

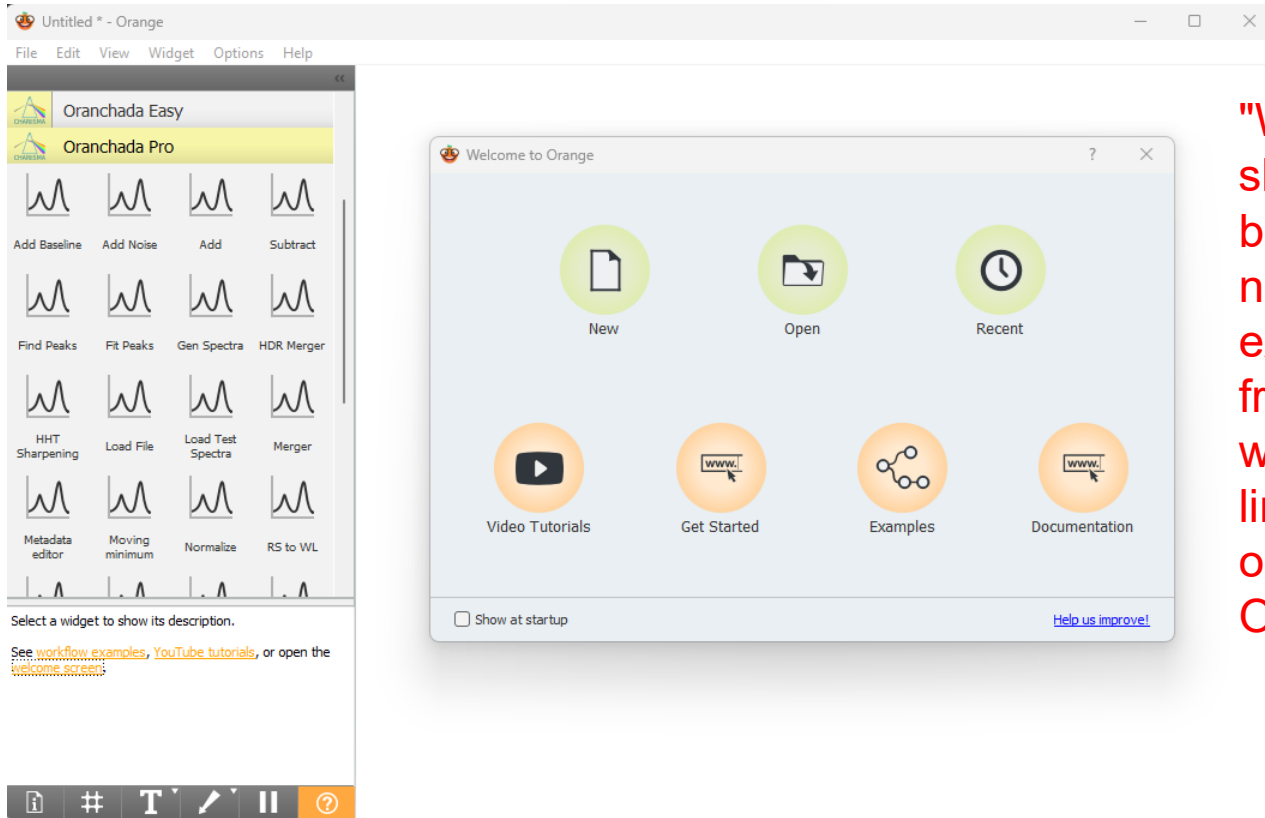
# ORANCHADA

## Widget usage examples

(visual guide ver.01, 2023 05 30)

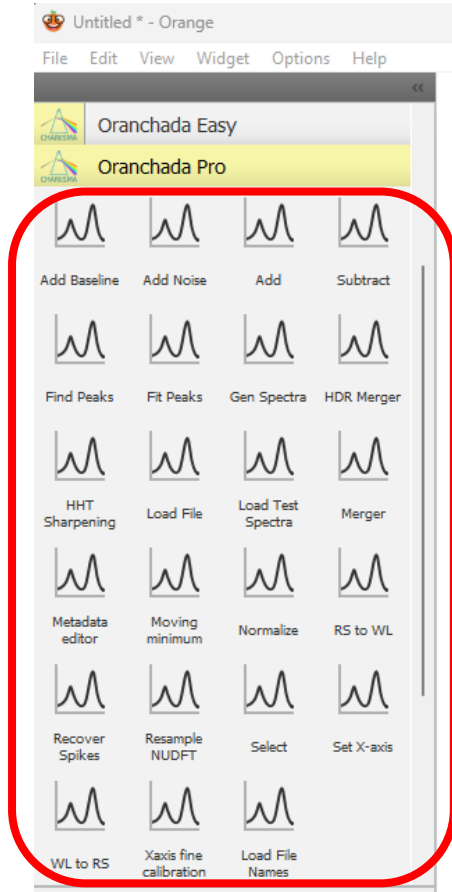
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Georgi Georgiev, Luchesar Iliev, Nina Jeliazkova  
IdeaConsult Ltd.

# Starting the program Orange



"Welcome to Orange" shows some important basic functions: create a new project, open an existing one, or choose from the ones we recently worked on. There are also links to helpful information on how to work with Orange.

After successful installation of **Oranchada** add-on, you should see a set of widgets.



**On the left you can see the main set of Oranchada Pro widgets:**

*Add Baseline, Add Noise, Subtract, Find Peaks, Fit Peaks, Gen Spectra, HDR Merger, HHT Sharpening, Load File, Load Test Spectra, Merger, Moving minimum, Normalize, RS to WL, Recover Spikes, Resample NUDFT, Select, Set X-axis, Xaxis fine calibration and Load File Names.*

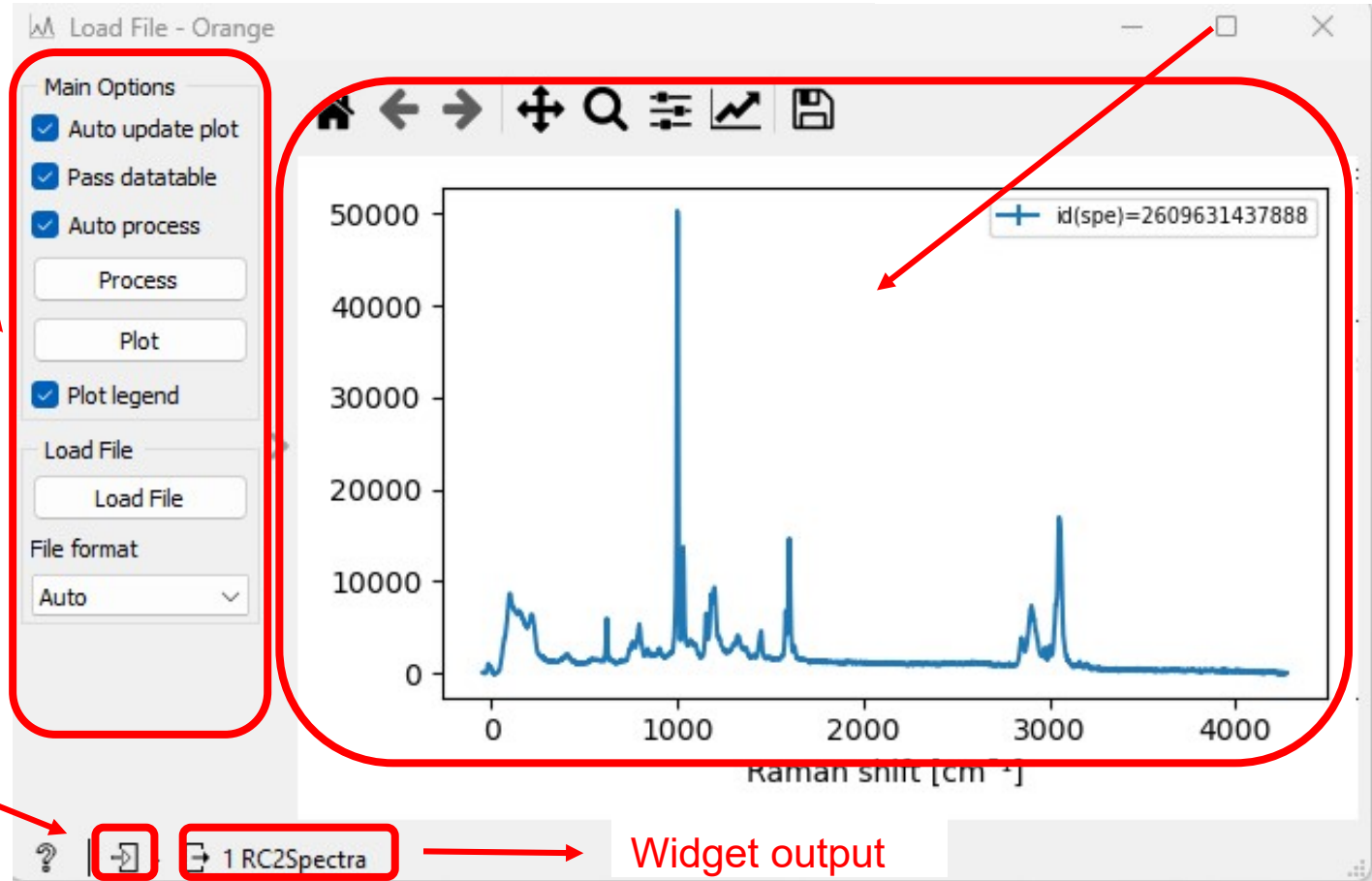
# Basic structure of all widgets

Widget options and settings

Resulting plot spectra

Widget input

Widget output



Load File - Orange

#### Main Options

- ☒ Auto update plot
- ☒ Pass datatable
- ☒ Auto process

Process

Plot

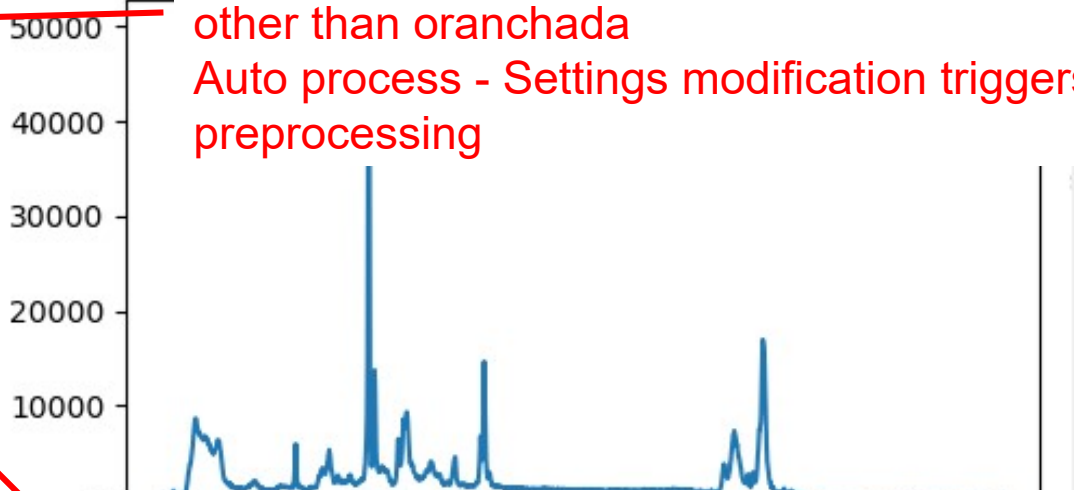
- ☒ Plot legend

#### Load File

Load File

File format

Auto



### Main options:

Auto update plot - Settings modification triggers plot update

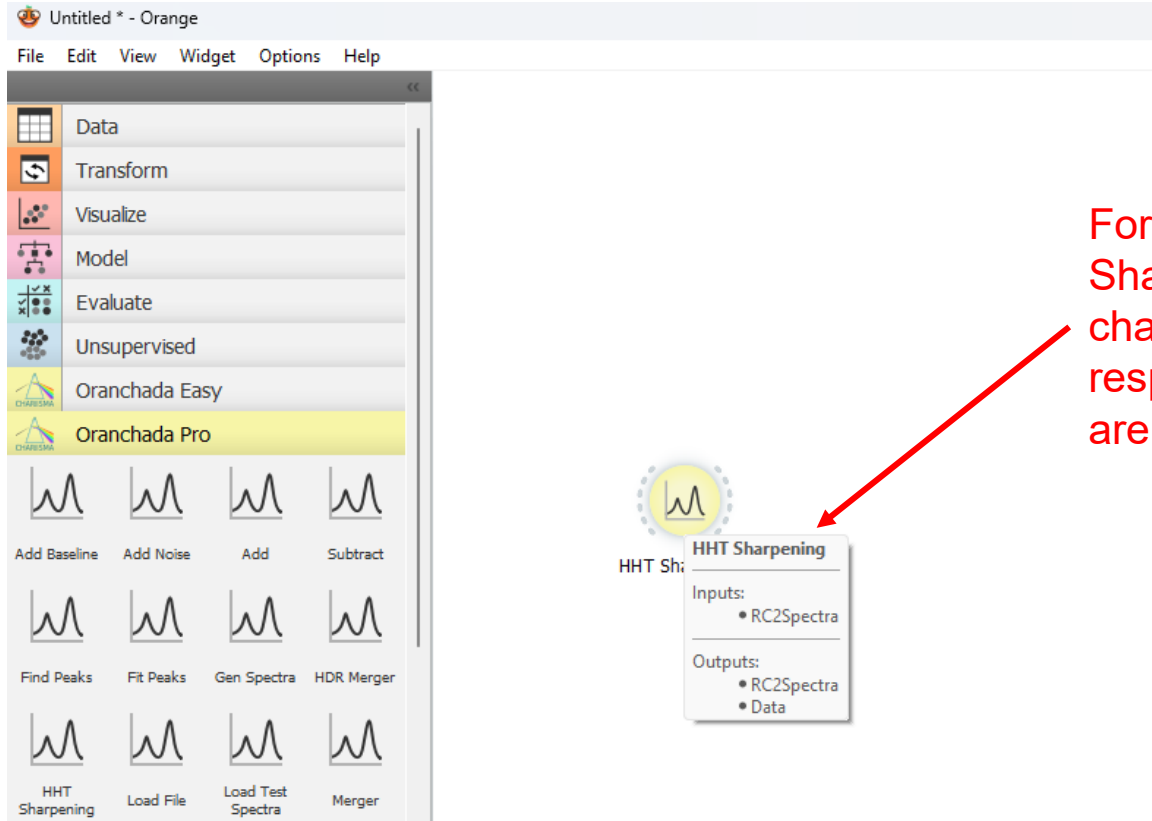
Pass datatable - Generate output compatible with widgets other than oranchada

