

Installation Guide For Bruker's Topspin 4.x

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This document attempts to guide the user through the intricacies and options of installing Topspin software. This is a work in progress; please let me know if you have any additions or corrections to make.

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The latest version of Topspin, version 4 has been released under a 'free for academic use license' and so the department no longer issues licenses; they are issued directly from Bruker.

There are various packages that not only process your data, but can do some quite in-depth analysis; including structure verification and elucidation. (With the addition of additional purchasable modules)

It is now available for Microsoft Windows (version 7 and above), Linux (Centos5) and Apple OS X (Intel based)¹ platforms. In the past year it has become free for academic use; this version has (*almost*) all the functionality of the commercial version.

¹ On Apple Mac's only Intel Core Two Duo chips are supported; the older (around 2007) Intel Core Two chips are not supported. As long as your computer isn't more than 8 or so years old; it should run.

Preparation

Before Installation

YOU WILL NEED TO REGISTER WITH BRUKER,²; fire up a web-browser and go to:-

² Previously Bruker used the 'Flexlm software to manage licenses; this has switched to software from 'CodeMeter.'

<https://www.bruker.com>

click 'login' and 'register'; then jump through all the hoops to create an account.

Once registered go to :-

<https://www.bruker.com/service/support-upgrades/software-downloads/nmr.html>

³ In the past there was a bug with certain web-browsers (Chrome and Edge) regarding the license activation through Topspin. If it doesn't work, the suggested fix is to use Firefox or Safari. Paste the url given into the new browser.

The click 'Free Academia License' and then 'Request personal license ticket now'.³

You do not need to download the software from Bruker. ⁴

⁴ If you have a departmental IP address you can access the server. If you configure access to the departmental VPN, you can gain access from anywhere in the world; this is my preferred method.

As long as you get access to the NMR backup server, 'nmr-fs'.

Obtaining The Software

In order that the bandwidth of the department is conserved (which does cost a reasonable amount per gigabyte), I've downloaded installation packages onto our backup server. You can find them in the location :-

```
\\nmr-fs.ch.private.cam.ac.uk\software\Topspin
```

To access the server, follow the instructions on :-

<https://www.ch.cam.ac.uk/analytical/nmr/data-backup-and-access>

COPY THE RELEVANT FILE TO YOUR COMPUTER. There is also an 'iso' file which provides a complete image of the installation DVD, which serves all platforms. You will need to read the manual of your DVD burning software to correctly write this to a disc. Just simply copying the file will not work. Or you can install software that will allow you to 'mount' the ISO file to your computer; it will appear like a disk drive and you can install the software from there.

Installation

General

Topspin comes with a 'super-user' account to administer topspin, this will default to the account you are logged into.

This is one of Topspins little quirks; it has its own security system to prevent tampering with the software; so it creates its own passwords that are separate from the operating system. The password you type here *doesn't have to be the same as your login password and probably shouldn't be, as the password is stored in a file on the disk and could be hackable.* Figure 1

Windows

Before you begin; you should log in to your system with an account that has administrator privileges. Double click on the .exe you downloaded above and follow the instructions to install the software. You will have to click through some issues related to the security of your system, before you can install the software.

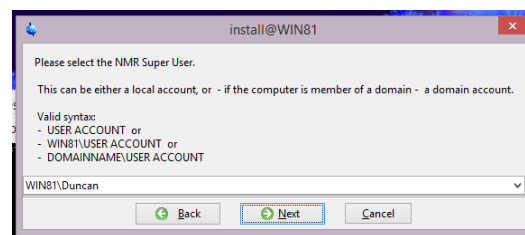


Figure 1: Topspin 'Super-User'

The installation will also pause to display a release letter and it may not continue until you close it!

You can chose to change the location of the installation if you wish; but unless you have good reason; its probably best to stick with the default. *Figure 2*

When asked, unless you have good reason choose the 'Data Processing' only option. (It is possible to change the install location, trim the size of the installation, or install a few extras by choosing customise, but unless you are certain of your needs, its best to go with processing only.) *Figure 3*

Mostly it is just a question of accepting the default options.

The installation will ask you if you wish the windows firewall to be configured. *Figure 4*

Unless you are familiar with how to administer the firewall and are prepared to spend some time doing it yourself; say yes here! If you mistakenly say 'no' my advice is to abort the install and start again. . .

