TopSpin

- Installation Guide

User Manual

Version 003

Innovation with Integrity

NMR

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1 Introduction

1.1 About this Manual

This manual is the TopSpin Installation Guide for Microsoft Windows, Linux and Mac OS.

This installation guide is available:

- as PDF file on the toplevel of the TopSpin DVD
- as the up to date version on the Bruker web server: *https://www.bruker.com/service/information-communication/user-manuals/nmr.html*

Note: This manual does not contain the TopSpin Release letter. This is a separate document delivered as PDF or HTML files on the TopSpin DVD and also on the Bruker web server.

Note: All text messages and graphics shown in this Installation Guide are taken from the current version of the respective software products. Small differences to other versions are possible.

1.2 Font and Format Conventions

Type of Information	Font	Examples
Shell Command, Commands, "All that you can enter"	Arial bold	Type or enter **fromjdx zg**
Button, Tab, Pane and Menu Names "All that you can click"	Arial bold, initial letters capitalized	Use the **Export To File** button. Click **OK**. Click **Processing**…
Windows, Dialog Windows, Pop-up Windows Names	Arial, initial letters capitalized	The Stacked Plot Edit dialog will be displayed.
Path, File, Dataset and Experiment Names **Data Path Variables** **Table Column Names** **Field Names (within Dialog Windows)**	Arial Italics	*$tshome/exp/stan/nmr/lists* *expno, procno,*
Parameters	Arial in Capital Letters	VCLIST

Program Code
Pulse and AU Program Names
Macros
Functions
Arguments
Variables
	Courier	`go=2`
		`au_zgte`
		`edmac`
		`CalcExpTime()`
		`XAU(prog, arg)`
		`disk2, user2`

AU Macro	Courier in Capital Letters	`REXPNO`

Table 1.1: Font and Format Conventions

Introduction

2 Installation

2.1 Preparation

The Linux distribution includes a built-in PDF viewer but it is preferred to have Acrobat Reader or Evince (on Linux) already installed. To display the TopSpin Online Help, for parts of the NMR-Guide and the Release Letter, a PDF viewer is required.

Acrobat Reader is not installed automatically as a part of TopSpin (on Linux, Mac OS and Windows). It is available from Adobe as download.

2.2 Packages on the TopSpin DVD

1	**TopSpin**	**Acquisition and Processing Software**	**3.6.x**	**4.x**
	TopSpin Plot Editor	Object oriented WYSIWYG plot editor. [3]	X	X
	Cygwin Tools	Used for compilation of TopSpin AU programs. [3]	X	X
	NMR-GUIDE	A web-based training and teaching tool providing a lot of theoretical and practical information on NMR spectroscopy and NMR methods for everybody interested in NMR. [2]	X	X
	NMR-Sim	Program for numerical simulation of NMR experiments. [3]	X	X
	CMC-q Viewer	Automation & Analysis [3]	X	X
2	**Central Audit File**	Enables a Central Audit File for activity recording in TopSpin.	X	X
3	**CMC-a**	CMC-assist, a tool for structure verification based on NMR data.	X	X
4	**IconNMR**	Icon-driven interface for Routine Spectroscopy and Automation.	X	X
5	**MICS**	Magnet Information & Control System.	X	X
6	**NMR-Data**	Example datasets	X	X
7	**CodeMeter Runtime**	License manager required to start TopSpin programs.	X	X
8	**AURELIA-AMIX-Viewer**	Multiple object viewer [1] During the installation the program is displayed as *AMIX*.	X	X
9	**SpectrOS**	Spectrometer operating system for AVANCE NEO. SpectrOS is needed for workstations controlling a spectrometer.		X
10	**Diskless**	Spectrometer operating system for AVANCE III. Diskless is needed for workstations controlling a spectrometer.	X	
11	**SBASE**	Spectra base for AMIX [1]	X	X
12	**Dynamics Center**	Analysis of NMR data containing non-frequency dimensions (incl. Protein Dynamics) [1]	X	X
13	**InsightMR**	Reaction Monitoring	X	X

[1] Requires a separate license.

[2] Package is integrated in TopSpin4.x, package is selectable in TopSpin3.6.x

[3] Installed by default together with the TopSpin package.

Packages available on a separate DVD:

	TopSpin	Acquisition and Processing Software	3.6.x	4.x
14	**AssureNMR**	The AssureNMR software provides automated multicomponent identity, quantification, classification, and detection of outliers with spectral databases and System Suitability Tests for GxP compliance. [1]	X	X
15	**AssureNMR-Methods**	This directory includes Analysis Methods, for use with AssureNMR, that automate the analysis of poloxamers, molar substitution, tire rubber, heparin, Aloe vera and other common materials. Some of these methods may require separate software licenses for use (heparin and Aloe vera).	X	X

[1] Requires a separate license.

2.3 Windows and Linux Installation

This chapter describes the installation of TopSpin, which requires local administrator permissions. There are two possibilities:

1. User Account Control (UAC) is enabled. If you are logged in an as a normal user for the installation of TopSpin, you will be prompted during the installation for the name of a local administrator as well as his password. If you are logged in as a user with administrative rights, you will only be prompted to confirm that you want to continue the installation with these rights.
2. User Account Control (UAC) is disabled. You must login as a user with administrator permissions and then install TopSpin. In that case, no question will be asked during the installation.

If a previous TopSpin installation exists on your Workstation either

- Install the new version in parallel to the previous one
  e.g. old in *C:\Bruker\TopSpin3.0* and the new in *C:\Bruker\TopSpin4.0* (Windows)
  e.g. old in */opt/topspin3.0* and the new in */opt/topspin4.0 (Linux)*

or

- Install the new version in the same directory as the previous one

  e.g. *both C:\Bruker\TopSpin* (Windows)
  e.g. *both /opt/topspin* (Linux)

Note: Bruker strongly recommends to always choose the parallel installation.

The installation in parallel has the advantage, that the previous version remains unchanged. After a parallel installation, start to work with the new version. If necessary, you can still go back to the previous TopSpin version.

Windows

- Close **all windows** on the desktop.
- Insert the TopSpin DVD and open the DVD drive with the Windows explorer.
- Double-click **Install.cmd**

Note: All current versions of Windows are initially installed with an option called Hide extensions for known file types enabled. In this case two files named *Install* are displayed. Click the one of type *Windows command script*.

A Command Prompt window displays the current installation process.

If you are logged in an as a normal user, a User Account Control window will be displayed. Enter the Administrator password.

Linux

- Insert the DVD to open a **cd-rom file** browser. If it will not be opened automatically click the now visible **DVD** icon on the Desktop.
- On KDE with konquerer, click **install**.
- On Gnome with Nautilus, double-click **install** in the right part of the window and then click **Run in a Terminal** in the newly opened window.

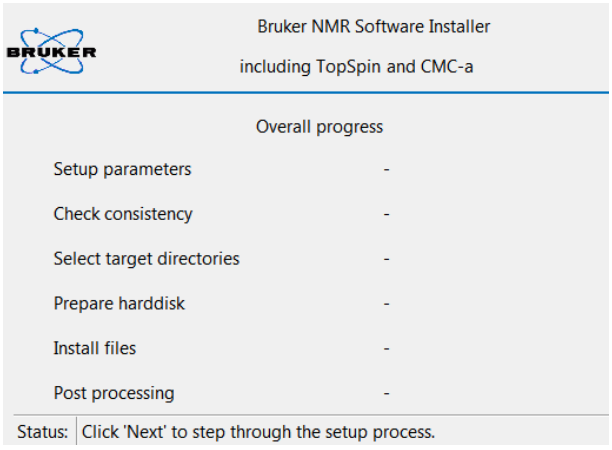
On CentOS 7 a shell window will be opened.

- Enter the Administrator (“root”) password here. The installation will start and and the location of the installation log file is displayed in the same shell described above on Windows.

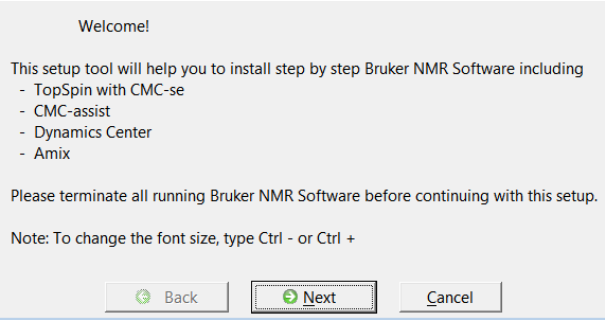
Windows and Linux

After a short time the installer opens two additional windows shown in the following figures.

The Overall Progress Information window will be visible during the whole installation .

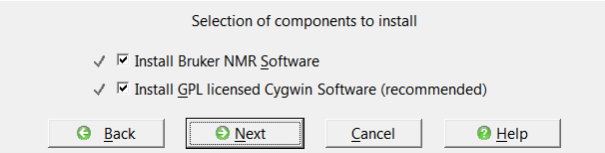


The second window displays a Welcome screen and lists the main programs that are part of the software distribution.

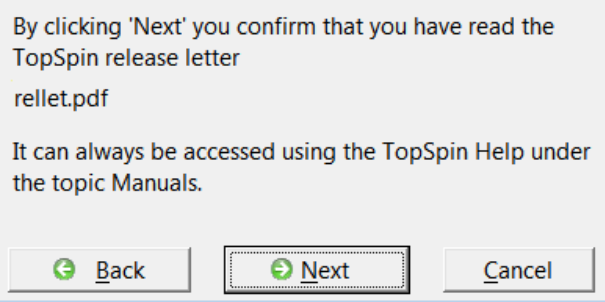


- Click **Next** to continue with the TopSpin installation.

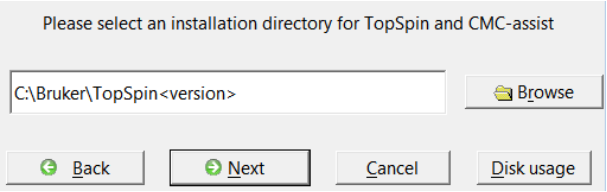
The installer offers either to install only the Cygwin tools, to install the NMR programs without Cygwin, or to install the NMR programs including the Cygwin tools which is recommended. The Cygwin tools are used for the compilation of AU programs.



The release letter will be displayed in a PDF reader in the background, so you can proceed with the installation while reading the release letter.



- Click **Next** to continue with the TopSpin installation.

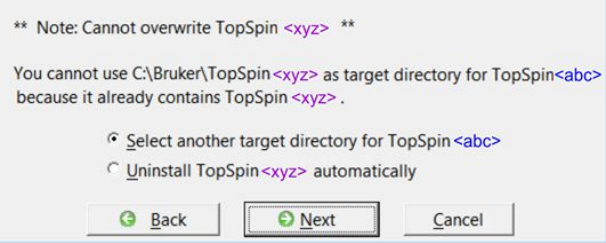


- Click **Browse** to change the installation folder or enter the path in the text field.
- Click **Next**.

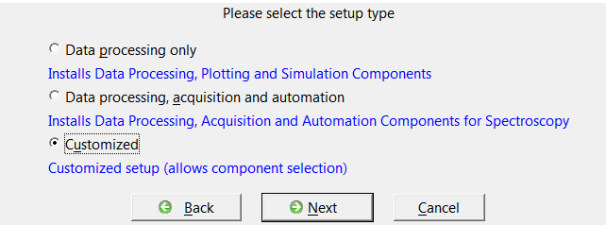
Note: This is also the directory where the installation log file will be located after the file extraction to the local hard disk has started. Please include the installation log file (install.log) in any request email concerning installation issues.

If the installation directory does not exist, the program asks if it should be created. The directory will be created only when the file extraction actually starts.

Exception: The installer will not allow to accidentally overwrite an existing installation of TopSpin with another version. If desired, the program can uninstall a previous version:



- When this exception note is displayed either
  - Check **Select another target directory for TopSpin<version abc>** and click **Next** to change the installation directory and continue with the setup type selection or
  - Check **Uninstall TopSpin<existing version xyz>** and Click **Next** to first uninstall the existing version and continue with the setup type selection.



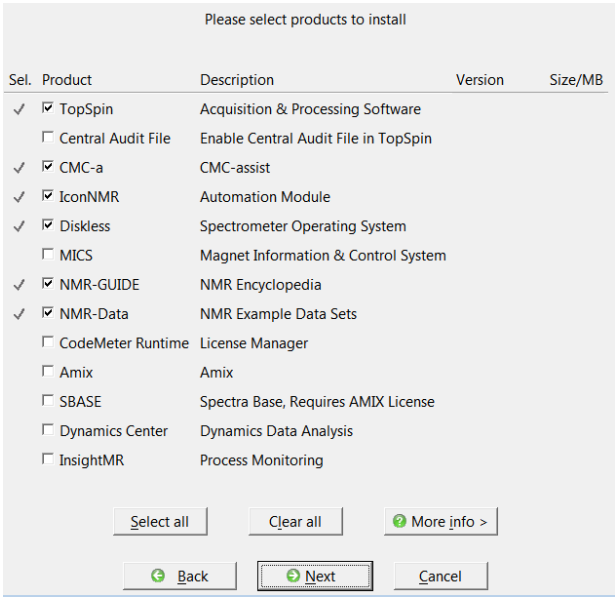
- Select one of the offered setup types:
  - Select **Data processing only** if you want to use TopSpin for data processing only. The packages TopSpin, NMR-Sim, NMR-Data, CMC-assist and CodeMeter will be installed.
  - Select **Data processing, acquisition and automation** if you want to use TopSpin for spectrometer control. This setup type provides the following packages: TopSpin, NMR-Sim, NMR-Data, CMC-assist, CodeMeter, IconNMR, SpectrOS and MICS.
  - Select **Customized** for a manual selection.

The Customize Products window has initial settings equal to the option **Data processing, acquisition and automation**.

Additionally:

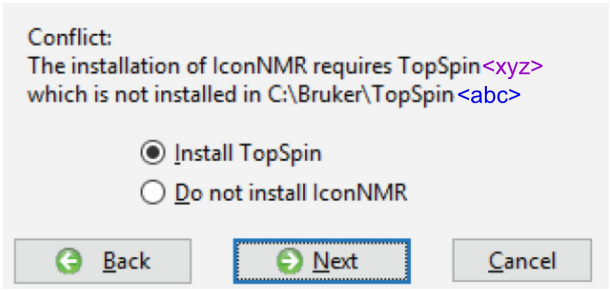
1. The option **SpectrOS** will be checked for the setup types *Data processing, acquisition and automation* and *Customized* if the current **SpectrOS** version on your spectrometer is outdated or equal.

2. The option **Codemeter Runtime** will be checked if the actual **Codemeter Runtime** version on your workstation is outdated.



- Click **More info** to check the already installed product versions.
- Click **Next**.

If a package dependency is not resolved correctly or the installation directory contains a TopSpin version that would be corrupted, the installer shows a dialog about the conflicts.



Linux:

Select whether the current TopSpin installation directory should be added to the global path. This allows to start TopSpin by typing **topspin** on the command line.

Windows and Linux:

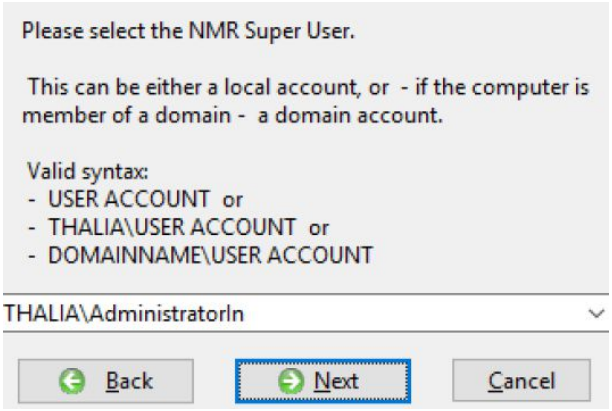
NMR products are configured with special access for the account selected as the so-called NMR Super User.

Linux:

Select a name for a user account. If the account does not exist, it will be created.

Windows:

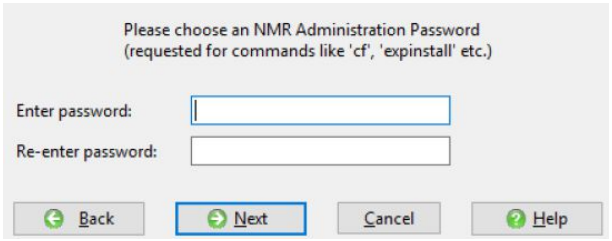
Select an existing account. This can be a local or a network account.