Auto process - Settings modification triggers auto preprocessing

### Preprocessing settings:

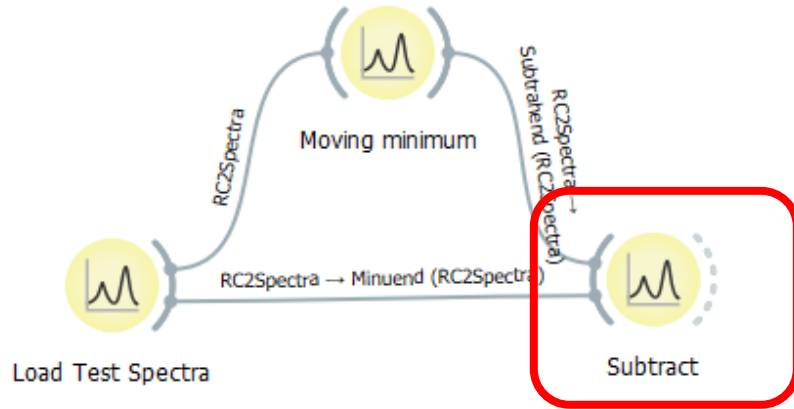
specific settings according to widget functionality

# When mouse is over a widget, Orange shows a tip with the input and output widget channels

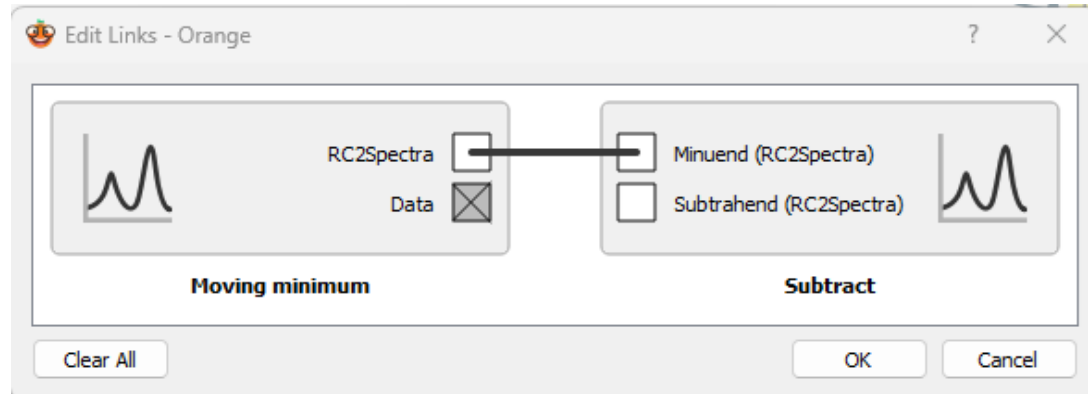


For example, the “HHT Sharpening” widget **Input** channels are “RC2Spectra” and respectively **Outputs** channels are “RC2Spectra” and “Data”.

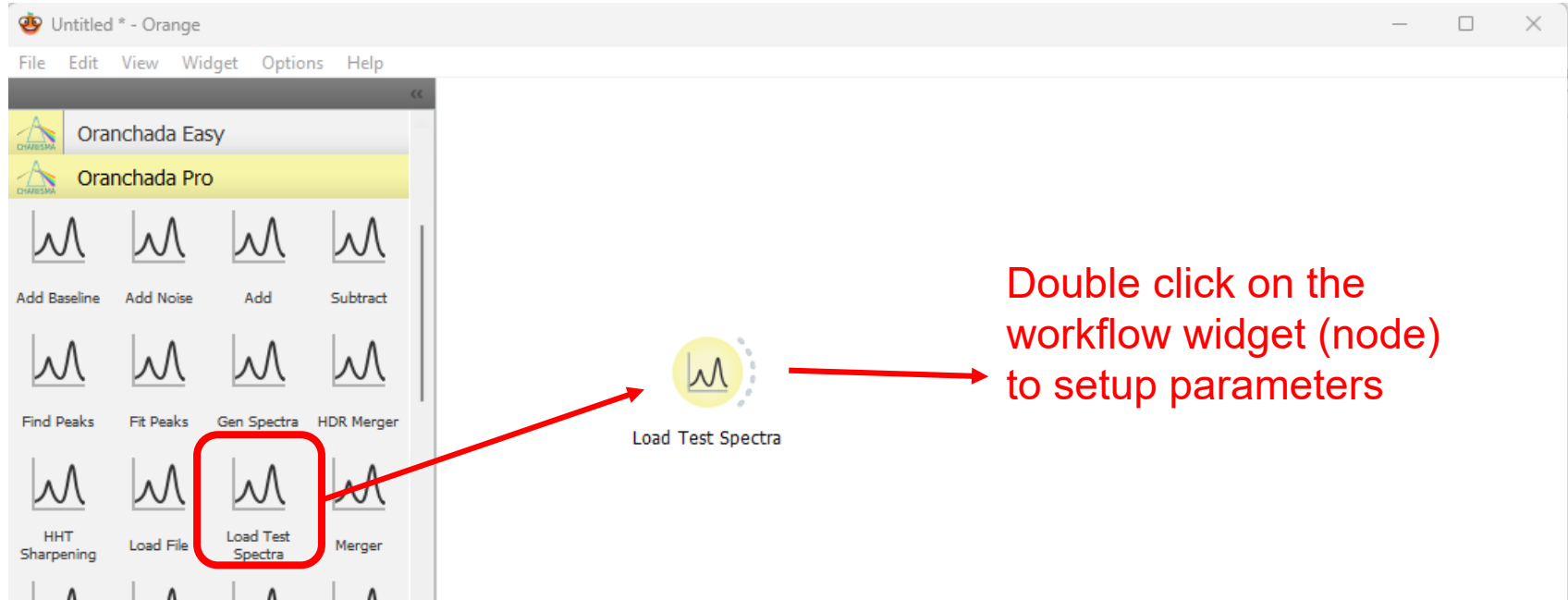
# Multiple channels widget



When connecting a widget to another multiple channels widget, as in the example workflow, we will get the following window asking users for information which channels to connect



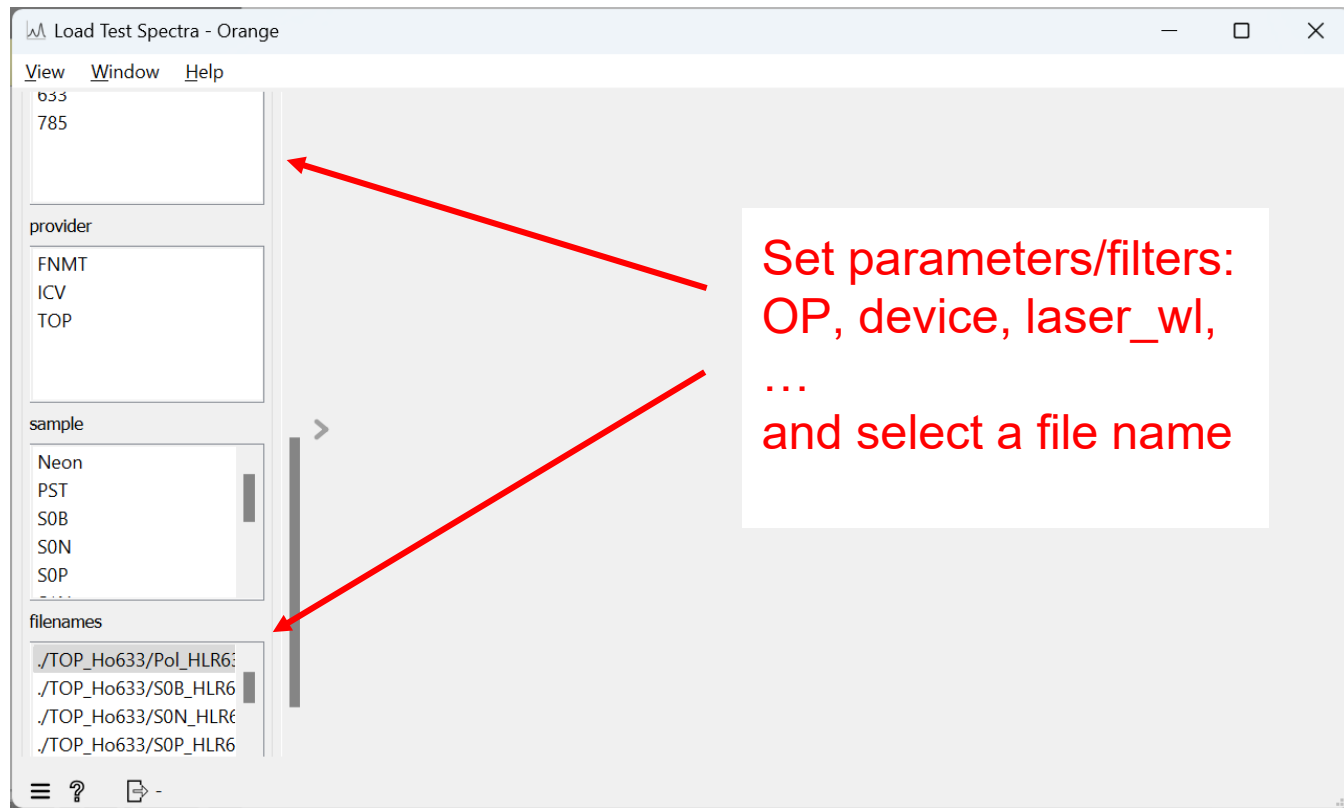
# 1. Load a test spectrum

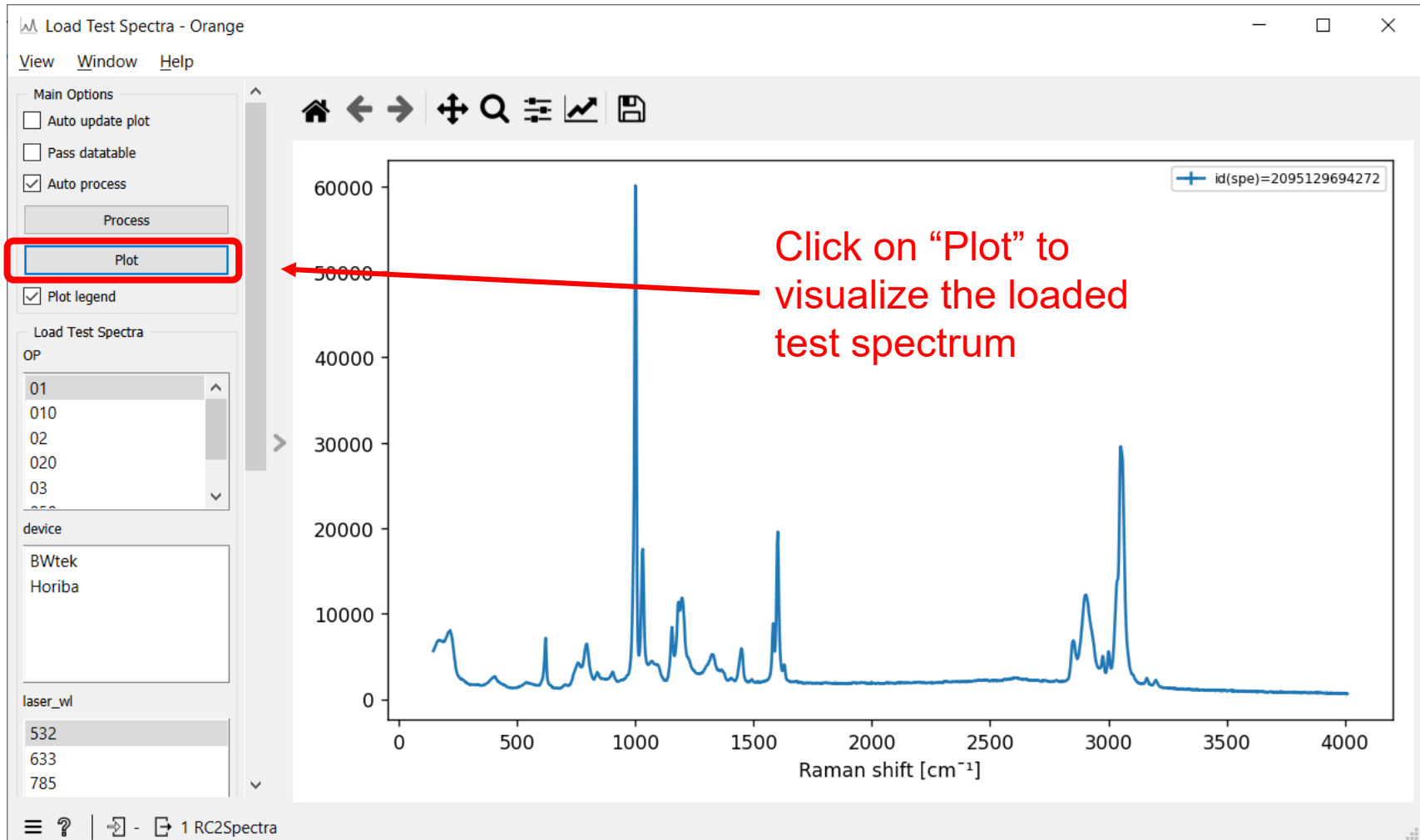


Click on the "Load Test Spectra" widget (or drag and drop) to put it on the main area of the Orange workflow

