# 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.
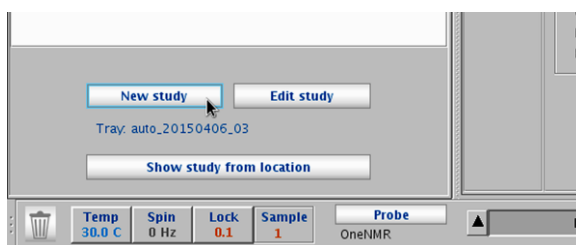
1. Sign into VnmrJ near the bottom of the screen with your NMR username and password.
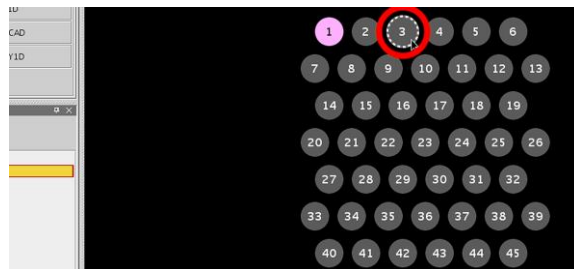

2. Select Automation →
   Automation Run [autodir] →
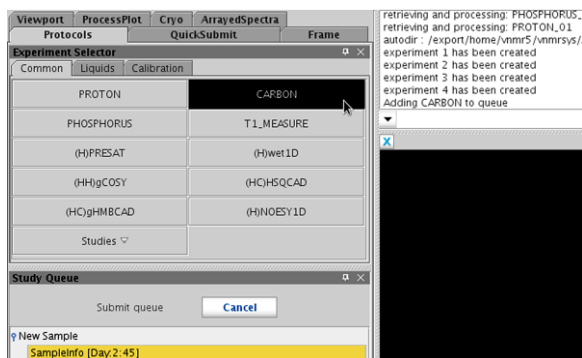   **New Automation Run**
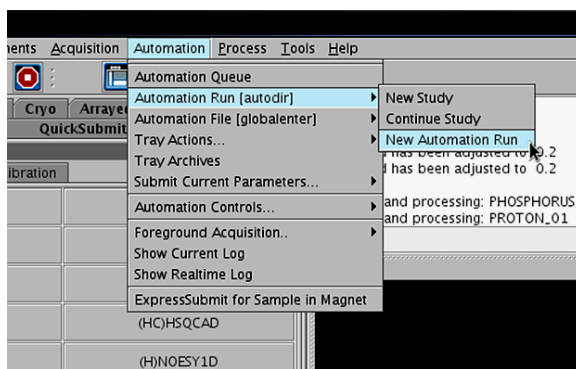
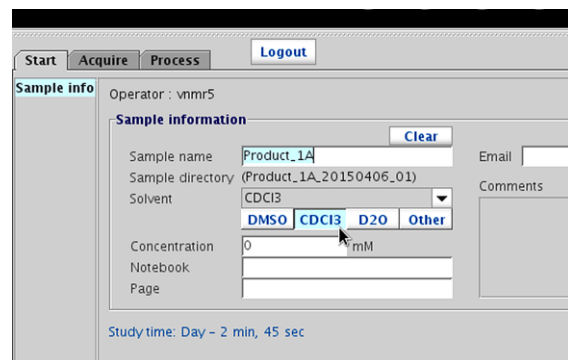3. Click the **New Study** button at the lower left corner of the screen.

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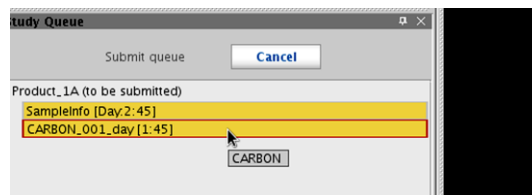

5. Select all the experiments you would like to run from the **Experiment Selector**.
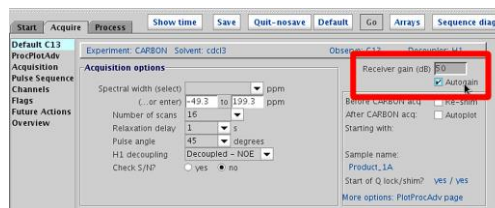

6. Enter a <u>sample name</u> (required) in the center window. Select your <u>solvent</u>.


7. Double-click an experiment to edit its parameters.

8. 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.)