Reboot your computer and test whether the software starts. Once it does, please now go to the section *First Use*

Mac OS X

Double click the mac-topspin.dmg to mount the installation image; then double-click the 'TopSpin 4.x.y.pkg' file to start the installation process.

Click continue until you get to the installation type. Here you can customise the type of installation if you wish; although there is actually little reason to do so. You can only really choose to not install a C complier and CMC Assist. There's no option to change the install location either, the software is put in /opt/topspin4.x.y⁵

Just click through the options.

The main problems occur with the security settings on OS X 'Catalina'. Bruker is not on the the 'approved' list of developers, and so the default security settings will prevent the installer running. To get around this problem, type 'Security' into the spotlight search, select 'Security and Privacy', go to the 'General' tab and allow the software to install.

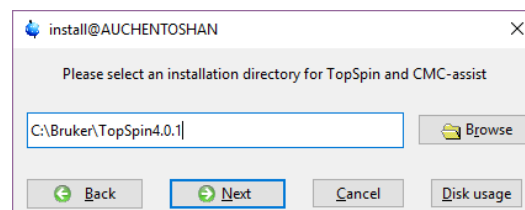


Figure 2: Install location

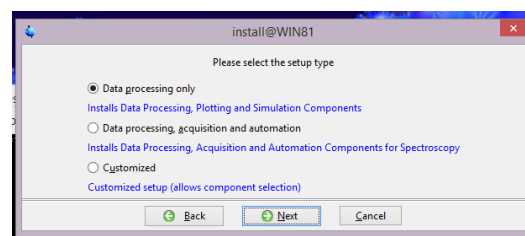


Figure 3: Customise Install

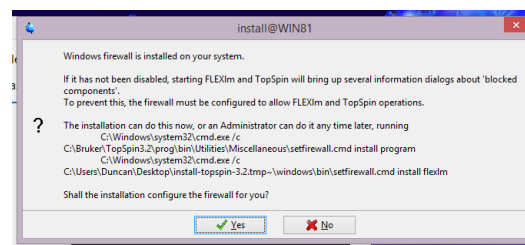


Figure 4: Configure firewall

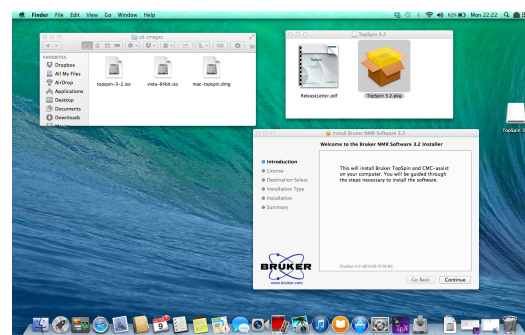


Figure 5: OS X install screen

⁵ This directory is hidden by default and you may not be able to browse to it. So in the finder window click 'Go' and 'Go To Folder' and type in /opt

Reboot your computer and check Topspin starts. Once it does, please now go to the section *First Use*.

Linux CentOS Installation

It is important that you install Topspin onto the correct Linux distribution; the supported versions are CentOS 7 and 5. Topspin is now a 64bit application, so you should install that version of linux. The CodeMeter software requires a linux distribution that supports 'RPM' packages. You can download it from the following location.

<http://mirror.centos.org/centos-7/7/isos/>

If you are determined to install it under your own non-supported distribution of Linux; I'd suggest installing into a virtual machine, you may have to fix a lot of dependencies, which might affect your standard operation. . . I've tried installing Topspin on various client OS virtual machines running under Open SUSE and OS X. ⁶

⁶ I used Oracle VirtualBox in all instances.

As to install, for the most part its just simply clicking through the default options; you can change the install location, and the customise the components you install; but I would recommend sticking with the defaults.

Reboot your computer and test whether the software starts. Once it does, please now go to the section *First Use*

First Use

The first time you start the software you'll need to register it. You can paste in the license code you received above; or request a new one. As of December 2017 there is still a bug when activating the it using Microsoft edge or Google Chrome. If it doesn't work, install Firefox, go through the process again and paste the URL from Edge or Firefox into Safari.

One it actually starts; there will be the usual license agreement you will need to click 'Ok' to.⁷

The software will now present you will the dialog box shown in *Figure 6* .

