

# FIVE steps to use IMSERC NMR

1. Login to [NUCORE](#) with your **netid** and logon to the instrument:
  - a) turn on the computer monitor at instrument,
  - b) your usage count starts
2. Login to instrument with your **operator id** (usually same as netid)
3. Load your sample and run your experiment
4. Logout from the instrument
5. Login to [NUCORE](#) and logout your instrument session:
  - a) turn off the computer monitor at instrument,
  - b) your usage count stops

Linux/IconNMR account: walkon

# Common Commands/Parameters in TopSpin

## Setting up experiments & Processing

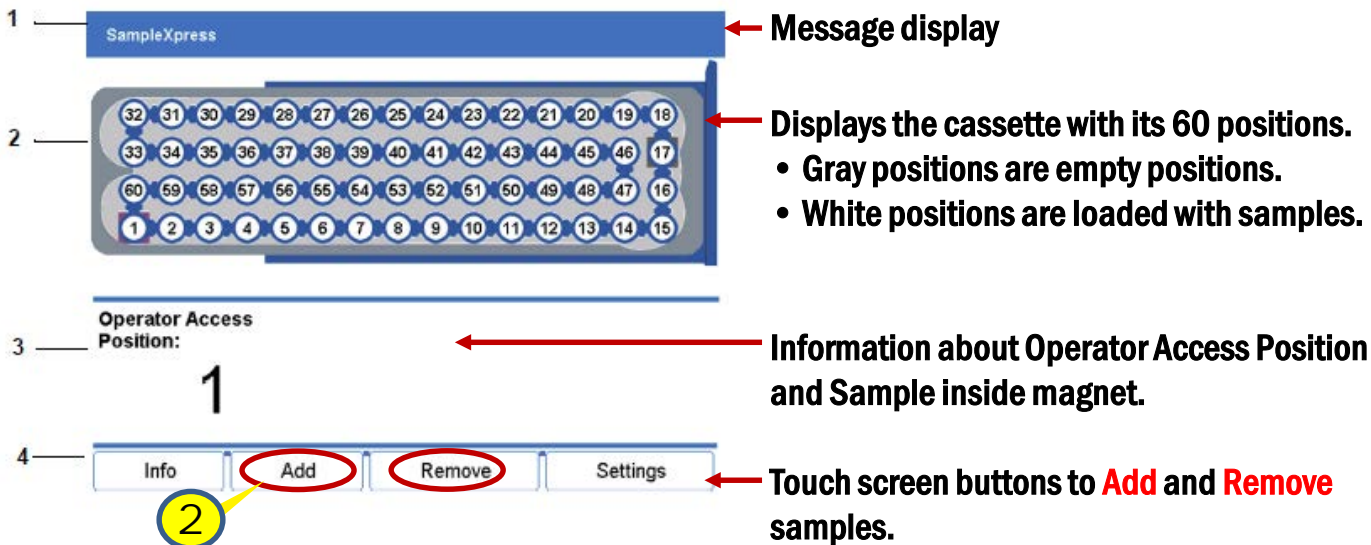
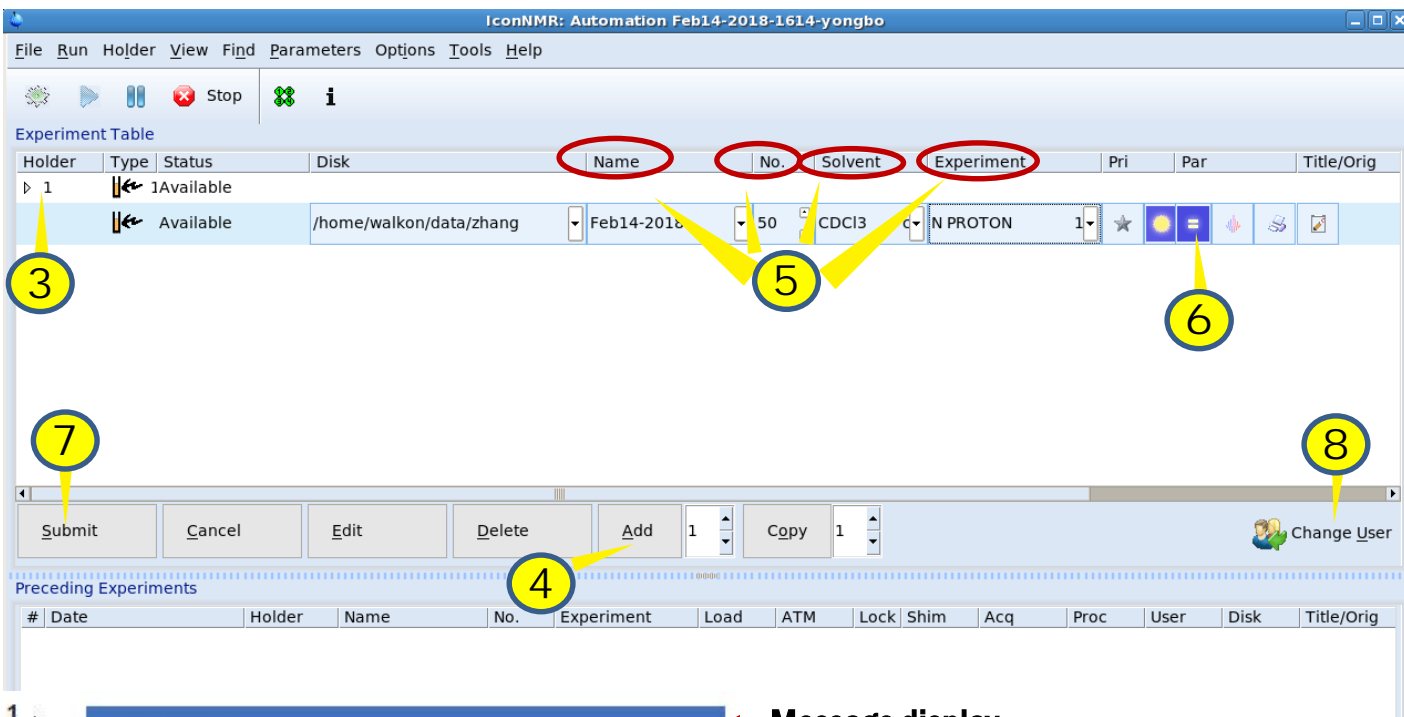
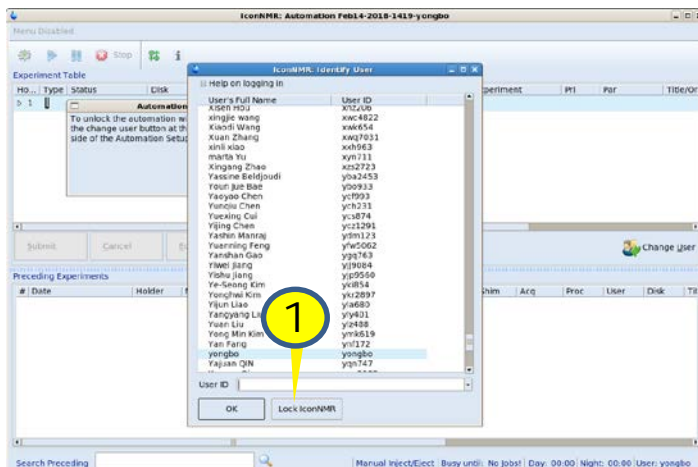
<b>sx 10</b>	to put #10 (could be any position) sample on the autosampler into magnet.
<b>sx ej</b>	to put sample inside magnet back to the autosampler
<b>rga</b>	automatically set receiver gain
<b>zg</b>	start acquisition
<b>tr</b>	transfer data (while acquisition is in progress)
<b>multizg</b>	start multiple acquisitions starting from current dataset
<b>go</b>	submit experiment to acquisition
<b>stop</b>	abort an acquisition, losing all the FID data recorded so far
<b>halt</b>	halt the running acquisition, saving the recorded FID data to hard disk
<b>efp</b>	weighted Fourier Transformation for 1D dataset
<b>apk</b>	do automatic phase correction
<b>abs</b>	automatically optimize baseline
<b>xfb</b>	weighted Fourier Transformation for 2D dataset

