

RAMAN DATA PROCESSING V6 QUICK MANUAL

J.Anaya

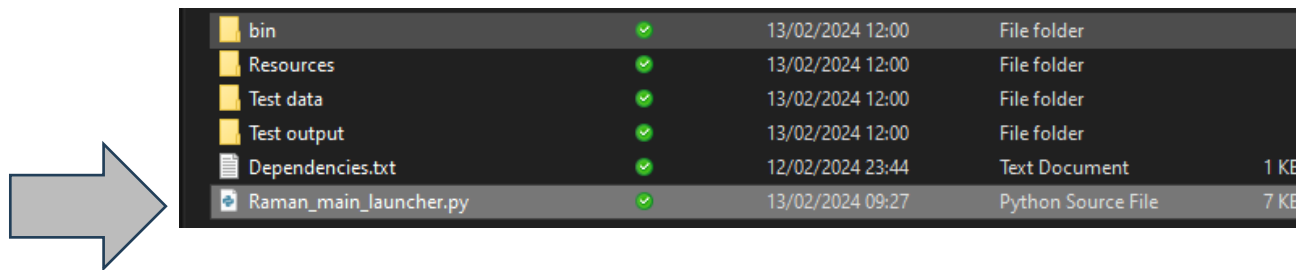
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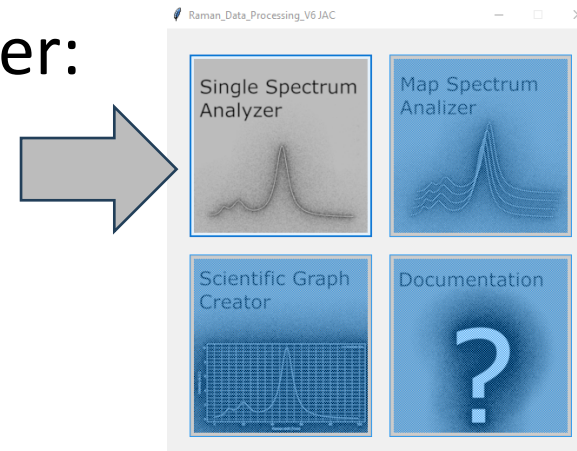
1. Install python $\geq 3.8.18$
2. Install the following libraries:
 - multiprocessing
 - sys
 - os
 - csv
 - re
 - pillow $\geq 10.2.0$
 - numpy $\geq 1.24.4$
 - matplotlib $\geq 3.7.4$
 - numexpr $\geq 2.8.6$
 - scipy $\geq 1.10.1$
 - lmfit $\geq 1.2.2$
 - tkinter ≥ 8.6



- Currently the software works for individual spectra taken in Horiba YobinYvon and B&W Tech spectrometers.
- Data must be saved as .txt files.
- Run the main launcher:

