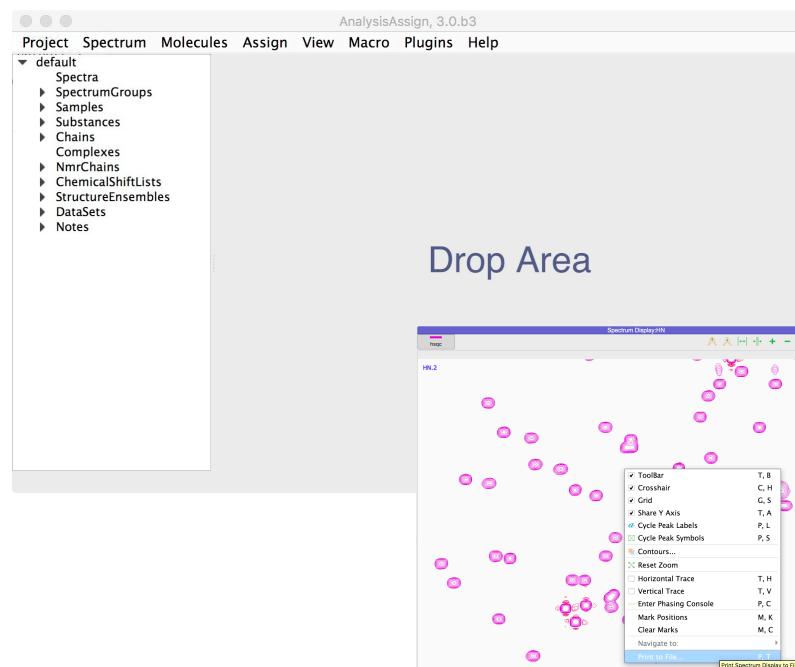


Beginner Tutorial



Introduction

This tutorial will guide you through some basic operations in CcpNmr Analysis Version 3 and help you to familiarise yourself with the program.

The tutorial is divided into sections, each of them has a set of simple actions. Each page of this tutorial corresponds to a single operation, you will see a descriptive image on top and a full description below. (Note that images are representative, and that there may be small differences between your setup and that shown in the tutorial.)

When you open the program you will see a large display area, with a sidebar to the left and a menu bar at the top. All the displays, tables, etc. which go into the display area are referred to as new “modules”. The sidebar shows the data in your project and lets you edit data items, create new ones, and drag the items into the display area to display them as a module. The menu bar lets you start actions and action modules. You can also start actions by two-key keyboard shortcuts (not case-sensitive), using the right mouse button, or from buttons and icons in the application.

Contents:

1. Loading Spectra
2. Displaying Spectra
3. Spectrum Settings
4. Rearranging Modules
5. Peak Picking
6. Working with Strips
7. Printing Spectra
8. Notes

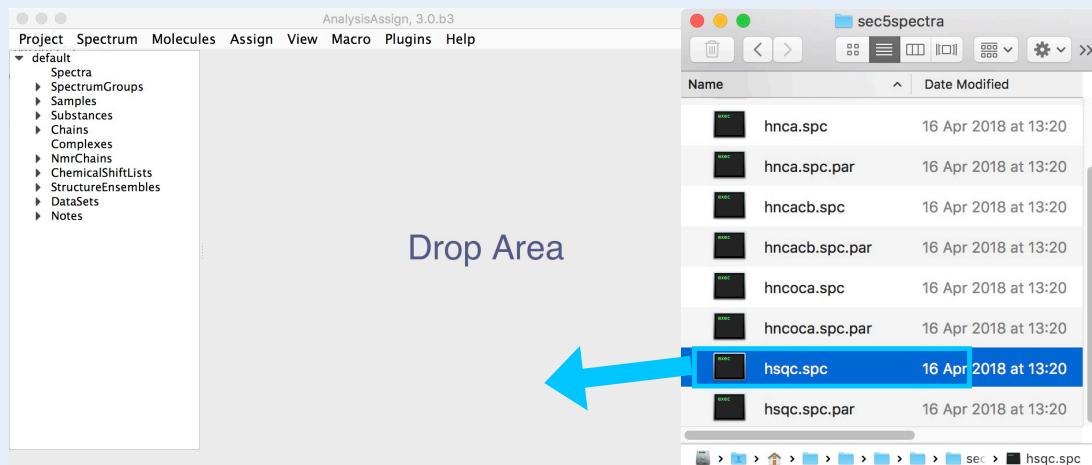
Start CcpNmr Analysis V3

Apple users by double clicking the icon 

Linux users by using the terminal command: *bin/assign*

Loading spectra

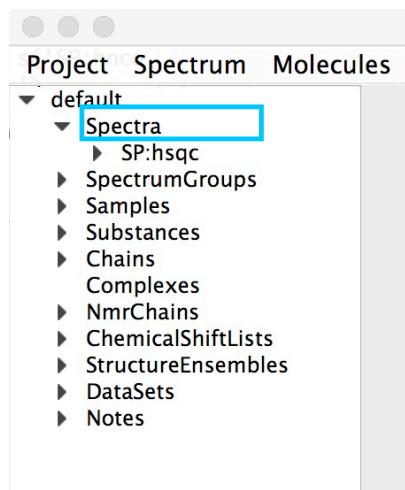
Spectra location : AnalysisV3/data/CcpnSec5BBTutorial/sec5spectra



1A Drag & drop the spectra into the sidebar or drop area.

- Find the hsqc in the demo spectra directory (AnalysisV3/data/CcpnSec5BBTutorial/sec5spectra)
- select it in finder and drag it onto the sidebar or drop area.

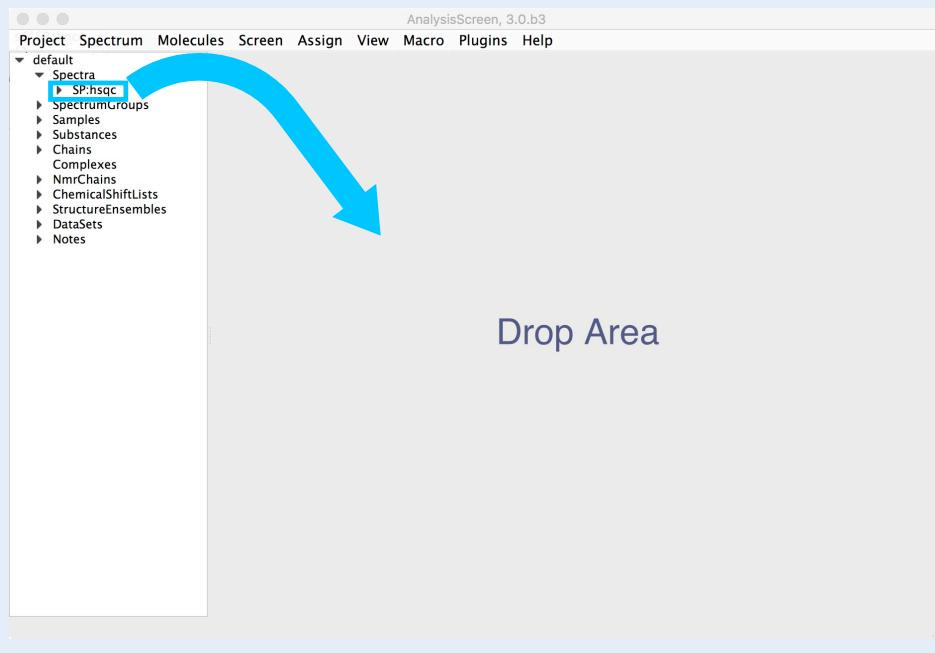
If you drop it onto the drop area, the spectrum will be displayed immediately, if you drop it on the sidebar you will need an extra step to display it (1B). You will also see an arrow appear next to the Spectra label in the sidebar showing that the spectrum has been loaded.



1

Loading spectra

Drag & drop from Sidebar



Drop Area

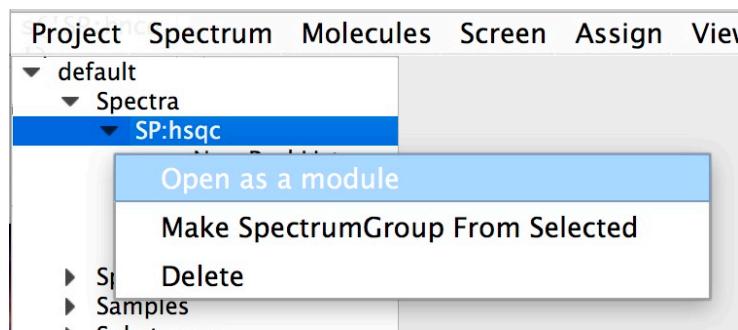
1B Drag & drop the spectra from the sidebar to the drop area.

