

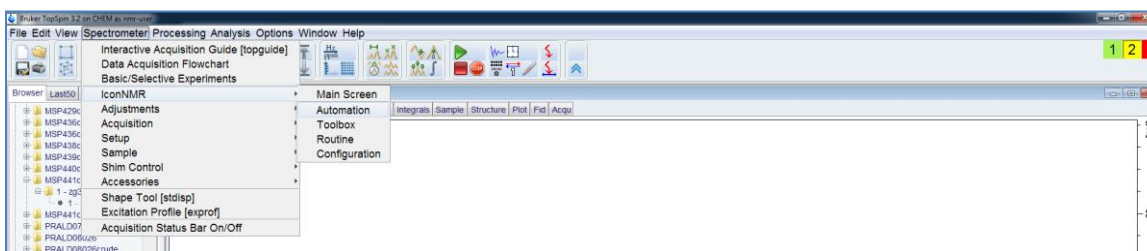
Use of ICON-NMR for Automated NMR Operation

It is essential that all group user time on the spectrometers is booked online using the NMR instrument booking sheet. Please include your name and contact details. Please note that the ICON-NMR interface may only be used for **ambient temperature** experiments.

As with manual Topspin operation, login to the spectrometer with the "nmr-user" domain account and open Topspin. It is advisable to check the probe temperature is properly equilibrated- the current probe temperature may be seen in the lower right status display panel and the default is 298K.

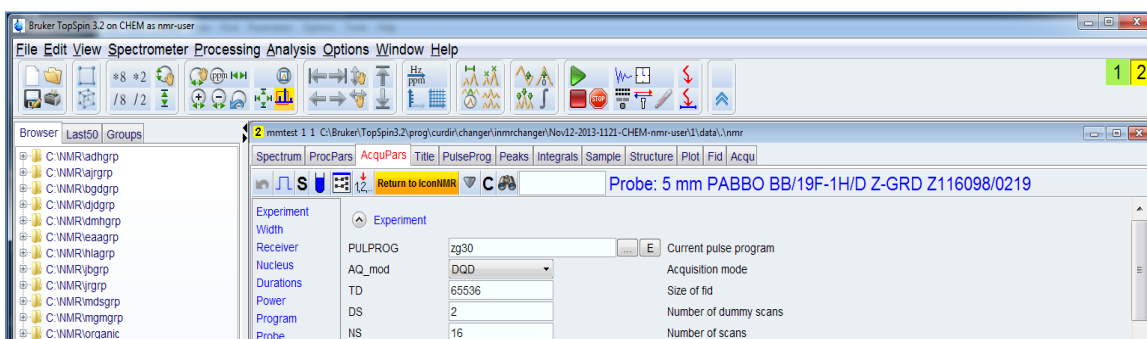
Fid Flash	Lock	Sample	Sample Temperature Corr. 298.0 K On <input checked="" type="checkbox"/> Reg. State: <input checked="" type="checkbox"/>	Spooler queued: 0 delayed: 0 cron: 0	Time 13:36:36 Nov 14
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Check whether ICON-NMR is already open. If necessary, open a new ICON-NMR interface window by clicking on **Spectrometer** and scroll down to **ICON-NMR** and across to **Automation**, as shown below. In the **ICON-NMR: Set User** window select the CHEM\nmr-user **User ID**, click **OK** and enter the password.

