

Bruker Icon NMR

UofA Chemistry Step-By-Step Visual Reference Guide

These instructions are currently specific for the new (*i.e.* 2023) Bruker Avance NEO i400 (Room SB-3E) with 60 position SampleCase robot, and will also be applicable to the Bruker Avance NEO ibd500, and 800MHz spectrometers with TopSpin Version 4.x ICON NMR and slightly smaller SampleCase robotic sample handling.



Table of Contents

Special Notes	3
How to Run a Bruker Automated NMR Sample	4
1.) Login ... but make sure the last user logged Out	4
2.) Your “password” is required.....	5
3.) Preparing and Loading your Sample.....	5
4.) Selecting Sample Position.....	7
5.) Free up a used Sample Slot (if all spots used)	8
6.) Add Experiments for the Sample.....	9
7.) Name the Sample Experiment in EACH Experiment Slot.....	9
8.) Select Solvent	10
9.) Select Experiments	11
10.) Edit Parameters	12
11.) Select Day or Night Queue	12
12.) Everything ready for submission	13
13.) Submit Experiments	13
14.) Do not forget to “Change User” (<i>i.e.</i> Log Out) – You are Done!	14
15.) How to retrieve a blocked sample from the carousel.....	14
Appendix – Colours of the Queue.....	15
Appendix – Another Example of Freeing up Slot for Complete Sample	16

See the subsequent pages for detailed explanation, examples with pictures.

Special Notes

Caps Lock Disabled

The caps lock button is disabled on all workstations and spectrometer. Users would leave on and cause havoc.

Do NOT reboot computers

If the computer is not working, frozen, or otherwise misbehaving tell NMR staff.

Do not try to fix yourself.

Processing, printing, annotating etc.

That is meant for workstations, please free up spectrometers as soon as you for other users.

Pick up samples when done.
Don't leave samples on the robots.

How to Run a Bruker Automated NMR Sample

1.) Login ... but make sure the last user logged Out

The screen should be asking for Login (See Identify User Panel in **Figure 1**). Scroll through the list or type your name to search and then select your account by double clicking the correct login or select and hit “OK” button.

If the last person has forgotten to logout, or entered the wrong password, you will see **Figure 2**.

If this is the case, please log them out and/or try the password again by using the “Change User” button in the top right. (**Figure 2** – see Red Box and Red Arrow indicating Change User Icon).

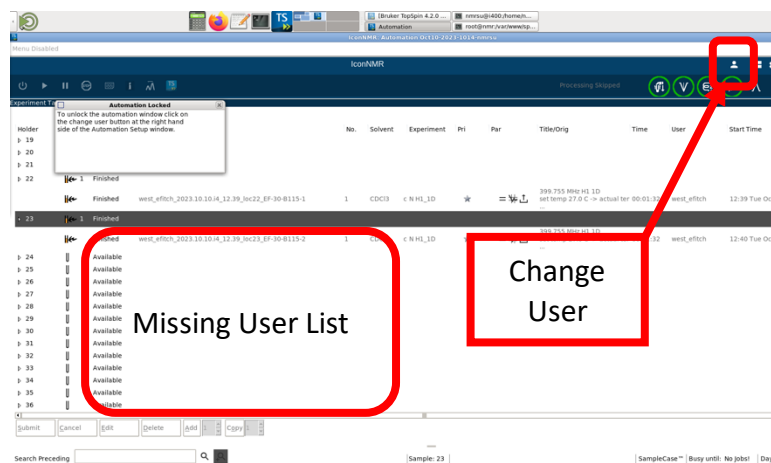


Figure 2 – Last User Forgot to Logout

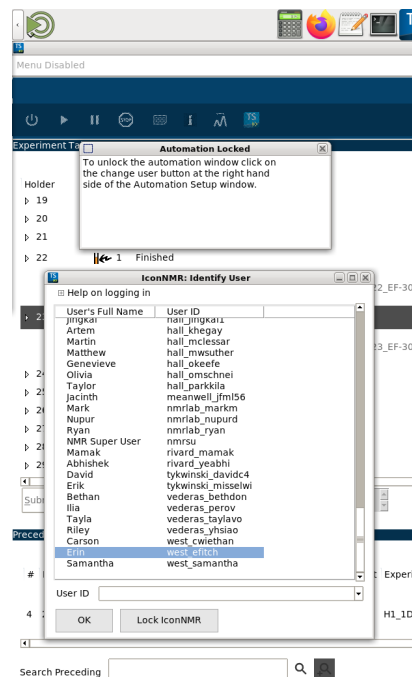


Figure 1 – Correct Start Screen

**** DO NOT FORGET TO LOGOUT when done with “Change User” every time, otherwise the next person could use the wrong account and your lab will be charged \$\$ for the experiments...¹**

¹ ...and users will never find their data...great sadness and confusion...re-invoicing of charges, ...etc.

2.) Your “password” is required.

Please enter your:

**Personal Online User Registration
Password**

NOT your lab’s account password.

*** This is different from the
Varian/Agilent Spectrometers**

Yes, the password you use to book spectrometers and entered when you registered. Forgot? Contact NMR staff.

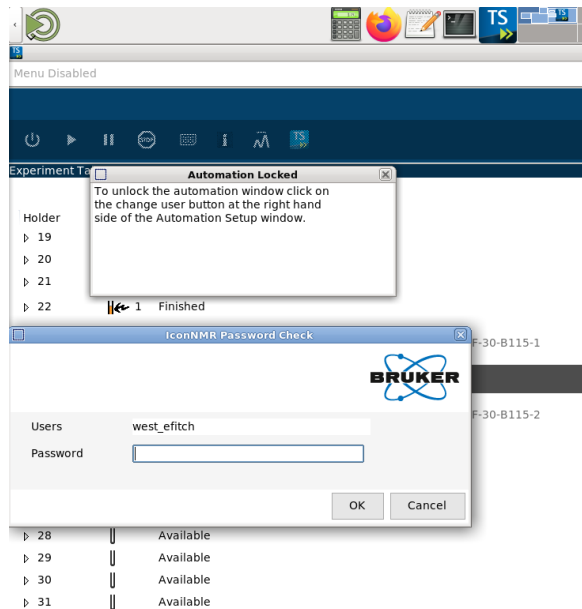


Figure 3 – Enter your online user password

3.) Preparing and Loading your Sample

Go over to the sample “Rack” (see **Figure 4**) and select an open position. Attach your label on the rack at the correct location of the spinner being used (see Spinner numbering in **Figure 5**). If all positions are used, you will have to retrieve a **finished** sample from the SampleCase robot and clear a space in the software (see below). Check the Bruker TopSpin-Icon software for which samples have run and are done. When you’ve found a finished sample, remove the sample from the spinner, reattach the corresponding label (if any) from the spinner rack back onto the NMR tube, and carefully place the re-labelled sample inside the sample return holder (**Figure 8**, next page). You may then use the spinner.

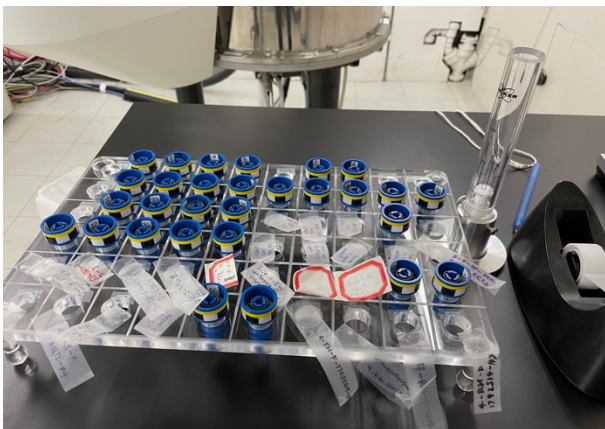


Figure 4 – Examples of spinners in use and labels at sample positions

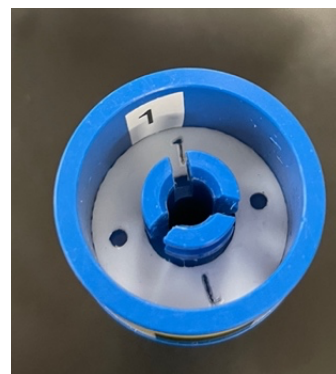


Figure 5 –Example of Spinner Numbering

Notice the spinner numbers. Always match the correct robot and storage rack position for the correct spinner number.