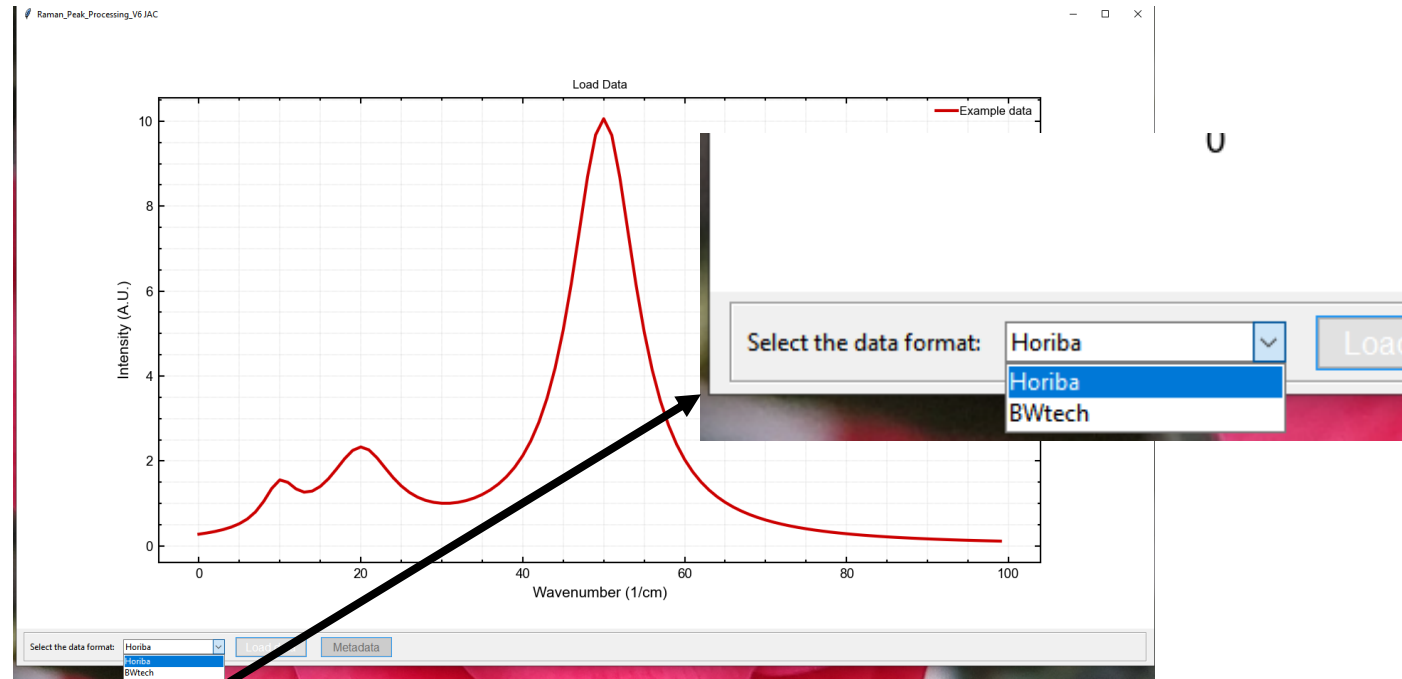


- Select the Single Spectrum Analyzer:



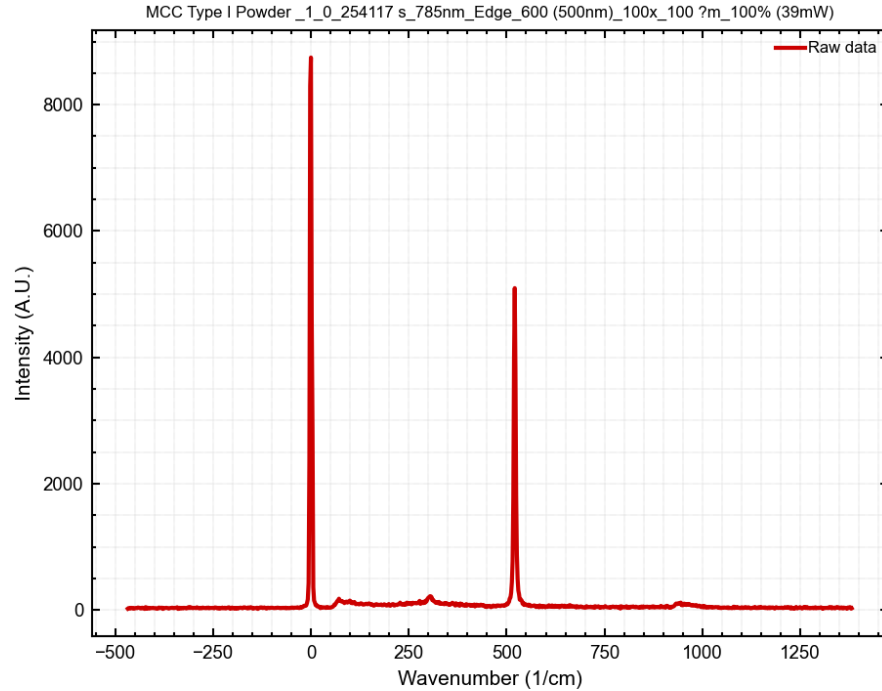


- Select the file format:



- Load data:

Raman_Peak_Processing_V6 JAC



Select the spectral range:

Min. wavenumber (1/cm): -465.794

Max. wavenumber (1/cm): 1380.1

Clip data

Baseline Correction:

Auto Manual

Baseline lambda: 1

Baseline fit

Subtract Baseline

Normalise

Peak detection and processing:

Max. number of peaks: 8

Peak detection

Add peaks

Smoothing window: 10

Peak threshold: 0.01

Peak separation: 4

Peak prominence: 0.05

Peak fitting menu

Batch processing of files in a folder

Load folder

Batch processing

Experiment metadata

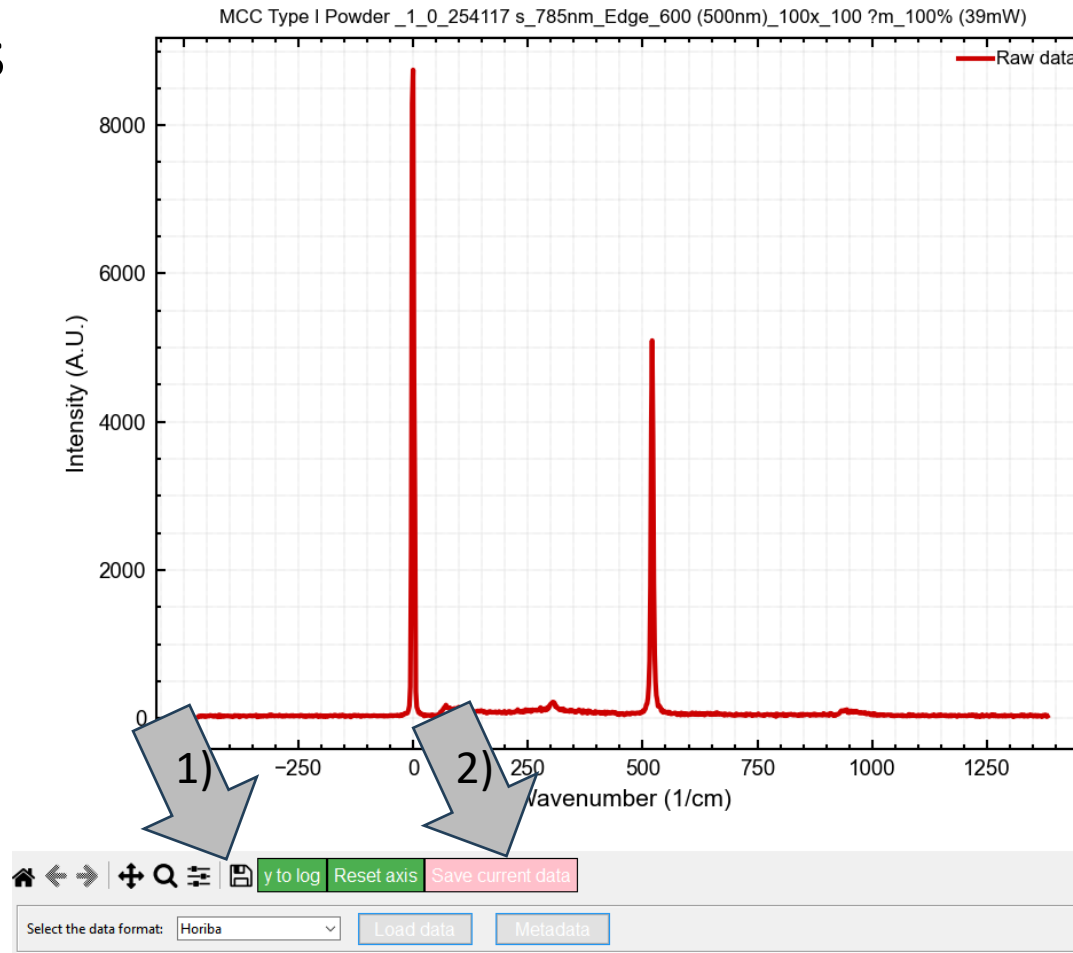
Acq. time (s): 0,254117
 Accumulations: 1
 Range: Off
 Autofocus: Off
 Macrospot: Off
 AutoExposure: Off
 Spike filter: Multiple accum.
 Delay time (s): 0
 Binning: 1
 Readout mode: Signal
 DeNoise: Off
 ICS correction: Off
 Dark correction: Off
 Inst. Process: Off
 Detector Gain: High Sensitivity
 Detector ADC: 45 kHz
 Detector temperature (°C): -60,1
 Instrument: LabRAM Soleil
 Detector: Sincerity
 Objective: 100x
 Grating: 600 (500nm)

Retrieve metadata:



- Image can be saved as a .png clicking in 1)
- The data that appears in the image can be saved as a .csv by clicking 2)

Raman_Peak_Processing_V6 JAC



Select the spectral range:

Min. wavenumber (1/cm)	Max. wavenumber (1/cm)
-465.794	1380.1

Clip data

Baseline Correction:

Auto Manual

Baseline lambda: 1

Baseline fit

Subtract Baseline

Normalise

Peak detection and processing:

Max. number of peaks: 8

Peak detection

=====

Add peaks

Smoothing window: 10

Peak threshold: 0.01

Peak separation: 4

Peak prominence: 0.05

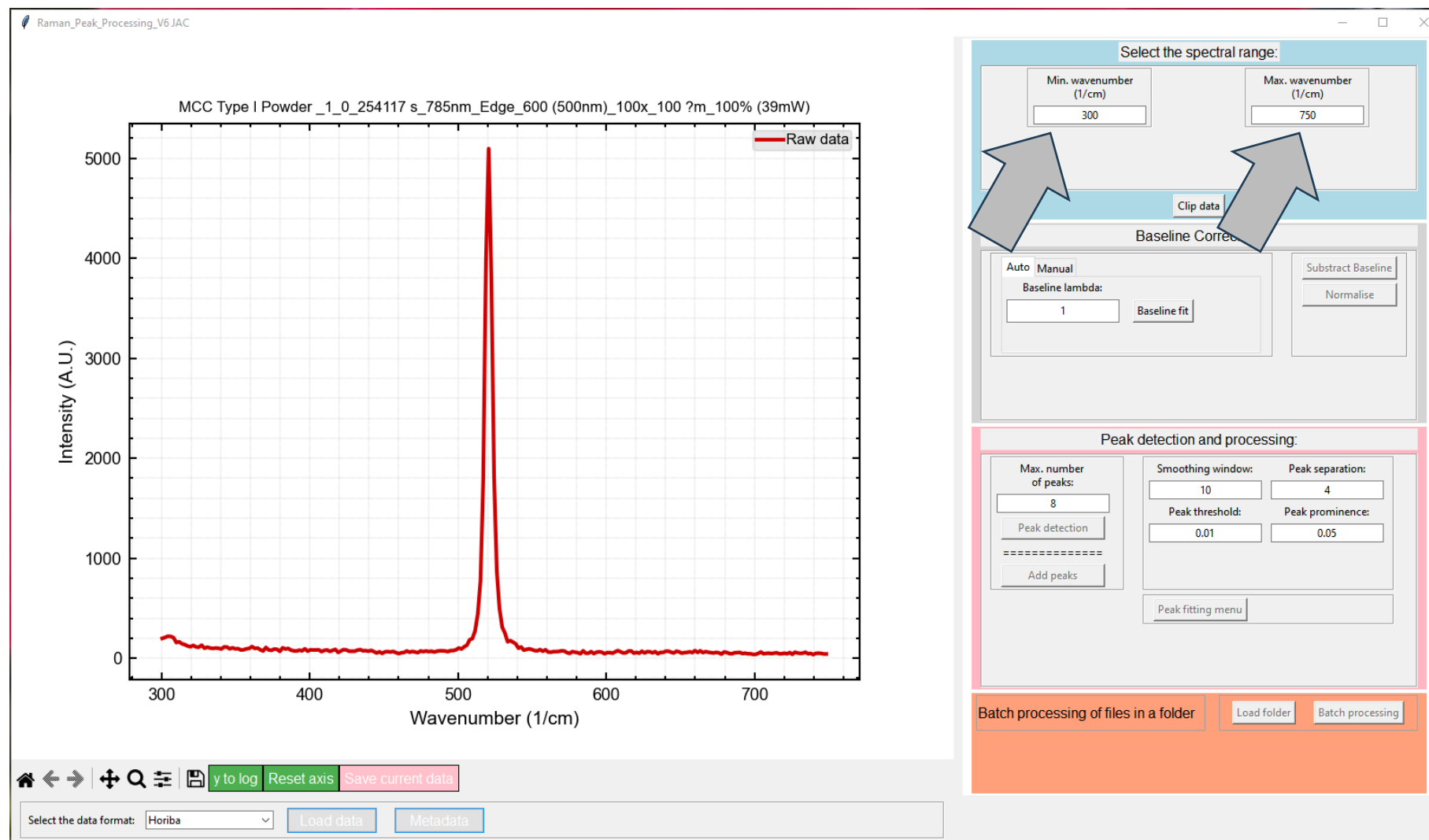
Peak fitting menu

Batch processing of files in a folder

Load folder Batch processing



- Select the region of interest for the analysis.