Windows and Linux:

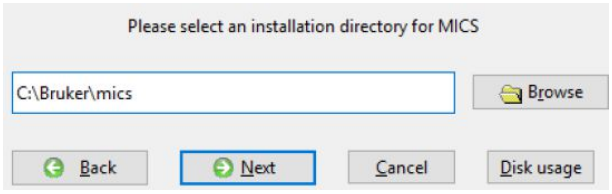
- Enter and re-enter the NMR administration password.

Note: The NMR administration password is not related to any system password. This password will be required later when configuration commands in TopSpin are run, such as **cf**.

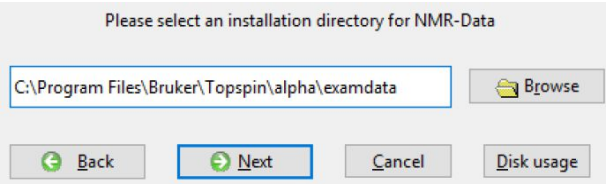


- Click **Next**.

Installation Directories for MICS, NMR-Data and SpectrOS



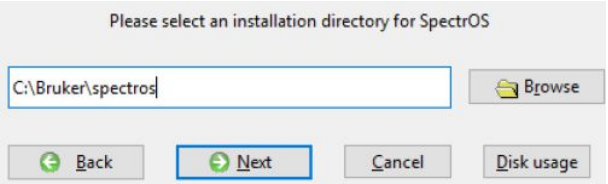
- Select the installation directory for MICS.



- Select the installation directory for NMR-Data.

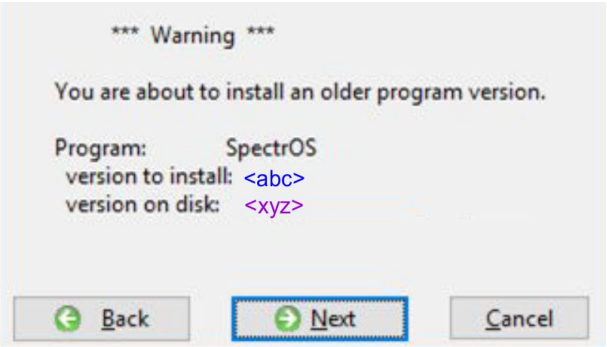
Note: The next four dialog windows are displayed only when SpectrOS is included.

Note: On Windows do not use a path that contains parentheses, e.g. *C:\Program Files (x86)*. Otherwise the firewall setup program will fail.



- Select the installation direcory for SpectrOS.

Note: The installer will warn when downgrading SpectrOS to an earlier program version.

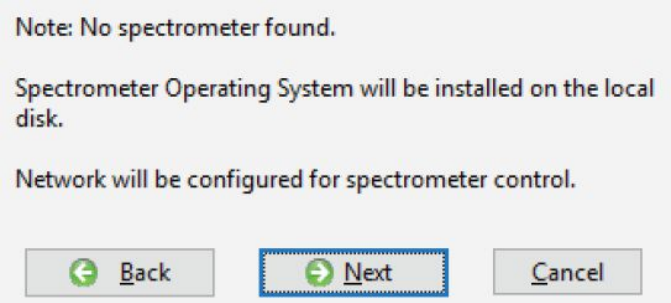


- Click **Next**, if this is intended.

Note: Though not recommended, the Spectrometer Operating System can be installed while no spectrometer is connected to the workstation. In this case the network settings of the workstation will be configured for spectrometer control and the Spectrometer Operating System is installed on the local hard disk. When a spectrometer will be connected later, the Spectrometer Operating System can be transferred to the spectrometer with the program *post/updatespectros.sh* in the SpectrOS installation directory.

If Windows displays the message **Don't know how to open this program, please choose a program ...** then select *GNU\bin\bash.exe* in the TopSpin installation folder.

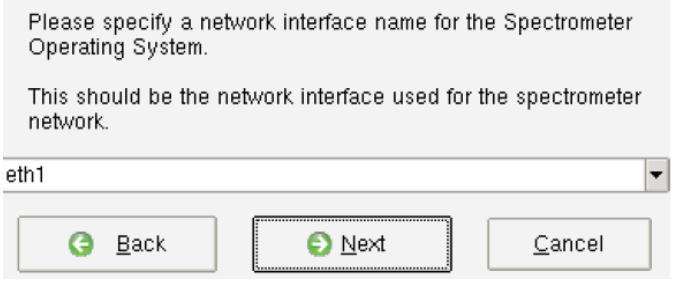
Exception: If the installation program cannot detect a spectrometer, it displays the following dialog window:



- Click **Next**.

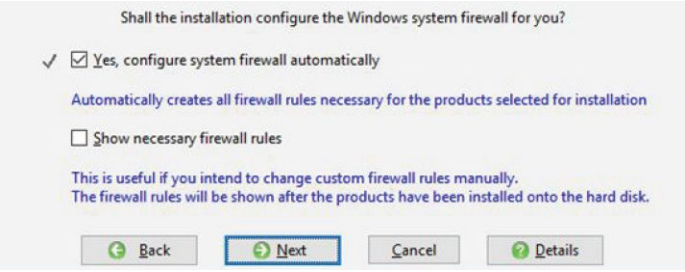
If the workstation controls a spectrometer, it should have two ethernet interfaces.

The installation tries to detect if manual changes have been made to the network interface configuration and to leave the file intact in that case. It will also save a copy of the original network interface configuration file in the SpectrOS installation directory.

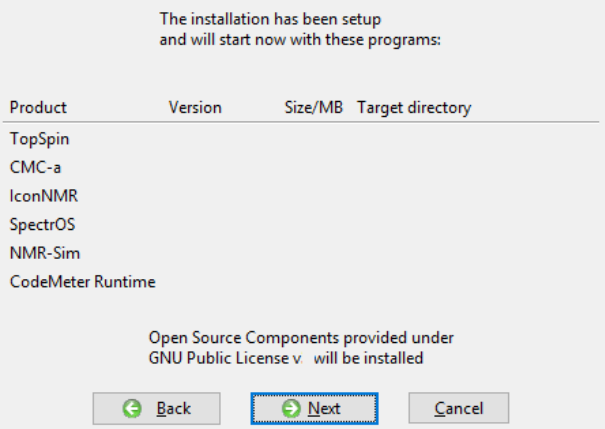


- Enter or select the name of the one connected to the spectrometer network.

Note: Bruker recommends to let the installer configure automatically the firewall for TopSpin commands. The firewall dialog is only displayed if a program was selected that requires firewall configuration, such as TopSpin on Windows, SpectrOS on Linux, CodeMeter on Linux, or MICS.



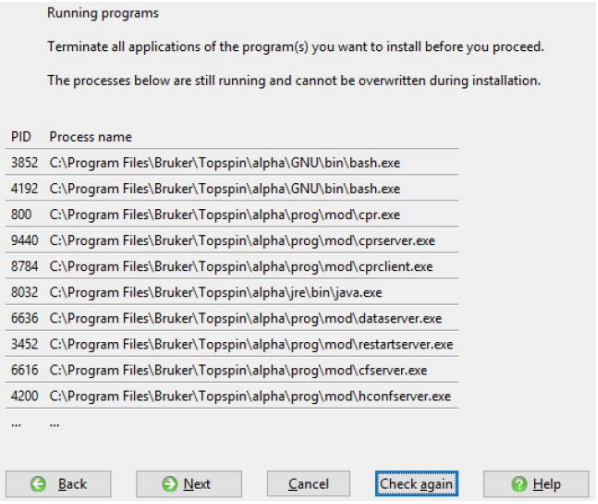
The last confirmation dialog is displayed before verification and file extraction to the local hard disk starts.



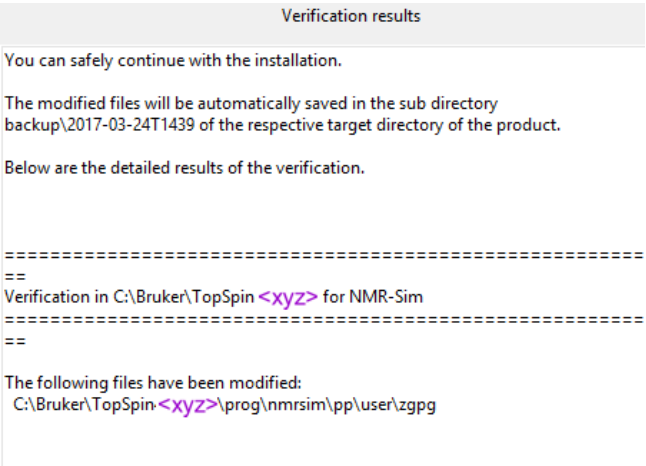
- Check the summary of the selected components and target directories, before the installation starts.
- Click **Next** to start the file extraction.

The installer performs some checks before file extraction starts. In case of an error or obstacle any of the following dialog windows may appear.

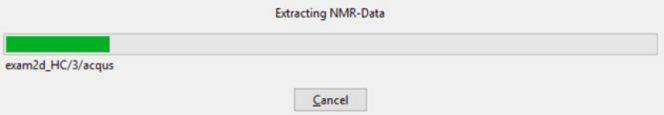
Note: When other TopSpin versions are running on the computer, they have to be closed. Otherwise the following error message will appear:



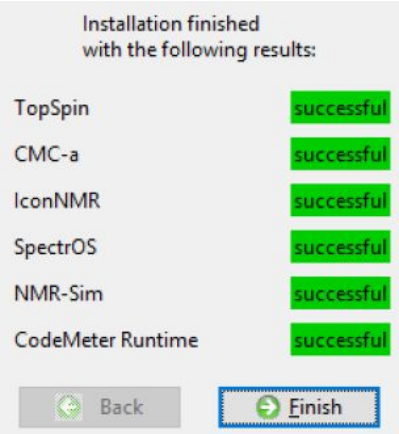
Note: If a path was selected with an already existing TopSpin installation, the verification checks if any of the previously installed files have been changed, e.g. as patch or workaround for a bug. If so, the affected files are saved into a backup directory and information is displayed as in the next figure. The backup directory contains the program *restorefiles.pl* that can be run to restore the backup files.



The installer displays the file extraction progress for each package.



The final dialog will display success or problems (during post installation) or errors if there are any. In that case please include the install.log in the TopSpin installation directory to your support request.



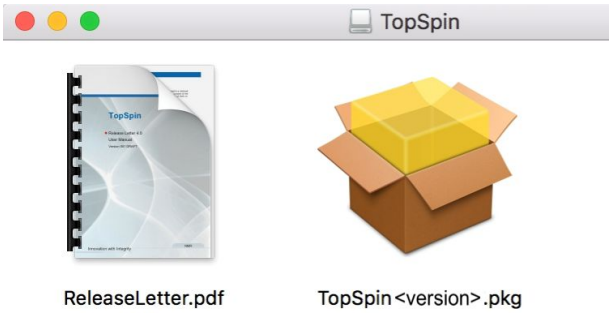
- Click **Finish**.

2.3.1 CodeMeter Installation on Linux and macOS

- The **Linux** version of the CodeMeter runtime delivered with TopSpin comes as an RPM package and thus can only be installed on RPM based distributions like Red Hat (CentOS, Fedora) or Suse. If you use a different, not directly supported, distribution (Debian, Ubuntu,…), please download the CodeMeter Runtime here: *https://www.wibu.com/support/user/downloads-user-software.html* and follow the given installation details.
- CM runtime for diverse **macOS** versions are available on the same site.

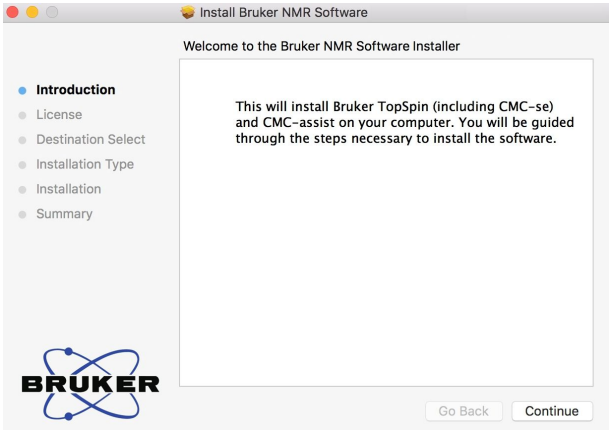
2.4 Mac OS Installation

Insert the DVD and use Finder to inspect its contents. TopSpin for Mac OS X comes as a DMG file that is located in the root folder of the DVD. Double click the file TopSpin-<version>.dmg to open it. When the DMG is opened for the very first time, Mac OS X will verify its checksum. Due to the rather large size (around 500 MB) this may take a while (usually 30s on an iMac, probably longer on MacBook or MacMini). But the verification will happen only once. It is recommended to wait and let the system finish the check. Mac OS X will then mount the disk image and automatically display a Finder window with the Release Letter and the installation package file.

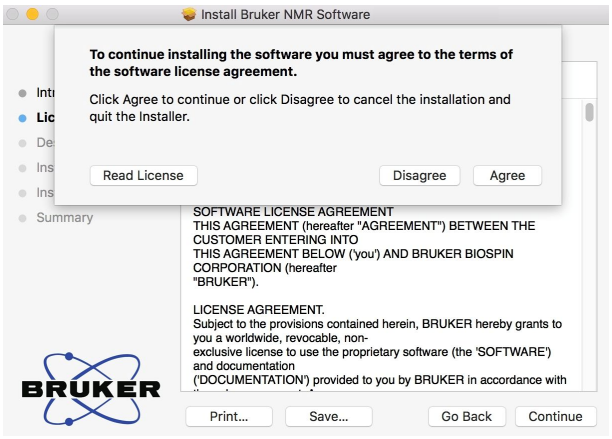


- Doubleclick **TopSpin<version>.pkg**.

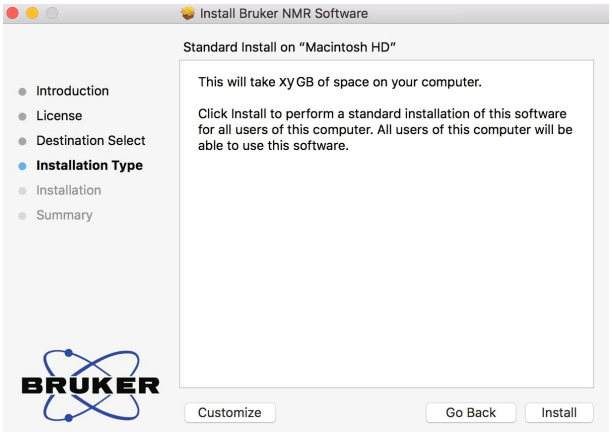
The Welcome screen is displayed.



- Click **Continue**.

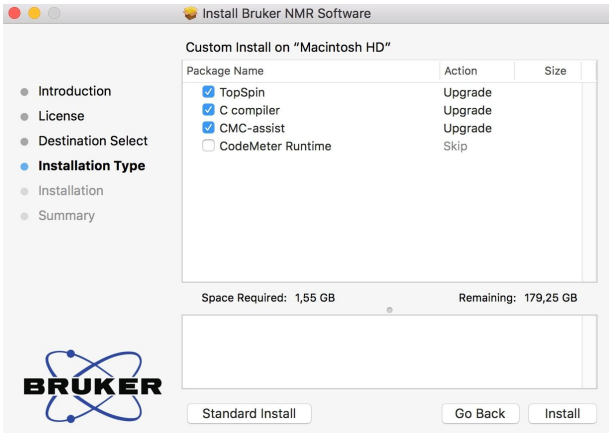


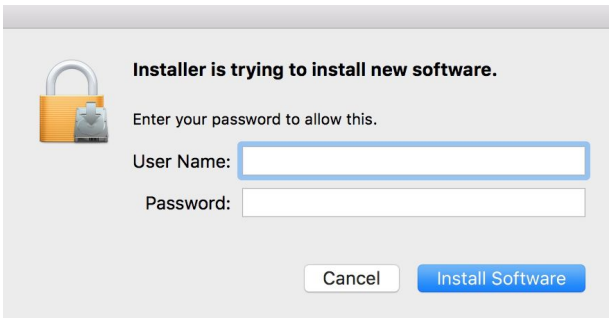
- Click **Agree**.



