Use of Hermes for Chem 636

Hermes is a Varian Mercury-300 NMR spectrometer, equipped with a sample changer robot and automation software. The spectrometer is located in room 2224A in the Chemistry Department's NMR Facility.

Normal Operation:

1. A *Login* screen should be present, with a large number indicating the lowest numbered position available on the sample trays.

   If the *Login* screen is not present, contact facility personnel.

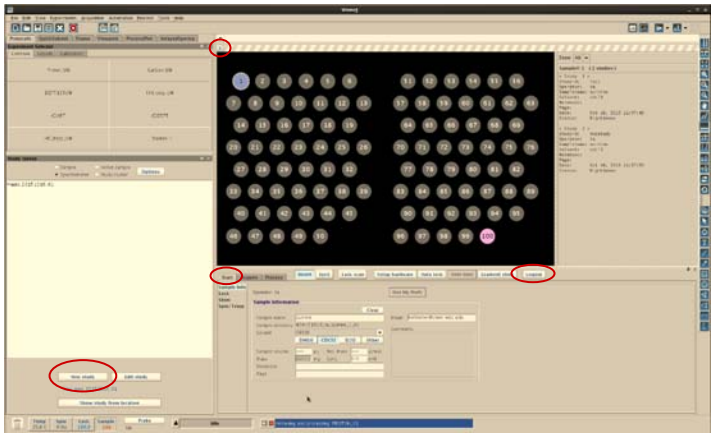
2. ***Login*** by typing your chem (or NMR facility) username and password. If one is not present on the dropdown, please contact Heike (hofstetter@chem.wisc.edu) to obtain password and training.

3. Set your sample tube depth using the gold depth gauge.
   - *Use standard NMR tubes, 9" being the maximum length. Longer tubes will be broken by the robot (special provisions exist to handle, e.g., J-Young tubes; ask staff about this).*
   - *If your sample is low on solvent (<600µl), make sure to center the sample about the dashed box in the depth gauge (marking the center of the magnetic field). Use of too little solvent (<450µl) will not shim properly or at all.*

4. ***Switch to tray view if not present.*** Click on  in the upper left corner of the spectrum window (it is an X in the tray window, as shown below) to switch to the tray position window.

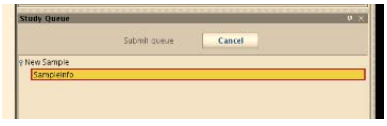
   Make certain tray position 0 is empty. Do not use position 100.

   Place your sample into an open tray position, being careful to note the position. *CAUTION: Make sure the autosampler arm is not moving when placing your tube.*

   In the program are different areas: the experiment selector, the study queue, the tray positions, and the sample setup.

5. To queue and experiment click on **New study** and the study queue window will change to display "new sample".

6. From the experiment selector choose the experiment you want to run.

   If you make a mistake so serious you are not sure you can correct it, e.g., clicking on the wrong protocol (you selected Carbon, but really want a Proton), you can remove the protocol by simply dragging it into the trashcan (lower left corner).

7. In the **Start → Sample info** panel (below the tray position/spectrum window):

   Choose your solvent.

   This panel is specific to your *sample*, not to the experiment. The information in it will carry over to all the experiments performed on this sample.

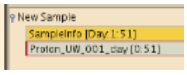
   a) ***Enter a sample name***

      This description will become part of the sample folder name (or *Studyname*), so keep it relatively short and ***do not* use special characters**. Hyphens (–) and underscores (_)are OK. Spaces will be automatically replaced with underscores _ .

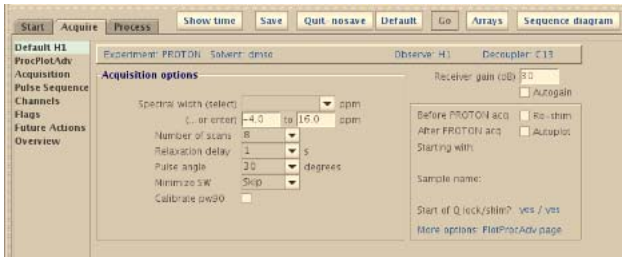
   b) ***Enter a notebook number and page number*** if you wish (can be left blank).

   c) If you would like to receive an e-mail when the sample is measured, make sure your e-mail address is correct and after queue → e-mail is ticked.

8. ***If you need to change parameters***, double-click on the experiment name in blue in the study queue window on the left, e.g., Proton_UW_001_day [0.51].



   The **Acquire tab – Default H1** will now be active and the sample tray on top will be exchanged with the pulse program.



   Common parameter changes:

   number of scans/transients (nt) → use a larger number for low sample concentrations; common for ^{13}C 1Ds.

   relaxation delay (d1) → use longer values, esp. for quantitative ^{1}H and ^{13}C 1Ds (**d1=4** is often more optimal for quaternary carbons).

   spectral width (sw) → can be optimized if desired. Left and right limits can be used here to position the spectral window.

   Click **Show time** to see a new estimate of the total experiment time.

   If you would like to change a parameter to a value that is not in the dropdown menu, or if you are looking for a different acquisition parameter, chose the **Acquire tab – Acquisition window**. Here you can change all acquisition parameters (including using the command

line to change them; e.g., **nt**=96). Remember that Varian and Bruker do not use the same language (e.g., Bruker dummy scans, **ds**, are Varian steady state scans, **ss**).

9. If you want to ***run more experiments on this sample***, go to step 6 and repeat.

10. Depending on the combined length of your experiments, in the study queue window the sample can be: **Submitted** to the **DayQ** (limited to 35 min) or **NightQ** (starts at 7pm; limited to 3h *per user*, i.e., not per sample but all samples combined from one user). The program will notify you when you exceed the allowed time limits.

11. ***Click on the tray position.*** Click on  if needed to switch to the tray position view. Click on **Zone 1**, **2**, or **all** as applicable and choose the position of your sample.

12. Submit your study queue using the **Submit** button towards the bottom of the study queue window.

13. ***If you have more samples***, go to 3 and repeat.

14. If you have to add more experiments to a study queue, right click on the tray position of the sample and select "edit study". This will take you back to the study queue window and you can edit, delete or add experiments. Then re-submit the queue.

15. If you would like to delete a study queue, right click on the tray position and select "Delete study". This will only work if the study has not started.

16. If you would like to run the same study (same sets of experiments) on multiple samples, set up the first sample and submit. Then right click on the sample number and "copy study". Click on the position of the next sample in the tray, right click and "paste study" to the new position. You will be asked to enter a new name for the sample. Once you click OK, the sample is submitted.

17. ***Logout*** using the logout button on the right side of the START menu: 

18. Your data will be located on the castor server (sftp:\\castor.chem.wisc.edu) under your user in the \hermes folder.