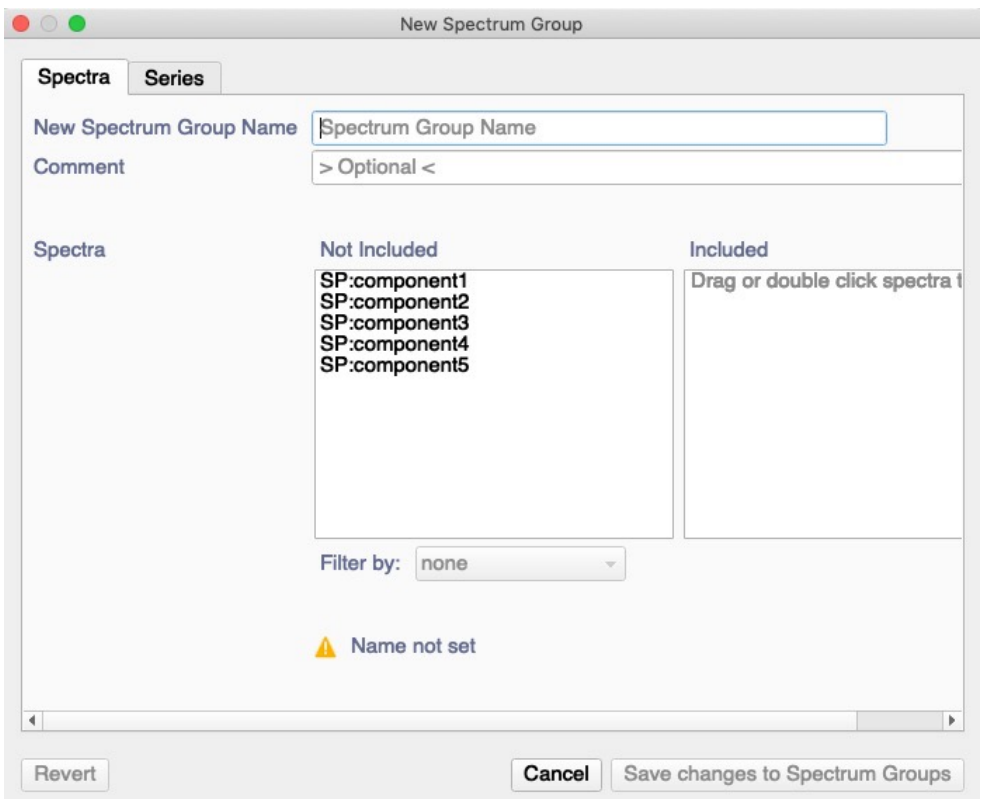
CCPN

CcpNmr AnalysisScreen Version 3

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:

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

1

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.

