Nuclear Magnetic Resonance Research Resource

Installing Free TopSpin 4 for Processing

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Bruker currently offers free processing TopSpin licenses to academic, governmental, and non-profit institutions[1]. Qualified users can download the free version of TopSpin and obtain the necessary license directly from the Bruker website. The purpose of this document is to help NMR[3] users navigate this process. At the time of this writing, the NMR[3] facility is still using the free version TopSpin 3.5 patchlevel 7. This version is set to expire March 31, 2019 at which point the facility will move to the most recent version of free TopSpin; TopSpin 4 (available for a period of 15 years). For this reason, the details of this document as well as included pictures refer to a TopSpin 4.0.5 installation.

Preliminary Note: Hardware and Software Requirements

Before installing free TopSpin 4 (TS4), please ensure your computer meets or exceeds the requirements recommended by Bruker. Bruker recommends a state-of-the-art PC computer or a MacBook, iMac or MacMini capable of executing 64-bit instructions. In addition, the following operating systems are supported:

- Windows 10 or 7
- CentOS 7 (minimum required version is 7.1)
- Apple macOS X 10.12 or higher

No additional software is required in order to run TS4. However, to view documents and manuals that come with the package, a PDF viewer is required.

Step 1: Pre-Installation Tasks

- Registration: You must register with Bruker in order to obtain a free academic license. If you do not have an account, create one by going to bruker.com, clicking on "Login", and then "Register for an Account". Provide the required information and then select "Register".
- Obtain the Software: Although you can download the software via the Bruker website[2], perhaps a simpler solution (and quicker) is to get your copy directly from the NMR[3] facility. Copies of the TS4 installation packages are available on the data server in the folder /Documents/nmrdata/Free TopSpin[3]. Simply bring a USB drive and copy the relevant package. Note that the total space required on your flash drive is ~ 1.5 GB for the Windows & Linux packages and ~ 750 MB for the Mac OS version.
- Obtain a License: Visit www.bruker.com/freetopspin and login. Click on "Request Personal License Ticket Now". On the next page you will be provided with a code which will allow you to activate your free academia license. Write it down, take a

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[1] NMR[3] used to provide and manage several processing licenses for TopSpin (and prior to that XWIN) for its user base. That slowly started to change ~2010 when Bruker announced an inexpensive 3-year license for academics with the launch of TopSpin 3.0. Many NMR[3] researchers began to purchase their own license. In 2016 with TopSpin 3.5, Bruker announced that the student & academic license was free.

[2] To download, visit: www.bruker.com/freetopspin, login and then click on the relevant download link.

[3] Also available is an ISO file which contains an image of the Bruker installation DVD.

picture or copy it to the clipboard for later use.

Step 2: Installing TopSpin

Windows

Before installing, ensure you are logged into your Windows system as Administrator or in an account with administrator privileges. Close all open windows. Launch the windows version of the installation package (windows-topspin4.0.5.exe). Once you see the Welcome window shown in **Fig 1,** perform the following steps:

- The Welcome screen lists the main programs that are part of the software distribution. Click →Next to continue with the install.
- A window entitled "Selection of Components to Install" appears. Accept the defaults and click → Next.
- Click → Next to confirm you have read the TopSpin release letter.
- Choose the destination directory for TS4 (see **Fig 2**). It is advised to simply use the default C:\Bruker\Topspin4.0.5 and click → Next (followed by selecting Yes to create the folder). If you have an older version of TS installed, please do not use the same directory for the installation of TS4!
- A window "Please select the setup type" opens. Go with the default option Data Processing Only and click → Next.
- A window entitled "Please Select the NMR Super User[4]" will appear as shown in **Fig 3**. The default will be the current account but an existing user or a specially created user like nmrsu can be used. In any event, if you change the default, what you use must be the name of an existing Windows login. Click → Next.
- Next (see **Fig 4**) you will be prompted for the NMR Administration Password[5]. This password is required for TS4 commands that make configuration changes to the installation. Enter the password (twice) and click →Next.
- Accept the default directory for NMR-Data and click → Next (followed by selecting Yes to create the folder).
- A window opens asking if the installation should automatically configure the Windows system firewall for you. Please select yes and click → Next.
- You are prompted to start the installation of the listed programs (see **Fig 5**); click → Next. Note that even though NMR-Sim and NMR-GUIDE are not specifically listed, you get these automatically with TS4 along with the TopSpin plot editor. Now consider getting a coffee…the installation takes on the order of 15-20 minutes.
- The final dialogue window states, "installation finished with the following results:" Successful should be highlighted in green beside each component. Click → Finish.
- You are advised to reboot your computer before proceeding to run the software. I had problems viewing pdf documents on my Windows system after installing but before rebooting.