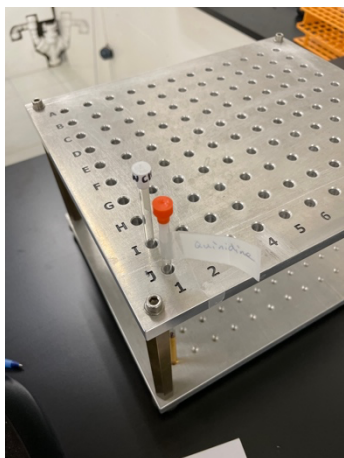


Figure 8 – Sample Holder

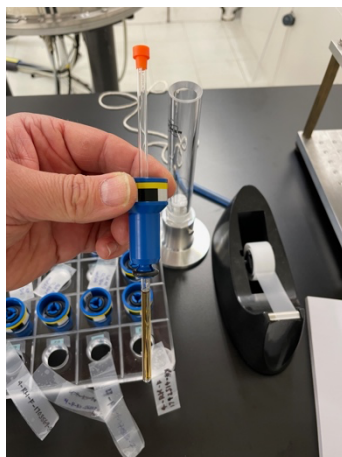


Figure 7 – Sample in Spinner

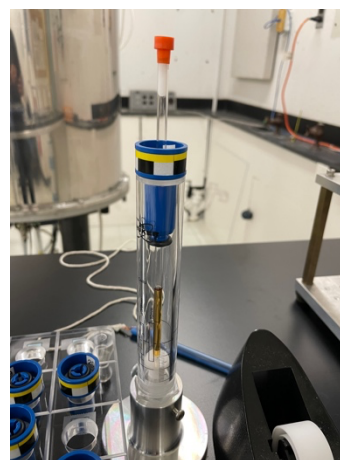


Figure 6 – Depth Gauge – sample set properly

Insert your sample in the spinner (**Figure 7**) and set the sample depth using the gauge (**Figure 6**). Then place your sample/spinner in the robot at the matching carousel number for your spinner number.

When placing the sample in the carousel, make sure the carousel is not moving. Gently lower sample into position, do not drop.



Figure 10 – Emergency Stop and Reset Button

Do NOT bump/hit the **Height Detect Bar (Figure 9 Red Box)**. If you do, everything will halt as the robot will panic, and the lights will be red.

Please contact NMR staff and get help.

Emergency Stop Button

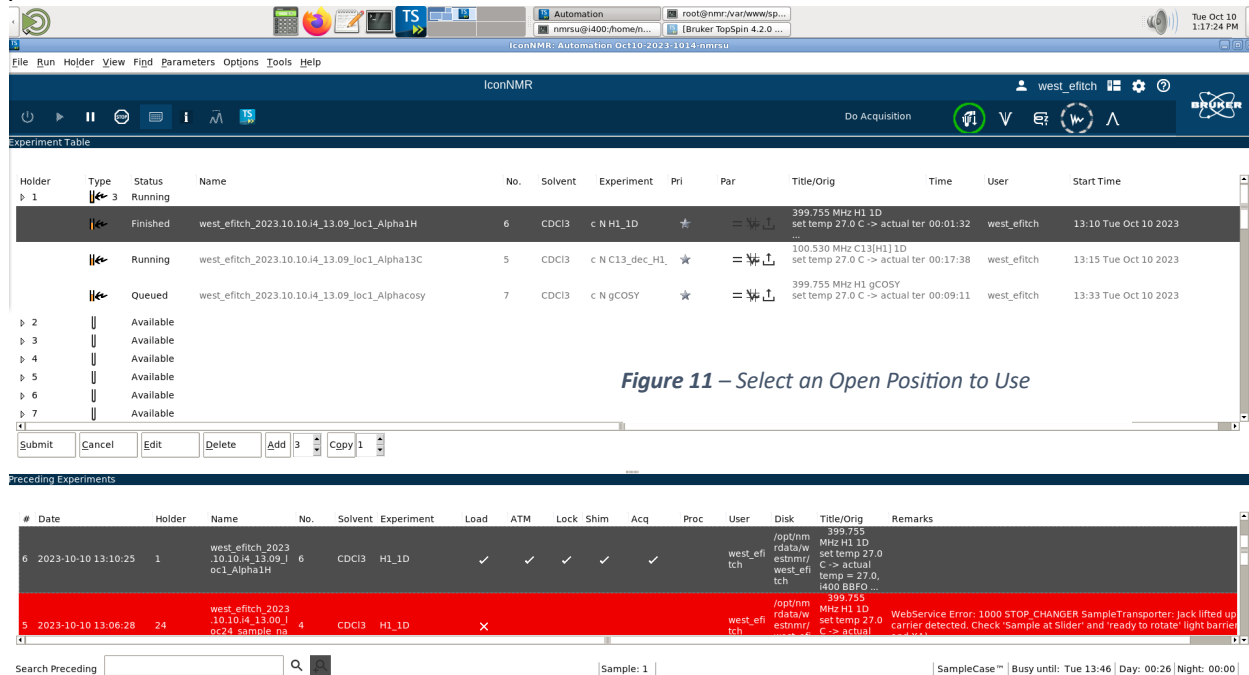
You may use the Emergency Stop (**Figure 10**) to halt operations if needed (e.g. robot is damaging equipment/misbehaving or hurting someone, etc.). Press the red button down, you'll hear a clunk. Contact NMR staff immediately.



Figure 9 – Height Detect Bar

4.) Selecting Sample Position

Back at the computer you will now need to select the carousel position where you have placed your sample. In the example below (**Figure 11**), Sample 1 is busy acquiring, but the other positions are available to select.

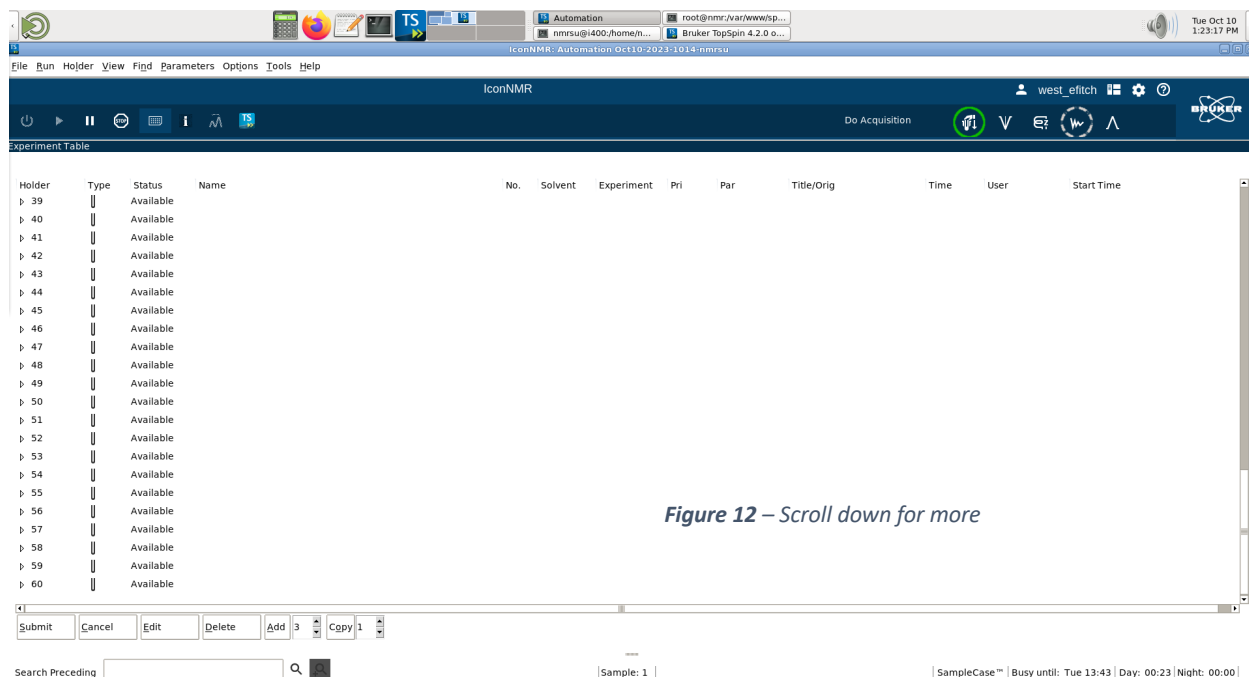


The screenshot shows the IconNMR software interface. The 'Experiment Table' section displays a list of experiments with columns for Holder, Type, Status, Name, No., Solvent, Experiment, Pri, Par, Title/Orig, Time, User, and Start Time. The first three rows are highlighted in grey, indicating they are selected. The first row is 'Finished', the second is 'Running', and the third is 'Queued'. The remaining rows (2-7) are 'Available'. The 'Preceding Experiments' section shows a list of previous experiments with columns for #, Date, Holder, Name, No., Solvent, Experiment, Load, ATM, Lock, Shim, Acq, Proc, User, Disk, Title/Orig, and Remarks. The second row in this section is highlighted in red, indicating it is the current experiment.

Holder	Type	Status	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
1	3	Finished	west_efitch_2023.10.10.i4_13.09_loc1_Alpha1H	6	CDCI3	c N H1_ID	*		399.755 MHz H1 1D set temp 27.0 C -> actual ter 00:01:32		west_efitch	13:10 Tue Oct 10 2023
	3	Running	west_efitch_2023.10.10.i4_13.09_loc1_Alpha13C	5	CDCI3	c N C13_dec_H1	*		100.530 MHz C13[H1] 1D set temp 27.0 C -> actual ter 00:17:38		west_efitch	13:15 Tue Oct 10 2023
	3	Queued	west_efitch_2023.10.10.i4_13.09_loc1_Alphacosy	7	CDCI3	c N gcOSY	*		399.755 MHz H1 gcOSY set temp 27.0 C -> actual ter 00:09:11		west_efitch	13:33 Tue Oct 10 2023
2		Available										
3		Available										
4		Available										
5		Available										
6		Available										
7		Available										

Figure 11 – Select an Open Position to Use

You may also scroll further down the sample list for more open positions (**Figure 12**).



