

# Bruker File Path Explanation

Revised August 2017

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## WHERE IS MY DATA?

The simplest answer - it is exactly where you put it. If you do not understand the file management utilized in the facility it is time to learn!

**NMR DATA IS NOT BACKED UP** - You alone hold this responsibility as of this date the department has not allocated a backup server for our large number of files.

**\*\*\*Data appearing randomly on any computer is subject to immediate removal without backup\*\*\***

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When the user types **new** – the user sets the file path where the data will be stored. Understand where your data is being stored so you can retrieve it at a later date.

The first thing that all users must do is type '**new**' or '**edc**' to create a directory, the dataset, which holds the NMR data. You are asked for the following items (in Topspin 1.3):

- NAME: - this will become the name of the directory; your sample or experiment name
- EXPNO: - typically this is '1', but by changing this you can save multiple experiments in the same directory which is useful for organizing your data
- PROCNO: just keep this as '1'. If you are running T1 experiments or pulse calibrations temporary data is stored in '999'.
- DIR: **\*\*\*IMPORTANT\*\*\* This is WHERE the data goes. See below\*\* for detailed instructions!**
- USER: your chemistry username ONLY

NMR data should be stored in a network drive location. It is preferred to have your data stored on a network drive so that you can easily access this data from any computer joined to the Chemistry domain. The network drives should be 'mapped' to your 'My Computer' everywhere you are logged into the Chemistry domain. You will only see the drives for the NMR to which you have been given access. When access is approved, the network location associated with that NMR appears in this list. If it does not please contact the NMR manager. The NMR manager or the NMR TA will assist you in setting up and explaining this to you during your training on each instrument.

As soon as you log into the instrument computer, open the 'My Computer' from the Start button. There are local drives (C:\ and D:\, etc.), devices (DVD drives, flash drives), and network drives (U:\, X:\, Z:\, etc.).

For example, osuguy.2 has access to the 250 MHz (NMR-Thyme) and the 400 MHz in 0083 (NMR-Paprika). When he logs onto either system his network drives should look something like:

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osuguy.2 (\\winsf) (U:\)
NMR-Thyme (\\winsf\nmr_nobackup) (X:\)
NMR-Paprika (\\winsf\nmr_nobackup) (Y:\)
profgroup (\\winsf) (Z:\)
```

**\*\*\*NOTE:** X:\ and Y:\ may flip at login such that NMR-Thyme could be mapped to Y:\ rather than X:\\*\*\*

**\*\*Check which mapped drive you need to save your data. In the case of NMR-Paprika from the example above.**

- DIR (in Topspin 1.3): Y:\
- DIR (in Topspin 3.5): Y:\data\ASC-osuguy.2\nmr

## HOW DO I COPY MY DATA?

If you need to copy your data from the local drive you may do so by using a flash drive device or saving to a network drive. If not already available, create a folder on the device on which you would like to copy your data; for example X:\250NMR. Within

this folder create another folder called \data\ so that the file path on your device is X:\250NMR\data\. Cut and paste the folder C:\Bruker\TOPSPIN\data\username\ into this \data\ folder.

The file path is important in order for Topspin to be able to recognize the data. Now you should have a file path on your device that looks something like: X:\250NMR\data\username\nmr\yourdata.

### **HOW DO I OPEN MY COPIED DATA IN TOPSPIN?**

Open Topspin and note the left side of the screen which displays the directories. Right click on the open space and select 'Add new data dir...'. Select the folder just above the \data\ folder. In this example, browse to and select X:\250NMR\. This directory will be added to the list on the left side. When you click the + all the usernames within the \data\ folder will be shown. Click the + by your username to access your files. Click and drag the file names into the large work space to open the spectrum. Process as usual.