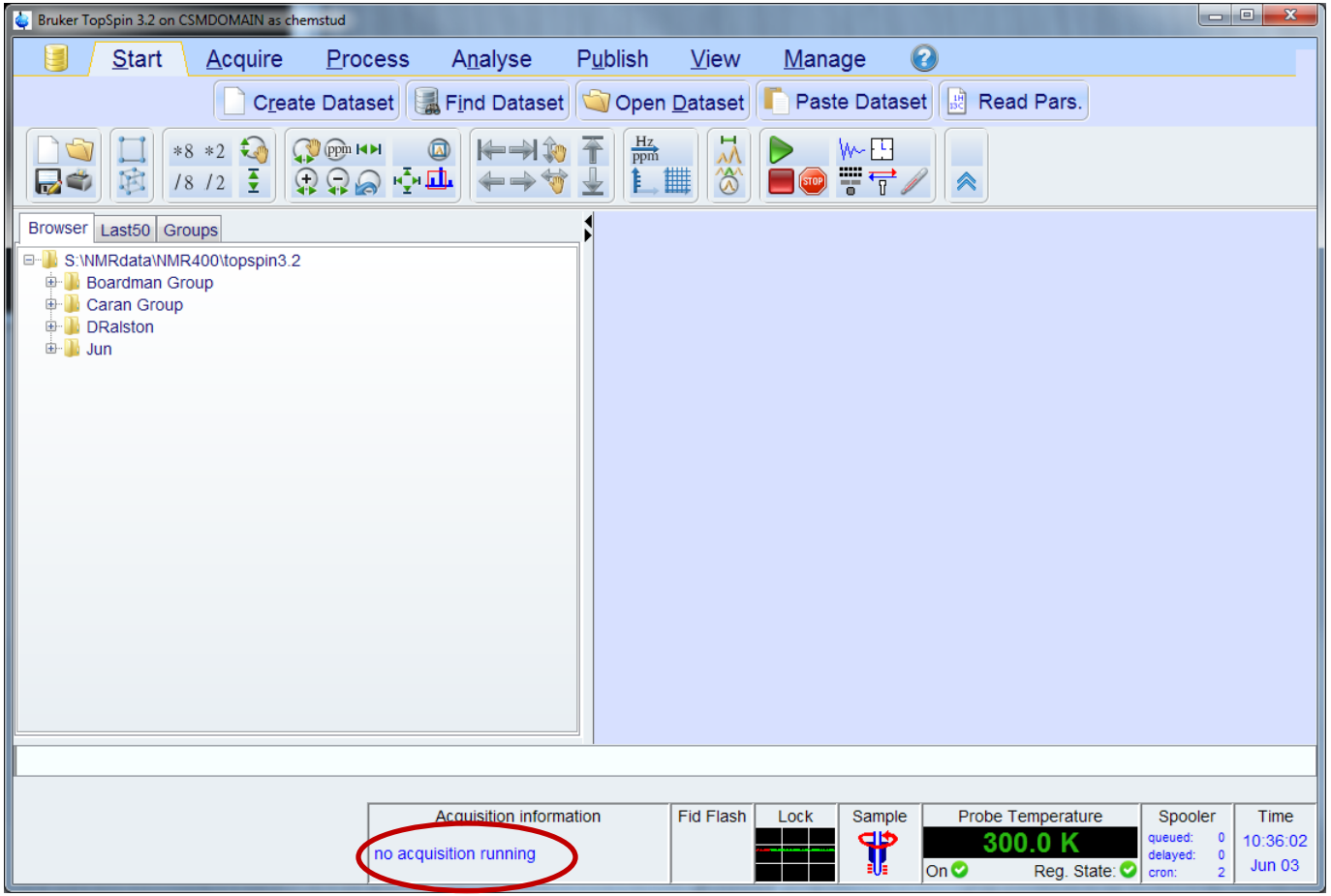
Operation instruction guide for topspin 3.2

This is assuming that you know the NMR basics and familiar with topspin 1.3 operation

