

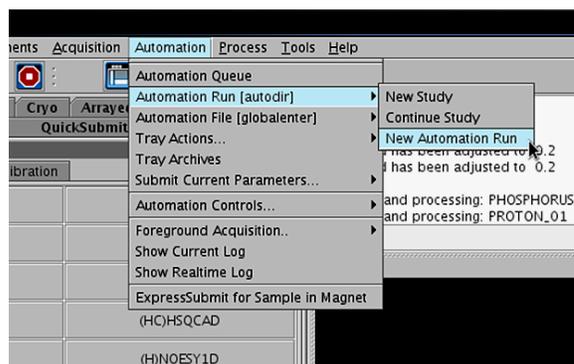
Running Samples on the Automated 500

Make sure your sample is 5 cm tall and is sealed **only** with a plastic cap. **Do not use parafilm, foil, or Teflon tape (alone or wrapped around a plastic cap) to cap your samples.** Load your sample into a spinner and use the depth gauge to set the sample height. This gauge is on the sample tray next to position 50 (black cylinder). **Do not place the spinner into the depth gauge before loading your sample.** This risks breaking your NMR tube. Load samples into spinners by hand making sure your hand is not more than 10 cm from the top of the spinner to avoid snapping your tube. Once you have set the height with the depth gauge, place the sample into an available location in the sample tray.

1. Sign into Vnmrj near the bottom of the screen with your UANet username and password (same as your UAkron email).

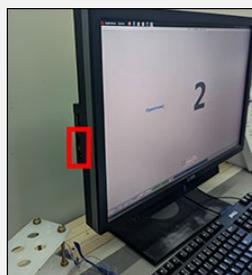


2. Select Automation →
Automation Run [autodir] →
New Automation Run

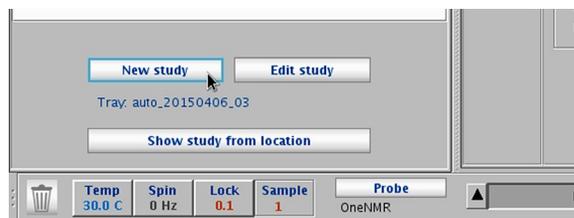


OPTIONAL :

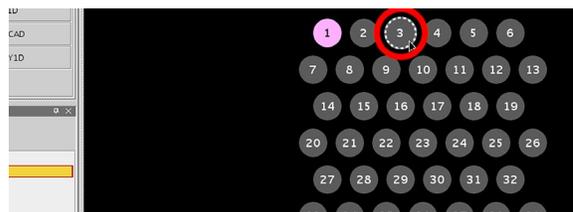
If you want to save data to a USB drive,, insert it into one of the USB ports located on the left side of the monitor or front of the tower on the floor. Then proceed to Step 3.



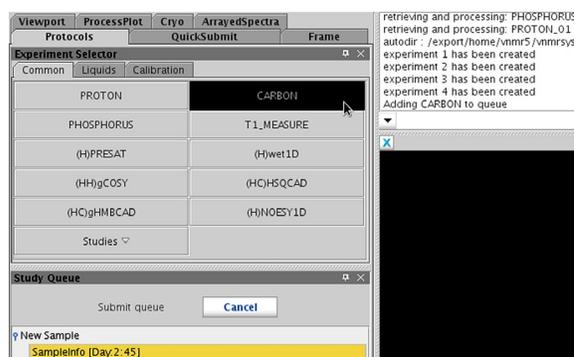
3. Click the **New Study** button at the lower left corner of the screen.



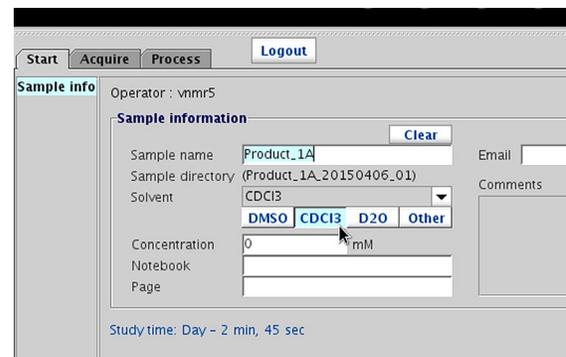
4. Select the location of your sample in the sample tray. The location will be highlighted with a white dotted line.



