

DCIF NMR Training Guide

IconNMR on the 401 MHz

Bruker AVANCE III HD b401

last edit 4/9/2015

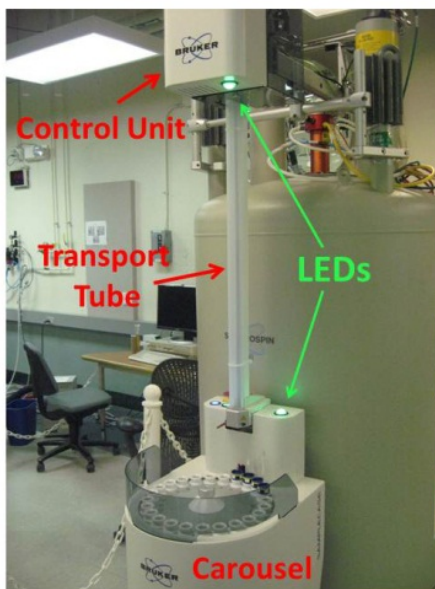
The Bruker AVANCE III HD 401 has a broadband (BBO) probe with a ^1H Channel and X-Channel tunable from (30-300 MHz). Both channels may be tuned automatically by the TopSpin 3.2 software. The 401 has variable temperature capabilities and has a SampleCase (sample changer) attached to it.

This training guide is for using the automation called **IconNMR**. You must have an account on the 401 in order to use IconNMR.

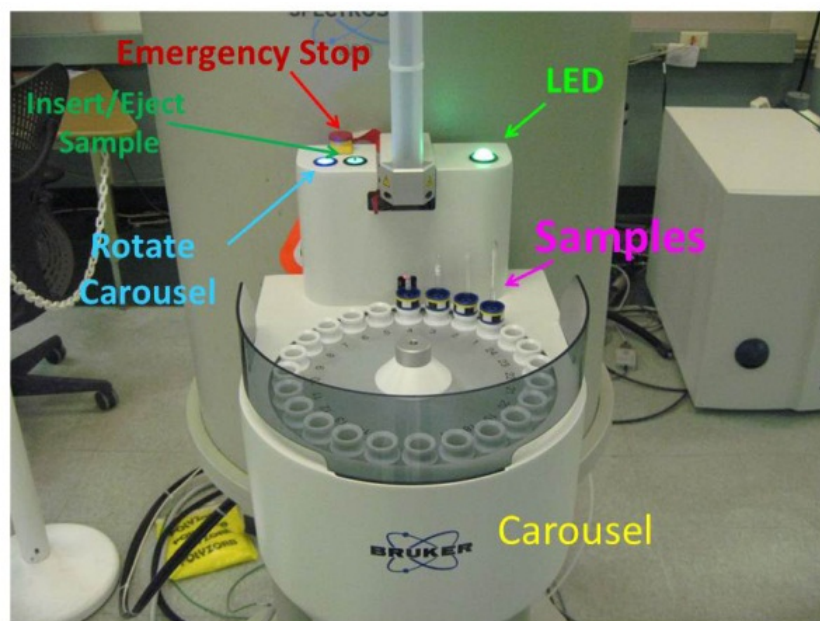
Loading your sample:

There is a *SampleCase* sample changer attached to the 401. Under NO circumstances is anything to be placed on the carousel of the *SampleCase*. Do not lean on any part *SampleCase*. Do not bump, jostle, or smack any part of the *SampleCase*.

Place your sample in any empty slot in the *SampleCase*'s carousel. Note the position number that you have placed your sample.