macOS

To launch the installation on a MAC, double-click on the .dmg file to mount the installation image. When opened for the first time, the checksum verification will start, and you should allow it to complete. Once finished, a Finder will be displayed with the release letter and the install .pkg file. Double click on the .pkg file. If it cannot be opened due to it being flagged as from an unidentified developer, go to System
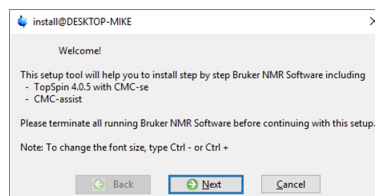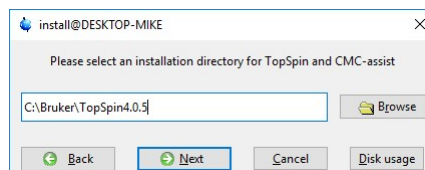

Fig 1: Welcome Screen
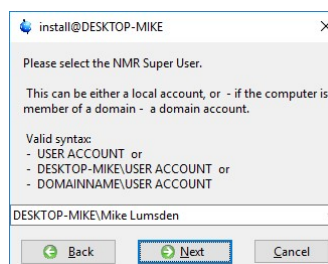

Fig 2: Location for the TopSpin Installation

Fig 3: Select the NMR Superuser

[4] The NMR Super User account need not have administrative privileges. After the installation, this account is the owner of all TS files. Logging into Windows as this user allows you to remove these TS files, change permissions, etc.
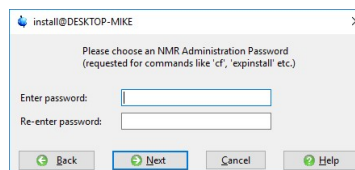

Fig 4: Select the TopSpin Administrative Password

[5] Note that this password does not need to be the same password associated with the current Windows login or Super User accounts. It is strictly a TS internal password which permits execution of configuration type commands such as cf or expinstall.
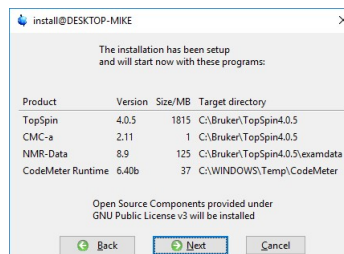

Fig 5: Programs to be Installed with Default Installation

Preferences → Security & Privacy and in the General tab in the "Allow apps downloaded from:" section, click "Open Anyway". Then proceed as follows:

- On the Welcome screen, click Continue
- Agree to the terms of the license agreement.
- There is no option to change the installation location; the software always resides in /opt/topspin4.x.y
- On the Installation Type screen, click Install.
- You will be prompted to enter a User Name and Password of a user with administration rights in order to proceed. Provide the input and select Install Software.
- Enter an NMR Admin password (twice).
- If the CodeMeter licensing package is not present, you will be prompted to install it. If you get a notice of a system extension blocked and signed by "WIBU-SYSTEMS AG", again go to your security and privacy settings to allow it.
- On the Summary Screen stating the installation was successful, click Restart.
- Once the system reboots, click Close to complete the installation.

Step 3: License Activation

Launch TS by double-clicking the shortcut on the desktop. A start window opens with details about the TopSpin version, installation directory and licensing. Since a valid license is not yet known to TopSpin, you will eventually see a dialogue window as shown in **Fig 6**. Proceed as follows:

- Select the option "Install License Ticket"[6]
- A web browser opens, and you should see "Welcome to CodeMeter License Central WebDepot". Enter the ticket number you obtained back in Step 1 in the Ticket field and click Next.
- The next screen shows "My Licenses" and should specify TopSpin4 Processing Only (academia license). Click Activate Licenses.
- On the next screen you select the "binding" for your license. Please choose the option on the right and bind to your computer (CmActLicense).
- The final screen before starting the activation shows the available license with a checkmark (TopSpin4 Processing Only) along with the CMContainer (do not change this). Click Activate Selected Licenses Now.
- Once activation is complete, you should see the Window shown in **Fig 7**. Click OK.

