How To’s:

Create Sidebar Objects
Introduction

In this How To’s you will learn how to create and edit object from the Sidebar.

Contents:
1. Spectrum Groups
2. Samples and Substances

Start CcpNmr Analysis V3

- Apple users by running Assign/Screen on the Launcher
- Unix users by using the terminal command: bin/assign or screen
- Windows users by double-clicking on the .bat file
Getting started, basic operations

Sidebar
All data contained in a project, such as spectra and peak lists are located in the sidebar. Double-clicking on an item will open its properties popup.

Display
A display can contain multiple overlaid spectra which share the same axes. To show/hide a single spectrum, click on its toolbar button. If you close a display, you can open a spectrum by dragging and dropping it into the drop area from the sidebar or by right-clicking on a sidebar item and selecting Open as module. You can also add additional spectra to a spectrum display module later on, or drag several spectra into the drop area together to open them simultaneously.

Mouse
• Pan  ->  Left-drag in display
• Zoom in/out  ->  Scroll wheel in display
• Context menu  ->  Right-click
• Select a peak  ->  Left-click on a peak symbol “X”
• Move a peak  ->  select first, then middle-click and drag

Shortcuts
The program uses several shortcuts, for example MK for creating a mark at the current mouse position. You will need to press the first letter on your keyboard e.g. M, followed by the second letter, e.g. K (case insensitive). Press Esc to cancel the first letter.

For more commands and operations
Main Menu → Help → Tutorials → Beginners Tutorial
OR
Main Menu → Help → Show Shortcuts
Drag & drop some spectra into the sidebar or drop area

Find some 1D spectra (e.g. in the ScreenTutorial/spectra/1Ds folder of the tutorial data folder) and drag them onto the sidebar or drop area.
Open the Spectrum Group Dialog

- On the Sidebar, find the `SpectrumGroups` item, expand the branch and **double-click** on `<New SpectrumGroup>`

OR
- Use the shortcut `SS`

OR
- Go to **Main Menu → Spectrum → Spectrum Groups**

OR
- Select the spectra in the sidebar, **right-click** and select **Make SpectrumGroup from selected**
Set up Spectrum Group

- Enter a name for your Spectrum Group.

- In the left-hand list of spectra, choose the spectra you want to add to your Spectrum Group and drag them into the right-hand box. If you wish, you can drag spectra back out of the Spectrum Group box, and you can drag spectra up and down to change their order within the Spectrum Group box.

- Click on Save changes to Spectrum Groups.

In the sidebar you will now see your new Spectrum Group and its constituent spectra.
Display Spectrum Group

- Drag your Spectrum Group from the sidebar into the drop area to display the spectra.

Note that when you drag a Spectrum Group into the drop area, the spectra are displayed as a single entity and the Spectrum toolbar simply contains one button for the group.

If you select all the spectra in the group and then drag them into the drop area, the spectra will be shown separately, with each spectrum having its own button in the Spectrum Toolbar.
Substances, Samples and Sample Components in CcpNmr Analysis V3 (Explanation only)

Within Analysis V3, **Substances** are essentially any kind of chemical - they could be biological macromolecules, small molecules, salts or solvents. Imagine your list of **Substances** to be your chemical store cupboard. If a **Substance** is a polypeptide or polynucleotide, it may also have a **Chain** associated with it. And if you create a **Chain** (e.g. by importing a FASTA file), a corresponding **Substance** will automatically be created for the polypeptide/polynucleotide.

As with a real chemical store cupboard, each **Substance** is associated with a particular type of isotopic labelling. You don’t have to specify the labelling and (unlike in V2), the specification of the labelling is not formalised. You can either choose a predefined labelling scheme or enter your own. **Substances** can have reference spectra associated with them.

**Samples** correspond to actual samples that you run experiments on. They have properties such as amount (e.g. in ml), ionic strength and pH and may contain **Sample Components**. **Sample Components** are based on and linked to **Substances**. You can either create **Substances** in advance and then create your **Sample Components** from the **Substances**, or, as you create new **Sample Components** for your **Sample**, equivalent **Substances** will be created for you by the programme. **Samples** can be linked to **Spectra** which were run on that sample.

Schematic diagram showing how objects are linked in CcpNmr Analysis. **Sample Components** are nested inside the **Sample** branch in the sidebar. All other objects are accessed at the top level. **Spectra** and **Reference Spectra** are containers for other objects rather than objects themselves.
2A Create New Substance

- Expand the Substances branch in the sidebar and double-click on <New Substance>.

- Enter a Substance Name, e.g. aspirin and, if you wish, also Labelling.

- By expanding the More options section you can view and edit many more properties such as empirical formula, molecular mass or atom and bond counts.

- Expanding Compound view will enable you to enter a small molecule SMILES, e.g. CC(=O)OC1=CC=CC=C1C(=O)O. Doing this will show the compound in the Compound View box.

- Click Ok to apply your changes and close the pop-up.
2B  Create New Sample
   • Expand the **Samples** branch in the sidebar and **double-click** on *<New Sample>*

2C  Open the Sample Properties Dialog
   • **Double-click** on *SA:sample* to open the **Edit Sample** dialog box.
   • Enter a **Name** for the sample and any other properties such as ionic strength and pH.

![Edit Sample dialog box]

**Enter a Name**
- *Mixture1_control*
- ionic strength: 0.00005
- pH: 5.5
Link Spectra to Sample

- Find a Spectrum in the sidebar, either under Spectra or Spectrum Groups
- Double-click the spectrum to bring up the Spectrum Properties pop-up
- Find the Sample pulldown entry and select your sample
Create New Sample Component from existing Substance

- Expand your Samples branch in the sidebar further and double-click on <New SampleComponent>

- Select the From Substances radio button to use a Substance that you have previously already added to your project
- Select the Substance you want to use from the drop-down menu and enter any other parameters you wish to add, e.g. role, concentration etc.
- Click on Ok

Your new Sample Component will now be shown as part of your Sample in the sidebar.
Create New Sample Component with new Substance

- In your Samples branch in the sidebar double-click on <New SampleComponent>

- Select the New radio button to add a new Substance to your sample that you don’t already have in your project
- Enter the substance Name and any other parameters you wish to add, e.g. role, concentration etc.
- Click on Ok

Your new Sample Component will now be shown as part of your Sample in the sidebar.

A new Substance is automatically created for you in the process which will be visible in the Substances branch.
Contact Us

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