Close-up of the Carousel

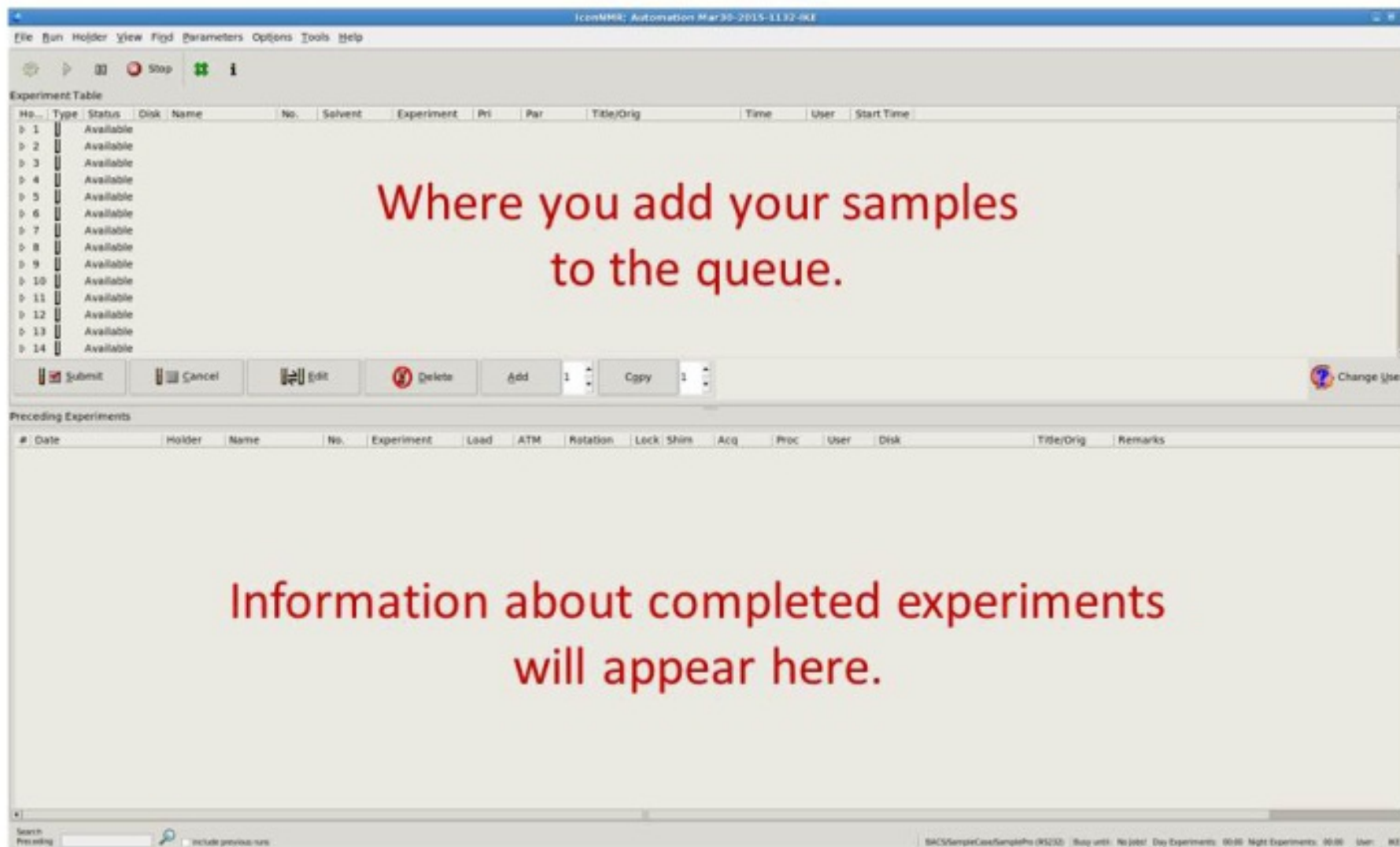


The carousel can hold 24 samples.

Make sure your sample is correctly adjusted in the depth gauge and does not exceed the maximum height.