- Select the spectrum you want to display in the sidebar
- Drag and drop it into the main drop area

Alternatively:

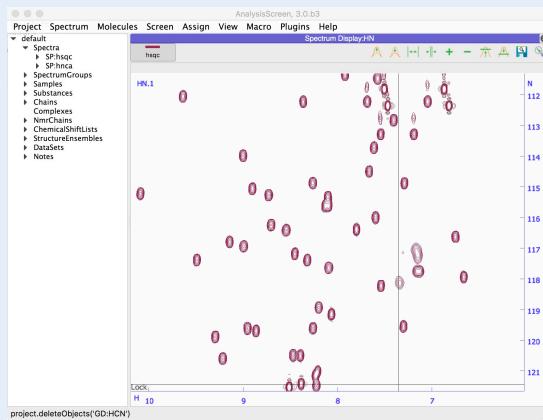
- right click on the sidebar item:
- click on open as module

Right Click on Sidebar Item

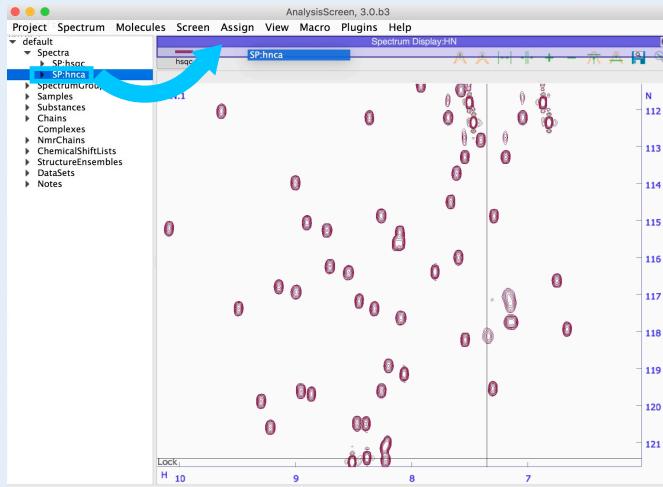


1

Loading spectra



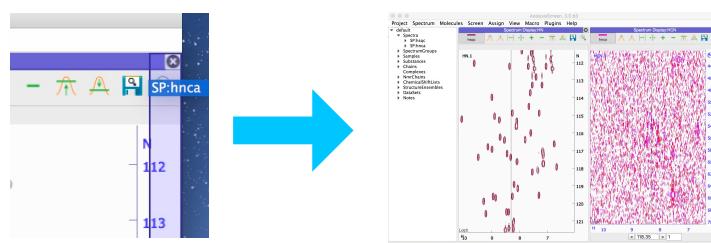
Drag over the purple bar then drop



1c Display more spectra

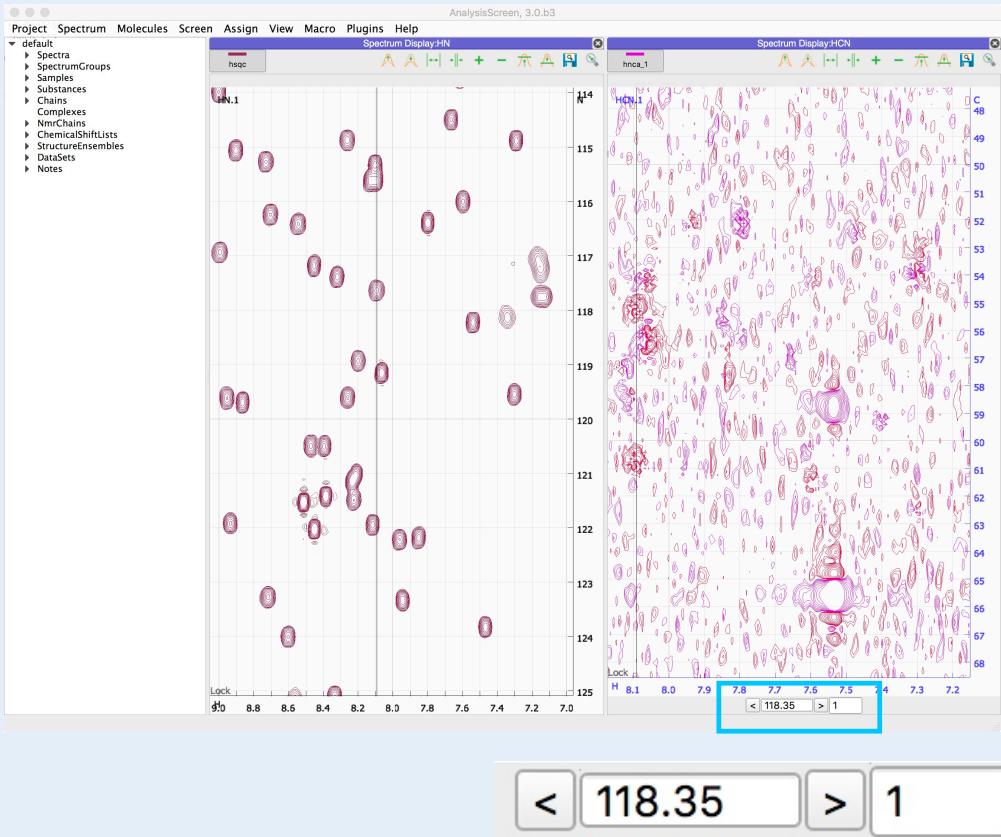
- Add a new spectrum to the project (like 1A), for example the hnca
- Select it on the sidebar, hold down the left mouse button and start to drag
- Drag it to the top bar of the currently displayed spectrum without dropping yet. When a semi-transparent purple box appears, the drop area is ready to accept the drop and you can release the button. If you keep holding you can choose another location where to display the spectrum.

The purple box represents the target location where the new module will be opened. Keep holding the left click and move at the edges of the target module (left, right, top or bottom) then drop the item to display it.



Displaying spectra

Change planes



2A Change planes in a 3D spectrum

At the bottom of the display is a Z toolbar; two arrows for changing planes, a box showing the ppm position of the z axis and a second box which shows how many planes are shown simultaneously.

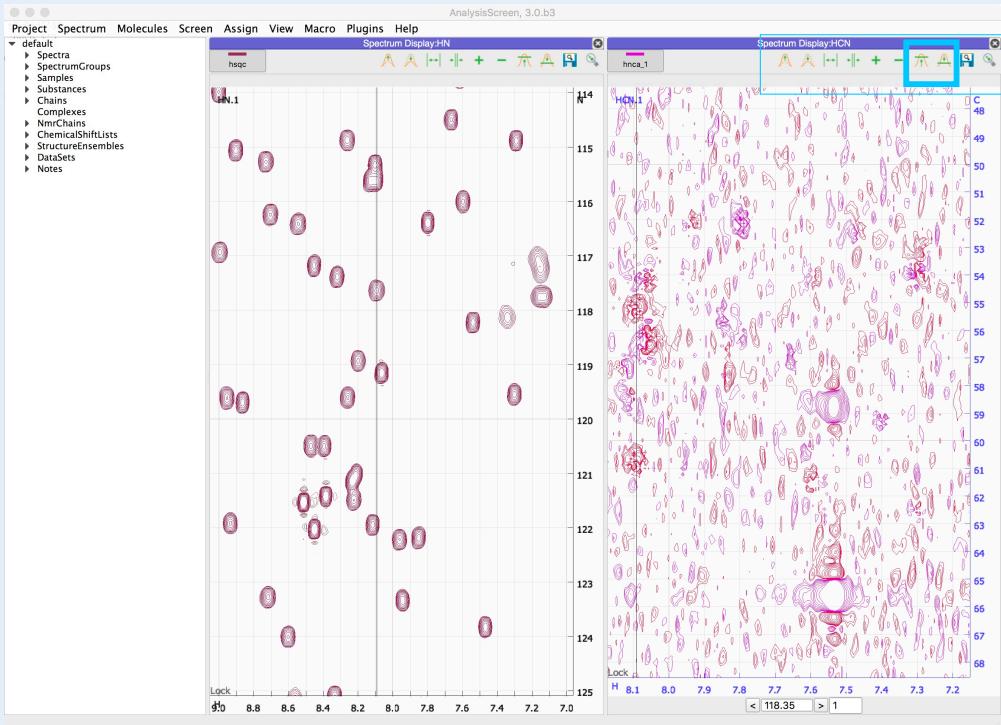
- The two arrows left and right of the z position box move the spectrum one plane at a time.
- The number of planes shown at a time can be changed by editing the plane count manually or by using the mouse wheel while hovering over the box. The z position can also be changed using the mouse wheel in the same way.