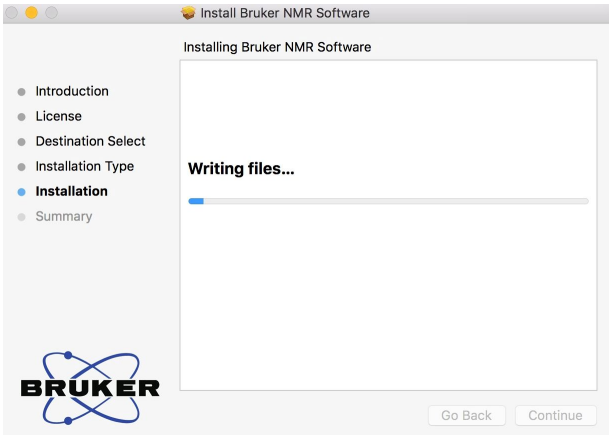
- Click **Customize** to change some default settings, otherwise continue with **Install.**

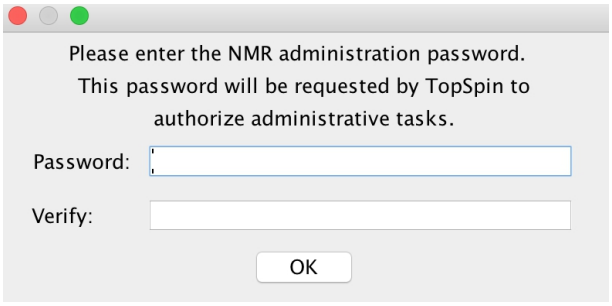
Note: CodeMeter is deselected if it is already installed.





- Enter user name and password of a user with administration rights.
- Click **Install Software**.

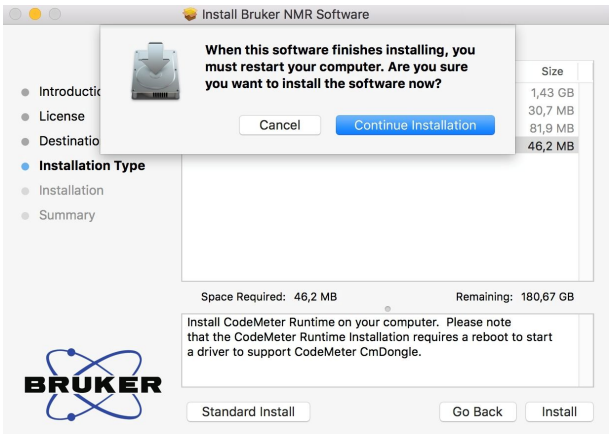




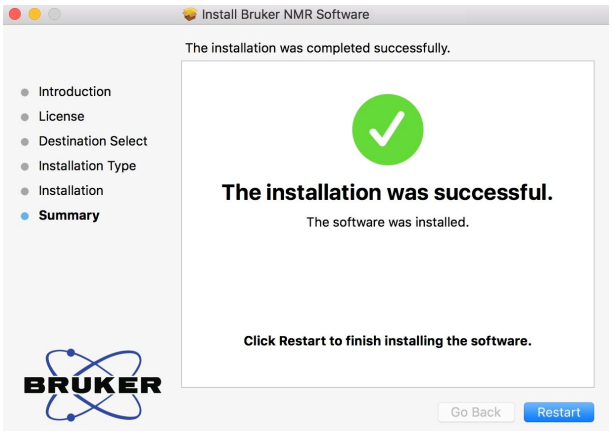
The NMR administration password is not related to any system password. This password will be required later when configuration commands in TopSpin are run, such as **cf**.

- Enter the NMR administration password and click **OK**.

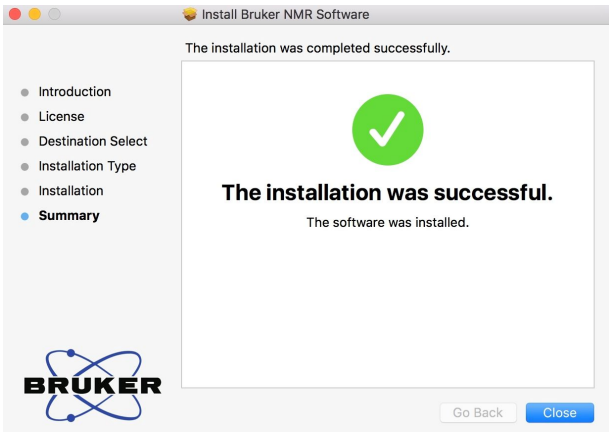
Exception: The next two dialog windows are displayed only, when CodeMeter was installed and therefore a restart is necessary.



- Click **Continue Installation**.



- Click **Restart** to finish the installation.



- Click **Close**.

2.4.1 Differences of the Mac Version Compared to Other Platforms

In accordance to the guidelines for Mac applications, no target directory can be chosen during the installation. Unlike on other platforms, a parallel installation of several TopSpin instances of the same version is not supported. Installation is possible only on the root volume.

TopSpin on Mac OS X is a processing-only installation. Support for NUS (non-uniform sampling) data is fully implemented and available. NMR-Sim and the full NMR-GUIDE are available as well.

There is no acquisition support, nor IconNMR present.

Example Data Sets

On Mac OS X, the TopSpin installer currently installs a subset of the full example data sets only. If required, you can find the full set on the TopSpin DVD in the following file:

noarch/pack/nmrdata.tar.xz

Use a Finder window to navigate to the sub folder *mac/bin* of the DVD and double-click nmrdata-extract. This opens a window and asks for a folder where to extract the data. The program *nmrdata-extract* can alternatively be run in a terminal.

2.4.2 TopSpin Utilities

Completing the installation, the *Applications* folder contains the TopSpin application as well as a separate folder *TopSpin Utilities*. You can find the following tools there:

- **SaveLogs**: Used to collect log files and more required information for support incidents.
- **Terminate TopSpin**: In case TopSpin does not start as expected, components of the application may not have been terminated correctly from the last session and may still be active in memory. Use this tool to stop all running components. TopSpin should start normally after that.
- **Uninstall TopSpin**: This tool will remove the TopSpin installation from the harddisk. Use this only if you want to delete TopSpin completely. Security questions will protect from an unintentional use.

2.4.3 Additional Notes

During the release testing it has been observed that the presence of at least one virus scanning tool for Mac OS X may delay the start of TopSpin significantly (up to a couple of minutes). If you notice similar behavior we recommend to temporarily disable the virus scanner. TopSpin should start very fast then.

When starting TopSpin for the first time, the firewall of Mac OS may ask whether you want to allow or deny **access to cprclient**. This request is displayed only once and we suggest to choose **Allow**. (The installation procedure cannot do that automatically for you.)

2.5 Installation Results

The installation stores its results in a log file named install.log.

When the installation is complete, the log file is stored in the TopSpin folder specified at the start of the installation or in */opt/topspin<version>* on MacOS. Under Windows and Linux, an existing log file is not overwritten, instead the new results are appended. On MacOS a new file is created every time a new TopSpin version is installed.

Before the installation begins to extract files to the hard disk, the log file is in the temporary folder

on Windows: *C:\Windows\Temp*

on Linux: */tmp*

The current location of the log file is displayed in the terminal that is shown during the installation.

Whenever you contact the support due to installation problems, please attach this log file.

2.6 General Comment Regarding the TopSpin Factory Default Configuration when Installed on a Bruker Standard Workstation

TopSpin on a Bruker delivered workstation is installed with two user groups called NmrSuperUser and NmrUser together with two users called nmrsu and nmr. The user nmrsu belongs to the group NmrSuperUser, the user nmr belongs to the group NmrUser. Any newly created user can be associated with either of these groups or any other group. The default TopSpin installation is owned by the user nmrsu (group NmrSuperUser). Hence, this user owns all the TopSpin files and any manipulations to the configuration of TopSpin can only be done as this user. It is in the responsibility of the system owner to decide whether the TopSpin installation should be assigned to a different NmrSuperUser than nmrsu. This could either be a different local user or even a domain user. A reassignment of TopSpin to a different user can be accomplished through the TopSpin **installnmr** command.

1. Procedure to change the NmrSuperUser of TopSpin under Windows:

   Login with an administrator (root) account and open a TopSpin command prompt by opening the "TopSpin Utilities" desktop icon and double-click the command prompt. In the command prompt, enter the command:

   perl\bin\perl prog\bin\installnmr <nmrsu>

2. Procedure to change the NmrSuperUser of TopSpin under Linux:

   Open a shell window and become superuser (user: root). Change to the installation directory of TopSpin. In this example, TopSpin is installed in */opt/topspin*:

   Enter the command:

   ./prog/bin/installnmr <nmrsu>

In both cases <nmrsu> refers to the name of the newly defined NmrSuperuser.

Under Windows, the user name for the so called NmrSuperUser must be the name of an existing user. Under Linux it can also be a non-existing user, which is then automatically created by the installation program. After running **installnmr**, the newly defined NmrSuperUser is the owner of all TopSpin program files. Logging in as this user allows you to remove files, change file permissions etc. The name of the NmrSuperUser is stored internally in TopSpin. Only the NmrSuperUser and users who belong to the administrator group are allowed to re-run installnmr (if that should be required).

In addition to this user, TopSpin also requires an NMR Administration password, which will be used for TopSpin internal configuration commands. This password can be freely chosen and is not connected to any user. It is asked for by TopSpin commands like **cf, expinstall** etc.

Note that the NmrSuperUser login password and the NMR Administration password have different purposes and are totally independent. Changing one of them does not affect the other.

Also note that the above described command **installnmr** also allows to change the NMR administration password.

The following table summarizes the groups and users and their meaning and rights:

Users belonging to	Install new software	Configure TopSpin	Run experiments
Windows/Linux Administrator-IT	Yes	Yes (if user belongs to group NmrSuperUser)	Yes
NmrSuperUser (Topspin Superuser/ Administrator)	No	Yes (requires NMR Administration Password)	Yes
NmrUser	No	No	Yes

2.7 Automatic Installation of TopSpin

It is possible to run an automatic installation of TopSpin (also known as unattended or silent installation). For that purpose

- On Linux run the shell script **install** with the command line option **-a**.
- On Windows run the batch file **install.cmd** with the command line option **-a**.

Other options that change the defaults can be added.

While you can launch install or install.cmd with any program, the examples below use the Command Prompt on Windows and a shell terminal on Linux. In that case the command and its options have to be typed in a single line.

Long lines can be split into several physical lines:

- On Linux type a backslash **** in the shell terminal as last character.
- On Windows type a caret **^** in the Command Prompt as the last character.

Note: When the automatic installation encounters an error or a warning, an appropriate error or warning message is displayed. After confirmation, the installation can be continued in interactive mode. Examples are:

- The installation directory cannot be used because there is already another TopSpin version.
- The verification check has detected modified files.
- There are processes running in the installation directory.

Note: If you use the options below without -a, the installation runs in interactive mode, but changes the defaults to the values specified on the command line. This allows for more easy clicking through the dialog windows without the need to change the settings when you have to attend a couple of installations.

Examples:

1. Scenario: The DVD is inserted in drive E:

- To list the available options, type:

  E:\install -h

- To install TopSpin and IconNMR into the directory *C:\Programs\Bruker\Topspin \<version>* , type:

  E:\install -a -s topspin -s iconnmr -x C:\Programs\Bruker\Topspin\<version>

- To install the Dynamics Center into the folder *C:\Bruker\DC*, type:
  E:\install -a -d dc=C:\Bruker\DC

2. Scenario: The DVD is mapped to *\\my-PC\my-share*

- To install the programs in the group **Data processing only**:
  \\my-PC\my-share\install -a --setup-type po

- To specify an empty NMR administration password via its md5sum:
  \\my-PC\my-share\install -a --nmradminpwenc d41d8cd98f00b204e9800998ecf8427e

3. Scenario: The DVD is mounted as */media/cdrecorder*

- To install the programs in the group **Data processing, acquisition and automation**:
  /media/cdrecorder/install -a --setup-type pa

- To specify the plain NMR administration password, type:
  /media/cdrecorder/install -a --nmradminpw TEDDY

- To install TopSpin without GCC, type:
  /media/cdrecorder/install -a -s topspin --gcc-off

- To specify not to add the installation directory to the global path, type:
  /media/cdrecorder/install -a --globalpath 0

- To get a list of valid program shortnames that can be used in the command line, type:
  /media/cdrecorder/install -s help

3 TopSpin License Management and Product Order

TopSpin uses the new Code Meter license management. A license can be ordered from the Bruker website. Just go to *https://www.bruker.com/nmr_license_requests.html* and fill out the request form. The License department will process the order details and generate an **activation ticket** and provide it to the customer. A ticket consists of a 25 character code like e.g.:

PH3T4-9D9U9-FNSGP-J9FXP-TTNXC

This code works as an access key to the purchased license package. It authorizes the customer to assign the license package to a computer of personal choice.

Install the software product on the computer system. During installation you may also be requested to install the package **CodeMeter Runtime**. This is the component of the license management system. Most installation routines will perform this task automatically.

A Free TopSpin Evaluation license can be ordered on the following web page:

https://www.bruker.com/service/support-upgrades/software-downloads/nmr/free-topspin-processing/topspin-demo-licences-generation.html

A Free TopSpin Processing license for Academia can be ordered on the following web page:

https://www.bruker.com/service/support-upgrades/software-downloads/nmr/free-topspin-processing/nmr-topspin-license-for-academia.html

For further information please look up the Code Meter License Management User Manual H162728.

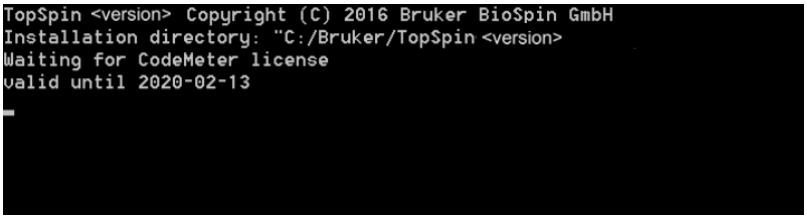
4 Basic Configuration of TopSpin

This chapter provides some guidelines to full spectrometer or processing-only configuration. Commands will not be discussed in detail here. For a full description please refer to the **Acquisition Commands and Parameters** Manual.

There are several ways to start TopSpin on Windows:

- Double-click the **TopSpin** icon on the desktop or
- Click **Start | All Programs | Bruker TOPSPIN | TOPSPIN<vers.>**

First of all a TopSpin start window will open with details about the program version, the installation directory and the valid license(s).



If there are any problems with the licenses or the license management you will be informed here. TopSpin will not start then.

If everything is OK, the TopSpin main window will be displayed and the window shown in the figure below disappears into the background but remains open.

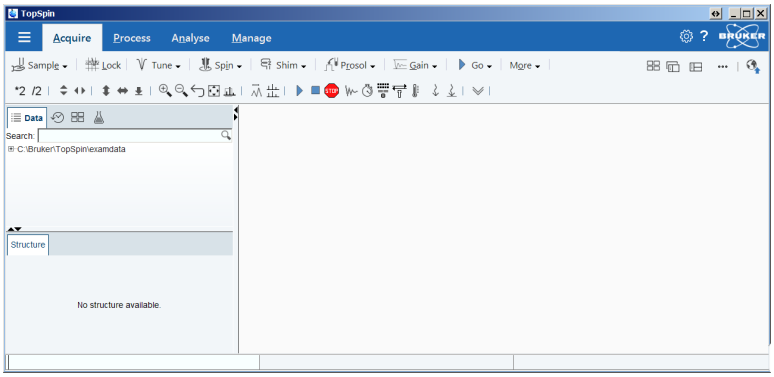
This procedure will be same with every start of TopSpin.

After the startup of TopSpin a LICENSE window will be displayed. Please read the license agreement for Bruker TopSpin.

