How to submit a sample to an existing automation.

#1) Insert you sample onto the autosampler. Make sure your NMR tube is tall enough and there is enough sample, using the guide on the wall. Take not 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 resonably sure they will work for any suitably concentrated samples. Please use the listed parameter sets. If you need additional experiments, let Justin know.

Experiment	Parameter Set	# scans	additional info	time
1D 1H	PROTON	16		1 min 29 sec
1D 13C w/1H decoupling	C13CPD	512	d1 = 1s	20 min 53 sec
1D 13C DEPT135 (CH,CH3-positive; CH2 negative)	C13DEPT135	256		14 min 46 sec
1D 13C APT	C13APT	256		14 min 47 sec
2D 1H COSY	AACOSY	2 x 256		14 min 49 sec
2D 1H NOESY	AANOESY	2 x 256	mixing time = 500 ms	23 min 51 sec
2D 1H-13C HSQC	AAHSQC	4 x 256		37 min 29 sec
2D 1H-13C HMBC	AAHMBC	16 x 128		1 hour, 7 min, 18 sec

Opening A New Automation Page – In Ten Easy Steps

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 auomation. 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.