Displaying spectra

Increase Contours



Contour base Up

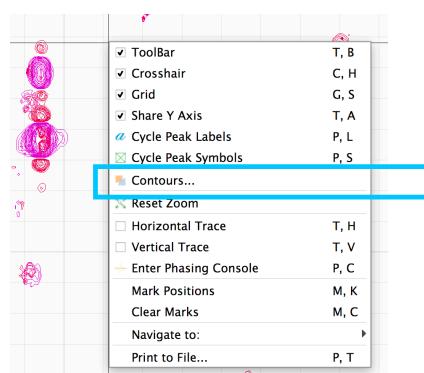


2B Adjust contours

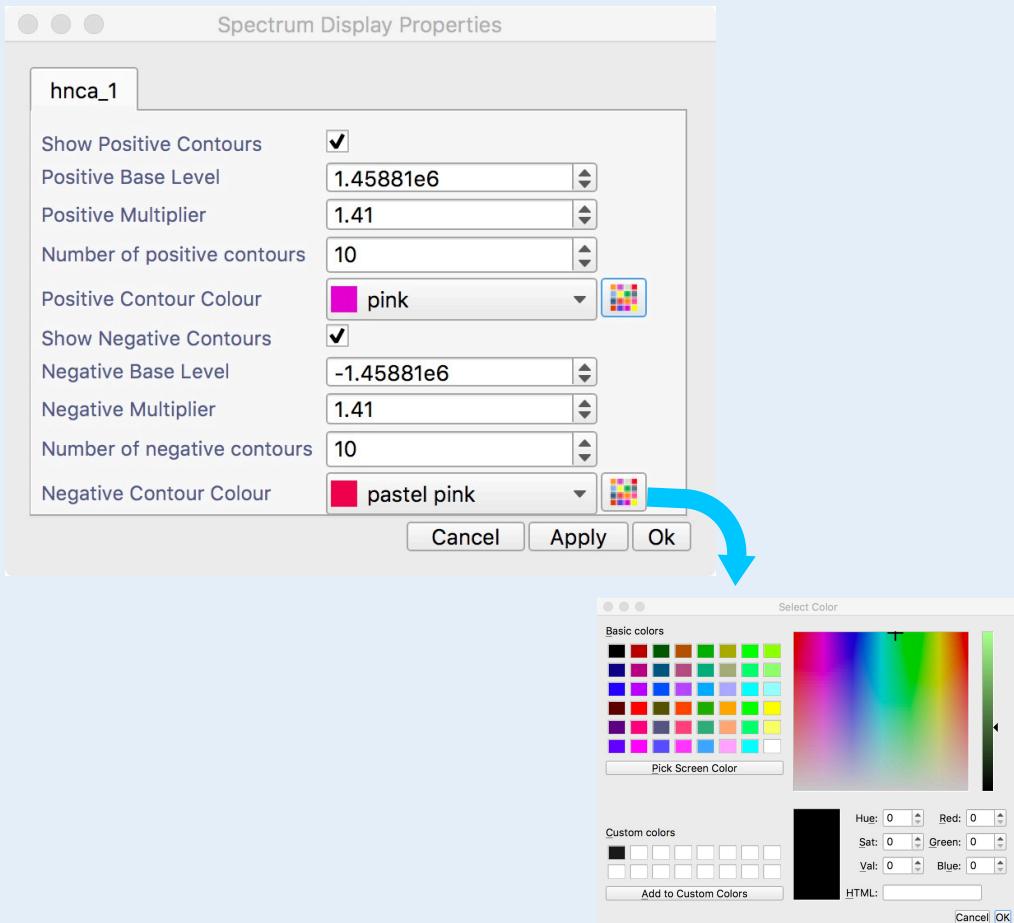
- Go to the HCN spectrum display
- locate the icons
- Raise the contour level by click on

This will increase by a default factor of 1.41. To have access to more settings:

- right-click on the spectrum display
- select Contours...



Customise Contours



2C Customise contours

This popup contains values that can be changed to manipulate how the contours are displayed for that spectrum.

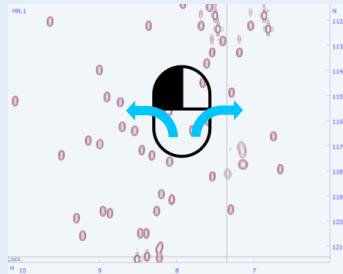
- Contour base levels, multipliers and the number of contours can be changed by adjusting the value with the mouse wheel or directly typing into the box.
 - Checking and unchecking the check boxes will show or hide the positive/negative contours. To change the colour of the contours, you can either select one from the list of standard colours using the drop down list or select one of your own by clicking the Multi-coloured button, which will pop up a Colour dialog.
- Once you have selected your colour and pressed OK the colour will appear in the drop down list as Colour + a number and will be stored for future use.

2

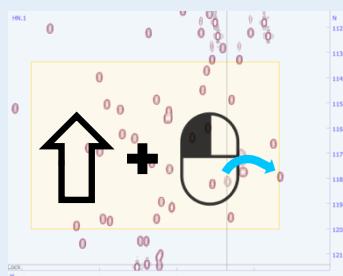
Displaying spectra

Mouse actions:

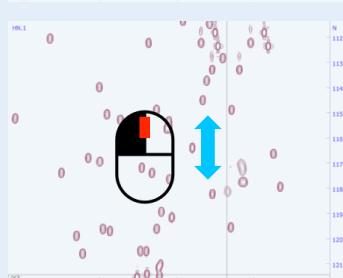
Pan the spectrum



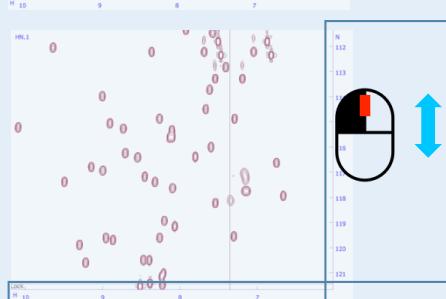
Zoom box



Zoom In – Out (all axes)



Zoom In – Out (one axis)