Step 4: First Use

Open TopSpin again. This time in the start window, upon reaching the licensing stage, below the line "waiting for codemeter license" you should see "valid until 20xx-xx-xx" which is 15 years from the time you activated the license. Then the TS4 GUI should open and you should also see a license window open automatically. Click on "I Accept. Do Not Show License Again".

You will see a configuration check window open as shown in **Fig 8**. It is from here you can launch the configuration routines cf and expinstall. Neither is strictly speaking necessary. The cf procedure would allow you to configure your installation to mimic one of the existing spectrometers at Dal but is not covered here. You are advised to execute expinstall as this will make available to you TopSpin parameter sets, pulse programs,
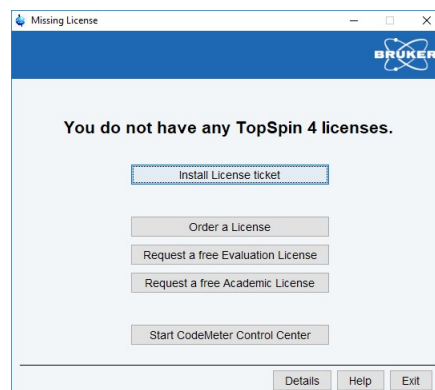

Fig 6: Dialogue Window to Start the License Activation

[6] Note that this is an online activation of your academic license and so internet connectivity is necessary.

[7] For decades, Bruker has used the license manager system flexlm. That changed with TopSpin version 3.6 in 2016 to the CodeMeter system. One of the nice new features is the ability to move your license to a different computer (re-hosting) without cost.
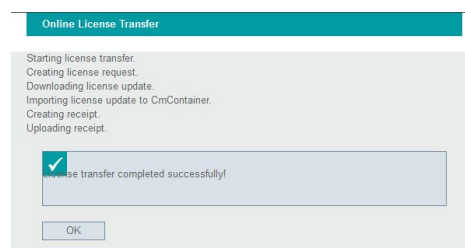

Fig 7: Window that Shows Successful Activation of License

Fig 8: Configuration Check Window

as well as automation programs (note that expinstall is normally invoked automatically on Macs). Proceed as follows:

- Click the check box "Do not show this message again" and then select expinstall.
- You will be prompted for the administration password you provided in Step 2 – Fig 4. Enter it here.
- An introductory "Expinstall" window opens. Click Next>
- Make sure "High Resolution Systems" is selected for the type of acquisition and click Next>.
- Close the warning window about only a default configuration available and click Next>
- Go with the defaults for the items you wish to install and click Next>.
- The next window is shown in **Fig 9**. Click Next>.
- Click Finish on the summary screen that opens which will start the expinstall procedure.
- At the end of the procedure, you will be prompted to setup an automatic backup of the TS installation. You can do this now or do it later via the command "NMR_Save". Expinstall is now complete.
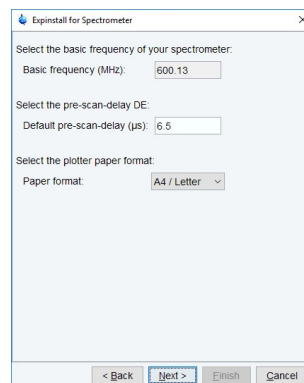

Fig 9

TS is now setup and configured and thus ready for NMR data processing.

Step 5: Organizing NMR Data on Your Disk

For those new to Bruker, please note that a Bruker NMR experiment does not consist of a single file. Instead, it exists as many files stored within a specific directory structure. This structure can be represented in one of two possible formats:

(1) <dir>/<name>/<expno>/<pdata>/<procnos>
(2) <dir>/data/<user>/nmr/<name>/<expno>/<pdata>/<procnos>

The part in blue is identical in both formats. The part in red will be addressed in Step 6. You must maintain one of these two directory structures for TS to open your data correctly and furthermore you must not use them interchangeably.