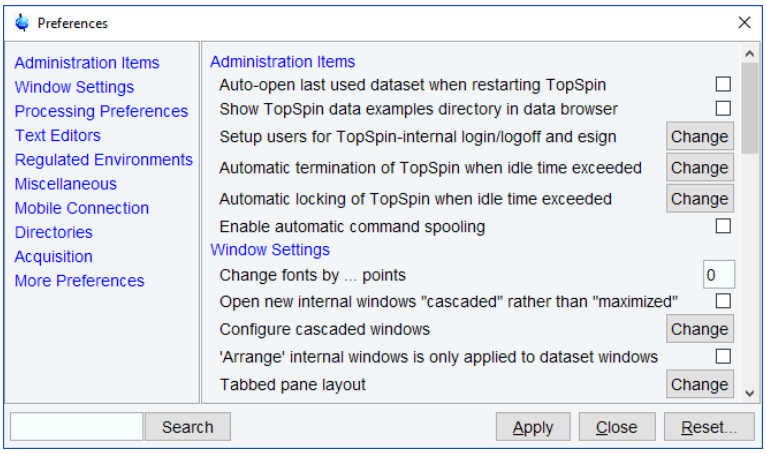
- Click **I Accept**.

If you do not wish to answer the License question again upon the next start of TopSpin, click **I Accept, Do Not Show License Again**.

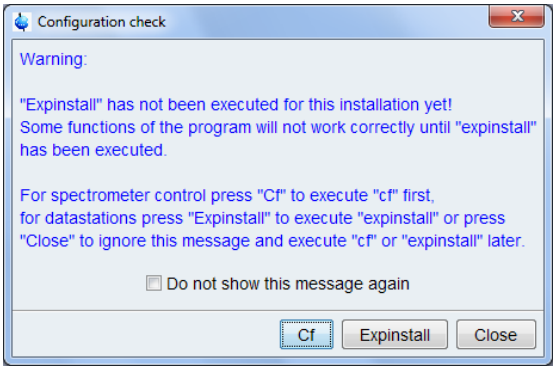
The TopSpin GUI is displayed.



The user interface can be changed with the command **set** or with the toolbar button  . This will open the User Preferences window. In the group Window Settings the window can be customized.



With the first start of TopSpin a Configuration Check window will be displayed:



Note: The TopSpin system configuration depends on the spectrometer hardware. Mainly three scenarios need to be considered:

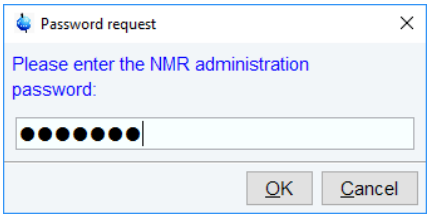
- Configuration of a Workstation to control a spectrometer
- Configuration of a processing-only Workstation using an existing spectrometer configuration.
- Configuration of a processing-only Workstation

4.1 Configuration of a Workstation to Control a Spectrometer

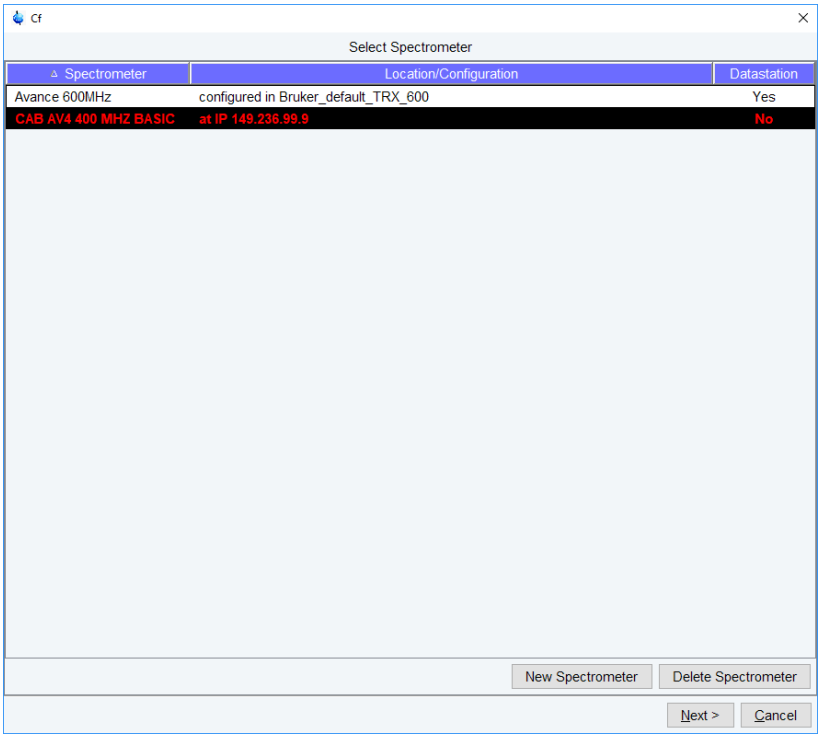
If the Workstation does control a spectrometer be sure that your spectrometer is booted.

- Click **cf** in the Configuration check window or type **cf** in the command line of the TopSpin main window.
- Enter the NMR administration password in the next window and click **Ok**.

Every time you want to access or change the configuration this password request will appear.



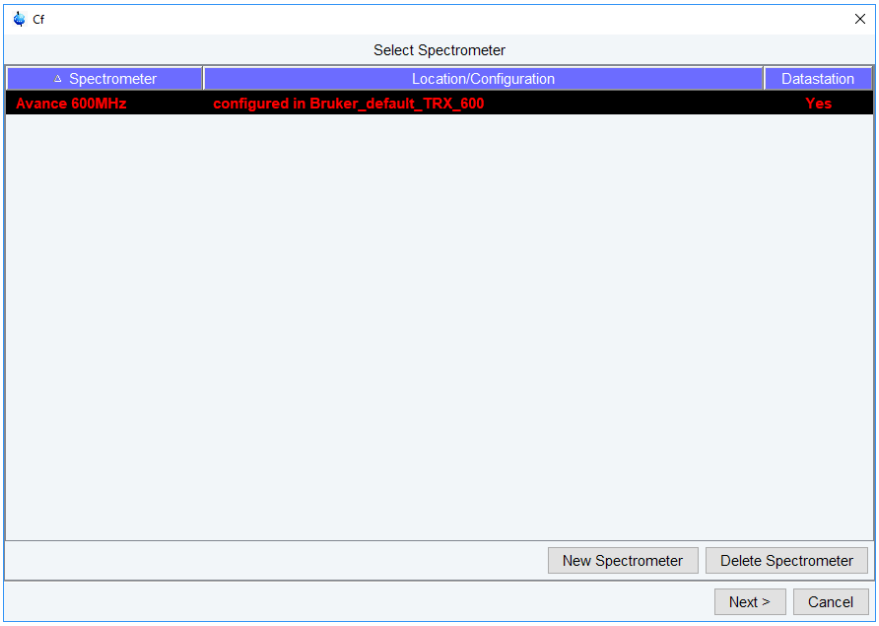
The first cf window is displayed.



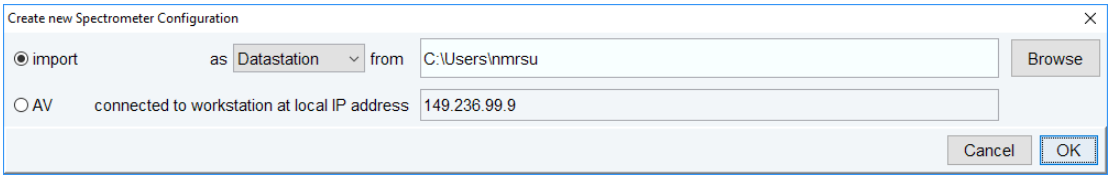
Most likely you will select an existing configuration and click **Next** to confirm this configuration. Click **New Spectrometer** to start a new configuration.

In this example the configuration CAB AV4 400 MHZ BASIC is an existing spectrometer configuration for an Avance Neo 400 MHz spectrometer.

If only the Bruker_default_TRX_600 configuration is shown (see below), then a previous configuration could either not be detected or does not exist.

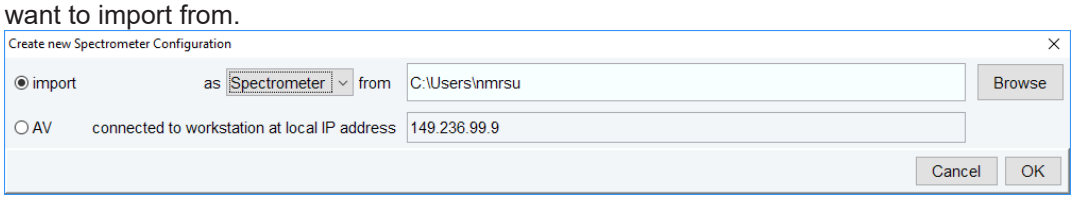


If an older TopSpin version with an appropriate configuration exists, then you can load it by clicking on **New Spectrometer**. The following window will be displayed:

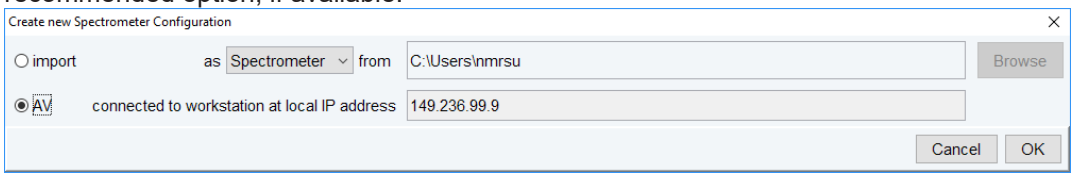


Select one of the following three options:

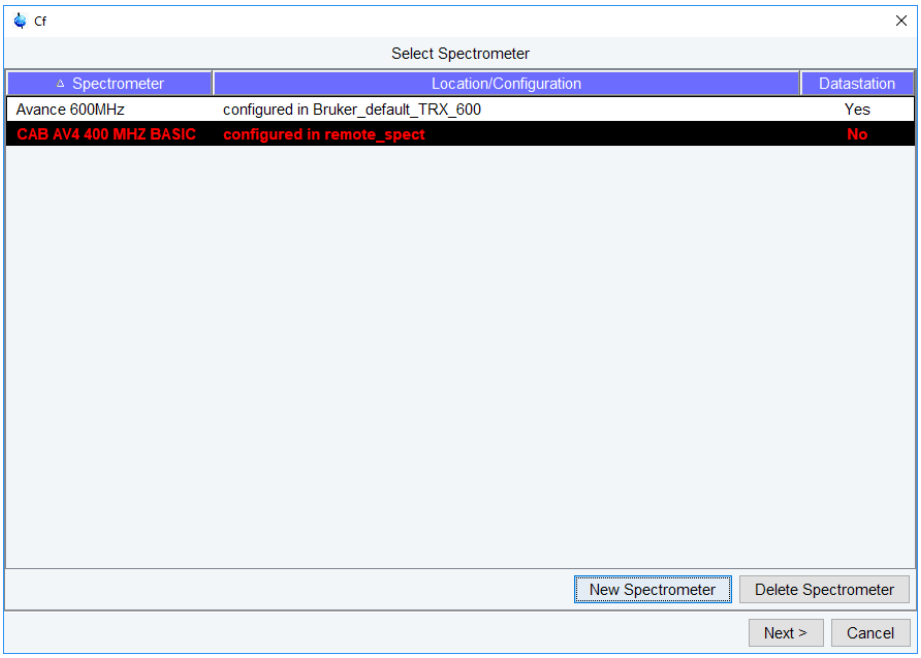
1. Import a datastation from … This will be explained in chapter *Configuration of a Processing-Only Workstation Using an Existing Spectrometer Configuration [▶ 44]* and *Configuration of a Processing-Only Workstation [▶ 48]* and only makes sense when you configure a processing-only workstation and not a spectrometer.
2. Import as spectrometer from... Browse to the TopSpin configuration directory where you want to import from.



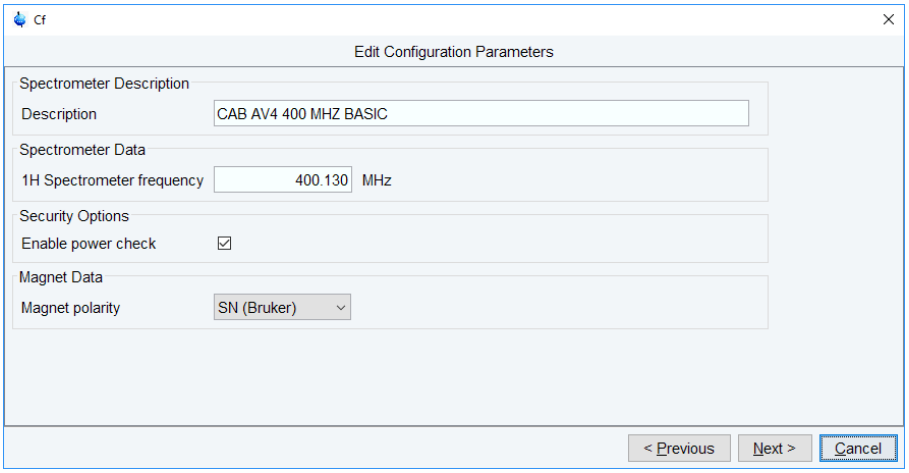
3. Use the option AV connected to workstation at local IP address 149.236.99.9. This is the recommended option, if available.



Both options 2 and 3 will bring you back to the main cf window. It will now show the imported configuration.



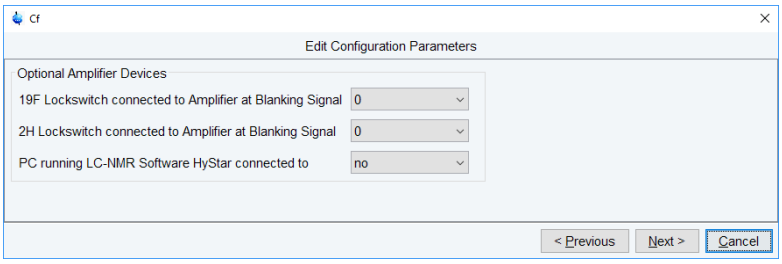
- Click **Next** to continue the configuration. A window with the basic spectrometer frequency will be displayed.



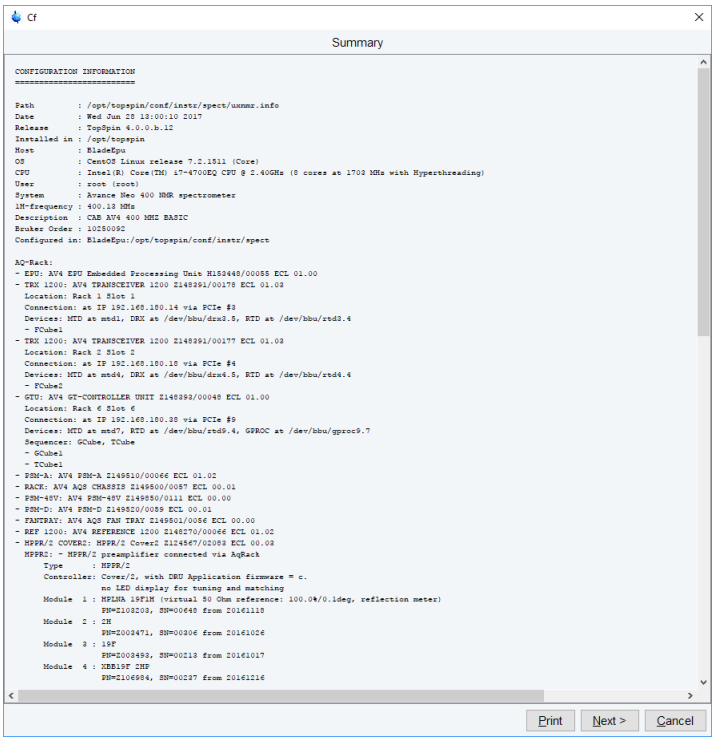
- Check or enter the spectrometer description, the 1H frequency of the magnet and magnet polarity. Enable **power check** and click **Next**.