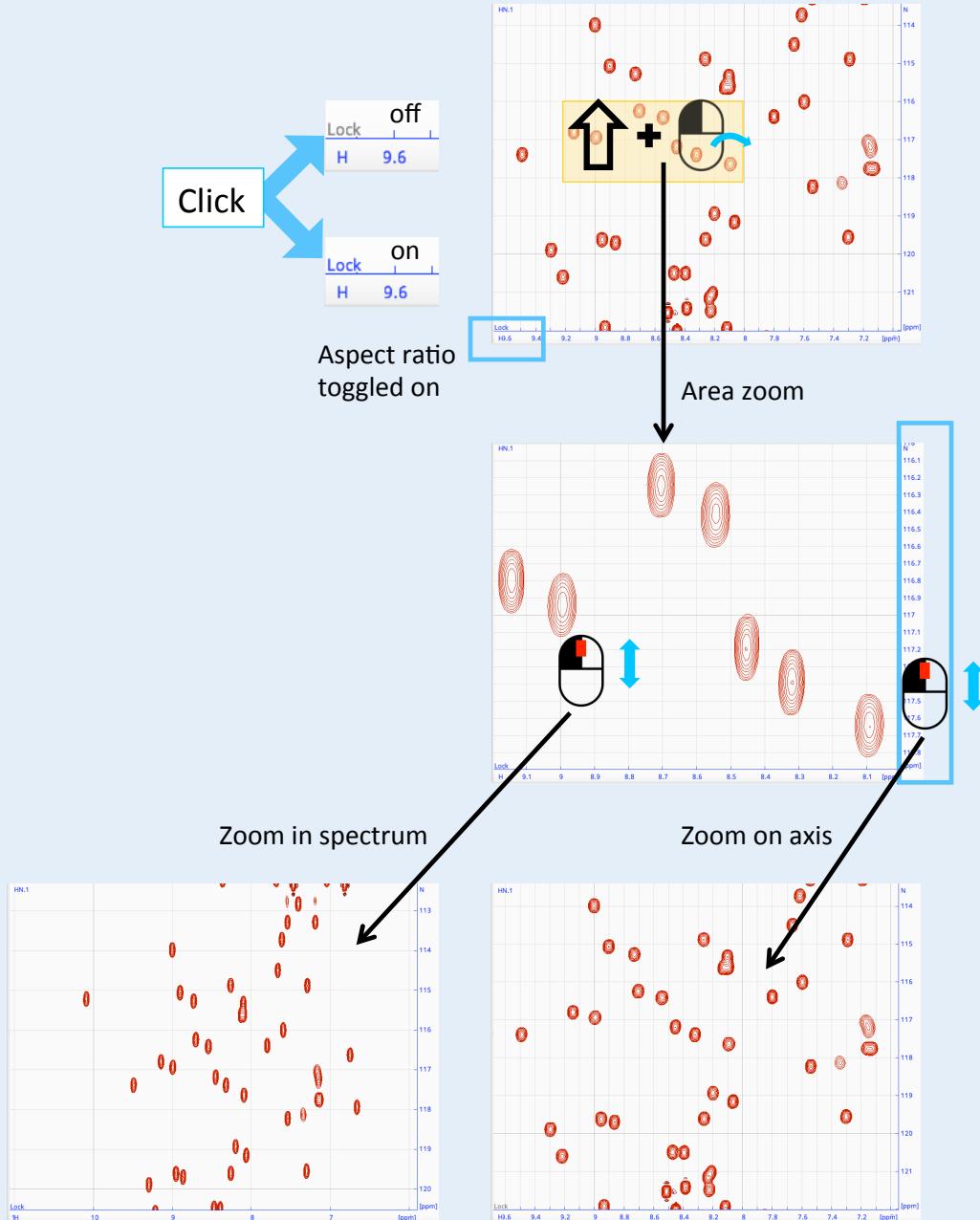


2D Mouse actions

Dragging the left mouse button around a spectrum display will pan the spectrum in the direction of movement and the mouse wheel will zoom the x and y axes simultaneously. If you want to zoom into a specific area, then using SHIFT+left-drag will cause a yellow box to be drawn on the display, which specifies the zoom region.

Displaying spectra

Zoom behaviour

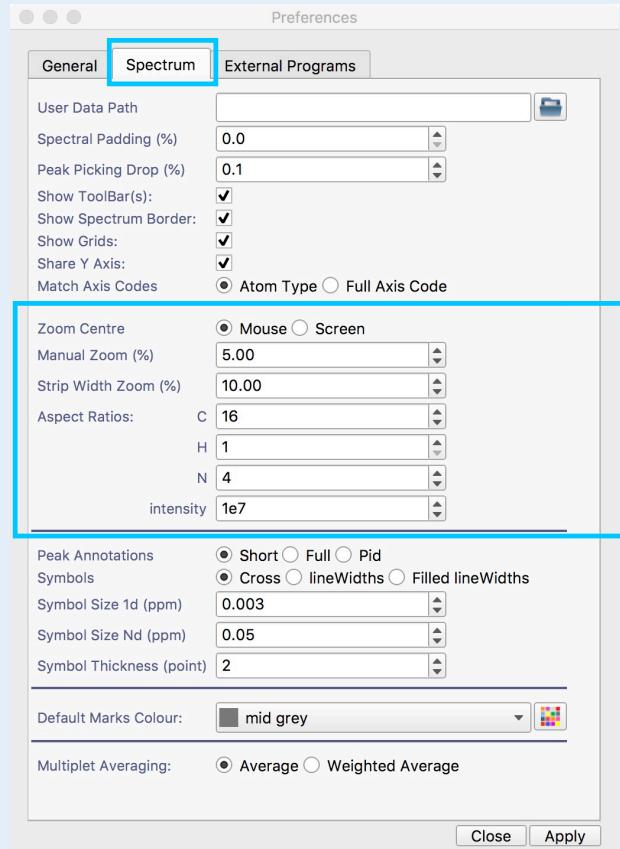


2E Zooming and Aspect Ratio Lock

You can lock the aspect ratio of your display by toggling the LOCK in the bottom left hand corner on.

- If you then do an area zoom, the aspect ratio will change in accordance with the area selected.
- Restore the aspect ratio by zooming on an axis with the middle mouse button or temporarily retain the new aspect ratio by zooming in the spectrum area with the middle mouse button

Spectrum display preferences



2F Zoom preferences

- Go to Main Menu → Project → Preferences...
- Select the Spectrum tab
- Modify the zoom behaviour from the middle section

2G Keyboard actions

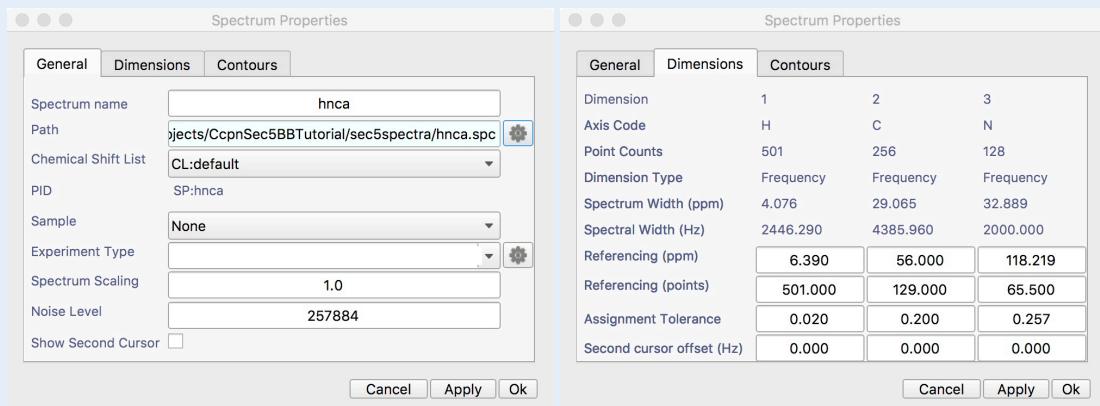
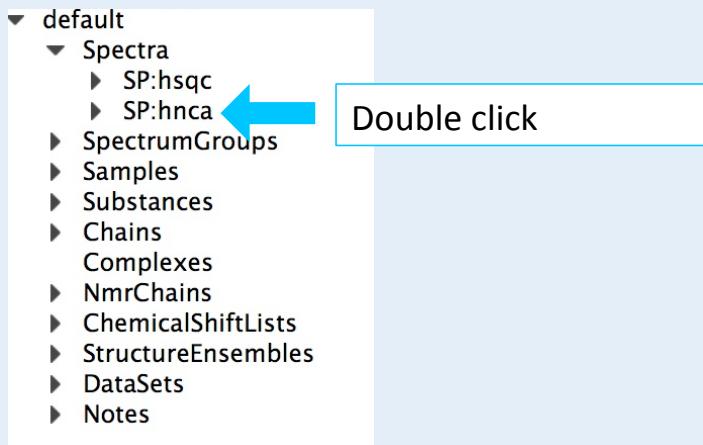
Select a spectrum display by clicking any point, this will set the strip as "current" and will highlight the axis.

- Use the keys "+" and "-" to zoom in and out
- Use the directional keys to move across the spectrum

3

Spectrum Settings

To change spectrum properties:

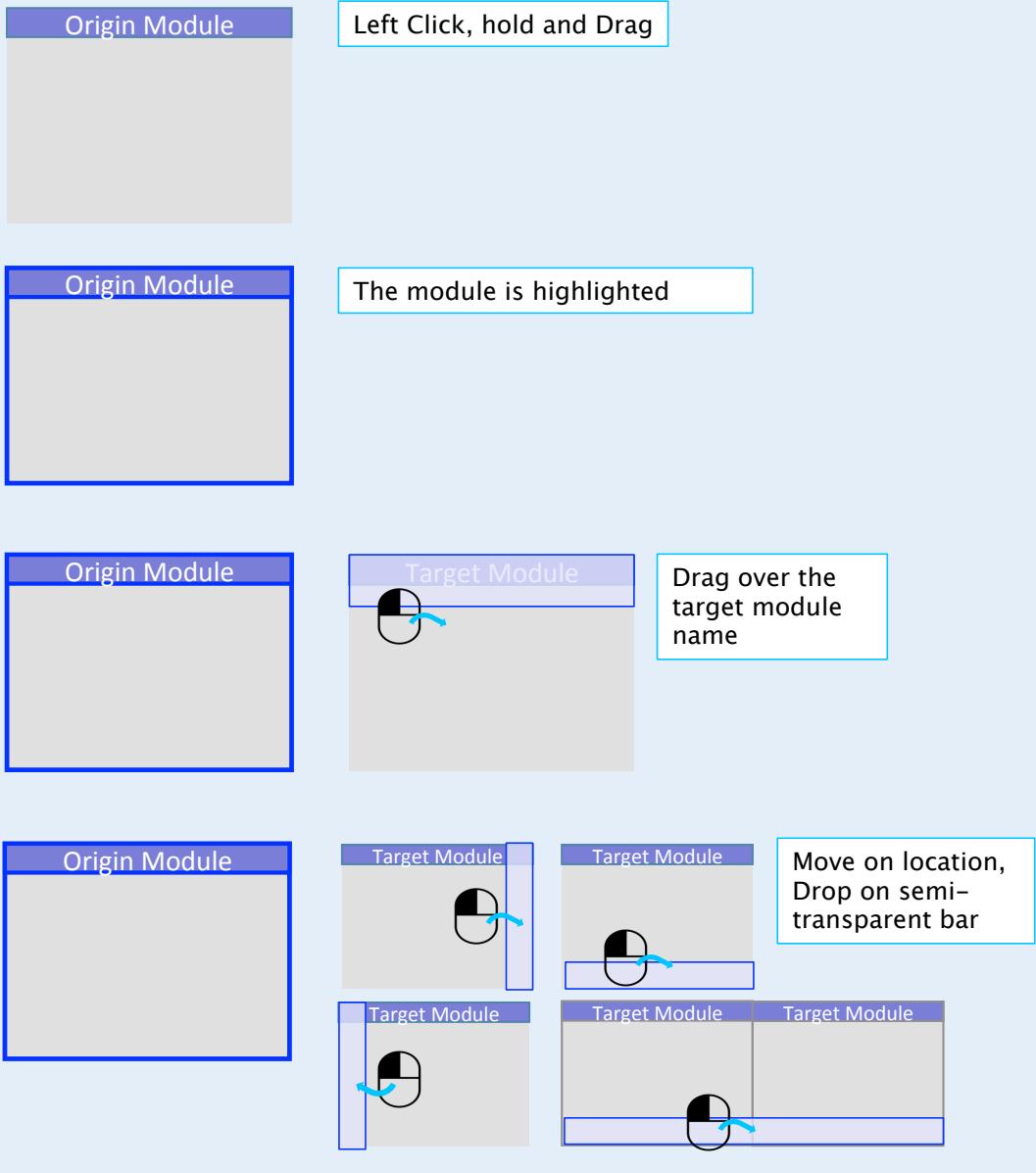


3A Change spectrum properties

To change the properties of a spectrum, including the contour colours, double click its name in the Sidebar and a dialog box will pop up with a series of tabs in it.

- In the first tab, you can set general parameters of the spectrum, such as the name, path, experiment type, scaling etc. Changing the values in each box and clicking Apply will change the parameter value.
- In the Dimensions tab, you can view information on each dimension of the spectrum and change referencing and assignment tolerances for each dimension.

Rearranging Modules



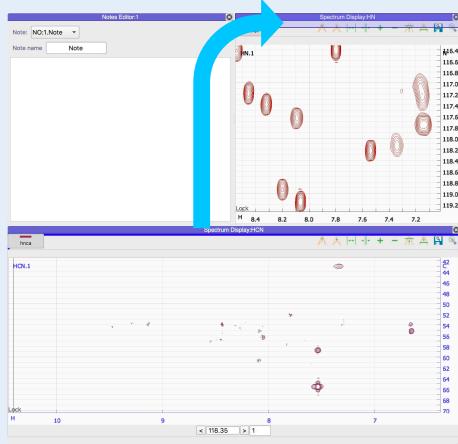
4A Rearrange a layout

To move a module:

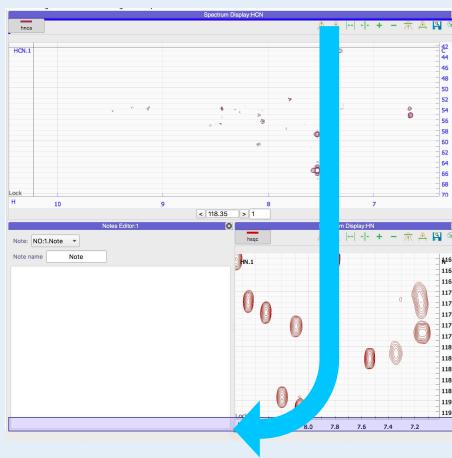
- hold the left mouse button down on the purple bar of the module (the module label). The module will be highlighted.
- drag it first over the top of any another module, this will activate the dropping area to accept the drop. A semi-transparent rectangle will appear
- keep holding the left mouse button down and move to either the top, bottom, left or right of another module, for each move the a new rectangle will appear, you can release the mouse to move the module to that position.

Rearranging Modules

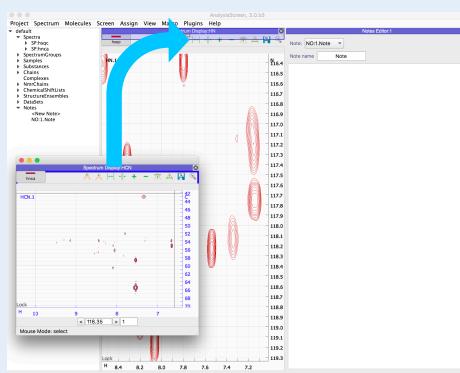
On top



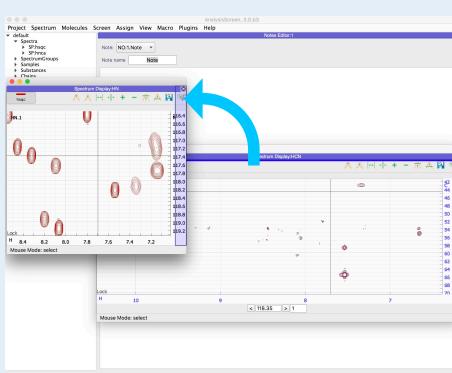
Under Two



Pop back into the main area



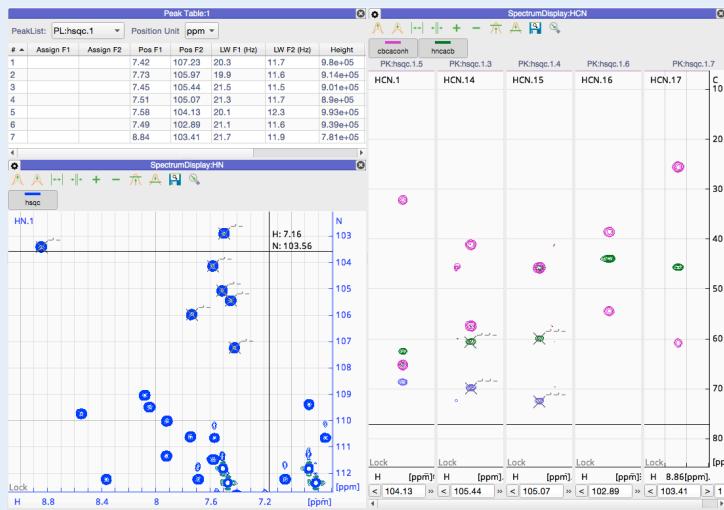
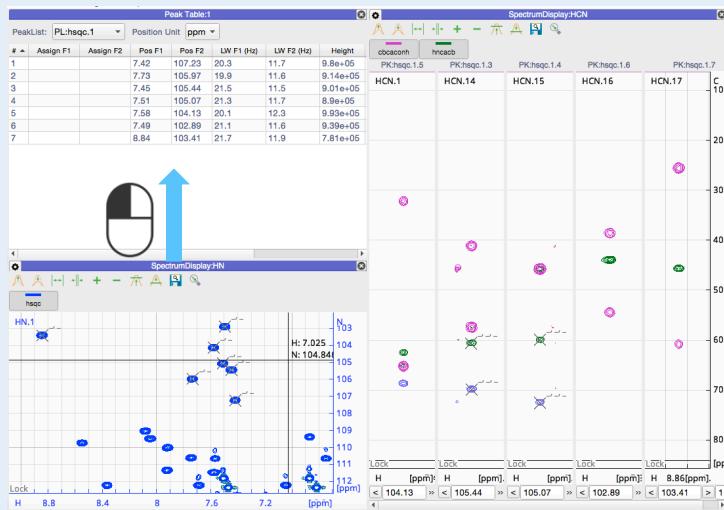
Move to a secondary area



In general, anything that is not a popup is a module and these can be easily rearranged in any way you want. Use the right click to see the available actions. You can also pop a module out; simply double click on the title bar. This will create a new window, containing the module and forms a secondary drop area. The secondary drop area has the same drag and drop features of the main drop area.