It prompts you do something called 'expinstall' and 'cf'. Its a good idea to do this, as some our automated processing requires it to work. 'Expinstall' sets up some standard parameter sets, automation programs and plot layout files for use with Topspin; 'cf' can configure a virtual spectrometer use by the simulation programs within the software. Its not strictly necessary to do a 'cf' to use the software, but I generally do; just in case.

Configuration-'cf'

Choose cf, then from the choose Avance 600 MHz (which is of a data station type) and click 'Edit' at the bottom of the window. You will now be shown a sequence of screens detailing information about this configuration mostly its just a question of finding the default 'Next' button to click.

The first screen has a short summary of the configuration; you can make changes here; but it probably isn't necessary. Click next to continue.

You will then be shown a slightly intimidating routing diagram; just click 'save and close. Next there's a summary of the hardware and software configured, just click 'Next' again.

The 'cf' configuration is now finished; you can now run through the 'expinstall' routine by clicking the button. You don't need to bother with the other options; 'edscon' and so forth.

⁷ This will actually keep appearing each time you start the software unless you click the 'Do not display' checkbox.

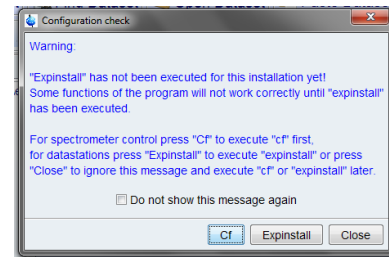


Figure 6: Expinstall

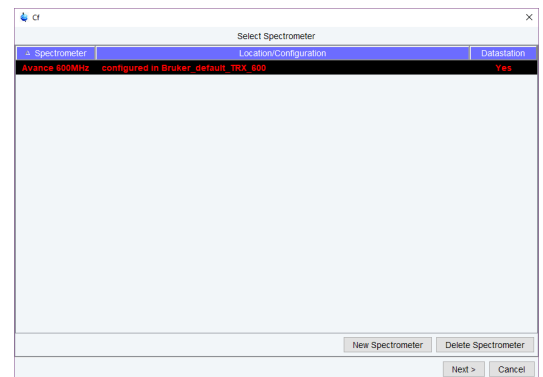


Figure 7: cf stage 1

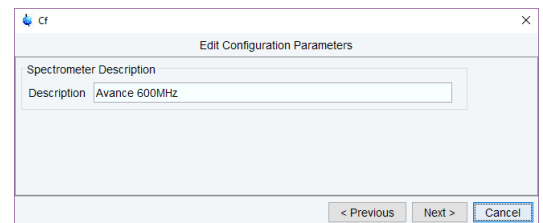


Figure 8: CF stage 2

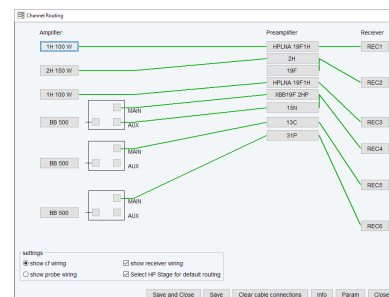


Figure 9: CF routing

Configuration 'expinstall'

Next you need to run through the 'expinstall' routine; *Figure 10* .

You probably came to this point by clicking a button; if you have no button to click, you can type `expinstall` at Topspin's command line.

Again its mostly just a matter of clicking 'Next' to go through each step. Note, you can run the command multiple times to install all the different types of acquisition.

Accept the default options of what to install.

Choose the paper format; I tend to choose A3 as that's what we use in our service layouts. The software will prepare the installation default layouts accordingly.

Click 'Finish'. It will take a bit of time to copy all the standard parameter sets, 'au' programs etc.

The last window of the routine prompts you to schedule a backup of the Topspin installation. This will be useful if you spend a lot of time getting your layouts and parameter sets just the way you like. You can safely ignore the option and click 'close'. Backups can be manually triggered by typing `nmr_save` at Topspin's command line.

