How to submit a sample to an existing automation.

#1) Insert your sample onto the autosampler. Make sure your NMR tube is tall enough and there is enough sample, using the guide on the wall. Take note of which sample holder your sample is in.
#2) In the ICON-NMR window, click the Change User button (right side, middle). Choose your username.
#3) Double click on the row corresponding to the sample holder. Enter the name for your dataset (generally the page number in a lab notebook), the solvent and the experiment (see list of approved experiments). To add additional experiments click the add button in the middle panel.
#4) Click the submit button to add your experiments to the automation.
#5) Click the Change User button and select the user "cmld-scc".
Approved Experiments for the CMLD-SCC NMR

CMLD/SCC users,

Unfortunately the NMR lab cannot guarantee that every NMR experiment works flawlessly 100% of the time. The following experiments have been tested using a sample of 1% heptanone in CDCl3 and 50 mg/ml of Cholesterol in CDCl3 and we are reasonably sure they will work for any suitably concentrated samples. Please use the listed parameter sets. If you need additional experiments, let Justin know.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Parameter Set</th>
<th># scans</th>
<th>additional info</th>
<th>time</th>
</tr>
</thead>
<tbody>
<tr>
<td>1D 1H</td>
<td>PROTON</td>
<td>16</td>
<td></td>
<td>1 min 29 sec</td>
</tr>
<tr>
<td>1D 13C w/1H decoupling</td>
<td>C13CPD</td>
<td>512</td>
<td>d1 = 1s</td>
<td>20 min 53 sec</td>
</tr>
<tr>
<td>1D 13C DEPT135 (CH,CH3-positive; CH2 negative)</td>
<td>C13DEPT135</td>
<td>256</td>
<td></td>
<td>14 min 46 sec</td>
</tr>
<tr>
<td>1D 13C APT</td>
<td>C13APT</td>
<td>256</td>
<td></td>
<td>14 min 47 sec</td>
</tr>
<tr>
<td>2D 1H COSY</td>
<td>AACOSY</td>
<td>2 x 256</td>
<td></td>
<td>14 min 49 sec</td>
</tr>
<tr>
<td>2D 1H NOESY</td>
<td>AANOESY</td>
<td>2 x 256</td>
<td>mixing time = 500 ms</td>
<td>23 min 51 sec</td>
</tr>
<tr>
<td>2D 1H-13C HSQC</td>
<td>AAHSQC</td>
<td>4 x 256</td>
<td></td>
<td>37 min 29 sec</td>
</tr>
<tr>
<td>2D 1H-13C HMBC</td>
<td>AAHMBC</td>
<td>16 x 128</td>
<td></td>
<td>1 hour, 7 min, 18 sec</td>
</tr>
</tbody>
</table>
1) Wait until all experiments have finished running. Click on red X on the top left of the automation window. This stops the current automation. Remember that if there are any additional experiments in the queue, those will be lost! It is your responsibility to resubmit those samples in the new automation.

2) Click on Change User in the box that pops open. Change to the CMLD-SCC account.

3) If prompted enter the CMLD-SCC password. Click YES to stop the run.

4) Go to FILE and select SAVE.

5) Close the automation window.

6) Select “Automation” from the ICON-NMR: Spect Window box

7) Select CMLD-SCC for User ID. Enter the CMLD-SCC password.

8) Click the green icon (looks like a gear) to start the automation. In the pop-up box, click the "Start" button.

9) Change User to your username.

10) Add experiments to the new automation.
NMR rules proposal 2

#1) Peak Hours, 10 AM to 6 PM

No more than 30 min per person counting lock and shim times (For example: using default settings this would be about 1 proton and 1 carbon or COSY experiment or 3 proton experiments). You cannot place more samples until after your first 30 min of samples have completed, so as to allow others the opportunity to place samples into the queue. Priority button will be disabled.

#2) Off-Peak Hours, 8 AM to 10 AM and 6 PM to 9 PM

No more than 45 min per person counting lock and shim times (For example 2 proton and 2 carbon experiments or 5 protons using default settings). You cannot place more samples until after your first 45 min of samples have completed, so as to allow others the opportunity to place samples into the queue. Priority button will be disabled.

#3) Overnight Hours, 9 PM to 8 AM

No more than 4 hours per person per night can be scheduled until after 6 PM. After 6 PM additional time can be scheduled in open slots. If more than 4 hours of time is required for a single experiment, use of the cryoprobe service is encouraged. Experiments must be finished by 8 AM.