BEFORE YOU START

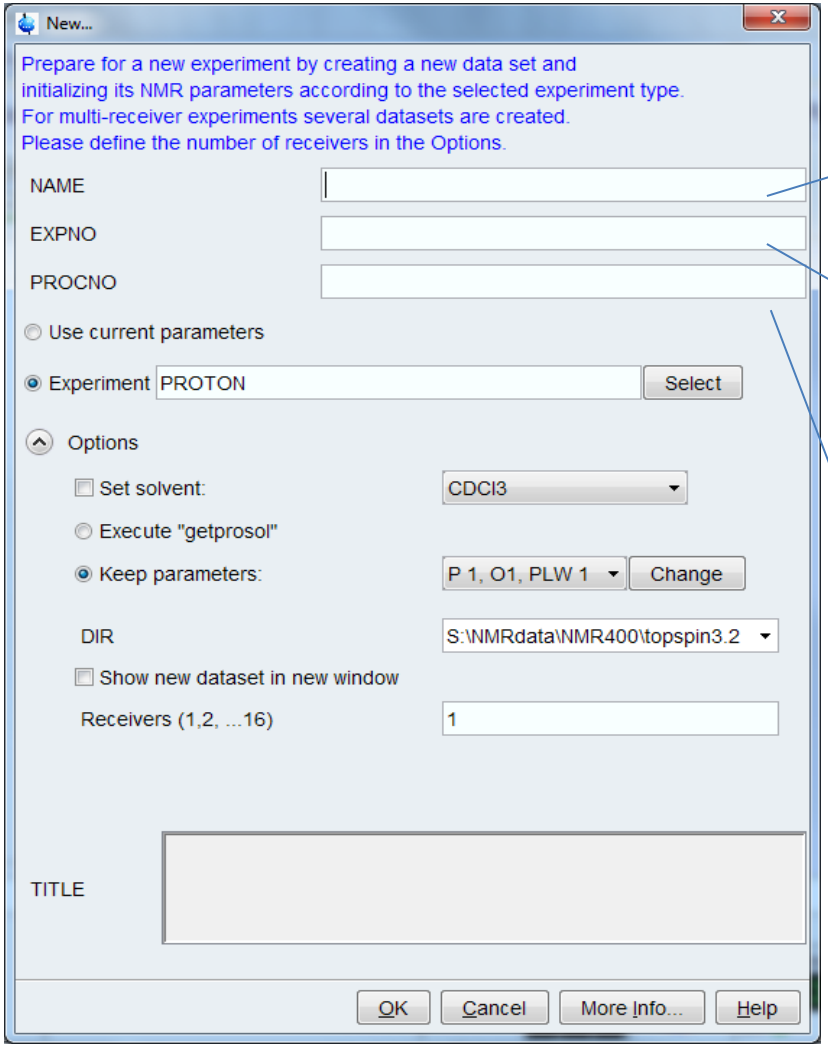
Double click on topspin 3.2 icon to start the program, if the program is already started.

Make sure no acquisition is running before you start your experiment !



CREATE NEW EXPERIMENT

Click "*Create Dataset*" or type "*edc*" or "*Ctrl+N*" in the command line to Create a new experiment.



(NAME) : Can be any name and should be used to identify the sample.

(EXPNO): Identifies the "raw" acquired data, meaning you may run a number of experiments under the same sample name.

