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School of Biological and Chemical sciences - NMR Service

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Welcome to the NMR Service

The QMUL NMR service is intended to provide researchers in the University with an NMR spectrum on as wide a range of nuclei as possible. We also provide a commercial NMR service to outside users (see [Submitting Samples](#)). The service is situated in the School of Biological and Chemical Sciences at Queen Mary, University of London (QMUL).

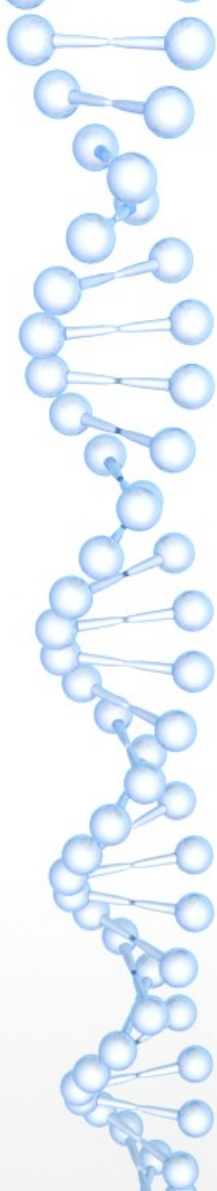
We have two Bruker NMR spectrometers operating at 400 MHz (^1H frequency) and one at 600 MHz. Please see [Available Equipment](#) for details of probes etc...



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Solution and solid state NMR

Programs for processing NMR data:

There are a variety of free programs available for processing NMR data, please select this [link](#)

Utility programs written at QMUL:

- [jdfutilities](#) - programs for converting Jeol NMR data into other formats (basically Bruker TopSpin format).
- [xep2csv](#) - programs for converting Bruker BES3T EPR data into ASCII "comma separated values".
- [ux2ascii](#) - programs for converting Bruker TopSpin data into ASCII format.

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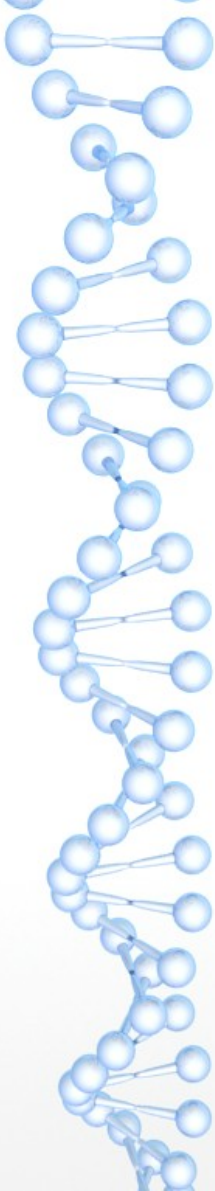
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Free Software for NMR data processing

Bruker Topspin

[Bruker TopSpin](#) (NMR data processing software, from Bruker, requires registration. Runs on Windows, Linux and MAC.) This is the program I recommend using for most general NMR data processing. **Note that to activate the license you cannot use the Chrome or Edge browsers, you must use Firefox, Safari or Internet Explorer.**

Kirk Marat's SpinWorks

[SpinWorks](#) (NMR data processing and simulation software from the University of Manitoba). There are .NET and Java versions that will run on Windows, Linux, MAC and *BSD (using MONO). This program has some very useful simulation options.

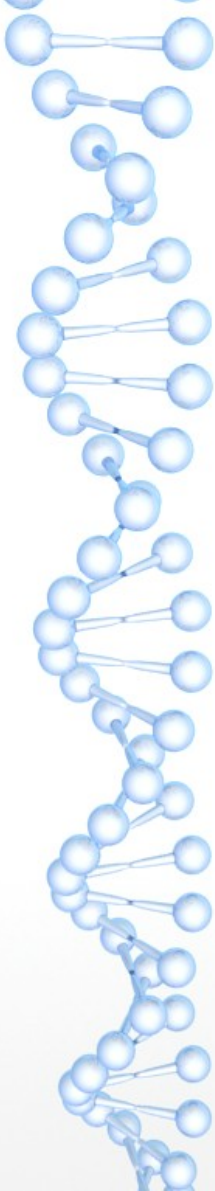
Mnova NMR Lite Software (version 6.21)

This software is licensed by SBCS for use by School staff and research students. The licence may be activated by anyone with a QMUL network connection. Once activated the software may be used on a laptop in any location for 90 days before re-activation is required.

Installation

- [Download the Licence File](#)
... download this file and save it to a local directory on your machine (PC/Mac).

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



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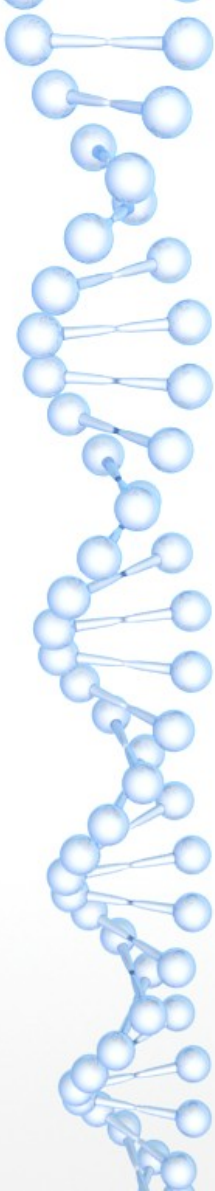
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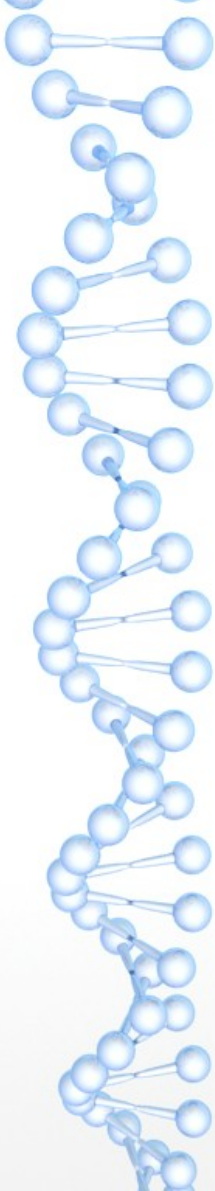
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Register for Bruker users account

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Please also note that the personal information that you enter in the form below may be screened against relevant sanction lists to ensure compliance with applicable export control laws.

*= These are mandatory fields

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Last Name: *

Country or Area: *

Email Address: *

Create Password: *


Confirm Password: *

Password must be at least 6 characters long

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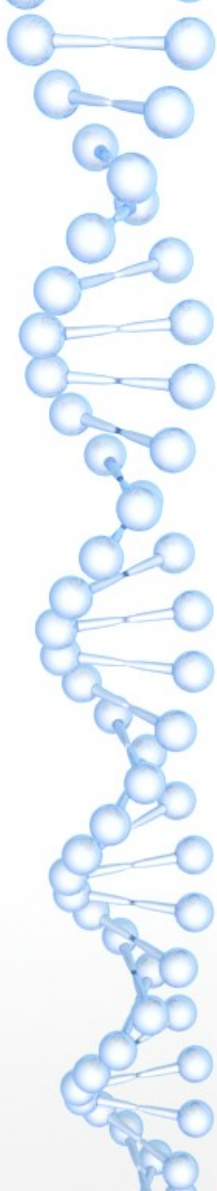
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- Mass Spectrometry
- Atomic Force Microscopy Materials Journal Club
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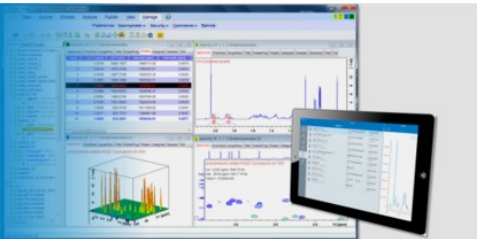
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NMR TopSpin License Processing for Academia

In order to provide students, researchers and teachers with unlimited access to the best tools for off-line NMR processing, Bruker is making their market leading NMR processing software TopSpin available free of charge for all academic users. In addition to Bruker NMR data, the software is able to process data acquired on Agilent, Varian and Jeol systems, as well as read any data provided in JCAMP format. We are happy to offer you a free Academia license for **TopSpin 4** and **TopSpin 3.6** ("Academia license").

[Request personal license ticket now](#)

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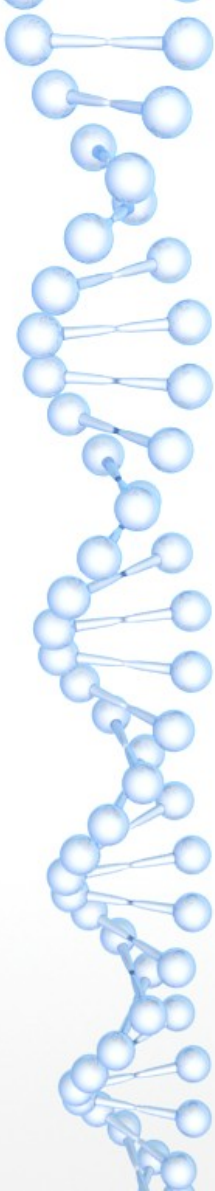
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TopSpin - Windows PC

Current versions:


- TopSpin 4.0.7 (for AVANCE NEO and processing in general)
- TopSpin 3.6.2 (for AVANCE III, III HD and processing in general)
- TopSpin 3.5 pl7 (for AVANCE III, III HD and processing in general)
- TopSpin 3.2 pl7 (for AVANCE II, III, III HD, Fourier 300 and processing in general)
- TopSpin 2.1 pl8 (for AVANCE I)
- TopSpin 1.3 pl10 (for AVANCE DRX, DPX, DMX, and DSX)

For detailed information refer to the corresponding [release letter and software support matrix](#).

(For information on acquiring the current version of TopSpin on DVD, contact your nearest [Bruker BioSpin office](#).)

To work with TopSpin a license is required. To download the current TopSpin version, click on the link and follow the instructions provided below. Please store the file on your hard disk and start the installation when the download is complete.