9. 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.
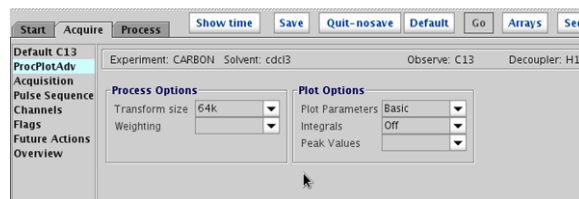
10. When you have finished editing the experimental parameters, click the **Save** button at the top of the panel. If you do not, the parameters will return to their default values.
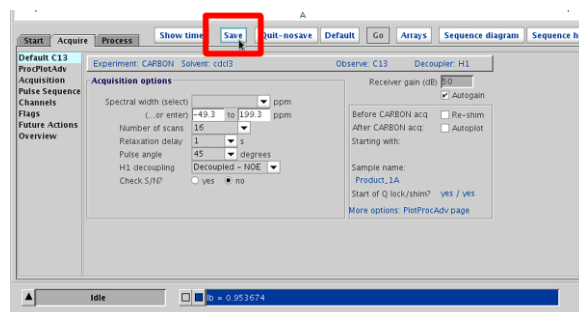
11. Continue steps 8-11 for the remaining experiments. After editing all experiments, make sure you have entered a sample name, solvent, and selected a location in the sample tray. Then click the **Submit** button at the lower left. The sample queue will automatically close.
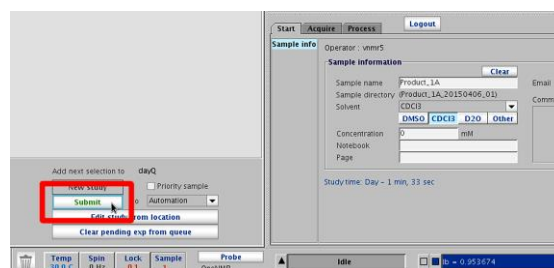
Note: **Once you have submitted a sample, you will not be able to edit the experimental parameters or add any additional experiments to it. You will have to wait for the sample to complete acquisition and return to the sample tray before you can submit any further experiments to that location. Please verify you have added all experiments you want to run on the sample before pressing the Submit button.**

12. Repeat steps **3-11** to add another sample location to the queue.

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

13. 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.
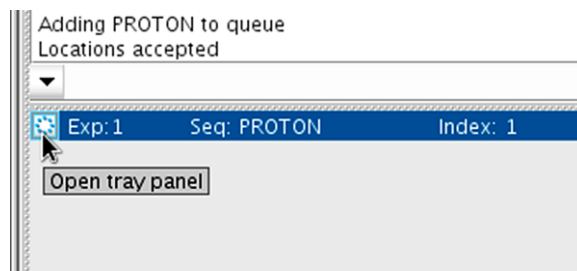

14. When the sample is loading (prescan) the location will be highlighted in violet. Queued experiments are shown in yellow.
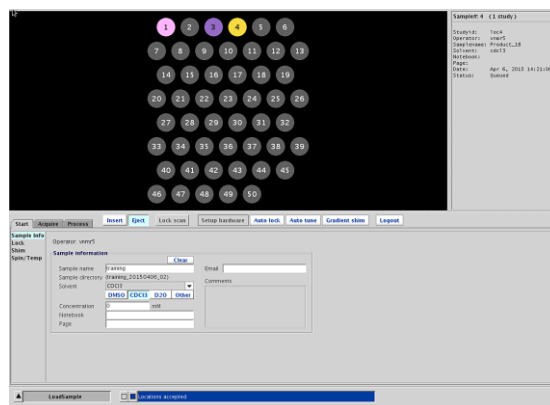

15. An active experiment will be shown in light blue. Completed experiments are shown in green. Any failed experiments will be shown in red.
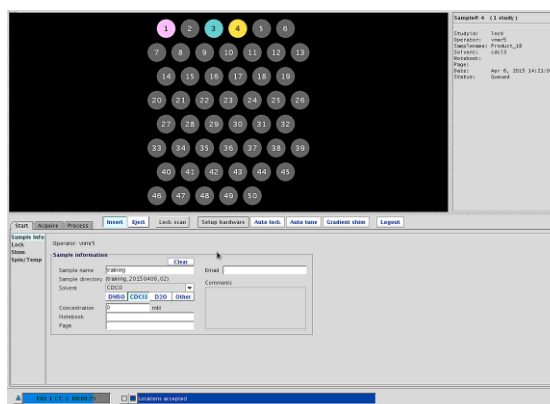
16. If you wish to view completed experiments, expand the Completed Studies tab on the left. Double-click on the green-highlighted experiment to view the spectrum. You may also view active experiments (light blue) once a block size has been collected.
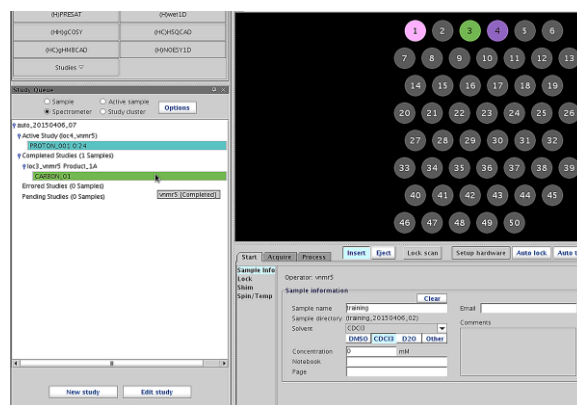
17. You may now adjust and print your spectrum. Completed experiments are automatically saved in your home folder for processing at workstations or on your own computer. The printing menu is accessed through the **Process** tab under the **Plot** sub-menu.
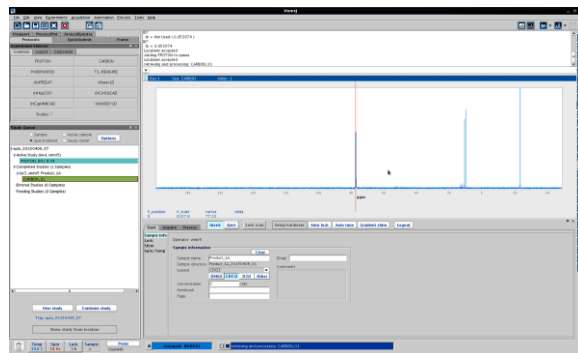
18. Your experiments will automatically be saved in your home folder when the experiment has completed. You will find a folder labeled with the sample name (e.g. Product_1A). Inside this folder will be the FID files of the experiments (e.g. PROTON_date_#.fid).