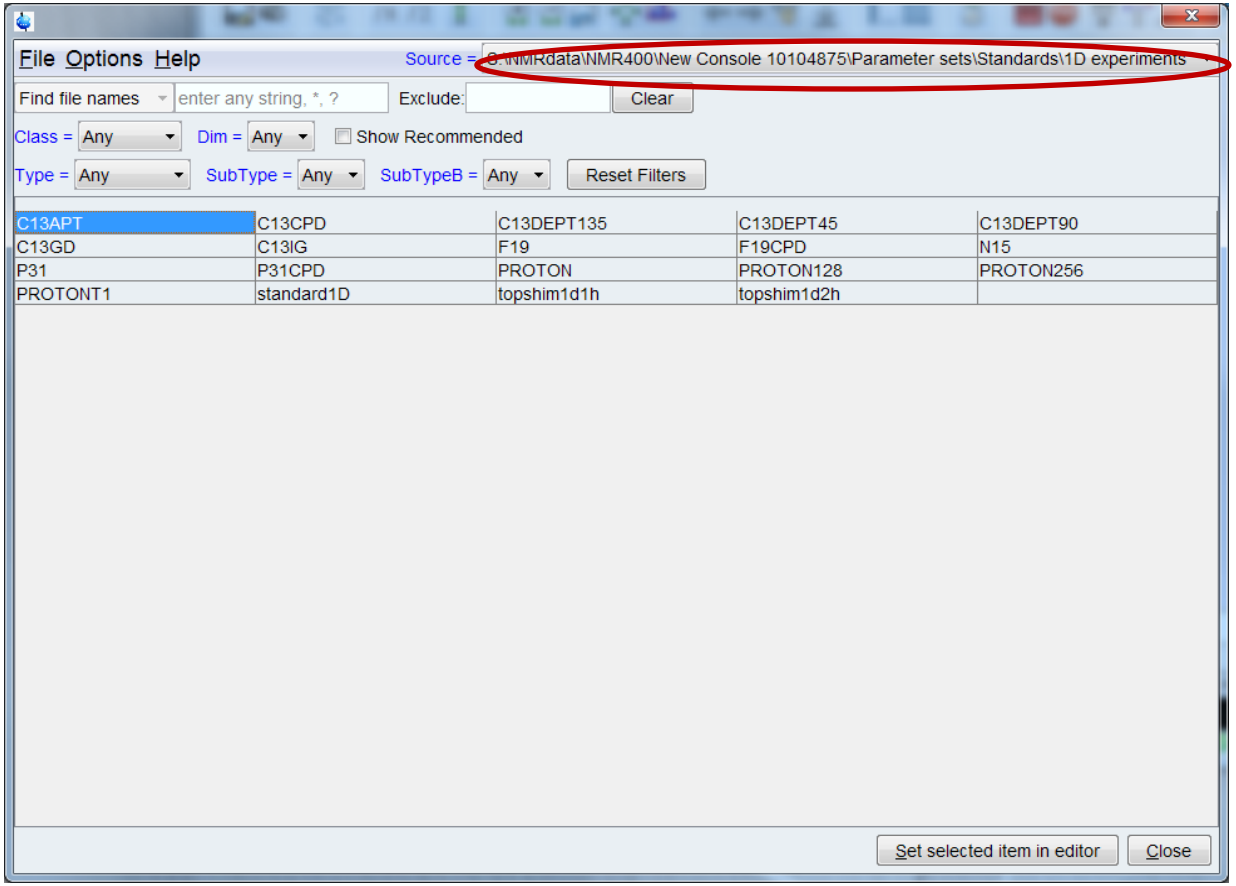
(PROCNO): Identifies the processed version of the raw data, allows you to process the raw data in a number of ways and to keep each processed data under a unique number.

In the DIR, select the directory to store your experiment data (make sure the data is in the topspin 3.2 folder)

CHOOSE PARAMETER SET

Under the experiment, click on "***select***" to choose a parameter set, select the source from

S:\NMRdata\NMR400\New Console 10104875\Parameter sets\Standards,
or from C:\Bruker\TopSpin3.2\exp\stan\nmr\par

