NMR NOTES #21
Managing Disk Space

The NMR fileserver provides disk space for all of the NMR spectrometers and workstations, and quotas are used to insure that there is sufficient disk space for everyone. They also encourage you to manage your NMR data before it becomes an undaunting task. One of the major sources of quota problems comes from the use of the firefox (mozilla) web browser – it can use up large amounts of disk space without warning. Following are some tips and guidelines for managing your disk space.

Pay attention to the warning box that starts popping up when you reach 60% of your quota. Once you reach 100% you will not be able to run either the X-window server (login) or run the NMR program. Address the issue before it becomes a problem'. You can also explicitly check your quota status at any time with the **quota -v** command in a teminal window.

If you do reach 100%, you can still login using the failsafe terminal (session button on the login screen) which will give you a unix terminal window that will let you clean up your file space. You can also telnet into your account from a remote PC, just like you do to reserve NMR time. Just use your username and password instead of 'reserve' to login;

The **du_summary** command can be run in a terminal window, and gives you a summary of disk usage by subdirectory (folder) in the current folder. This includes hidden files, so you will see how much space is taken up by **.mozilla** (web browser) and **.Trash**;

The **.mozilla** folder can safely be deleted - it will be automatically recreated the next time you use the browser. To delete it, use "**rm -rf .mozilla**" in a unix window;

Using the desktop GUI to drag unwanted files to the Trash Can does not delete them - you have to empty trash can to do that. Do not delete the **.Trash** folder - it is part of the X-Windows desktop. Rather, simply empty the trash from the X-window system or delete the contents of the folder from a unix terminal window;

DO NOT REMOVE THE vnmrsys FOLDER!! - It is essential for the operation of VnmrJ! If a large amount of disk space is being taken up in vnmrsys, go to that folder and run the du_summary command (**cd vnmrsys; du_summary**) to see where the disk space is going. It will almost certainly be in one or more of the experiment files (e.g. **exp3** or **exp4**....). These can be safely deleted (**rm -rf exp3**) but of course you will lose any data in that experiment that has not been saved. Also, you must not delete all of your experiment files, you need at least one as a template to create new experiments.

Running 2D NMR can result in some disk usage problems as well. The most common problem has to do with the size of the transformed data. Someof the Varian processing has a tendancy to do a lot of zero filling – such as transforming 8k data points for 256 collected points. After you start a 2D experiment check and make sure that **fn**~=**np** and that **fn1**~=2***ni**.

If you use the automatic 2D plotting macros like plcosy, there will be subexperiment space created to hold copies of the 2D and 1D data for easy plotting. VnmrJ neither tells you that this space has been created nor deletes it when finished plotting. This too can occupy significant amounts of disk space. Within VnmrJ, the **explib** command will list all of your experiment files and show which ones, if any, have subexperiments. To remove the subexperiments, simply go to that experiment and run the cleanexp command (e.g. **jexp3 cleanexp**). You can only clean the experiment that you are joined to. In the unix window, you can simply delete the subexp folder within an experiment folder (**cd exp3; rm -rf subexp**).

Once you have saved your 2D data, it is still occupying disk space in the experiment file as well. You can reclaim this space by returning a small 1D dataset **and transforming it**. It is necessary to transform it so that the 2D spectrum is replaced with the small 1D spectrum.