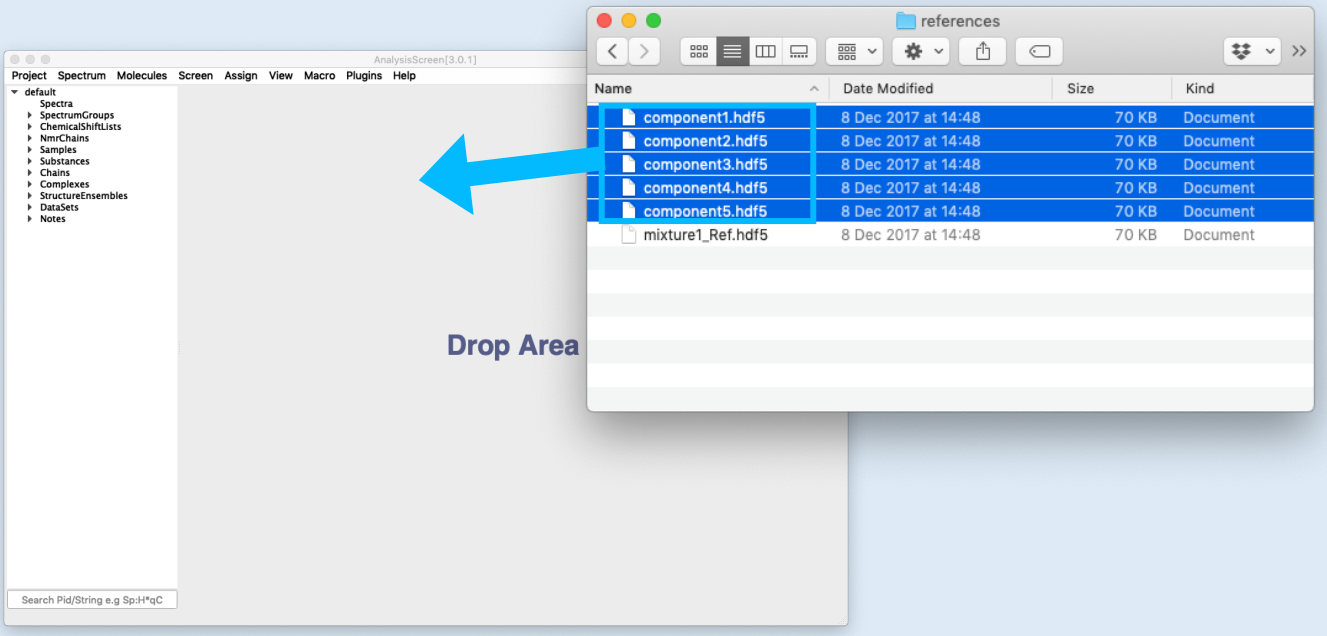
For more commands and operations

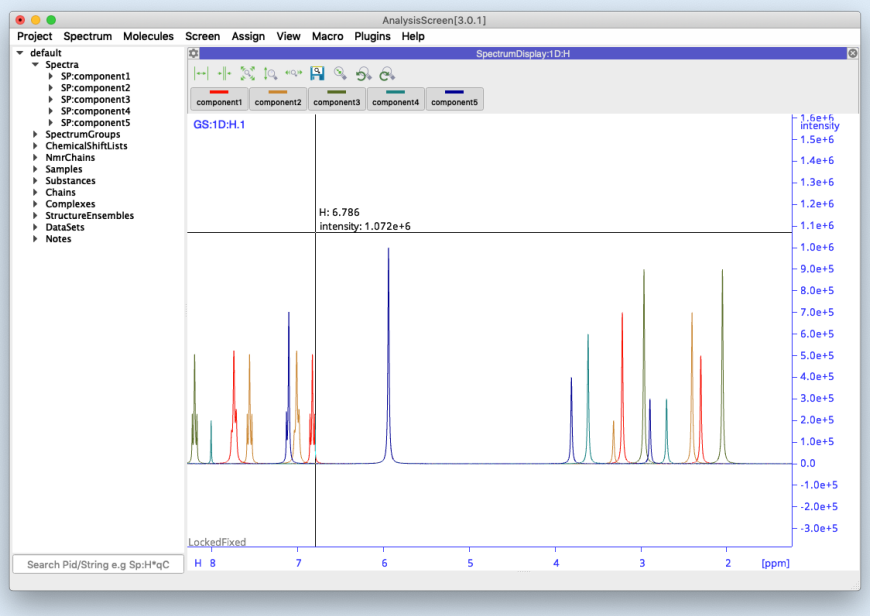
Main Menu ⟶ Help ⟶ Tutorials ⟶ Beginners Tutorial

OR

Main Menu ⟶ Help ⟶ Show Shortcuts

1 Spectrum Groups

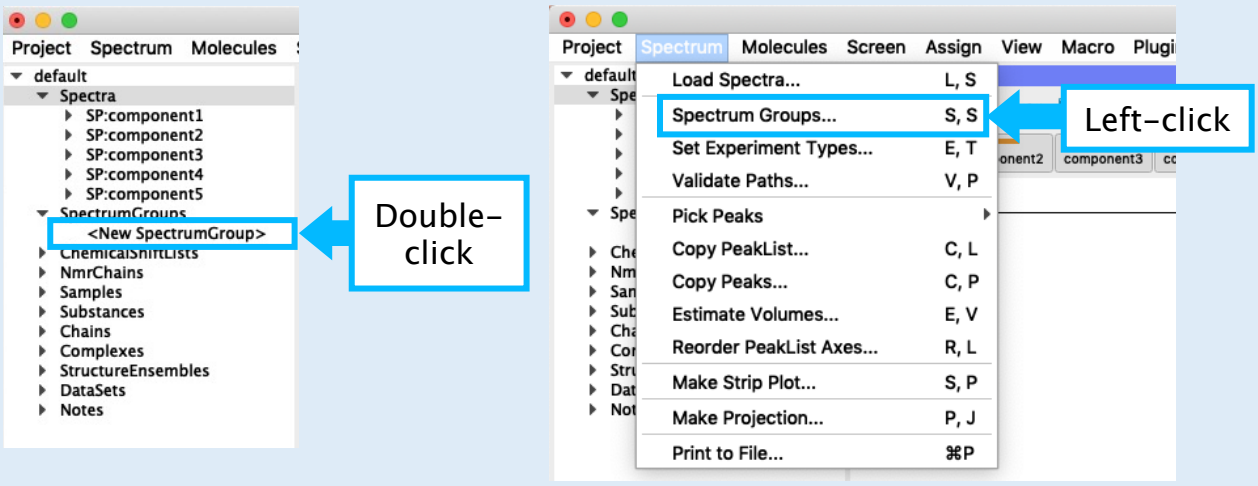




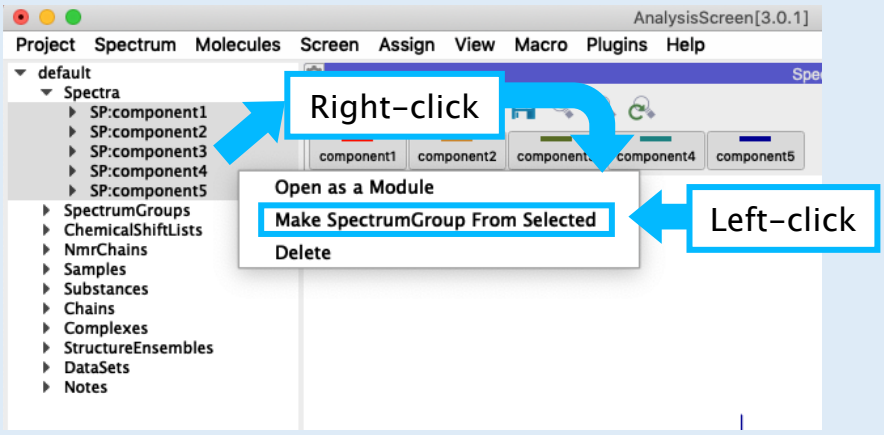
1A • **Drag & drop some spectra into the sidebar or drop area**

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.