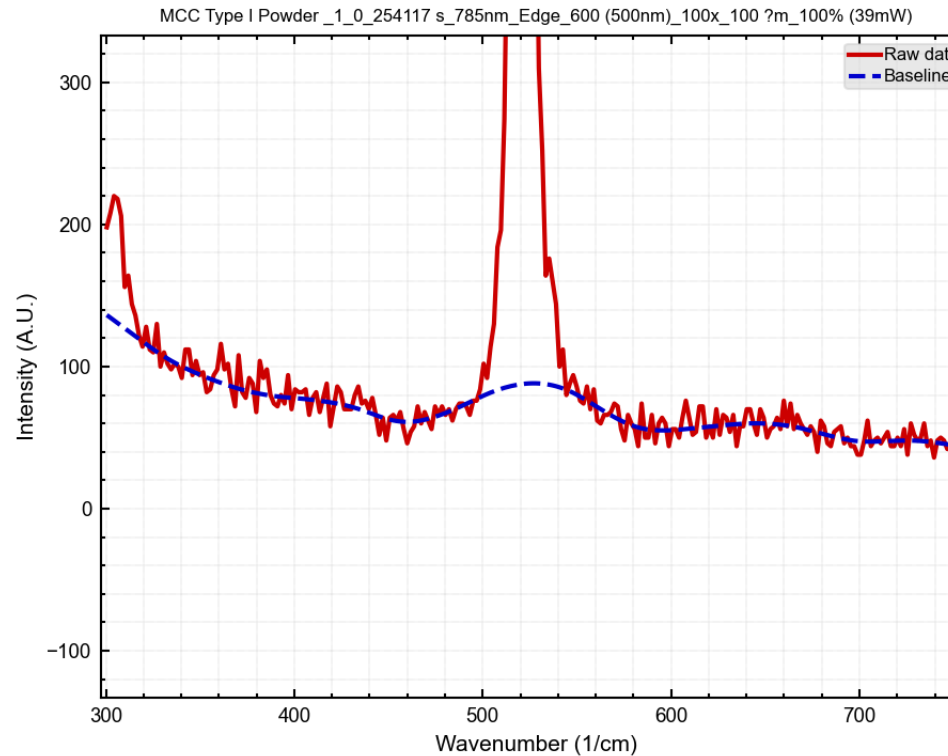
• Remove baseline:

• Auto:

- Uses the asymmetrically reweighted penalized least squares (arPLS) baseline correction on the given spectrum.* Adjust lambda (0-1e6), closer to 1 less sensitive to peak, higher values more sensitive to peaks
- Subtract baseline.
- Normalise the data to the highest peak if needed.

*Sung-June Baek, Aaron Park, Young-Jin Ahna and Jaebum Choo: "Baseline correction using asymmetrically reweighted penalized least squares smoothing", Analyst, 2015,140, 250-257

Raman_Peak_Processing_V6 JAC



Navigation icons: Home, Back, Forward, Zoom In, Zoom Out, Full Screen, Print, Save, y to log, Reset axis, Save current data

Select the data format: Horiba Load data Metadata

Select the spectral range:

Min. wavenumber (1/cm)	Max. wavenumber (1/cm)
300	750

Clip data

Baseline Correction:

Auto ☐ Baseline lambda: 0.01 Baseline fit

Subtract Baseline Normalise

Peak detection and processing:

Max. number of peaks: 8	Smoothing window: 10	Peak separation: 4
Peak detection	Peak threshold: 0.01	Peak prominence: 0.05
Add peaks	Peak fitting menu	

Batch processing of files in a folder

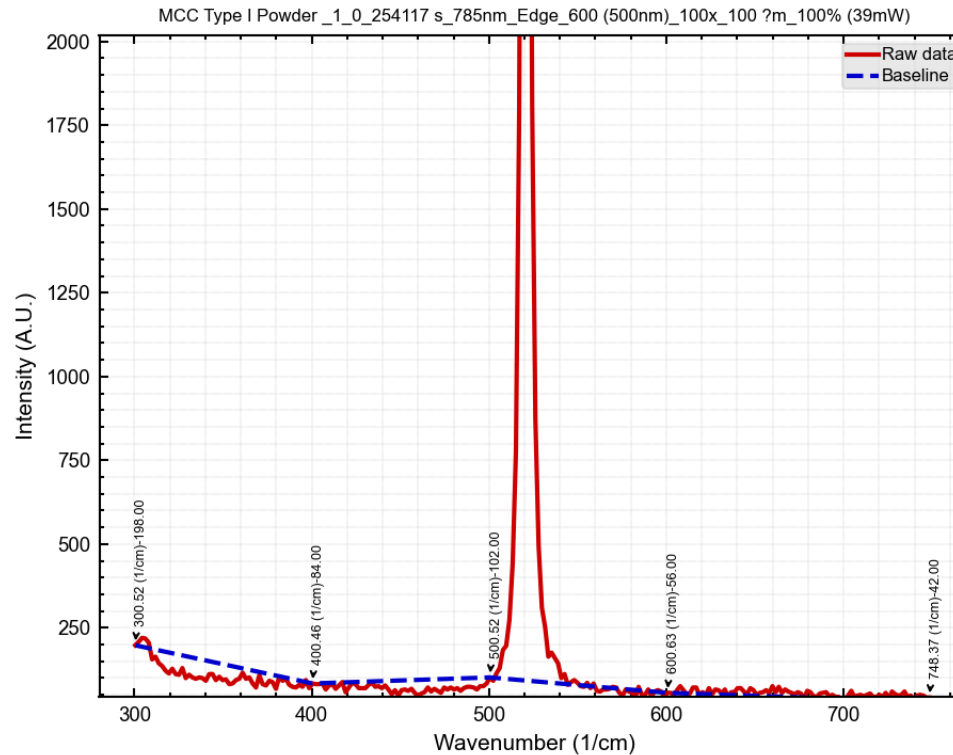
Load folder Batch processing

• Remove baseline:

• Manual:

- Uses baseline defined by the user.
- Add manually as many wavenumber points as need 1).
- Choose the order of the baseline 2).
- The user can save the baseline as a .csv file and load that file for other datasets 3).
- Subtract baseline.
- Normalise the data to the highest peak if needed.

Raman_Peak_Processing_V6 JAC



Home Left Right Zoom Fit Save y to log Reset axis Save current data

Select the data format: Horiba Load data Metadata

Select the spectral range:

Min. wavenumber (1/cm): 300 Max. wavenumber (1/cm): 750

2) 3)

Baseline action:

Auto Manual
linear Load file Save points
Add point (x coord): 0.0 Add Reset
Subtract Baseline
Normalise

1)

Peak detection and processing:

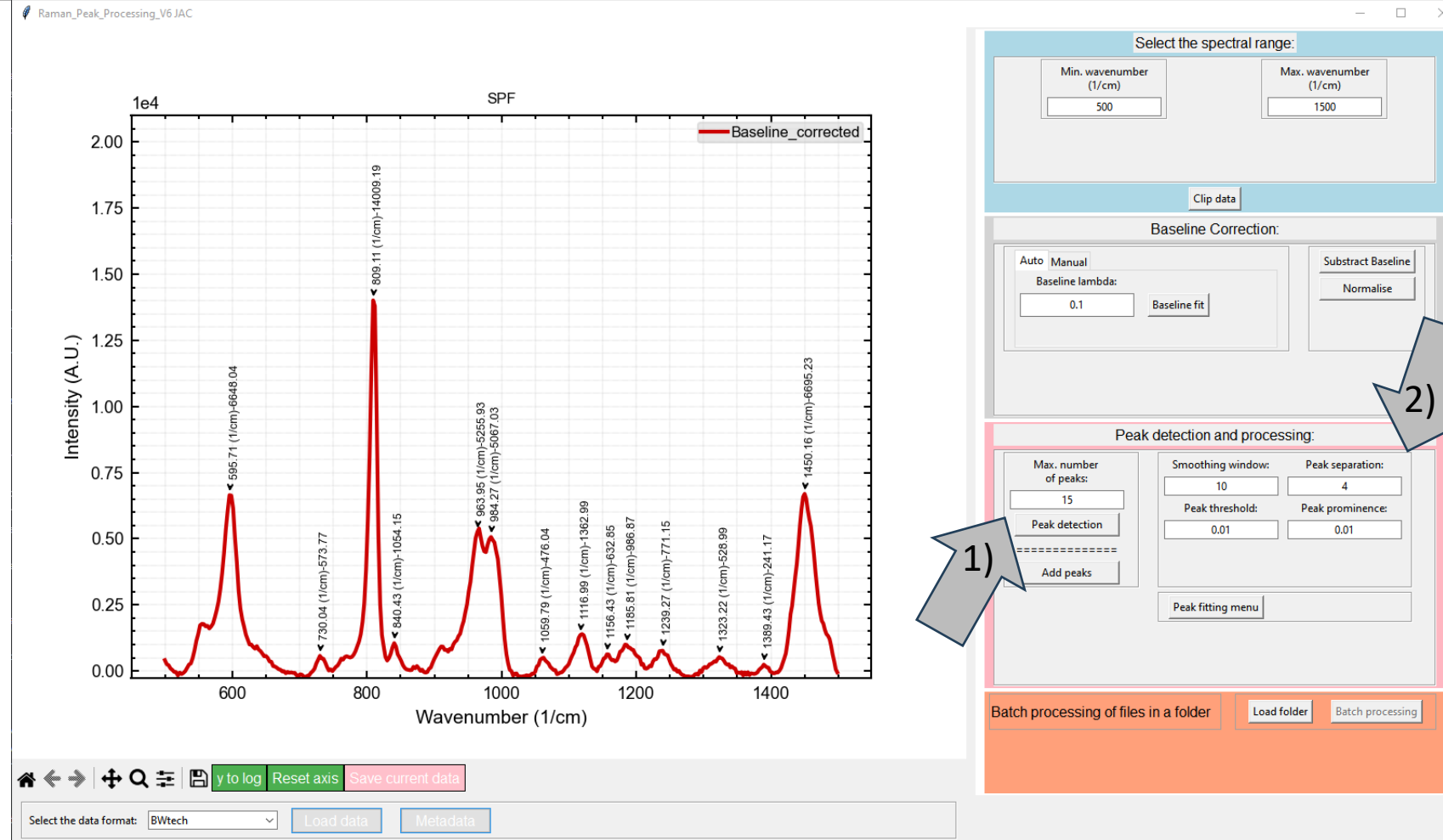
Max. number of peaks: 8
Peak detection
Add peaks
Smoothing window: 10
Peak threshold: 0.01
Peak separation: 4
Peak prominence: 0.05
Peak fitting menu

