

# NUCLEAR MAGNETIC RESONANCE RESEARCH RESOURCE

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## Installing TopSpin 2.1 for Windows

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The NMR<sup>3</sup> facility has three TopSpin (TS) 2.1 licenses available. All researchers trained in the use of a NMR<sup>3</sup> spectrometer are invited to install the software on their personal desktop/laptop to create what is known as a TS datastation. However, a maximum of 3 computers can be using the software at any one time. Please note that TS for Windows has been tested by Bruker (and is therefore supported) on Windows 2000, XP Pro, and Vista - the instructions/screen shots that follow are taken from an installation performed on an XP Pro computer. Please note that although not supported, users have reported successful use of the software on a Windows XP Home datastation.

### **\*\*Windows 7\*\***

TS 2.1 is NOT compatible with the Windows 7 operating system. Having said that, I have been informed it can be installed on these systems provided you also have "XP Emulator" software. Please note this has not been tested by the NMR<sup>3</sup> facility and is therefore not supported.

### **Preliminary Note: Windows Accounts/Passwords & TopSpin**

There are a number of configuration-type commands and scripts within TS that require authorization before execution. As a result, TS requires two pieces of information to be supplied during the installation that ultimately controls who can run these scripts and make configurational changes to the installation:

1. **NMRSUPERUSER**: during the installation, you must declare a NMRSUPERUSER which must be an existing Windows account on your computer. The default is Administrator but note that this account need not have administrative privileges. After the installation, the NMRSUPERUSER is the owner of all TS files. Logging into Windows as this user allows you to remove these TS files, change permissions, etc.
2. **NMR ADMINISTRATION PASSWORD**: this password must also be supplied during the installation. TS configuration commands like cf and expinstall require this password before execution. Note that this password has nothing to do with the Windows login password for the superuser, although they can be the same. Knowledge of this password allows any user to execute configuration type commands during his/her login session.

On a computer with multiple Windows accounts, the users must decide who will be the NMRSUPERUSER. The solution recommended by Bruker is to create a new Windows account called "nmrsu". This account does not need admin privileges; standard privileges are sufficient. Subsequently, the password for the nmrsu account can be made known to only those authorized to make changes to the TS configuration.

### **Step1: Pre-Installation Notes & Checks**

Before installing TS 2.1, you should ensure your computer meets or exceeds the hardware requirements recommended by Bruker. As well, supporting pieces of software will need to be installed to ensure you benefit from the full functionality of your TS datastation.

#### Hardware Requirements:

- x86 based PC (64 bit architecture is not supported)
- CPU processor  $\geq$  1 GHz
- $\geq$  512 MB of RAM
- $\geq$  64 MB of video memory
- Ethernet card and a local network configuration (Check by going to Start --> All Programs --> Accessories --> Command Prompt and then typing the command ipconfig /all).

Note that if your system does not meet these specifications, TopSpin may still run but you can expect degraded performance. In addition to the above list, your display resolution should be set to 1280 x 1024 or better.

#### Software Requirements:

- Windows Vista, Windows XP Pro (SP2) or Windows 2000 (SP4)
- FlexIm License Manager (available during the TS installation)
- Internet Explorer (IE) version 6.x or higher (for NMR GUIDE only): to configure IE, go to *Tools* → *Internet Options* → *Advanced* and make sure that the following options are enabled (1) Java console (2) Java logging and (3) JIT compiler for virtual machine. If any of these options had to be enabled on your system, you should restart your computer before proceeding with the install.
- A PDF Viewer like Acrobat Reader (for TS Help and/or NMR Guide)

Note that TS requires a NTFS filesystem on the partition where TS is installed as well as on all partitions where TS data are stored. To check your system, go to "My Computer", right click on the appropriate disk, select properties, and ensure filesystem says "NTFS". If it says "FAT", I'm told it is possible to convert from FAT to NTFS but this is not something supported by NMR<sup>3</sup>.