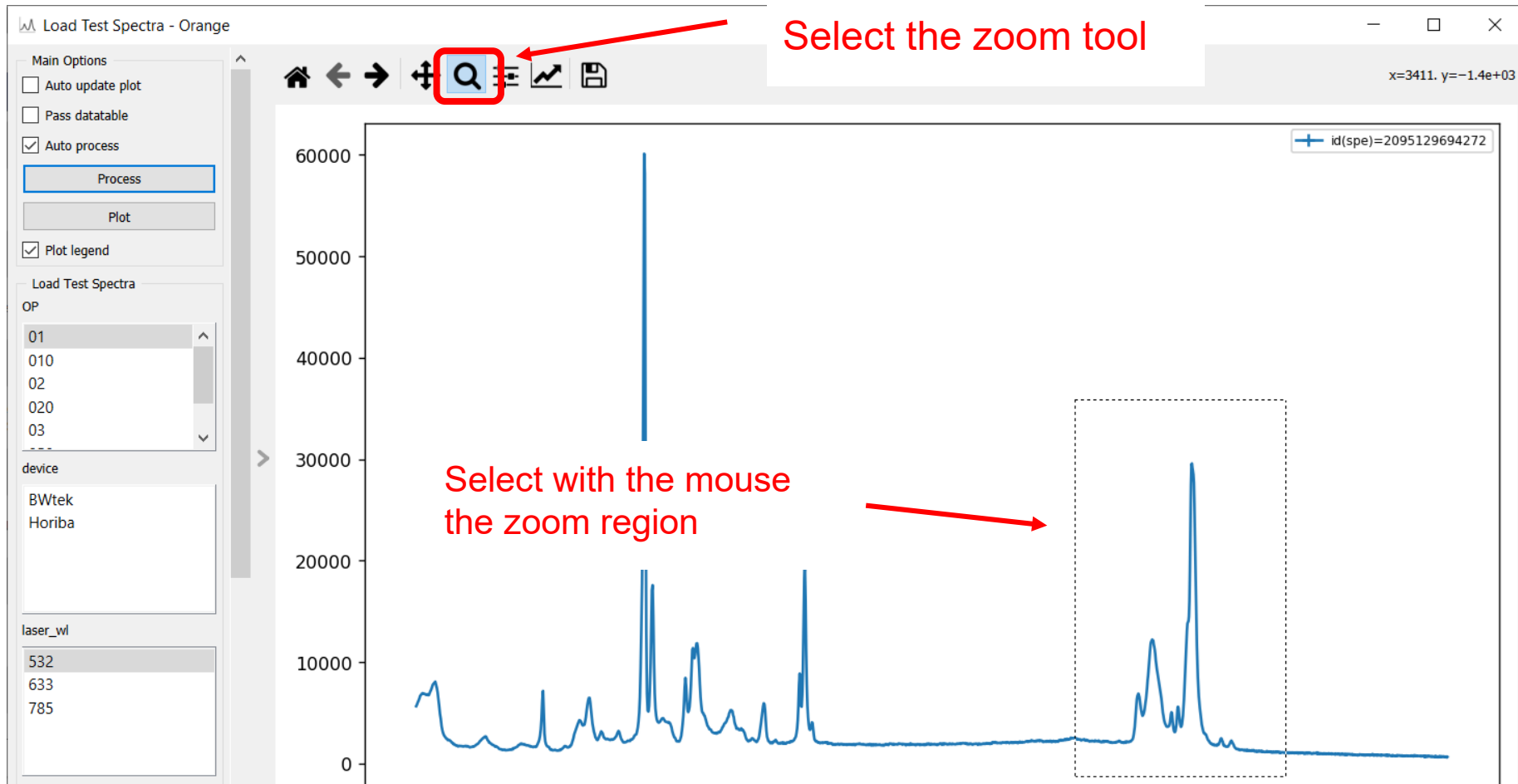
Double click on the workflow widget (node) to setup parameters

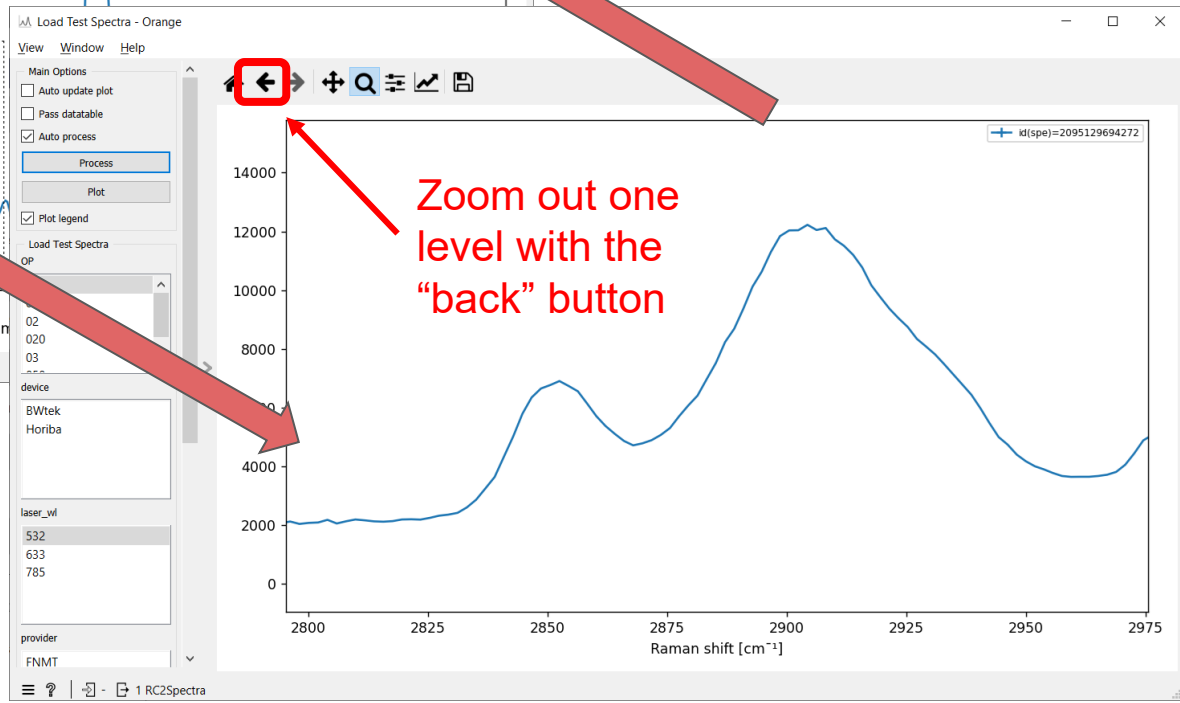
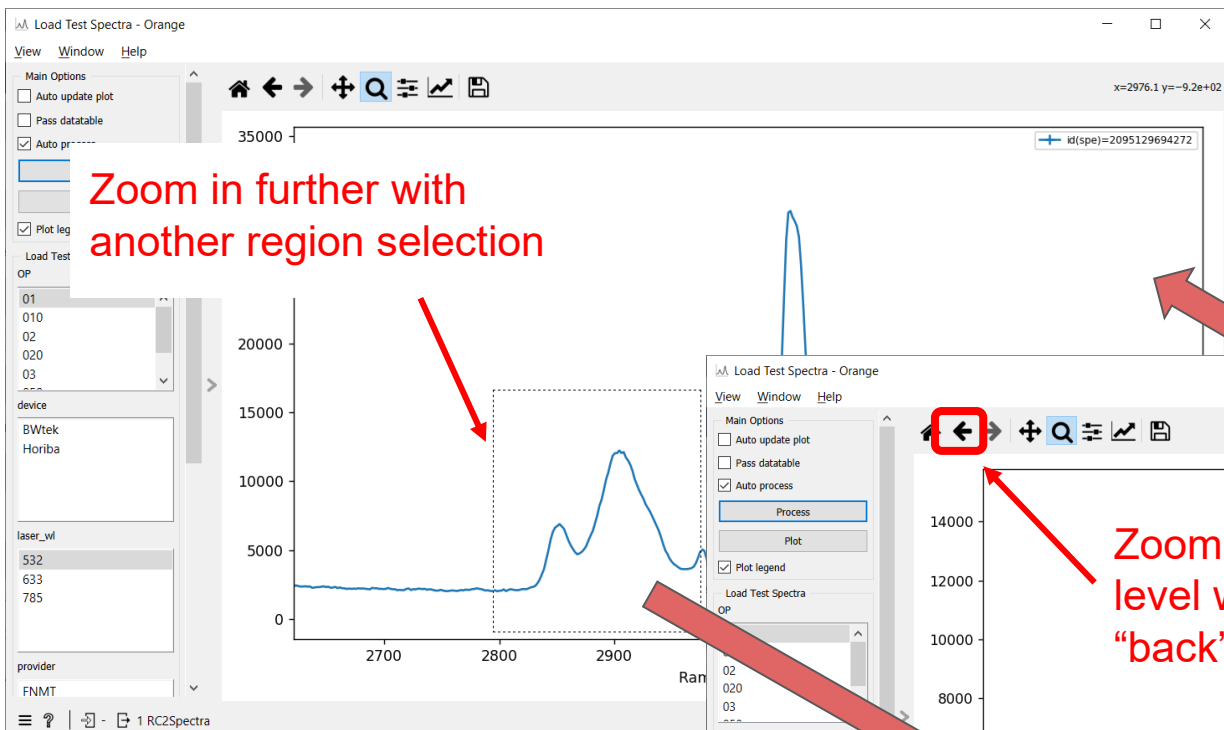




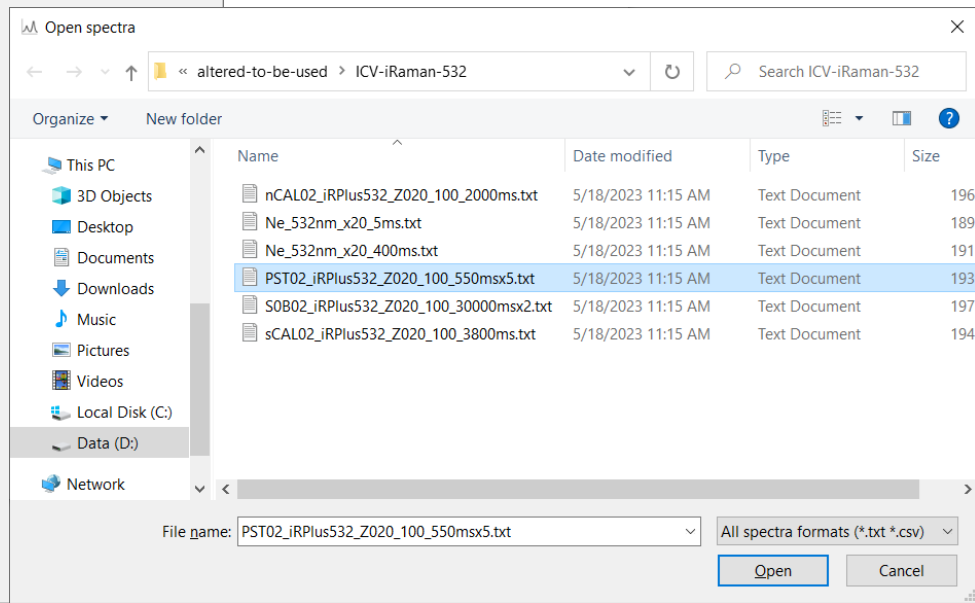


## 2. Zoom-in spectra (inspect a specific region)





The screenshot shows the 'Load File' widget in the Orange3 software. The widget has a 'Main Options' section with checkboxes for 'Auto update plot', 'Pass datatable', 'Auto process' (checked), and 'Plot legend' (checked). Below these are buttons for 'Process', 'Plot', and 'Load File'. The 'Load File' button is highlighted with a red rectangle. A red arrow points from the text 'Select a file from a user specified path' to the 'Load File' button. Another red arrow points from the 'Load File' button to a file explorer window that is open, showing the 'Data (D:)' drive selected. The file explorer shows a list of folders including 'This PC', '3D Objects', 'Desktop', 'Documents', 'Downloads', 'Music', 'Pictures', 'Videos', 'Local Disk (C:)', 'Data (D:)', and 'Network'. The 'Data (D:)' drive is highlighted. The file explorer also shows a 'File name' field at the bottom.