1 Spectrum Groups



SS



1B 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**

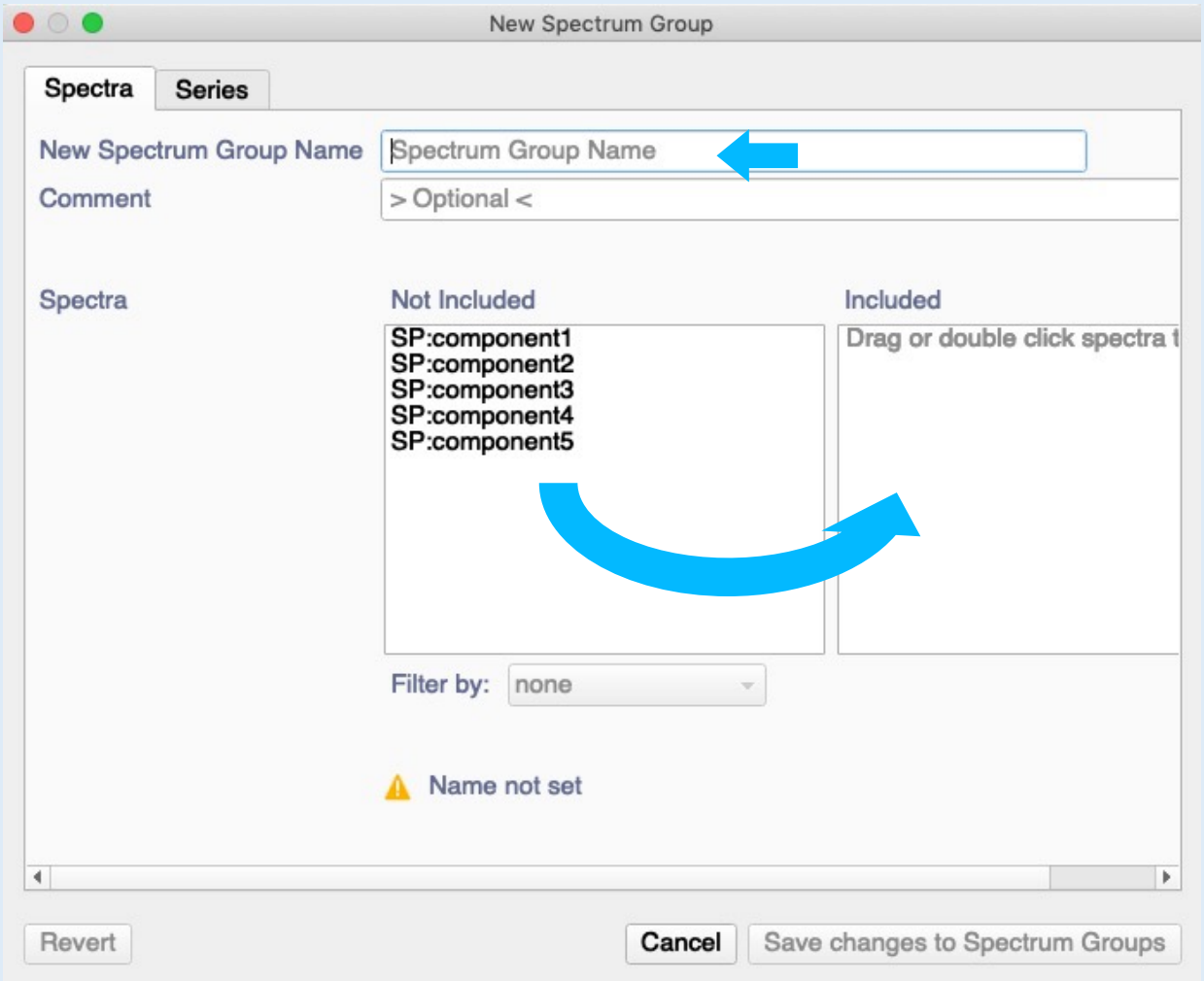
OR

- Go to **Main Menu ⟶ Spectrum ⟶ Spectrum Groups**

OR

- Select the spectra in the sidebar, **right-click** and select **Make SpectrumGroup from selected**