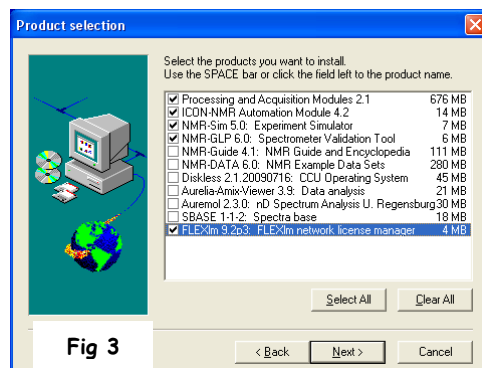
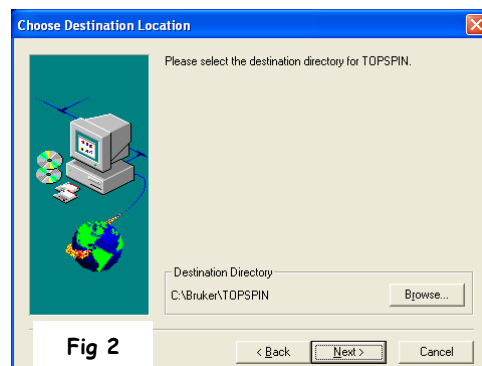
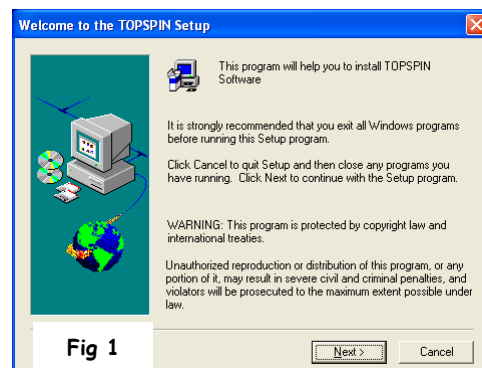
#### Step2: Obtaining a Copy of the Software

The installation files are available on the NMR<sup>3</sup> fileserver in Room 426B in a folder called D:\armrc\TS2.1. You can make your own installation DVD by burning a copy of the files or alternatively, you can copy the installation directly to your usb flash drive. The total space required on your flash drive is ~ 1.2 GB.

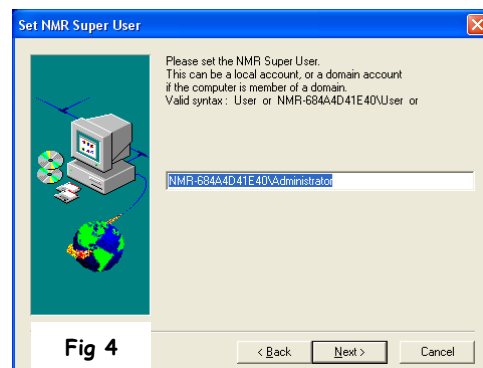
#### Step3: Installing TopSpin

Before installing, ensure you are logged into Windows as Administrator or in an account with administrator privileges. Close all open windows and insert your TS installation cd/dvd or usb flash drive. If using a cd/dvd, the software may launch automatically. If not, explore the contents of the cd/dvd or flash drive and run the program "install.cmd". If that doesn't work, drill down into the Windows folder and double click on "setup.exe". Once you see the window shown in Fig 1 entitled "Welcome to the TOPSPIN Setup", the installation has started successfully and you should now perform the following steps:

- Click Next > at the bottom of the Welcome screen.
- The TS release letter should open next. When you are done reading the letter, close it by clicking the red X in the upper right corner.
- Choose the destination directory for TS (see Fig 2). Please do not use the default and also do not use an existing directory from a previous TS/XWIN installation. Instead, use C:\Bruker\TopSpin2.1 by clicking the Browse... button. When finished, click Next>.
- A window "Select the setup type" opens. Choose the option "Customized setup (allows component selection)" and click Next >.
- A "Product selection" window opens. If TS/XWIN was previously installed on your system, you should select the 4 components shown in Fig 3. However, if this is the 1<sup>st</sup> installation, you must also install the **FLEXIm 9.2p3 product for licensing purposes**. You can also install NMR Guide 4.1 if desired. This product is an NMR encyclopedia containing a wealth of information about NMR pulse sequences, experiments, etc. When done, click Next >.
- If running XP SP2 or higher, a "Question" window opens asking if the installation should automatically configure Windows firewall. Please select yes.
- If another version of TS/XWIN is installed on your system, a "Select Components" window opens allowing you to import a spectrometer configuration, browse for one, or skip the import of a spectrometer configuration all together. Normally, you will choose the first option: "No, I don't want to import a spectrometer configuration".



- A window entitled "Set NMR Super User" will appear as shown in **Fig 4**. The default will be Administrator (as shown in the figure) but an existing user or a specially created user like nmrsu can be used for this purpose. In any event, if you change the default, what you use must be the name of an existing Windows login. Click Next>.
- A window called "Password Input" (see **Fig 5**) will prompt you for the NMR Administration Password. This password is required for commands like cf and expinstall that make configuration changes to the installation. You can use the Windows login password for the account you specified in the previous step or a password of your choice. Click Next>.

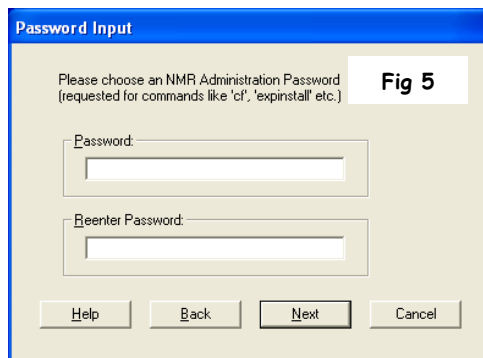


Now go grab a coffee...the installation takes awhile. It will take on the order of 20 - 30 minutes or even longer if you are installing NMR Guide. Note that if you are installing FLEXlm 9.2p3, you will be prompted part-way through for the directory to use for the software - please accept the default path.

#### Step4: Setting Up the TS 2.1 License

The NMR<sup>3</sup> facility has a single computer acting as a license server which monitors usage of the three TS2.1 licenses. To set the licensing up on your computer, please complete the following steps (all required files are in your TS2.1 installation folder):

1. Copy topspin2.dat into the folder "C:\flexlm\Bruker\licenses\".
2. Copy topspin2.cmd into the folder "C:\Bruker\TopSpin2.1\".
3. Delete the "TOPSPIN 2.1" shortcut on your desktop that was created during the installation.
4. Copy the "TOPSPIN 2.1" shortcut provided into the folder "C:\Documents and Settings\All Users\Desktop\".



#### Step5: An Extra Step for Nitrogen Referencing

Bruker automatically references nitrogen spectra to liquid ammonia. However, in keeping with the conventions of IUPAC, nitromethane should be the nitrogen reference compound. In order to ensure all nitrogen spectra (both direct and indirect detection) are referenced to nitromethane, please copy the file "nuclei.all" in your TS2.1 installation folder to the destination folder C:\Bruker\Topspin2.1\exp\stan\nmr\lists, overwriting the existing file.

#### Step6: Configuring TopSpin

Launch TS by clicking the desktop shortcut. If the licensing has been setup properly and there is a license available, TopSpin will launch. During the initial launch, a "LICENSE" window will appear. Once you have read and can confirm the agreement, click on the "I Accept" button at the bottom. Now complete the following steps:

- A window entitled "Configuration check" (see **Fig 6**) should appear that allows you to perform cf and expinstall. Cf is used to install a specific spectrometer configuration - for routine manual and interactive processing this is not required. TS will use "Bruker\_default\_av500"; a default configuration automatically added during installation. Expinstall installs pulse programs, AU programs, parameter sets, as well as a variety of other resources. For routine processing, this is also not needed UNLESS you plan on using Bruker AU programs. So, if you plan on using AU programs, click Expinstall. If not, click "Do not show this message again" check box and click "Cancel".
- Assuming you wish to use AU programs and therefore clicked Expinstall, a window entitled "Experiment installation and AU compilation" will appear. Just click Next>.
- Select the type of installation by selecting "Installation for Datastation (Default)", as shown in **Fig 7**. Then click Next>.
- Select the type of acquisition by placing a check mark in the High Resolution Systems option, as shown in **Fig 8**. Again, click Next>.