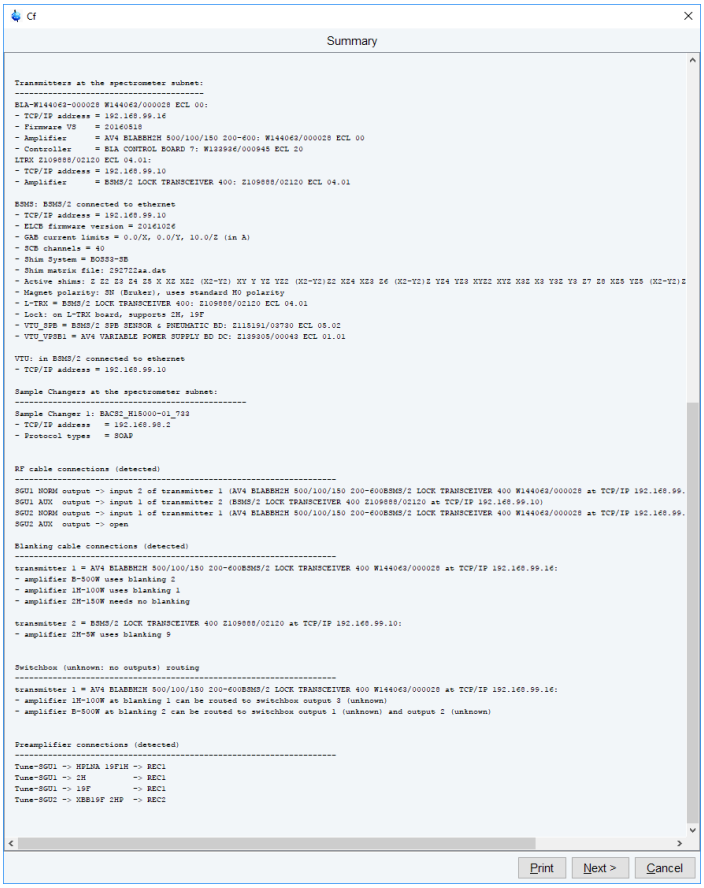
The progress of the configuration procedure is displayed.

Depending on the hardware configuration optional devices will be displayed. Please keep in mind that this is an example. Specific entries may be different.

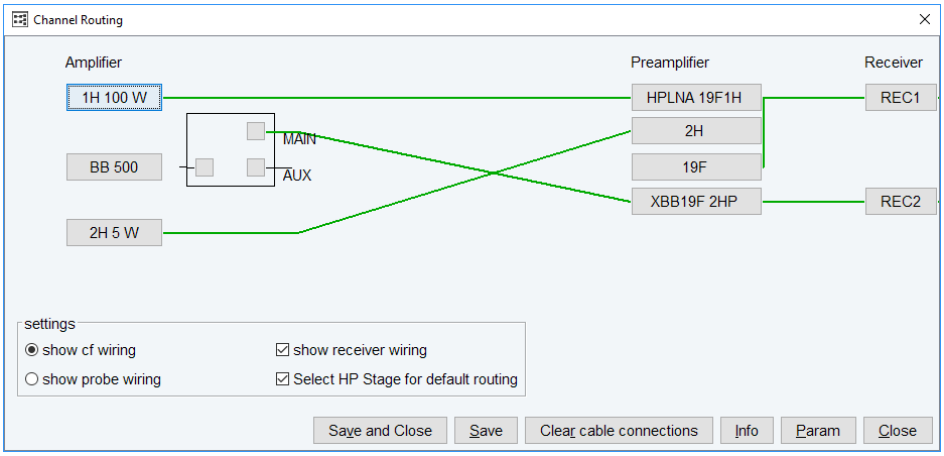


- When finished, click **Next**. A summary window will be displayed.

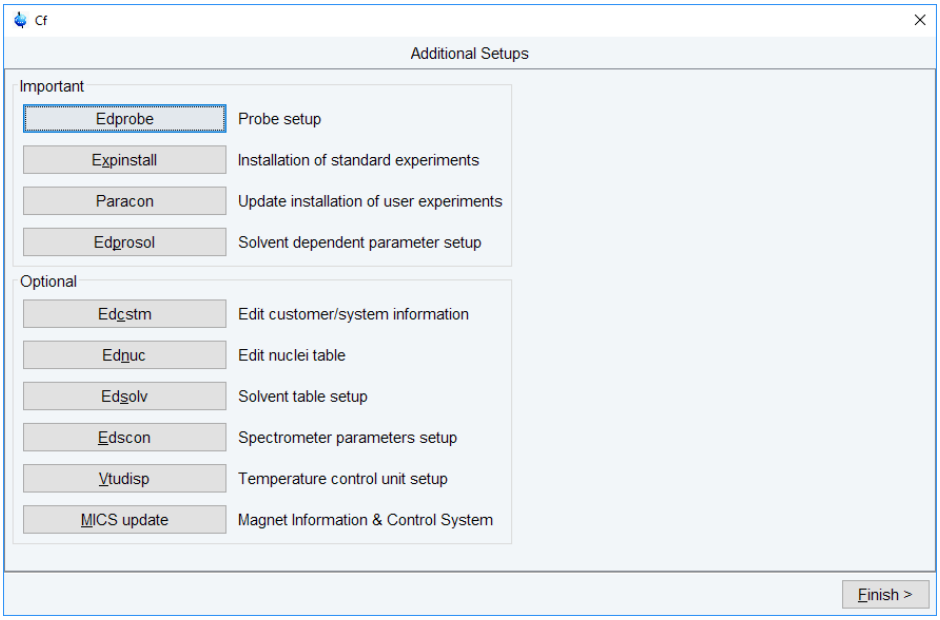




- Click **Next**. The channel routing window will be displayed. Check and correct it, if necessary.



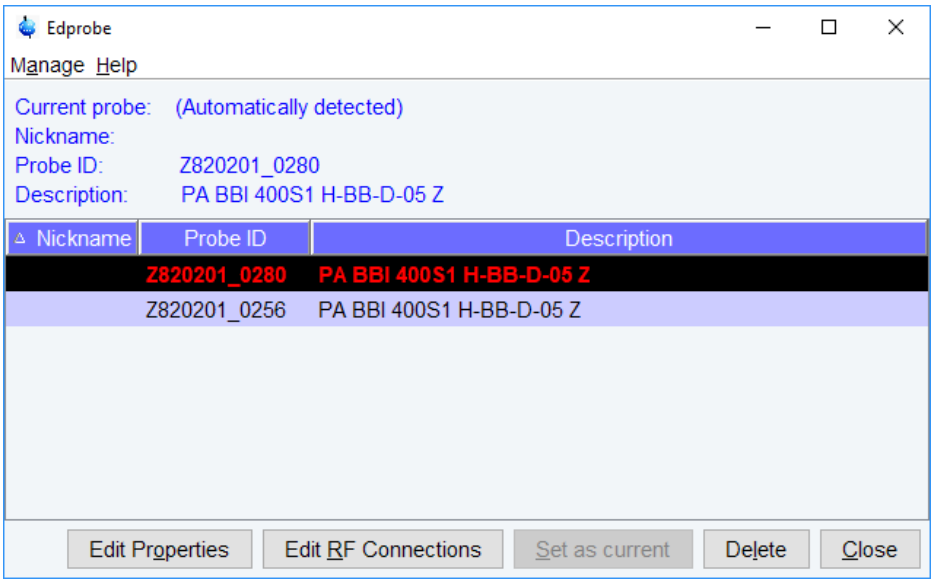
- Check and correct the connections, if necessary. Click **Save and Close** or **Close**. The Additional Setups window will be displayed:



- **Note:** The most important next configuration steps are **Edprobe**, **Expinstall** and **Edprosol**.

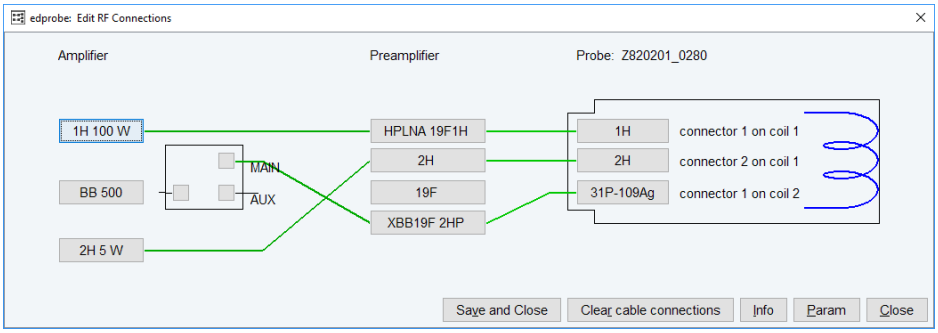
Edprobe

- Click **Edprobe**. The Edprobe window will be displayed.



If the current probe is recognized through the PICS (Probe Identification Control System), then it will automatically be selected.

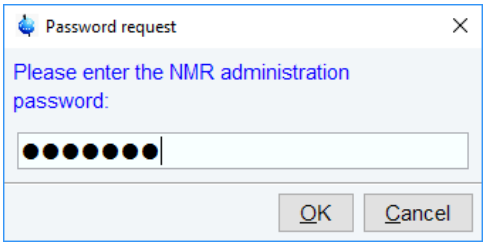
- Click **Edit Properties** to check or set the properties. Click **Close**. The probe RF connections will be displayed.



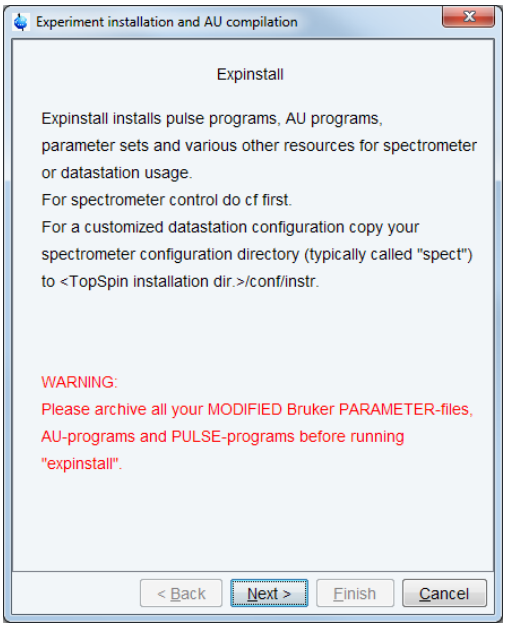
- Check and correct them, if necessary. Click **Save and Close** or **Close**.

Expinstall

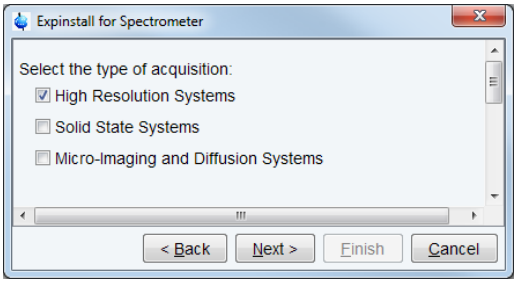
- In the Additional Setups window, click **Expinstall**. A Password request window is displayed.



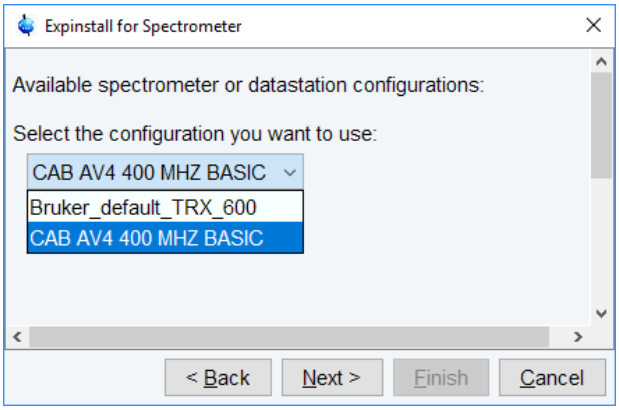
- Enter the NMR administration password to display the first Expinstall window.



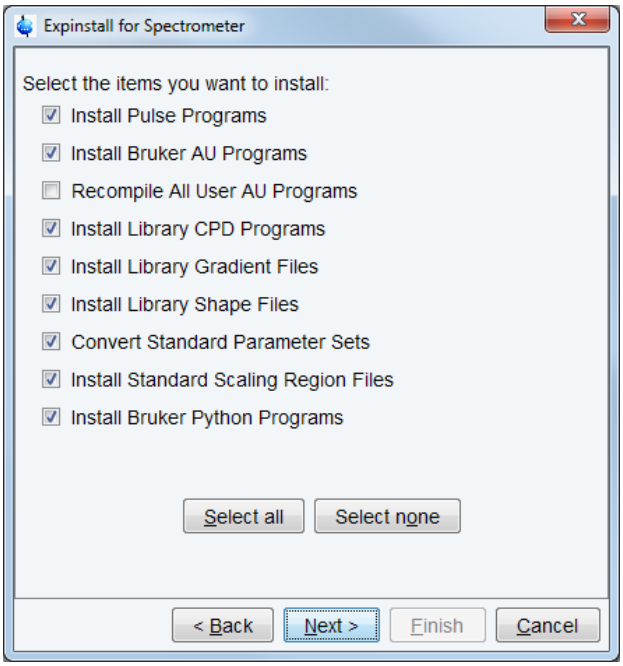
- Click **Next**. If there are no modified Bruker-Parameter files, AU-programs and Pulse-programs or files and programs are archived in a different directory. Individual Parameter files, AU-programs and Pulse-programs with different names to the original Bruker files will not be affected during the installation.
- In the next window select the type of acquisition. In the example a High Resolution System has been checked.



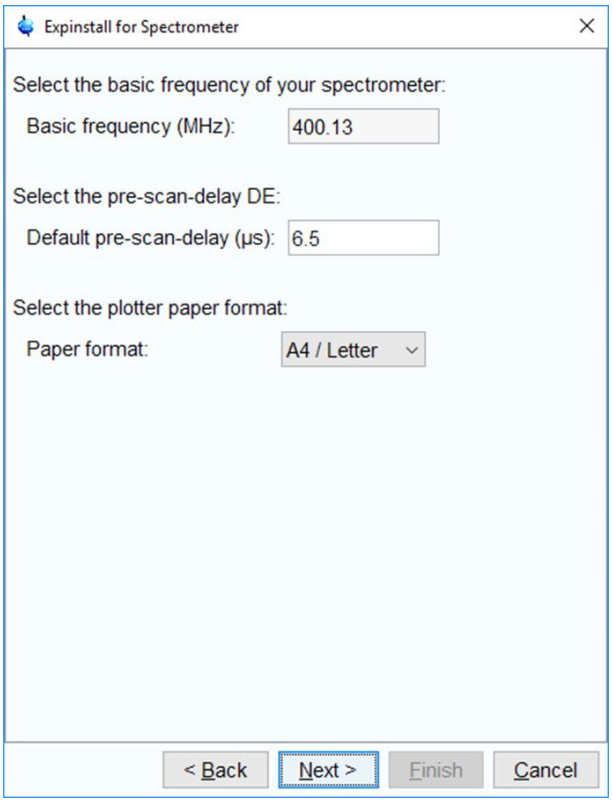
- Click **Next**.



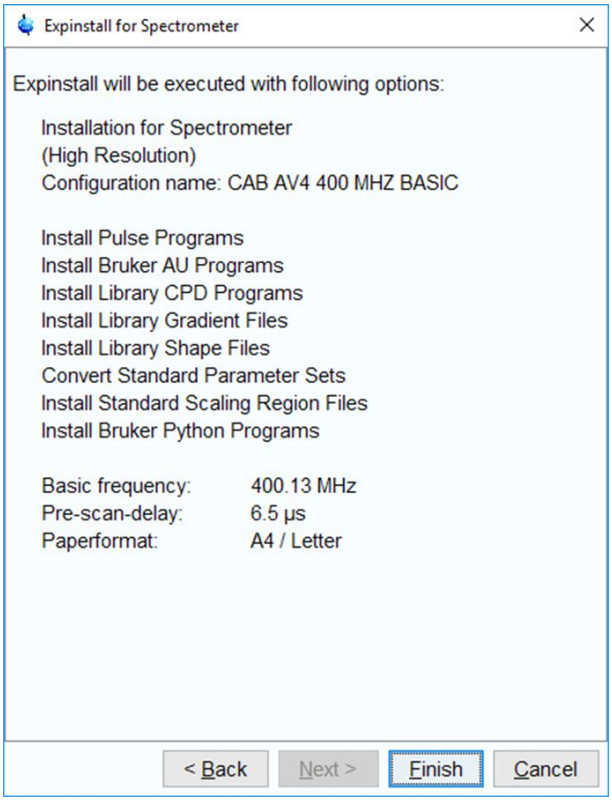
- Select the spectrometer or data station configuration for **expinstall**. Here the **CAB AV4 400 MHZ BASIC** has been selected. If this window is not displayed, then TopSpin has found only one valid configuration, namely the one for the current spectrometer, and immediately continues with the next window. Click **Next**.
- In the next window select the items to use for the spectrometer or the processing-only Workstation configuration. Accepting the default settings is a good choice. Then click **Next**.



