How To’s:

Pick 1D Peaks
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**
1D Peak Picking

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 a peak symbol:
1D Peak Picking

Automatic Peak Picking

• Go to Main Menu → Peak Picks → Pick 1D Peaks
• 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.
**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).
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:
  ```python
  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.