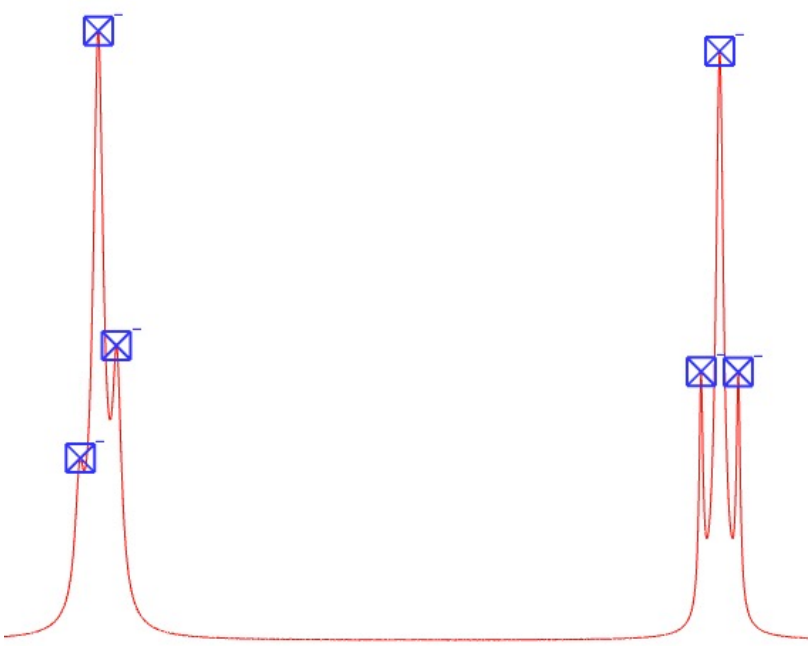
CCPN

CcpNmr AnalysisScreen Version 3

How To's:

Pick 1D Peaks



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.

