

**User Guide for Setting Up NMR Workstations  
(Located in 045 BRL)**

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# PREFACE

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## **Purpose of This Document**

This user guide aims to help you to setup the NMR workstations (located in 045 BRL) when logging in for the first time. The document does not cover data processing procedures of the Bruker TopSpin NMR software.

## **Intended Audience**

This document is intended for users of the AV 400 MHz and AVIII 600 MHz NMR spectrometers. The user may use AV400 MHz and AVIII 600 MHz NMR spectrometers for data acquisition and use the workstations for data processing.

# 1 Introduction

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The NMR workstations in 045 BRL are mounted to the NMR server through network. When the NMR data is collected on the AV 400 MHz NMR and the AVIII 600 MHz spectrometers, the data will be automatically transferred to the NMR server. The workstations in 045 BRL can be used to access the NMR data collected on AV400 and AVIII 600 NMR spectrometers without interrupting data acquisition on these instruments. The NMR workstations are preloaded with Bruker TopSpin software and other NMR data processing software.

Login information, including login name and password, will be provided by the NMR spectroscopist when the NMR training on the AV 400 MHz or the AVIII 600 NMR has been completed.

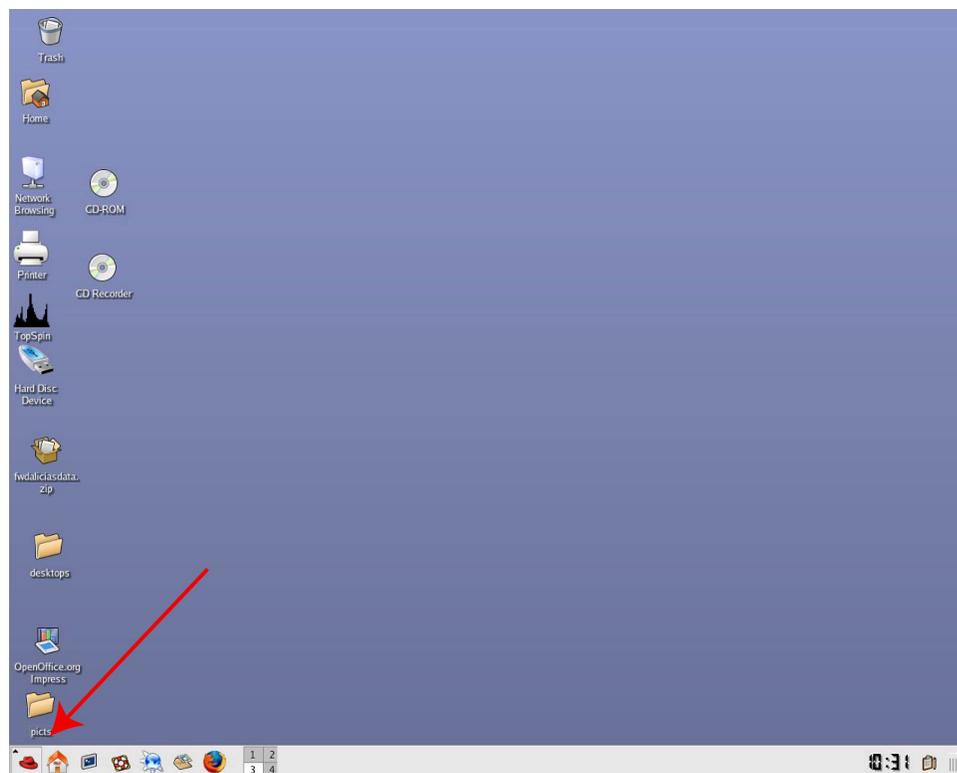
This guide is intended to help user to setup the workstation when logon for the first time. The procedure described in this guide only need to be carried out once for each workstation.

## 2 Disable Screen Saver

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Follow these steps to disable the screen saver when you logon to the workstations for the first time.

1. After login, the KDE desktop is shown in Figure 1. Click on the **Redhead** icon (located in the left lower corner) as indicated in Figure 1. Select **Control Center** in the pull-up menu.



**Figure 1: The KDE Desktop**

2. The **Control Center** interface is shown in Figure 2. Click on + sign in front of **Appearance & Themes** as circled in Figure 2, then select **Screen Saver** in the index panel on the left. The window is expanded as shown in Figure 3.

