**j**ect sample	`ij`	check temperature before this!
lock	`lock`	**[90% H_2O/10% D_2O]** or **[D_2O]** or **[Methanol-d4]**
optimize lock feedback loop	`loopadj`	`loopadj N` where `N` is from 1-10 gives slow to fast reaction time
automatic **t**une/**m**atch **m**odule	`atma`	option `exact` slower but more accurate
manual tune/match module	`atmm`	adjust both tune & match to shift curve from left to right last to avoid drifting
read **sh**ims	`rsh *.eth`	read a recent shim
automatic **top**spin **shim**ming	`topshim gui`	`topshim` (runs without opening gui)
manually adjust lockphase & shims	`bsmsdisp`	software version of the lock panel
	Experiments	
edit **c**urrent experiment	`edc`	`NAME EXPNO PROCNO DIR /opt/topspin/user/nmr` change **user** if copying parameters from another user **Do not select checkbox "Keep parameters"!**
read **par**ameters	`rpar *.all`	can filter e.g: `rpar NA_*.all` also switch from bruker to user dir!
write **p**rocessed & **a**cquired data	`wrpa`	**can overwrite nmr data!**
edit pulsesequence parameters	`ased`	calculated parameters are shown in grey
edit **a**cquisition parameters	`eda`	includes parameters for indirect dimensions of 2D,3D
edit **p**rocessing parameters	`edp`	
go **s**et up adjust parameters during measurement	`gs`	adjust `o1`, `rg`, flipback pulses interactively
display cnst array	`cnst`	all constants
display power level array	`pl`	all hard power levels
display pulse length array	`p`	all pulse lengths (in us)
display shaped pulse power array	`spdb`	all shaped pulses (name, power, etc)
zero **g**o (measure data)	`zg`	delete current experiment buffer and start experiment
	Calibrations	
temperature calibration	`calctemp`	first process methanol spectrum
	Calibrations	
90° hard pulse calibration	`HCN90`	enter logbook power levels to calibrate afterwards write calibrations in logbook!
set up DOTALL experiment	`xxx90` `geteth`	set 90° hard pulses (p1,p3,p5 & pldb 1-3) set params e.g. shape pulse & dec pwr
set up Bruker experiment	`getprosol 1H p1 pldb1 13C p3 pldb2 15N p5 pldb3`	

Standard high power pulses			
Channel	Power level	90° pulse	180° pulse
1: H1	**pldb1**	**p1**	**p2**
2: C13	**pldb2**	**p3**	**p4**
3: N15	**pldb3**	**p5**	**p6**
3: N15 (Bruker pulseq.)	**pldb3**	**p21**	**p22**
See logbook for standard values			

Action	Command‡	Comment
Processing data		
exponential **m**ultiply	**em**	**lb** is linebroadening in Hz
sine window multiply	**sin**	phaseshifted by π/**ssb** but ssb=0 is unshifted sine)
quadratic **sin**e window multiply	**qsin**	see above
fourier **t**ransform 1D	**ft** **fp** **ef** **efp** **qfp**	fourier transform only ft+pk em+ft em+ft+pk qsin+ft+pk
phase correction (interactive)	**.ph**	**.sret** (store phases, end phasing mode)
apply **p**hase correction	**pk**	apply **phc0** and **phc1** to spectrum
automated phase correction	**apk**	only for simple spectra like methanol
Baseline correction	**abs**	**absf1** & **absf2** are range in ppm
2D spectra		
display params of indirect dim	**eda**	displays **sw**, **td**, offsets **o1** in all dims **td1 (# of fids) must be an even number!**
fourier transform 2D	**xfb** **xfb n** **xf2** **xf1**	FT both dimensions **xfb** and discard imaginary data FT direct dim (F2) FT indirect dim (F1)
Baseline correction	**abs2** **abs1**	baseline correct F2 dimension baseline correct F1 dimension
3D spectra		
Fourier transform	**tf3 n;tf2 n;tf1 n** **ftnd 0** **ftnd 0 dlp**	FT dim F3,F2,F1 **n**=no imaginary data FT all dims in **AQORDER** FT all dim with delayed linear pred. (**dlp**)
Baseline correction	**tabs3;tabs2;tabs1**	Baseline correct dim F3,F2,F1
Extract data		
Extract fid from 2D ser file	**rser N M**	read fid N and store in expno=M
read serial row	**rsr N M**	read row N and store in procno=M
read serial column	**rsc N M**	read column from processed 2D
If **M** is not included: fid/row/column is transferred to ~TEMP/1, overwriting what is there		

‡Many additional standard topspin commands are available as documented in the acquisition and processing manuals available from the Topspin's help button, or the BNSP website. In addition, there are a number of BNSP specific commands documented on the BNSP website. A few are given in the above table: **HCN90, xxx90, geteth**

Common procedures

Calibrate temperature

1. Create new experiment (**edc**)
2. Load parameter-set for temperature calibration (**rpar methanol4.eth**)
3. eject sample (**ej**)
4. insert methanol4.eth sample with yellow label (**ij**)
5. lock on methanol (**lock**) select [methanol-d4]
6. set temperature (**edte**)
7. read a recent shimfile (**rsh *.setup**)
   Steps 8-12 can be performed on one line: **atma;topshim;zg;ef;apk;calctemp**
8. tune/match (**atma**)
9. shim (**topshim**)
10. measure data (**zg**)
11. process 1D (**ef;apk**)
12. calculate temperature (**calctemp**)
13. Adjust target temperature in edte and wait a few minutes
14. Repeat steps 7 to 10 until calibrated temperature = desired temperature
    - Now you can use this set temperature for all your samples
    - Temperature may still deviate from your desired value if experiment heats (e.g. decoupling, TOCSY)