1 Spectrum Groups

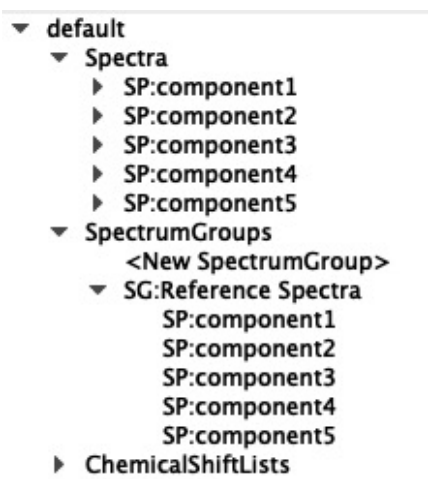


1c Set up Spectrum Group

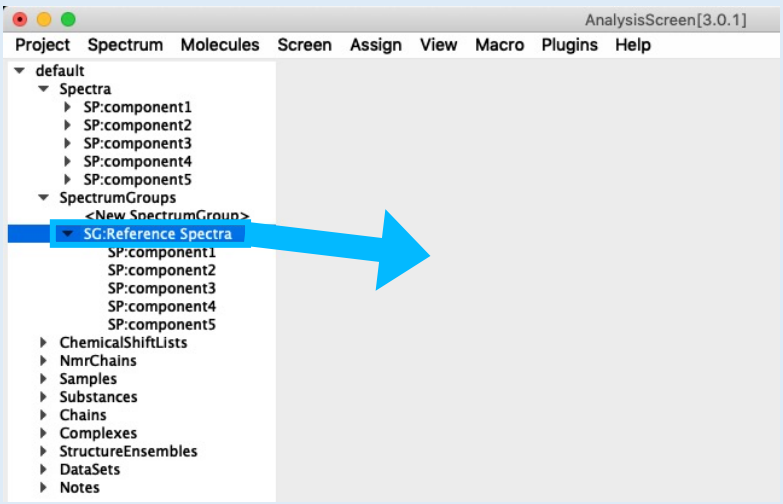
- **Enter a name** for your Spectrum Group.

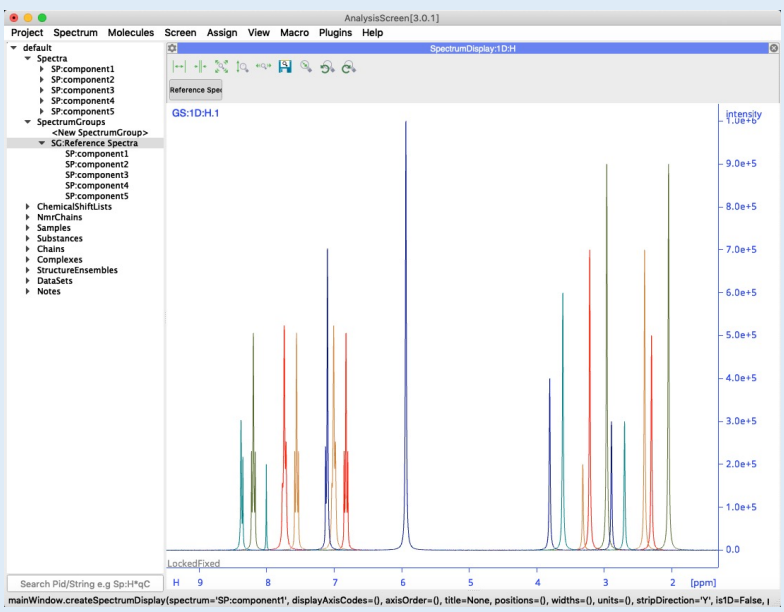
- In the left-hand list of spectra, choose the spectra you want to add to your Spectrum Group and **drag them into the right-hand box**.
  If you wish, you can drag spectra back out of the Spectrum Group box, and you can drag spectra up and down to change their order within the Spectrum Group box.
-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

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



1 Spectrum Groups

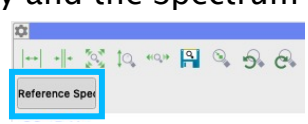




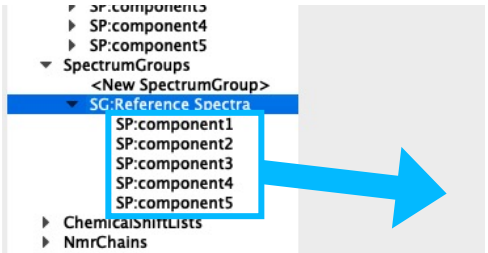
1D Display Spectrum Group

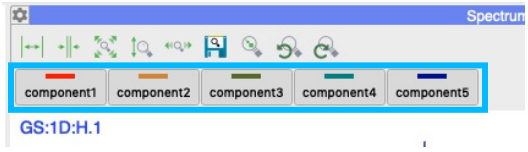
- **Drag** your Spectrum Group from the sidebar into the drop area to display the spectra.

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.