5. Select all the experiments you would like to run from the **Experiment Selector**.



6. Enter a sample name (required) in the center window. Select your solvent.

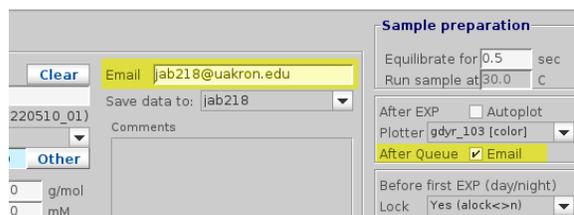


7. Configure file saving options

Email:

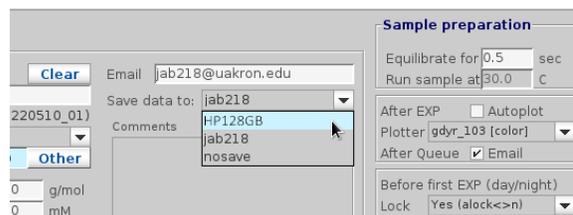
To have the instrument email you your data as a .zip file, enter an email address in the Email text box.

NOTE: This must end in @uakron.edu or the campus spam filter will block it.



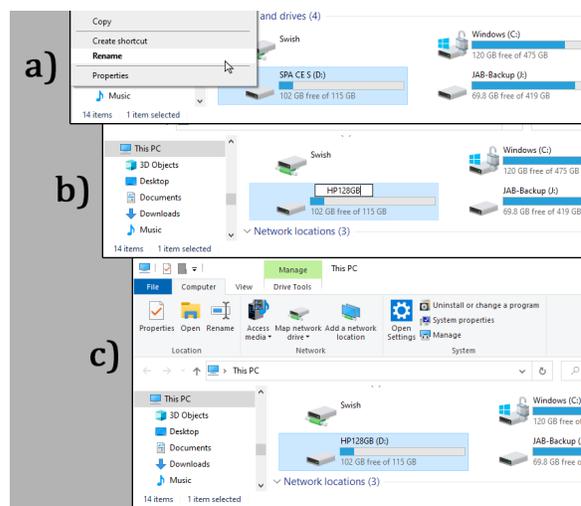
USB:

By default, the instrument will save to your home directory on the chemistry server. You may change this to a USB drive by selecting it from the drop-down menu. If your drive is not in the list, you will need to click **Cancel** in the Study Queue, insert the drive, and then continue with Step 3. Choosing the 'nosave' option will disable saving and should only be used if you are emailing the data instead.

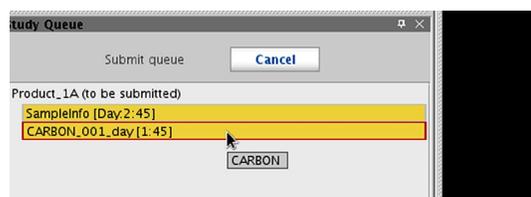


NOTE: You can only use USB drives without spaces or other special characters in their name. You can change your drive's name in Windows within the Properties dialog.

- Right-click on the drive and select Rename
- Enter a new name. You should only use letters, numbers, dashes, and underscores.
- Press Enter/Return to set the new name

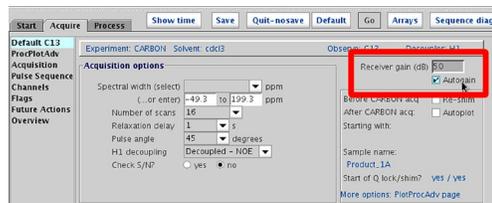


8. Double-click an experiment in the Study Queue list to edit its parameters.

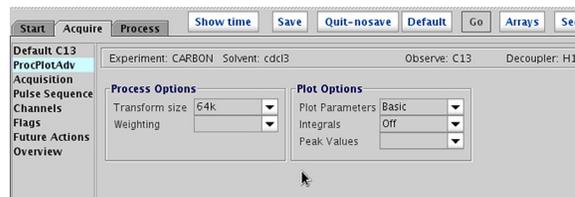


9. Enter the basic acquisition parameters in the Default menu. For 1D experiments, check the **Autogain** checkbox, unless a specific gain is desired.