The screenshot shows the IconNMR software interface with the 'Experiment Table' section. The list of experiments is scrolled down to show positions 39 through 60. All positions in this range are listed as 'Available'. The 'Preceding Experiments' section is also visible at the bottom of the screen.

Holder	Type	Status	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
39		Available										
40		Available										
41		Available										
42		Available										
43		Available										
44		Available										
45		Available										
46		Available										
47		Available										
48		Available										
49		Available										
50		Available										
51		Available										
52		Available										
53		Available										
54		Available										
55		Available										
56		Available										
57		Available										
58		Available										
59		Available										
60		Available										

Figure 12 – Scroll down for more

5.) Free up a used Sample Slot (if all spots used)

If all sample positions are used, you will need to release a “Finished” sample spot. **Figure 13** shows an example of us selecting Sample 24 (i.e. not the experiment slots) then going down to the “Delete” option to remove the entire sample selection (e.g. we changed our mind). You may remove “Finished” samples (see Status window below), or a sample you were about to submit. Another option is to right-click the Holder Number, and select “Delete” if finished.

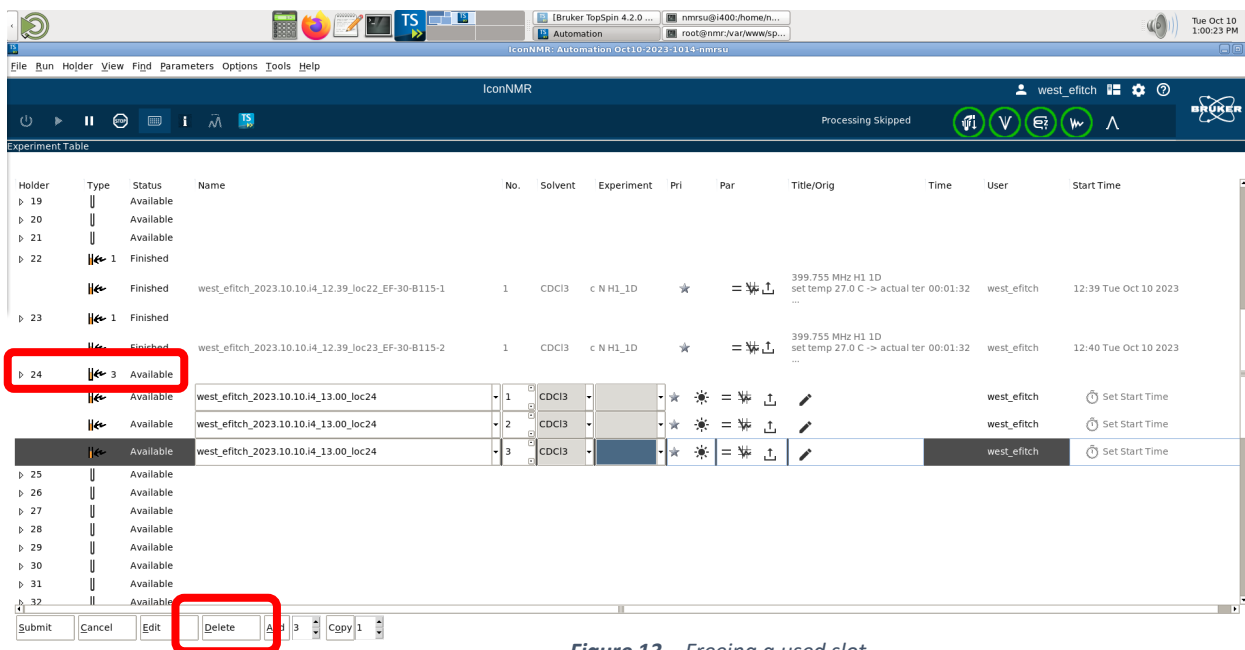
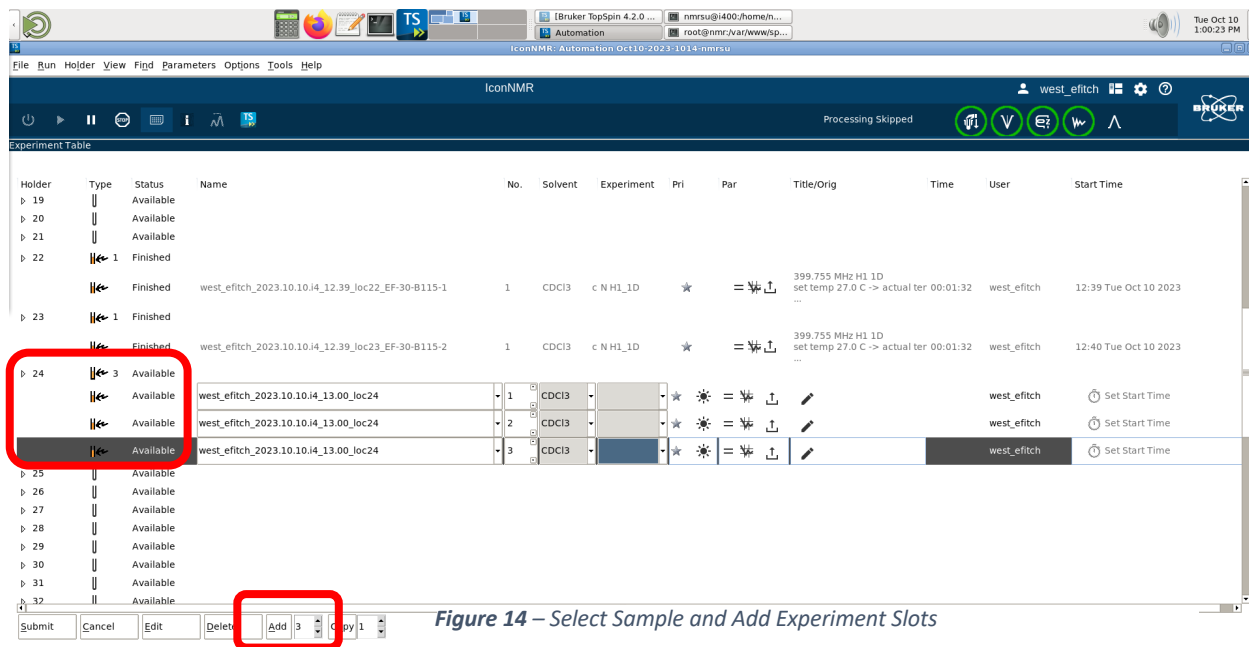


Figure 13 – Freeing a used slot

ONLY remove Status = “Finished” samples. Never try to interfere with a running sample, or samples submitted to the queue.

6.) Add Experiments for the Sample

In this example we have clicked on and chosen position 24 (left box) in the list, then opened “3” slots by selecting three experiments (bottom box) then hitting the “Add” button (see **Figure 14** red boxes). We now have 3 open experiment slots to use, we can add more, cancel, remove later, or modify as desired.



The screenshot shows the IconNMR software interface. The Experiment Table is visible, with position 24 selected. Three experiment slots are added to position 24. The 'Add' button is highlighted with a red box.

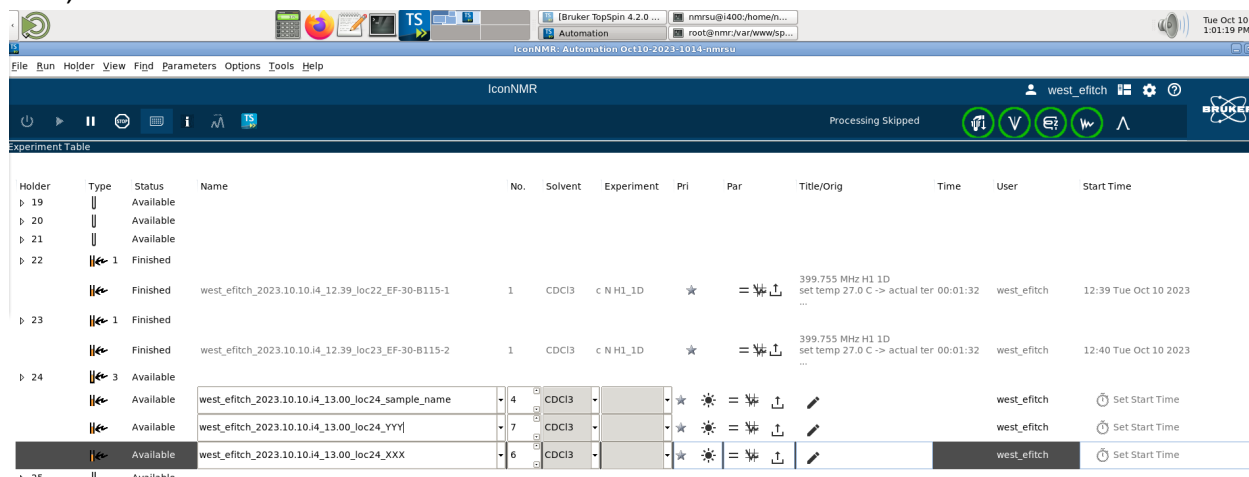
Holder	Type	Status	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
p 19	U	Available										
p 20	U	Available										
p 21	U	Available										
p 22	U	Finished										
p 22	U	Finished	west_efitc_2023.10.10.i4_12.39_loc22_EF-30-B115-1	1	CDCI3	c N H1_1D	*	=	399.755 MHz H1 1D set temp 27.0 C -> actual ter 00:01:32		west_efitc	12:39 Tue Oct 10 2023
p 23	U	Finished										
p 23	U	Finished	west_efitc_2023.10.10.i4_12.39_loc23_EF-30-B115-2	1	CDCI3	c N H1_1D	*	=	399.755 MHz H1 1D set temp 27.0 C -> actual ter 00:01:32		west_efitc	12:40 Tue Oct 10 2023
p 24	U	Available										
p 24	U	Available	west_efitc_2023.10.10.i4_13.00_loc24	1	CDCI3		*	=			west_efitc	Set Start Time
p 24	U	Available	west_efitc_2023.10.10.i4_13.00_loc24	2	CDCI3		*	=			west_efitc	Set Start Time
p 24	U	Available	west_efitc_2023.10.10.i4_13.00_loc24	3	CDCI3		*	=			west_efitc	Set Start Time
p 25	U	Available										
p 26	U	Available										
p 27	U	Available										
p 28	U	Available										
p 29	U	Available										
p 30	U	Available										
p 31	U	Available										
p 32	U	Available										

Figure 14 – Select Sample and Add Experiment Slots

It is important to note that the position number itself (e.g. 24) doesn’t let you do anything until you add experiments.

