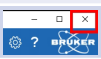
Commands for routine experiments on Topspin

Links to :

Booking SOP ISIC-NMRP

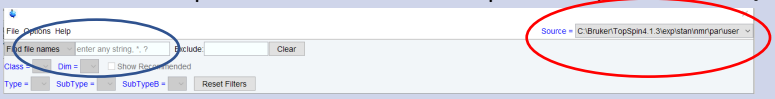
1) Setup and run a ^{1}H NMR experiment

Command	Action	Options / Remarks
	Start topspin program	On the computer desktop
newnmr	Generate a new ^{1}H experiment	Enter your sample name If asked, enter your user (Gaspar) name.
ej/ij	Inject or eject the sample	1. Start the N_2(g) flux (or eject the sample) : **ej** 2. Place your sample in the magnet (⚠ check that the spinner is floating !) 3. Stop the N_2(g) flux (or inject the sample) : **ij** Rem: the lift will not start if the black cap close the magnet (you will need to enter the command again after removing it) 
(Optional) rhs shim	Load a reference shim file	This step can be skipped, especially if you pass many samples in a row You can load later this reference shim if your spectrum looks poorly shimmed
lock	Lock spectro. to your d-solvent	Select the solvent in the list (ask us if it does not appears)
atma	Tune and match the probe	Tune only to the frequency of the nucleus set in the experiment (here ^{1}H) ⚠ If later you setup a new nucleus, you will need to do this step again
Topshim	Automatic shimming	Your shim will be **bad** if : - There is not enough sample in the coil (optimal : 500-600 uL) - Your sample is not well dissolved / precipitate / too concentrated (π-stacking) - Your solvent is viscous - Your tube is damaged / reused (consider throwing away CHF 2.– tubes) - In presence of paramagnetic species
(Optional) ns **expt**	Change the number of scans Estimate the experimental time	By default ns = 16. If your sample conc. is around 1-10 mM it should be enough Increase ns if you want more sensitivity (to double the SNR you need 4x ns) Consider using high sensitivity magnet if the SNR is too small
zg	Start the acquisition	Use the command **multizg** to start multiple experiments (from the 1st one)
(Optional) efp	Fourier transform	If you use MestreNova, the raw data will be processed in this soft by default (ask us if you want to transfer the Topspin processed data)
(Optional) apk , apbk	Automatic phase / baseline correction	If you use MestreNova, the raw data will be processed in this soft by default (ask us if you want to transfer the Topspin processed data) Use the command **.ph** and **bas** to correct phase / baseline manually
ej / ij	Eject the sample / Stop the lift	
	Close Topspin program	Wait until Topspin is fully closed (no more command prompt)
	Log out from your session	⚠ Do NOT : switch off the computer / lock your session