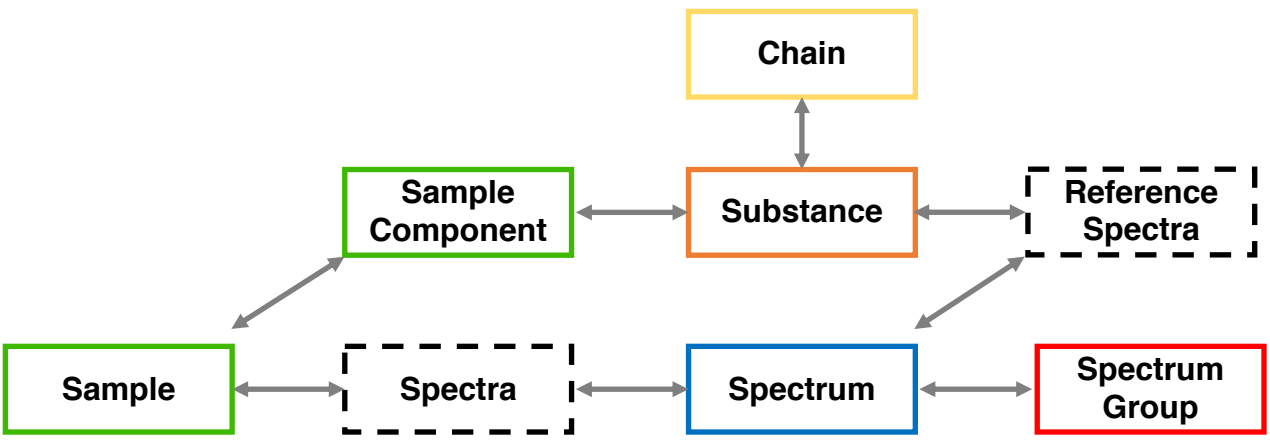
2 Substances and Samples

Substances, Samples and Sample Components in CcpNmr Analysis V3 (Explanation only)

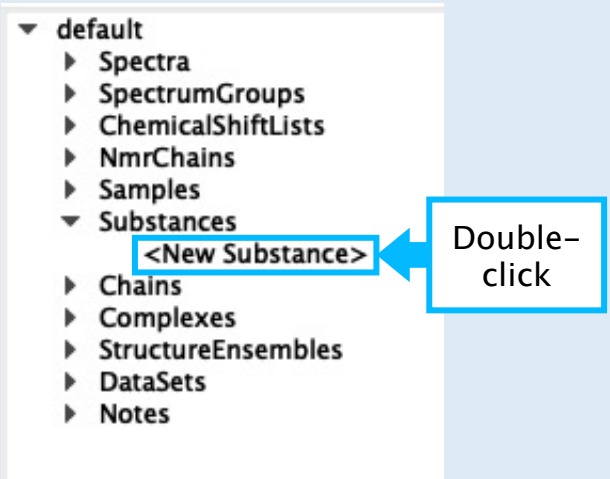
Within Analysis V3, **Substances** are essentially any kind of chemical – they could be biological macromolecules, small molecules, salts or solvents. Imagine your list of **Substances** to be your chemical store cupboard. If a **Substance** is a polypeptide or polynucleotide, it may also have a **Chain** 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.

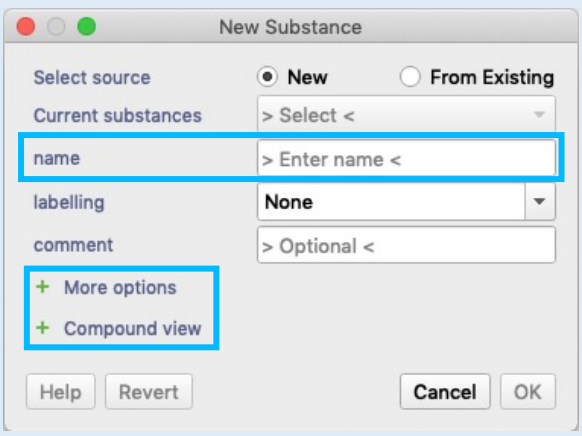
Samples correspond to actual samples that you run experiments on. They have properties such as amount (e.g. in ml), ionic strength and pH and may contain **Sample Components**. **Sample Components** are based on and linked to **Substances**. You can either create **Substances** in advance and then create 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.

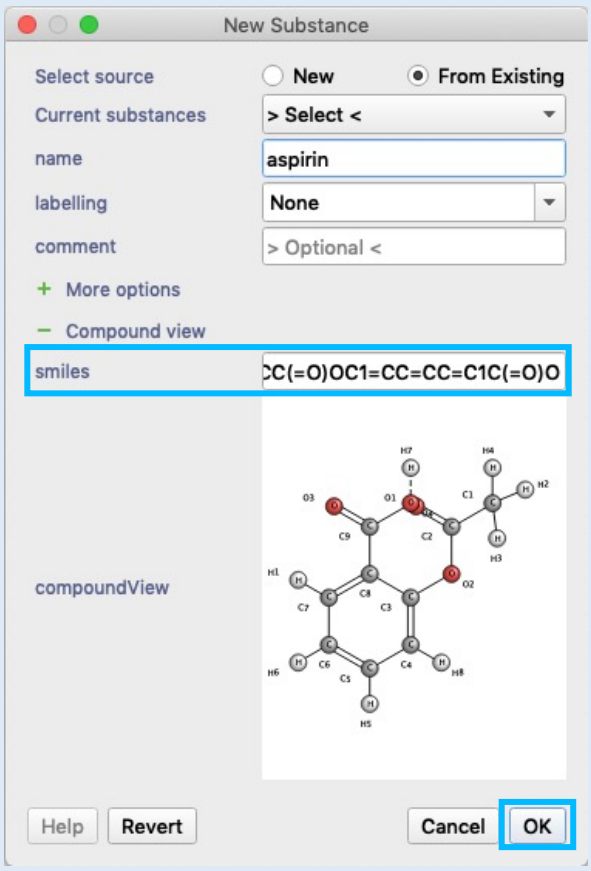
Schematic diagram showing how objects are linked in CcpNmr Analysis.
Sample Components are nested inside the **Sample** branch in the sidebar. All other objects are accessed at the top level.
Spectra and **Reference Spectra** are containers for other objects rather than objects themselves.