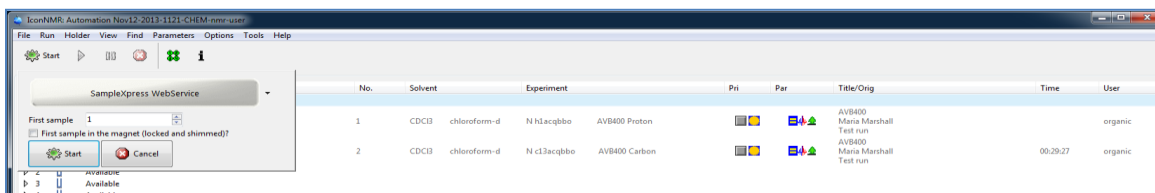
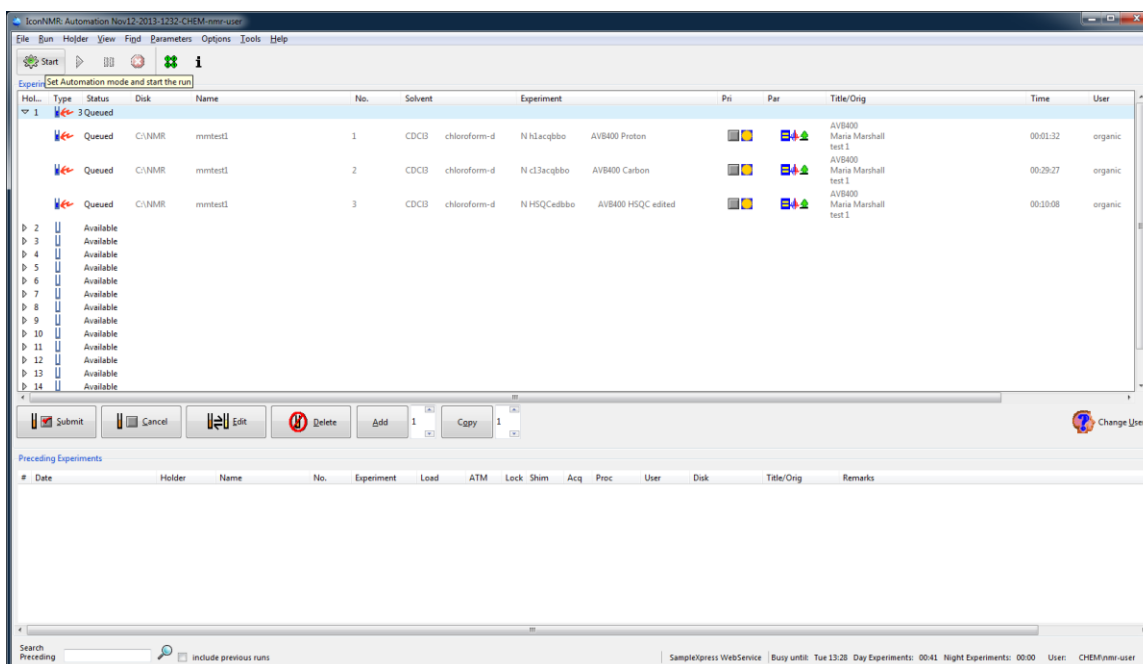


To submit your first sample, double click on **Available** next to an available Holder position (e.g. 1) which will open the sample entry menus. Enter your sample name, starting with your initials (**DO NOT** include non-standard characters such as * ! " ; etc and it is advisable not to include spaces in data set names). Select your solvent and experiment. If you wish to edit the number of scans (NS) click on the **Parameter** icon (blue box with yellow strips). Click on the **Notepad** icon to enter your details and experiment title; **Set and Copy** this to save for all experiments.

To view/edit the full acquisition parameter set, click on **Parameters** (top left) and scroll down to **Edit all Acquisition Parameters**. To return to ICON-NMR, **YOU MUST** click on **Return to ICON-NMR**, as shown below:



Now place your sample in the corresponding position on the carousel. To queue your sample, click on the **Submit** icon (bottom left). Check that all the experiments for your sample have been queued. To start the run in ICON-NMR, change to the *nmr-user* account click on the green **Start** icon (top left cog wheel, see below). In the **Initialise Run** window check that the **First sample** is set to your holder position. [If you have already collected data on your sample (eg to check the ^1H is OK) and it is already in the magnet locked and shimmed you may also select “**First sample in magnet (locked and shimmed)?**” to skip these processes]. Next, click on the **Start** button.



ICON-NMR will now perform automatic tuning, locking, and shimming of your sample and automatic acquisition and processing of data. All data produced through ICON-NMR will be archived to group folders on the departmental NMR data server (within the appropriate instrument folder).

To open the **ICON-NMR Online Controls** window, click on the **i** icon (top left). Here you may view the current experiment information. Also, you may use the control buttons to halt acquisitions, after which the spectra will be processed as usual and any following experiments executed. Data may be viewed in TOPSPIN by double-clicking on any experiment in the lower history window.