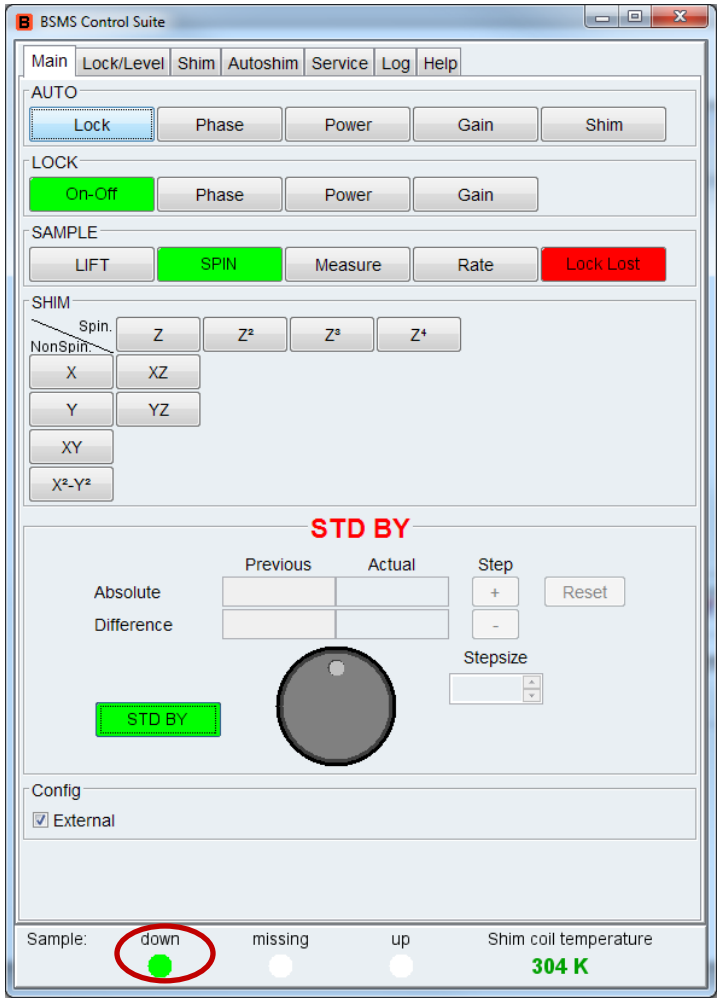


Typically select a proton experiment, or other nuclei experiments.
If you are not sure about the parameter set, highlight the parameter name and click "help"
To search in the NMR guide.

INSERT YOUR SAMPLE

Type "*ej*" in the command line, or choose LIFT under PROCEDURE to lift an existing sample.
Type "*ij*" or click INJECT to insert your sample.

Under the BSMS Suite, you will notice the sample is down in the magnet. If BSMS is not available , Type "bsmsdisp" to bring up BSMS window.



LOCK YOUR SAMPLE

Type "*lock*" in the command line or select LOCK in the PROCEDURE. Then choose the solvent you wish to lock. Notice the change in the lock display (If lock display in not available, type "lockdisp" to bring it up.