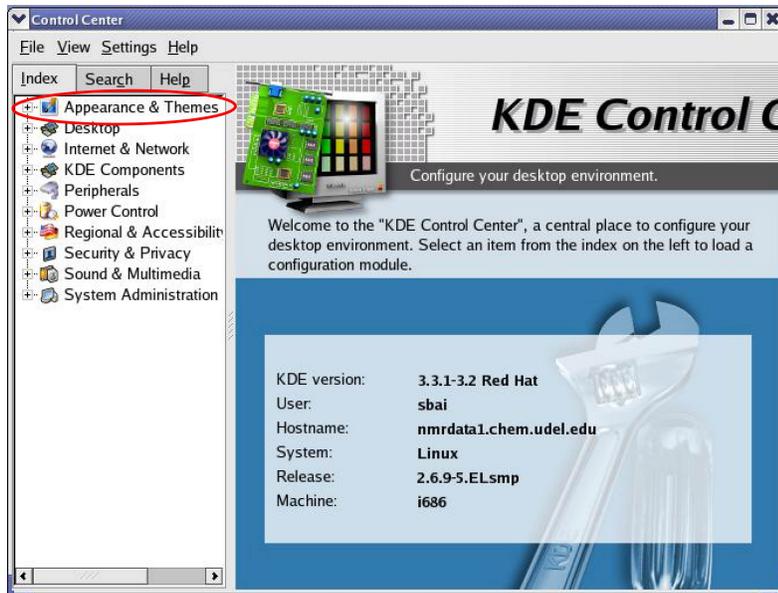


Figure 2: KDE Control Center

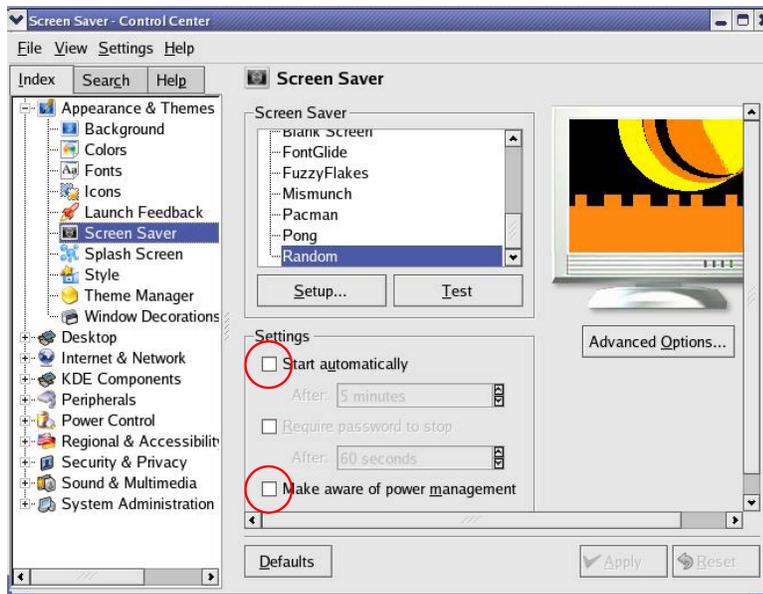


Figure 3: Screen Saver Option

3. In Screen Saver Option window, uncheck the box labeled as “*Make aware of power managemnet*” and then uncheck the box of “*Start automatically*” as indicated two red circles in Figure 3.
4. Finally click on **Apply** button to save the setting. To exit **Control Center**, click on **File** and select **Quit**.

### 3 Setup Directory Path for TopSpin File Browser

When TopSpin software is activated for the first time, a correct path of NMR data directory must be set so that the program will be able to locate the data directory automatically when it is started next time. Follow these steps to set up a file path for the TopSpin file browser:

1. Start TopSpin program by double clicking on the TopSpin icon (  ) on the desktop. Answer “*I agree*” to the software license question. The TopSpin interface is shown in Figure 4.

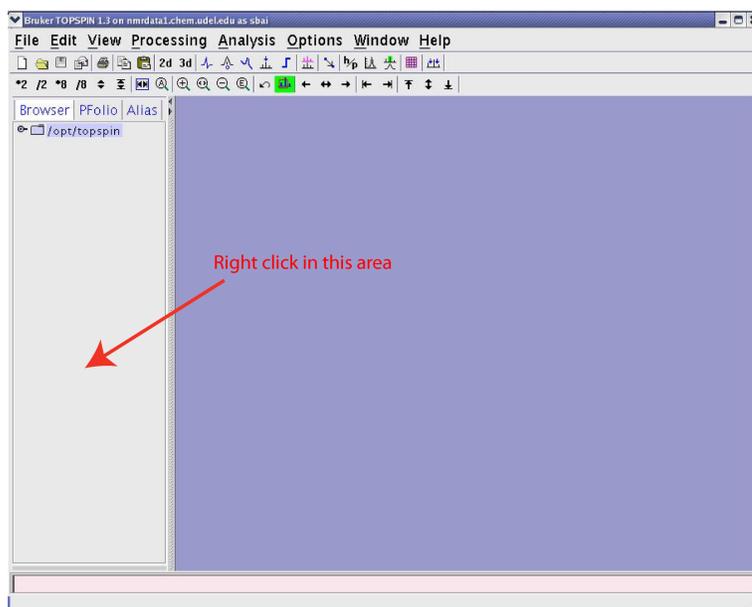
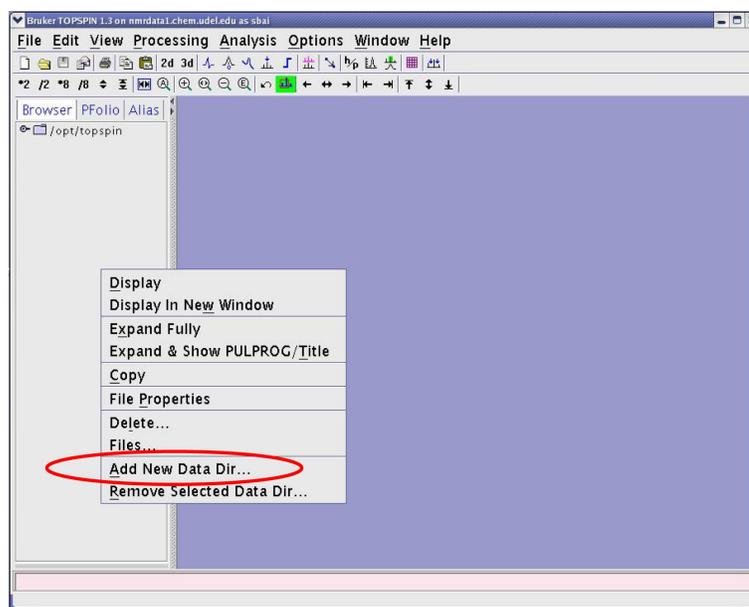


