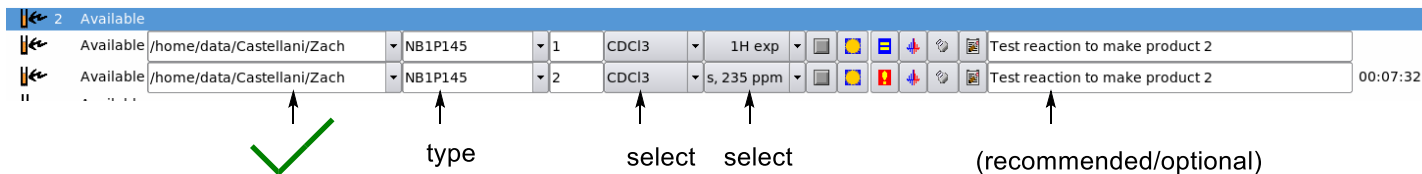
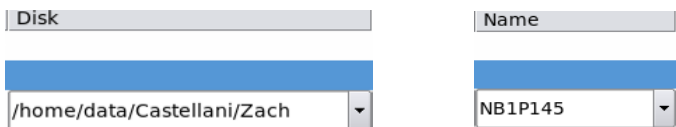


Using the automation program IconNMR

Each sample holder in the carousel has a line associated with it in Icon NMR. Selecting the user “218H” will automatically write the data to the correct folder in the file system. You can run multiple experiments for a single sample using the “add” button.



1. Select the user for your research group or class (). If someone else's user is already selected, use the change user icon to bring up the selection menu (). The file destination folder is determined with the user. Only create experiments and folders in your research group's folder. If you have your own subfolder (such as a folder named after a student doing research in a professor's research group), you can type it after the professor's name under “Disk.”
2. Select or type your subfolder for your group under “disk.” Only create experiments and folders in your research group's folder. Spelling and the use of capital and lowercase letters is important.
3. Type your experiment name under “Name.” Research students should use a logical system for finding files. See your professor for guidance.



4. The experiment number should automatically fill under “No.” You may change this if you wish. If you create two or more datasets with the same name, you must increment the number under “No.”
5. Select the solvent from the dropdown list.
6. Select the experiment from the dropdown list. Each experiment has a name and description. Be cautious that some experiments are long, and others further down the list require certain experiments to be run first. If the experiment name begins with the letter “C” you will see several experiments added under the one on top.
7. You may choose to decrease or increase the number of scans “NS” by clicking on the blue and yellow equal symbol (). A red and yellow exclamation point () will let you know that you changed something.
8. You may set a title with additional information, if you wish, or you may leave this area blank.
9. Click “Add” to create more experiments for the same sample or “Copy” if the next slot has a similar sample that will have the same parameters (). Click “Submit” to add the experiment(s) to the queue ().
10. If you are the last person to run a sample in automation, and you want to retrieve your

sample from the magnet, run a PROTONRO for the NMR standard “EtPh” in holder one.

In the bottom window of IconNMR, you will see which samples have been run and even which steps have been done. It is usually sorted by the date. When all of the check marks are there or when it goes to the next sample, you may double click that line. It will automatically open the data in TopSpin. If somebody forgot to click the save and return button when they last processed data in TopSpin, it will return an error that says “illegal operation.” It will not open your data in this case. You need to save and return, then go back to IconNMR and double click the sample name again.

Preceding Experiments														
#	Date ▾	Holder	Name	No.	Experiment	Load	ATM	Rotation	Lock	Shim	Acq	Proc	User	Disk
68	2020-01-14 18:07:47	17	1JM115cr	1	PROTONRO								Markiewicz	/home/data/Markie
67	2020-01-14 18:03:15	16	1JM114cr	1	PROTONRO	✓	✓	✓	✓	✓	✓	✓	Markiewicz	/home/data/Markie

If all of the holders contain samples, feel free to remove samples for your class but please do not move samples from other classes or research groups. If all slots are filled, please see your professor. You can highlight the holder number in icon and click “delete” to clear the information. This does not delete the NMR data. It will not let you clear information from another user unless the sample already completed.