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

- `sx 10` to put #10 (could be any position) sample on the autosampler into magnet.
- `sx ej` to put sample inside magnet back to the autosampler
- `rga` automatically set receiver gain
- `zg` start acquisition
- `tr` transfer data (while acquisition is in progress)
- `multizg` start multiple acquisitions starting from current dataset
- `go` submit experiment to acquisition
- `stop` abort an acquisition, losing all the FID data recorded so far
- `halt` halt the running acquisition, saving the recorded FID data to hard disk

- `efp` weighted Fourier Transformation for 1D dataset
- `apk` do automatic phase correction
- `abs` automatically optimize baseline
- `xfb` weighted Fourier Transformation for 2D dataset

Important parameters for acquisition

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

### General Channel f1

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PULPROC</td>
<td>egpr</td>
<td>Pulse program for acquisition</td>
</tr>
<tr>
<td>TD</td>
<td>32768</td>
<td>Time domain size</td>
</tr>
<tr>
<td>SWH [Hz, ppm]</td>
<td>9615.38, 16.0212</td>
<td>Acquisition width</td>
</tr>
<tr>
<td>AQ [sec]</td>
<td>1.7093860</td>
<td>Acquisition time</td>
</tr>
<tr>
<td>RG</td>
<td>203</td>
<td>Receiver gain</td>
</tr>
<tr>
<td>DW [usec]</td>
<td>52.000</td>
<td>Dwell time</td>
</tr>
<tr>
<td>DE [psec]</td>
<td>6.50</td>
<td>Pre-scan-delay</td>
</tr>
<tr>
<td>D1 [sec]</td>
<td>2.0000000000</td>
<td>Relaxation delay, 1-5 * T1</td>
</tr>
<tr>
<td>d12 [sec]</td>
<td>0.00002000</td>
<td>Delay for power switching [20 usec]</td>
</tr>
<tr>
<td>NS</td>
<td>4</td>
<td>Number of dummy scans: NS * TDO</td>
</tr>
<tr>
<td>TDO</td>
<td>1</td>
<td>Number of averages in 1D</td>
</tr>
</tbody>
</table>

### Channel f1

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SF01 [MHz]</td>
<td>600.1678208</td>
<td>Frequency of ch. 1</td>
</tr>
<tr>
<td>Q1 [Hz, ppm]</td>
<td>2820.78, 4.700</td>
<td>Frequency of ch. 1</td>
</tr>
<tr>
<td>NUC1</td>
<td>1H</td>
<td>Nucleus for channel 1</td>
</tr>
<tr>
<td>P1 [usec]</td>
<td>12.700</td>
<td>F1 channel - 90 degree high power pulse</td>
</tr>
<tr>
<td>PLW1 [W, dB]</td>
<td>31.823, -15.00</td>
<td>F1 channel - power level for pulse (default)</td>
</tr>
<tr>
<td>PLW9 [W, dB]</td>
<td>0.00020402, 36.30</td>
<td>F1 channel - power level for presaturation</td>
</tr>
</tbody>
</table>

### Experiment

#### F2

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PULPROC</td>
<td>hsqetgdp</td>
<td>Current pulse program</td>
</tr>
<tr>
<td>AQ_mode</td>
<td>DOD</td>
<td>Acquisition mode</td>
</tr>
<tr>
<td>FnTYPE</td>
<td>traditional</td>
<td>nD acquisition mode for 3D etc.</td>
</tr>
<tr>
<td>FnMODE</td>
<td>Echo-Antiecho</td>
<td>Acquisition mode for 2D, 3D etc.</td>
</tr>
<tr>
<td>TD</td>
<td>1024</td>
<td>Size of fid</td>
</tr>
<tr>
<td>DS</td>
<td>16</td>
<td>Number of dummy scans</td>
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<tr>
<td>NS</td>
<td>8</td>
<td>Number of scans</td>
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<tr>
<td>TDO</td>
<td>1</td>
<td>Loop count for ‘tD0’</td>
</tr>
<tr>
<td>TDav</td>
<td>0</td>
<td>Average loop counter for nD experiments</td>
</tr>
</tbody>
</table>

#### F1

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SW [ppm]</td>
<td>20.0264, 165.0000</td>
<td>Spectral width</td>
</tr>
<tr>
<td>SWH [Hz]</td>
<td>12019.230, 24902.283</td>
<td>Spectral width</td>
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</tbody>
</table>

### Nucleus 1

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td>NUC1</td>
<td>1H</td>
<td>Observe nucleus</td>
</tr>
<tr>
<td>O1 [Hz]</td>
<td>2820.78, 4.700</td>
<td>Transmitter frequency offset</td>
</tr>
<tr>
<td>O1P [ppm]</td>
<td>75.00</td>
<td>Transmitter frequency offset</td>
</tr>
<tr>
<td>SF01 [MHz]</td>
<td>600.1678208</td>
<td>Transmitter frequency</td>
</tr>
</tbody>
</table>