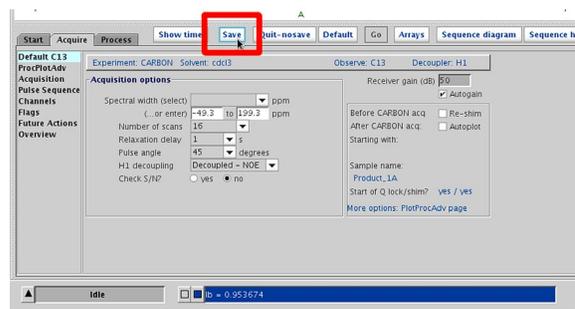
NOTE: If you set the gain too high, the experiment will fail.



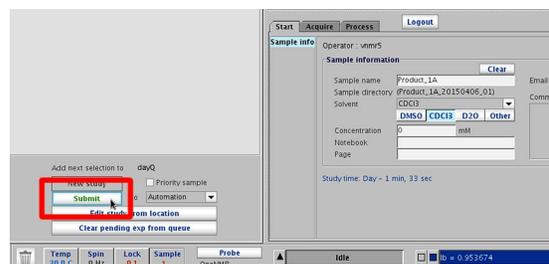
10. The transform size can be found in the ProcPlotAdv menu. If a specific lb value is wanted, you may enter lb=## on the command line to set it.



11. When you have finished editing the parameters, click the **Save** button at the top of the panel. If you do not, the parameters will return to their default values.



12. Continue steps 8-12 for the remaining experiments. After editing all experiments, make sure you have entered a sample name, solvent, and selected a location in the sample tray. Then click the **Submit** button at the lower left. The sample queue will automatically close.

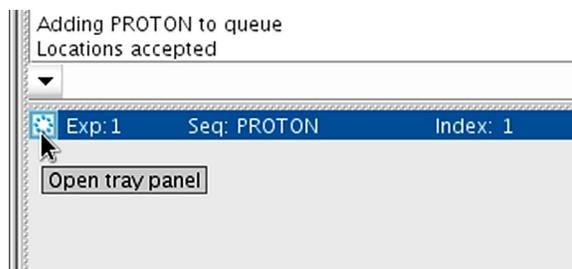


NOTE: Once you have submitted a sample, you will not be able to edit the experimental parameters or add any additional experiments to it. You will have to wait for the sample to complete acquisition and return to the sample tray before you can submit any further experiments to that location. Please verify you have added all experiments you want to run on the sample before pressing the **Submit button.**

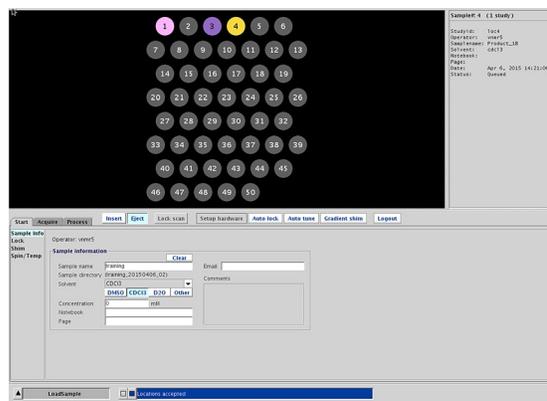
13. Repeat steps 3-12 to add another sample location to the queue.

You do not need to submit the standard (sample 1). It will automatically return to the magnet after your last experiment has finished.

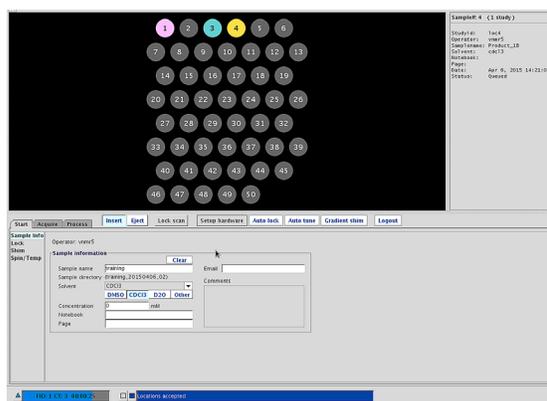
14. While the experiments are running, you may monitor the process in the Study Queue by clicking the “Open tray panel” button at the upper left of the main window.



