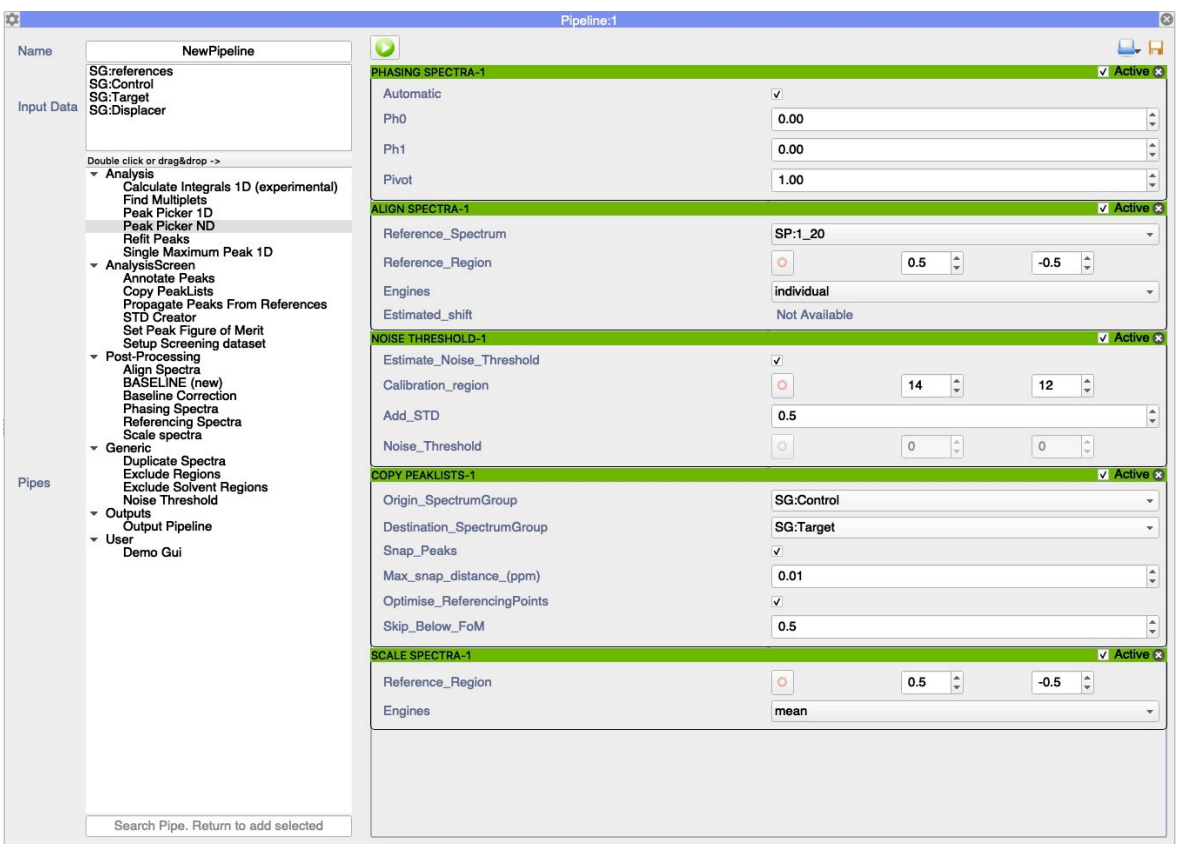
CCPN

CcpNmr AnalysisScreen Version 3

How To's:

Pipelines



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

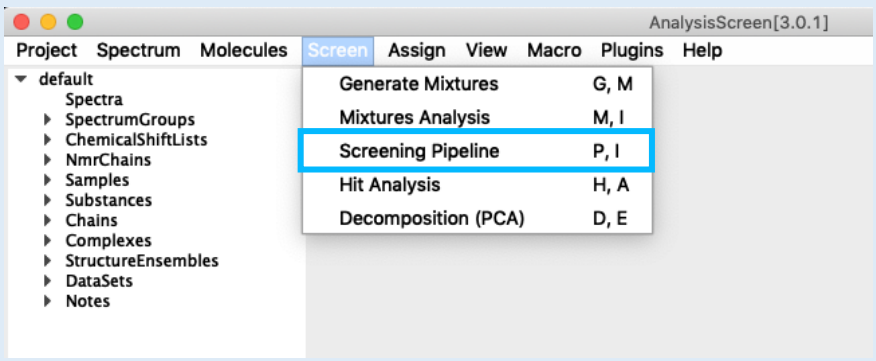
1 Pipelines

The Pipeline is the core module of AnalysisScreen. It allows you to apply several tasks or algorithms, called pipes, to single spectra or groups of spectra (SpectrumGroups).