Rearranging Modules

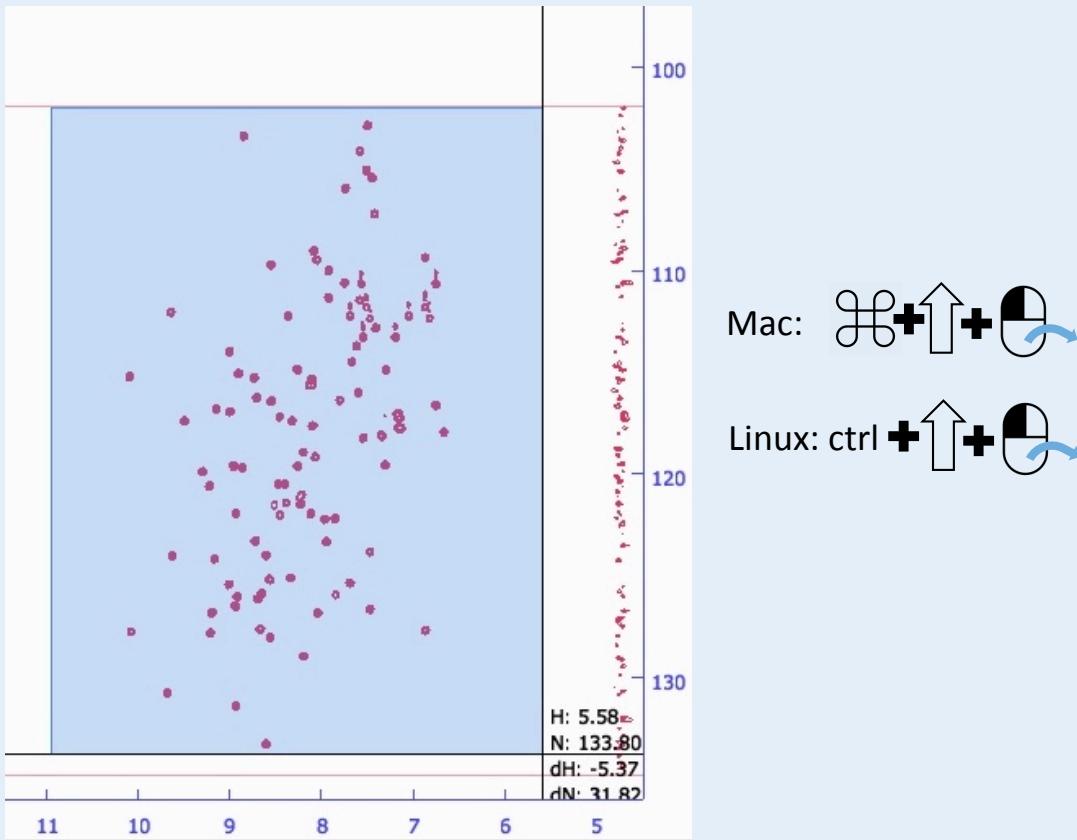
Re-size a module



4B Re-size a module

You can easily resize modules by left-dragging the edge of one into another.

Picking Peaks



The “Peak Picking Drop” parameter in the “Preferences” popup (Menu: Project → Preferences, tab Spectrum) affects peak picking. This parameter defines the percentage the intensity must drop from a local maximum (for positive peaks) in each dimension in each direction, in order for the position of the local maximum to be considered to be a peak. If this percentage is too high then some actual peaks might be missed, and if it is too low then too many peaks might be picked.

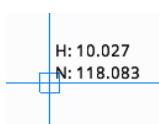
5A Manual Peak Picking:

CTRL (or CMD for Mac) + SHIFT + Left-drag

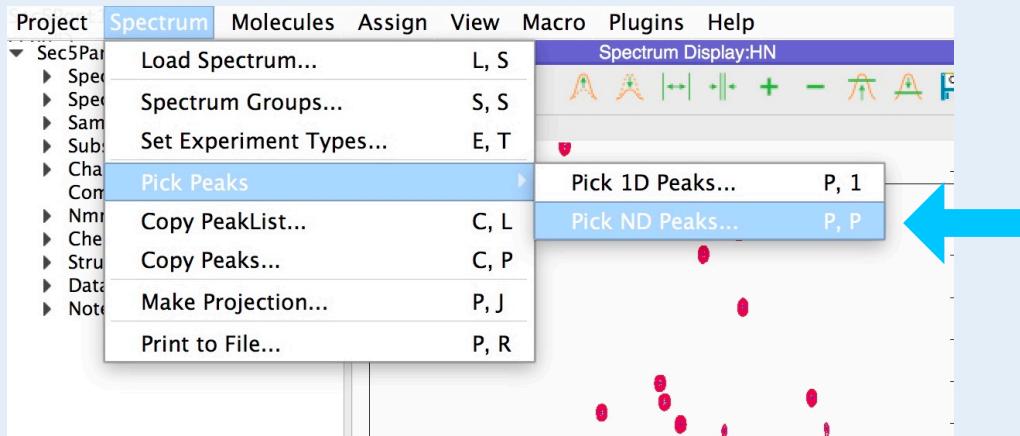
Click on the spectrum display, hold down CTRL(or CMD for Mac) plus SHIFT and left-drag the mouse to create a blue peak picking box.

You can place a single peak at a position of your choice by holding down CTRL / CMD plus SHIFT and left-clicking the mouse.

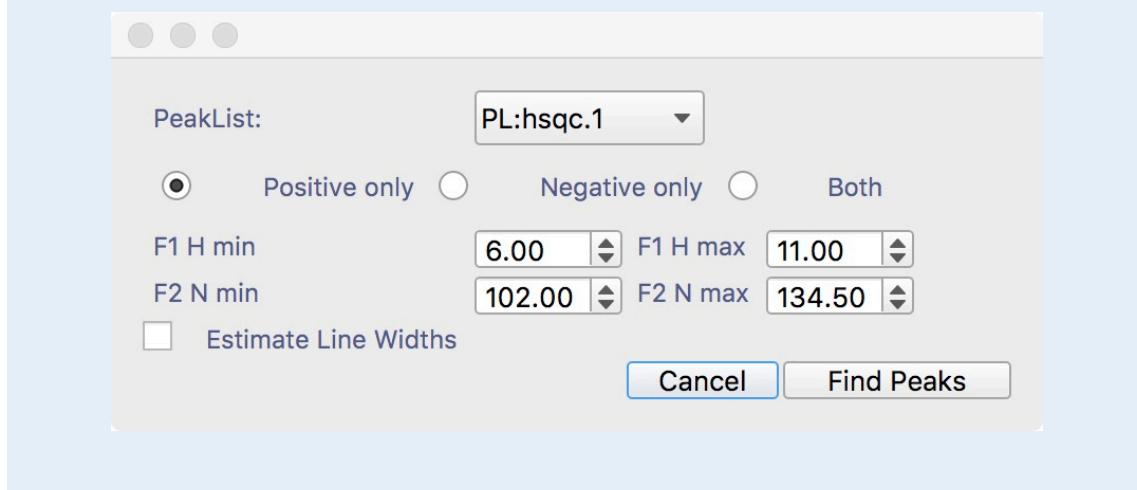
Alternatively, you can toggle the mouse into peak picking mode by typing the ‘MM’ shortcut and then you can repeatedly place peaks at positions of your choice. ‘SE’ will snap the peak to the nearest extremum.



Picking Peaks



or Shortcut ‘PP’



5B Automatic Peak Picking

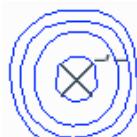
Main Menu → Spectrum → Pick Peaks → Pick ND Peaks...

shortcut ‘PP’

- Select types of peak to pick and the region
- Click Find Peaks

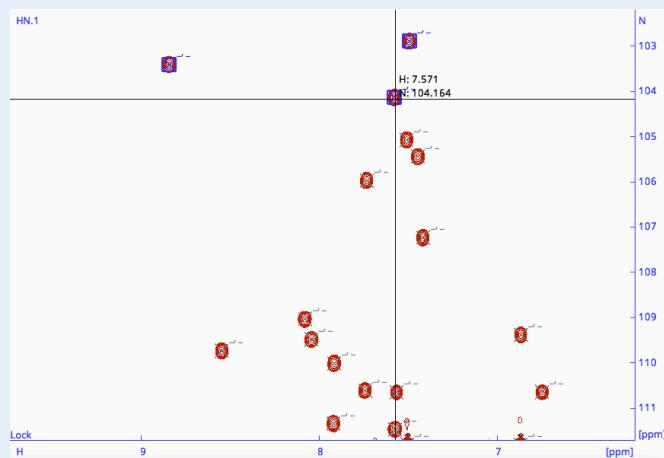
Result:

The crosses in the spectrum mark the peak positions picked. The hyphens separated by a comma indicate that the dimensions of these peaks are unassigned