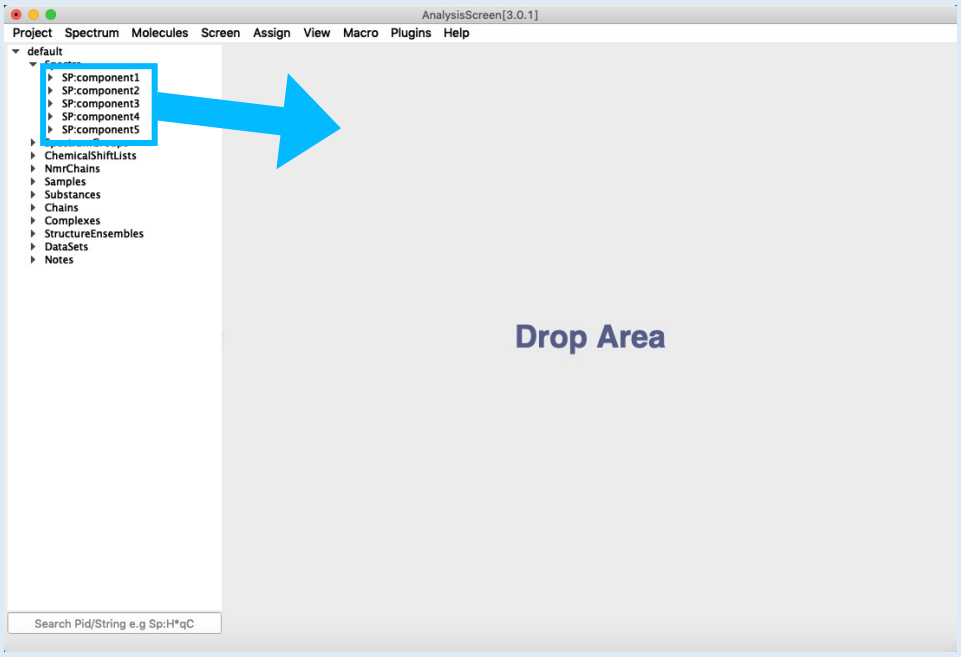
For more commands and operations

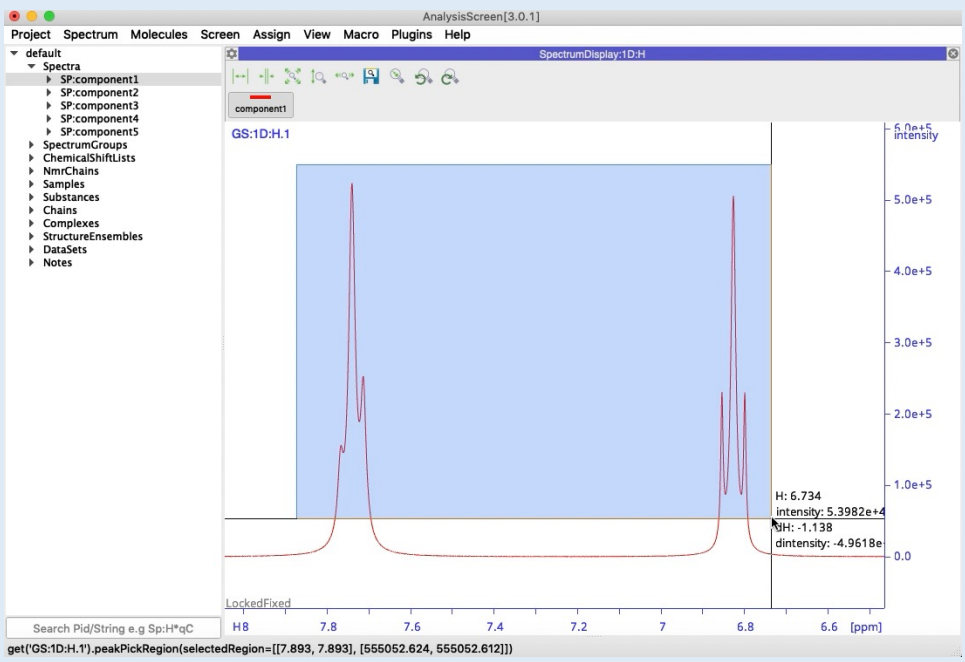
Main Menu ⟶ Help ⟶ Tutorials ⟶ Beginners Tutorial

OR

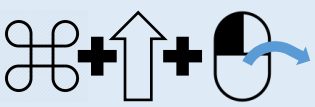
Main Menu ⟶ Help ⟶ Show Shortcuts

1 1D Peak Picking



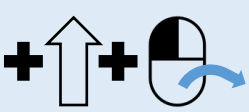


Mac:



Linux/Windows:

Ctrl



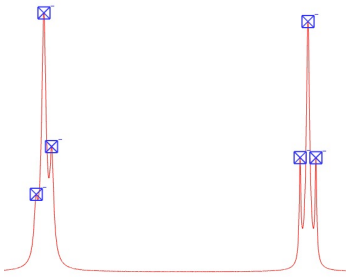
1A Drag Spectrum into Display

- Drag one or more 1D spectra from the sidebar into the drop area.

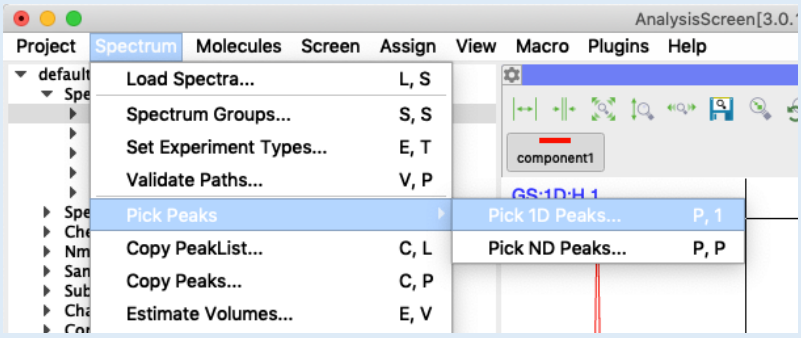
1B Pick Peak Manually

- Adjust the displayed region of the spectrum by changing the zoom or aspect ratio if necessary.
- Press **Shift** + **Ctrl** (**Cmd** on Mac) while **left-dragging** the mouse over the peaks you would like to pick. The region will be highlighted in blue.