## Main Options

☐ Auto update plot☐ Pass datatable☒ Auto process

Process

Plot

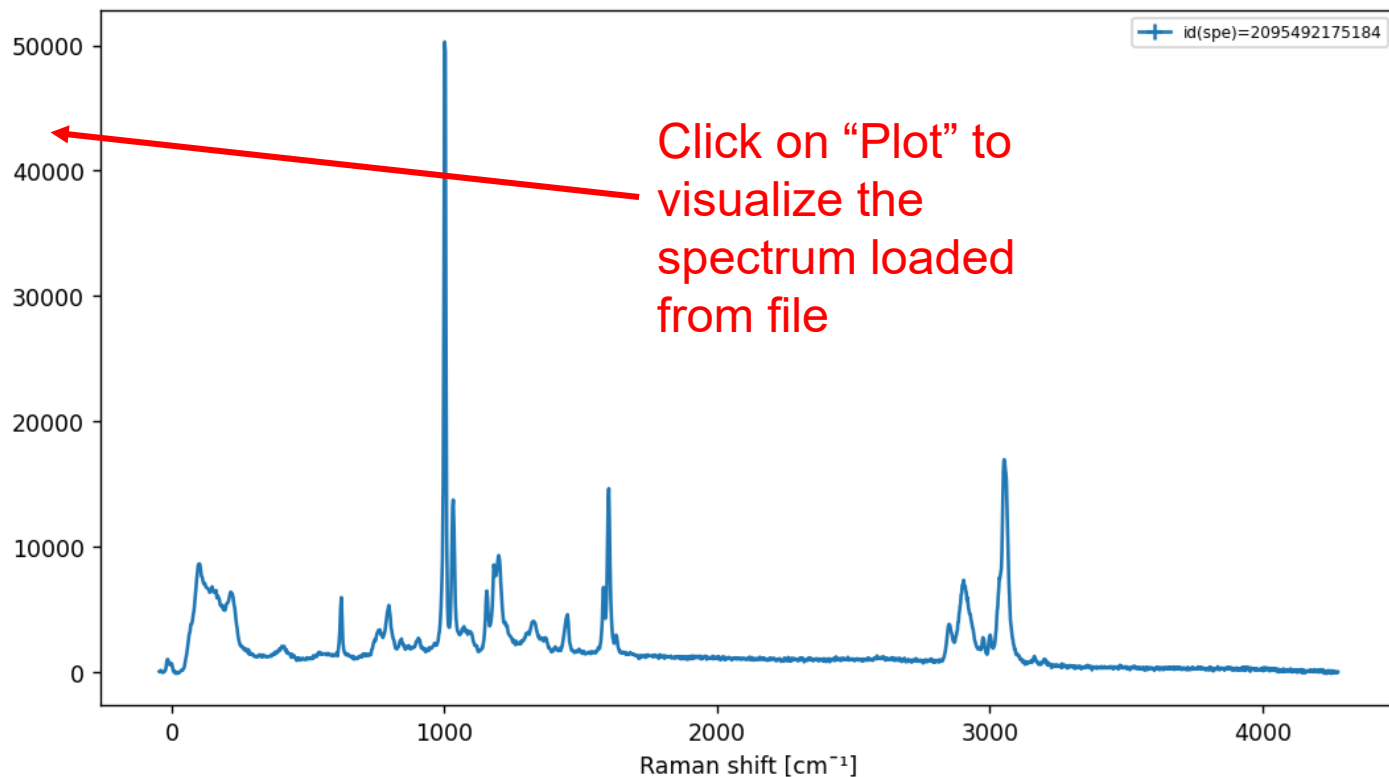
☒ Plot legend

## Load File

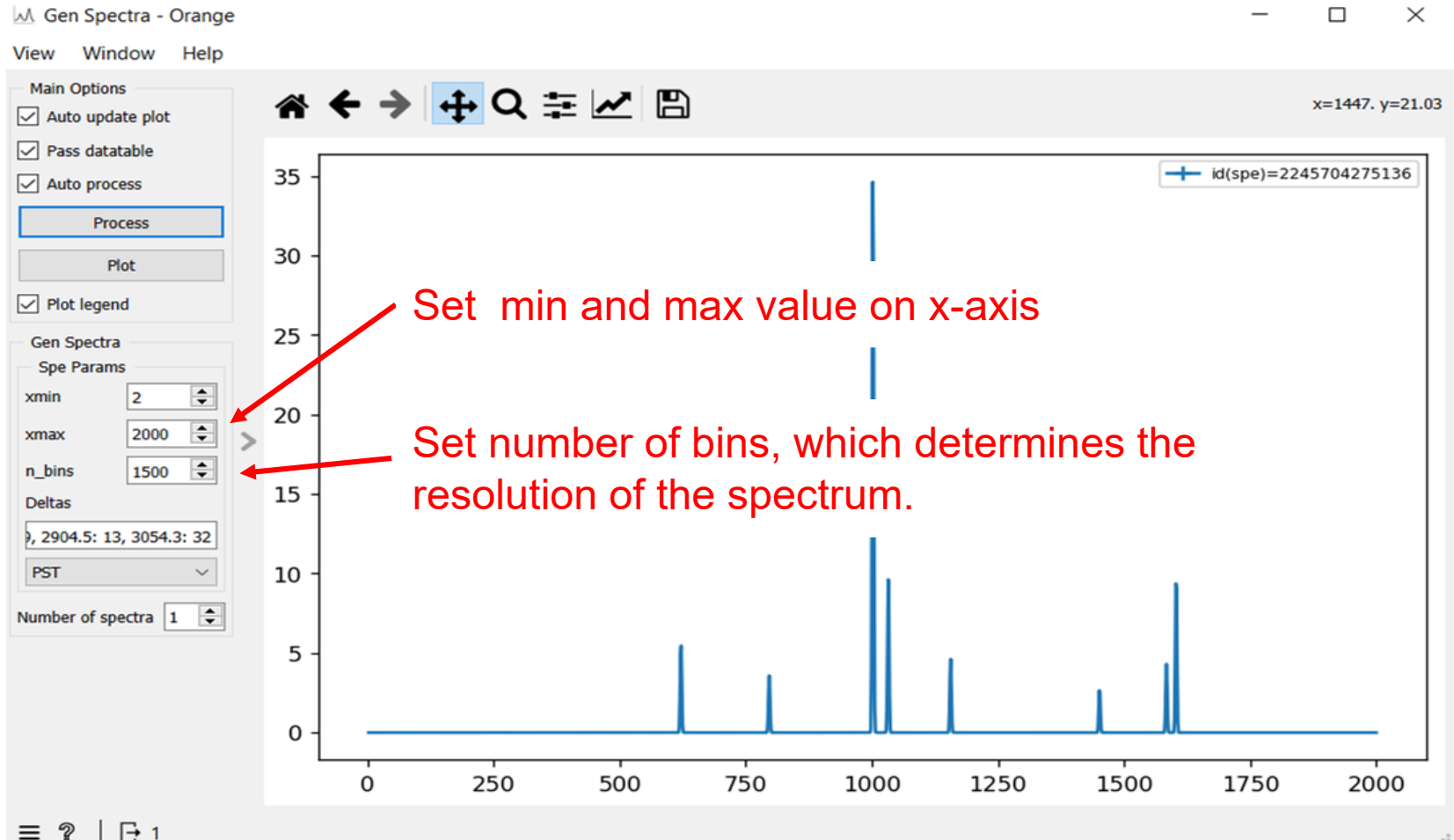
Load File

File format

Auto



## 4. Generate synthetic Spectra v2



## Main Options

☒ Auto update plot☒ Pass datatable☒ Auto process

Process

Plot

☒ Plot legend

## Gen Spectra

## Spe Params

xmin 2

xmax 2000

n\_bins 1500

Deltas

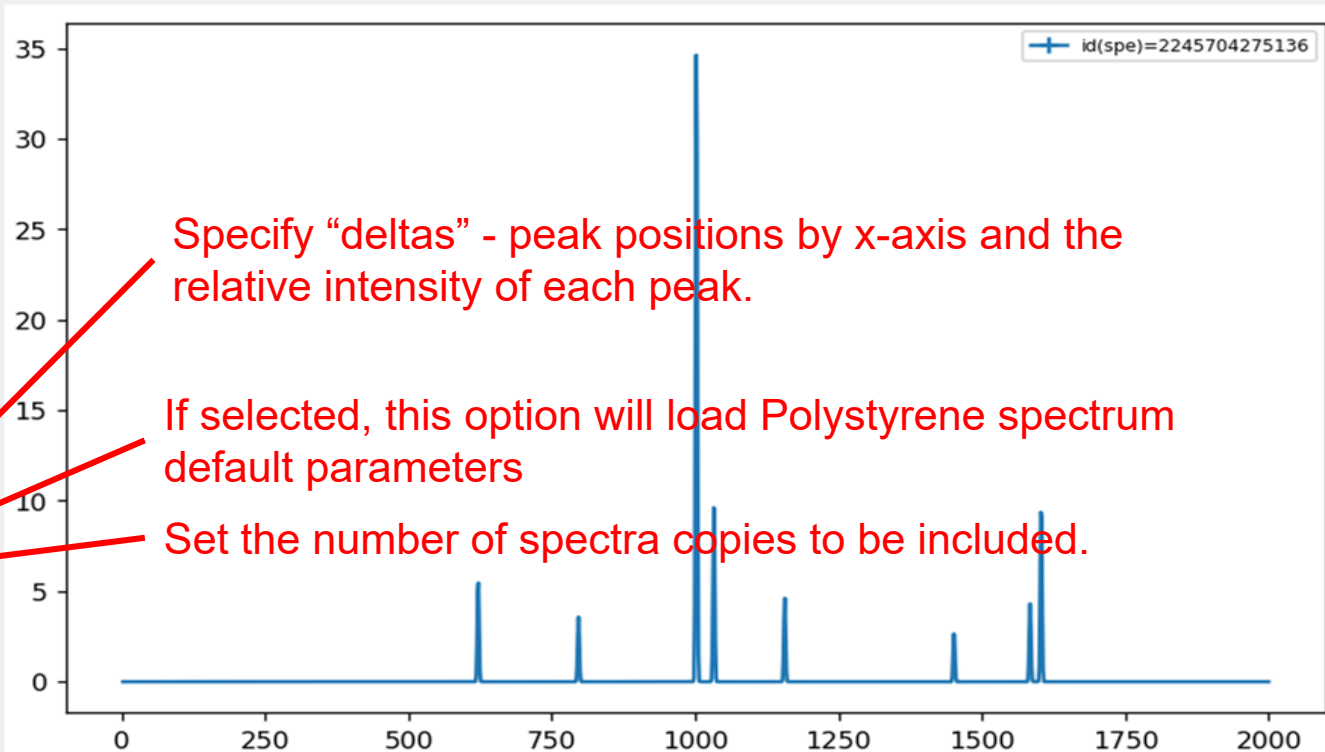
9, 2904.5: 13, 3054.3: 32

PST

