List of commands to use within the TOPSPIN program

Below is a list on common keyboard commands to use in the command window in the TOPSPIN program. A more comprehensive list can be found under the question mark icon (? – Commands) in the top right of the program interface.

	TopSpin Commands	Brief description	Additional information
Spectrometer Calibration and parameter sets			
Injecting / ejecting the sample	sx 10	Inject sample from position 10	Ensure the sample is in the correct position prior to entering the command. Check temperature of spectrometer before this command.
	sx ej	Eject sample from the NMR spectrometer	Check temperature of spectrometer before this command.
	ij	Inject sample	Recommended only for manual mode. Check temperature of spectrometer before this command.
	ej	Eject sample	Recommended only for manual mode. Note an error message may appear on some spectrometers and fail to eject the sample. If this occurs, use ‘sx ej’
Changing temperature	edte	Brings up temperature interface	This can be brought up by double clicking the temperature in the TOPSPIN interface.
Creating new experiment	new	Define a new dataset.	When generating a new experiment, it is recommended to locate a recent previous experiment to ensure the file location of the new data is correct.
	edc	Define a new dataset	Command is comparable to ‘new ‘however ‘new’ is recommend by TOPSPIN.

	rpar	Read parameters	Pop up window appears with all available parameter sets.
Locking to a solvent	lock	Lock the magnetic field to the deuterium signal of the solvent.	Brings up a window detailing the possible solvents the NMR spectrometer is set up to lock to. The spectrometer can be set up to lock to non-deuterated solvents.
	Lock cdcl3	Lock the magnetic field to the deuterium signal in $CDCl_3$.	The solvent can be replaced by any solvent under the column BLANK set up in the 'lock' window of TOPSPIN
Tuning and matching	atma	Automatic tuning and matching of ATM probeheads.	Will only tune and match those nuclei specified within the pulse program / experiment. Good tuning and matching will improve the SNR of your experiment compared to poor tuning and matching.
	atmm	Manual tuning and matching of the ATM probeheads	The manual version of atma. Recommended for fine adjustments and for checking the tuning and matching after atma.
Shimming	tshim	AU macro which uses the topshim command, then adjusts the phase of the lock.	NMR facility specific command.
	topshim	1D shimming	Topshim typically takes < 5 minutes to complete. This shimming should be sufficient for general samples.
	tshimvt	AU macro which uses tshim with convection compensation.	Should be used for variable temperature samples. Each spectrometer will have a VT tshim macro however may be spelt differently.

Experiment Acquisition			
Running the experiment	getprosol	Reads the probeheads and solvent dependent parameters into the experiment.	Examples of parameters read in: pulse durations, pulse shapes, delays and decoupling sequences.
	rga	Determines the optimal value for the receiver gain (rg) and sets it to that value in the experiment.	An optimal value ensures the highest SNR for your experiment without causing a receiver overflow.
	zg	Start acquiring raw data	'zero go'
Stopping the experiment prematurely	stop	Stops the experiment.	1D: Does not save any data! 2D: Does not save the current increment.
	halt	Halts the experiment after completing the next scan/increment.	1D: Halt 32: Halts the experiment after the next multiple of 32 scans 2D: Halt 32: halts the experiment after the next multiple of 32 increments

1D processing commands			
Fourier transform of the dataset	ft	FT of the FID	
	fp	FT and phase correction using predefined values of PHC0 and PHC1	PHC0 and PHC1 values are defined under 'PROCPARS – Phase correction'
	fmc	FT and magnitude calculation	
	ef	Exponential window multiplication + FT	Exponential window multiplication is defined under 'PROCPARS - Window function'
	efp	Exponential window multiplication, FT + phase correction	
	gf	Gaussian window multiplication + FT	
	gfp	Gaussian window multiplication, FT + phase correction	
Phase correction	apk	Automatic phase correction of the spectrum.	Determines the optimal values of PHC0 and PHC1
	apbk	Combined automatic baseline and phase correction.	
	pk	Phase correction according to predefined PHC0 and PHC1	
	.ph	Opens manual phase correction interface	
Baseline correction	abs	Automatic baseline correction and integration of major signals in spectrum.	
	abs n	Automatic baseline correction only. No integrating of signals.	
	.basl	Opens manual baseline correction interface.	

	2D processing commands		
Fourier transform of the dataset	xfb	FT both dimensions	
	xf1 (xf2)	FT F1 only (FT F2 only)	
Phase correction	apk2d	Automatic phase corrections in both dimensions	If a command ends in 1 or 2, it corresponds to a processing command in the F1 or F2 dimension, respectively.
	.ph	Manual phase correction for both dimensions	
Baseline correction	abs2d	Automatic baseline correction in both dimensions	
	abs1	Automatic baseline correction in F1	
	abs2	Automatic baseline correction in F2	
Other	prguide	Opens the processing guide (1D/2D)	Contains a workflow for processing data, highlighting the crucial steps.