Batch processing of files in a folder Load folder Batch processing

• Peak detection:

• Auto:

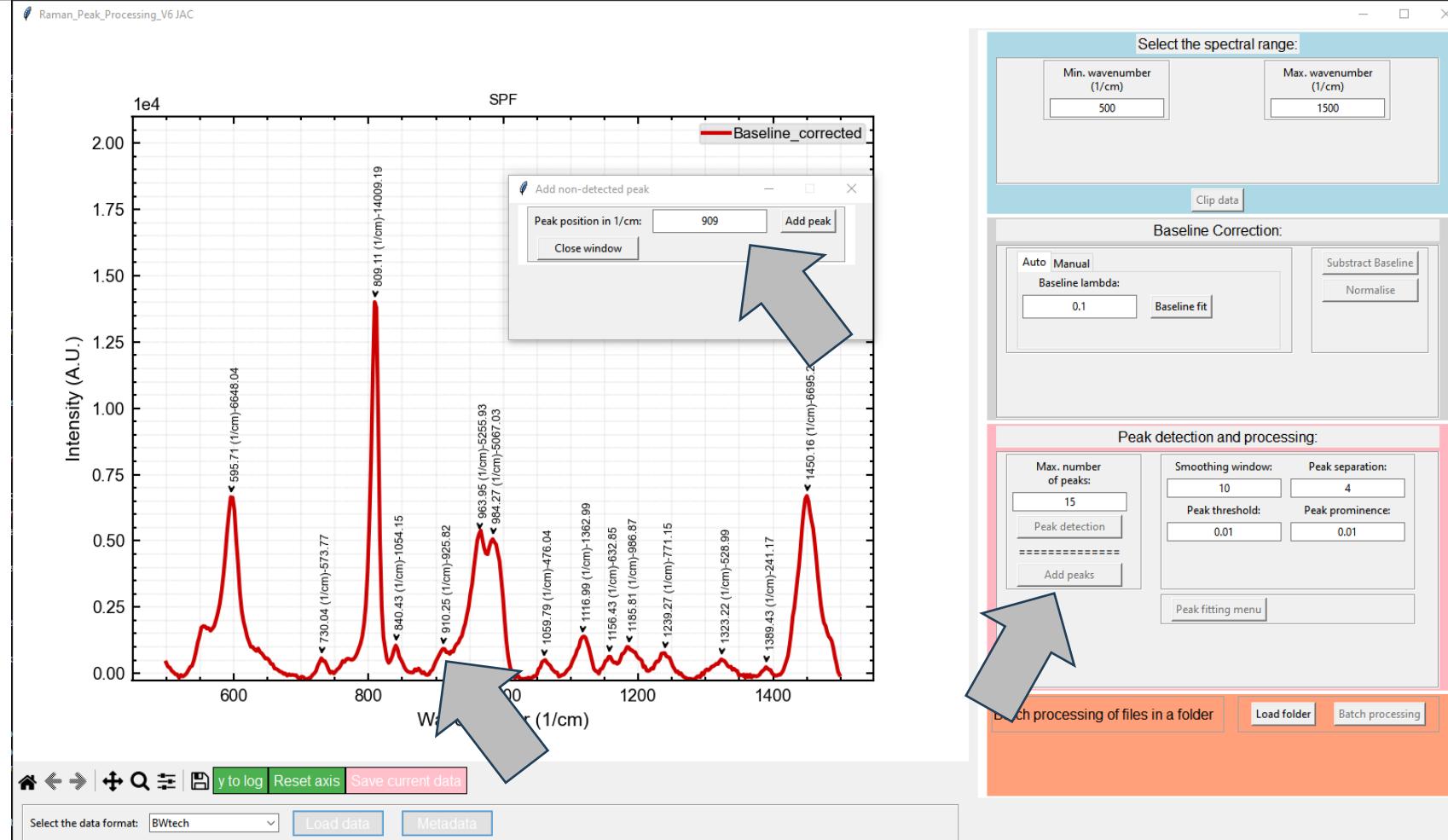
- Select maximum number of peaks to be detected (maximum 25) 1).
- Tweak the detection parameters to find the peaks 2).
 - Smoothing window: Size of the smoothing window to produce a smooth and continuous dataset for derivative-based peak finding algorithm).
 - Peak separation: in pixels, minimum of 3 pixels to detect contiguous peaks.
 - Peak Threshold: Ratio from minimum peak height to max peak height to be detected.
 - Peak prominence: Parameter to be more or less sensitive to shoulders.