7.) Name the Sample Experiment in EACH Experiment Slot

In the example below (**Figure 15**) we’ve named the first experiment “_sample_name”, the second “YYY”, third “XXX”. Name yours appropriately, and remember we add date, instrument, time, etc.



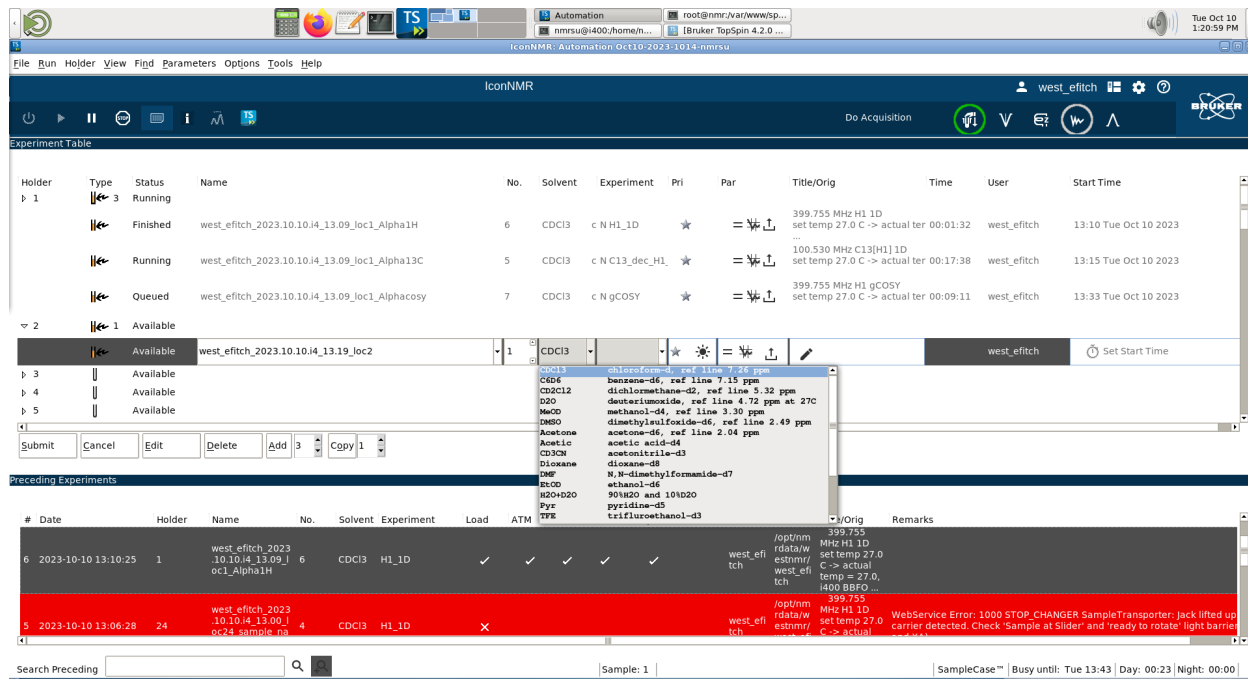
The screenshot shows the IconNMR software interface. The Experiment Table is visible, with position 24 selected. Three experiment slots are added to position 24, each with a unique name.

Holder	Type	Status	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
p 19	U	Available										
p 20	U	Available										
p 21	U	Available										
p 22	U	Finished										
p 22	U	Finished	west_efitc_2023.10.10.i4_12.39_loc22_EF-30-B115-1	1	CDCI3	c N H1_1D	*	=	399.755 MHz H1 1D set temp 27.0 C -> actual ter 00:01:32		west_efitc	12:39 Tue Oct 10 2023
p 23	U	Finished										
p 23	U	Finished	west_efitc_2023.10.10.i4_12.39_loc23_EF-30-B115-2	1	CDCI3	c N H1_1D	*	=	399.755 MHz H1 1D set temp 27.0 C -> actual ter 00:01:32		west_efitc	12:40 Tue Oct 10 2023
p 24	U	Available										
p 24	U	Available	west_efitc_2023.10.10.i4_13.00_loc24_sample_name	4	CDCI3		*	=			west_efitc	Set Start Time
p 24	U	Available	west_efitc_2023.10.10.i4_13.00_loc24_YYY	7	CDCI3		*	=			west_efitc	Set Start Time
p 24	U	Available	west_efitc_2023.10.10.i4_13.00_loc24_XXX	6	CDCI3		*	=			west_efitc	Set Start Time
p 25	U	Available										

Figure 15 – Name the Sample in Experiment Slots

8.) Select Solvent

For each experiment slot, please specify the solvent for your sample (see **Figure 16** and **Figure 17**).



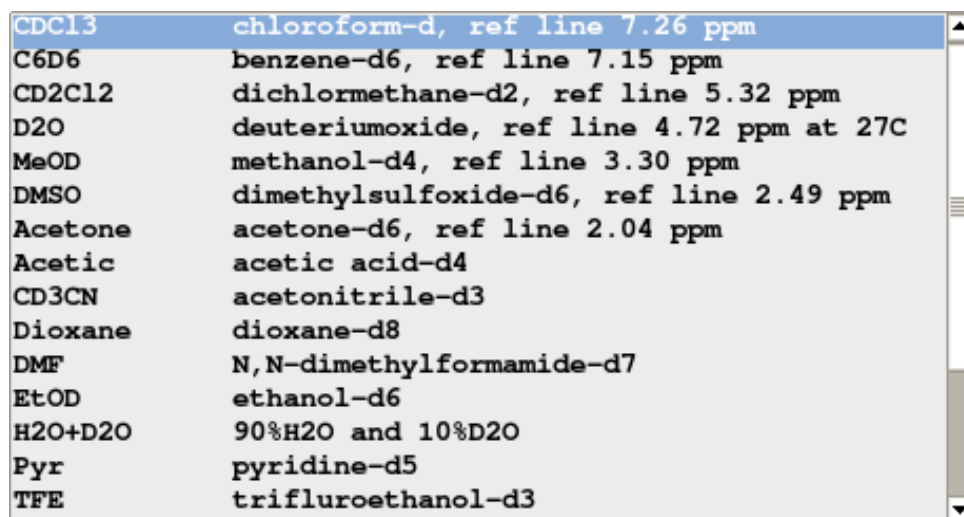
The screenshot shows the Bruker IconNMR software interface. The 'Experiment Table' is visible, listing several experiments with their respective solvents and statuses. A dropdown menu is open, showing a list of available solvents with their corresponding reference lines. The 'Preceding Experiments' table is also visible, showing the history of experiments.

Holder	Type	Status	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
1	3	Running	west_efitch_2023.10.10.i4_13.09_loc1_Alpha1H	6	CDCl3	c N H1_1D	*	=	399.755 MHz H1 1D set temp 27.0 C -> actual ter 00:01:32	00:01:32	west_efitch	13:10 Tue Oct 10 2023
		Finished	west_efitch_2023.10.10.i4_13.09_loc1_Alpha13C	5	CDCl3	c N C13_dec_H1	*	=	100.530 MHz C13[H1] 1D set temp 27.0 C -> actual ter 00:17:38	00:17:38	west_efitch	13:15 Tue Oct 10 2023
		Queued	west_efitch_2023.10.10.i4_13.09_loc1_Alphacosy	7	CDCl3	c N gCOSY	*	=	399.755 MHz H1 gCOSY set temp 27.0 C -> actual ter 00:09:11	00:09:11	west_efitch	13:33 Tue Oct 10 2023
2	1	Available	west_efitch_2023.10.10.i4_13.19_loc2	1	CDCl3						west_efitch	Set Start Time

#	Date	Holder	Name	No.	Solvent	Experiment	Load	ATM	V/Orig	Remarks
6	2023-10-10 13:10:25	1	west_efitch_2023_10.10.i4_13.09_loc1_Alpha1H	6	CDCl3	H1_1D	✓	✓	399.755 MHz H1 1D set temp 27.0 C -> actual temp = 27.0, 1400 B8FO...	
5	2023-10-10 13:06:28	24	west_efitch_2023_10.10.i4_13.09_loc24_sample_na	4	CDCl3	H1_1D	✗	✗	399.755 MHz H1 1D set temp 27.0 C -> actual	WebService Error: 1000 STOP_CHANGER SampleTransporter: Jack lifted up carrier detected. Check 'Sample at Slider' and 'ready to rotate' light barrier

Figure 16 – Solvent selection

Close up view of solvents, scroll down for more options.