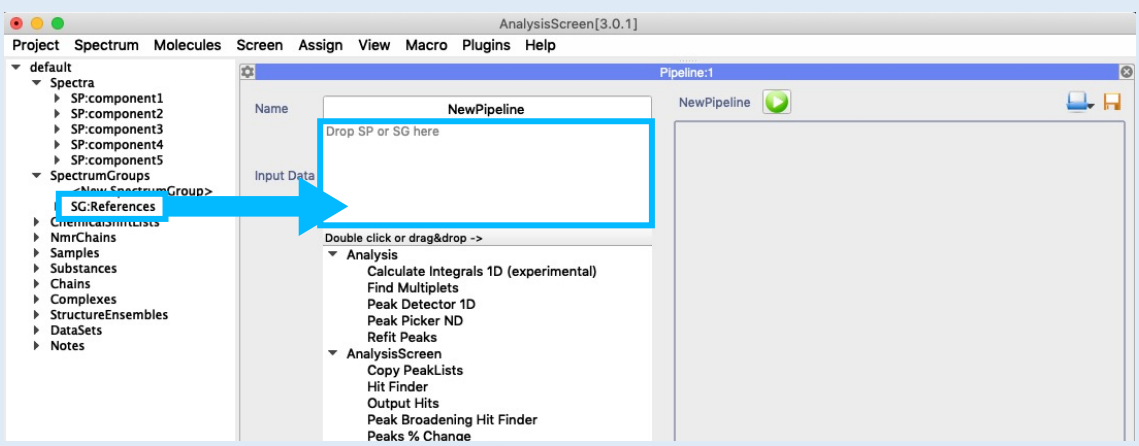
You can run single pipes or a queue of pipes, where the output from each pipe will be the new input for the next pipe.

The pipeline module has been built to be a flexible tool, and this tutorial will show you only a few of the features available for 1D spectra. We will be continually adding new pipes, including pipes for 2D spectra.

Information about pipes not shown here is available within the software.