Figure 4: TopSpin GUI

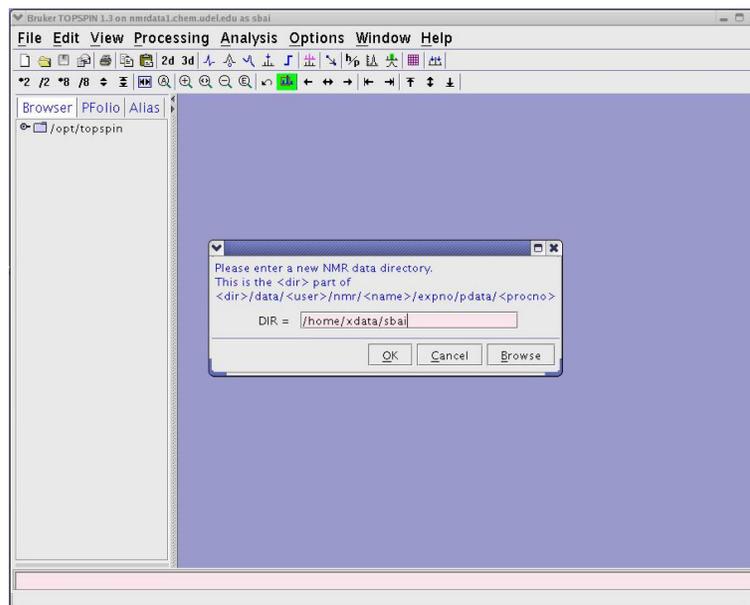
2. Right click on the left data browser panel as indicated by the red arrow in Figure 4. A selection menu appears as shown in Figure 5.



**Figure 5: Selection Menu**

3. Select “**Add New Data Dir...**” by clicking on it. A pop-up window appears that allows you to enter a path of data directory. The correct sequence for NMR data directory is `/home/xdata/username`, where the username is the same as the login name. For example, Steve Bai's login name is `sbai`, so the correct path for him is therefore `/home/xdata/sbai`, as it is shown in Figure 6 as an example.

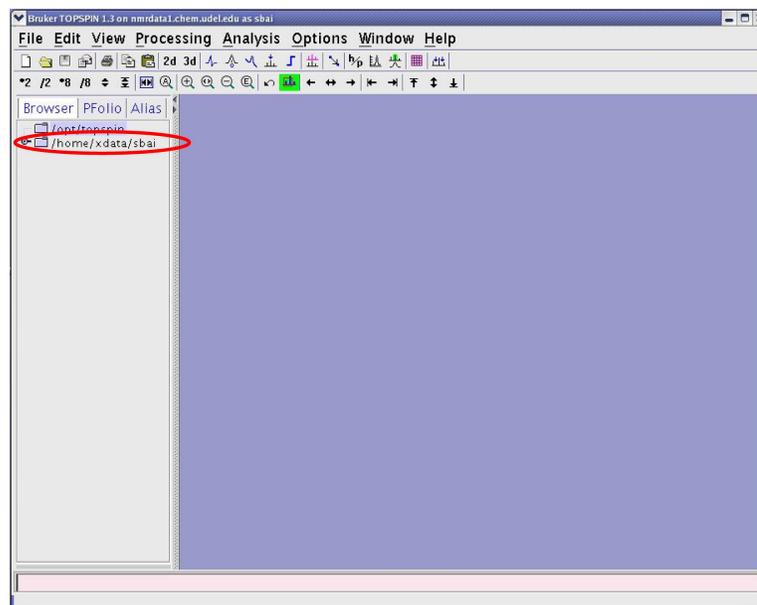
*Note: the first part of the path `/home/xdata/` should not be altered.*



**Figure 6: Path for NMR Data Directory**

4. After a correct path is entered, click on **OK** to continue. On the left data browser panel, a new data directory as circled in red appears (Figure 7).

*Note: clicking on a switch icon in front of the folder will allow user to browser the NMR data saved in this folder.*



**Figure 7: Appearance of New Data Directory**