Number of spectra 1

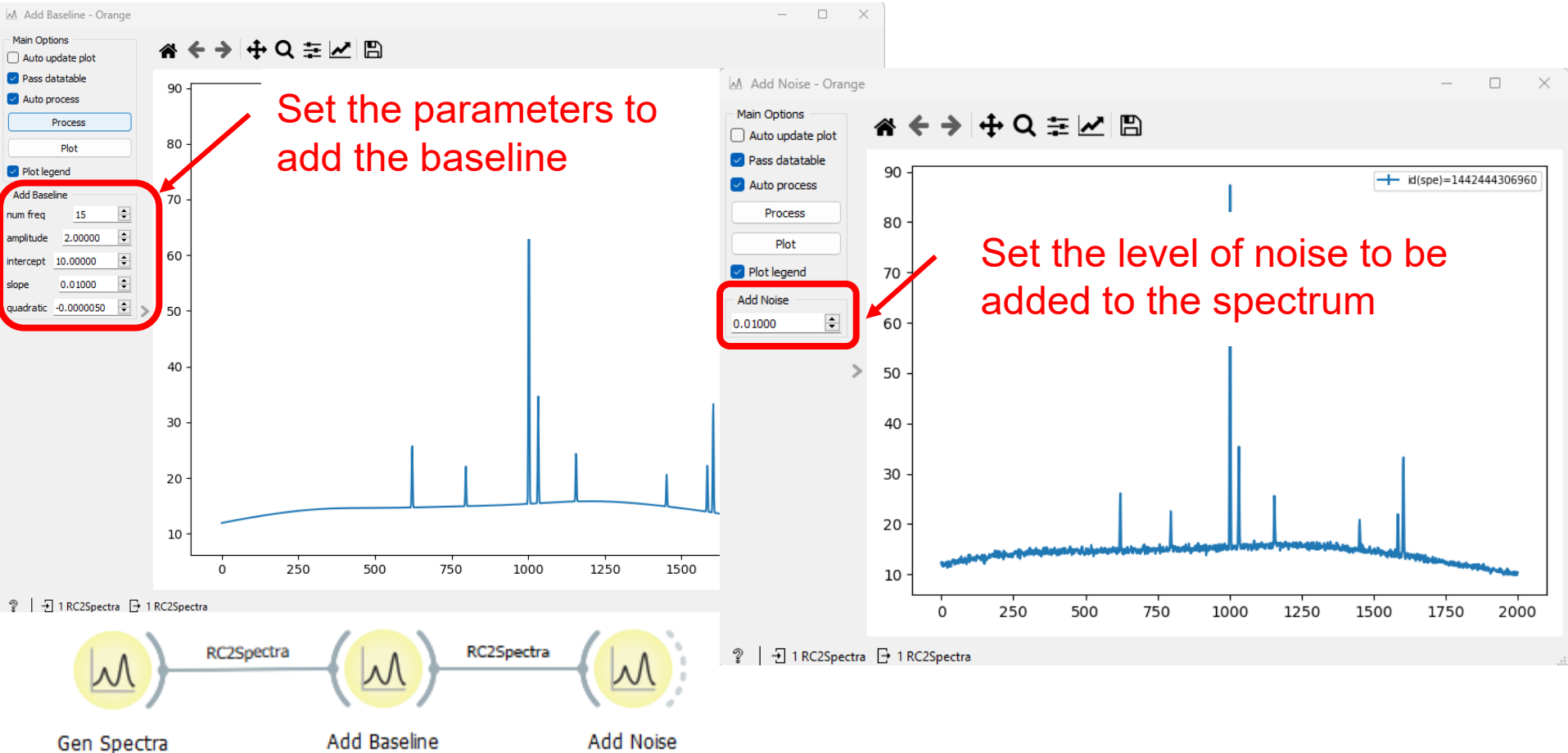


x=1447. y=21.03



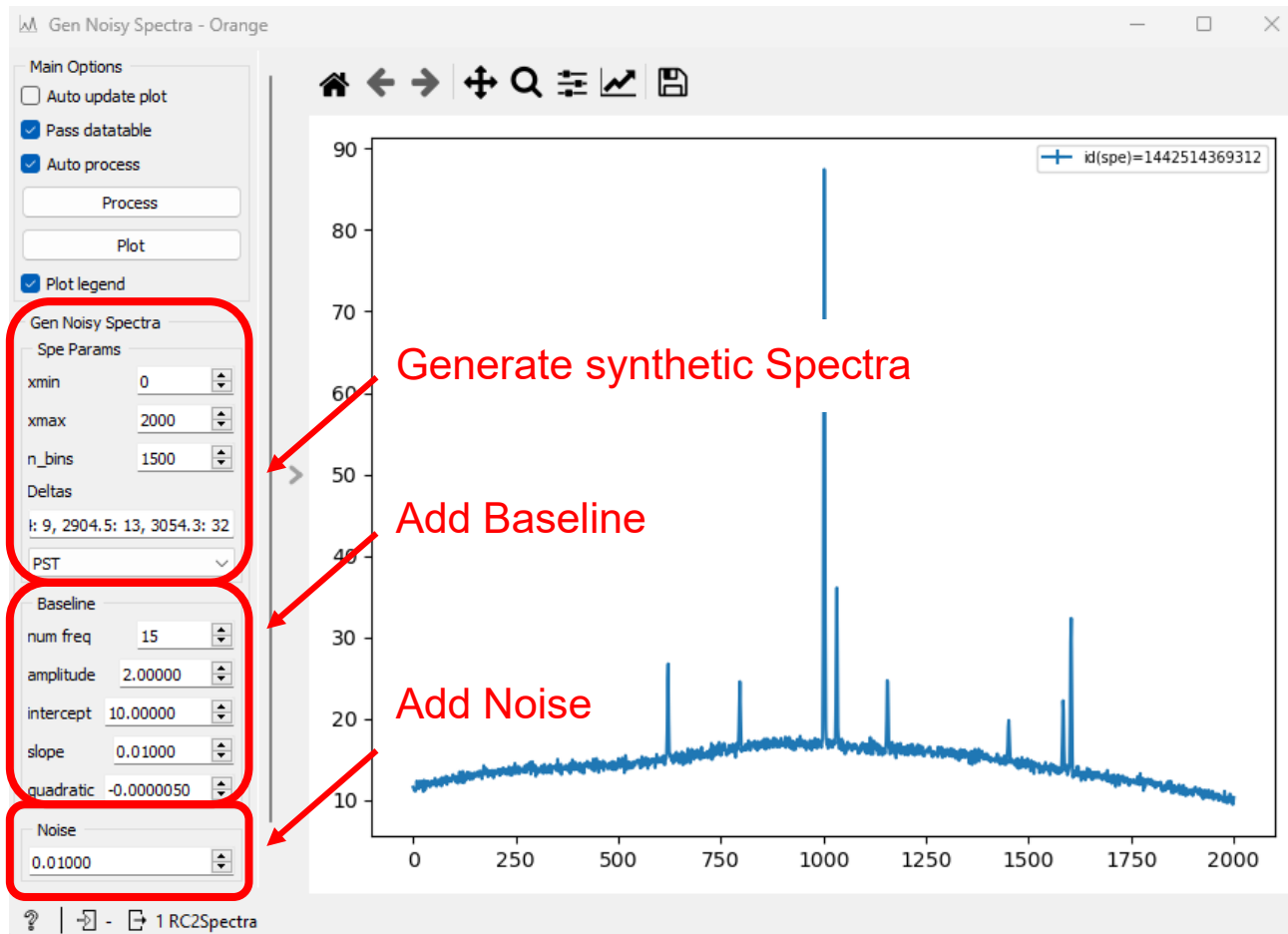
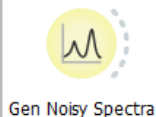
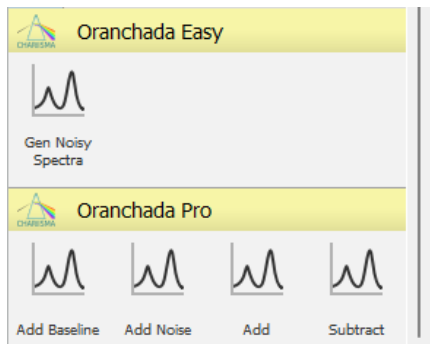


# 5. Add Baseline and Noise to synthetic spectra

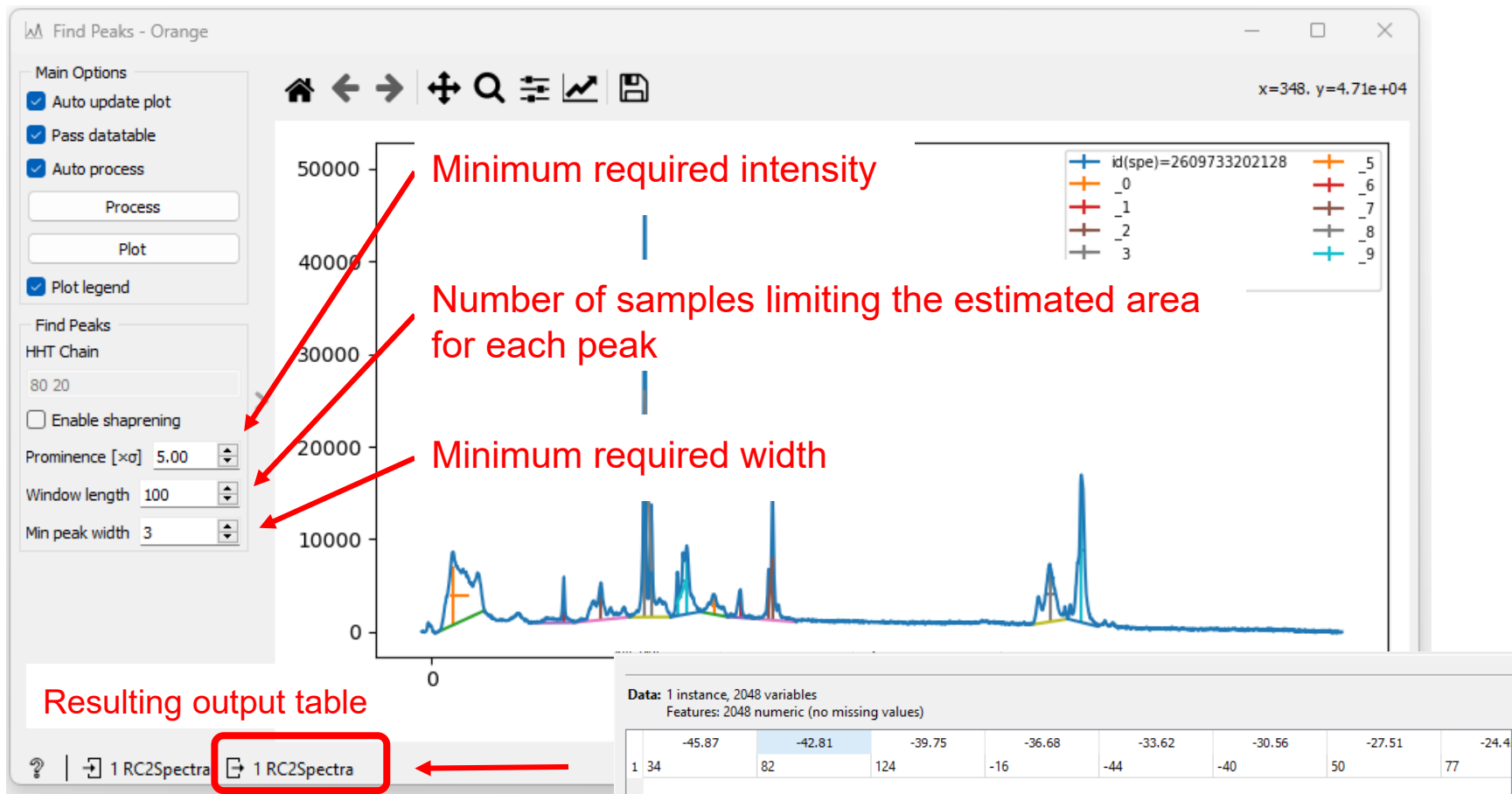


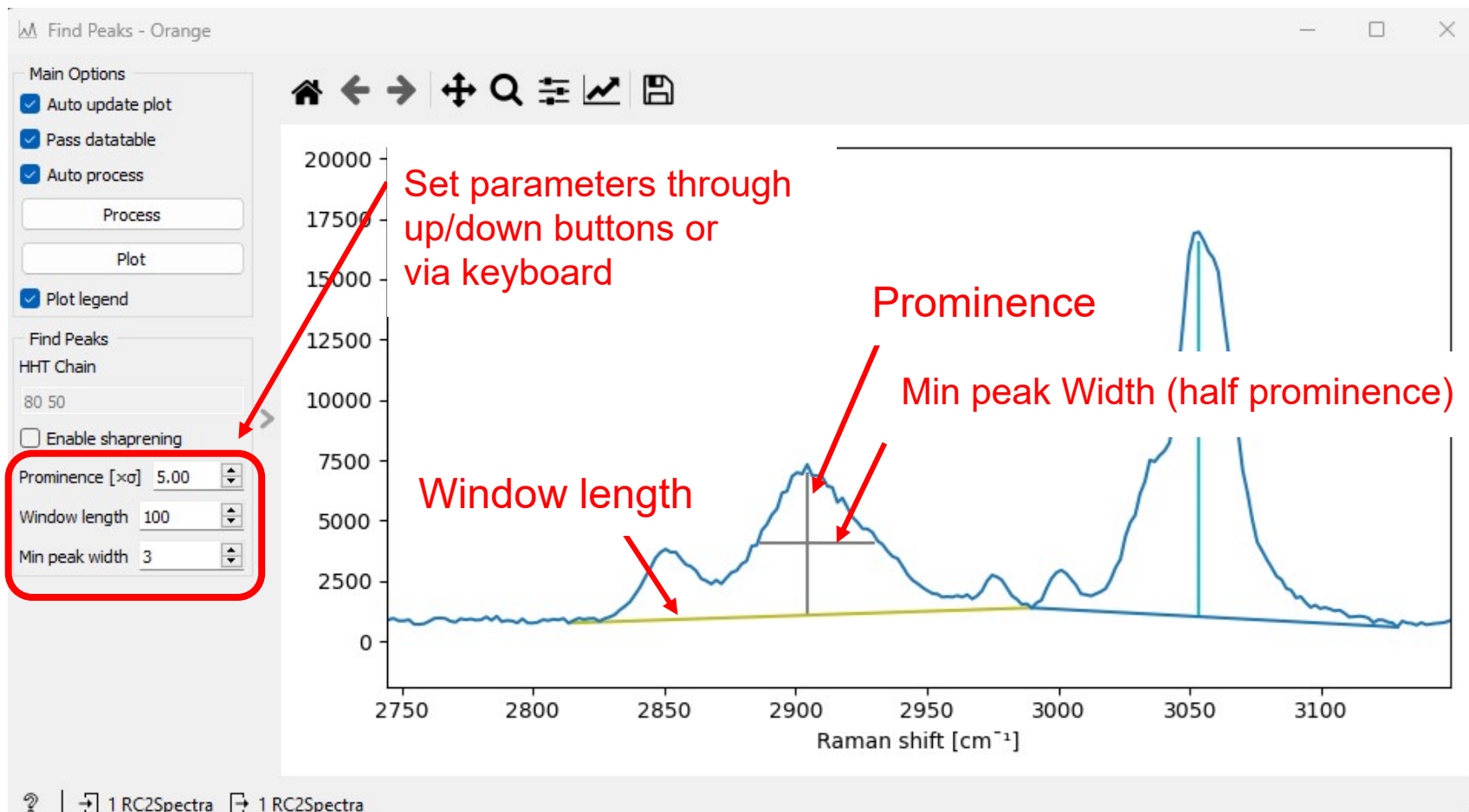
# 6. Generate synthetic Spectra with added Baseline and Noise

Generate synthetic spectra with Baseline and Noise with one widget from "Oranchada Easy" Category



