Installing and setting up Topspin

1. Insert the Topspin CD and the installation wizard will guide you. Select processing only. The only question will be to identify the NMR superuser. You can select any valid account on the computer. You will then be asked to input a password. Be sure to write down what user and password you selected. You will need to know this for later customization.

2. Set up the license file.

    a. You will receive an email from Bruker with several lines of text that constitute the license. (Directions from Bruker sometimes refer to these lines of text as a "password".)

    b. The directory C:\flexlm\Bruker\licenses will be created during the Topspin installation. First copy the file with the name **example_license.dat** to a file called **license.dat**, then insert the lines into **license.dat**.

    c. If you do not allow file extensions to be shown, these files will appear to be named **example_license** and **license**. If you don't pay attention to this detail, you may end up with the actual name of your license file being **license.dat.dat**, which WILL NOT WORK! To avoid this problem, make sure you are aware of whether you are displaying extensions or not. You can check by opening a Windows Explorer window. Select Tools → Folder Options → View →. There is a check box labeled "Hide extensions for known file types". If this is checked, you will not see the **.dat** extension.

    d. The first two lines of the **license.dat** file that you just created will be:

        SERVER your_computer_name your_hostid 1700
        DAEMON bruker_ls c:\flexlm\Bruker\bruker_ls.exe

        1) Replace the string 'your_computer_name' by the hostname of your computer. (Directions for obtaining this information were given in the Topspin_Info.doc write-up.)

        2) Replace the string 'your_hostid' by the hostid of your computer, the "physical address" used to obtain the license.

        3) Append the FEATURE lines which your received from Bruker after the DAEMON line. Never change the FEATURE lines; no extra blanks, tabs etc. are allowed! The 12-digit number at the end of each FEATURE line must be the same as the hostid in the SERVER line.

3. Once you have the license file set up properly, you will have to boot the computer before Topspin will run.

4. There are a few things that you may want to do to customize the installation.

    a. To locate data using Topspin, the main data directory where your data reside must be added to the data browser area at the left side of the main window. Position the mouse in

this data browser area, right-click, and select **Add New Dir**. Enter the name of the main data directory where you have put data on your computer.

b. Type expinstall. You will be asked to input the NMR administration password. (Same as "NMR superuser" in step 1. above.)

1) Don't worry about the caution, select Next.
2) Choose "Installation for Datastation (Default), then select Next.
3) Choose "High Resolution Systems", then select Next.
4) Choose all the defaults, then select Next.
5) A window displaying all your choices will come up. Select Finish. This will take some time to complete.

c. There are a few files that we have written that we suggest you use in the write-ups. They have all been placed on the linrl1 computer in the home directory of the username "nmr". If you do not ever acquire data manually and therefore don't know how to access this computer, see the NMR lab staff. You will need to use ssh transfers to get these files. The archiving write-up tells you how to get the program needed for the ssh transfer if you do not already have it.

1) Mostly these files are layouts for plotting spectra with the Plot Editor.

a) On the computer where you will run Topspin, put the layouts in the directory **C:\Bruker\TOPSPIN\plot\layouts**.

b) In the ssh transfer program, set the directory for the linrl1 computer to the Topspin_customization_files directory, then the **layouts** directory. Bring over all the files.

2) If you plan to process 2D spectra, you should bring over the pulse programs and some automation programs that we use that were not provided by Bruker.

a) On the computer where you will run Topspin, put pulse programs in the directory **C:\Bruker\TOPSPIN\exp\stan\nmr\lists\pp**.

b) In the ssh transfer program, set the directory for the linrl1 computer to the Topspin_customization_files directory, then the **pp** directory. Bring over all the files.

c) On the computer where you will run Topspin, put automation programs in the directory **C:\Bruker\TOPSPIN\exp\stan\nmr\au\src**.

b) In the ssh transfer program, set the directory for the linrl1 computer to the Topspin_customization_files directory, then the **au** directory. Bring over all the files.