PI



1A Open Pipeline Module

- Go to **Main Menu ⟶ Screen ⟶ Pipelines**

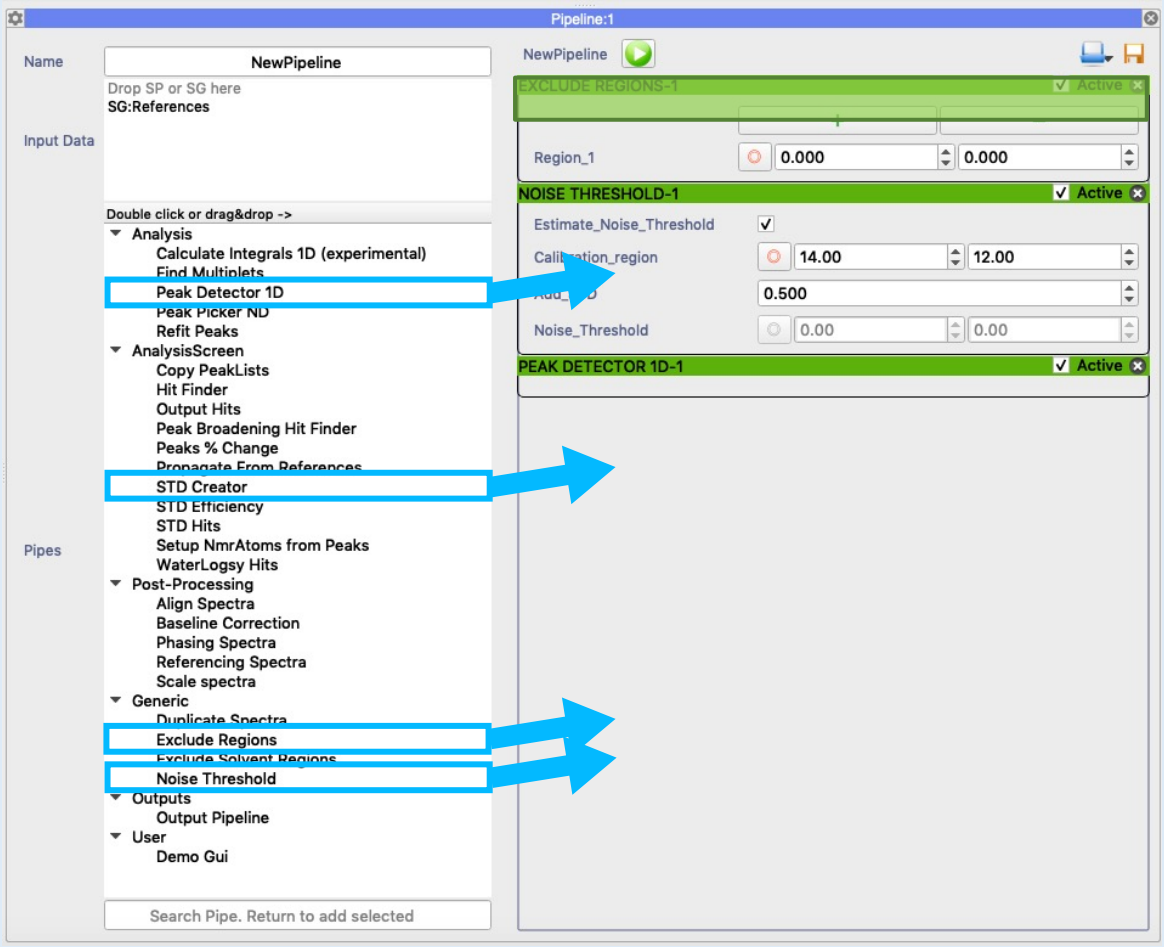
OR

- Use the shortcut **PI**

1B Select Spectra to apply Pipeline to

- **Drag and Drop** one or more **Spectra** or **Spectrum Groups** from the sidebar into the **Input Data** box.

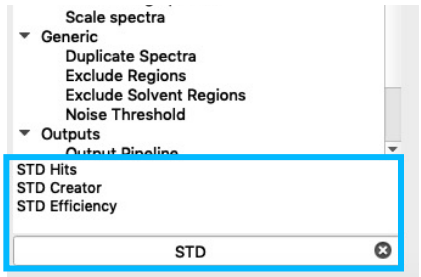
1 Pipelines



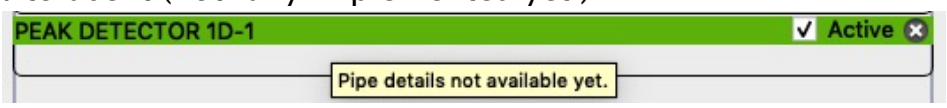
1C Add Pipes to Pipeline

- **Drag and Drop** pipes from the left-hand side of the module to the right (or **double-click** pipes on the left) in order to add pipes to your pipeline. Similar to when dragging modules, you will see a green box appear once you start to drag your pipe, showing you where your pipe will be dropped, e.g. above, below or in between other pipes that are already present.

You can search for pipes using the **Search Box** and **drag** pipes directly from the search results Box, or add a selected pipe by pressing **Enter**.



If you hover over the top bar of a pipe you will see information about what the pipe does and how to use it (not fully implemented yet!).



