

Saving data

When you log in as an automation user (username = chemlab, organic, plnu, miramar or grossmnt) your data is automatically archived when the experiment finishes. The data is stored in a directory: /home/username/vnmrsys/data/studies/ with the name you give it in step II.b. and that shows up in the automation window.

To archive your data in your personal folder, do the following after you have collected your data and have exited **vnmrj**:

- 1) From the Desktop, open the folder (double click) labeled “Link to automated data storage”. This opens a window in **/home/username/vnmrsys/data/studies/** where you can locate a folder named by the date on which you acquired the data (e.g. “auto_2005.month.day). Open this folder to locate a folder containing your experimental data (the folder is named by the sample name you supplied).
- 2) From the Desktop, open the folder (double click) labeled “Link to personal data storage”. This opens a window in **/home/username/vnmrsys/data/yourname** where you can store your personal data.
- 3) At this point, with both windows open, you may simply “drag and drop” your experiment folders (take the entire folder) into your personal folder.

Retrieving stored data

Once you have stored data in your personal folder, you may wish to view it again from within VNMJRJ. You do this in the following way:

- 1) Launch **vnmrj** as usual.
- 2) At the top of the far left panel of the screen, there is a window that displays the current path for data storage (should look like: **/home/username/vnmrsys/rest of last path viewed/**). On the top edge of this window is a small blue arrow (pointing up). If you click the arrow, you will change the directory path (it moves “up” in the “tree”) until you get to **/home/username/vnmrsys/data** (which is where your personal folder lives).
- 3) You can then scroll down and find your personal folder/directory from the list in the window. When you find it, double click on your personal directory, and then double click on the filename of the sample you wish to view. This opens to another list of files from you can locate a folder named **data**; open the **data** folder and locate a file with the name “**solvent_#.fid**” (where solvent is literally the solvent you ran the sample in and # is an identifying number such that if you collected only a proton spectrum it would be 01, if you collected a proton and carbon spectra you would see two files, solvent_01.fid and solvent_02.fid, etc.)
- 4) From the list there, you can either double click or drag and drop your experiment **solvent_#.fid** into the spectral window. It should automatically process.