# 7.Find peaks





## Main Options

- ☒ Auto update plot
- ☒ Pass datatable
- ☒ Auto process

- ☒ Plot legend

## Find Peaks

## HHT Chain

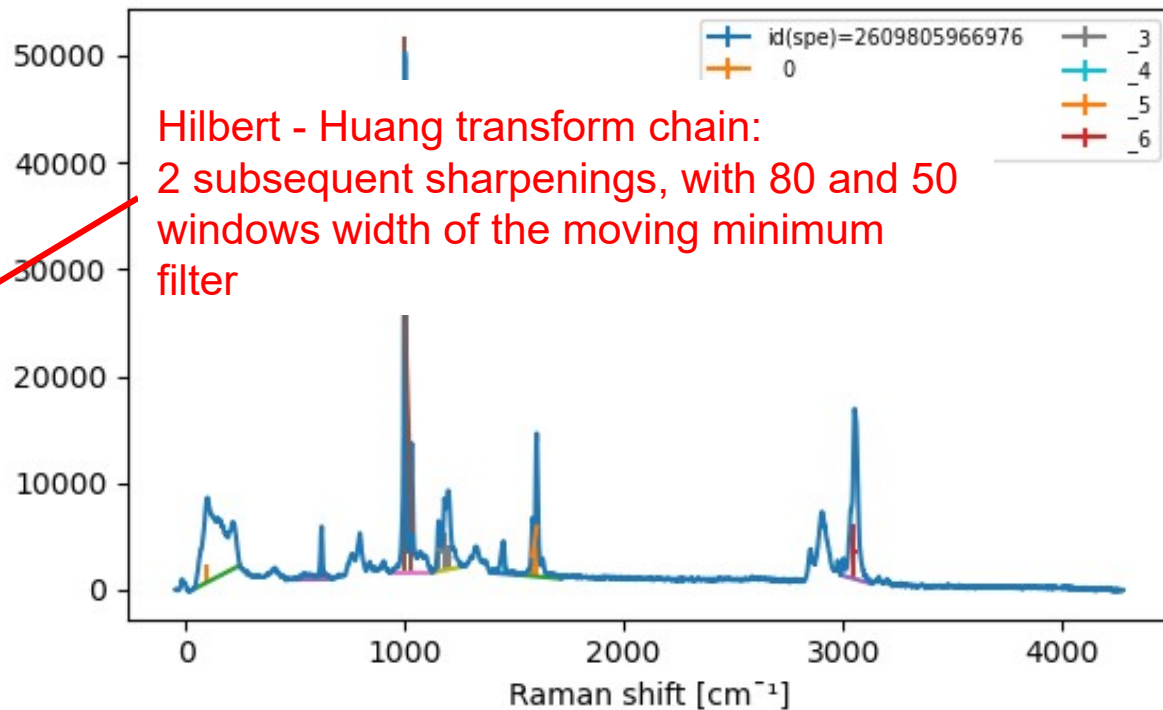
80 50

- ☒ Enable sharpening

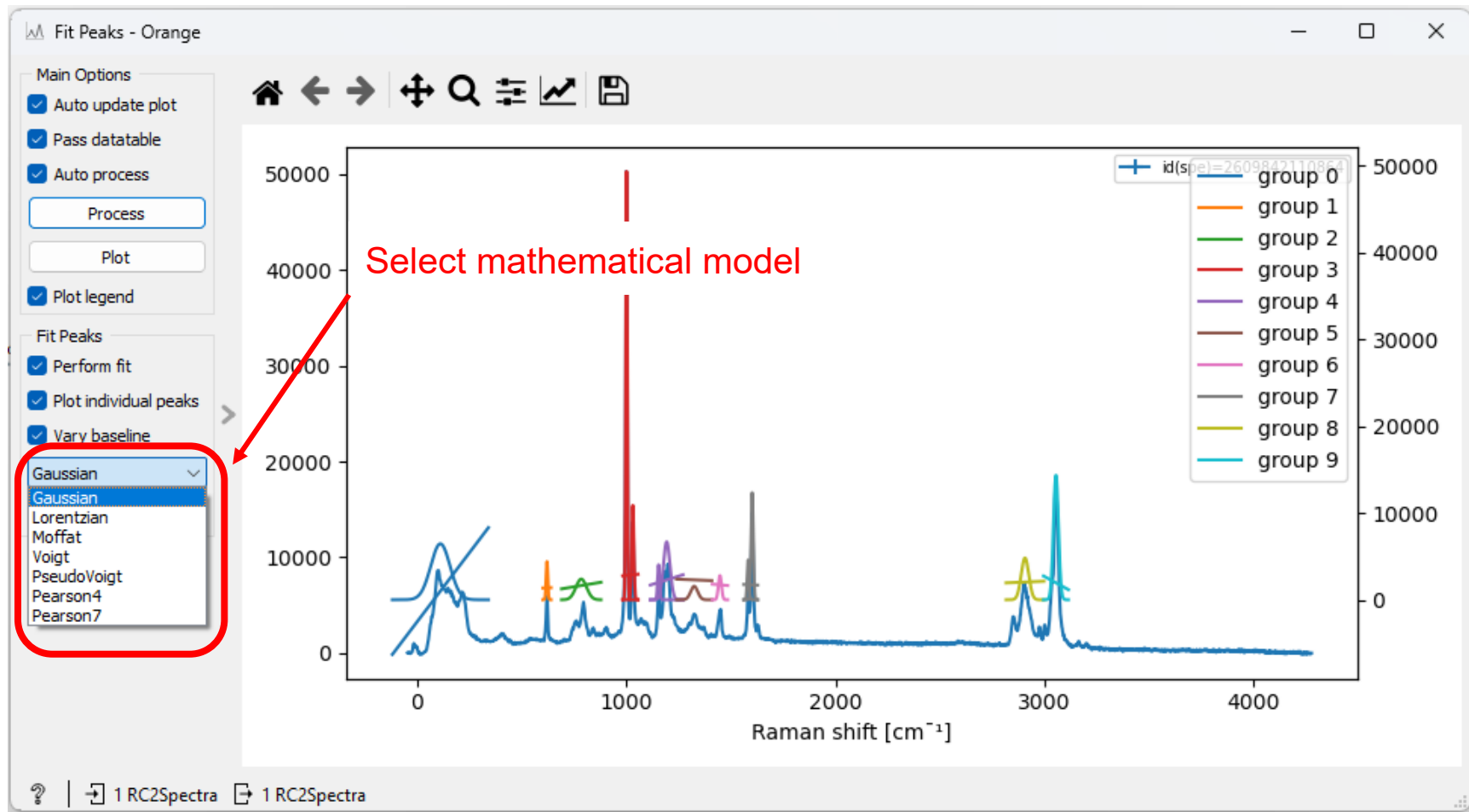
Prominence [ $\times\sigma$ ] 5.00

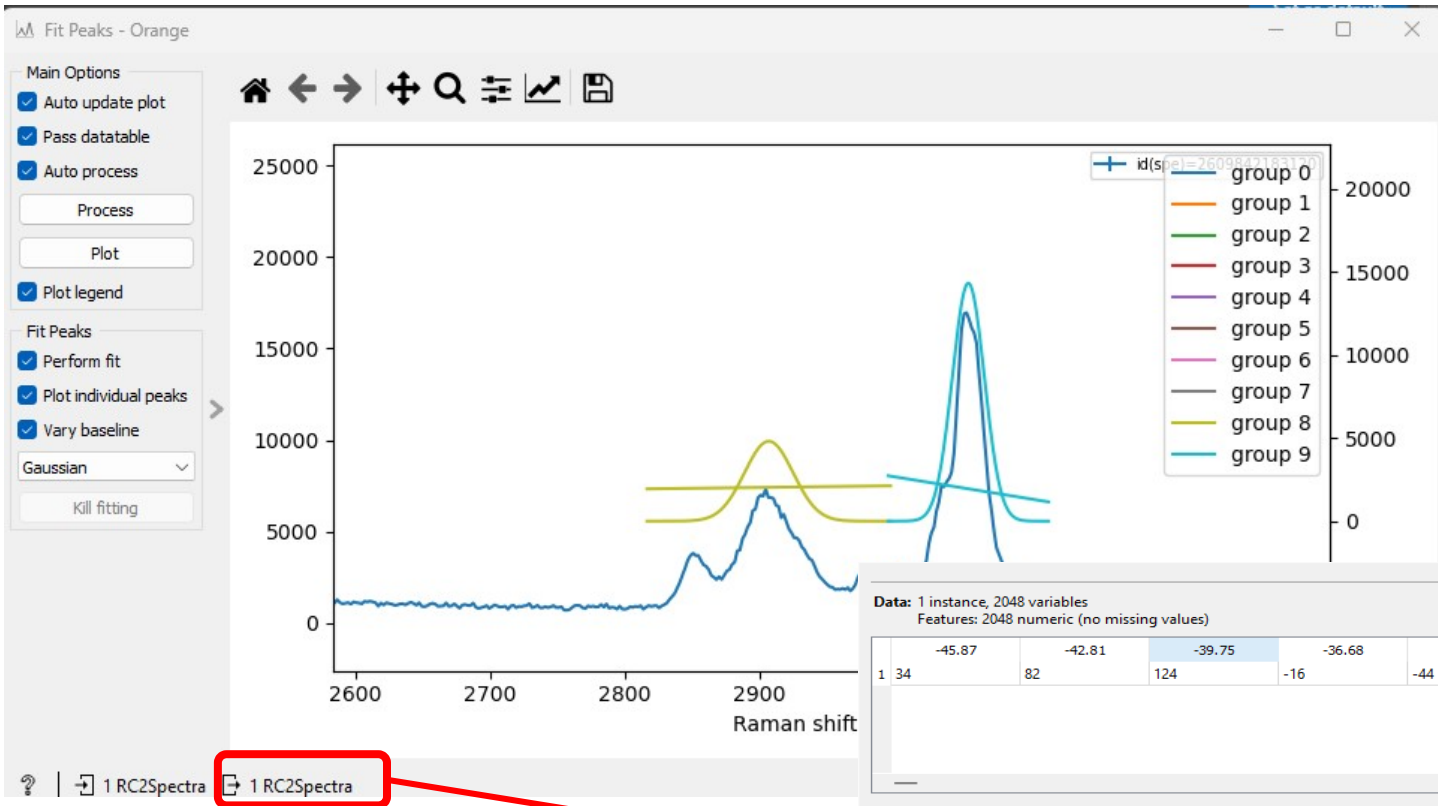
Window length 100

Min peak width 3



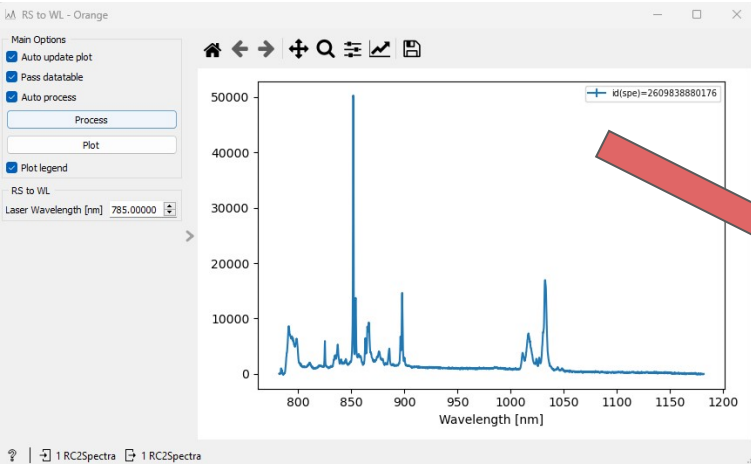
## 8. Fit peaks - can be placed only after Find peaks widget



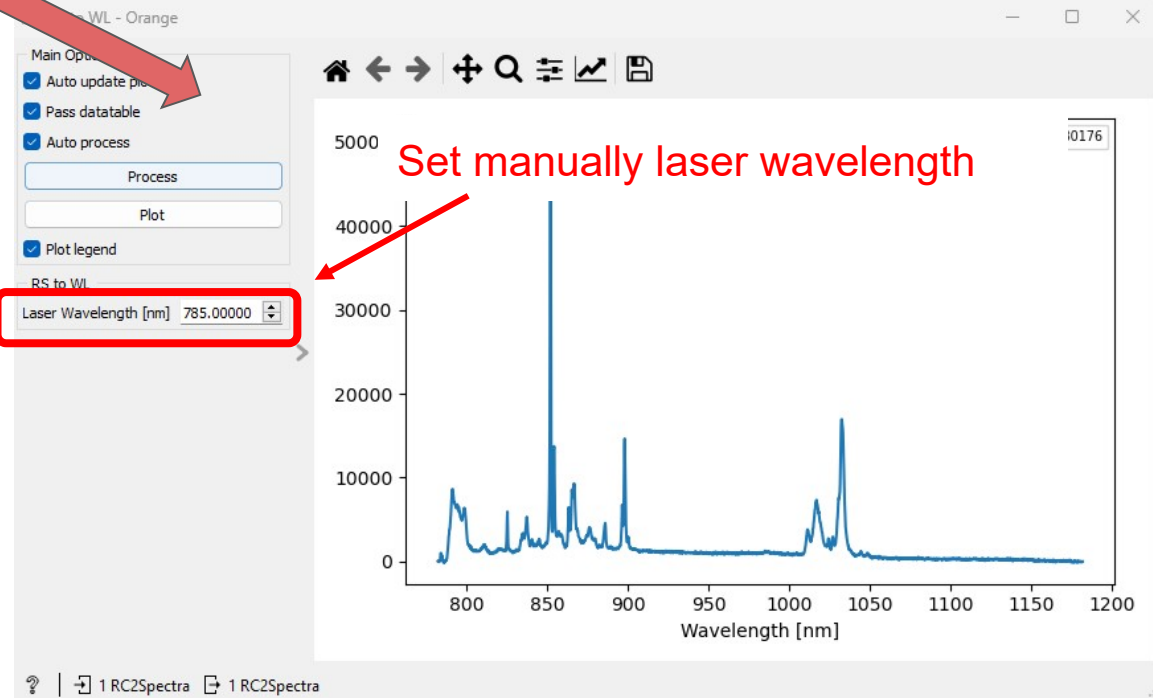


Resulting output table with calculated parameters for fitted peaks indexed based on each specific peak group