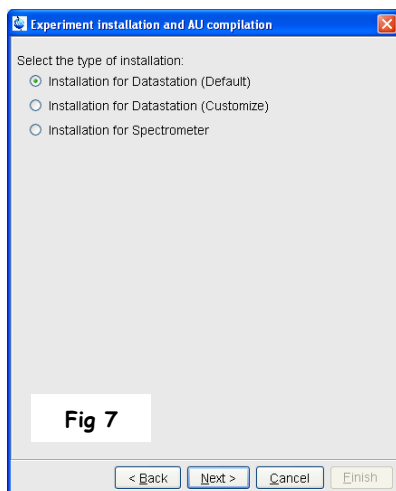


Fig 7

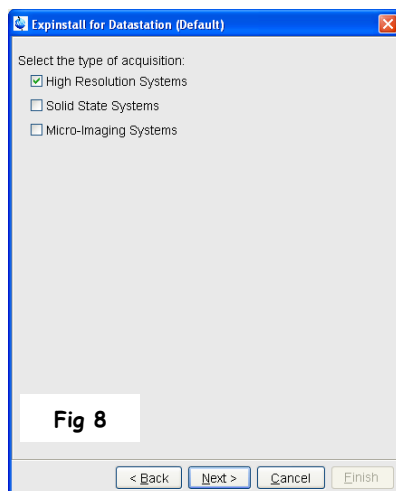


Fig 8

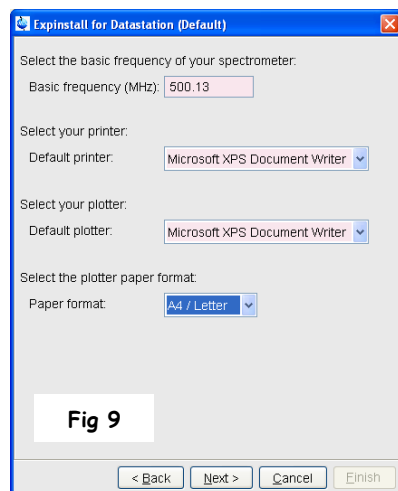


Fig 9

- You will now be asked to select your basic frequency as well as the default printer, plotter, and paper format (see Fig 9). Select these options appropriately for your desktop/laptop and then click Next >. Do not make any changes to the "Basic frequency (MHz):" field.
- A summary screen will appear (see Fig 10); click Finish and Expinstall will start.
- Once expinstall is complete, a window entitled "Cron check" appears that allows setup of a periodic backup of your TS2.1 configuration (see Fig 11). You can either select "Automatic Backup" to configure it or click Close.
- TS is now setup and configured and so is ready for NMR data processing.

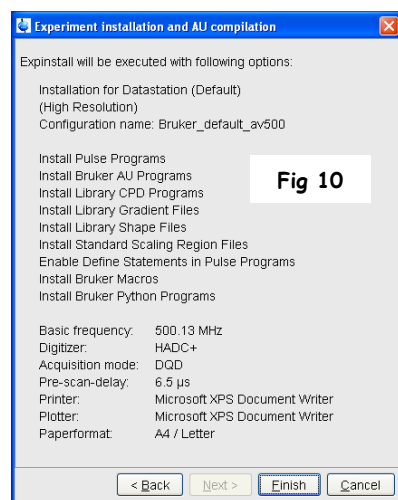


Fig 10

### Step7: Opening NMR Data in TS

TS requires a rigidly defined directory structure in order to access data. The data MUST reside in a directory structure that follows a specific format. It can be represented as `\DISK\data\USER\nmr`. Both "DISK" and "USER" are customizable whereas "data" and "nmr" are not. For example, let's suppose that Mary and I share a TS datastation in NMR<sup>3</sup> to process NMR data. We want to keep our data in a folder on drive "C" called "nmr\_users" (which is the name used on both the AV300 and AV500 spectrometers). Since we want to keep our data separated, we must create the following two folders on drive C:

- C:\nmr\_users\data\mike\nmr\
- C:\nmr\_users\data\mary\nmr\

Subsequently, all data that Mary and I acquire on the spectrometer should be copied to our individual folders on the datastation for processing.

Note you can and should add your folder to the TS dataset browser so that you can browse for the data sets you wish to open and work with. To do this, launch TS and with your mouse in the browser area (typically the left side of the main TS interface), right click and choose the "Add New Data Dir..." option. In the window that opens, type "c:\nmr\_users" in the DIR= field.

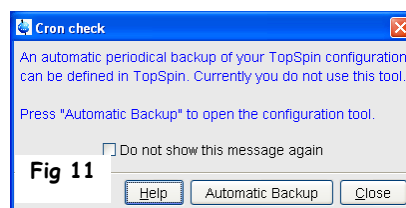


Fig 11

# Additional Information about Installing TS 2.1

## (1) Configuring Your TS Datastation like a Spectrometer Workstation

Advanced users of TS may wish to configure their datastation to mimic the configuration on the workstations of either the AV300 or AV500. This can prove useful in certain circumstances such as when setting up experiments, processing and/or plotting. To accomplish this, folders in your installation directory are available named "AV300 Stuff" and "AV500 Stuff". These folders contain many configuration files from the 300 and 500 MHz NMR<sup>3</sup> spectrometers, respectively. To configure your datastation like a spectrometer configuration, proceed as follows:



Fig 12

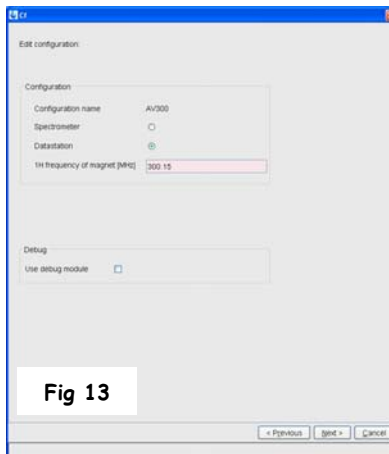


Fig 13



Fig 15

- Copy the AV300 folder (in "AV300 Stuff") or the AV500 folder (in "AV500 Stuff") to C:\Bruker\TopSpin2.1 on your datastation (or whatever your directory is for TS 2.1). The instructions and figures that follow assume use of the AV300 configuration folder.

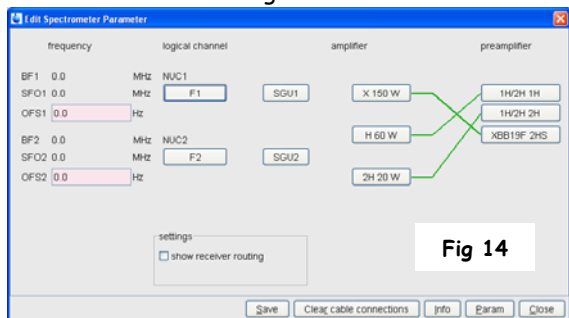


Fig 14

- Start TS as Administrator and open any dataset. If none are available, type "new" to create one.
- Enter the command "cf" and type in the NMR Administration Password.
- A window entitled "Cf" opens (see Fig 12). Select the AV300 configuration and click Edit.
- Another "Cf" window opens (see Fig 13). The selected configuration is displayed. Select Datastation rather than Spectrometer and click Next >.
- The next "Cf" window that appears is a table of nuclei. All

should be correct so click Next > at the bottom of the window.