Current Release Download

 [TopSpin 4.0.7 & CMC-assist 2.14 \(1718.9 MiB\)](#)

(Created: 2019-05-07)
TopSpin for AVANCE NEO and processing in general.
This link allows for the direct installation of a complete acquisition/processing version for Windows 7 and Windows 10.
MD5 checksum:
ed3bb65b45ac8759970e481e6a46d75d


ISO - Downloads

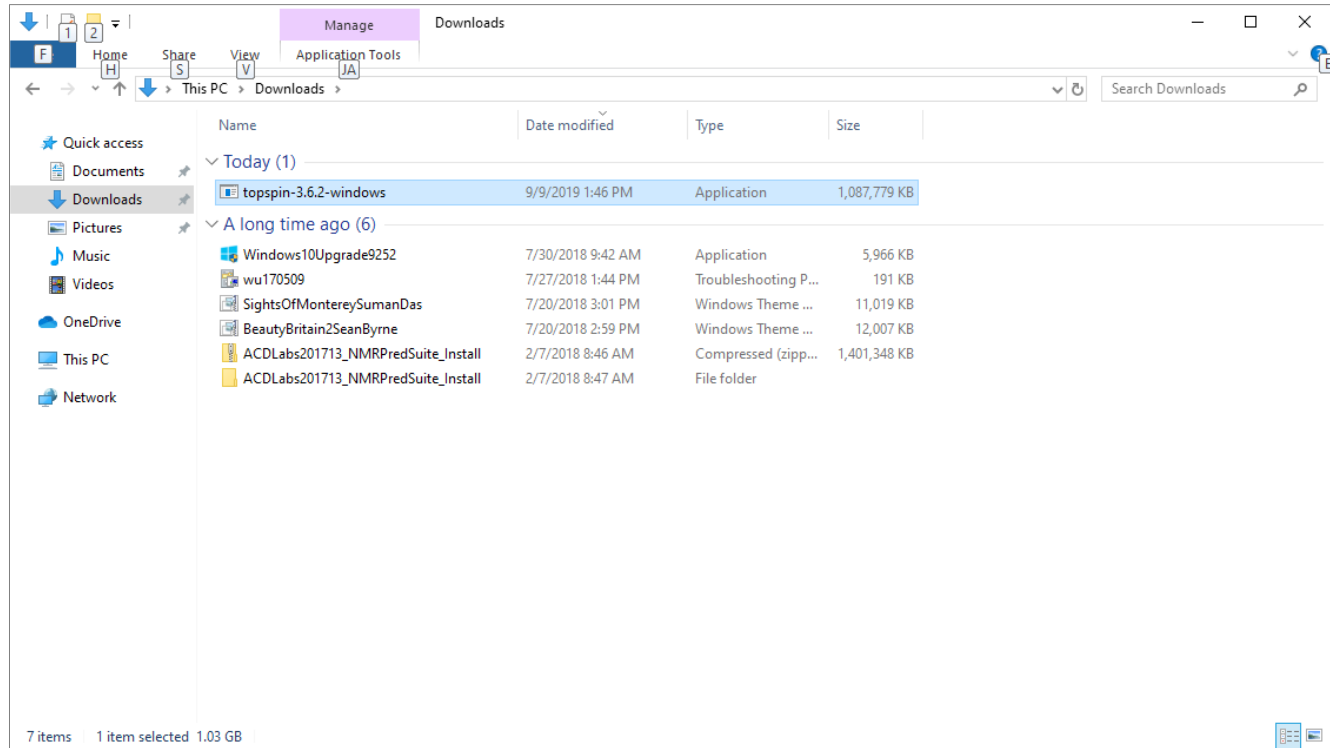
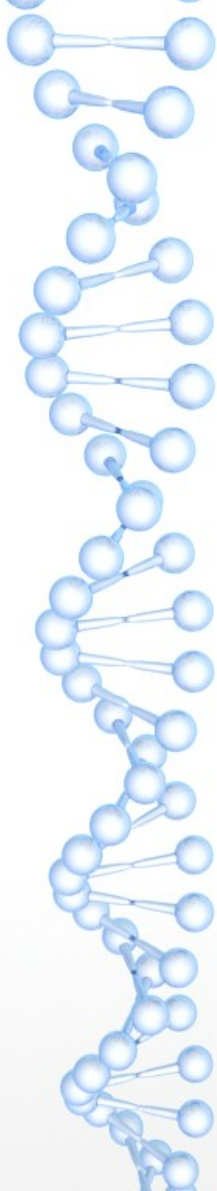
These images contain everything that you would also see on a DVD when you order it from Bruker. They contain all programs for all supported operating systems and also all additional software like AMIX, AURELIA and CMC-assist. For programs that are supported on the MAC, the MAC version is also contained in this image.

 [TopSpin 4.0.7 \(6441.5 MiB\)](#)

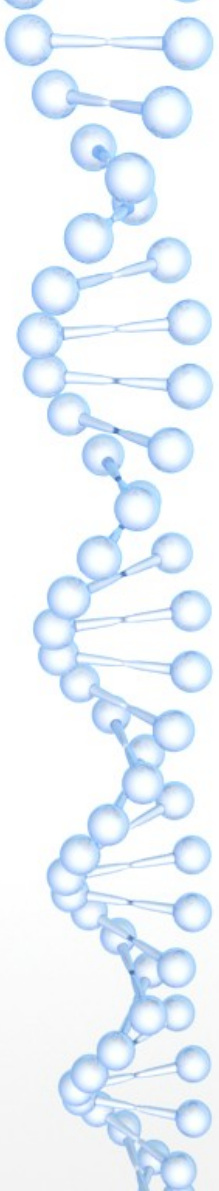
(Created: 2019-05-07)

EN



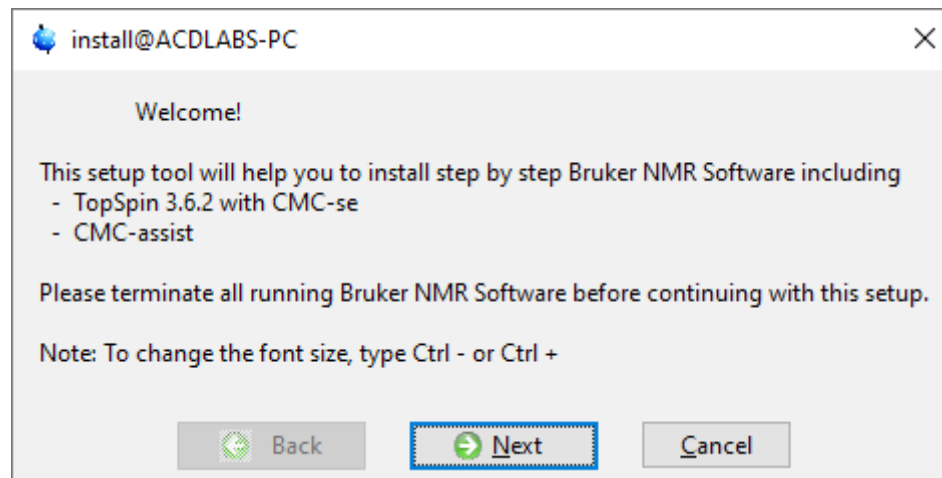
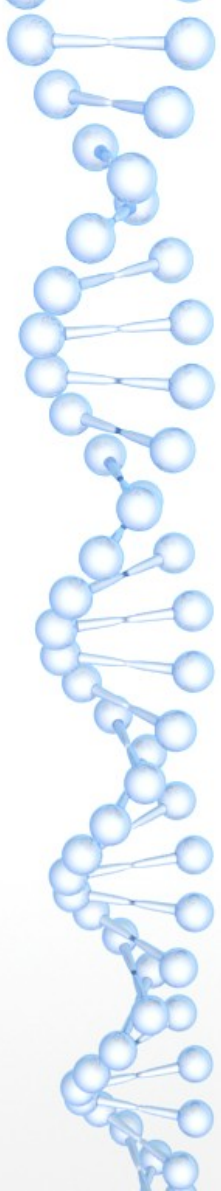


There are two versions of TopSpin supported (3 & 4). I recommend version 3 which is a smaller download and matches the version on the spectrometers and the lab. workstation and is used in the handouts.