2 Substances and Samples





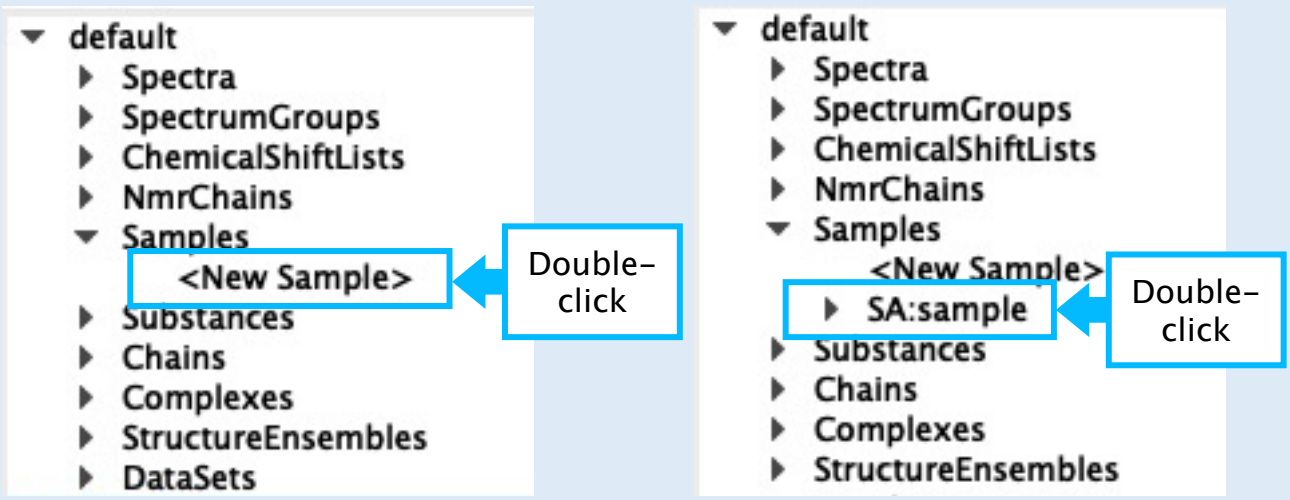


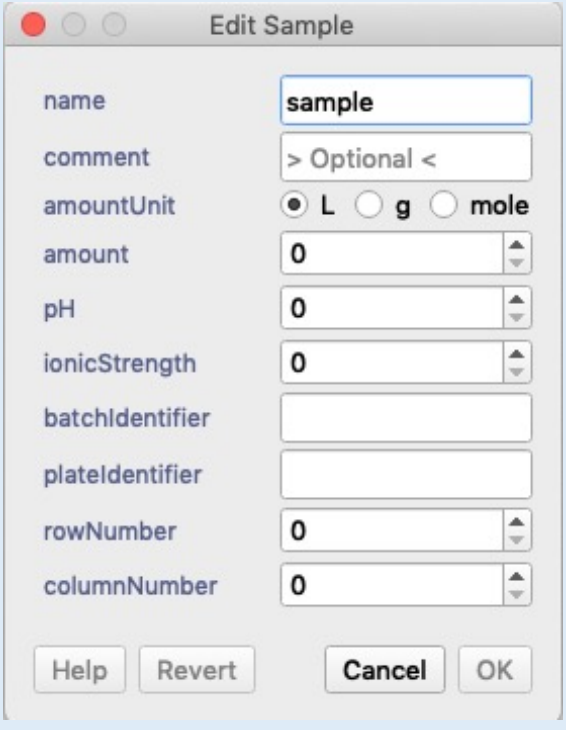
2A Create New Substance

- 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.

