

Processing NMR Spectra Remotely with TopSpin

The Chemistry Department employs a workstation serving three copies of TopSpin for remote access via X-windows.

To access via a Mac running OS 10.5.7 or later:

1. Launch the application *X11*. Under the *Applications* menu, select *Terminal*
2. In the terminal window type `ssh -X nmr@nmr.chem.hmc.edu`
3. When prompted, type the password for *nmr*
4. When you get a prompt from the workstation, type `topspin`
5. If TopSpin will not run because someone else is already using this copy,
 - a. logout by typing `<control-D>`
 - b. log in again via `ssh -X nmr2@nmr.chem.hmc.edu` or `ssh -X nmr3@nmr.chem.hmc.edu`
 - c. go to step 3
6. Do your business. Your data files are located at `/opt/topspin3.0.a/`
7. When finished,
 - a. exit *TopSpin*
 - b. type `<control-D>` to log out of the workstation
 - c. exit *X11* on your local machine.

To access via a PC running Windows XP or Vista:

1. Launch *Xming* (freeware available at www.straightrunning.com/XmingNotes)
2. Launch *PuTTY* (freeware, available on Charlie)
3. In *PuTTY*, under Host, type `nmr.chem.hmc.edu`
4. Select the SSH radio button
5. In the menu on the left, select *SSH-tunnels*, then check the *enable X11 forwarding* box
6. Click on OPEN
7. When asked "login as", reply with *nmr*
8. When prompted, type the password for *nmr*
9. When you get a prompt from the workstation, type `topspin`
10. If TopSpin will not run because someone else is already using this copy,
 - a. logout by typing `<control-D>`
 - b. Goto step 3. When you get to step 7, use *nmr2* or *nmr3*
11. When finished,
 - a. exit *TopSpin*
 - b. type `control-D` to log out of the workstation
 - c. exit *PuTTY* on your local machine.

Please note: any changes you make via the workstation are made to your original data on the spectrometer. To process your data in a new, different way without changing your original data:

1. within TopSpin type *edc*
2. increment *PROCNO* by one
3. reprocess your data