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

19. To end an experiment, press the Stop button in the top system menu. **Only stop an experiment during <u>acquisition</u>.** 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.
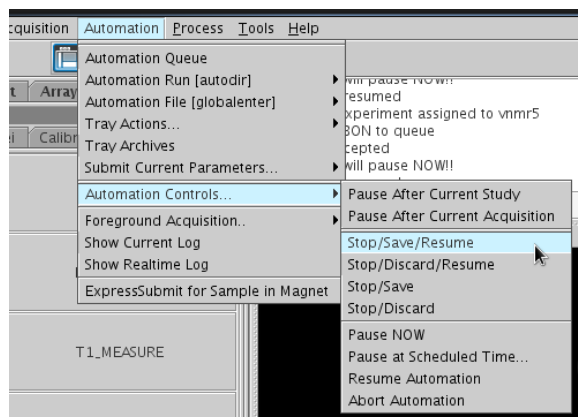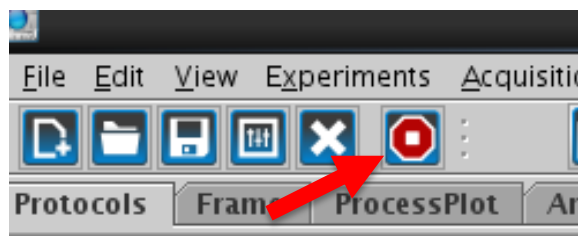
***** DO NOT USE THE** aa **COMMAND ON THE AUTOMATED 500! *****

20. If an experiment is stopped before a block size of scans are 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).
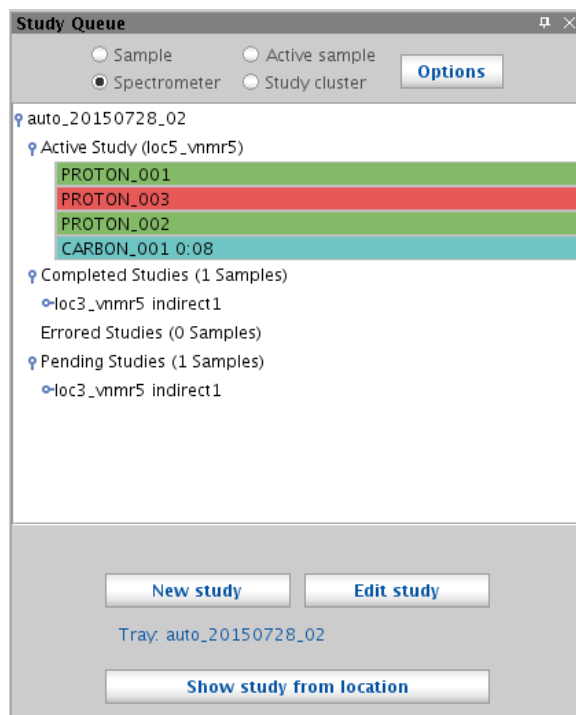
21. If you want to stop the active experiment without saving it,

    Select Automation →
    Automation Controls →
    Stop/Discard/Resume
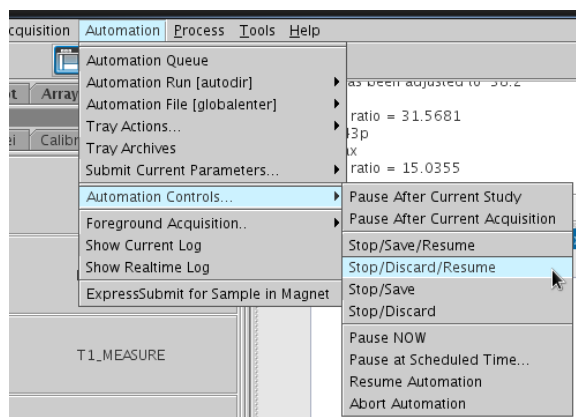
22. When you are finished, click the **Start** tab in the lower panel. Then click **Logout** button at the top of lower panel.