

Using the NMR workstation

The NMR workstation runs VnmrJ 2.2C using a Red Hat operating system. Both the software and the operating system are different from what is on the acquisition machine for the NMR

Logging on:

Your username and password is the same as the NMR acquisition machine

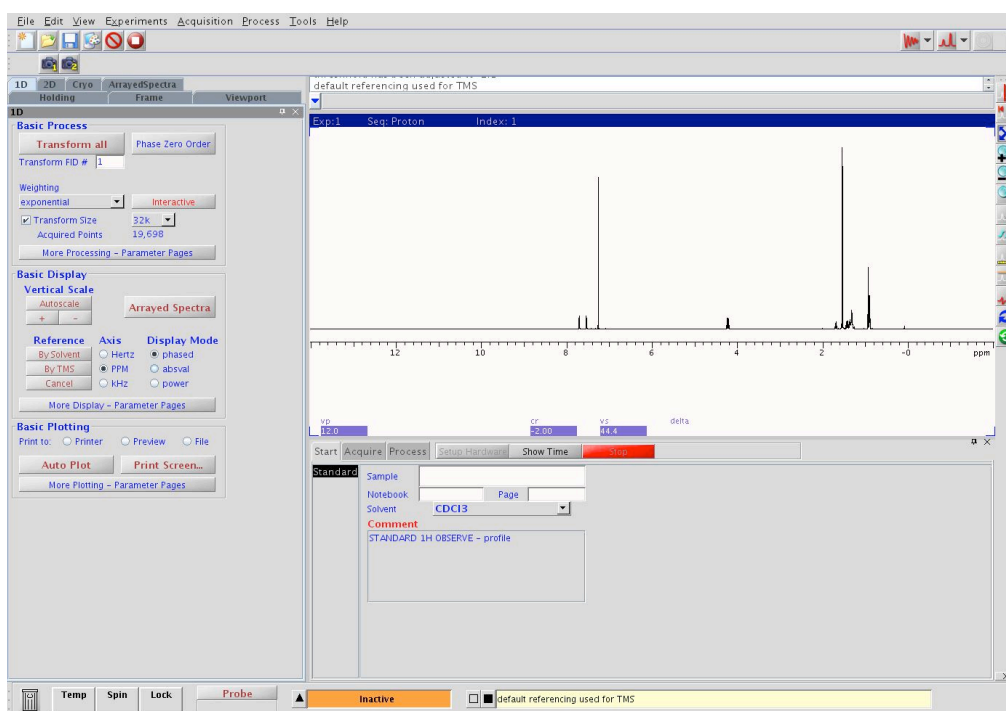
Using the workstation:

Red Hat is a much friendlier OS than Unix. It looks and feels more like a windows type environment. Once you log in you will see a folder icon labeled “home” two icons for the VnmrJ software, one in English, one in Chinese and a trash can. Clicking the VnmrJ icons starts up the software.

There is no sign up to use the workstation, and there is no fee for it’s use.

Using VnmrJ 2.2C:

VnmrJ 2.2C looks pretty close to VnmrJ 2.1B (which is what we are using to acquire data) two major items of note. First the graphics display has changed to black on white instead of blue on black. This is so if you can capture a jpeg image of your spectra, place it in a report and have it be a black on white image. If you want to revert your graphics to the traditional display you can find that setting by clicking the Display Options button. Second the left hand side of the interface has changed. You can now tab through various options for 1D, 2D, arrayed spectra and so on. I encourage you to look at what they have placed there, it is quite useful.



The button menu that used to be on the left hand side of the graphics window is now on the right hand side, and there are some new buttons as well. Holding the mouse over any of them will display a “hint tab” as to what their function is.

Additional note: when loading or saving spectra though VnmrJ 2.2C for the first time you may have to change your file location. The default location to save/load data is /home/username/vnmrsys/data. You will probably want to change that to /home/username.

Transferring Data:

Unfortunately I am unable to make a link to the NMRdata server. If you want to transfer your data from the server you must find it manually.

You can find the server from the following: Applications-Network services-windows Network-Microbiology-NMRdata-NMRdata. At this point it will ask you to log in. Enter your username and password. The ‘domain’ portion of the login should be left blank. at this point you can open your labs folder on NMRdata and copy your data to your home folder

You can also use FTP or secure copy to copy your data. the name of this workstation is nmrwkstn2.med.harvard.edu. you can open a terminal window by using right click-open terminal

Copying using secure copy:

- 1) Select the file you want to copy to the workstation
- 2) Once you have logged in to your account on the workstation, right click the mouse. This will bring up a window.
- 3) Select Tools>terminal. A white window with a prompt “NMRWKSTN2 username>” will appear
- 4)At the prompt type exactly the following (spaces included) substituting user with your username and filename with your filename

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scp -r user@nmr:./filename ./filename
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- 5) If it asks you to verify a key connection, type “yes” to proceed.
- 6) It will ask for your password at NMR:user, enter it.
- 7)Some text graphs will appear indicating the file transfer.

That’s it! Your file is now in your account at the workstation

Using flash drives:

Unlike the Sun workstations, the new workstation will support plugging in a thumb drive into the USB port, and copying your data on to it.