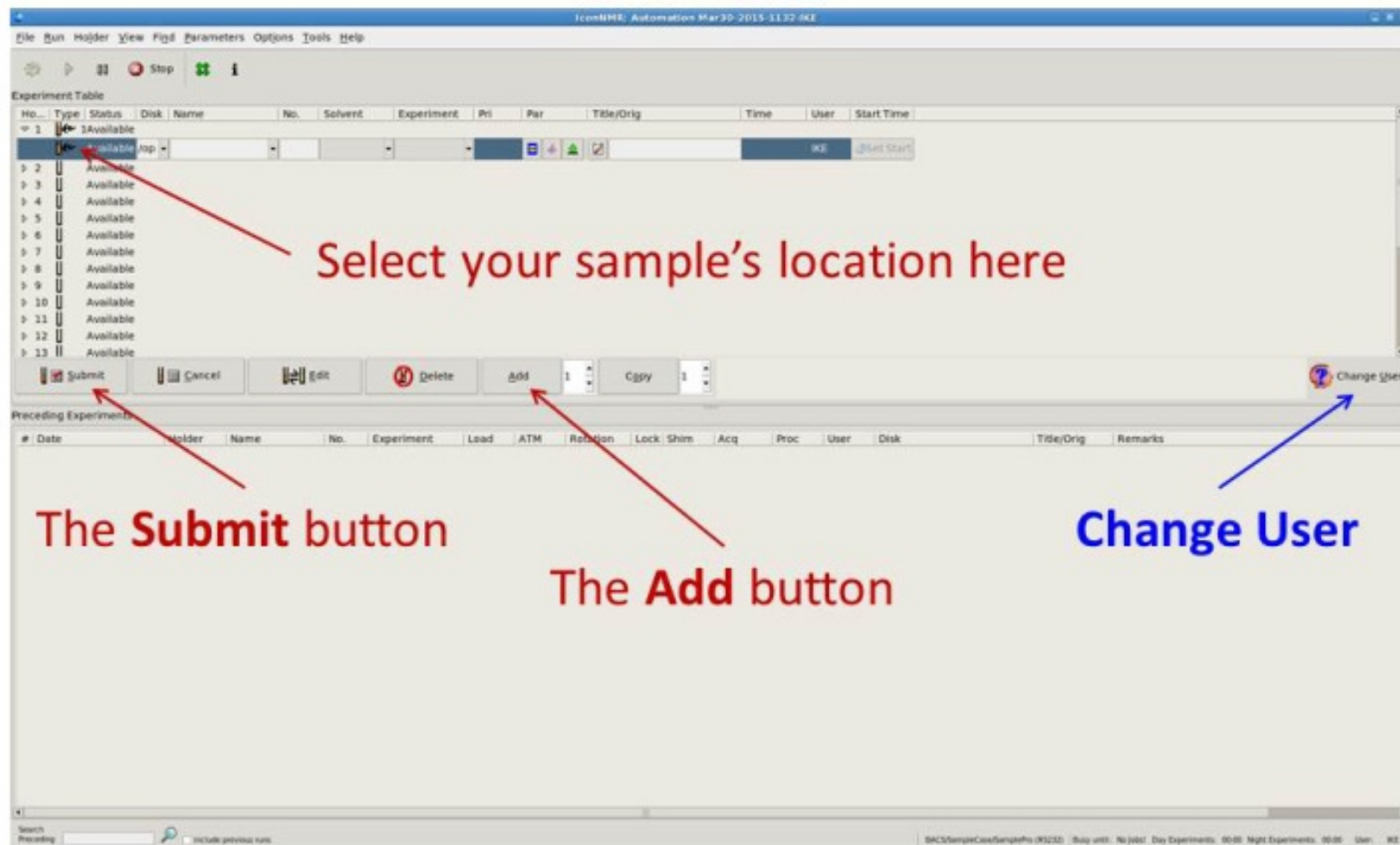


The IconNMR window should already be open. Do not attempt to close, shrink, move, or adjust the size of this window.



If you have a question about what a button does, you can hover your mouse over the button without pressing it, and it will tell you what it does.