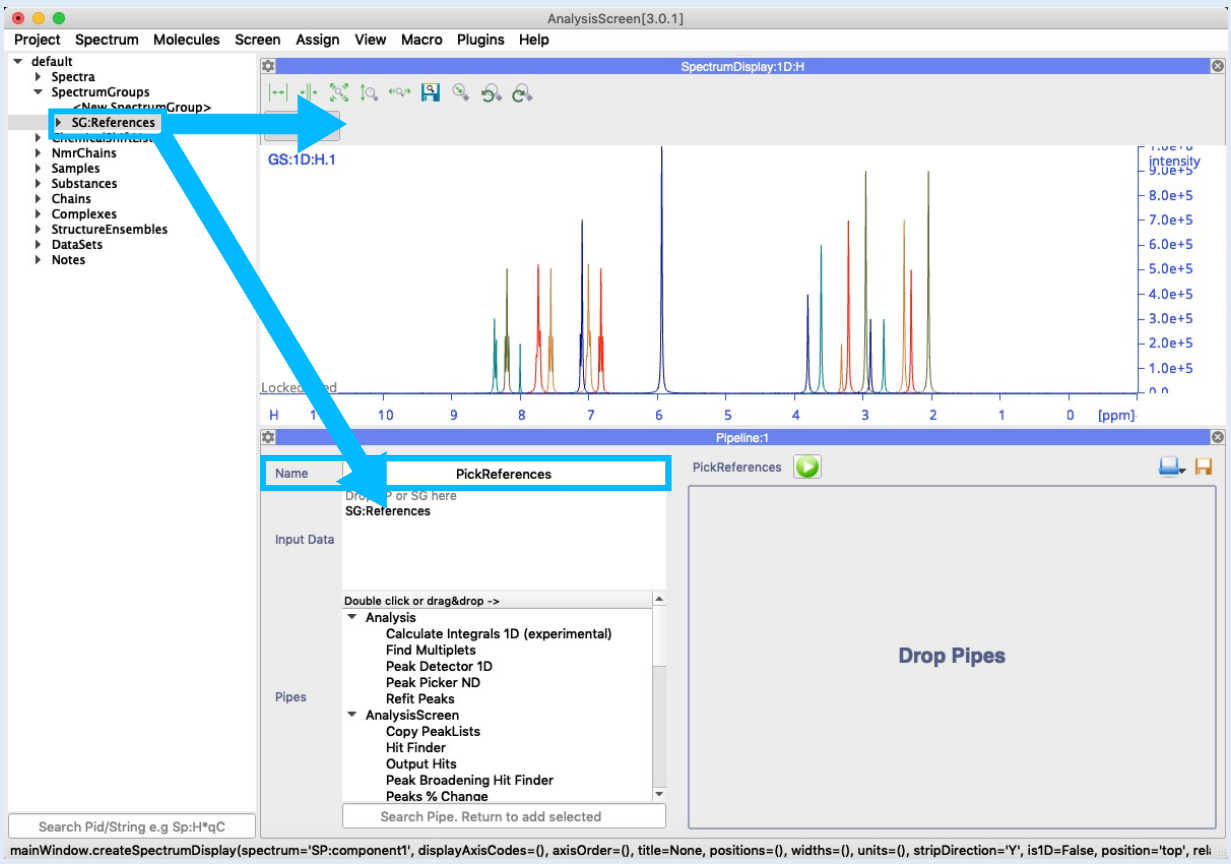
1D Saving and opening pipelines

You can save a pipeline as a .json file for later use, for use in another project or you can pass it on to a colleague to use.

- **Click** on the  icon in the top right-hand corner to save your pipeline as a .json file.
- **Click** on the  icon to open a saved pipeline.

2 Picking Reference Peaks Pipeline

This Pipeline will help you pick the peaks in all your reference spectra.