Next page : other useful commands; setup ^{13}C, 2D, … experiments

Commands for routine experiments on Topspin

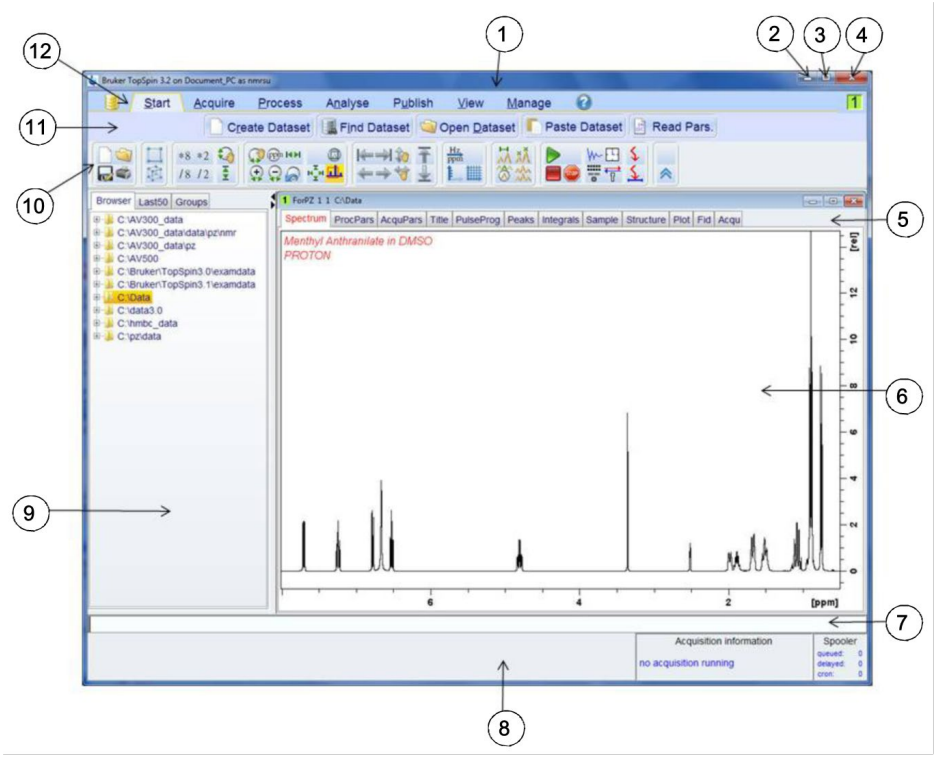
2) More useful commands

Command	Action
tr	Import the data already acquired from the console to the PC to be processed Use **tr #** to import the data after a defined number of scans (ex tr 4)
halt	Stop the experiment before its end and save the data on the disk ⚠ If you use the command **stop** (in 1d) your data will be lost !
go	Restart the acquisition and continue to accumulate signal. This is helpful to improve the SNR by acquiring more scans
xfb	Fourier transform 2D data
xf2	Fourier transform "pseudo 2D" data only in F2 dimension (useful for kinetic, T1/T2, DOSY measurements)
expt / multiexpt	Calculate the duration of the experiment / of multiple experiments
edc	Create a new experiment in the same folder (new expno) or in a new folder - If "Use current parameters" is selected: copy the current experiment - If " Read parameterset" is selected : load the parameter of a different experiment (⚠ source : …**/user**) 
rpar **rpar *keyword***	Read a set of parameter to load a new experiment (⚠ source : …**/user**) You can restrict / search for precise experiment / experiment type putting between *-* some keywords (ex: rpar *2d*, rpar*13C*, rpar *HSQC*, rpar *dosy*, …)

3) Setup and run additional experiment(s)

Command	Action	Options / Remarks
See 1)	Acquire ^{1}H spectrum	Start by acquiring a ^{1}H spectrum - to check your sample (degradation, concentration, shim, etc …) - to reference your spectrum using secondary referencing
newexp	Create a new experiment	Indicate the new experiment number You can specify a keyord (1H, 13C, 1d, 2d, HSQC, DOSY, …) Select the desired NMR experiment in the list (→ Select→Ok)
atma	Tune and match the probe	Tune only to the frequency of the nucleus set in the experiment ⚠ The probes can only be tuned simultaneously to 2 sometime 3 frequencies - 1504r: ^{1}H and ^{19}F and BB (^{109}Ag – ^{31}P), possible to do BB{^{1}H,^{19}F} - 1516 : ^{1}H OR ^{19}F and BB (^{109}Ag – ^{31}P, no ^{19}F{^{1}H}) - 1508 : ^{1}H and ^{13}C and ^{15}N (only, no other BB nuclei) - 1510 : ^{1}H and ^{13}C and ^{15}N (only, no other BB nuclei) - All the other 400MHz : ^{1}H and BB (^{109}Ag – ^{19}F)
(Optional) **ns, o1p, sw, …**	Optimize selected parameter	Don't hesitate to ask us for information
(Optional) **newexp** **multiexpt**	You can prepare as many NMR experiments as you need Calculate experiments duration	No need to tune the probe again (no need for atma) But you can have only one frequencies configuration for a set of experiments
zg	Start the acquisition	Use the command **multizg** to start multiple experiments (from the 1st one)

The TopSpin Window



1. Title bar
2. Minimize button
3. Maximize button
4. Close button
5. Data Set tabs
6. Data Display window
7. Command line
8. Status bar
9. Browser window
10. Tool bar
11. Workflow button bar
12. Workflow menu bar