## Important parameters for acquisition

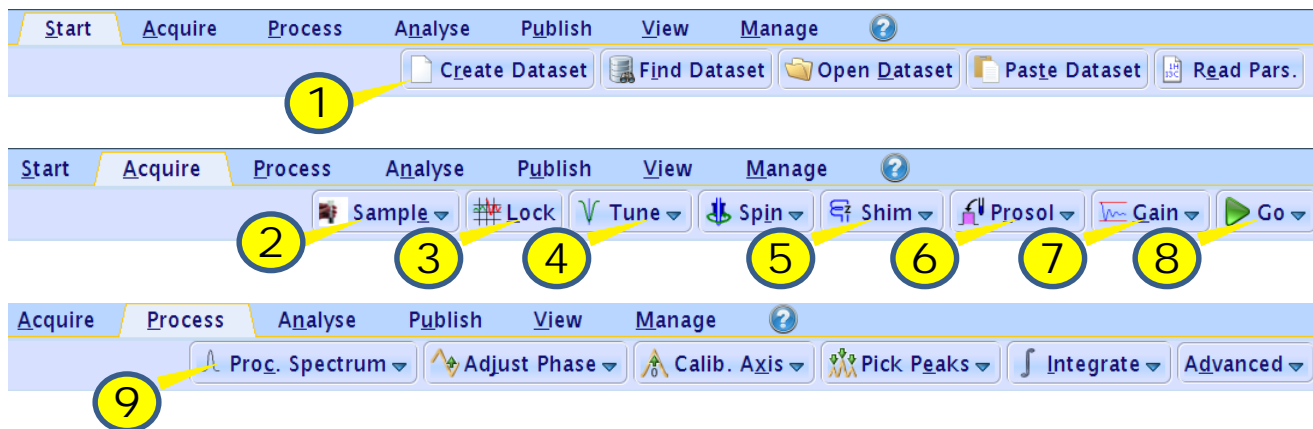
<b>P1</b>	F1 channel 90° pulse width, micro seconds
<b>P2</b>	F1 channel 180° pulse width
<b>RG</b>	Receiver gain
<b>D1</b>	relaxation delay, 1 to 5 times T1
<b>2TD</b>	Time domain data points for F2 (direct dimension)
<b>2SW</b>	spectral width in ppm for F2 (direct dimension)
<b>1TD</b>	Time domain data points for F1 (indirect dimension)
<b>1SW</b>	spectral width in ppm for F1 (indirect dimension)
<b>AQ</b>	Acquisition time in seconds
<b>NS</b>	Number of scans
<b>DS</b>	Number of dummy scans
<b>NUC1 – NUC8</b>	Nucleus observed (1H, 13C, 31P, 19F, etc.)
<b>O1 – O8</b>	Frequency offset for channel 1 – 8 in Hz
<b>O1P – O8P</b>	Freq. offset for channels 1 – 8 in ppm
<b>SFO1 – SFO8</b>	Freq. for channels 1 – 8 in MHz

# Setup experiment using ICONNMR w/ SampleXpress

1. Login with your operator ID
2. Load your sample to SampleExpress
3. Click the Holder # where you sample is loaded.
4. Click Add
5. Fill in following fields: Name, No., Solvent, and Experiment
6. Change parameters if needed
7. Click Submit
8. Logout ICON by clicking on "change user"



# Workflow to interactively setup experiment with TopSpin



1. Create new dataset and setup initial parameters
2. Insert/Eject Sample
3. Lock on your selected Solvent
4. Tune/Match the Probe to the nucleus of your expt
5. Shim
6. Load probe related parameters
7. Auto set receiver gain
8. Acquire fid
9. Process data

The red arrowed fields below need to be filled, red circled parameters in next page can be changed based on your need

- Sample name
- Experiment number
- Experiment to run
- Solvent used
- Directory for the dataset (your folder under your group name)

Prepare for a new experiment by creating a new data set and initializing its NMR parameters according to the selected experiment type. For multi-receiver experiments several datasets are created. Please define the number of receivers in the Options.

