

Transferring Files

IP Addresses:

CDD nmr600: 160.94.71.50

MDCH medicinal2 (offline): 160.94.172.205

1. *To a PC (Windows) from the Drug Design workstation:*

Winscp program for file transfer:

<http://winscp.net/eng/download.php>

This program will allow a simple arrow transfer from Drug Design a PC running windows.

2. *Move files from Med Chem offline workstation to CDD workstation:*

Method 1: UNIX window

While logged into CDD workstation:

- a. Open a UNIX terminal by right clicking on the wallpaper: **Tools->Terminal**
- b. Change directories to the Med Chem offline (Medicinal 2):
>**cd /net/medicinal2/export/home/username/vnmrsys/data**
Use the medicinal2 username if it is different than CDD. This will go to the DATA directory on the medicinal2 where data is typically stored.
- c. View the data directories in a list by >**ls**
- d. To copy the data back to the home directory of CDD, use
>**cp -r directoryname ~/.**
Other examples of use:
>**cp -r *2005* ~/.** (copies everything with 2005 in the name)
>**cp -r abc* ~/.** (copies every directory starting with abc)
>**cp -r directoryname ~/vnmrsys/data/.** (copies into the vnmrsys/data on CDD)

The **cp -r** means copy a directory. The **~/.** means go back to the home directory on nmr600 and give the directories the same name.

- e. Use >**cd** to return to the home directory on nmr600. The files that were copied should now be on the CDD workstation and can be loaded there.

Method 2: File Manager window

While logged into CDD workstation:

- a. Open a File Manager window by right clicking the wallpaper **Files->File Manager**
- b. Change the path name in the box to **/net/medicinal2/export/home/username/vnmrsys/data**
- c. Highlight the directory to copied and choose **Selected->Copy To**
- d. A box will open and change the destination folder to **/net/nmr600/export/home/username/vnmrsys/data**
- e. Hit OK and the file directory should be copied back to the CDD workstation. Make sure if the usernames on the two workstations are different to use the appropriate one for each specific path.
- f. Close the file manager windows when finished.

3. Move files from CDD workstation to Med Chem offline workstation:

Method 1: UNIX window

While logged into medicinal2 (offline):

- e. Open a UNIX terminal by right clicking on the wallpaper: **Tools->Terminal**
- f. Change directories to the CDD nmr600:
>**cd /net/nmr600/export/home/username/vnmrsys/data**
Use the medicinal2 username if it is different than CDD. This will go to the DATA directory on CDD nmr600 where data is typically stored.
- g. View the data directories in a list by >**ls**
- h. To copy the data back to the home directory of medicinal2, use
>**cp -r directoryname ~/.**
Other examples of use:
>**cp -r *2005* ~/.** (copies everything with 2005 in the name)
>**cp -r abc* ~/.** (copies every directory starting with abc)
>**cp -r directoryname ~/vnmrsys/data/.** (copies into the vnmrsys/data on medicinal2)

The **cp -r** means copy a directory. The **~/.** means go back to the home directory on medicinal2 and give the directories the same name.

- e. Use >**cd** to return to the home directory on medicinal2. The files that were copied should now be on the medicinal2 workstation and can be loaded there.

Method 2: File Manager window

While logged into medicinal2:

- g. Open a File Manager window by right clicking the wallpaper **Files->File Manager**
- h. Change the path name in the box to **/net/nmr600/export/home/username/vnmrsys/data**
- i. Highlight the directory to copied and choose **Selected->Copy To**
- j. A box will open and change the destination folder to **/net/medicinal2/export/home/username/vnmrsys/data**
- k. Hit OK and the file directory should be copied back to the medicinal2 workstation. Make sure if the usernames on the two workstations are different to use the appropriate one for each specific path.
- l. Close the file manager windows when finished.

To View a file from Med Chem on the CDD workstation (does not copy!):

Within VNMRj in the file system window, use the **^** button and go up to **/** directory. Then select the **/net** directory. Select the **/medicinal2** directory etc. and go to the **/net/medicinal2/export/home/username/vnmrsys/data** directory. Select the directory containing the data file Drag the **.fid** file into the window to be processed.