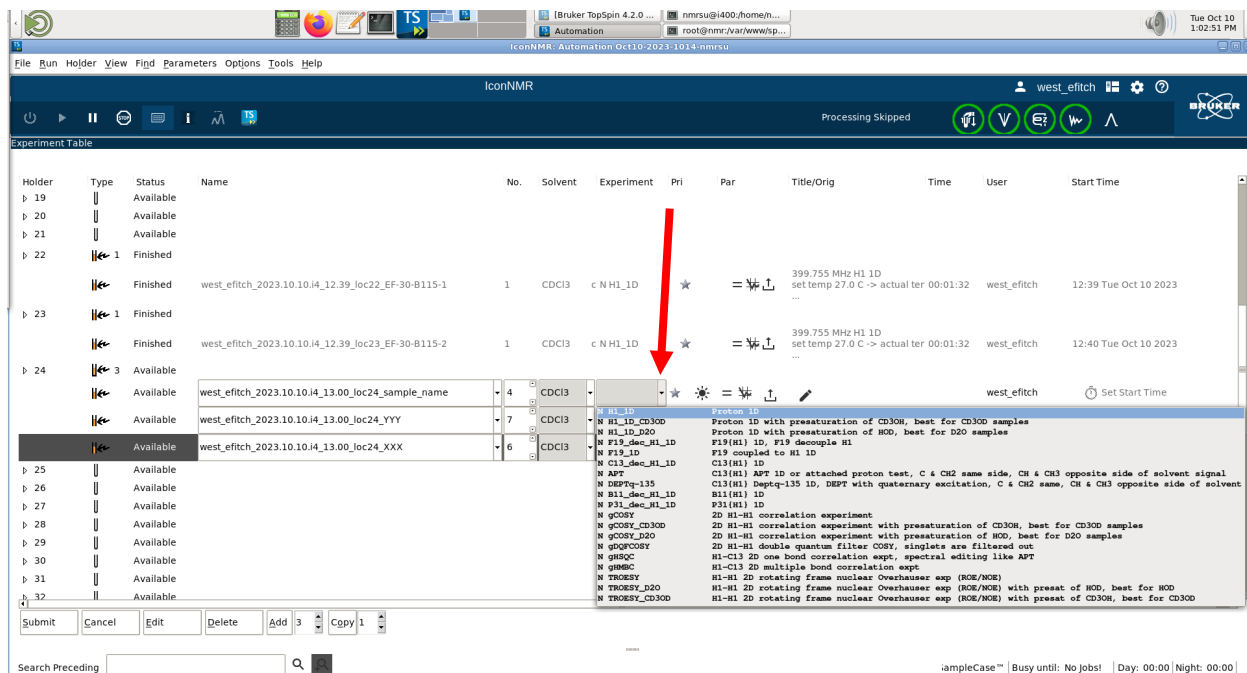
This image shows a close-up of the solvent selection dropdown menu. The list of solvents is as follows:

- CDCl3 chloroform-d, ref line 7.26 ppm
- C6D6 benzene-d6, ref line 7.15 ppm
- CD2Cl2 dichloromethane-d2, ref line 5.32 ppm
- D2O deuteriumoxide, ref line 4.72 ppm at 27C
- MeOD methanol-d4, ref line 3.30 ppm
- DMSO dimethylsulfoxide-d6, ref line 2.49 ppm
- Acetone acetone-d6, ref line 2.04 ppm
- Acetic acetic acid-d4
- CD3CN acetonitrile-d3
- Dioxane dioxane-d8
- DMF N,N-dimethylformamide-d7
- EtOD ethanol-d6
- H2O+D2O 90%H2O and 10%D2O
- Pyr pyridine-d5
- TFE trifluoroethanol-d3

Figure 17 - Zoom in of available solvents

9.) Select Experiments

From the drop-down list (**Figure 18** and **Figure 19**), select the desired experiment for each slot. If you want more experiments, add more slots.



The screenshot shows the IconNMR software interface. The 'Experiment Table' is visible, listing various experiments. A red arrow points to a dropdown menu in the 'Experiment' column, which is currently set to 'c N H1_1D'. The dropdown menu is open, showing a list of available experiments for selection.

Holder	Type	Status	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
▷ 19	U	Available										
▷ 20	U	Available										
▷ 21	U	Available										
▷ 22	U	Finished										
	U	Finished	west_effch_2023.10.10.i4_12.39_loc22_EF-30-B115-1	1	CDCl3	c N H1_1D	★	=	399.755 MHz H1 1D set temp 27.0 C -> actual ter 00:01:32	00:01:32	west_effch	12:39 Tue Oct 10 2023
▷ 23	U	Finished										
	U	Finished	west_effch_2023.10.10.i4_12.39_loc23_EF-30-B115-2	1	CDCl3	c N H1_1D	★	=	399.755 MHz H1 1D set temp 27.0 C -> actual ter 00:01:32	00:01:32	west_effch	12:40 Tue Oct 10 2023
▷ 24	U	Available										
	U	Available	west_effch_2023.10.10.i4_13.00_loc24_sample_name	4	CDCl3		★	=			west_effch	Set Start Time
	U	Available	west_effch_2023.10.10.i4_13.00_loc24_YYY	7	CDCl3		★	=				
	U	Available	west_effch_2023.10.10.i4_13.00_loc24_XXX	6	CDCl3		★	=				
▷ 25	U	Available										
▷ 26	U	Available										
▷ 27	U	Available										
▷ 28	U	Available										
▷ 29	U	Available										
▷ 30	U	Available										
▷ 31	U	Available										
▷ 32	U	Available										

Figure 18 - Select Experiments

Below is shown a zoom-in of the available experiments pre-approved for Chemistry samples.

N H1_1D	Proton 1D
N H1_1D_CD3OD	Proton 1D with presaturation of CD3OH, best for CD3OD samples
N H1_1D_D2O	Proton 1D with presaturation of HOD, best for D2O samples
N F19_dec_H1_1D	F19(H1) 1D, F19 decouple H1
N F19_1D	F19 coupled to H1 1D
N C13_dec_H1_1D	C13(H1) 1D
N APT	C13(H1) APT 1D or attached proton test, C & CH2 same side, CH & CH3 opposite side of solvent signal
N DEPTq-135	C13(H1) Deptq-135 1D, DEPT with quaternary excitation, C & CH2 same, CH & CH3 opposite side of solvent
N B11_dec_H1_1D	B11(H1) 1D
N P31_dec_H1_1D	P31(H1) 1D
N gCOSY	2D H1-H1 correlation experiment
N gCOSY_CD3OD	2D H1-H1 correlation experiment with presaturation of CD3OH, best for CD3OD samples
N gCOSY_D2O	2D H1-H1 correlation experiment with presaturation of HOD, best for D2O samples
N gDQFCOSY	2D H1-H1 double quantum filter COSY, singlets are filtered out
N gHSQC	H1-C13 2D one bond correlation expt, spectral editing like APT
N gHMBC	H1-C13 2D multiple bond correlation expt
N TROESY	H1-H1 2D rotating frame nuclear Overhauser exp (ROE/NOE)
N TROESY_D2O	H1-H1 2D rotating frame nuclear Overhauser exp (ROE/NOE) with presat of HOD, best for HOD
N TROESY_CD3OD	H1-H1 2D rotating frame nuclear Overhauser exp (ROE/NOE) with presat of CD3OH, best for CD3OD

Figure 19 - Zoom of available experiments

10.) Edit Parameters

Experiments can be modified (see “=” icon, **Figure 20**). Please note that 2D parameters will still appear but are not applicable to 1D experiments so leave alone as unexpected results may occur.

