

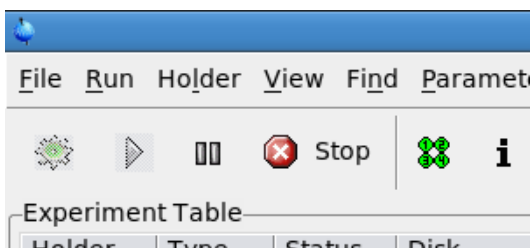
# NMR Programs – Automation vs. Manual Mode

- Do not close windows using the “X” in the corner of the program window. This may delete someone’s experiment. It will also cause people to lose track of which holder has their samples.
- Do not remove the sample “EtPh” from sample holder number 1. This standard is used frequently during automation.
- Do not remove an NMR tube with a plastic cap from the carousel. This will likely disrupt a researcher’s experiment or cause them to lose his or her sample. If the carousel is full, see a professor to empty it for you. Students in CHM 218H may remove samples for this class as long as they verify that a classmate has not queued it to run later in automation (see the queue on IconNMR).
- If you run a sample in manual mode, you must restart automation when you are done.

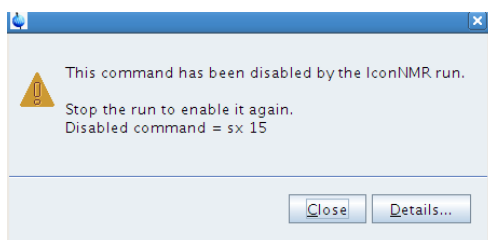
The program you use to run the NMR in manual mode is called “TopSpin 3.2.” There is a sub-program, called “IconNMR,” that runs TopSpin in automation. When Icon is in “run” mode, you can process previously acquired data in TopSpin, but you cannot run new samples in manual mode. With the automation program, it is possible for many users to submit samples to run in a queue because you simply input information to run your experiment, and the robot runs it for you while you are away. You can submit multiple experiments, go away, and come back later to collect the data. If someone uses manual mode, s/he must stop and restart automation. The following instructions will show you how to do this without disrupting the automation sequence.

**There are several ways to tell if the instrument is running in manual mode or automation.**

- 1) The easiest is to look at the green cog or red stop sign in the top left-hand corner of Icon. If the green cog is greyed out, automation is running. If the stop sign is greyed out, the instrument is in manual mode.



- 2) Another way to know that the instrument is running in automation is that it will give an error if you enter a command that deals with acquiring a new sample. In the example below, the user entered “SX 15.” The instrument will tell you that IconNMR is in control. You can still process data that has already been acquired while automation is running.



**Switching from automation to manual mode**

# NMR Programs – Automation vs. Manual Mode

First, you must stop the run. **You should first verify that the instrument is not actively running a sample.** There are several ways to check this.

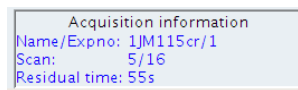
In IconNMR, you will see a blinking box around one of the steps in the top right-hand corner, such as loading the sample, locking field, tuning, shimming, receiver gain adjustment (RGA), acquisition and spectrum processing.



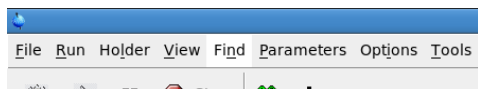
In TopSpin, you will see information displayed on the bottom panel. Just under the command line, it tells you what the instrument is doing (receiver gain adjustment in the example below).



The longest part of running a sample is acquiring the FID. It will tell you how much time is left, but only for the sample that is currently running.



If more than one sample is queued to run, you will have to wait for all of them to finish before switching to manual mode. You can simply look through the queue to see when the last sample will run. Sometimes the queue looks busy.



- 1) You can use the “Find” function to make it easier to find the last sample.
- 2) Highlight row 1, which should have the sample “EtPh.”
- 3) “Find available holder” will automatically shift the highlighted bar to an empty holder. “Find active holder” will highlight the sample that is currently being used to acquire data.
- 4) “Find queued holder” will find the next queued sample. The start time and duration is written to the right of the sample information. You may have to cycle through several queued samples to find the last one.

Time	User	Start Time
00:01:32	218H	12:49 Wed Dec 04 2019
00:01:32	Markiewicz	13:45 Fri Dec 06 2019
00:01:32	Markiewicz	13:56 Fri Dec 06 2019
00:01:32	Markiewicz	15:00 Sat Dec 21 2019
00:01:32	Markiewicz	20:33 Fri Jan 03 2020
00:01:32	Markiewicz	17:26 Wed Jan 08 2020
00:01:32	Markiewicz	18:25 Thu Jan 09 2020

# NMR Programs – Automation vs. Manual Mode

If no samples are actively running, you may switch to manual mode.

To switch to manual mode, click the red stop sign on the top left-hand corner of Icon. It will ask you **Do you really want to stop the run?** Double check that the instrument is not running a sample. Then click “yes.”



There may be samples queued to run later that day or at night, so **be sure to return the instrument to automation if you are the last one to run a sample.** To restart automation, click the green cog in IconNMR. You may always start at line one. Researchers typically run longer experiments at night and over the weekend to allow the NMR to be free during the day for CHM 218H and 361H.