## 9. RS to WL - Raman shift to Wavelength

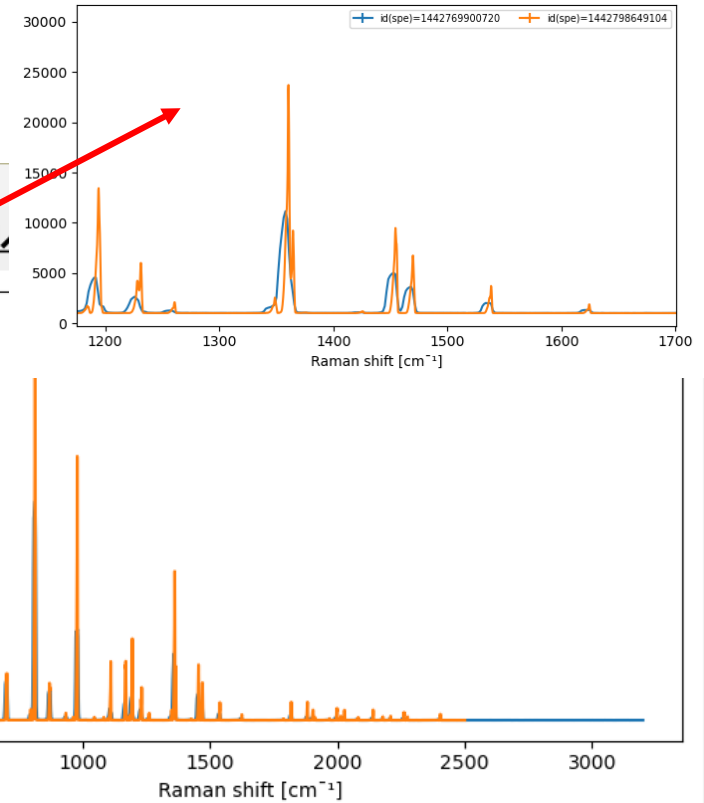
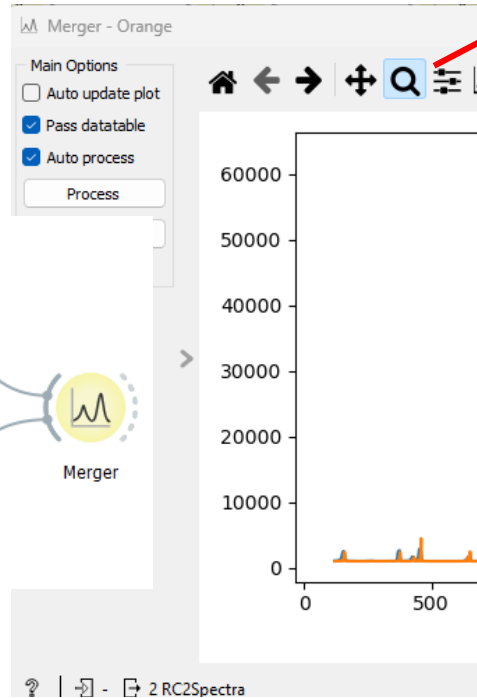
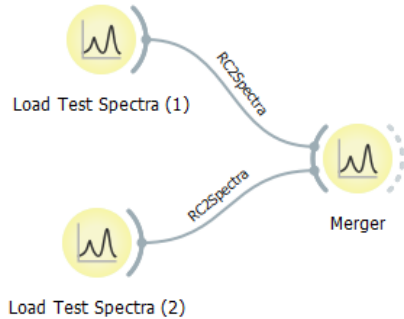
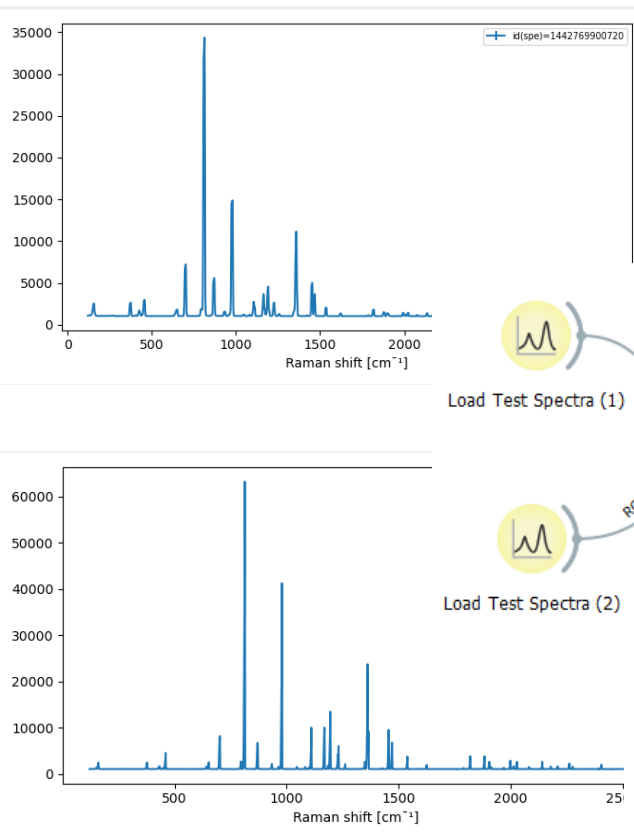


The reverse functionality in:  
“WL to RS” widget  
(Wavelength to Raman shift)



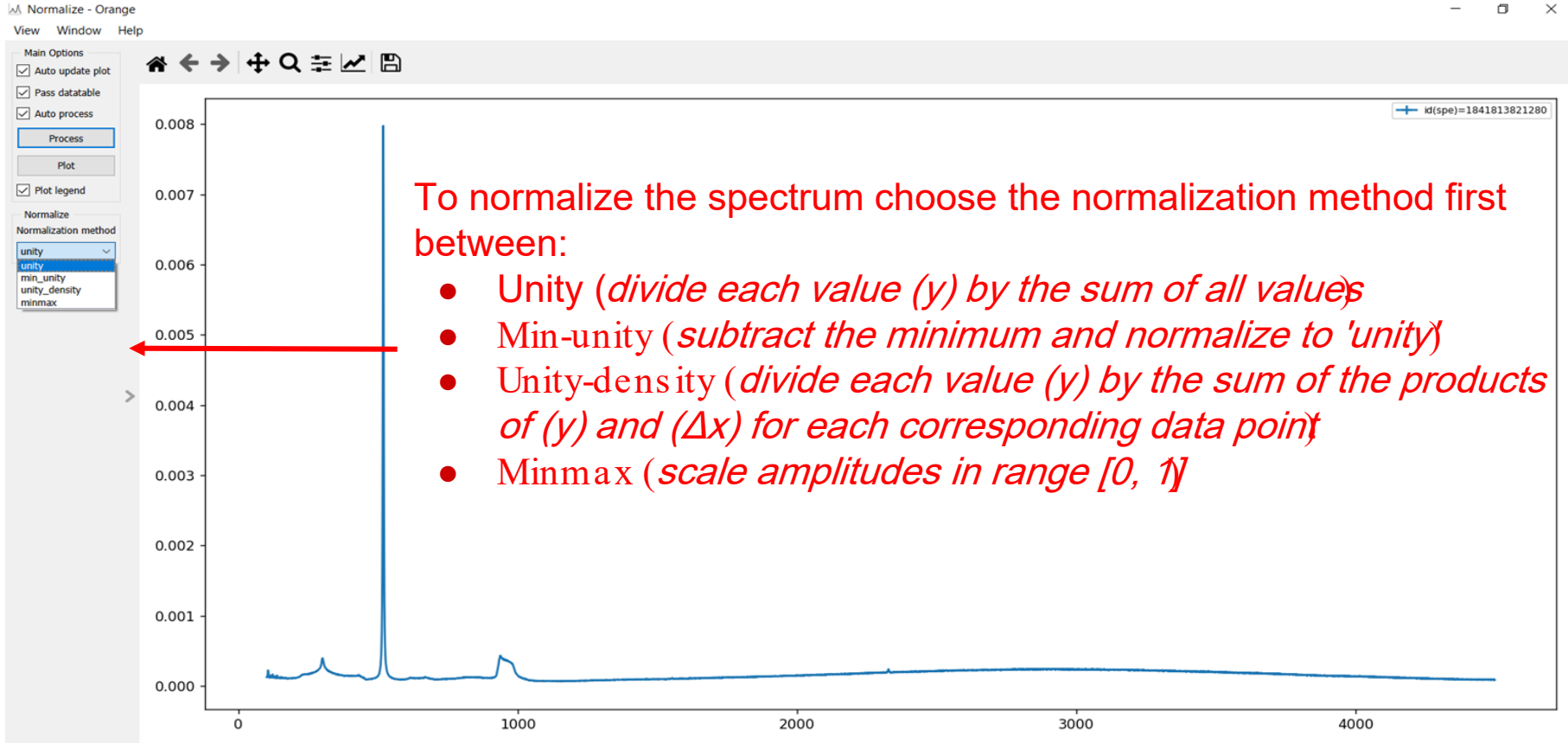


# 10.Merger

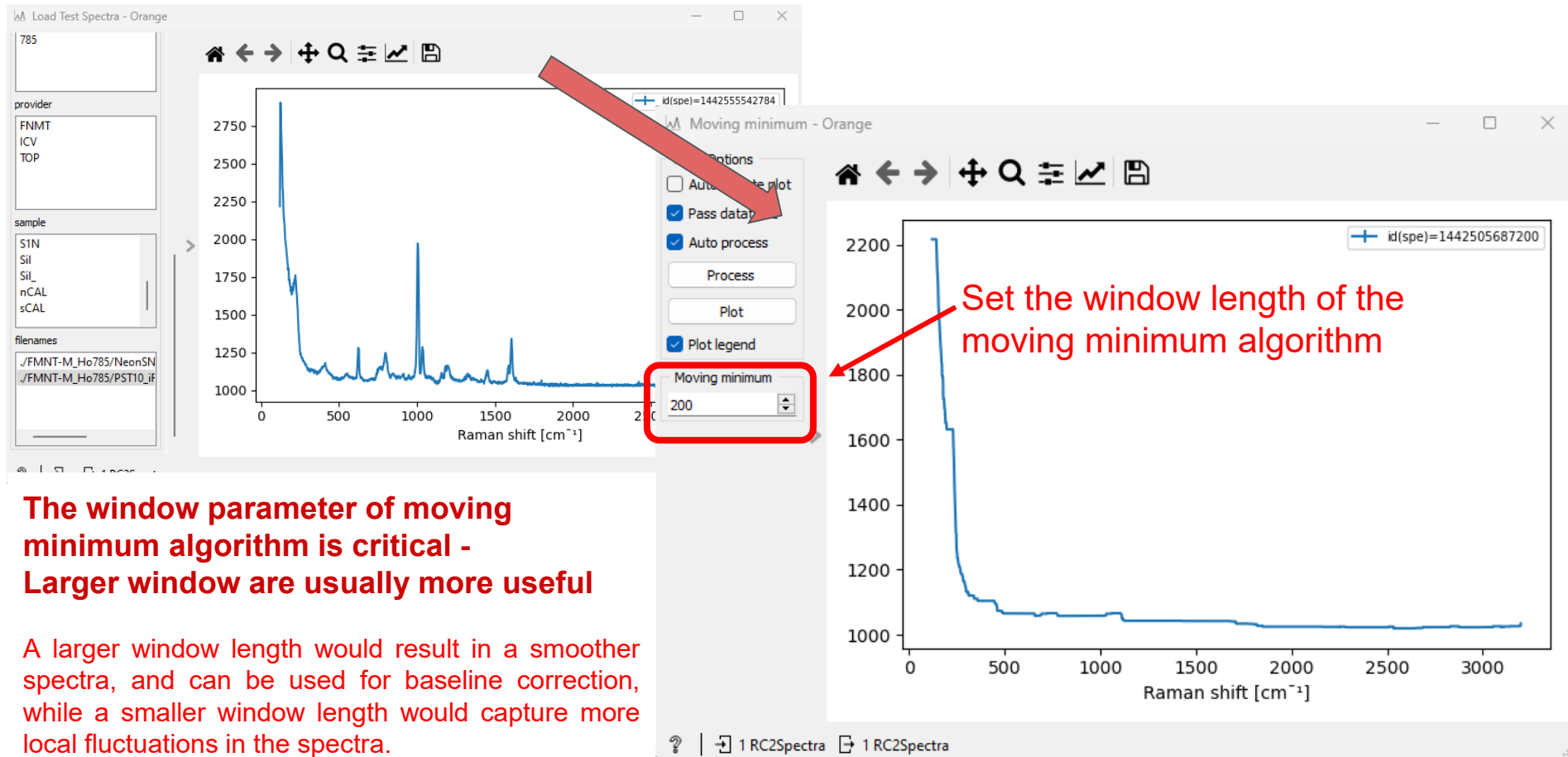


The resulting spectrum is merged from the input spectra and each spectrum is shown in a different color

# 11.Normalize



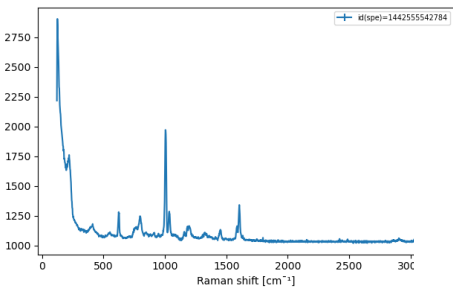
# 12. Moving minimum (estimates baseline via moving minimum)