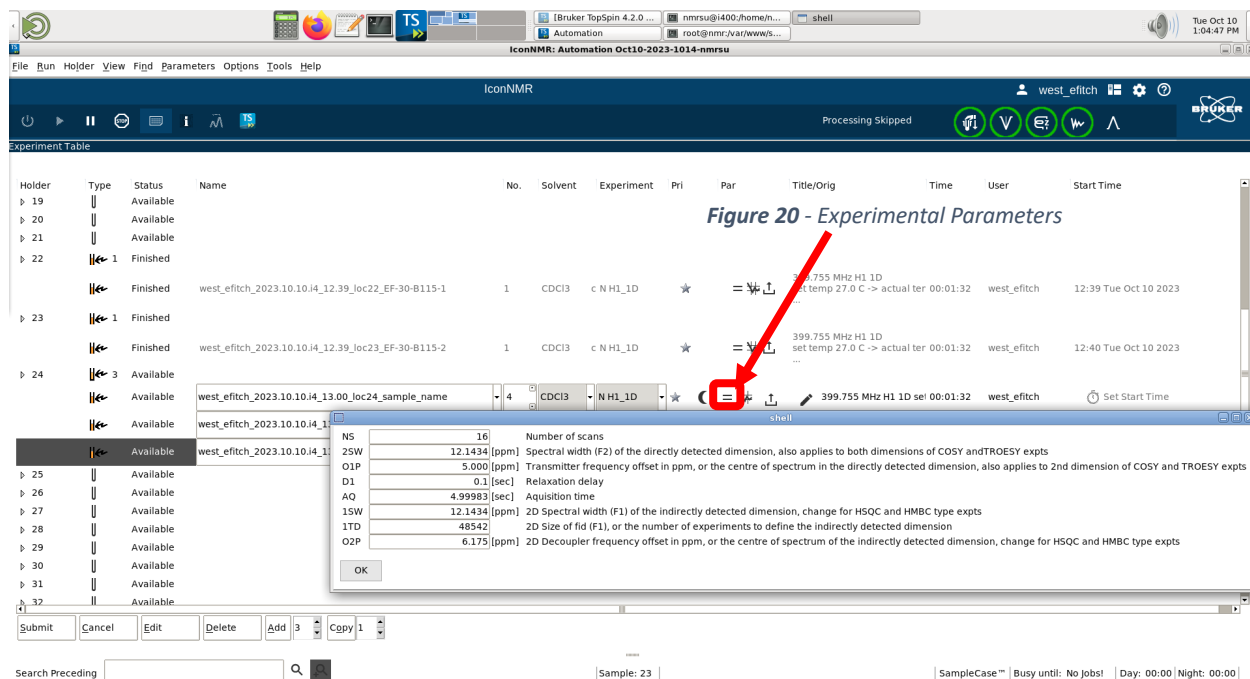


Figure 20 - Experimental Parameters

Holder	Type	Status	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
19		Available										
20		Available										
21		Available										
22	1	Finished										
		Finished	west_efitch_2023.10.10.i4_12.39_loc22_EF-30-B115-1	1	CDCI3	c N H1_1D	★	=	399.755 MHz H1 1D set temp 27.0 C -> actual ter 00:01:32	00:01:32	west_efitch	12:39 Tue Oct 10 2023
23	1	Finished										
		Finished	west_efitch_2023.10.10.i4_12.39_loc23_EF-30-B115-2	1	CDCI3	c N H1_1D	★	=	399.755 MHz H1 1D set temp 27.0 C -> actual ter 00:01:32	00:01:32	west_efitch	12:40 Tue Oct 10 2023
24	3	Available										
		Available	west_efitch_2023.10.10.i4_13.00_loc24_sample_name	4	CDCI3	N H1_1D	★	=	399.755 MHz H1 1D set 00:01:32	00:01:32	west_efitch	Set Start Time
		Available	west_efitch_2023.10.10.i4_13.00_loc24_YYY	7	CDCI3	N C13_dec_f	★	=				
		Available	west_efitch_2023.10.10.i4_13.00_loc24_XXX	6	CDCI3	N gCOSY	★	=				

11.) Select Day or Night Queue

Select the queue based on the length of experiment time required (**Figure 21**).

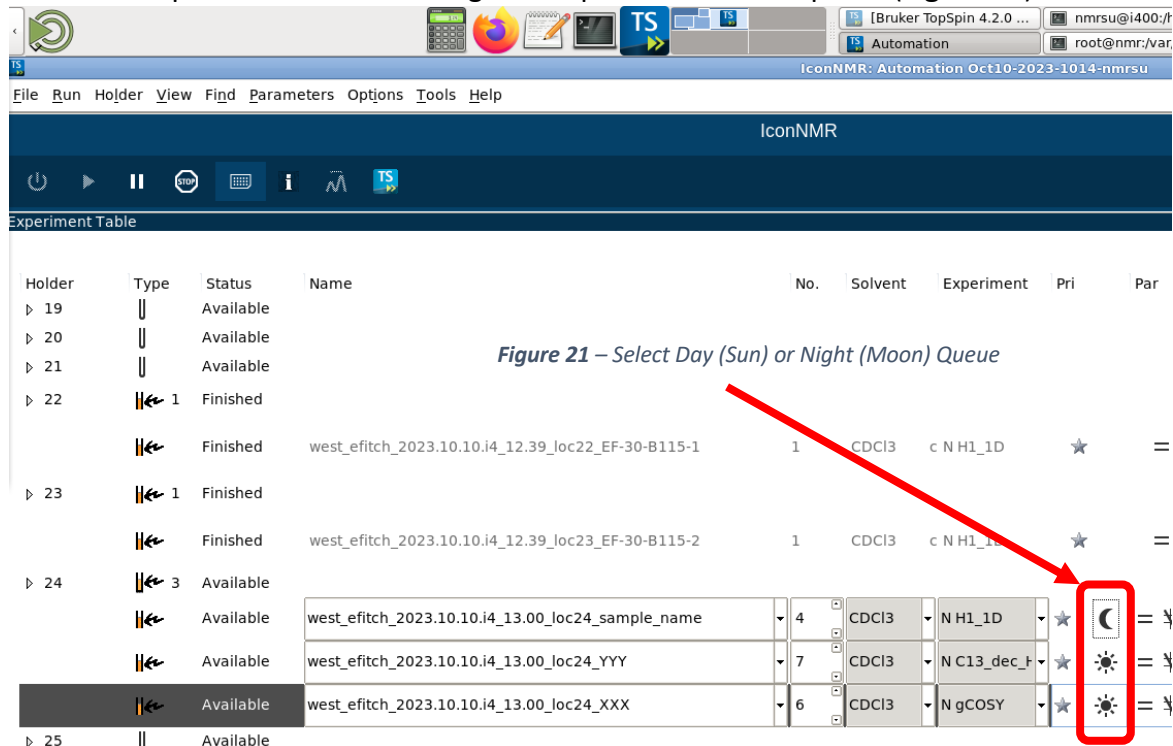
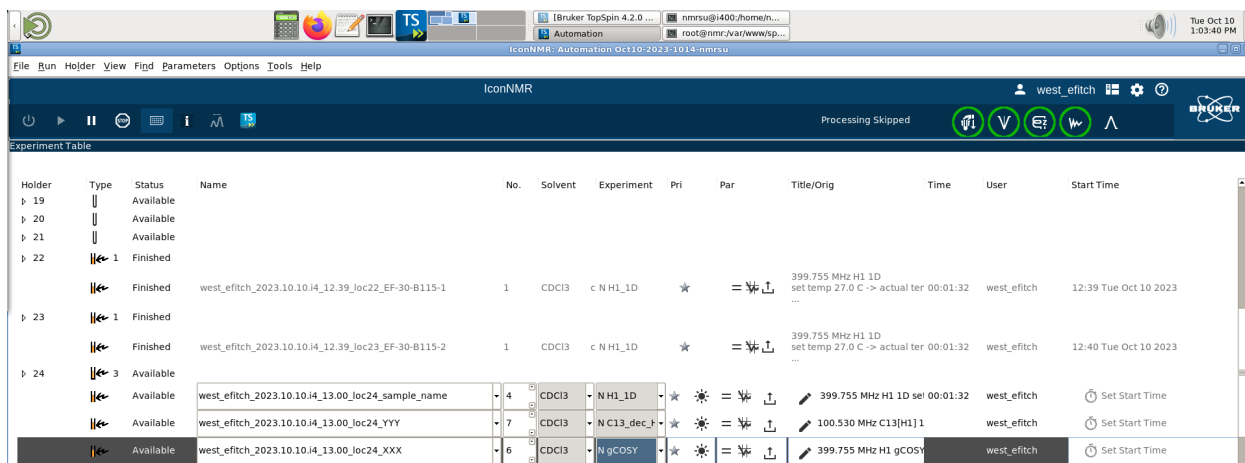


Figure 21 – Select Day (Sun) or Night (Moon) Queue

Holder	Type	Status	Name	No.	Solvent	Experiment	Pri	Par
19		Available						
20		Available						
21		Available						
22	1	Finished						
		Finished	west_efitch_2023.10.10.i4_12.39_loc22_EF-30-B115-1	1	CDCI3	c N H1_1D	★	=
23	1	Finished						
		Finished	west_efitch_2023.10.10.i4_12.39_loc23_EF-30-B115-2	1	CDCI3	c N H1_1D	★	=
24	3	Available						
		Available	west_efitch_2023.10.10.i4_13.00_loc24_sample_name	4	CDCI3	N H1_1D	★	☾ =
		Available	west_efitch_2023.10.10.i4_13.00_loc24_YYY	7	CDCI3	N C13_dec_f	★	☀ =
		Available	west_efitch_2023.10.10.i4_13.00_loc24_XXX	6	CDCI3	N gCOSY	★	☀ =
25		Available						

12.) Everything ready for submission

Figure 22 below shows a sample ready for submission to the study queue. The sample position and experiments are chosen, named, and ready to go.