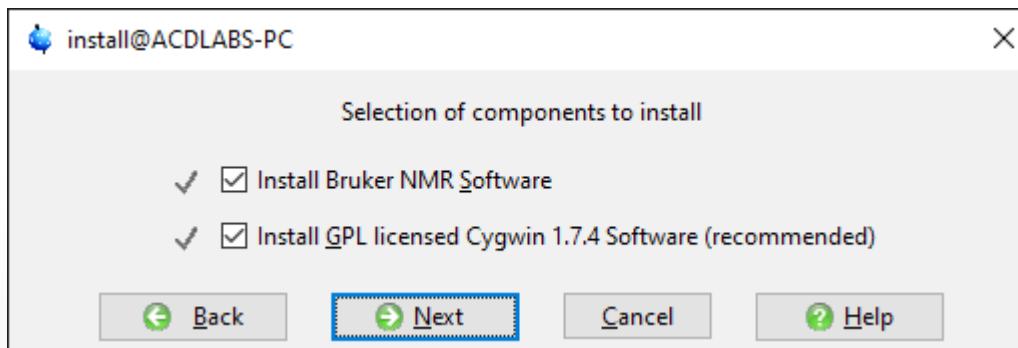


```
C:\Users\ACDlabs\Downloads\topspin-3.6.2-windows.exe
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extracting: install-topspin-3.6.2.tmp/noarch/pack/centralaudit.vsn
inflating: install-topspin-3.6.2.tmp/noarch/pack/remotecq.md5
inflating: install-topspin-3.6.2.tmp/noarch/pack/tsdocu.tarx
inflating: install-topspin-3.6.2.tmp/noarch/pack/docpr.tar.xz
extracting: install-topspin-3.6.2.tmp/noarch/pack/reporttemplates.size
inflating: install-topspin-3.6.2.tmp/noarch/pack/docpr.tarx
inflating: install-topspin-3.6.2.tmp/noarch/pack/tsinstr.tar.xz
extracting: install-topspin-3.6.2.tmp/noarch/pack/iconnmrdocu.size
extracting: install-topspin-3.6.2.tmp/noarch/pack/nmrguide.vsn
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extracting: install-topspin-3.6.2.tmp/noarch/pack/gplfonts.vsn
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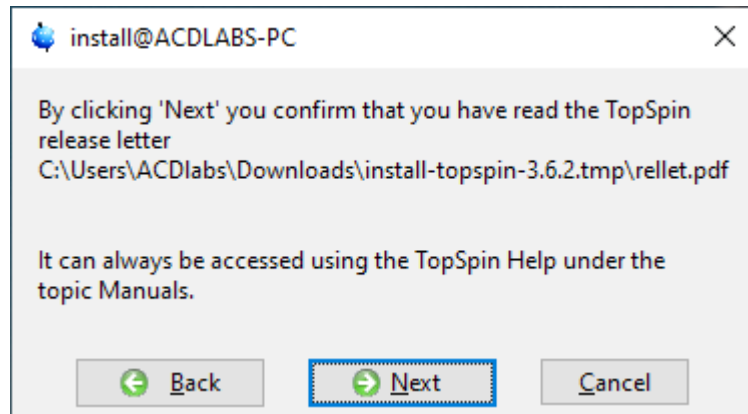
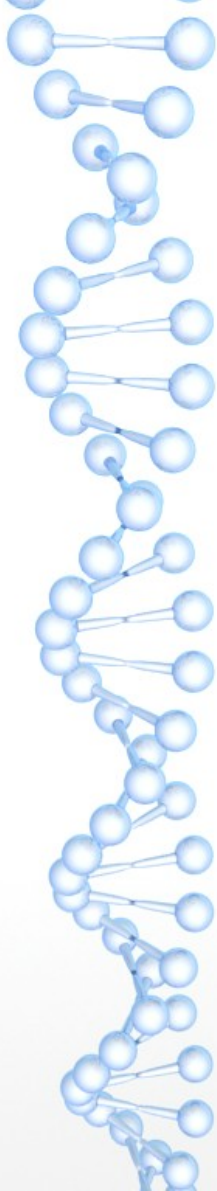
When you run the TopSpin installer, various temporary windows will be opened, when the installation finishes they will all be closed automatically.



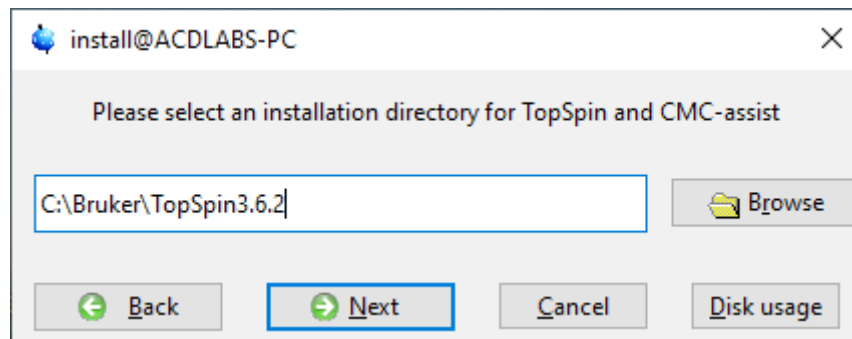
Once the installer has loaded, there will be a series of windows which will require input of some type. The first window (above) Just needs you to click on Next.



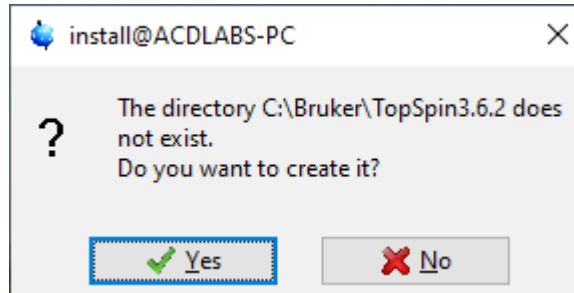
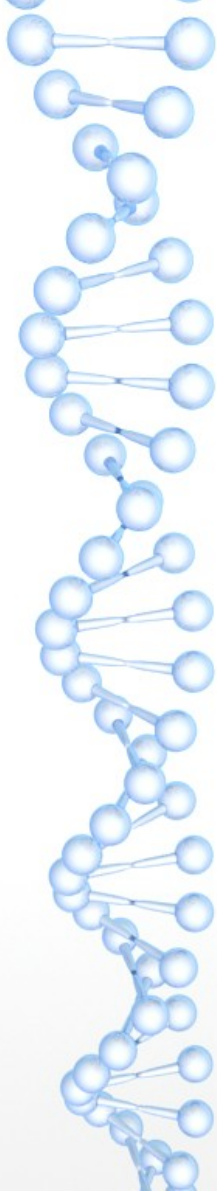