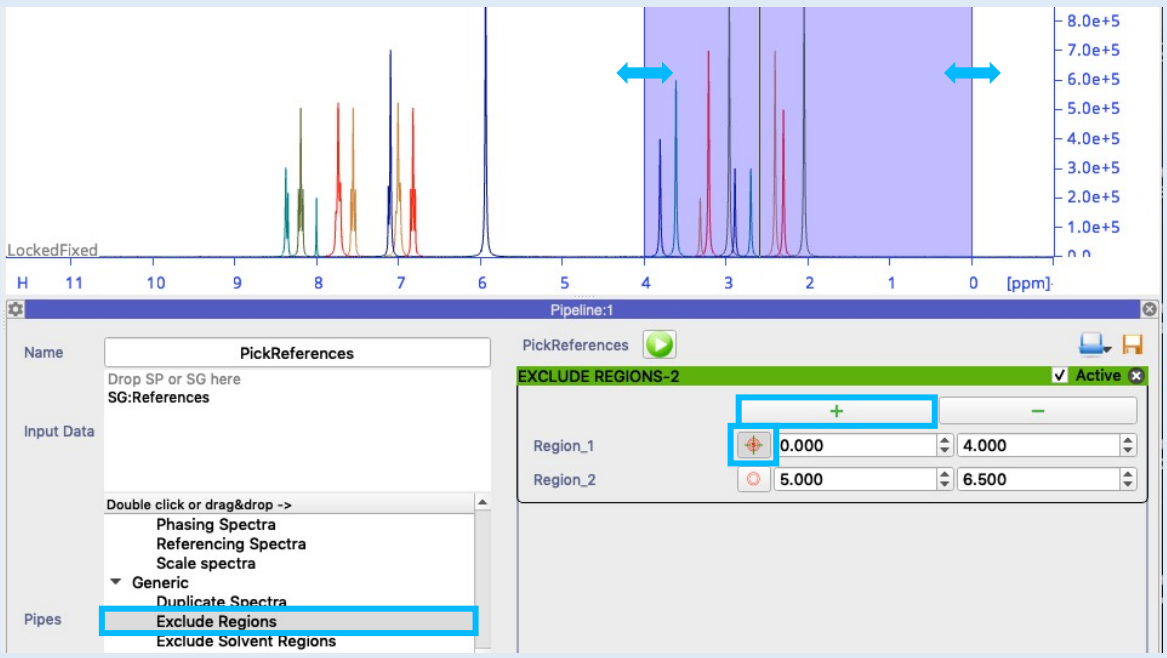
2A Open Project

- **Drag** the **ScreenTutorial/Projects/PickReferencePeaks.ccpn** project into the Drop Area.
- Drag and drop the **References Spectrum Group** into the **Drop Area.**

2B Set up Pipeline

- Open the pipeline module with **PI** or **Main Menu → Screen → Pipelines** and place it below your spectra.
- Give your new Pipeline a name if you like.
- **Drag** the **References Spectrum Group** from the sidebar into the **Input box**.