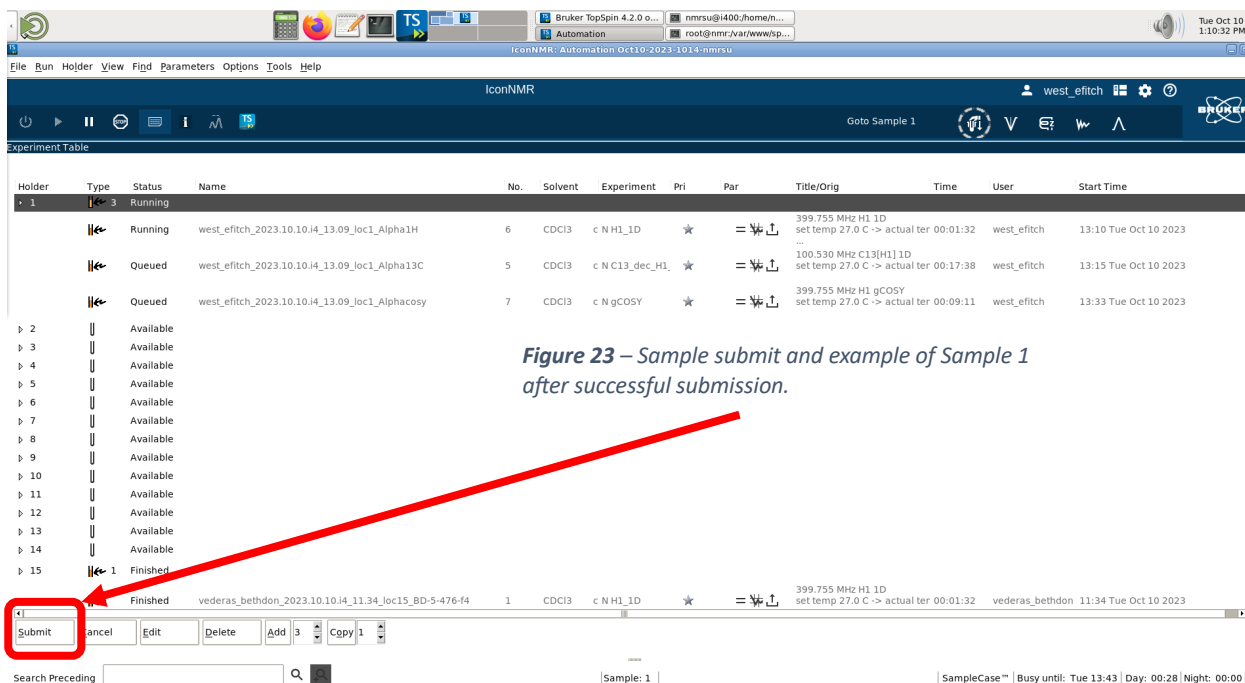


Holder	Type	Status	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
19		Available										
20		Available										
21		Available										
22	1	Finished	west_effitch_2023.10.10.i4_12.39_loc22_EF-30-B115-1	1	CDCI3	c N H1_1D	★	=	399.755 MHz H1 1D set temp 27.0 C -> actual ter 00:01:32	00:01:32	west_effitch	12:39 Tue Oct 10 2023
23	1	Finished	west_effitch_2023.10.10.i4_12.39_loc23_EF-30-B115-2	1	CDCI3	c N H1_1D	★	=	399.755 MHz H1 1D set temp 27.0 C -> actual ter 00:01:32	00:01:32	west_effitch	12:40 Tue Oct 10 2023
24	3	Available	west_effitch_2023.10.10.i4_13.00_loc24_sample_name	4	CDCI3	N H1_1D	★	=	399.755 MHz H1 1D set 00:01:32	00:01:32	west_effitch	Set Start Time
		Available	west_effitch_2023.10.10.i4_13.00_loc24_YYY	7	CDCI3	N C13_dec_1	★	=	100.530 MHz C13[H1] 1		west_effitch	Set Start Time
		Available	west_effitch_2023.10.10.i4_13.00_loc24_XXX	6	CDCI3	N gCOSY	★	=	399.755 MHz H1 gCOSY		west_effitch	Set Start Time

Figure 22 – Ready for submission to queue

13.) Submit Experiments

Once you've made all your selections, click the **Submit** button to finalize (Figure 23). The figure below shows Sample#1 successfully in the queue after hitting the Submit button (red box bottom).



Holder	Type	Status	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
1	3	Running	west_effitch_2023.10.10.i4_13.09_loc1_Alpha1H	6	CDCI3	c N H1_1D	★	=	399.755 MHz H1 1D set temp 27.0 C -> actual ter 00:01:32	00:01:32	west_effitch	13:10 Tue Oct 10 2023
		Queued	west_effitch_2023.10.10.i4_13.09_loc1_Alpha13C	5	CDCI3	c N C13_dec_H1	★	=	100.530 MHz C13[H1] 1D set temp 27.0 C -> actual ter 00:17:38	00:17:38	west_effitch	13:15 Tue Oct 10 2023
		Queued	west_effitch_2023.10.10.i4_13.09_loc1_Alphacosy	7	CDCI3	c N gCOSY	★	=	399.755 MHz H1 gCOSY set temp 27.0 C -> actual ter 00:09:11	00:09:11	west_effitch	13:33 Tue Oct 10 2023
2		Available										
3		Available										
4		Available										
5		Available										
6		Available										
7		Available										
8		Available										
9		Available										
10		Available										
11		Available										
12		Available										
13		Available										
14		Available										
15	1	Finished	vederas_bethdon_2023.10.10.i4_11.34_loc15_BD-5-476-f4	1	CDCI3	c N H1_1D	★	=	399.755 MHz H1 1D set temp 27.0 C -> actual ter 00:01:32	00:01:32	vederas_bethdon	11:34 Tue Oct 10 2023

Figure 23 – Sample submit and example of Sample 1 after successful submission.

14.) Do not forget to “Change User” (i.e. Log Out) – You are Done!

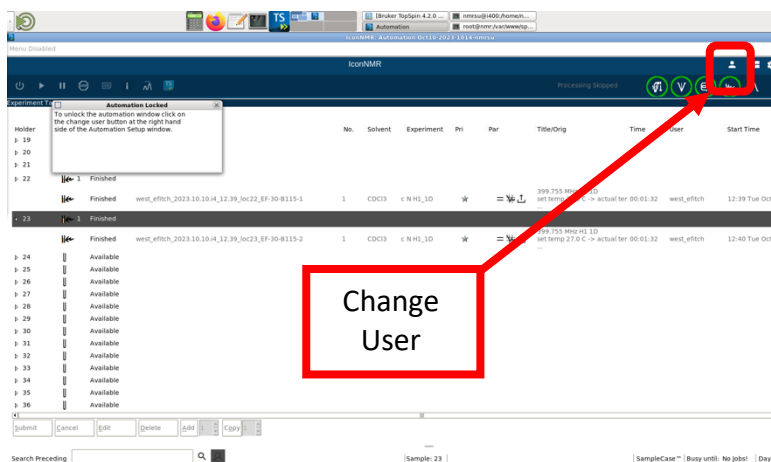


Figure 24 – The last part of submission is to logout using the Change User Icon.

Remember that last thing you need to do is log out using the “Change User” (Figure 24) button so the next person can proceed.

15.) How to retrieve a blocked sample from the carousel.



Figure 25 – The tube prevents access when a sample is in the magnet. Leave that spot alone.

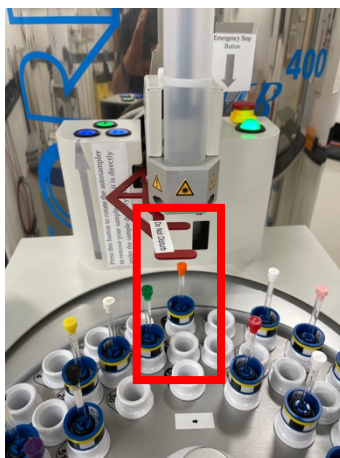


Figure 27 – When done your sample will be returned to the carousel but may be blocked (red box in center above).

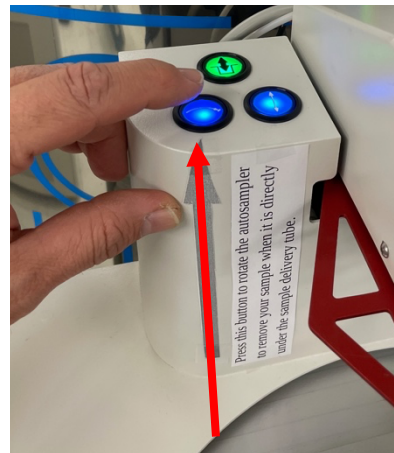
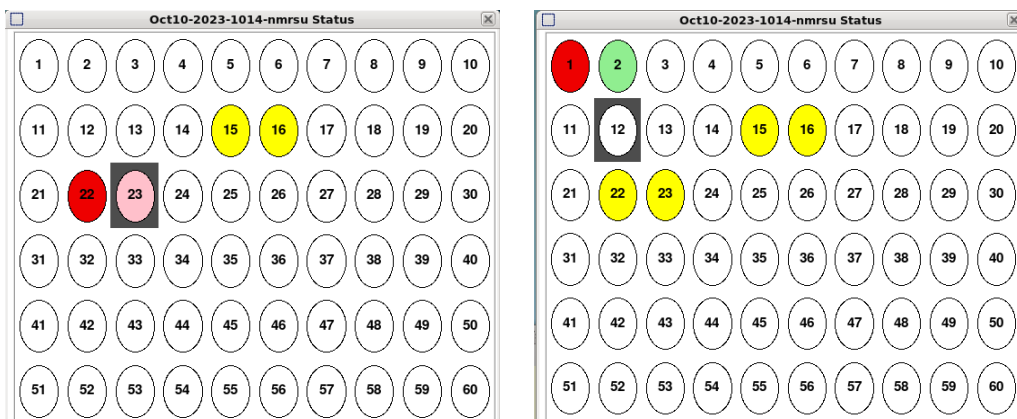


Figure 26 – To move the carousel position, press the blue tray advance button (i.e. button with left-right arrows) as in the picture above.