Do not change these options, again just choose Next.



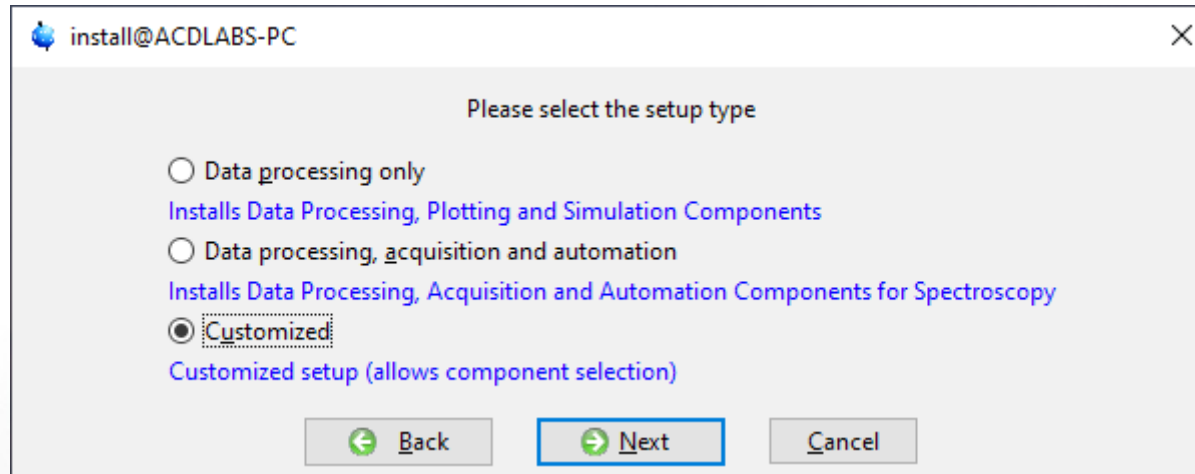
It is not necessary to read the TopSpin release letter, again just choose Next.



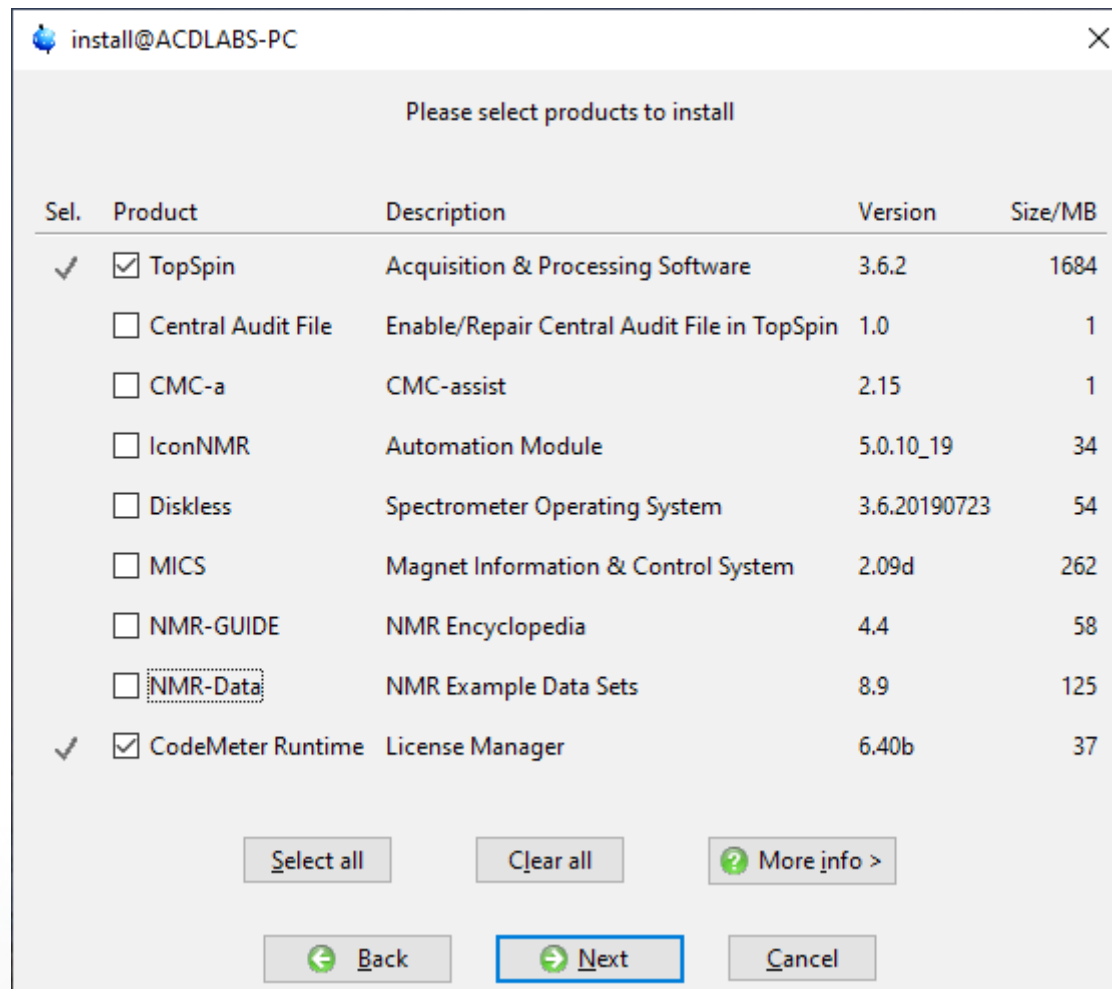
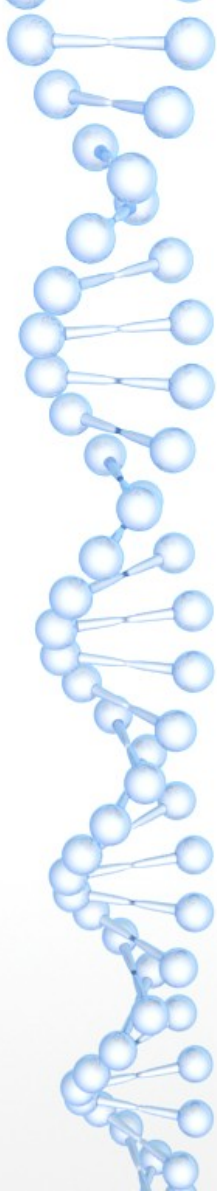
The default installation directory is usually fine, so again just choose Next.



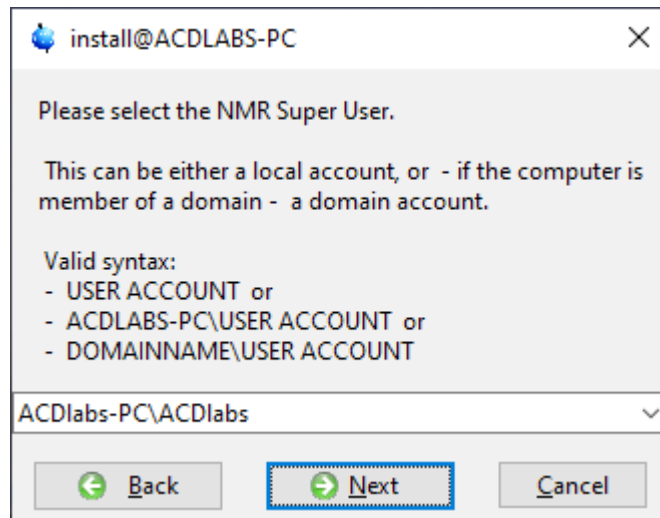
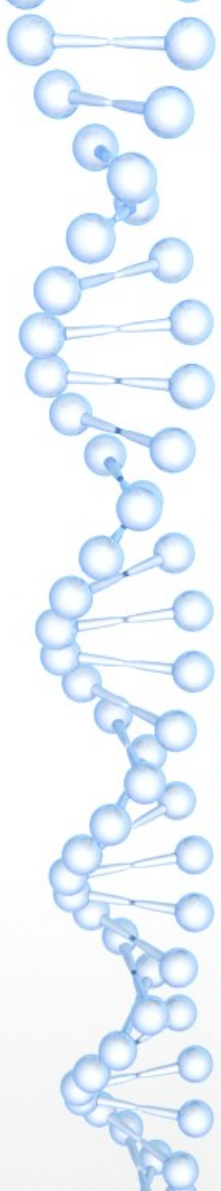
The installer will ask you to confirm the directory creation.



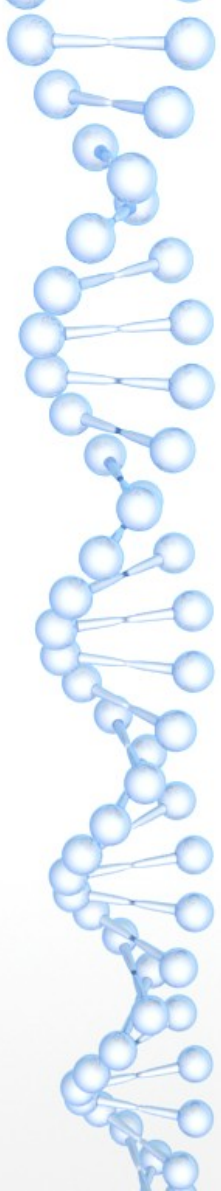
To avoid installing software you will not need, select Customized.



The only products you need are TopSpin and CodeMeter.



You will need to choose an account on your computer as the NMR Super User (i.e. administrator). Usually you would select your own login account.



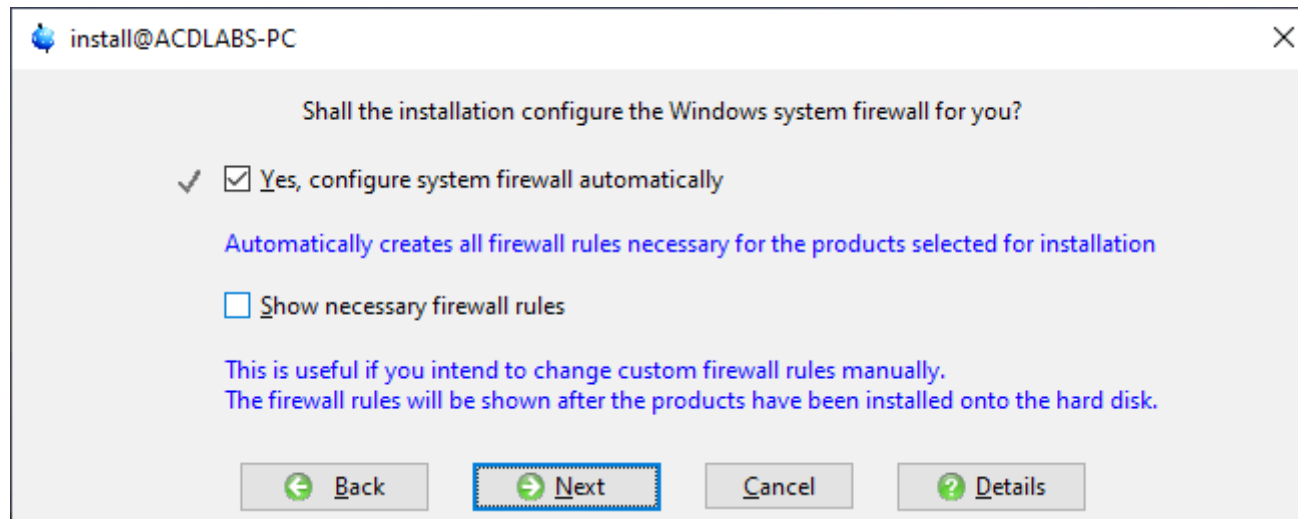
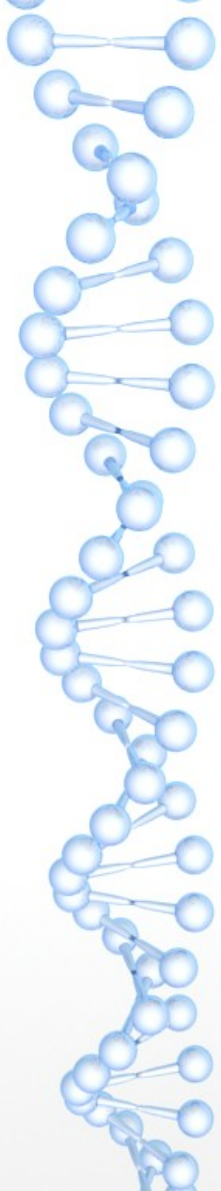
install@ACDLABS-PC

Please choose an NMR Administration Password
(requested for commands like 'cf', 'expinstall' etc.)

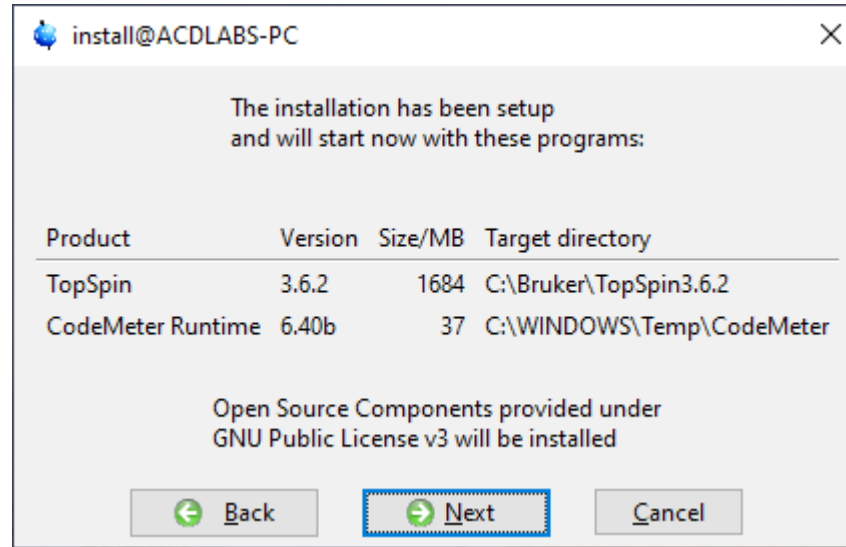
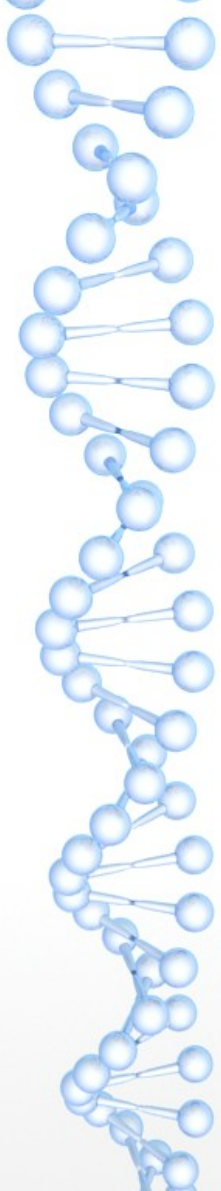
Enter password:

Re-enter password:

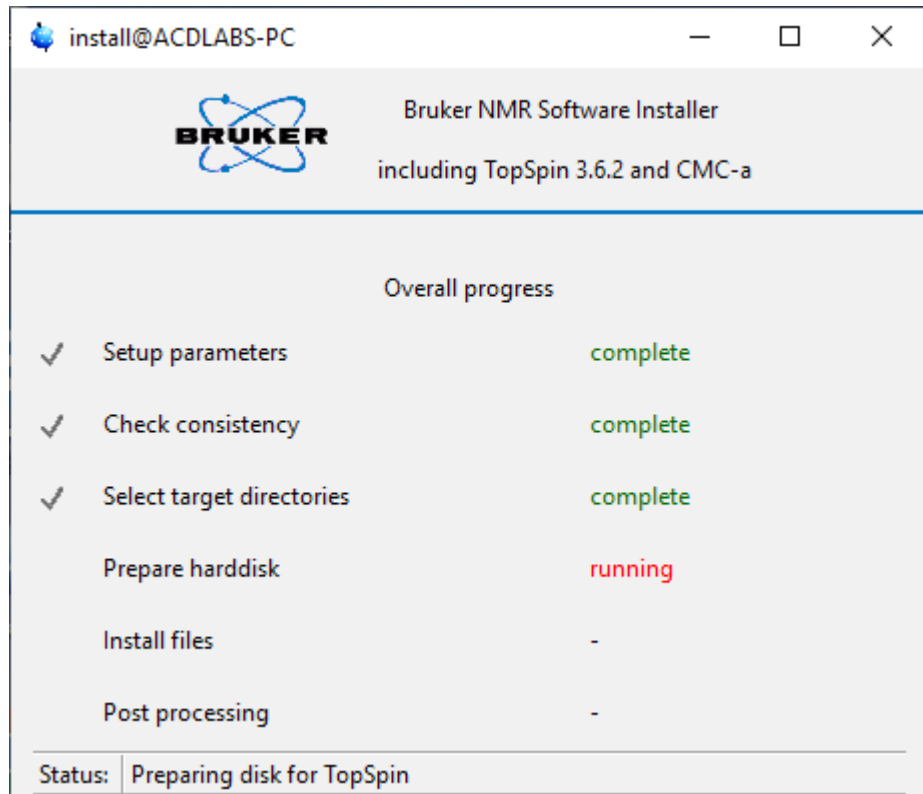
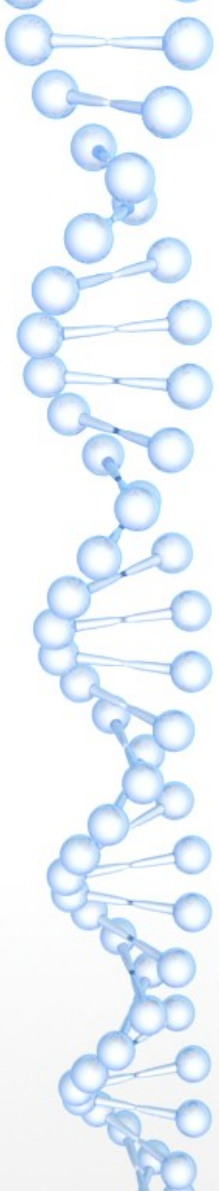
You will need to set a password for programme administration.
Note that this is asking for you to choose a password, not asking for an existing password!