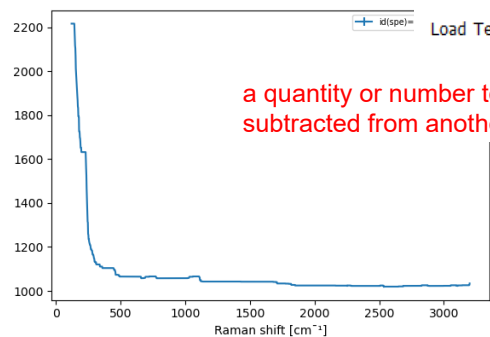
# 13.Subtract

$$\text{Difference} = \text{Minuend} - \text{Subtrahend}$$

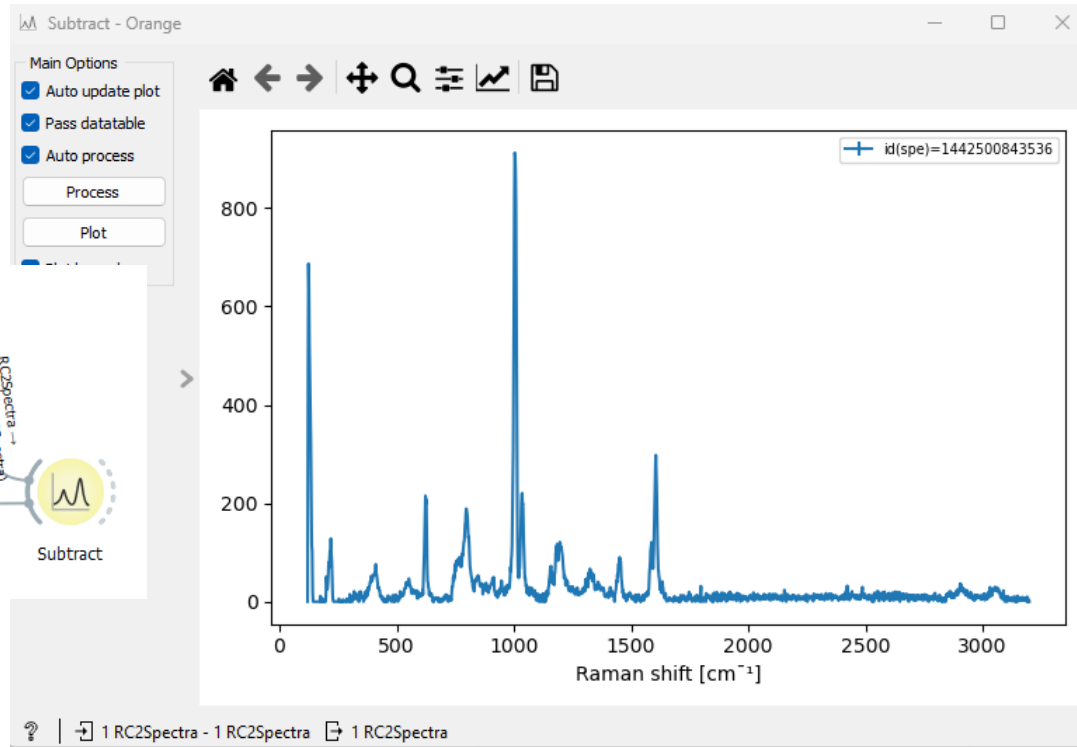
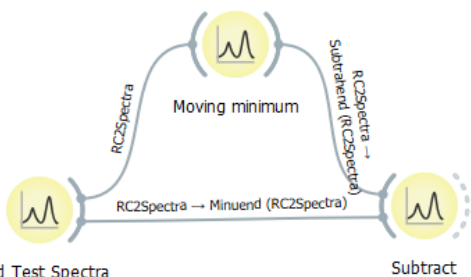
**Minuend** a quantity or number from which another is to be subtracted



**Subtrahend**

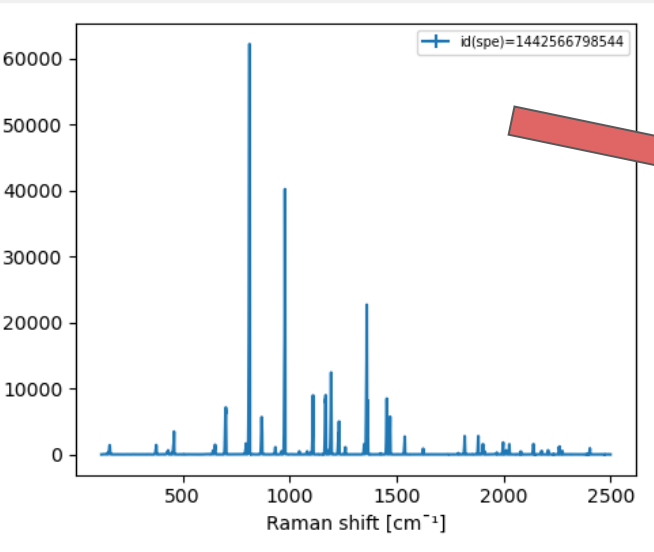


a quantity or number to be subtracted from another



The two spectra need to be with equal length and same x-axis

# 14. Resample NUDFT (Non-Uniform Discrete Fourier Transform)



Resample NUDFT (1) - Orange

Main Options

- ☐ Auto update plot
- ☐ Base datatable
- ☒ Auto process

Process

Plot

☒ Plot legend

Resample NUDFT

x-min: 0

x-max: 3000

n-bins: 3000

window

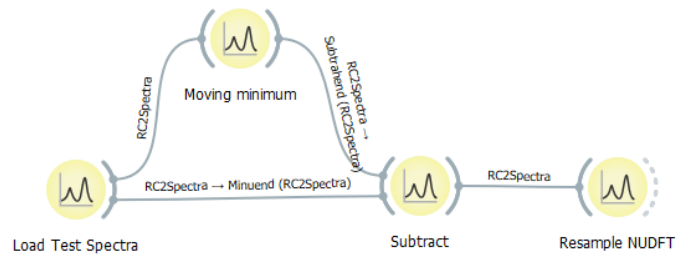
- bartlett
- barthann
- bartlett
- blackman
- blackmanharris
- bohman
- boxcar
- hamming
- hann
- nuttall
- parzen

Set the Resample parameters:

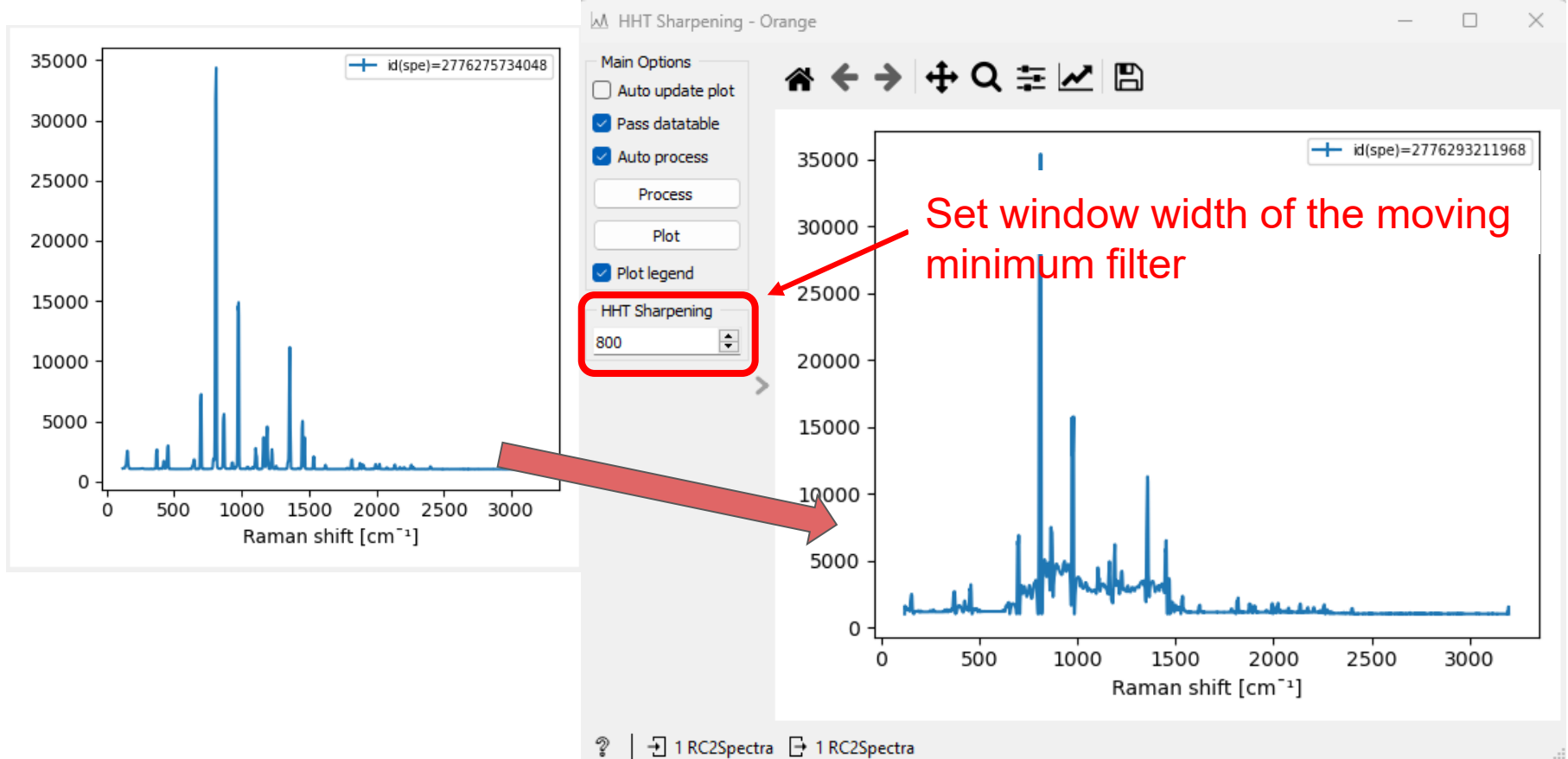
- x-min - min value of new x-axis
- x-max - max value of new x-axis
- n-bins - number of bins

Select window function

A line plot showing Raman shift in cm<sup>-1</sup> on the x-axis (ranging from 0 to 3000) and intensity on the y-axis (ranging from 0 to 140,000). The plot displays several sharp peaks, with the most prominent ones around 800, 1000, and 1300 cm<sup>-1</sup>.



# HHT Sharpening (Hilbert - Huang Transform)



# HDR Merge

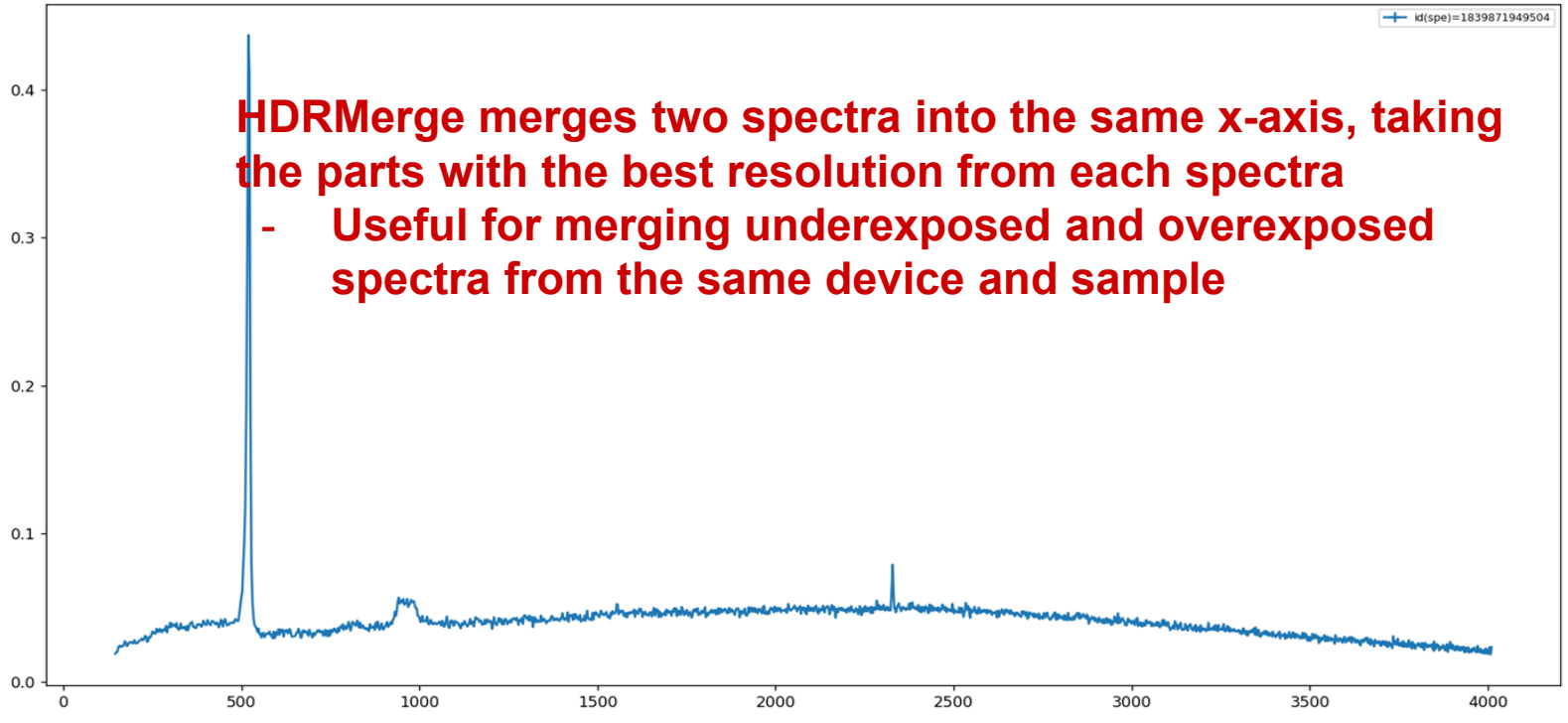
HDR Merger - Orange

View Window Help

- Main Options
- ☒ Auto update plot
  - ☒ Pass datatable
  - ☒ Auto process
- Process
- Plot
- ☒ Plot legend



x=1518, y=0.2481



**HDRMerge merges two spectra into the same x-axis, taking the parts with the best resolution from each spectra**

- Useful for merging underexposed and overexposed spectra from the same device and sample

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