

Data Management Using a UNIX Shell

Commands:

> cd	change directory
> pwd	print working directory
> cp and > cp -r	copy files, copy directories
> ls	list files
> mkdir	make directory
> rm and > rm -r	remove files, remove directories
> pwd	print working (current) directory

To open a UNIX shell, on the wallpaper hold down the right mouse button. Select **[Programs]** then **[Terminal]**.

To close the shell, type >**exit** at the prompt in the terminal window.

Copying or removing large amounts of data may take some time. WAIT for the prompt to come back. The desktop bar (bottom of the screen) will indicate whether the disk is running.

To move files from medicinal1 (online) to medicinal2 (offline) while logged into medicinal2 (offline):

1. Open a UNIX terminal.
2. Go to the directory where the data will be moved to: >**cd vnmrsys/data**
3. Copy the directories from the online to this directory on the offline:

>**cp -r /net/medicinal1/data/username/vnmrsys/data/directoryname .**

The cp command specifies source and then destination. The space and period after the directory name specifies put the data in the current directory with the same name.

Hints for usage:

Try moving bigger blocks of data by specifying a date or name. For example, move all of data from July 2002 by:

> **cp -r /net/medicinal1/data/username/vnmrsys/data/*Jul2002* .**

The * is a wildcard meaning select everything that contains “Jul2002” regardless of what it starts or ends with.

As a second example, move all data including the compound name “benzene”:

> **cp -r /net/medicinal1/data/username/vnmrsys/data/*benzene* .**

To remove files from the data directory:

1. Open a UNIX terminal.
2. Go to the directory containing the data to be deleted: >**cd vnmrsys/data**
3. Look at the data directories: >**ls**
4. Delete the data directory: >**rm -r directoryname**

Hints for usage:

Try removing larger blocks of data by specifying a date or name. For example, remove all the data from July 2001 by:

>**rm -r *Jul2001***

The * specifies select any directory containing “Jul2001” regardless of what the name starts with or ends with.

Remove larger blocks of data based on a compound designation like “epoxy”:

```
>rm -r *epoxy*
```

WARNING: Be careful removing things using *. Entering a command like `>rm -r *` will remove everything in the current directory.

Sort data into individual directories:

Keeping all data in one directory becomes cumbersome to manage and locate a specific file.

1. Open a terminal and go to the data directory: `>cd vnmrsys/data`
2. As an example, all ethyl compound spectra will be stored in a directory called “ethyl”. Make a directory for the specific data sets. `>mkdir ethyl`
3. List the files and confirm the creation of the new directory. `>ls`
4. Copy the data sets into the new directory: `>cp -r *ethyl* ethyl/`.

This command copies all directories containing the string “ethyl” into the directory ethyl and give them the same name (note the period at the end).

5. View all the data in the new directory: `>cd ethyl` `>ls`
6. To make another directory, go back up one directory `>cd ..`

The data will also still be in the top vnmrsys/data directory. After confirming that it has been copied to the new directory. The files can be removed the top vnmrsys/data directory.