

IconNMR PROGRAMMING PROTOCOL

AV 400 MHz and AVL 500 MHz

- 1 - In the IconNMR window, click on 'Change User' (1) in the right-hand corner of the table.
- 2 - Double-click on your login name (2).
- 3 - Enter your password.

The screenshot displays the IconNMR software interface. The main window shows an 'Experiment Table' with columns for Holder, Type, Status, Name, No., and Solvent. A dialog box titled 'IconNMR: Identify User' is open, showing a list of users with columns for 'User's Full Name' and 'User ID'. The user 'NMR Super User' is highlighted. A red arrow labeled '2' points to this user. In the bottom right corner of the main window, a 'Change User' button is visible, with a red arrow labeled '1' pointing to it. Below the main table is a 'Preceding Experiments' table with columns for #, Date, Holder, Name, No., Experiment, Load, ATM, Lock, Shim, Acq, Proc, User, Disk, and Title/Orig.

Holder	Type	Status	Name	No.	Solvent
1					
2					
3					
4					
5					
6					
7					
8		Available			
9		Available			
10		Available			
11	1	Finished			
		Finished	HL2054B	2	CDCl3 chloroform
12	1	Failed			
		Failed	TDM-OXE1-PYRUVIC SEC+CONCENTRE	3	CDCl3 chloroform
13	1	Finished			
		Finished	TDM-OXE1-PHENYLGLYO	1	CDCl3 chloroform
14	1	Finished			
		Finished	MM211	1	CDCl3 chloroform
15	1	Finished			
		Finished	BA275-D	1	CDCl3 chloroform
16	1	Finished			
		Finished	TDM-OXE1-PYRUVIC SEC+CONCENTRE	2	CDCl3 chloroform-d
17	1	Finished			
		Finished	BA273-V3	1	CDCl3 chloroform-d

#	Date	Holder	Name	No.	Experiment	Load	ATM	Lock	Shim	Acq	Proc	User	Disk	Title/Orig
2460	2024-09-12 14:14:54	11	EDF-147-Brut	1	Proton-jour	✓	✓	✓	✓	✓	✓	commeira	/opt/topspin3.6.2/data/commeira/nmr	
2459	2024-09-12 08:40:07	15	BA279-dl	1	Proton-jour	✓	✓	✓	✓	✓	✓	martinez	/opt/topspin3.6.2/data/martinez/nmr	
2458	2024-09-12 08:16:14	38	ALF086_all	3	13C-decouple-jour	✓	✓	✓	✓	✓	✓	amatore	/opt/topspin3.6.2/data/amatore/nmr	
2457	2024-09-12 08:13:13	38	ALF086_all	2	13C-DEPTQ135-jour	✓	✓	✓	✓	✓	✓	amatore	/opt/topspin3.6.2/data/amatore/nmr	
2456	2024-09-12 08:05:42	38	ALF086_all	1	Proton-jour	✓	✓	✓	✓	✓	✓	amatore	/opt/topspin3.6.2/data/amatore/nmr	
2455	2024-09-11 18:16:08	11	SH-70	1	Proton-jour	✓	✓	✓	✓	✓	✓	ouari	/opt/topspin3.6.2/data/ouari/nmr	
2454	2024-09-11 17:47:35	15	BA279	1	Proton-jour	✓	✓	✓	✓	✓	✓	martinez	/opt/topspin3.6.2/data/martinez/nmr	
2453	2024-09-11 17:36:17	11	BA277	3	Proton-jour	✓	✓	✓	✓	✓	✓	martinez	/opt/topspin3.6.2/data/martinez/nmr	
2452	2024-09-11 17:16:08	30	HSLB1-416	2	29Si-DEPT31.5-jour	✓	✓	✓	✓	✓	✓	hysilabs	/opt/topspin3.6.2/data/hysilabs/nmr	

4 – Double-click on the position number on which you want to place your sample.

5 - Enter a name in the 'Name' cell without spaces, full stops or semicolons. Separate the characters with the dash 6 (3).

6 - Click on the 'Solvent' cell and choose the solvent in which you have prepared your sample (4).

7 - Click on the 'Experiment' cell and choose the experiment you want to carry out (5).

8 - Click on the 'Title/Orig' icon and write your text, all characters are allowed (6).

9 - If you want to add an extra experiment for the same sample, click on the 'Add' button. (A) An extra experiment Table will be added and the experiment number will be incremented with the same name.

10 - Click on the programming number to highlight the position and click on 'Submit' (7).

11 - Click on 'Change User' to log out (8).

The screenshot shows the IconNMR Automation software interface. The main window displays an 'Experiment Table' with columns for Holder, Type, Status, Name, No., Solvent, Experiment, Pri, Par, Title/Orig, Time, User, and Start Time. The table contains several rows of experiment data, including 'Finished' and 'Failed' entries. Red arrows labeled 3 through 8 point to specific fields: 3 points to the 'Name' field, 4 to the 'Solvent' field, 5 to the 'Experiment' field, 6 to the 'Title/Orig' field, and 8 to the 'Change User' button. A green arrow labeled 'A' points to the 'Add' button. A red arrow labeled 7 points to the 'Submit' button. Below the main table is a 'Preceding Experiments' table with columns for #, Date, Holder, Name, No., Experiment, Load, ATM, Lock, Shim, Acq, Proc, User, Disk, and Title/Orig. The status bar at the bottom shows 'Sample: 20', 'BACS/SampleCase/Pro (RS232)', 'Busy until: No Jobs!', 'Day: 00:00 Night: 00:00', and 'User: nmrsu'.