- In the next window enter the basic frequency of the spectrometer and the pre-scan delay. All settings should be correct. Nevertheless in case of a configuration to control a spectrometer they should be checked. Click **Next**.



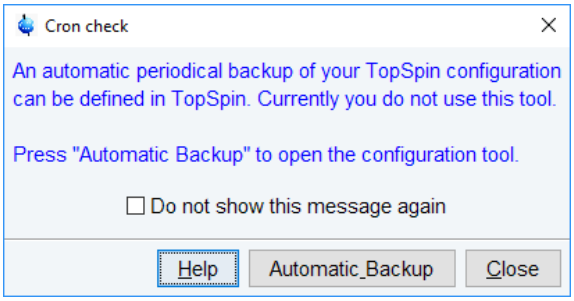
- Click **Next** to display a summary of options executed by **expinstall**.



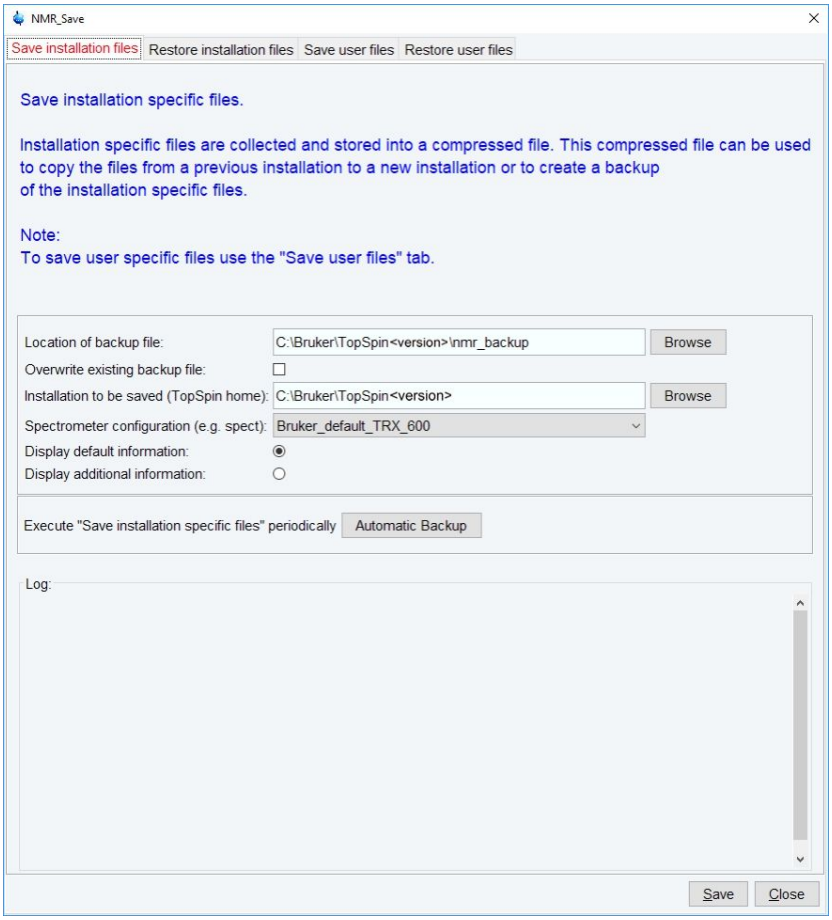
- Check this list.

- To change an option, click **Back** to the window(s) where corrections have to be done. Then click **Finish**.

The installation of the selected items will start now. Wait until this process has finished. In the TopSpin status line the progress of the installation is monitored. At the end of expinstall a Cron check window is displayed.



- Click **Automatic Backup** to open the NMR Save window.

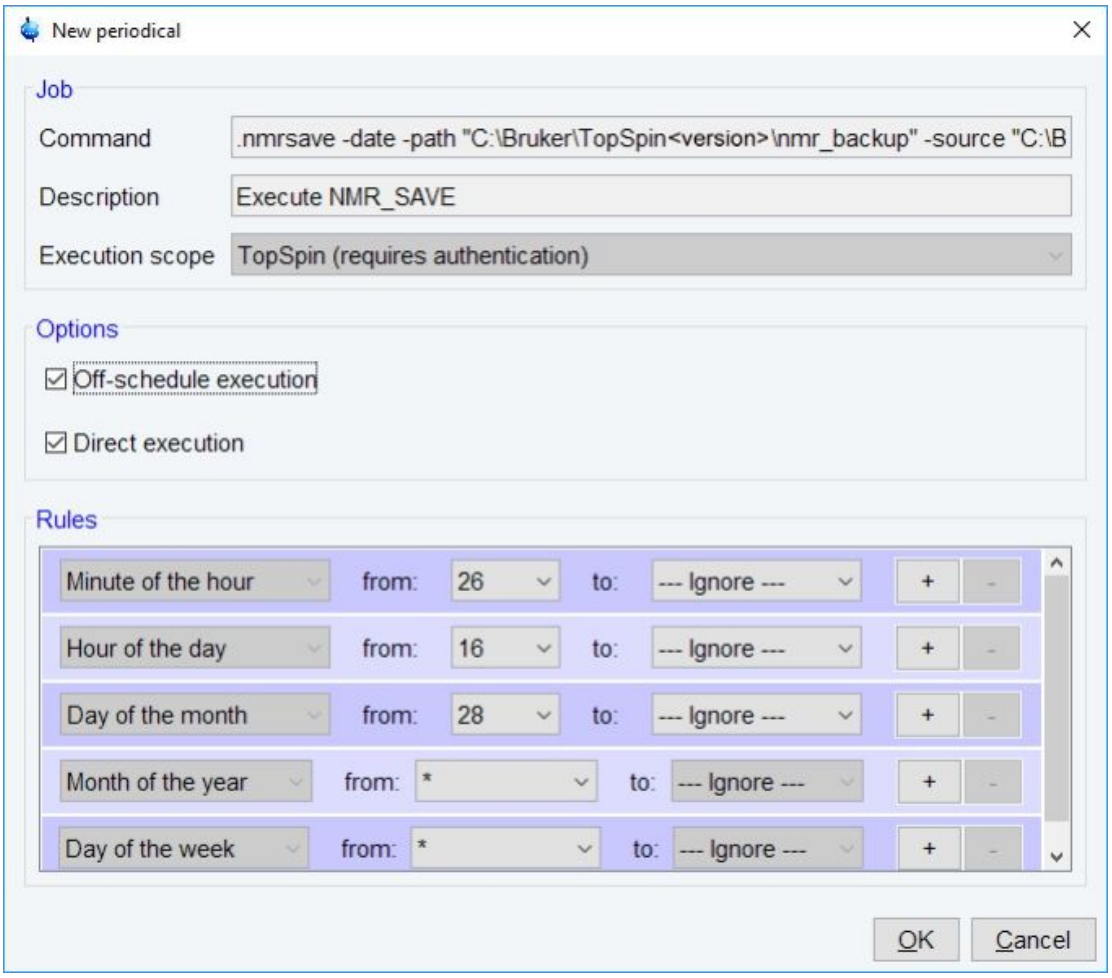


- Define the locations for saving and restoring the installation and user files.
- Click **Automatic Backup** to periodically save the configuration specific files.

It might be useful to save the periodical backups on a network drive. Enter the network drive as location of backup file in the NMR_Save window. Click **Automatic Backup**, the chosen drive is set and cannot be edited anymore. For more information see *Backup and Restore of Important Files [▶ 49]*.

- Set job, options and rules for an periodical backup.

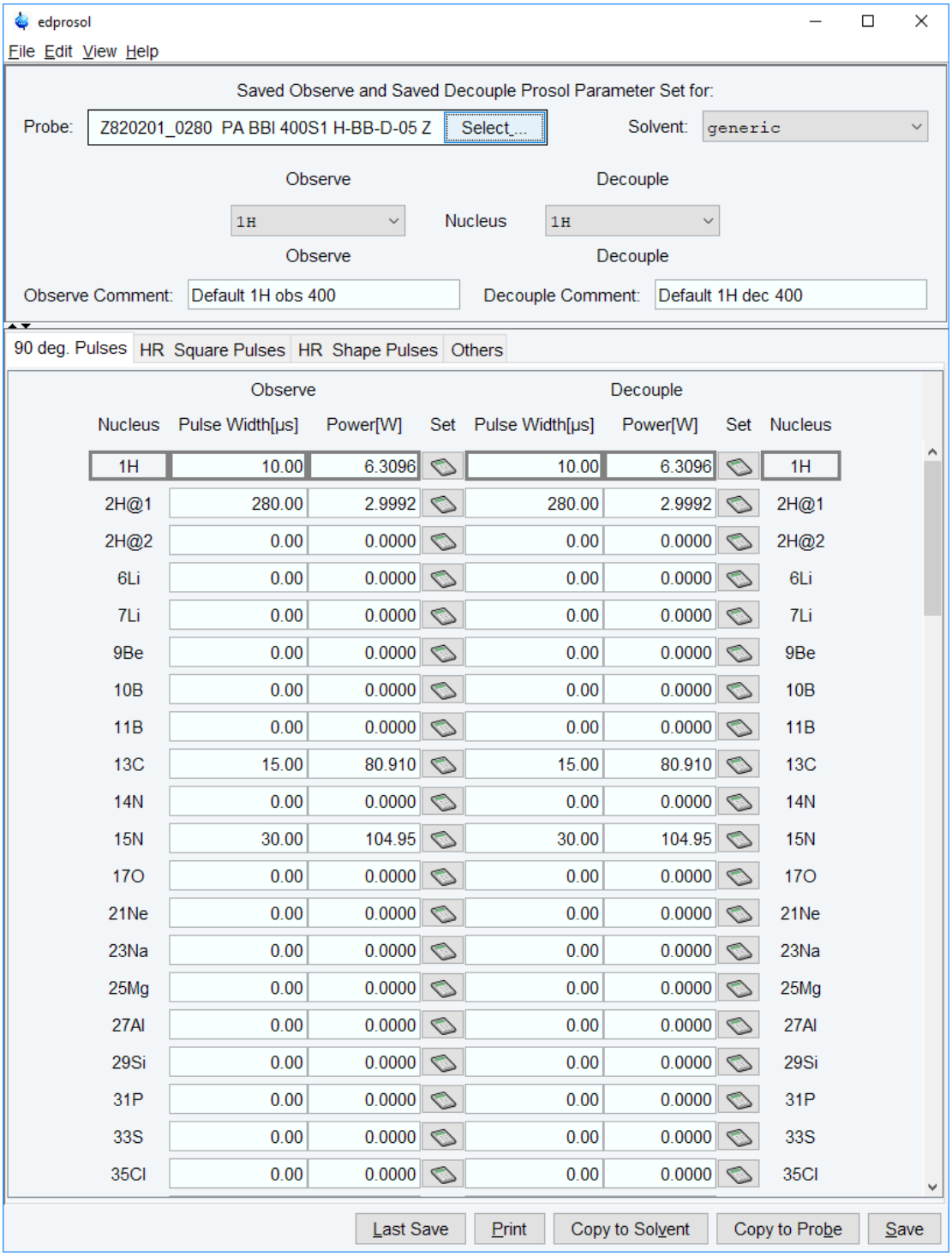
Note: The command box cannot be edited!



- Click **OK** and enter the NMR administration password.
- In the NMR Save window, click **Save**. The compilation of **xauw** will start. When this process is finished the Additional configuration programs window is displayed.

Edprosol

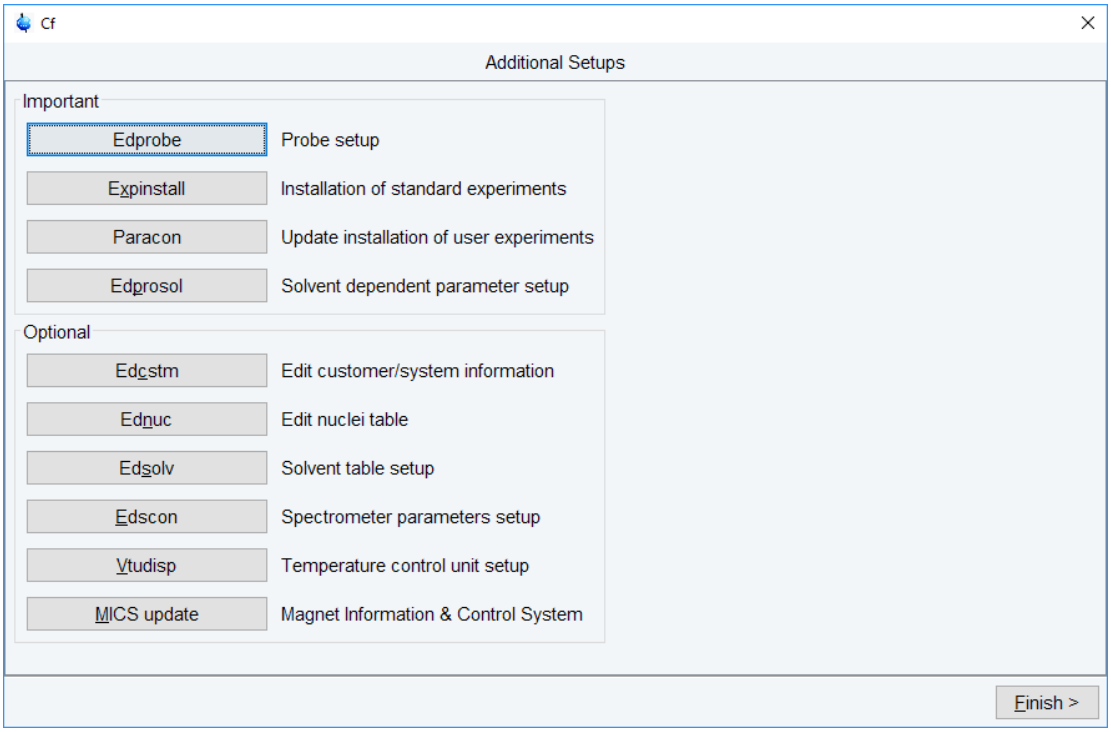
- Click **Edprosol** to enter the probe and solvent dependent parameters. It is necessary to execute Edprobe first (see above) because the probe parameters are needed.



For detailed information about the parameters and how to define them please refer to the Bruker Edprosol manual.

Optional commands

You may want to check the optional configuration commands as listed below in the last cf window.