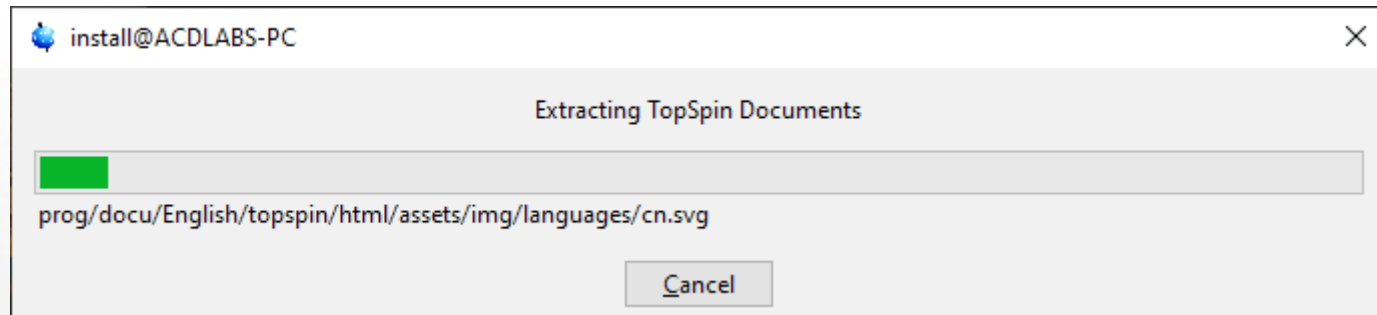
Let the installer configure the Windows firewall for you.

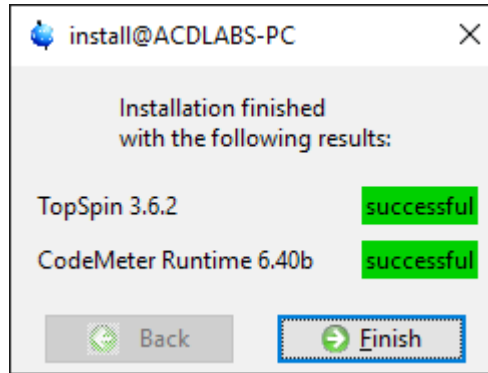
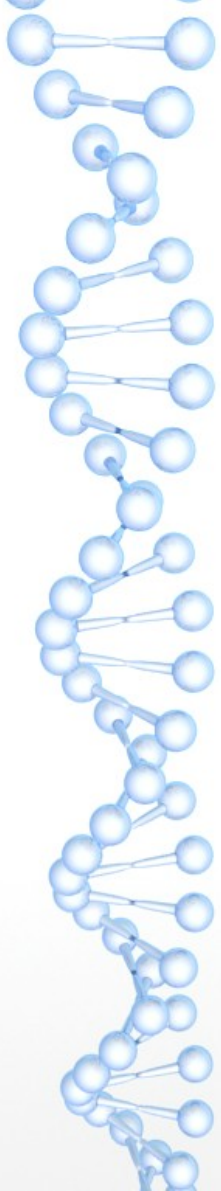


When you choose next, TopSpin will be installed.

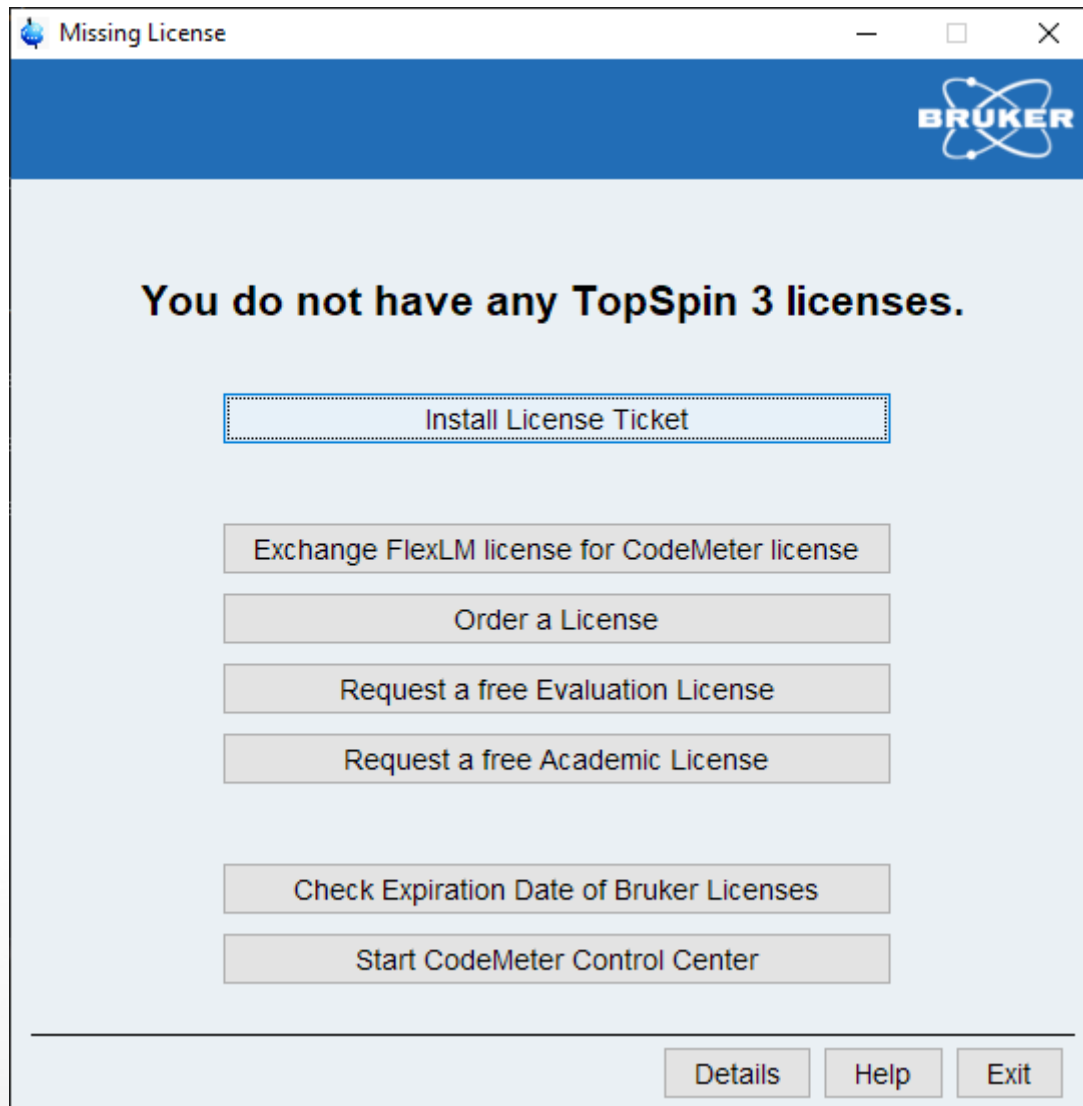
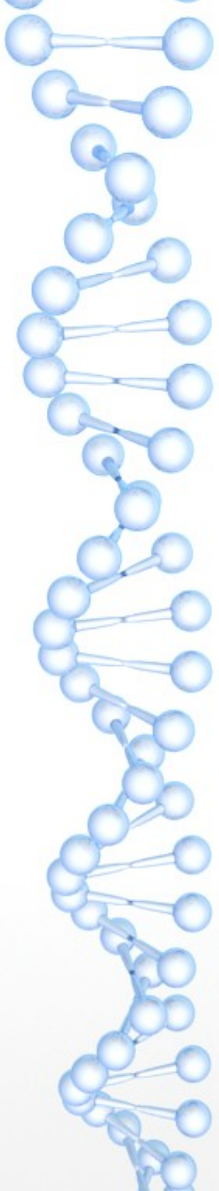


The installation will take a long time, typically about 15 minutes. Various progress bars will appear as the components are un-packed on to your computer.

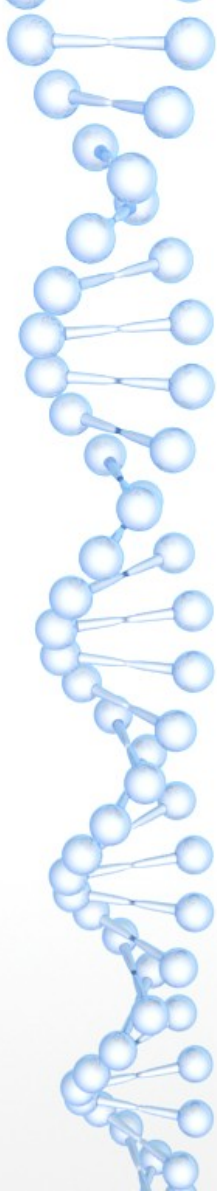




When finished, you should see the results. If anything fails you may have problems later when you try to use the program. An installation logfile is created, so you can try and find out why something failed. You should now find TopSpin as an option on the Start menu.



The first time you run the program you will get this window. Choose the option to request a free academic licence. This should take you to the Bruker website.



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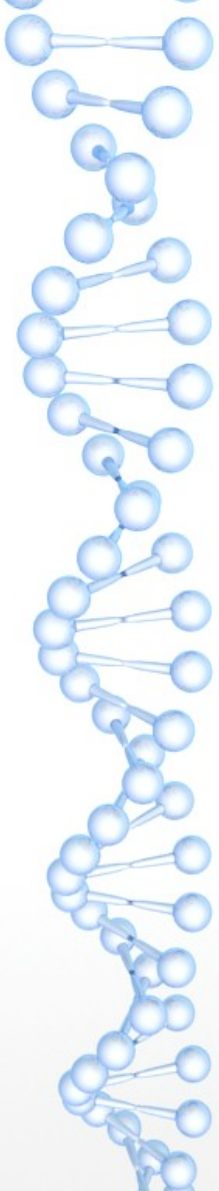
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NMR TopSpin License Processing for Academia

In order to provide students, researchers and teachers with unlimited access to the best tools for off-line NMR processing, Bruker is making their market leading NMR processing software TopSpin available free of charge for all academic users. In addition to Bruker NMR data, the