Processing of XWINNMR-data from DPX200, DPX300 and DRX500, and TOPSPIN-data from AV600 and AVII600 with TOPSPIN 1.3 on a Windows 2003 Server.



University of Oslo

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The datasets from all of our NMR-instruments except DMX200 (forester.uio.no) and Varian Gemini 200 (wittig.uio.no) are copied from the PCs controlling the instruments to a central Windows 2003 server once a day.

The name of this computer is: pauling.uio.no

- 1. You log on to pauling.uio.no with the "remote desktop connection program" on your local XP PC. Click on "Start" at the lower left corner of your XP PC desktop followed by: "programs", "accessories", "communications", "remote desktop connection", click on options, experience and choose the speed of your connection, LAN (10Mbps when at UiO), if you are sitting at home use your connection speed. Type in your username and password and click on connect.
- 2. You should locate the TOPSPIN (topspin 1.3 pl6) icon on Paulings desktop and double click on it to start TOPSPIN.
- 3. You then look at the data disks at the left side of the TOPSPIN window and do realize that the disks with your NMR data are not in the list.
- 4. You click on one of the other disks and realize that the connection to that disk is broken.
- 5. You decide to clean up the list and get "your" disk(s) (for instance DPX200, DPX300 or DRX500) in the list.
- 6. You do realize that you do not know how to do this.
- 7. You have a bright moment and you left click on one of the disks to be removed, it becomes highlighted and then you right click on the disk and drag down to REMOVE SELECTED DATA DIR. The disk is gone and you repeat the procedure for all other unwanted or corrupted disks. (If you hold down CTRL key you can remove many disks at a time).
- 8. You are in a hurry and cannot wait till tomorrow to get access to nmr-data generated today. You then have a second bright moment and do realize that you can connect the disks on the DPX200 and DPX300 spectrometers directly and you double click on "MyComputer" on Paulings desktop.
- 9. You click on "Tools" and "Map Network drive".

- 10. You type in \cunskis\D\$2 or only \cunskis\D\$ (for mounting the DPX300 data disk) in the folder area. (\\augner\D\$2 or only \\augner\D\$ for DPX200 data)
- 11. You then click on "Finish".
- 12. You then go back to the TOPSPIN program and right click in the data part of the window.
- 13. You do select Add New Data Dir....
- 14. You browse in the new small window (desktop, My computer D\$2 or D\$ on Augner or D\$2 or D\$ on Cunskis. and do highlight it and click OK.
- 15. The disk comes up in the data window in TOPSPIN named with the letter the disk was mounted as.
- 16. If your data was acquired more than 24 hours ago the data is already copied to pauling.uio.no and do reside on one of the local disks.
- 17. You right click in the browser/data window in topspin and use "Add new Data Dir.." and type in one of the following: D:\DPX200, D:\DPX300, F:\dataDRX500. Other data disks do also exist. Please ask.
- 18. You click on the dataset you want to process in TOPSPIN.
- 19. You can use the same commands as you are used to in Xwinnnmr. Integration is easier since there is no middle mouse button involved.
- 20. Plotting can be done by starting "Xwinplot" or "plot" in the command line in TOPSPIN.
- 21. You most likely have a lot of trouble with connecting to a plotter near you. You have to try to install a printer on your local PC. Click on Start, run and type in \winprint2\kj_o316 and click enter/return. If you want to use another printer exchange "kj_o316" with the other printer-name. Parts of the Campus are served by other printer servers than winprint2. Ask you local IT personnel if you have no idea about this.
- 22. Or you give up and do click on COPY under EDIT in TOPSPIN and do paste the spectrum in a Word document which is opened on your local computer before you do COPY.
- 23. Click on file in upper left corner in TOPSPIN and then Exit at the bottom of the list that comes up.

- 24. Click on Start in lowe left corner in the Pauling remeote desktop window. Selct "Log Off"
- 25. Never close the "pauling.uio.no Remote desktop" by clicking on the X in upper right corner.
- 26. If you don't exit TOPSPIN or leave the remote desktop in the wrong way you will block other people from using TOPSPIN. We have only 5 TOPSPIN licenses exiting wrongly blocks the licenses.
- 27. If you get strange error messages when trying to open a data set, close Topspin and start again. If it still does work OK close Topspin and log out of pauling.uio.no and log on once more and start Topspin one more time. If you still have trouble cry for help.
- 28. Good Luck