- A window entitled "Edit Spectrometer Parameter" appears next (see Fig 14). Click Save.
- A summary of the cf procedure appears in the next window (see Fig 15). Click Next >.
- After finishing cf, a window specifying "Additional configuration programs" will appear. Click on expinstall and

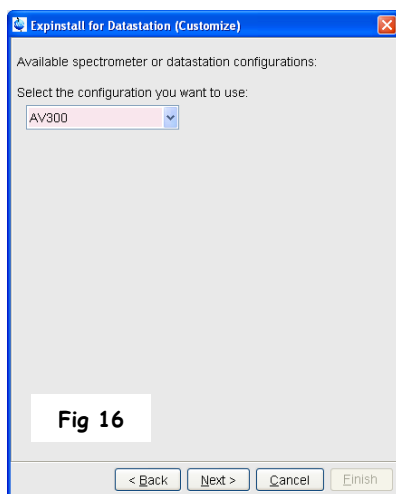
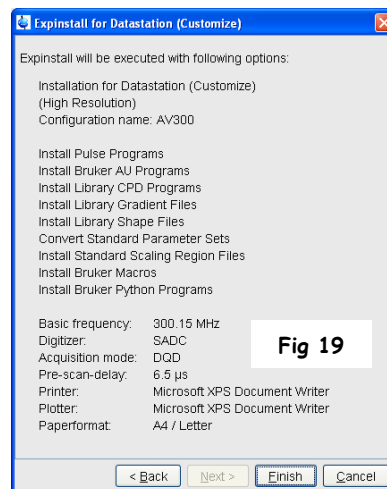
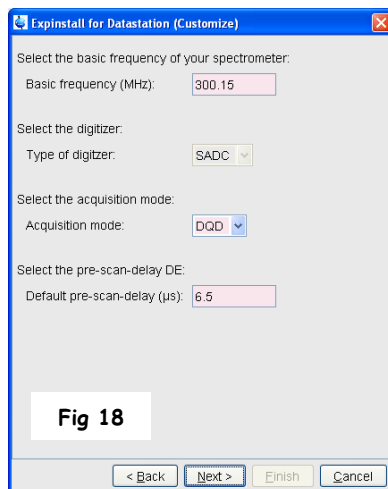
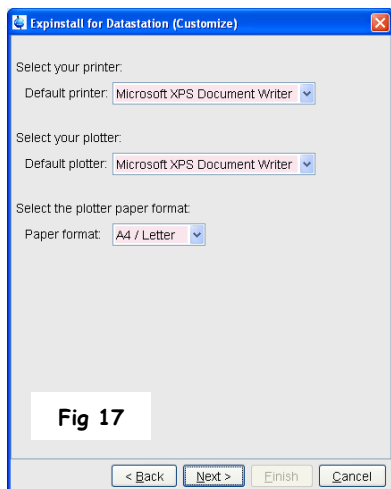


Fig 16

- enter the NMR ADMINISTRATION PASSWORD.
- A window entitled "Experiment installation and AU compilation" will appear. Just click Next>.
- A window similar to that shown in Fig 7 is displayed. Instead of selecting the default installation for a datastation, select "Installation for Datastation (Customize)".
- A window similar to that shown in Fig 8 is displayed. Choose the "High Resolution Systems" option.
- Next you will be asked to choose the configuration you wish to use. Select the AV300 configuration in the drop-down (see Fig 16).
- In the next window, you will be asked to select the items you want to install. You should use the default choice where all items are selected except for the "Recompile All User AU Programs". Click Next >.
- In the next window (see Fig 17), you will be asked to select your default printer, default plotter, and the desired paper format. When these three items are set properly, click Next >.



- The next window (see Fig 18) asks for information on the basic frequency, type of digitizer, acquisition mode, and default pre-scan delay. All of these items should be set properly so proceed by clicking Next >.
- A summary box will appear (see Fig 19) summarizing the options and values you've chosen which will be used during the expinstall procedure. Click Finish.
- Once expinstall is complete, a window entitled "Cron check" appears (see Fig 11) that allows setup of a periodic backup of your TS2.1 configuration. You can either select "Automatic Backup" to configure it or click Close.