Double click on the number that corresponds to your sample's position in the carousel. It should read **Available**. Do not change *Disk* (where your data will be stored). In the *Name* box, give your sample a filename (no spaces or funny characters like \$ # @ or *). Use the arrow to open a drop down menu and select the *Solvent* and what *Experiment* you would like run. If you click the blue and yellow equal sign, you can adjust parameters like **ns**, **sw**, **aq**, and **o1p**. In *Title*, type whatever information you want.



If you want to run multiple experiments on the same sample, make sure you have that position selected and click the Add button. Fill out the necessary information. Once you have entered all of the samples you want run, hold down the Shift button and select all of the experiments you want run. Then click the Submit button. This will start the run.

Click the **Change user** button when done. Once you do so, no other user can edit or change your sample's information.

If an experiment has finished and the sample has been removed from the carousel by a DCIF staff member, you can load your sample. You will have to click **Change user** and enter your password. In the top window, you left click to select the finished experiment that is in the slot you want to use. A window should open up. Right click on *Delete*. The slot should now read *Available*. You can now enter the information for your sample and submit it.

The screenshot shows the IcenHMR Automation software interface. The main window displays the 'Experiment Table' with columns: No., Type, Status, Disk, Name, No., Solvent, Experiment, Pri, Par, Title/Orig, Time, User, and Start Time. The table lists three experiments: 1 (Finished), 2 (Finished), and 11 (Finished). Experiment 11 is highlighted in blue. A red arrow points to the 'Finished' status of experiment 11, with the text 'Finished experiment' overlaid in red. Below the table is a toolbar with buttons: Submit, Cancel, Edit, Delete, Add, Copy, and Change User. The 'Preceding Experiments' section at the bottom shows a list of previous experiments with columns: #, Date, Holder, Name, No., Experiment, Load, ATM, Rotation, Lock, Shim, Acq, Proc, User, Disk, Title/Orig, and Remarks. The status bar at the bottom indicates the current user is 'IKE' and the system is ready for the next experiment.

No.	Type	Status	Disk	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
1	1	Finished	/opt/test406	10	CDC13	1H-dcl				test406	00:01:32	IKE	10:17 Mon
2	2	Finished	/opt/test406a	10	CDC13	1H-dcl				test406a	00:01:32	IKE	10:19 Mon
11	1	Finished	/opt/test406a	11	CDC13	13C-CPD-dcl				test406a	00:02:03	IKE	10:24 Mon
3		Available											
4		Available											
5		Available											
6		Available											
7		Available											
8		Available											
9		Available											
10		Available											
11		Available											

#	Date	Holder	Name	No.	Experiment	Load	ATM	Rotation	Lock	Shim	Acq	Proc	User	Disk	Title/Orig	Remarks
3	2015-04-06 10:29:06	2	test406a	11	13C-CPD-dcl	✓	✓	✓	✓	✓	✓	✓	IKE	/opt/data/IKE/nmr	test406a	sref: reference peak not found default calibration done
2	2015-04-06 10:24:07	2	test406a	10	1H-dcl	✓	✓	✓	✓	✓	✓	✓	IKE	/opt/data/IKE/nmr	test406a	sref: reference peak not found default calibration done
1	2015-04-06 10:17:59	1	test406	10	1H-dcl	✓	✓	✓	✓	✓	✓	✓	IKE	/opt/data/IKE/nmr	test406	sref: reference peak not found default calibration done

NOTE: All data from samples run in IconNMR can be found in
/opt/data/<UserID>/nmr

In you want to see your IconNMR data in TopSpin on the spectrometer computer, you need to add a new data directory. In the left Browser window, right click anywhere. A window will appear. Select **Add New Data Dir....**

DIR = /opt/data/<UserID>/nmr

Alias = Icon Data

Click ok.

If you have a problem with IconNMR or the SampleCase, please let a DCIF staff member know. If it is after hours, you can email dcifhelp@mit.edu. This goes to a group of student volunteers that may be able to help you.