On a privately owned desktop or laptop, it is recommended to use format 1. For <dir>, create the folder c:\nmrdata. To further subdivide and organize (for example by project or spectrometer), create additional folders below c:\nmrdata. For example, to organize your data according to spectrometer, you would have to create the following two paths:

- c:\nmrdata\av300
- c:\nmrdata\av500

Format 2 offers a built-in organizational structure that could be used by multiple users who share a single computer, for example, or in ways mentioned above. To use this format to organize data according to spectrometer again, you would have to create the following two paths:

- c:\nmrdata\data\av300\nmr
- c:\nmrdata\data\av500\nmr

macOS
From a Finder window menu, choose Go → Home and then File → New Folder. Create the folder "nmrdata" and then proceed with either of the two formats outlined in the preceding section.

Step 6: Opening NMR Data in TS4

TS provides a "data browser" to facilitate finding and opening NMR data. It is located on the left-hand side of the main TS window. By default, you should see a data folder with example NMR data supplied by Bruker (<INSTALL DIRECTORY>/examdata). To add your individual folder(s), move your mouse into the browser, right click and select "Add New Data Dir…". What you specify and the result depends on whether you are using format 1 or 2 as explained in section 5:

- Format 1: specify everything before the part in blue. Shown in the top part of **Fig 10** is the browser after adding two different format 1 data directories: one for each of the AV300 and AV500 spectrometers. Clicking a + sign in this case expands the folder to show the individual experiment names.
- Format 2: the part shown in red is assumed to be present and thus must not be directly specified. Specify everything before the part in red (everything before "/data"). Shown in the bottom part of **Fig 10** is the browser after adding a single format 2 directory. Clicking a + sign in this case first displays the organizational folders (in this case spectrometer name) before drilling down further to see experiment names.
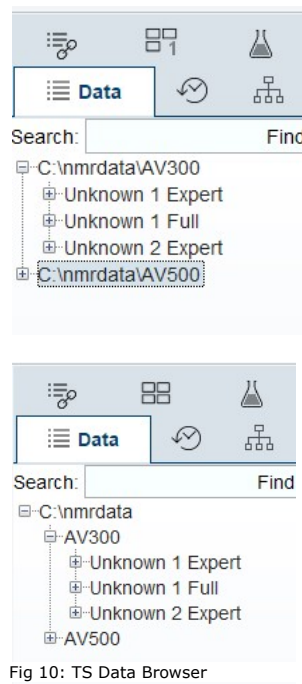

Fig 10: TS Data Browser

macOS

Right click in the browser and again select "Add New Data Dir…". Click on the triple ellipse to browse for the nmrdata folder. If you followed the instructions above, the directory should be /Users/<username>/nmrdata where <username> is the name of your MacOS user account and home folder. It is specified in the sidebar of a Finder window beside the home icon.

macOS Workaround → Problems Opening NMR Data

Mac users have often reported permission problems when trying to open NMR data in TS4. The issue seems to plague several macOS and TS4 version combinations. If you experience permission problems, try starting TopSpin using the following procedure (instead of using the application shortcut):

- Open a new Finder window and go to "Macintosh HD". If Macintosh HD is not present, go to Finder -> Preferences… and under Locations check the option "Hard disks".
- Show hidden files by pressing the keys CMD + SHIFT + period.
- Drill down into the folder opt/topspin4.x.x and double-click the "topspin" file. This will open topspin through a terminal. The first time doing this, you will be asked to allow terminal to access your file system (select OK). By granting this permission, you should be able to use topspin normally.

Note that for convenience, you can place a shortcut to this "topspin" file on your desktop. To do so, right-click on the file and choose "Make Alias" and then move the alias to your desktop.

Step 7: User Preferences

TS can be configured in a variety of ways to suit the needs or preferences of the user. These can be viewed by selecting the gear icon. Some of the most popular and useful settings are as follows:

- Administration Items
  - choose whether to auto open (or not) the dataset used the previous time TS was open.

- Processing Preferences
    - Choose whether to automatically process (or not) data that TS opens.

There are many useful settings within "Spectra Display Preferences".
- It is from here you can control what is visible when viewing NMR data, such as titles, integrals, peaks labels, etc.
- Customize the display fonts and colors.
- Customize the number of digits shown for peak picking and integrals.