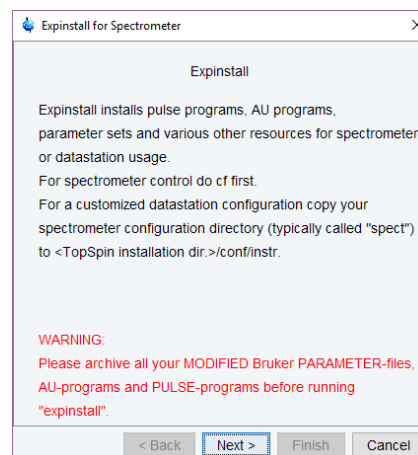


Figure 10: Experiment Installation

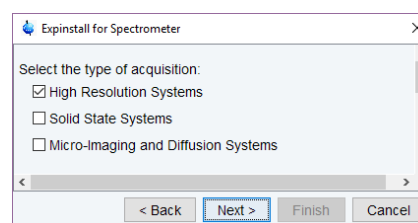


Figure 11: Expinstall Type

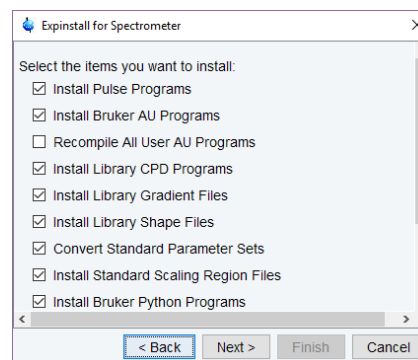


Figure 12: Expinstall options

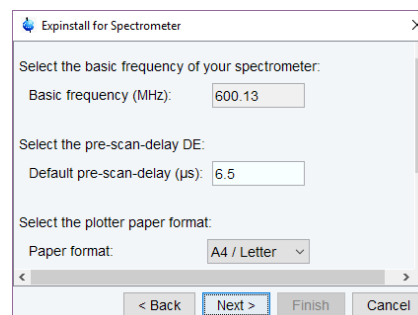


Figure 13: Expinstall Format

Advanced Installation

Installation to a virtual machine

I have installed Topspin to Windows and Linux virtual machines running under Windows, Linux and OS X operating systems using Oracle's 'Virtualbox' software. It works very nicely; as long as your computer has enough RAM installed. As the virtual machine is portable;⁸it makes it possible to transfer your working environment between computers if you wish.

⁸ I have a Centos one that takes up less than 32GB of space; enough to fit on a USB stick

Installing service plot layouts and au programs

We have a number of layouts and au programs to automate your work flow; to install them follow the instructions below.

These will periodically be updated; so please occasionally check back. Also there is no guarantee that they will work flawlessly with your data; always work with a copy of important data as we accept to liability of loss from using these programs. Any bugs or requests for features; please contact djh35@cam.ac.uk.

Install plot layouts

Copy all the layouts beginning with 'service' from :-

```
\\nmr-fs.ch.private.cam.ac.uk\software\service-plot
```

To :-

```
$TOPSPINHOME$/plot/layouts/
```

Where \$TOPSPINHOME\$ is :-

```
c:\Bruker\Topspin4.x.y on a Windows PC and
```

```
/opt/topspin4.x.y on OS X or Linux.
```

Install "au" programs

Copy all the files beginning with 'serv' from :-

```
\\nmr-fs.ch.private.cam.ac.uk\software\service-au
```

To :-

```
$TOPSPINHOME$/exp/stan/nmr/au/src/user/
```

Using the 'au' programs

Typing the name of the 'au' program will run it.

Try the `service-master-proc`⁹ first. It will examine the experiments in your data set and process them one-by-one.

⁹ It calls different sub-au programs to process each different type of experiment

It will also load a defined layout and create a pdf in the `/pdata/1` directory.

`service-def-proc` will process the experiment number you're currently in.

`service_nohump` does a baseline correction on multiply regions; defined by the argument passed to it. So `service_nohump 17` will split the spectrum into 17 sections; performing a baseline correction on each. Useful for carbon spectra.

Troubleshooting

This is an ongoing work-in-progress section; as problems are found and fixed; I'll add the to the document.

Won't Start

Most of the problems I've found stem from the Virus checkers on computers. The way Topspin works is the buttons and commands you type issues commands via an internal network to little server programs running behind the scenes. . . This can make virus checkers/firewalls twitchy and cause them to disable/remove parts of Topspin. Each virus scanner will be different, but I'd recommend allowing an exception rule to prevent scanning of the entire Topspin directory.

Let me know any problems you have however!

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