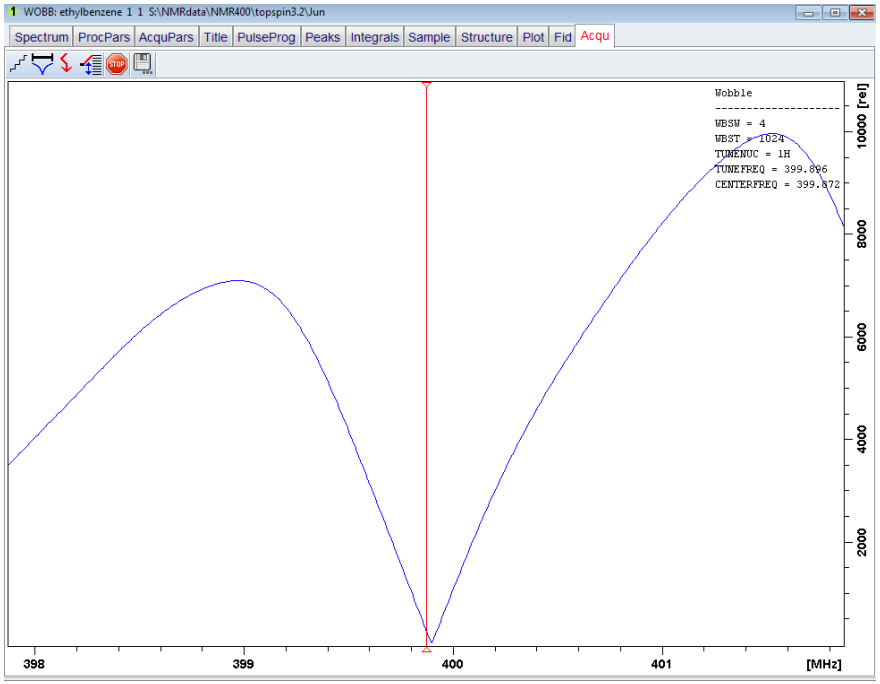
Solvents table

Solvent	Description
Acetic	acetic acid-d4
Acetone	acetone-d6
C6D6	benzene-d6
CD2Cl2	dichlormethane-d2
CD3CN	acetonitrile-d3
CD3CN_SPE	LC-SPE Solvent (Acetonitrile)
CD3OD_SPE	LC-SPE Solvent (Methanol-d4)
CDCl3	**chloroform-d**
CH3CN+D2O	HPLC Solvent (Acetonitril/D2O)
CH3OH+D2O	HPLC Solvent (Methanol/D2O)
D2O	deuteriumoxide
Dioxane	dioxane-d8
DMF	dimethylformamide
DMSO	dimethylsulfoxide-d6
EtOD	ethanol-d6
H2O+D2O	90%H2O and 10%D2O
HDMSO	90%DMSO and 10%DMSO-d6
Juice	fruit juice
MeOD	methanol-d4
Plasma	blood plasma
Pyr	pyridine-d6
T_H2O+D2O+Me4NCl	(CD3)4NCl in 90%H2O and 10%D2O, for NMR thermometer
T_H2O+D2O+NaAc	sodium acetate in 90%H2O and 10%D2O, for NMR thermometer
T_H2O+D2O+Pivalate	pivalate-d9 in 90% H2O and 10% D2O, for NMR thermometer
T_MeOD	methanol-d4, for NMR thermometer
TFE	trifluroethanol-d3
THF	tetrahydrofuran
Tol	toluene-d8
Urine	urine

OK Cancel

TUNE and MATCH the probe

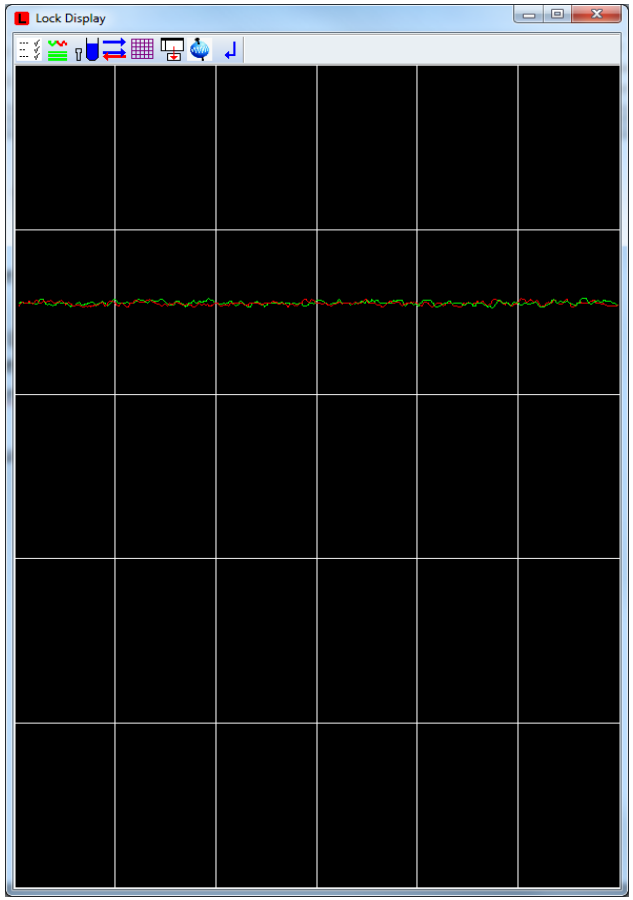
Type "***atma***" in the command line or select TUNE in the PROCEDURE.
The command "atma" allow you to automatically tune and match the probe.
You will see the process flash on the screen