software is able to process data acquired on Agilent, Varian and Jeol systems, as well as read any data provided in JCAMP format. We are happy to offer you a free Academia license for **TopSpin 4** and **TopSpin 3.6** ("Academia license").

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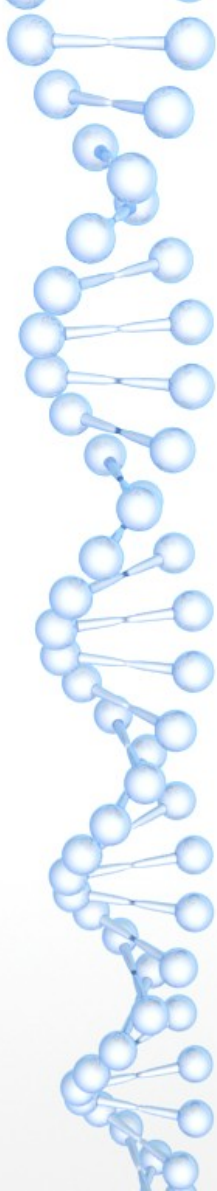
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Free License For Academia

With the following code you can activate your free academia license:

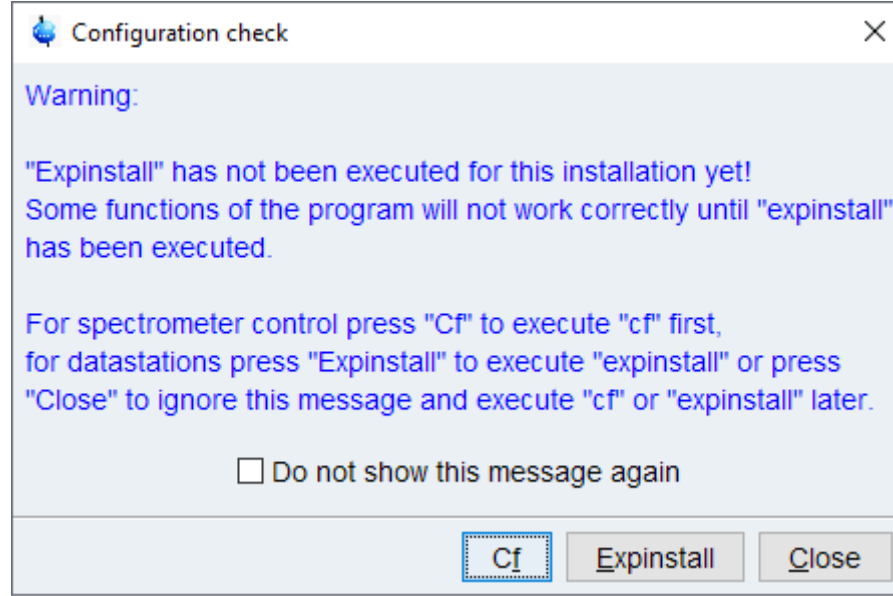
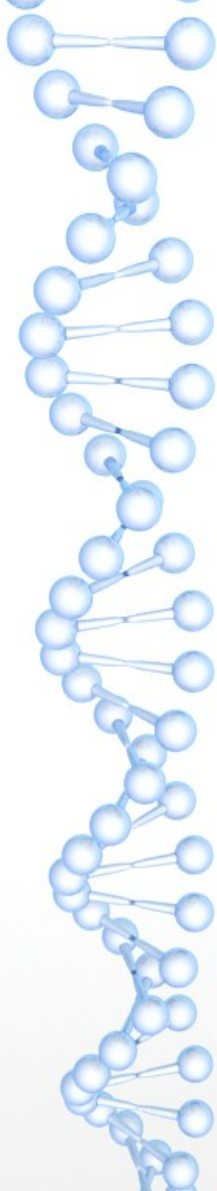
KTGNM-KZXUF-2X3HC-ZVPUG [REDACTED]

Just write it down (or copy it to the clipboard), start TopSpin, choose the option "Activate this installation now" and follow the instructions. If you have not installed TopSpin already you can download it [here](#).

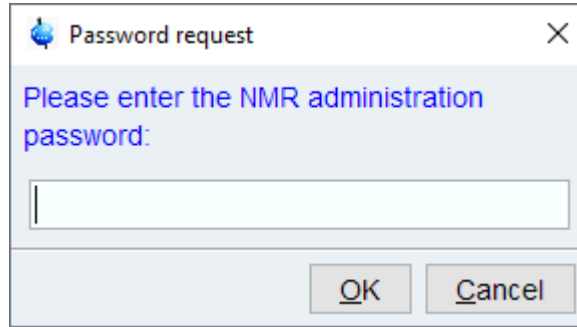
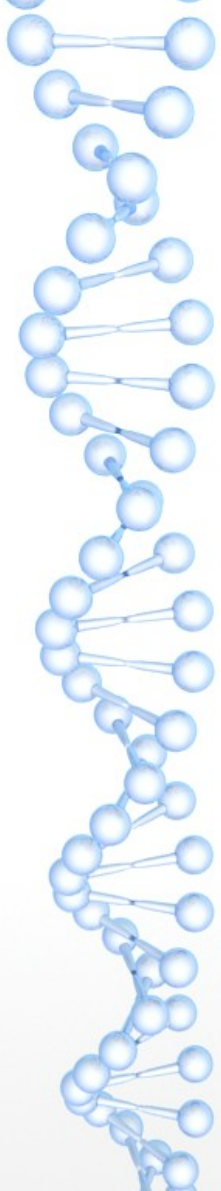
Your license is valid for 15 years. You can use it on a compatible computer of your choice and you can move it to another system if needed. See the section "Rehosting of license" in the license management manual for details.

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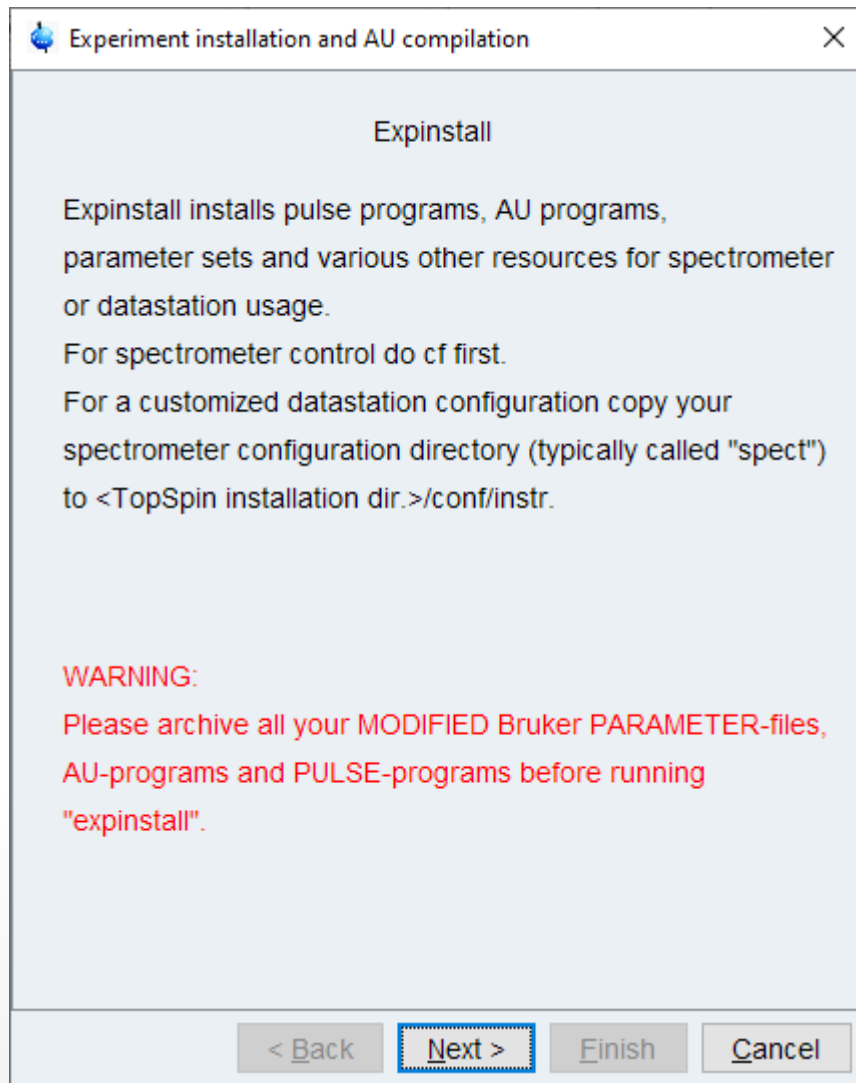
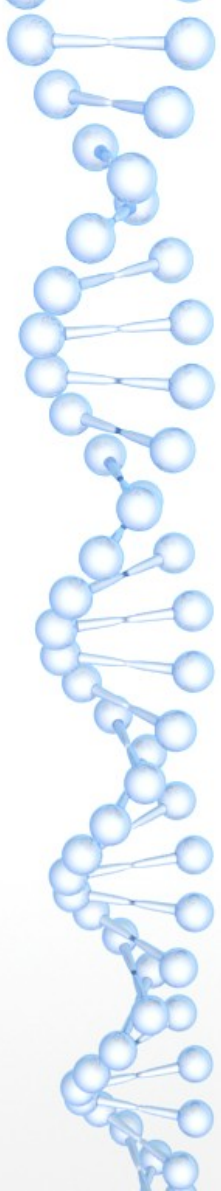