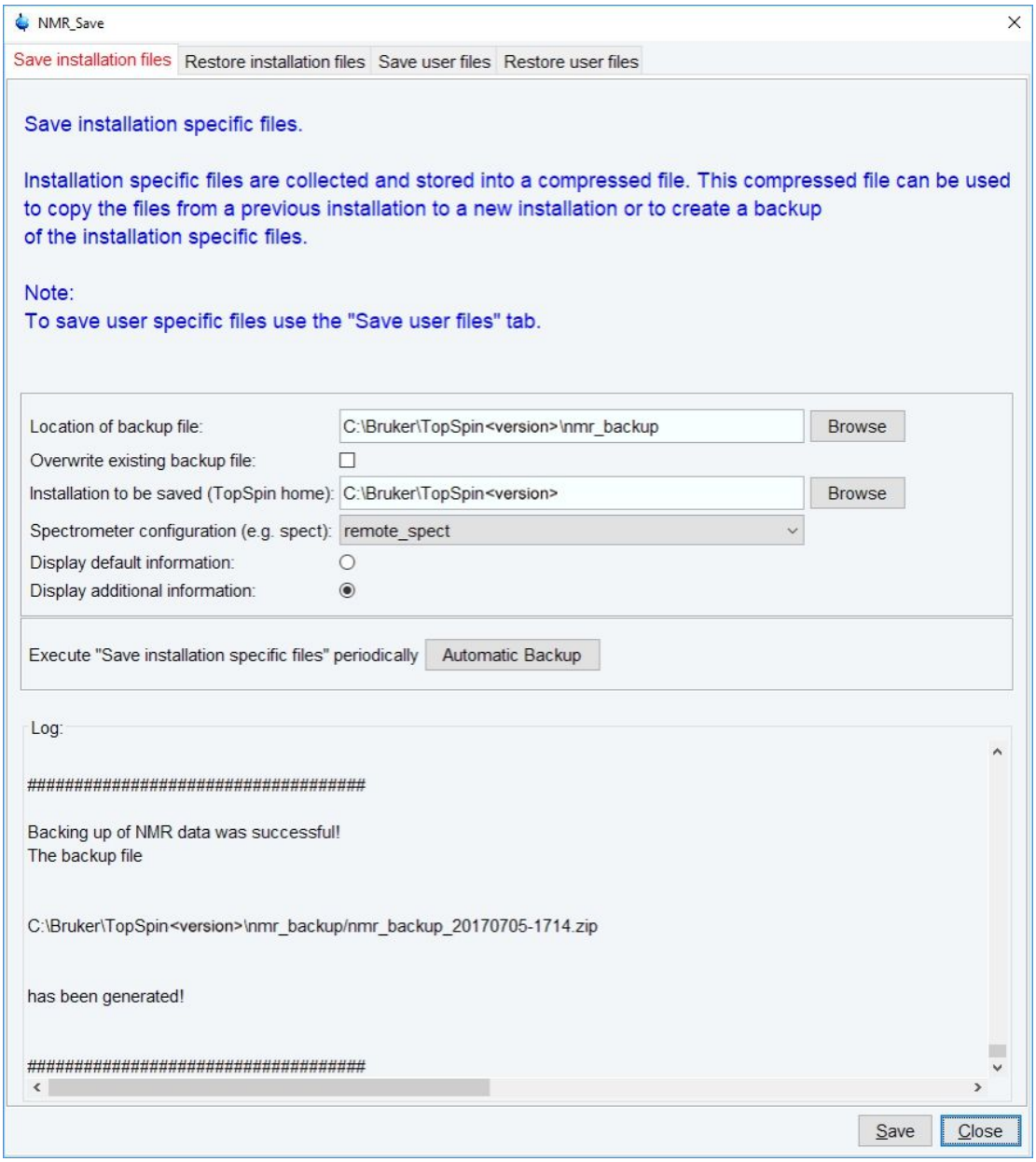
- When done, click **Finish**.

4.2 Configuration of a Processing-Only Workstation Using an Existing Spectrometer Configuration

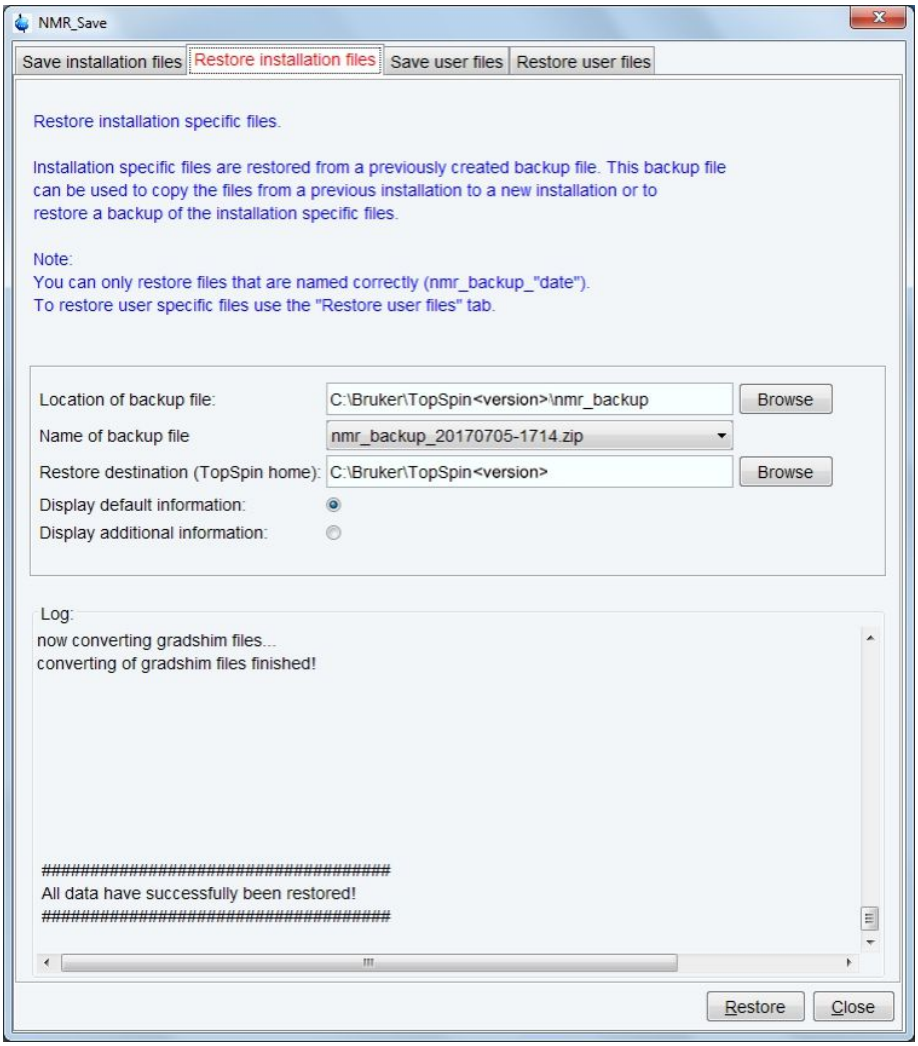
If the Workstation does not control a spectrometer but is used in connection with a particular spectrometer, e.g. for setting up experiments, processing or plotting you should configure it like that spectrometer.

To transfer the configuration of the spectrometer to the processing-only Workstation execute the following steps:

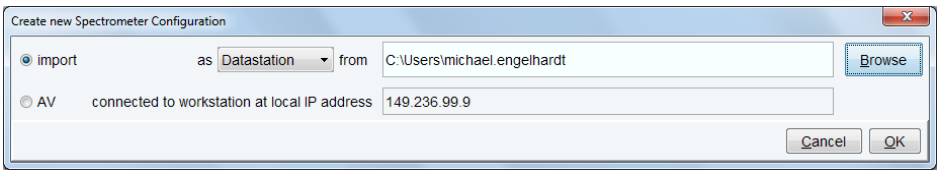
- Save the desired configuration on your spectrometer Workstation with **nmr_save** (see *Backup and Restore of Important Files [▶ 49]*)



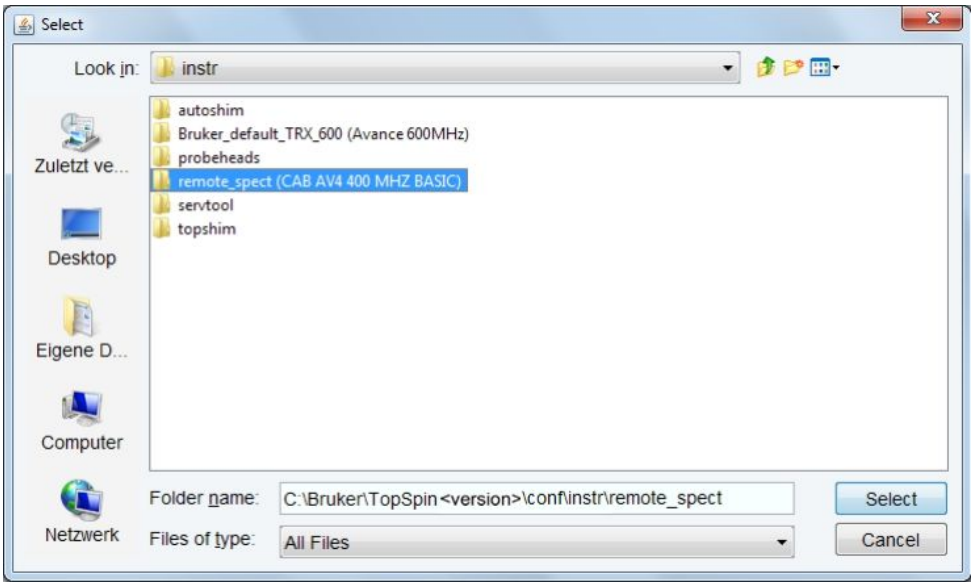
- Copy this archive file to the processing-only Workstation.
- Restore the configuration with the **nmr_restore** command to the processing-only Workstation (see *Backup and Restore of Important Files [▷ 49]*)



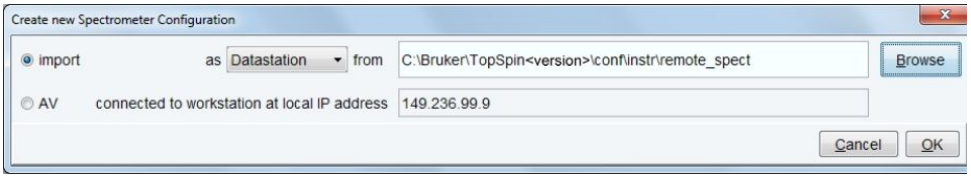
- The spectrometer configuration is now available. It will appear in the expinstall window and can be used to configure the Processing-only system.
- Click **cf** in the Configuration check window or type **cf** in the command line of the TopSpin main window. Enter the NMR administration password when prompted for it. In the **cf** window, click **New Spectrometer**. Enter the pathname to the above imported spectrometer configuration or click **Browse** to select it.



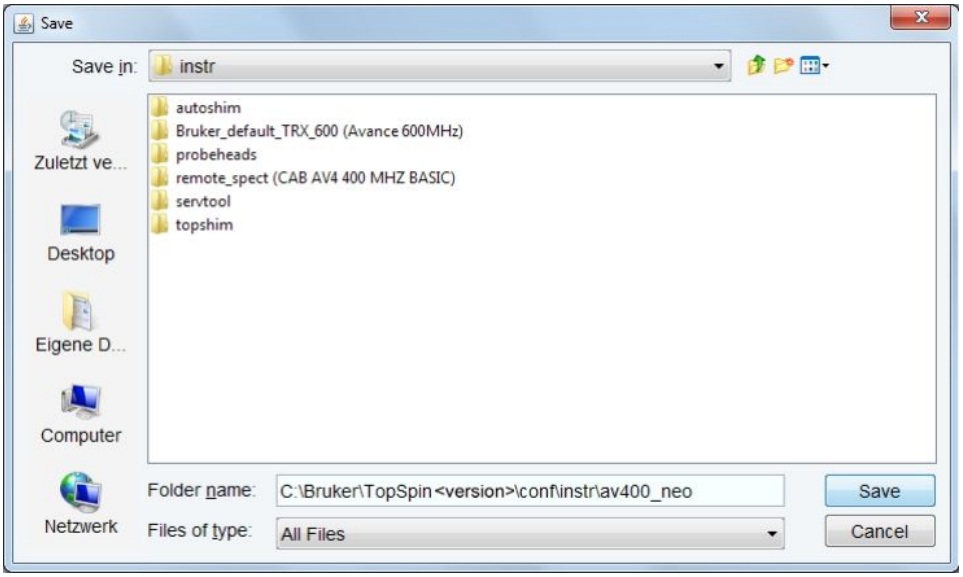
Here the configuration stored as remote_spect has been selected:



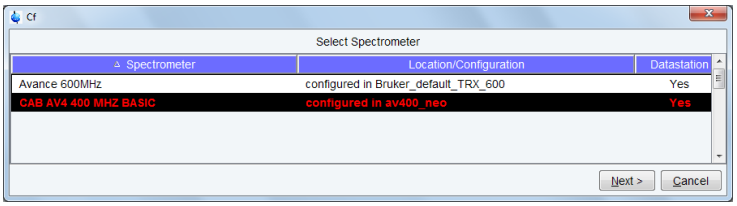
- Click **Select**, the name will be entered in the *from* field:



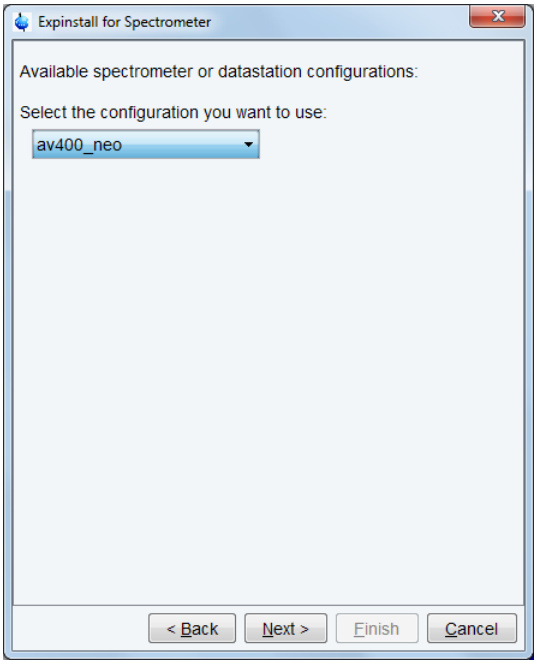
- Click **OK** and enter a suitable name for the spectrometer configuration to describe it in a meaningful way, e.g. av400_neo:



- Click **Save**.



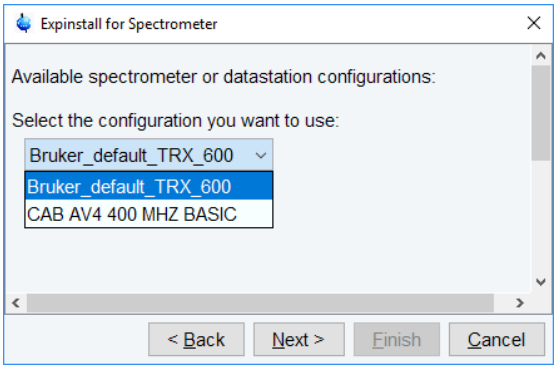
The **cf** window will be displayed. Click **Cancel** and continue with **edprobe** and **expinstall**.



In the **expinstall** window, the available spectrometer list should show the av400_neo entry. Select it and continue as outlined in the previous chapter.

4.3 Configuration of a Processing-Only Workstation

If the Workstation does not control a spectrometer and is just used for processing only, then only expinstall needs to be executed. Proceed as outlined in the previous chapters and for instance select **Bruker_default_TRX_600** as an example configuration.



5 Backup and Restore of Important Files

It is strictly recommended to frequently create a backup of the important files of your configuration of TopSpin.

There are many good reasons for weekly or monthly backup of important data, e.g. head crash or theft of hard disk. It will allow to restore the spectrometer configuration in a short time.

TopSpin offers the command **nmr_save** for saving those important files. With **nmr_save** all installation specific files, like spectrometer information, licenses etc. are saved. Even the default directories listed in the source directories, like e.g. *pp* are saved. All these files will be stored in one archive file.

Note: The commands **nmr_save** and **nmrsave** have identical functions.

With **nmr_save** installation specific files can be saved periodically at a specific time and date.

The same function as nmr_save is available for user-specific files with the command **user_save**. Only user-specific configuration files will be saved with this command. The additional directories, added by user which are listed in the source directories as defined in the user preferences, and the user specific directory *<USER_HOME>/.topspin-/<Workstation_NAME>/prop* are saved. All these user specific files will be stored in one archive file.

