

ICON-NMR USER GUIDE (SampleExpress)

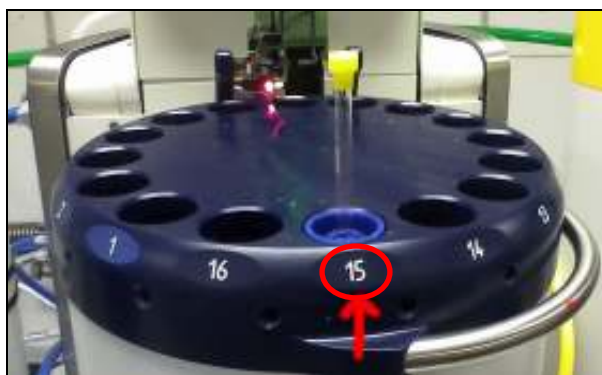
Starting IconNMR:

If IconNMR is not open, start TopSpin. Enter the command "iconnmr". Click the Automation button to begin.



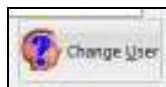
Experiment Setup:

- 1.) Place your sample into any open compartment of the NMR carousel. Remember which sample holder number you used.




Now that nighttime experiments have been enabled, please do NOT remove other users' samples without first checking the IconNMR queue to make sure the sample is marked Finished!

- 2.) Click the "Change User" button to make sure the correct user is selected.



- 3.) In the Experiment Queue, find the experiment with the same sample holder number as you used on the carousel. Enter the information for your experiment.



- Name – enter your sample name here
- Experiment types:
 - N PROTON – 1H experiment with 16 scans
 - N 13CCPD – 13C experiment with 1024 scans
 - N 13CDEPT135 – DEPT135 with 1024 scans
- (Optional) Change the number of scans with the  button. The software will automatically reject the experiment if it is too long.
- (Optional) If you wish to run more than one experiment on the sample, (i.e. a proton and a carbon) right click on the experiment and choose "Add". Enter the details for your additional experiment.

4.) Click the **Submit** button to queue your experiment(s). If yours is the first experiment, make sure the **Start** button has been clicked.



Processing:

Data from the experiments will be automatically transferred to the left processing computer. You can access it by opening TOPSPIN and finding your group's name under the "C:\400A" directory.

Night-time experiments:

- 301B Night-time hours are 11PM to 8 AM.
- 400A Night-time hours are 9PM to 9AM
- Night experiments can be longer than daytime experiments
 - 4 hours maximum on 400A
 - 6 hours maximum on 301B
- Night-time experiments can be submitted before night-time begins!
 - To submit your experiment as a night-time experiment, click the sun icon beside the experiment. The sun should change to a moon.
- Your experiment will be added to the night queue. The experiments in the queue will automatically begin once the night-time hours begin.