SHIM the magnets

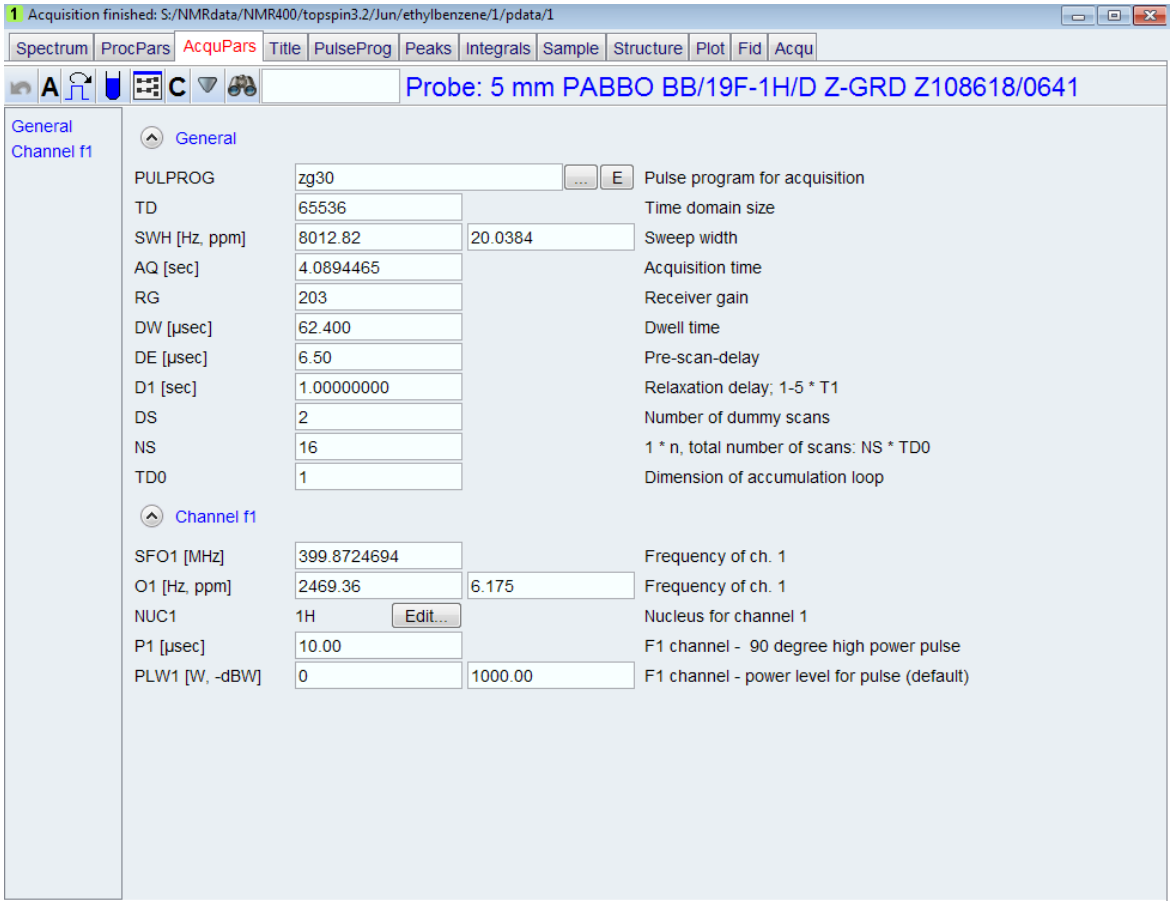
Type "***topshim***" in the command line or select shim in the PROCEDURE.
The command "topshim" performs a gradient shimming on the magnets, you will see the lock signal increased after the topshim.

After topshim completed, you may check the experimental condition again and
Start data acqusition.



Adjust parameter

Type "***ased***" to adjust some of the experimental parameters if you wish.
You may change the number of scan, sweep width and different pulse program, etc.



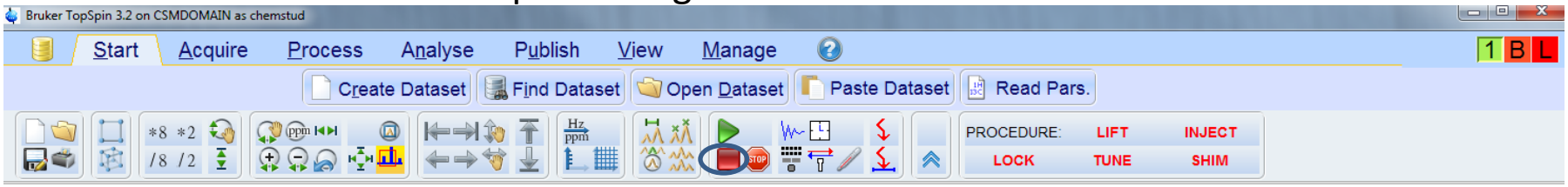
Start an acquisition

Type "*zg*" or click on the green button in the tab to start a acquisition.

Click on the clock icon to see how much time is remaining for each experiment.

Stop, halt an acquisition

To stop the acquisition before reaching the specified number of scans, enter "***halt***", which will write your data to the disk at the end of the current scan and allow processing.



Enter "***stop***" or clicking the stop icon, will terminate acquisition immediately but will not save your data, your data will be lost!

If you wish to process and examine the data already acquired and you wish to leave the acquisition running e.g to check the S/N ratio, you most force the data onto disk from the computer memory, where it's held during the acquisition. Use the transfer command for this: "***tr***".