As the instructions say, you can either write down the activation code, or copy it (CTRL-C) and then paste it into TopSpin (CTRL-V) The option is "Install License Ticket" which will open a Browser window. You must use either Internet Explorer or Firefox! Not Edge/Chrome.



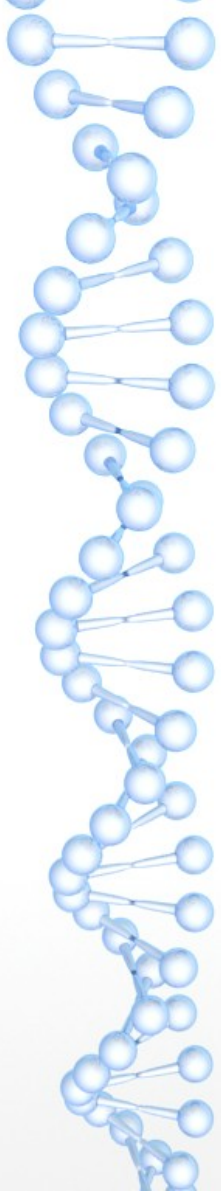
Topspin will now run, and the first thing it will do is request that you configure the program. If you skip this step then lots of things wont work... so don't omit it. You do not need the "Cf" command (which is for running spectrometers) you need the "Expinstall" option which will configure your computer as a datastation.



You will be asked for the administrator password that you set earlier.



Choose Next.



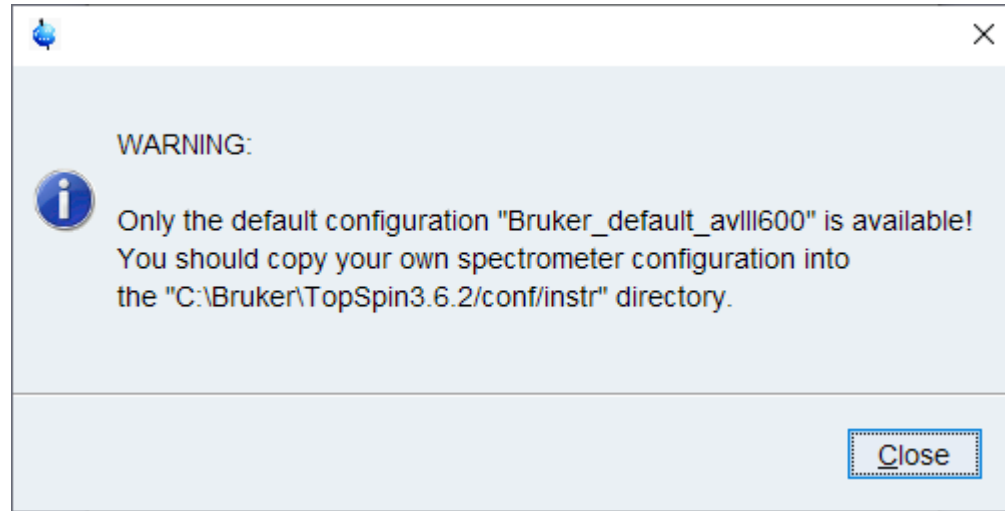
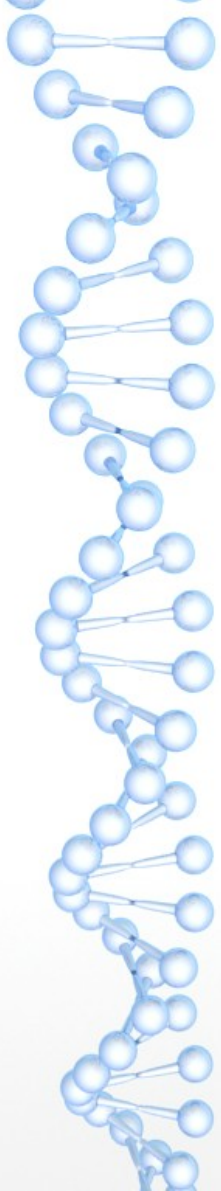
Expinstall for Spectrometer

Select the type of acquisition:

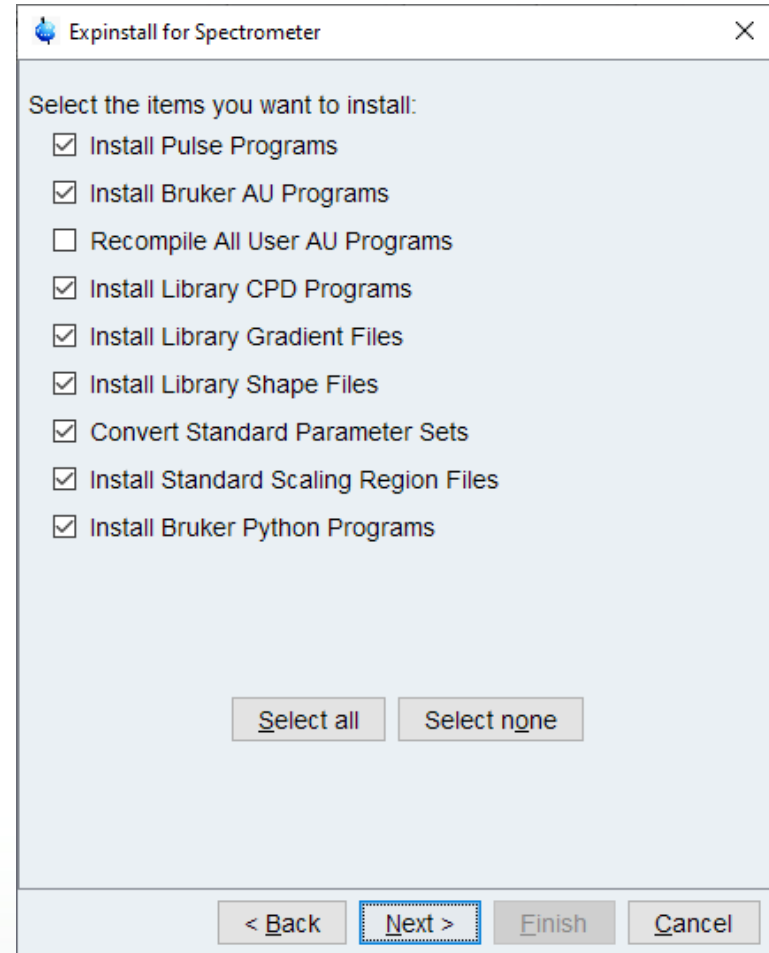
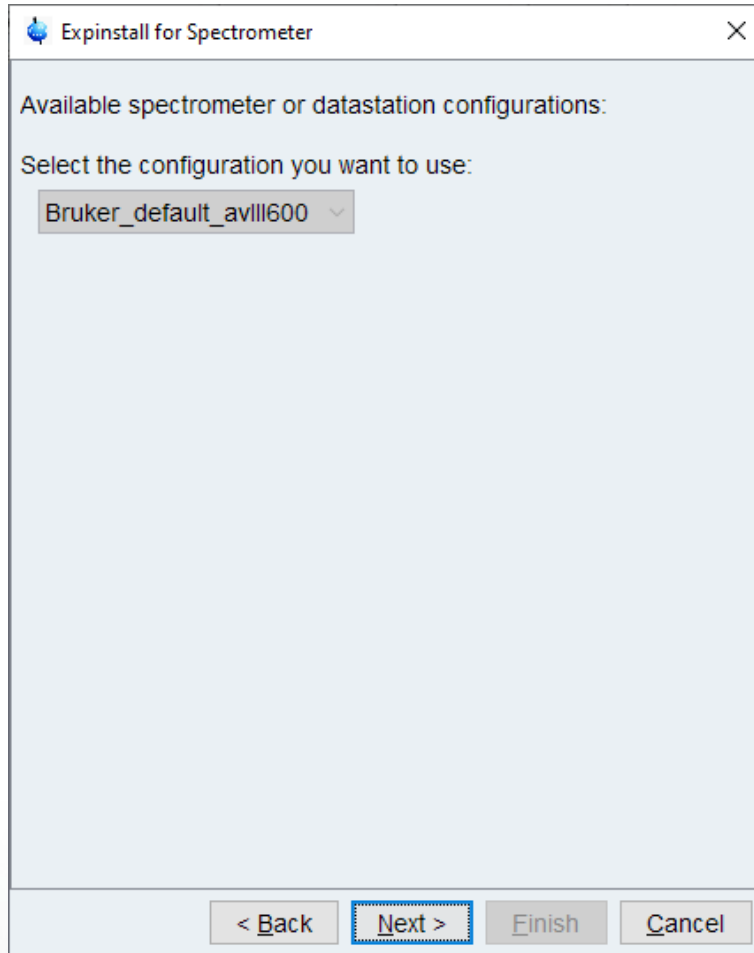
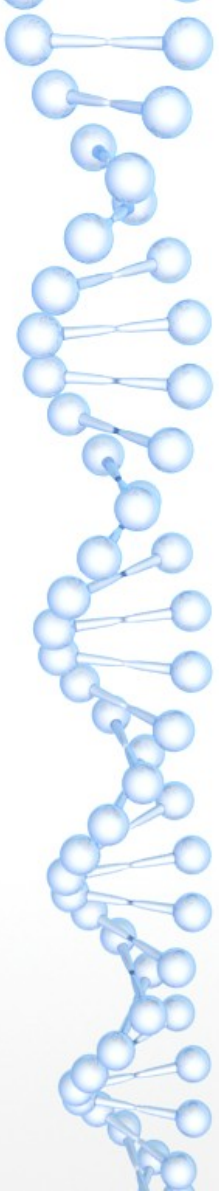
- High Resolution Systems
- Solid State Systems
- Micro-Imaging and Diffusion Systems

< Back Next > Finish Cancel

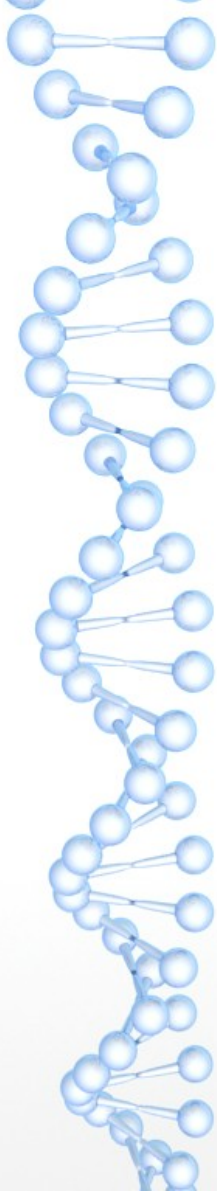
The default option (for high resolution systems is fine.



The default configuration “Bruker_default_avIII600” is also fine.



Choose next (with default options) for both these dialogue windows.



Expinstall for Spectrometer

Select the basic frequency of your spectrometer:

Basic frequency (MHz):

Select the pre-scan-delay DE:

Default pre-scan-delay (μ s):