NAME: yw1-042

EXPNO: 3

PROCNO: 1

Use current parameters

Experiment: 13C [Select]

Options

Set solvent: C2D2Cl4

Execute 'getprosol'

Keep parameters: P 1, O1, PLW 1 [Change]

DIR: /home/walkon/data/Marks/ygq763

Show new dataset in new window

Number of additional datasets: (1,2, ...16): 1

TITLE: [Empty]

[OK] [Cancel] [More Info...] [Help]

# Parameters setting for 1D and 2D experiments

1 presat 1 1 /home/walkon/data/zhang

Spectrum ProcPars **AcquPars** Title PulseProg Peaks Integrals Sample Structure Plot Fid Acqu

Probe: PA BBO 600S3 BB-H-D-05 Z BTO

General Channel f1

General

PULPROG	zgpr	...	E	Pulse program for acquisition
TD	32768			Time domain size
SWH [Hz, ppm]	9615.38	16.0212		Sweep width
AQ [sec]	1.7039360			Acquisition time
RG	203			Receiver gain
DW [µsec]	52.000			Dwell time
DE [µsec]	6.50			Pre-scan-delay
D1 [sec]	2.000000000			Relaxation delay; 1-5 * T1
d12 [sec]	0.00002000			Delay for power switching [20 usec]
DS	0			Number of dummy scans
NS	4			1 * n, total number of scans: NS * TD0
TD0	1			Number of averages in 1D

Channel f1

SFO1 [MHz]	600.1678208			Frequency of ch. 1
O1 [Hz, ppm]	2820.78	4.700		Frequency of ch. 1
NUC1	1H	Edit...		Nucleus for channel 1
P1 [µsec]	12.700			F1 channel - 90 degree high power pulse
PLW1 [W, dB]	31.623	-15.00		F1 channel - power level for pulse (default)
PLW9 [W, dB]	0.00020402	36.90		F1 channel - power level for presaturation

1 tp35 12 1 /home/walkon/data/zhang

Spectrum ProcPars **AcquPars** Title PulseProg Peaks Integrals Sample Structure Plot Fid Acqu

Probe: PA BBO 600S3 BB-H-D-05 Z BTO

Experiment Width Receiver Nucleus Durations Power Program Probe Lists NUS Wobble Lock Automation Miscellaneous User Routing

Experiment

PULPROG	hsqcetgp	...	E	Current pulse program
AQ_mod	DQD			Acquisition mode
FnTYPE	traditional(planes)			nD acquisition mode for 3D etc.
FnMODE		Echo-Antiecho		Acquisition mode for 2D, 3D etc.
TD	1024	256		Size of fid
DS	16			Number of dummy scans
NS	8			Number of scans
TD0	1			Loop count for 'td0'
TDav	0			Average loop counter for nD experiments

Width

SW [ppm]	20.0264	165.0000		Spectral width
SWH [Hz]	12019.230	24902.283		Spectral width

2 RR 3 1 /home/walkon/data/zhang

Spectrum ProcPars **AcquPars** Title PulseProg Peaks Integrals Sample Structure Plot Fid Acqu

Probe: PA BBO 600S3 BB-H-D-05 Z BTO

Experiment Width Receiver Nucleus Durations Power Program

Nucleus 1

NUC1	1H	Edit...	13C	Observe nucleus
O1 [Hz]	2820.78		11318.37	Transmitter frequency offset
O1P [ppm]	4.700		75.000	Transmitter frequency offset
SFO1 [MHz]	600.1678208		150.9229277	Transmitter frequency