NMR HANDS-ON PROTOCOLS – COMMON COMMANDS AND PARAMETERS FOR TOPSPIN

COMMANDS

Sample related commands

Commands	Brief description	Additional Information
ej	• Eject sample from the NMR spectrometer. • Exchange your sample for the standard sample on the column of air	• Used in manual mode spectrometers (no autosampler) • Even if there isn't any sample in the spectrometer this is required. • Check the temperature before this command
sx <#> **sx ej**	• injects sample from a specific sample position number (#) of an autosampler • ejects the current sample in the magnet back into the autosampler	• Commonly used for spectrometers with autosampler.
ij	• lowers your sample (inject)	• Recommended only for manual mode.

Acquisition related

Commands	Brief description	Additional Information
ased	Opens acquisition parameters page	Show and allow editing of the limited set of parameters, relevant to the current experiment
eda	Opens acquisition parameters page	displays all data acquisition parameters.
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.
atmm	Manual tuning and matching of the ATM probeheads	The manual version of atma.
edte	Opens temperature interface	This can also be opened by double clicking the temperature in the TOPSPIN interface.
getprosol	Reads the probehead and solvent dependent parameters into the experiment	Note that entering getprosol is equivalent to clicking the AcquPars tab and the clicking button.
getprosol 1H p1 pl1	reads in parameters for a specific p1 and pl1 into the experiment	Update pulses related to measured p1

Commands	Brief description	Additional Information
halt	Halts the experiment after completing the next scan/increment.	
lock	Lock the magnetic field to the deuterium signal of the solvent.	Brings up a window detailing a solvent list set up in the NMR spectrometer to lock to. Select the solvent and click **OK**.
new or **edc**	Create a new experiment	• When setting up a new experiment, it is recommended to check a recent one you made to make sure you're saving the new data in the correct directory. • Fill in the required fields of the dialogue box: ○ experiment name ○ experiment number ○ your user ID directory ○ choose experiment from the parameters list or "use current parameters" ○ choose your solvent from the drop-down menu ○ enter a title that will appear at the top of your spectrum (optional) Click **OK** to close the dialogue box
rg	Check the set receiver gain value	
rga	sets receiver gain automatically	
rpar	load an existing parameter set	Pop up window appears with all available parameter sets.
stdisp	Shape tool for handling RF shapes and gradients	opens the shape tool window where you can create, manipulate, and analyse RF shapes and gradients
stop	Stops the experiment.	1D: Does not save any data! 2D: Does not save the current increment. Serves as an emergency stop.
topshim	1D shimming	Topshim typically takes < 5 minutes to complete. This shimming is sufficient for general samples.
topshim gui	enter topshim interface	See acquisition protocols
tr	transfer data during acquisition	follow with ef; apk
zg	Start acquiring raw data	"zero go"

Processing related

Commands	Description
.all	zoom out to display full spectrum
.basl	Opens manual baseline correction interface.
.cal	open interactive 0 ppm referencing window
.int	opens dialogue box for integration options - most common is to define integral regions manually. See processing handouts
.md	enter multiple display mode
.ph	open interactive phase correction window
.ph	Manual phase correction for both dimensions
.pp	open interactive peak picking window
abs1	baseline correct F1 dimension
abs2	baseline correct F2 dimension
absn	Automatic baseline correction only. No integrating of signal
apk	Automatic phase correction of the spectrum using a polynomial function (1D). Determines the optimal values of PHC0 and PHC1
apk0	Zero-order automatic phase correction (1D)
apk2d	Automatic phase correction 2D. If a command ends in 1 or 2, it corresponds to a processing command in the F1 or F2 dimension, respectively.
bas	Open baseline correction dialog box (1D,2D)
bc	Baseline correction of the FID (1D). The type of correction is determined by the processing parameter BC_mod in the PROCPARS tab.
edp	edit processing parameters
ef	**E**xponential window multiplication + **F**T
efp	**E**xponential window multiplication, **F**T + **p**hase correction
ft	**F**ourier **T**ransform of the FID
gf	Gaussian window multiplication + FT
gfp	Gaussian window multiplication, FT + phase correction
rser #	Read row # from 2D raw data and store as 1D FID (2D,1D)
sref	automatically perform spectrum calibration based on lock solvent and TMS info. Set the TMS/DSS/TSP to zero ppm.
xfb	Fourier transform 2D exp

Parameters

Parameter	Type	Description
P1	pulse	F1 channel 90° pulse width
D1	delay	relaxation delay or recycling delay. 1 to 5 times T1 in 1D-NMR
D8		NOESY mixing time (50 ms – 1s)
D9		TOCSY mixing time (range: 15 ms to 120 ms)
AQ	Acquisition related	Acquisition time. The total time during which data is collected in a single scan. It is determined by the number of data points and the dwell time.
DS		Number of dummy scans. Several sets of pulses which are identical to those used for acquisition are sometimes transmitted to the sample before any FID is recorded. This procedure is employed to allow the sample to reach a stable or equilibrium state.
DW		Dwell Time. The time spent sampling each data point in the time domain. It is inversely related to the spectral width and is crucial for determining resolution.
FIDRES		FID resolution (1/AQ). smaller number for the digital resolution corresponds to better resolution.
NS		number of scans of a given experiment
O1		Offset of the spectrum center (Hz) with respect to the base frequency (BF) of the spectrometer.
O1p		offset of the spectrum center in ppm units. - CHANNEL F1
O2		Same as previous but on the F2 channel (Hz)
O2p		Same as previous but on the F2 channel (ppm)
RG		Receiver Gain. The amplification factor applied to the received NMR signal to optimize the signal-to-noise ratio. It adjusts the sensitivity of the receiver.
SI		number of points in the spectrum (4k to 64K for ^{1}H)
SW		spectral width ppm units. Depends on the nucleus studied.
SW1		spectral width ppm units in the F1 dimension
SW2		spectral width ppm units in the F2 dimension
SWH		spectral width Hz units. Depends on the nucleus studied and the spectrometer's base frequency
TD		number of FID points (value range 4k to 64K)
TD1		number of FID points in the F1 dimension
TD2		number of FID points in the F2 dimension
GB	Processing related	Gaussian broadening factor for Gaussian window multiplication
LB		line broadening parameter can be set with the **lb** command and execution of the window function is done with **em** Values: 0.3 – 1 Hz (^{1}H); 2.0 – 5.0 Hz (^{13}C)
maxi		Height of the largest peak considered for peak picking.

Parameter	Type	Description
mi	Processing related	The minimum relative height of peak to be picked
pc		peak picking sensitivity factor (range 0.1 to 100): pc < 1 will pick more peaks; pc > 1 will pick less number of peaks; pc = 1 is default
PH_mod		Phase correction mode. Mode for processing the phase of the data No: no phase correction pk: Phase sensitive ps : power mode
Ph0		zero order phase correction factor
Ph1		first order phase correction factor
F2QLIST	Miscelaneous	Irradiation Frequency Lists. Can be set from **eda** (submenu Lists) by entering a name or by clicking the down arrow and selecting a name from the appearing list. Or **fq2lis**t on the command line.
NBL		Number of irradiation frequencies in the STD NMR experiment
L4		Loop counter in the STD NMR experiment. Can be set from **eda** (submenu Program parameters) or writing **l4** in the command line.
D20		Saturation time in Bruker stddiff pulse sequence (0.5 – 4 s)