## (2) Custom-Made TS Files on Your Datastation

Advanced users may also be interested in having datastation access to a number of custom-made TS files directly from the spectrometer workstation. Custom made files that could be of interest include pulse programs, parameter sets, AU programs, plot layouts, shim files, etc. The majority of these files reside in directories in the TS2.1 home directory under either \exp or \conf. Consequently, in your installation directory under "AV300 Stuff" and "AV500 Stuff" you will find copies of both the "exp" and "conf" folders obtained from the spectrometer workstations. Provided you know the path to the desired files, you can copy them from your installation folder to the proper TS directory on your datastation. The below table details the majority of the customized files available within TS 2.1 along with the TS commands used to access them and the appropriate path.

Type	TS Commands	Path	File(s) to Copy
Amplifier Correction Tables	cortab	\conf\instr\<instrument>\cortab\	Entire Folder
Probe/Solvent Dependent Parameters	edprosol	\conf\instr\<instrument>\prosol\	Entire Folder
Spectrometer Constants	edscon	\conf\instr\<instrument>\	scon
Edit Solvent Table	edsolv	\exp\stan\nmr\lists\	solvents & solvents.all
Edit Lock Table	edlock	\exp\stan\nmr\lists\	2Hlock
		\conf\instr\<instrument>	2Hlock
Edit Tune Files	edtune	\exp\stan\nmr\lists\group\	Desired Files
View Shim Files	vish	\exp\stan\nmr\lists\bsms\	Desired Files
User Defined Parameter Sets	rpar	\exp\stan\nmr\par\user\	Desired Files
User Defined AU programs	edau	\exp\stan\nmr\au\src\user\	Desired Files
User Defined Pulse Programs	edpul/edcpul	\exp\stan\nmr\lists\pp\user\	Desired Files
User Defined Macros	edmac	\exp\stan\nmr\lists\mac\user\	Desired Files
User Defined Shaped Pulses	edshape/stdisp	\exp\stan\nmr\lists\wave\user\	Desired Files
User Defined Gradient Pulses	edgp	\exp\stan\nmr\lists\gp\user\	Desired Files
User Defined Decoupling Programs	edcpd	\exp\stan\nmr\lists\cpd\user\	Desired Files

### **(3) Adding Users to the Group NmrUser**

For Windows 2000 or Windows XP Professional (not "XP Home"), TS creates two new groups during installation called "NmrSuperUser" and "NmrUser". Every user who wants to run TS must be a member of the group NmrUser. In order to add users to the NmrUser group, first login as Administrator and then do the following:

- Click "Administrative Tools" in Control Panel
- Double-click on "Computer Management"
- Within Computer Management, go to System Tools --> Local Users and Groups --> Groups
- Highlight the NmrUser group (right side of window) and right mouse click and select "Add to Group..."

### **(4) Miscellaneous Information**

- During the TS installation, you are given the chance to automatically configure the Windows firewall. However, there may be times in the future when the firewall needs reconfiguration (i.e. firewall is reset, TS is installed to a new location, or changes in Service Pack status). An administrator can configure the firewall anytime by running the setfirewall.cmd script, found in the TS home directory under /prog/bin/Utilities/Miscellaneous. The script applies all required changes to the firewall (related to Bruker software) without user interaction.
- To change the NMR Administrator Password, login as NMR Superuser or Administrator, open Bruker Utilities on the desktop, and double click on the command prompt. Type in perl\bin\perl prog\bin\installnmr C:\Bruker\TopSpin2.1 nmrsu (replace nmrsu with the name of the NMRSUPERUSER account if necessary). Enter the old password and new password as requested.
- If you have forgotten the old NMR administrator password, login as Administrator and delete the file nmradminpassword found in C:\Bruker\TopSpin2.1\conf. Then run the installnmr script as above.
- Note that TS offers a so-called security mode where configuration files are only read and writeable for the NMR SUPERUSER.