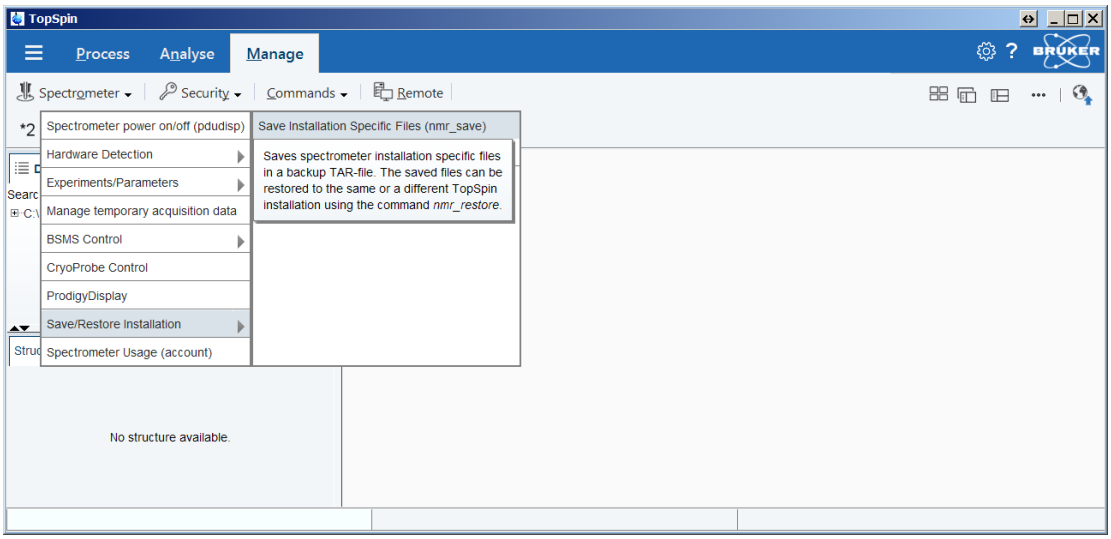
The command **nmr_restore** and **user_restore** respectively restore installation and user-specific files to the same or a different installation.

5.1 How to Save Information with nmr_save

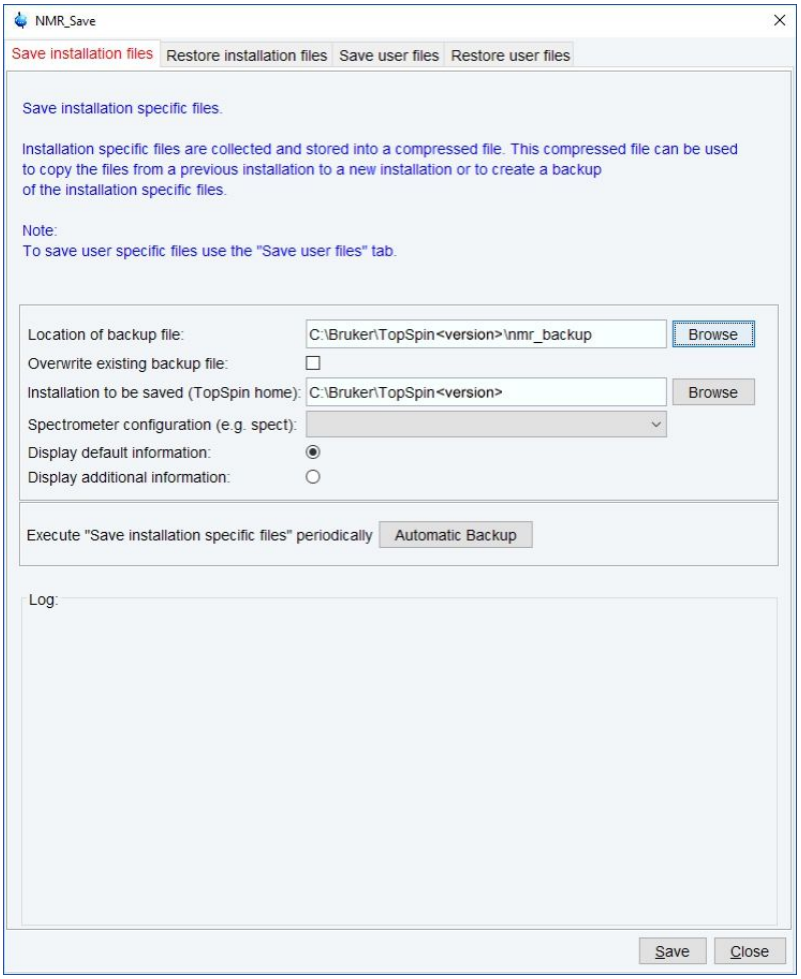
- Start TopSpin and enter **nmr_save** or **nmrsave**

or

- Start TopSpin and click
  Manage | Safe/Restore installation | Save installation specific files



The NMR_Save window will be displayed.



- Accept or modify the location of the backup file.
- Enter the location of the installation to be saved.
- **nmr_save** will then offer a list of all available spectrometer configurations which are located in this installation. Select the correct spectrometer name, e.g. **BRUKER_default_TRX_600**.
- For a periodical backup click **Automatic Backup**. This will open a window for a command scheduling. Click **OK** to accept the default values to execute **nmr_save** once a month.
- Click **Save**.

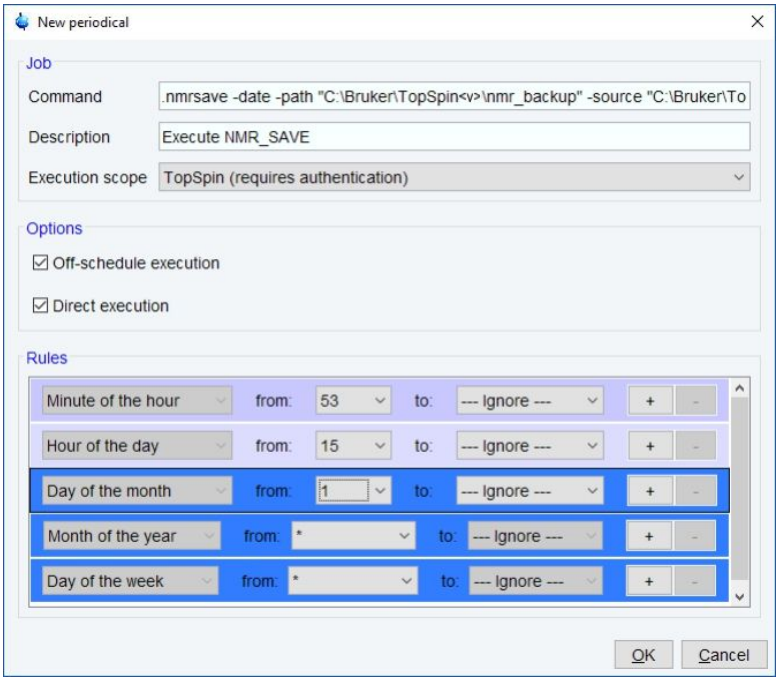
This will create an archive file of all necessary information from the selected installation/ spectrometer configuration. It is called:

nmr_backup_<date>-<time>.tar

and is stored in the directory you selected above, typically:

<TOPSPINHOME>\nmr_backup

The command **cron** performs command scheduling. It allows to execute commands periodically at predefined date/time in planned intervals. These intervals can be defined user-specific or by default. It offers full flexibility in time definition, off-schedule execution and user control. When called from **nmr_save**, the fields contain default values as in the next figure.



The following fields are available:

- **Command:** The command to be executed
- **Description:** A description of the command
- **Execution scope:** The scope of the command execution, User of TopSpin
  For scope *User*, the scheduled command will only be executed if TopSpin is running by the same user that is active during cron definition. If the scope is *TopSpin*, the scheduled command will be executed for any user. Scheduled command with *TopSpin* execution scope can only be defined, cancelled or modified after entering the NMR administration password.
- **Off-schedule execution:** This flag allows you to execute commands that were scheduled to run at the time when TopSpin was off. These commands are executed after the next TopSpin startup.

Note: Commands that were scheduled to run multiple times during TopSpin downtime are only executed once.

The following time scheduling rules exist:

- Minute of the hour: between 00 and 59
- Hours of the date: between 00 and 23
- Month of the year: January to December
- Day of the week: Sunday to Saturday

For each of these fields, you can define an interval by selecting a value in the **from** and a value in the **to** field. Setting the **to** field to *ignore* schedules the command for execution only at the time/date in the **from** field. An asterix (*) in the **from** field indicates all possible times. Clicking the **+** button to the right of the field, adds an an extra field of the same type, allowing multiple interval definition. Clicking **-** removes the extra field.

5.2 Which Information is Stored with nmr_save

You can save (or restore all) Topspin user defined files. This includes:

- Spectrometer configuration files (cf)
- Parameter sets (rpar, wpar)
- Pulse program (edpul, edcpul)
- AU programs (edau)
- Plot editor layouts (plot, autoplot)
- Shim files (rsh, wsh)
- Gradient shimming field maps (gradshim)
- IconNMR user information (iconnmr)
- Program Licenses (Topspin, Nmr-sim, NMR Guide)
- Various lists like scl, f1, ds (edlist, zg, gs)
- Topspin macros (edmac)
- Probehead and solvent dependant parameters (edprosol)
- Lock parameters (edlock)
- Probehead information (edprobe)
- Nucleus information (ednuc)
- RF Shapes and gradients
- etc.

Furthermore the files:

prog/logfiles/heliumlog

prog/logfiles/heliumloig.err

Bruker/licenses/license.dat

will be saved with the ending .backup. Please note that these files will be stored in the folder *conf/instr/*, no longer in the original folder.

Furthermore the whole directory *<diskless>/crco_data/cryotool_log/* will be saved.

5.3 How to Restore Information with nmr_restore

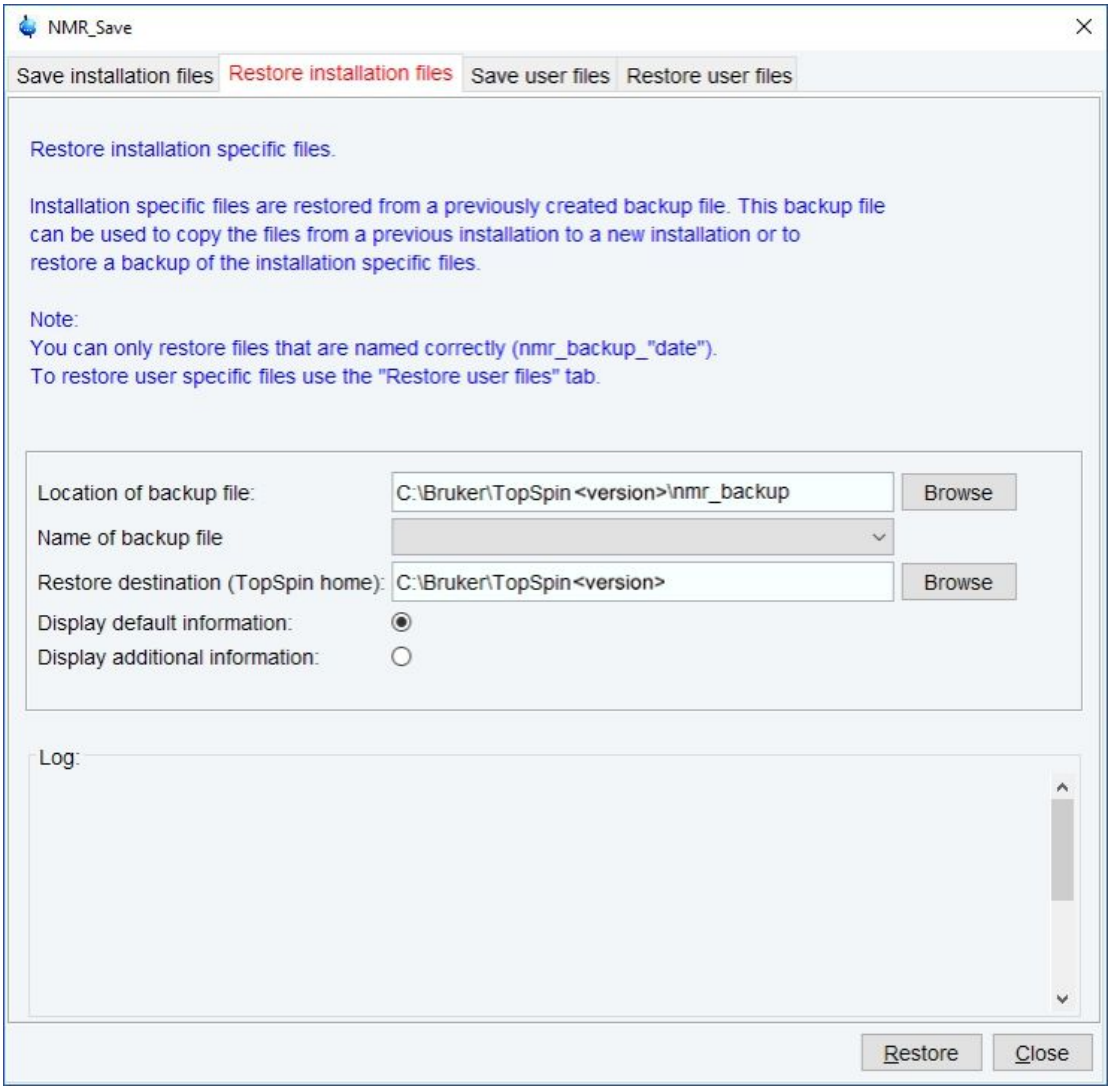
Note that this will overwrite your complete TopSpin configuration plus spectrometer configuration. Restore from a backup file only if you are absolutely sure that this is necessary. If in doubt do not restore or at least create a backup of the current state before.

- Start TopSpin and enter **nmr_restore**

or

- Start TopSpin and click **Manage Configuration | Spectrometer | Safe\Restore installation | Restore installation specific files**

The NMR_Save window will be displayed.



- Enter the path where your archive file is stored in the field **Location of backup file**. The default path is *<TOPSPINHOME>\nmr_backup.* A backup file created by **nmr_save** will be shown in the field **Name of backup file** if available. They always look like:
  nmr_backup_20120206-1428.zip
  where the first number represents the date and the second the time
- Enter the location of the **Restore destination**, the default is: *<TOPSPINHOME>*
- Click **Restore** and enter the NMR administration password in the upcoming Password request window.
- Execute the command **cf**

Backup and Restore of Important Files

6 Deinstallation of TopSpin

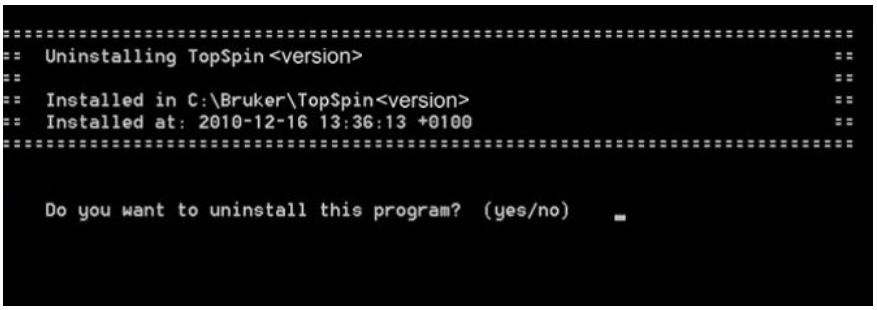
6.1 Deinstallation on Windows

During the installation of TopSpin also a deinstallation routine *deinst.exe* is copied to your system.

- Click the Windows **Start** button.
- Open the **Control Panel**.
- Click **Programs and Functions.**
- Select the TopSpin Version to uninstall and click **Uninstall/Change.**

This will cleanly shut down running services and deinstall the software package. On the other hand, configuration files and acquired data will be left on the disk.

The following window will be displayed:



- Enter **yes**.

The deinstallation starts and might take a few minutes. When the deinstallation is finished, all programs and icons of the TopSpin version are removed from the Workstation.

6.2 Deinstallation on Linux

During the installation of TopSpin also a deinstallation routine is copied into the sub folder uninstall.

- Open a file browser like konqueror or a shell window.
- Open the program directory.
- Open the sub folder **uninstall** and start *uninstall-<program>.sh*.

This will cleanly shut down running services, delete files in other directories and remove the entries in the GNOME or KDE menu. On the other hand, configuration files and acquired data will be left on the disk.

Examples:

- To deinstall TopSpin and all dependent programs, run
  /opt/topspin<version>/uninstall/uninstall-topspin.sh
- To deinstall SpectrOS only, run
  /opt/Bruker/spectros/uninstall/uninstall-spectros.sh

Deinstallation of TopSpin

7 Contact

Manufacturer

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Germany

E-Mail: *nmr-support@bruker.com*
http://www.bruker.com
WEEE DE43181702

Bruker BioSpin Hotlines

Contact our Bruker BioSpin service centers.

Bruker BioSpin provides dedicated hotlines and service centers, so that our specialists can respond as quickly as possible to all your service requests, applications questions, software or technical needs.

Please select the service center or hotline you wish to contact from our list available at:

https://www.bruker.com/service/information-communication/helpdesk.html

Contact

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info@bruker.com
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Order No: H9168SA2