2 Substances and Samples



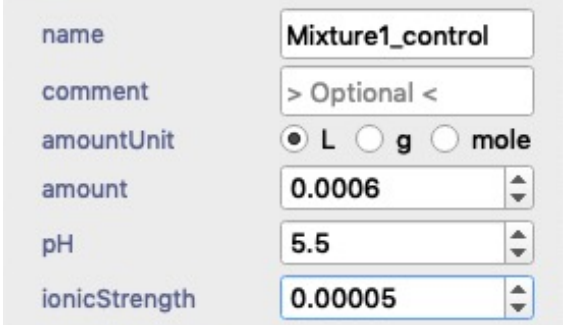


2B Create New Sample

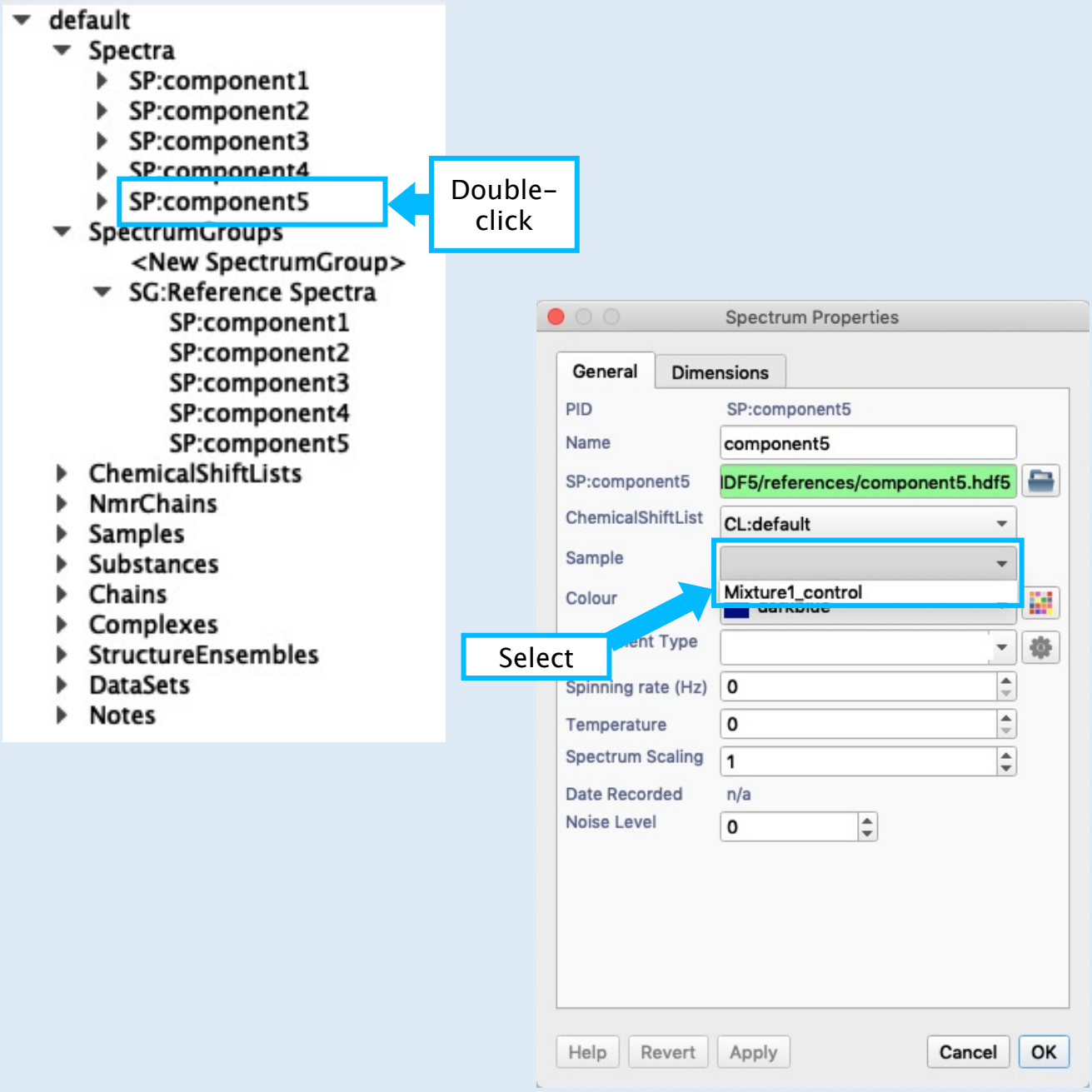
- Expand the **Samples** branch in the sidebar and **double-click** on **<New Sample>**

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**.