2 Picking Reference Peaks Pipeline



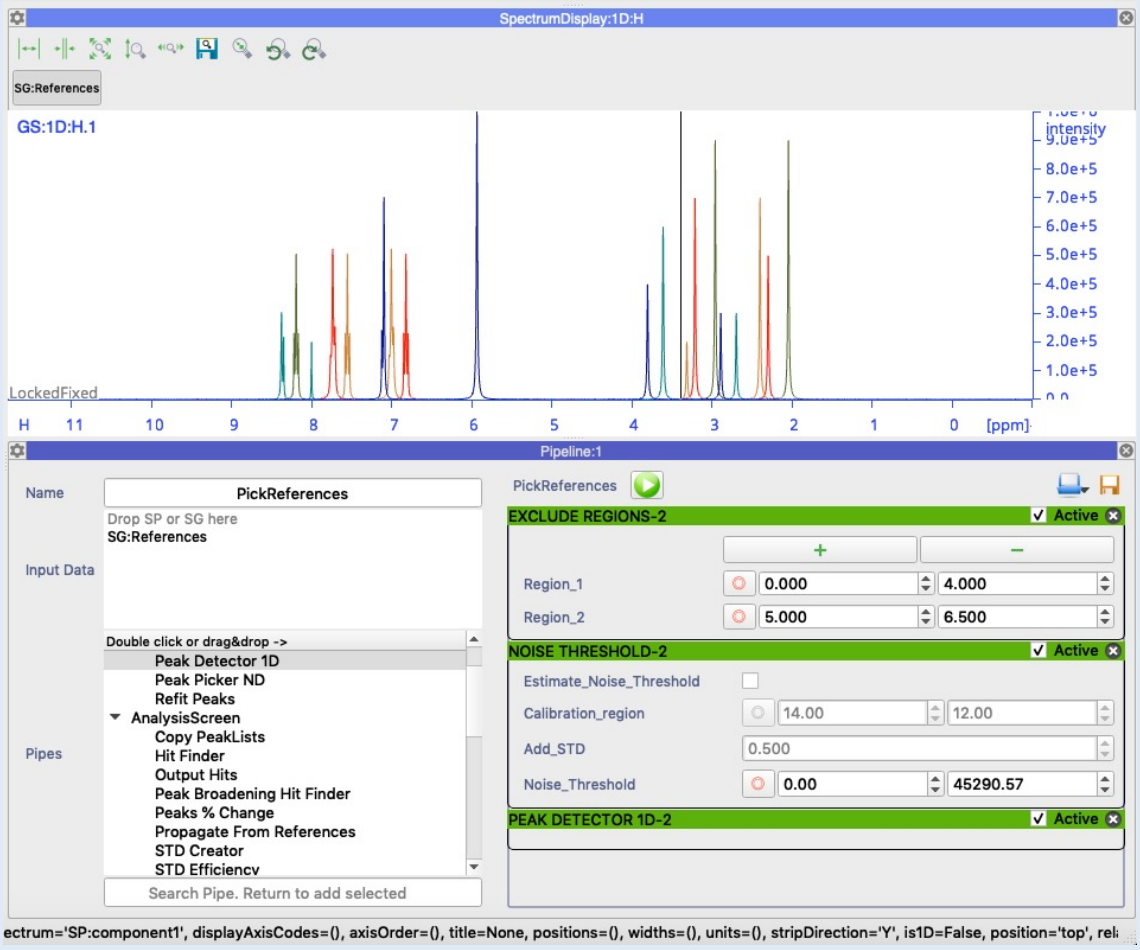
2C Add Exclude Regions Pipe

- **Drag** the **Exclude Regions** pipe into your pipeline.
- Set a region from 0-4ppm to be excluded from peak picking by entering the values into the boxes, or clicking on the icon and using the mouse to adjust the region in the Spectrum Display.
- **Click** on the + to add a second exclusion region at 5-6.5ppm

2D Add Noise Threshold Pipe

- **Drag** the **Noise Threshold** pipe into your pipeline.
- To use automatic Noise Estimation, leave **Estimation** ticked and select a region of the spectrum to be used for the estimation.
- To set a threshold manually, **untick Estimation** and set the noise level using the box or via the icon and the moue in the display.

2 Picking Reference Peaks Pipeline

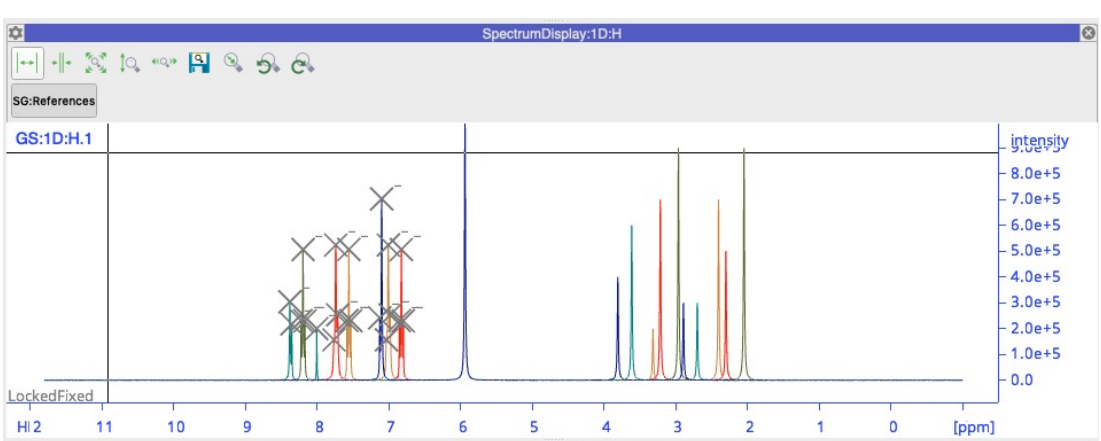


2E Add Peak Detector Pipe

- **Drag** the **Peak Detector** pipe into your pipeline. This works fully automatically with no manual adjustments required.

2F Run the Pipeline

- **Click** the green **Play button**  . You should now see that the peaks in your reference spectra are picked (in the regions you did not exclude).



Contact Us

Website:
www.ccpn.ac.uk

Suggestions and comments:
ccpnmr3@gmail.com

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)