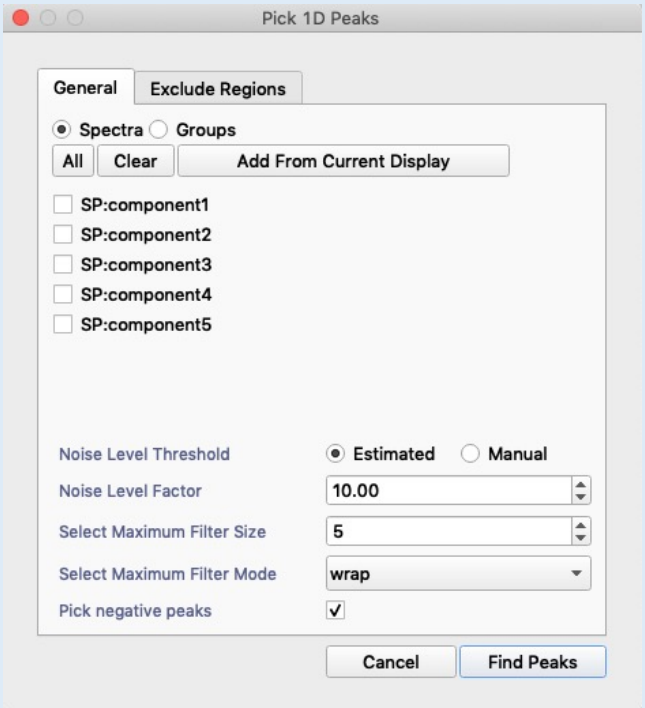
All picked peaks will be marked with with a peak symbol:

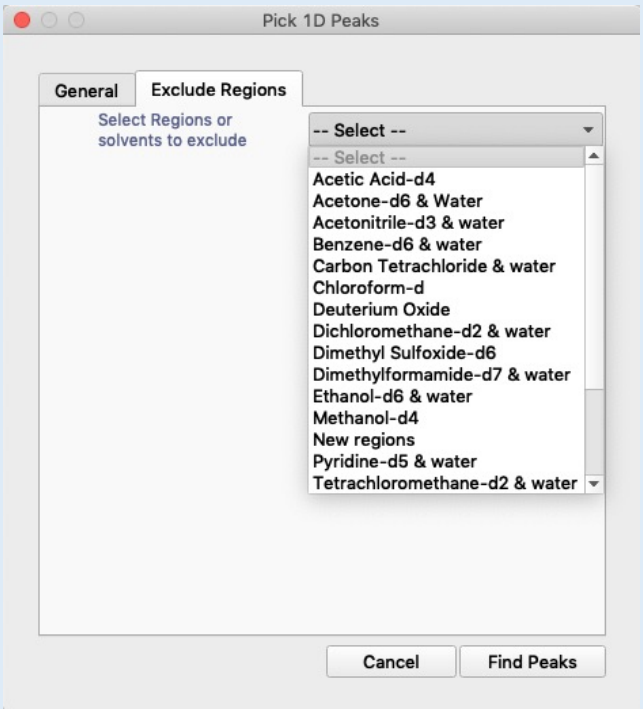


1 1D Peak Picking



P1





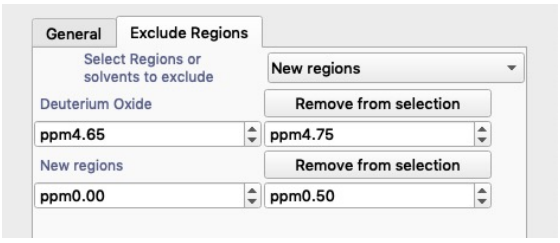
1C Automatic Peak Picking

- Go to **Main Menu ⟶ Peak Picks ⟶ Pick 1D Peaks**

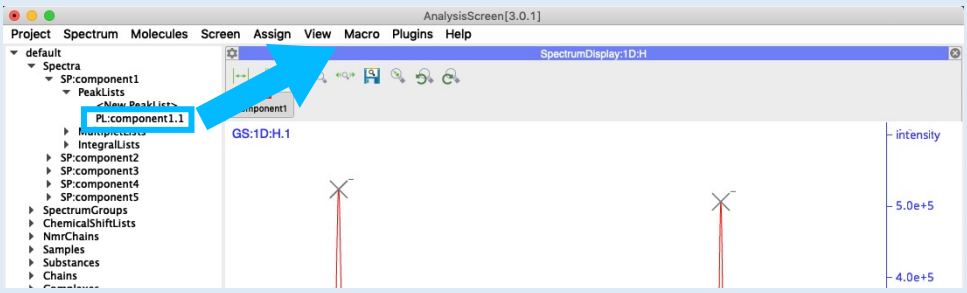
OR

- Use shortcut **P1**

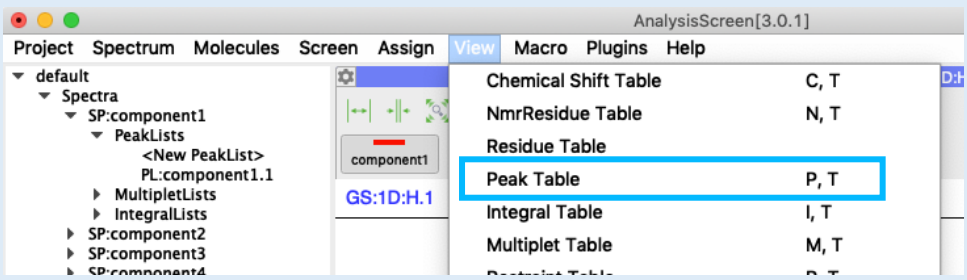
- Select the required **Spectra** or **SpectrumGroups**.
- Leave the **Noise Level Threshold** as **Estimated** if you have different types of noise across all the spectra you have selected.
- Increase the **Maximum Filter Mode** if you have very noisy spectra or spectra with a large number of "shoulder" peaks.
- In the **Exclude Regions** tab you can select regions of the spectrum where you don't want to pick peaks. Add regions by selecting solvent(s) from the list or add your own bespoke region by selecting **New regions**. Make multiple selections to add multiple regions.
- Click **Find Peaks** to pick the peaks.

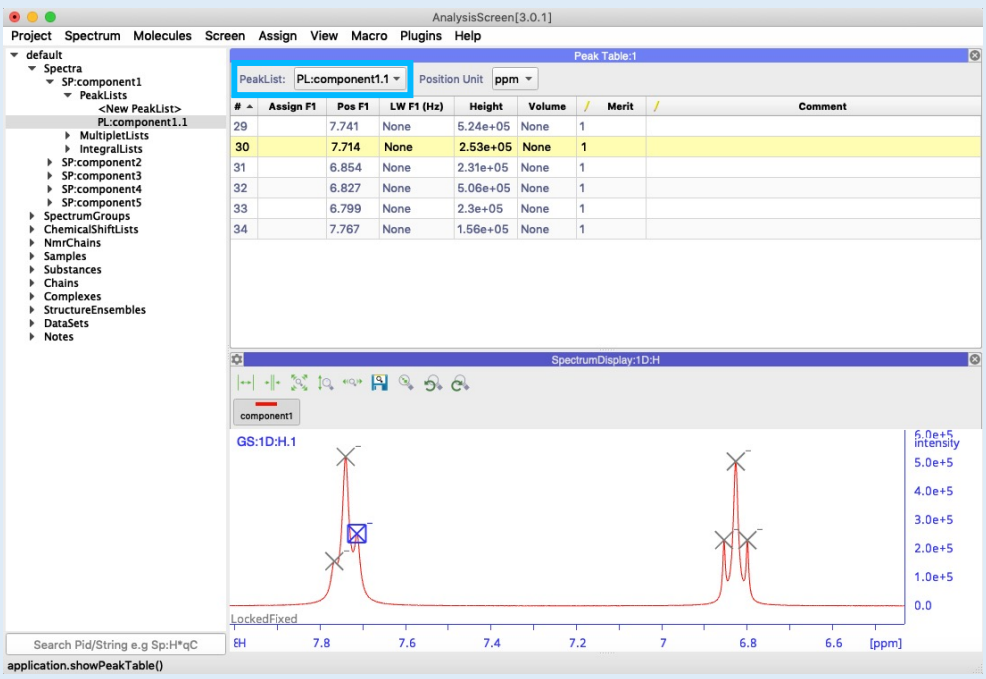


1 1D Peak Picking



PT





1D Open Peak Table

- Expand the **Spectra** branch in the sidebar and then the **Peak Lists** branch.
- **Drag** a peak list into the drop-area.