If you can not retrieve your sample under the robot (Figure 27), use the move sample button (Figure 26).

Appendix – Colours of the Queue



Queue Window

Red = Sample Running – Do not use

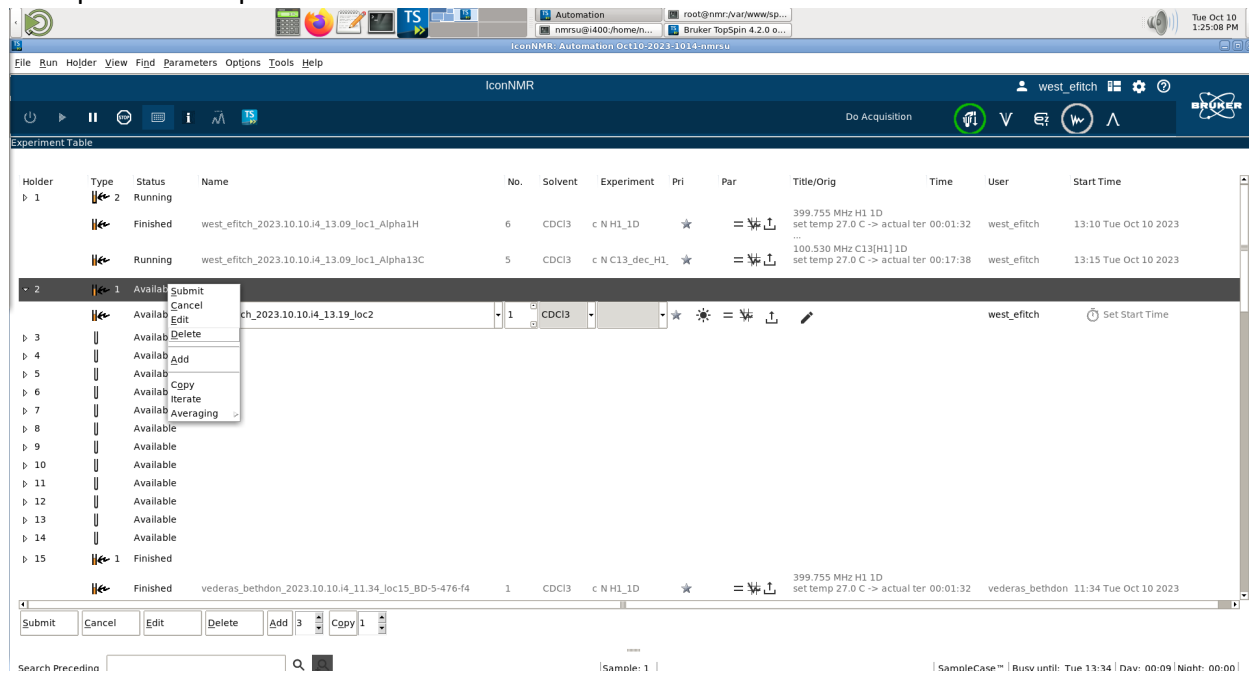
Green = Submission in Progress (not complete)

Yellow = Complete and safe to remove from queue/use spinner

Pink = XXX

Appendix – Another Example of Freeing up Slot for Complete Sample

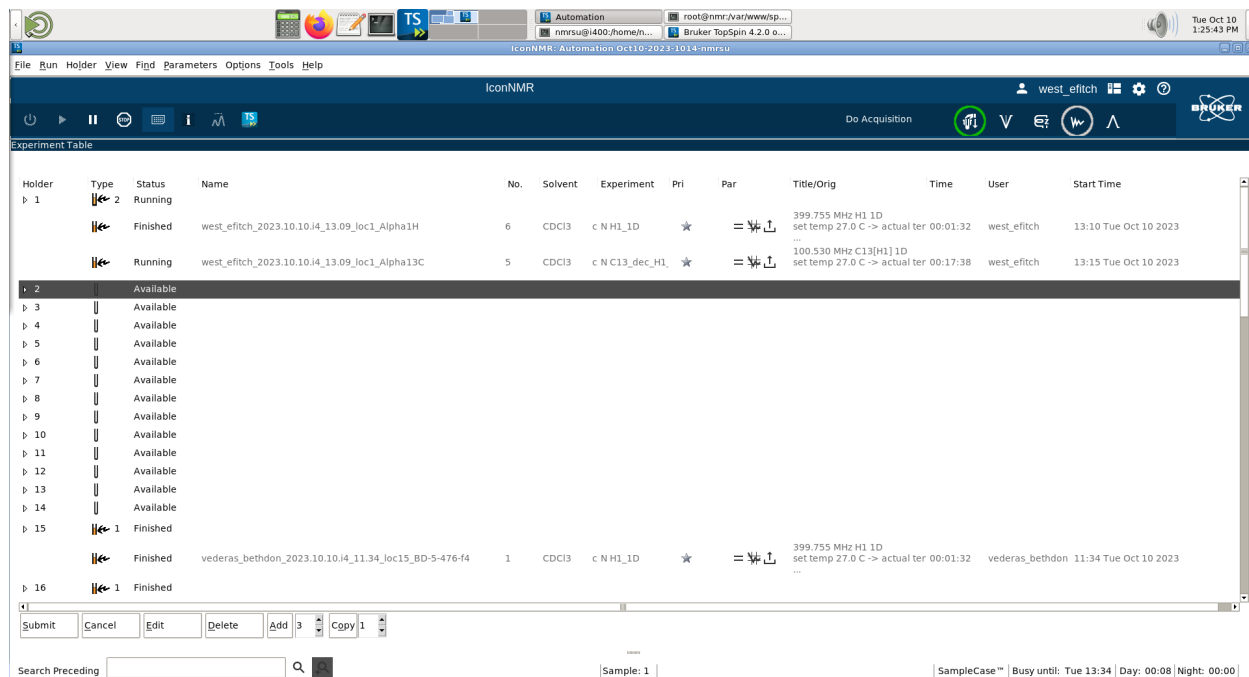
Example Freeing up used slot – control-click or right-click the completed Sample number, example below is position #2. Select “Delete”



The screenshot shows the IconNMR software interface. The 'Experiment Table' is visible, listing various samples. Sample #2 is highlighted, and a context menu is open over it, with 'Delete' selected. The table contains the following data:

Holder	Type	Status	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
1	2	Running										
		Finished	west_efitch_2023.10.10.i4_13.09_loc1_Alpha1H	6	CDCI3	c N H1_1D	★		399.755 MHz H1 1D set temp 27.0 C -> actual ter 00:01:32		west_efitch	13:10 Tue Oct 10 2023
		Running	west_efitch_2023.10.10.i4_13.09_loc1_Alpha13C	5	CDCI3	c N C13_dec_H1	★		100.530 MHz C13[H1] 1D set temp 27.0 C -> actual ter 00:17:38		west_efitch	13:15 Tue Oct 10 2023
2	1	Available	ch_2023.10.10.i4_13.19_loc2	1	CDCI3		★				west_efitch	Set Start Time
3		Available										
4		Available										
5		Available										
6		Available										
7		Available										
8		Available										
9		Available										
10		Available										
11		Available										
12		Available										
13		Available										
14		Available										
15	1	Finished										
		Finished	vederas_bethdon_2023.10.10.i4_11.34_loc15_BD-5-476-44	1	CDCI3	c N H1_1D	★		399.755 MHz H1 1D set temp 27.0 C -> actual ter 00:01:32		vederas_bethdon	11:34 Tue Oct 10 2023

Successfully Removing Completed Sample #2 to Free up Spinner



The screenshot shows the IconNMR software interface after sample #2 has been removed. The 'Experiment Table' is visible, and sample #2 is no longer present. The table contains the following data:

Holder	Type	Status	Name	No.	Solvent	Experiment	Pri	Par	Title/Orig	Time	User	Start Time
1	2	Running										
		Finished	west_efitch_2023.10.10.i4_13.09_loc1_Alpha1H	6	CDCI3	c N H1_1D	★		399.755 MHz H1 1D set temp 27.0 C -> actual ter 00:01:32		west_efitch	13:10 Tue Oct 10 2023
		Running	west_efitch_2023.10.10.i4_13.09_loc1_Alpha13C	5	CDCI3	c N C13_dec_H1	★		100.530 MHz C13[H1] 1D set temp 27.0 C -> actual ter 00:17:38		west_efitch	13:15 Tue Oct 10 2023
2		Available										
3		Available										
4		Available										
5		Available										
6		Available										
7		Available										
8		Available										
9		Available										
10		Available										
11		Available										
12		Available										
13		Available										
14		Available										
15	1	Finished										
		Finished	vederas_bethdon_2023.10.10.i4_11.34_loc15_BD-5-476-44	1	CDCI3	c N H1_1D	★		399.755 MHz H1 1D set temp 27.0 C -> actual ter 00:01:32		vederas_bethdon	11:34 Tue Oct 10 2023
16	1	Finished										