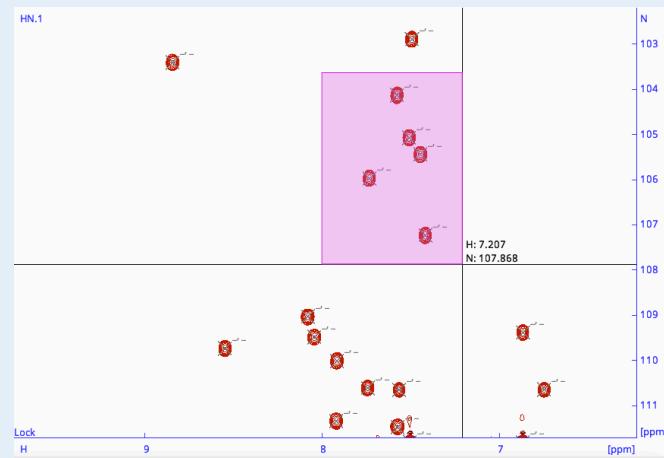
Picking Peaks

Selecting peaks



Mac:

Linux:



Mac:

Linux:

5C Selecting Peaks

To select a single peak:

left-click

on it with the mouse

To select several peaks at the same time:

Ctrl or Cmd (for Mac) + left-click

on peaks to select and/or deselect them

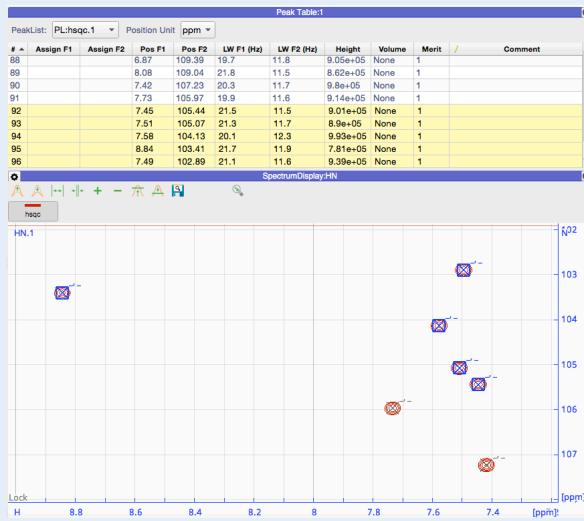
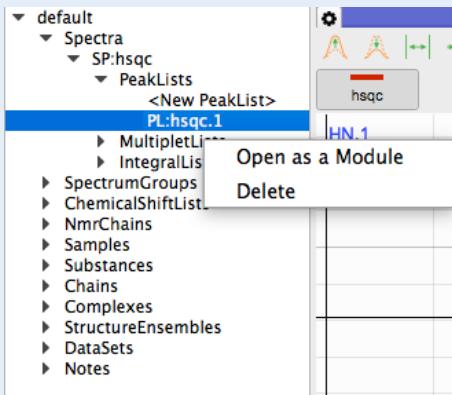
To select several peaks in an area:

Ctrl or Cmd (for Mac) + left-drag

A pink box will indicate the area in which you are selecting peaks.

Picking Peaks

Peak Lists

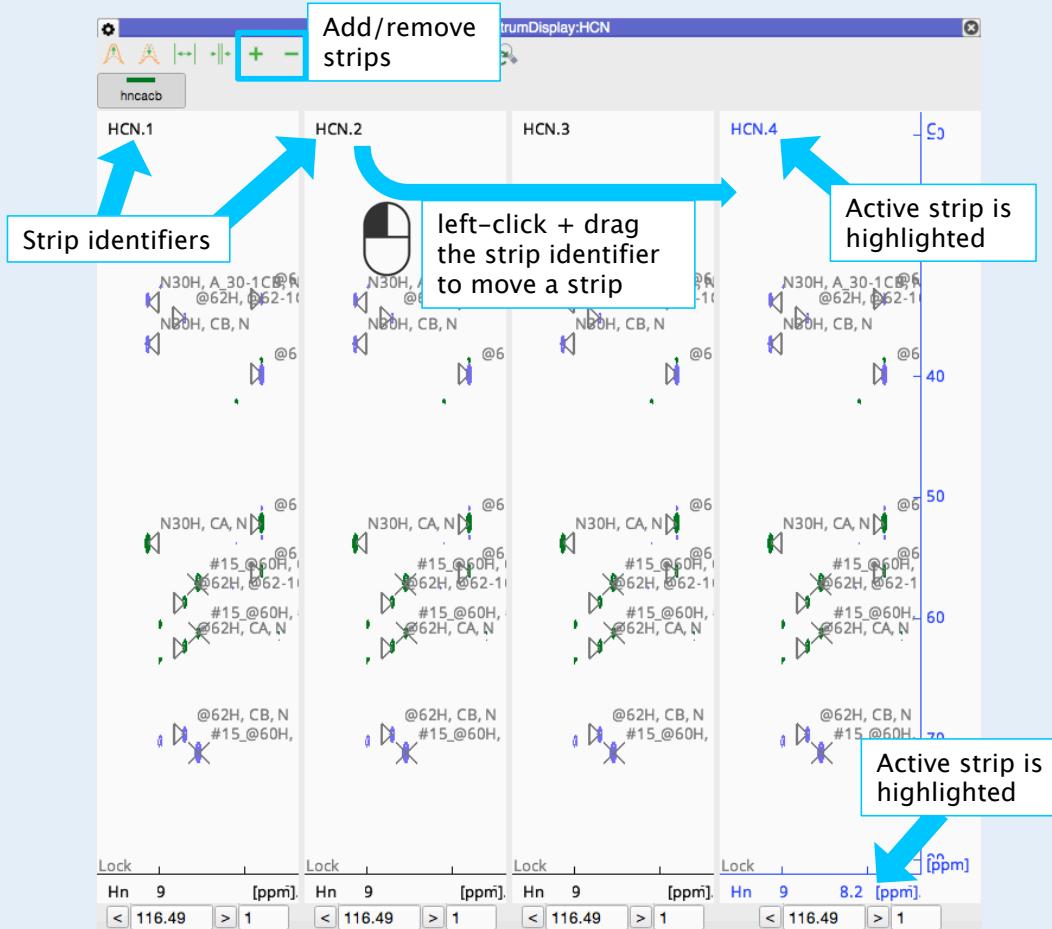


5D Peak Lists

Peak lists are nested underneath your spectra in the sidebar. If you right-click on a peak list you can open it as a module in the display area, or simply left-click and drag the peak list into the display area to the desired position.

If you select peaks in the peak list, this will automatically select them in the spectrum and vice versa.

If you double-click on a peak in the peak list, the spectrum will automatically jump to that peak and place it in the middle of the spectrum display.



By default the strips in a module share the y-axis of the last strip. If you want to give each strip their own y-axis you can toggle 'Share Last Axis' on and off in the right hand mouse menu or with the 'LA' shortcut.

6A Adding and removing strips

You can add or remove strips to/from any display with the '+' and '-' buttons in the display toolbar.

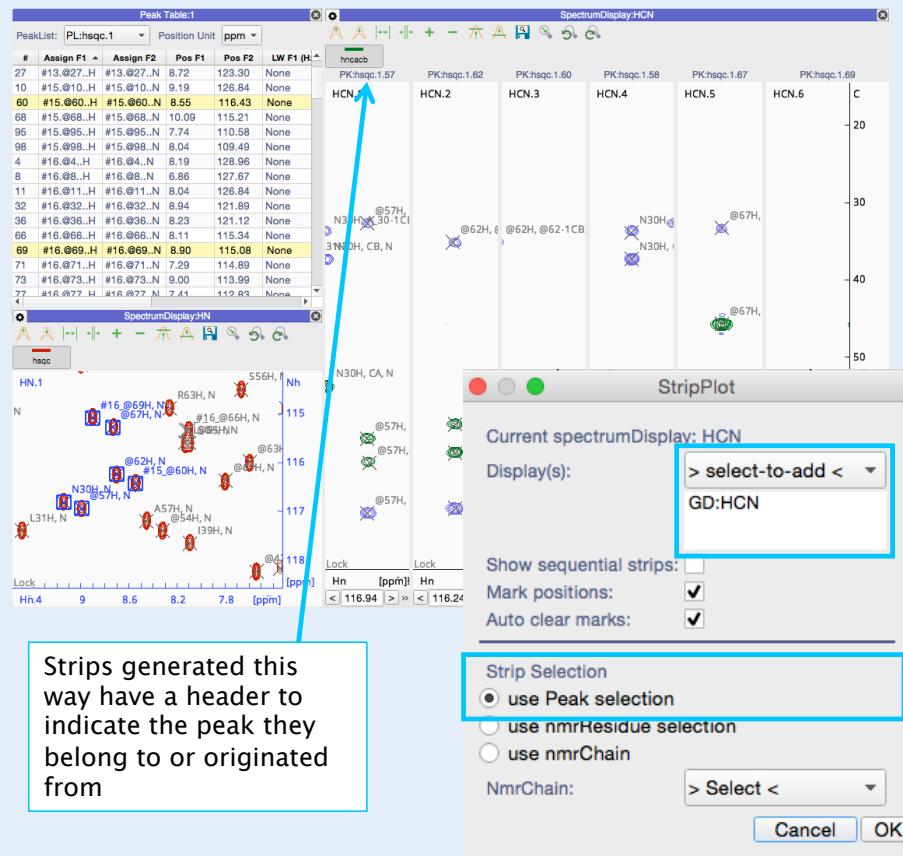
6B Moving Strips

You can move a strip by left-clicking the strip identifier and then dragging it to the desired position where you release it.