OR

- Go to **Main Menu → View → Peak Table**

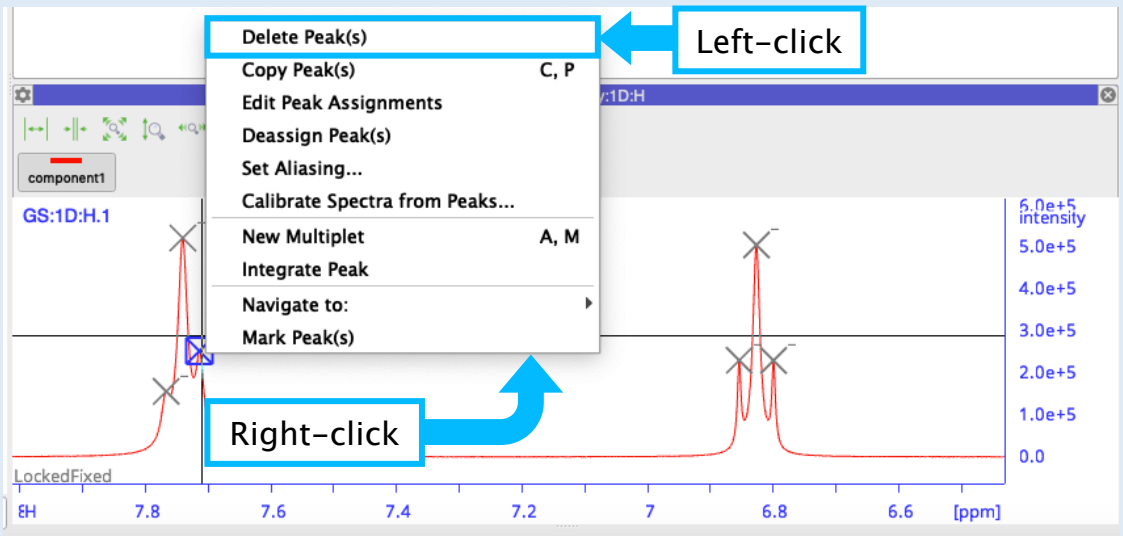
OR

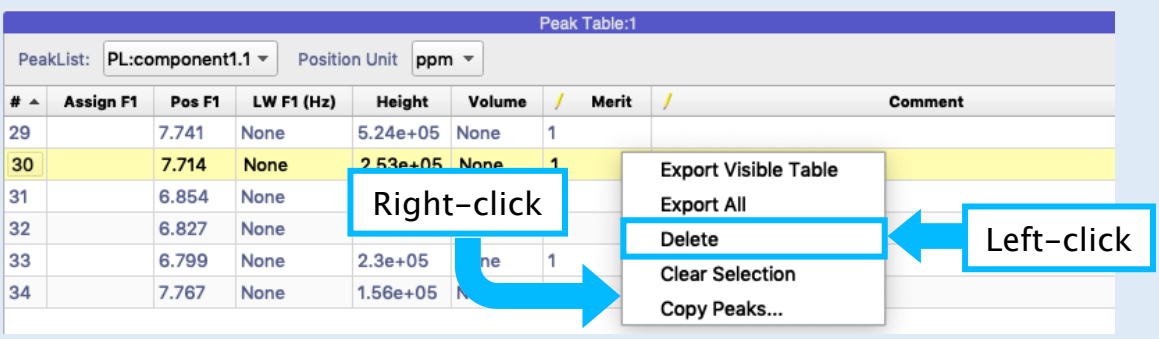
- Use the shortcut **PT**

The peak table will open. You can use the drop-down menu to view a different peak table in that module.

Note that peaks selected in the table are also selected in the spectrum and *vice versa*.

1D Peak Picking





1E Deleting Peaks in the Spectrum Display

- **Select a Peak** by **left-clicking** on it. Press **Ctrl** (**Cmd** on a Mac) to select multiple peaks.
- **Right-click** on a selected peak and select **Delete Peak(s)**.