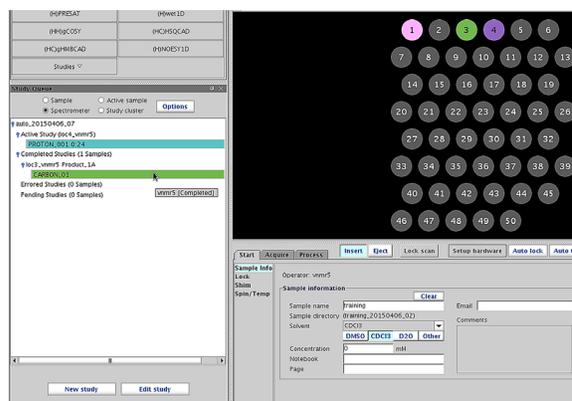
15. When the sample is loading (prescan) the location will be highlighted in violet. Queued experiments are shown in yellow.



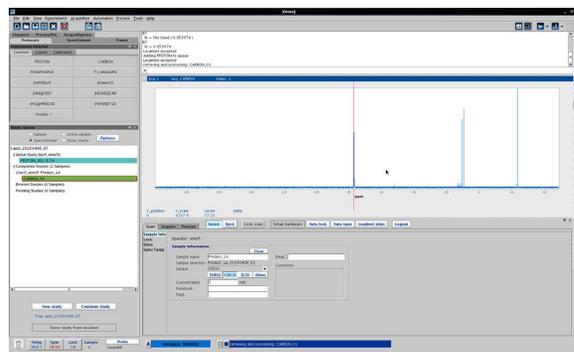
16. An active experiment will be shown in light blue. Completed experiments are shown in green. Any failed experiments will be shown in red.



17. If you wish to view completed experiments, expand the Completed Studies tab on the left. Double-click on the green-highlighted experiment to view the spectrum. You may also view active experiments (light blue) once a block size has been collected.



18. You may now adjust and print your spectrum. Completed experiments are automatically saved in your home folder or USB drive for processing at workstations or on your own computer. The printing menu is accessed through the **Process** tab under the **Plot** sub-menu.



19. If selected, data will automatically save to your home folder or USB drive when the experiment has completed. You will find a folder labeled with the sample name (e.g. Product_1A). Inside this folder will be the FID files of the experiments (e.g. PROTON_date_#.fid).

If your data was not copied to your home folder/USB drive, notify the MRC staff. We will correct your account and email you any FID's that are missing in your home folder.

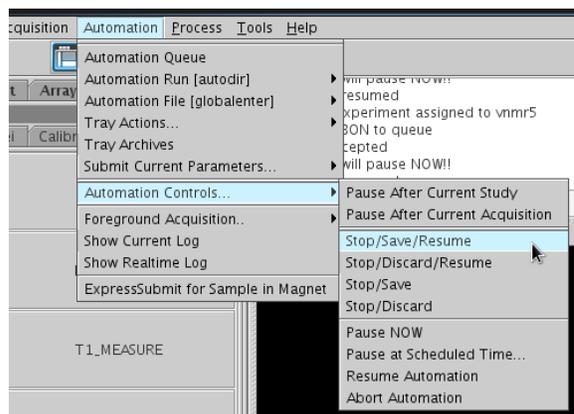
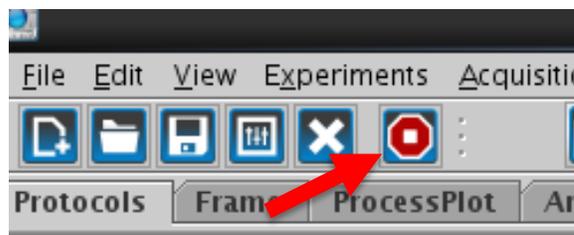
20. To end an experiment, press the Stop button in the top system menu. **Only stop an experiment during acquisition.**

Stopping during prescan (sample tray color violet) will cause errors.