Select the plotter paper format:

Paper format:

< Back Next > Finish Cancel

Expinstall for Spectrometer

Expinstall will be executed with following options:

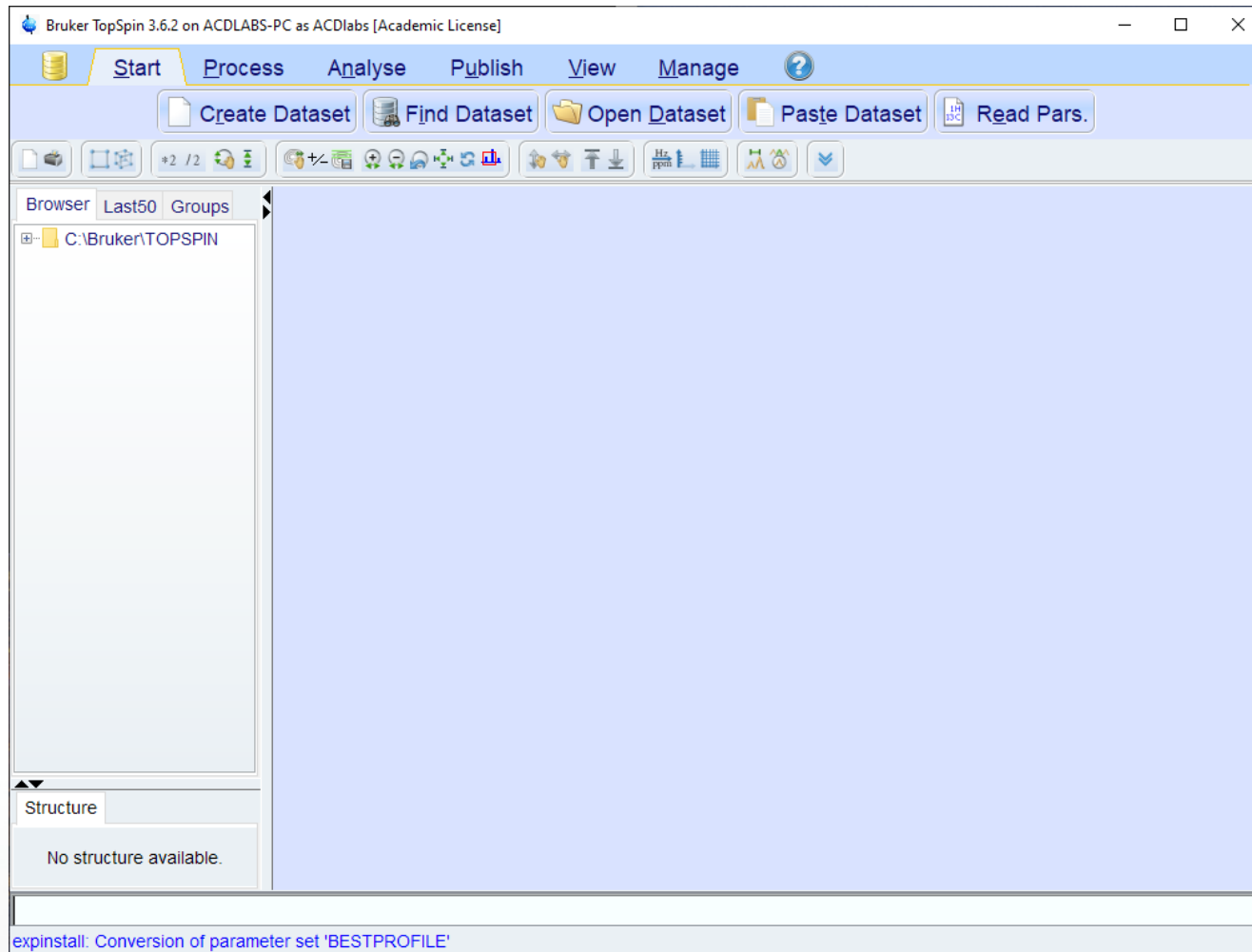
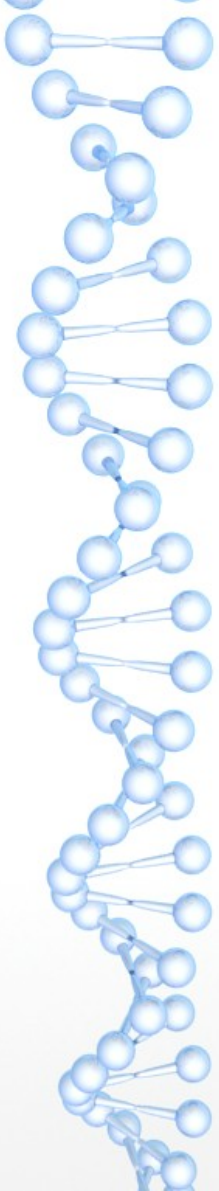
Installation for Spectrometer
(High Resolution)
Configuration name: Bruker_default_avlll600

Install Pulse Programs
Install Bruker AU Programs
Install Library CPD Programs
Install Library Gradient Files
Install Library Shape Files
Convert Standard Parameter Sets
Install Standard Scaling Region Files
Install Bruker Python Programs

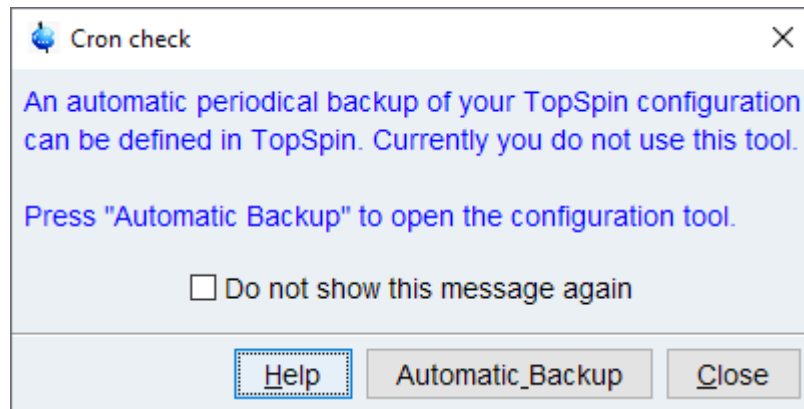
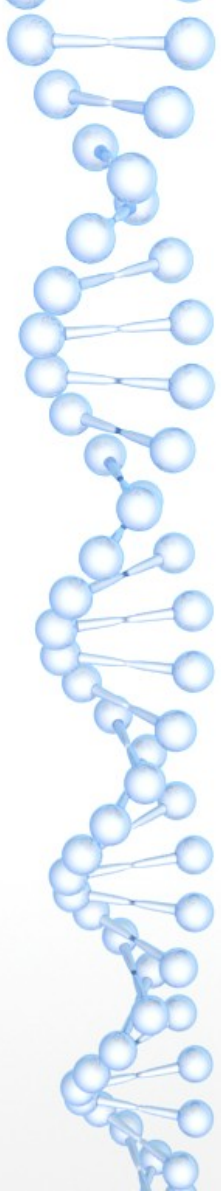
Basic frequency: 400.23 MHz
Pre-scan-delay: 6.5 μ s
Paperformat: A4 / Letter

< Back Next > Finish Cancel

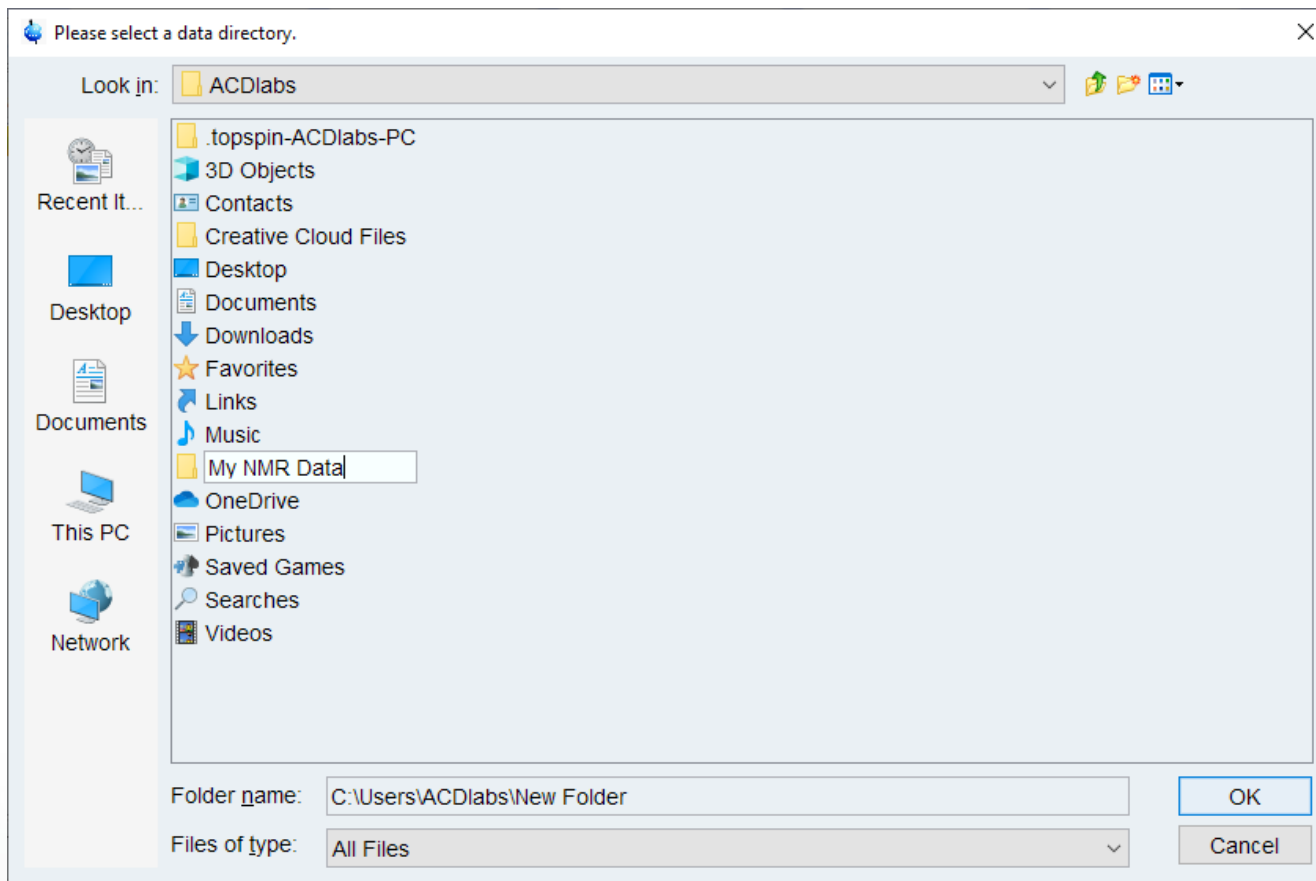
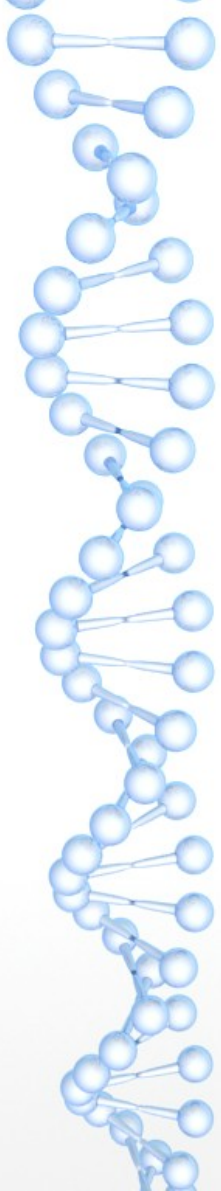
The Basic frequency for our 400 MHz spectrometers is 400.23.



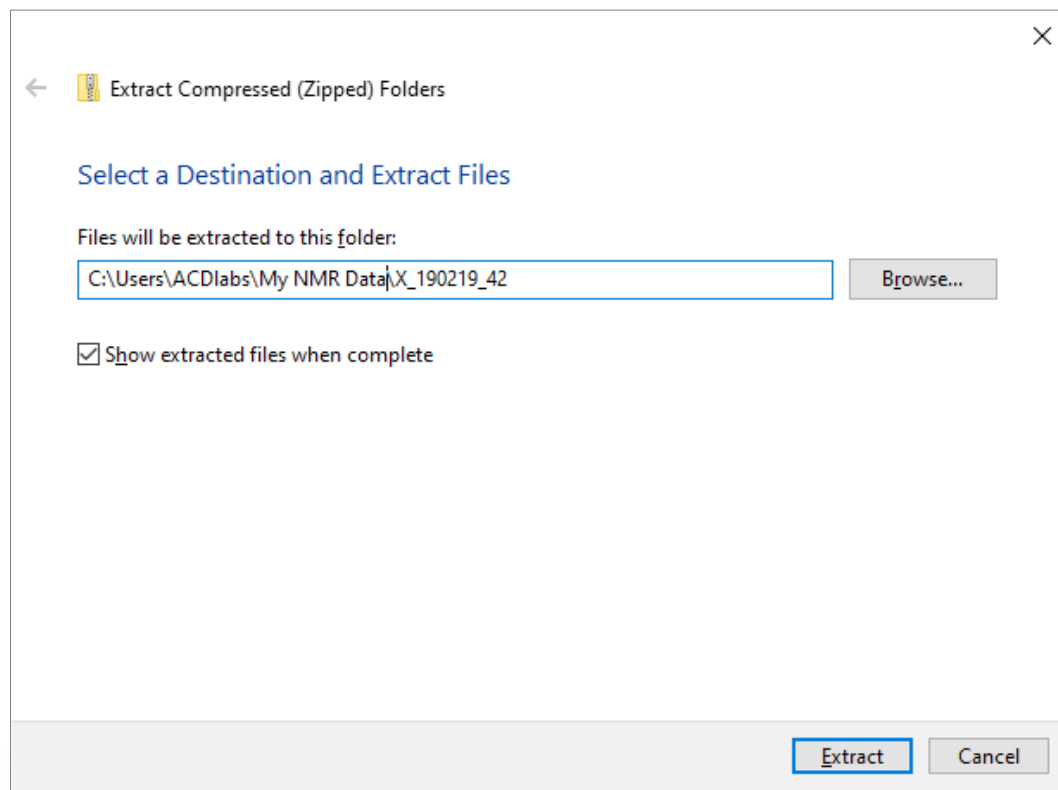
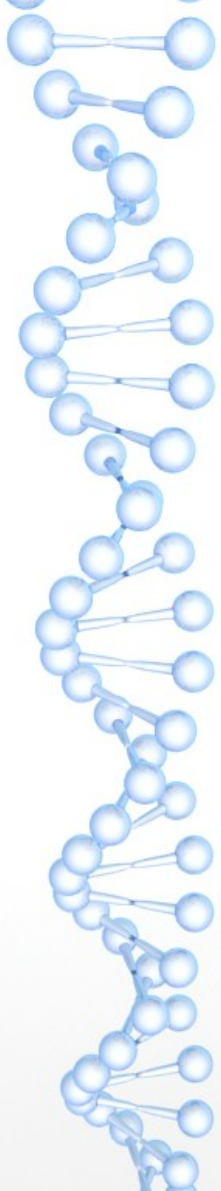
Do not quit the program until “Expinstall has finished (a few minutes).



You will see this message when Expinstall finishes, choose "Close".



If you right-click on the Browser window in Topspin you will get the Option to permanently add the folder for your NMR spectra.



When you download zipped data from the NMR website you can then Extract it (right click on the downloaded file in Explorer) into your NMR folder.