Insert sample and set up 1D ^{1}H measurement

1. Create a new experiment (**edc**)
2. load experiment parameters (**rpar *.eth**) select `zgpr.eth` or `zg-wg3919.eth`
3. lock display (**lockdisp**)
4. eject sample (**ej**)
5. set temperature (**edte**)
6. insert sample (**ij**)
7. lock on H2O/D2O (**lock**)
8. optimize lock parameters for sample (**loopadj**)
9. tune and match probe (**atmm**)
10. read shims (**rsh *.eth**)
11. adjust lock or shims manually (**bsmsdisp**)
12. start automatic shimming (**topshim gui**)
13. set power levels: **pldb1** (^{1}H), **pldb2** (^{13}C), **pldb3** (^{15}N)
14. pulse length determination (**HCN90)**
    - If it fails due to low s/n, increase **ns**
    - After running **HCN90**, calibrate high pwr pulses for `DOTALL` or `ETH` datasets: **xxx90**
15. check and optimize experimental setup (**ased**)
16. interactively adjust parameters (**gs**)
    - Optimize **o1** for solvent suppression
    - Optimize **rg** to be large, but avoid receiver overflow
17. record a spectrum (**zg**)
18. stop experiment (if lock drops rapidly stop measurement: **stop**)
19. end experiment early after completing current phase cycle: **halt**)
20. process the spectrum (1D: **efp,** 2D: **xfb**)
21. phase correct if necessary (**.ph** to start, **.sret** to store results)

Calibrate selective pulses for solvent flip-back

1. Calibrate hard 90deg ^{1}H pulse using HCN90 (see procedure above)
   On 900 do this manually use zg experiment to measure 360° pulse & divide by 4.
2. Create a new experiment (**edc**)
3. Read flipback calibration parameter-set (**rpar flips.all**)
4. Enter hard 90deg ^{1}H pulse calibration (**xxx90**)
5. Display important parameters and adjust them (**ased**)
   - p11 flipback pulselength – set to value appropriate for spectrometer
   - o1 – set to optimized value determined in zgpr.eth experiment using **gs**
   - ZGOPTNS :

Type of flip pulse	ZGOPTN	Shape name *	Shape power	Phase correction
flip down	-DDWN	spnam1	spdb1	phcor1
flip up	-DUP	spnam2	spdb2	phcor2
flip watergate	-DWG	spnam3	spdb3	phcor3
* Use gauss128_5, Sinc1000, or rect1000 and geteth for *approximate* calibration Other shapes are possible, but then you must use **stdisp** for *approximate* calibration.				

6. Calibrate shaped pulse powers to *approximate* values (**geteth**)
7. Interactively adjust shaped pulse pwr & phase correction to minimize solvent (spdb1, phcor11) (**gs**)
8. Write down the shaped pulse power and phase correction
9. Change to next type of flipback pulse (ZGOPTN: –DDWN, -DUP, DWG) and repeat steps 7-8

Setup and measure 2D (for bruker expt replace steps 3-4 with getprosol – see bottom of p.1)

1. Create a new experiment (**edc**)
2. Read 2D parameter-set (**rpar *.all**) and select 2D: E.g. HSQC15N.all
3. Enter high power pulse calibrations (**xxx90**, uses calibration from 1D above)
4. Setup 2D experiment automatically (**geteth**, calibrates decoupling, shapes, td1, td2)
5. Check main acquisition parameters (**ased**)
6. Check indirect dim acquisition parameters (**eda**)
   Important are:
   - decoupling should not be too high ~4W, for 123ms
   - No negative calculated delays
   - Indirect dim carrier (**o3p** for experiments with 15N in indirect, **o2p** for 13C)
   - Indirect spectral width in ppm (**sw**) F1
7. Run 2D (**zg**)
8. Extract fid from 2D series (**rser N**) where **N** is fid number
   - FID is copied to 1D parameterset in ~TEMP/1
   - You can process this like the 1D described above, and store phases to 2D
   - Close window when done using x in upper right corner
9. Process direct (^{1}H) dimension of 2D (**xf2**)
10. Process indirect (^{15}N) dimension (**xf1**)
11. Process both dimensions (**xfb**)
12. After initial 2D run with small number of scans (ns), adjust
    - **sw** (F1) and **o3p** (^{15}N) or **o2p** (^{13}C) to optimize spectral width to sample

Setup and measure 3D:

1. Steps 1-8, same as for 2D
2. process a 2D plane of 3D (with no evolution in one dim (**xfb**)
3. select orientation 13 or 23, and processing number 13 or 23
4. phase as usual for a 2D and store to 3D, close 2D by clicking on x at top right
5. revise **STSI** and **STSR** so strip FT selects region of interest in direct dim3
6. Enter **STSI** and **STSR** from step 2c above in 3D processing parameters
7. Process direct (^{1}H) dim (**tf3 n**)
8. Process indirect dim (**tf1 n** or **tf2 n**)
9. Process other indirect dim (**tf2 n** or **tf1 n**)
10. Steps 2-4 can be replaced by **ftnd N** or **ftnd 0 dlp**
11. The 3D can be viewed with 3D viewer after steps 4-7 to inspect results