- OR -

Select Automation →
Automation Controls →
Stop/Save/Resume

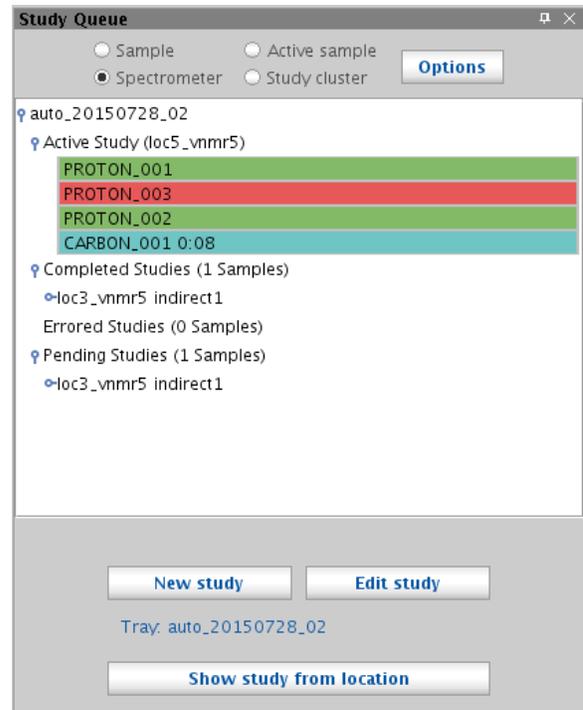
This will stop the current experiment and save the results (if one or more block sizes have been collected) before proceeding to the next experiment or sample in queue.



***** DO NOT USE THE aa COMMAND ON THE AUTOMATED 500! *****

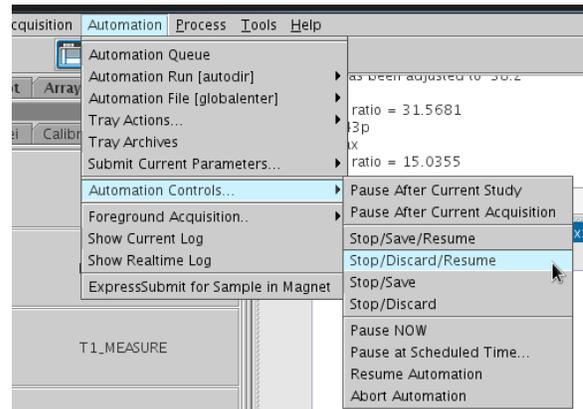
21. If an experiment is stopped before a block size of scans is collected, it will appear red in the study queue (see PROTON_003) and no data is saved.

Stopped experiments with one or more block sizes will appear green (see PROTON_002).



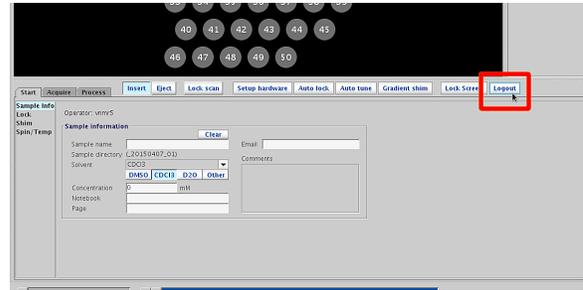
22. If you want to stop the active experiment without saving it,

Select Automation →
Automation Controls →
Stop/Discard/Resume



23. When you are finished, click the **Start** tab in the lower panel. Then click the

Logout button at the top of lower panel.



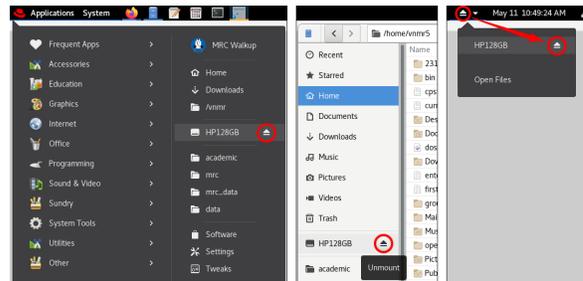
24. Ejecting Your USB Drive

To avoid corrupting your drive, you should eject the drive before removing it.

You can eject from the

1. main menu *
2. file browser
3. top right drive menu *

* These will display over the login screen and can be used after logging out.



Click on the eject icon and wait for the popup message at the top center of the screen to confirm it is safe to remove the drive.

NOTE: If you eject the drive before logging out, it may tell you the drive is busy. Log out and you should soon get confirmation that it is safe to remove the drive.