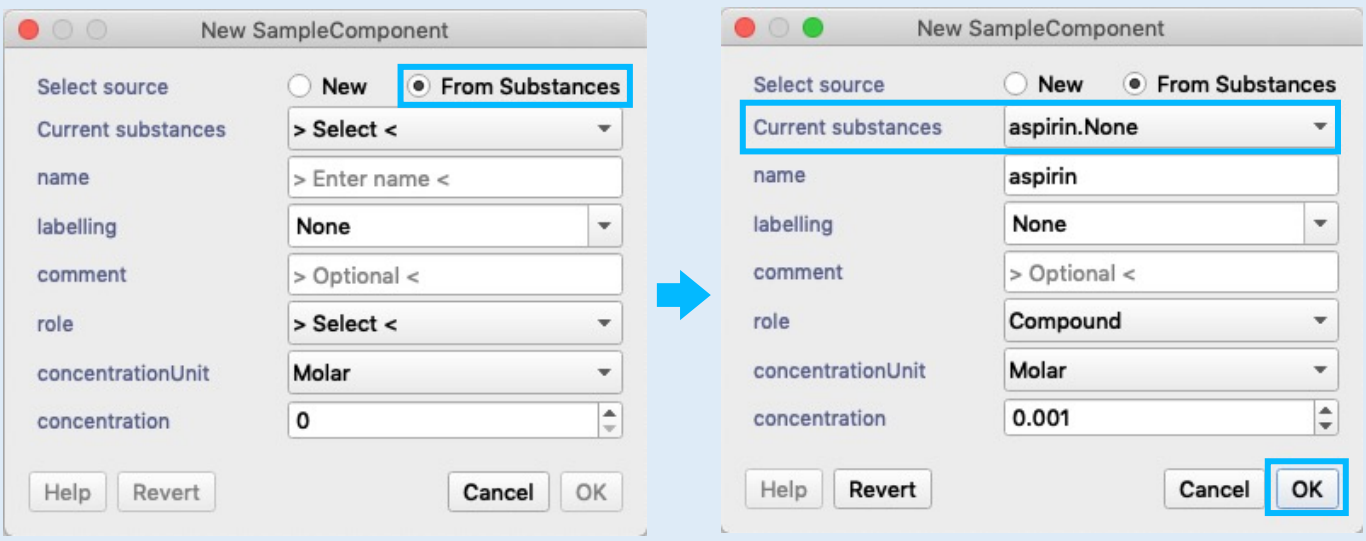
2 Substances and Samples



2D 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

Substances and Samples

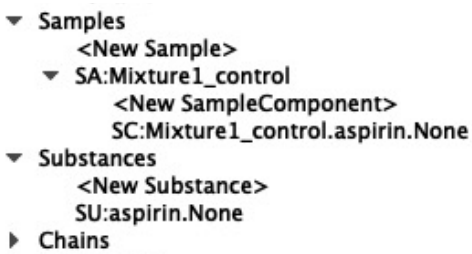


2E Create New Sample Component from existing Substance

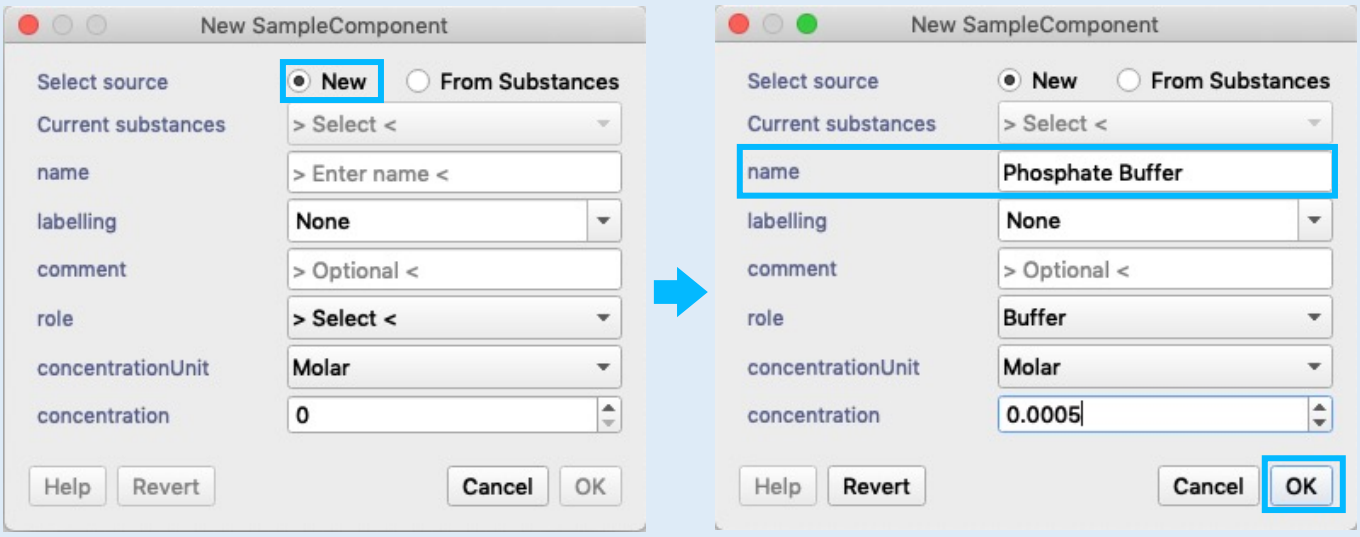
- Expand your **Samples** branch in the sidebar further and **double-click** on **<New SampleComponent>**

- 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.



Substances and Samples



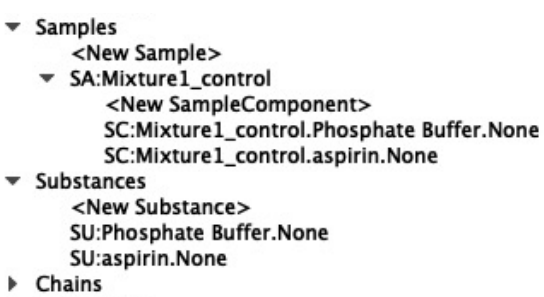
2F Create New Sample Component with new Substance

- 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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https://www.ccpn.ac.uk/forums

Cite Us

Skinner, S. P. et al. CcpNmr AnalysisAssign: a flexible platform for integrated NMR analysis. J. Biomol. NMR 66, (2016)

Mureddu, L. et al. CcpNmr AnalysisScreen, a new software programme with dedicated automated analysis tools for fragment-based drug discovery by NMR. J. Biomol. NMR (2020)