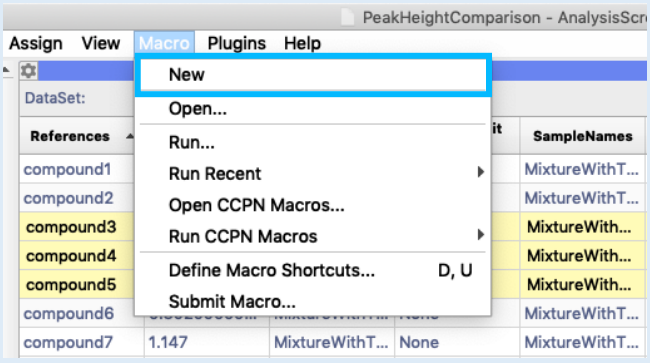
1F Deleting Peaks in the Peak Table

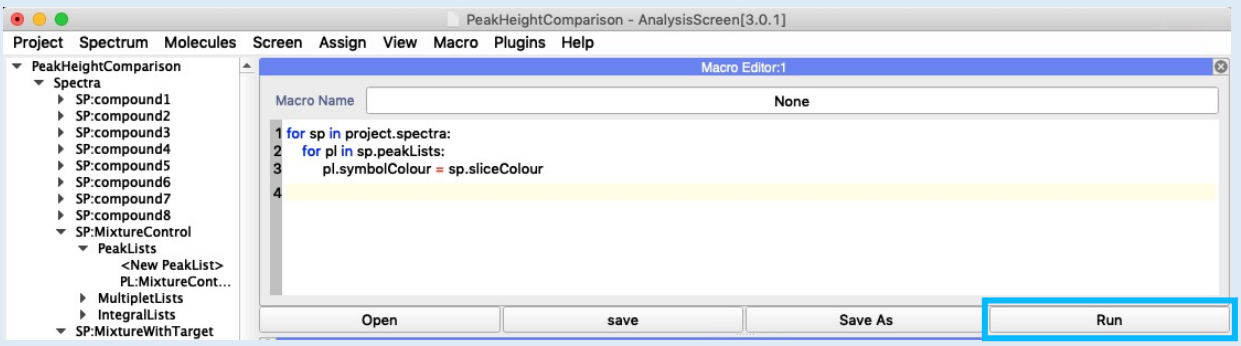
- Select the peak(s) you want to delete in the table. Use **Shift** or **Ctrl** (**Cmd** on Mac) to select multiple peaks, or **Ctrl**/**Cmd**+**A** to select all peaks in the table.
- **Right-click** and select **Delete**.

OR

- Use the **Delete** button on your keyboard (**fn** + **Backspace** on Mac).

1 Peak symbol colours





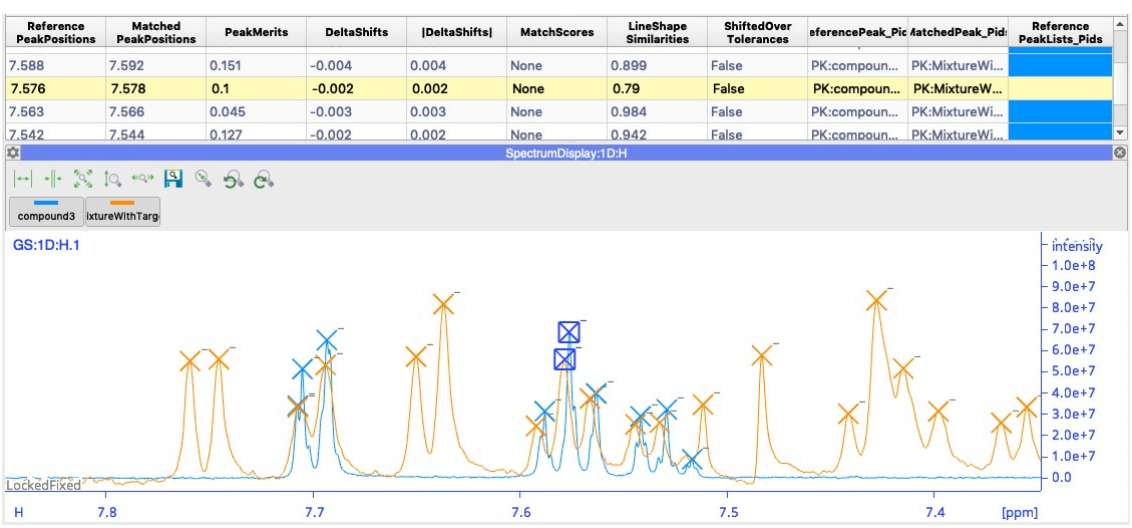
Change peak symbol colours

You may find it easier to examine your data if the peak symbols have the same colour as your spectra. You can easily change the peak symbol colour using a short Macro:

- Go to **Main Menu ⟶ Macro ⟶ New**
- **Copy and Paste** the following text into the **Macro Editor** window:

```
for sp in project.spectra:
    for pl in sp.peakLists:
        pl.symbolColour = sp.sliceColour
```

  making sure that the indentations are retained correctly.
- **Click** on the **Run** button. Your **Hit Analysis** and **Spectrum Display** modules should update with the new peak list colours:



- Now close the **Macro Editor** module again, saving the macro if you wish.

Contact Us

Website:
www.ccpn.ac.uk

Suggestions and comments:
support@ccpn.ac.uk

Issues and bug reports:
https://www.ccpn.ac.uk/forums

Cite Us

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)

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