6

Working with Strips

Creating Strip Plots from selected peaks



Shortcut 'SP'

6C Creating Strip plots automatically

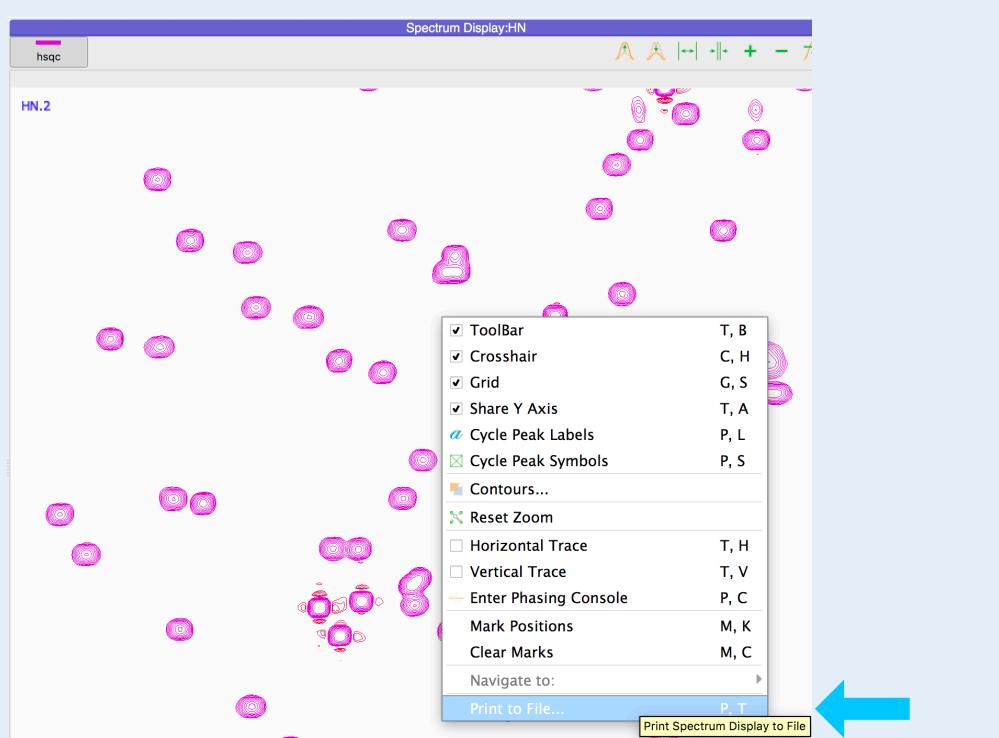
First select 4 or 5 peaks in your HSQC spectrum
To create a set of strips automatically from these peaks, go to
Main Menu → Spectrum → Make Strip Plot
shortcut 'SP'

You will see a pop-up in which you can select the display in which you want to show your strip plot – choose the HCN display.
For your strip selection choose ‘use Peak selection’.

Click OK and the strips will be generated automatically and they will each be given a header to indicate which peak they belong to and originated from.

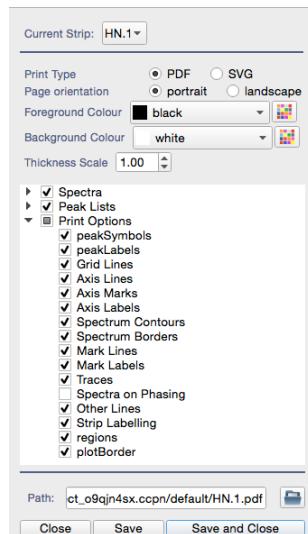


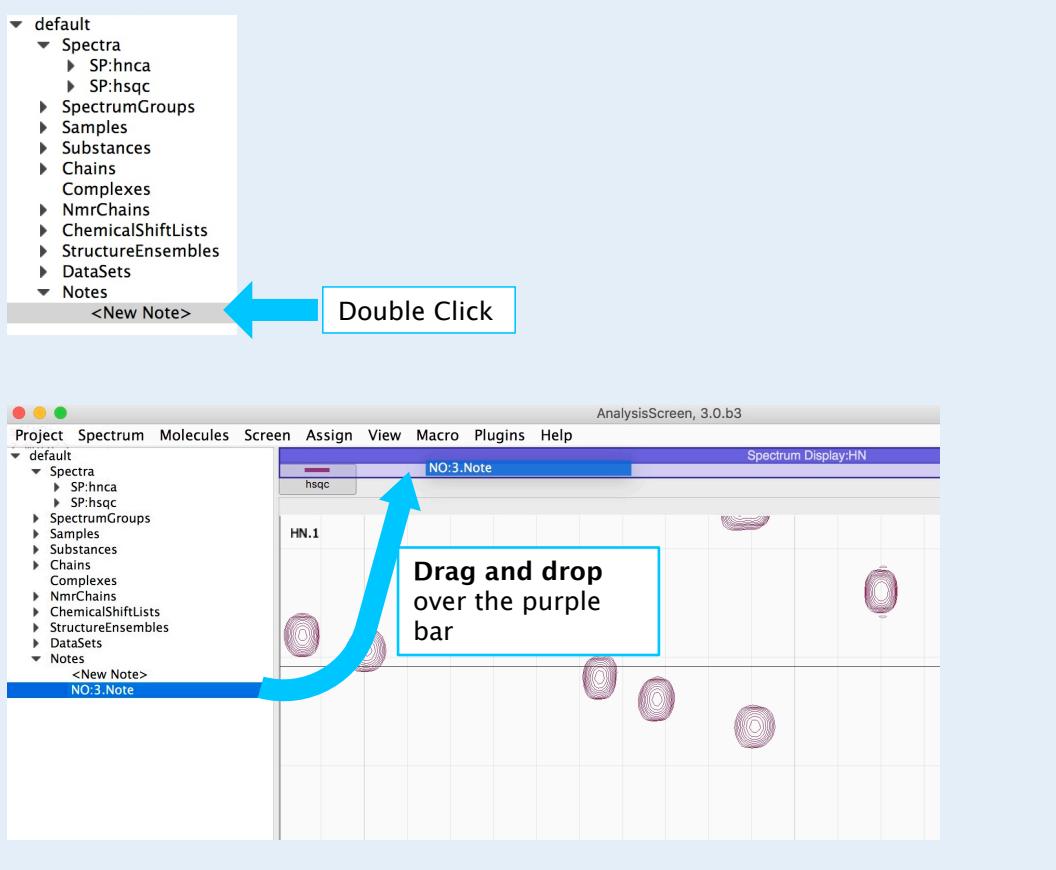
Printing spectra



7A Print to file

- Right click on a display to print
- Click on Print to File... The popup will appear
- Select the strip. You can select a single strip or all strips in the spectrum display.
- Select the other options as desired.
- Select a file name and path for the print file using the folder icon.
- Click Save or Save and Close.





8A Create a note

Analysis V3 also provides a means to make free text notes and store them with the project. To create a note:

- Go to the sidebar
- click on the Note arrow to expand the branch
- double click on on <New Note>. This will create a new note

To open it:

- Select the new item and drag it to the edge of any existing module and drop it as soon as you see a transparent purple box; alternatively, right click on the sidebar item and select “open as a module”
- You can write any text and all changes will be automatically saved in the project.

Contact Us

Website:

www.ccpn.ac.uk

Suggestions and comments:

ccpnmr3@google.com

Issues and bug report:

<https://bitbucket.org/ccpnmr/issue-tracker/>

Cite Us

Skinner, S. P. et al. CcpNmr AnalysisAssign: a flexible platform for integrated NMR analysis. *J. Biomol. NMR* (2016). doi:10.1007/s10858-016-0060-y

Tutorial Version History:

beta1 (SS): First version

beta2 (GWV): Minor changes

beta3 (LGM): Re-designed and added several steps

beta5 (VAH): Added more steps