• Peak detection:

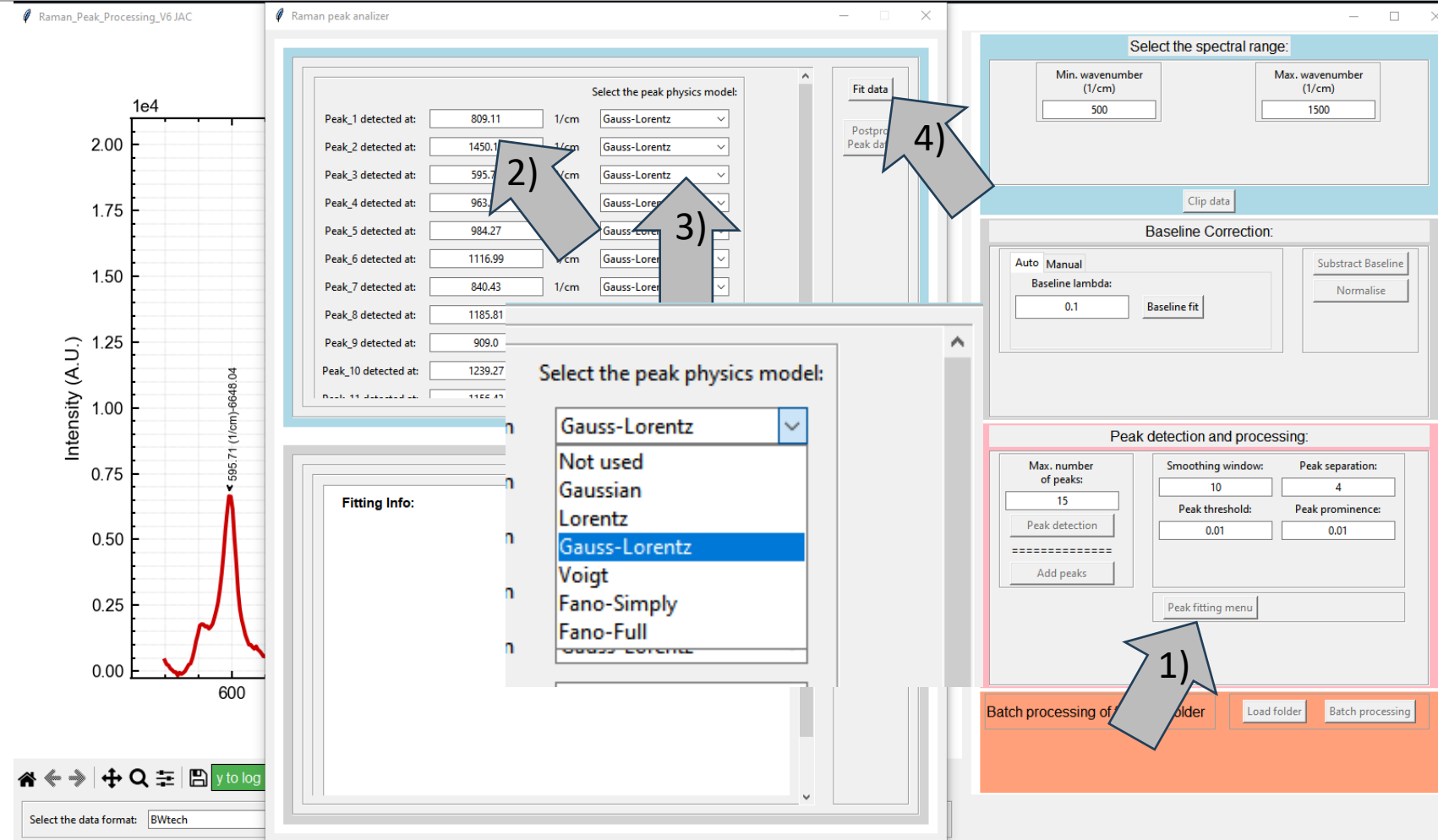
• Manual:

- Peaks can be added by introducing their wavenumber.
- This can be combined with the automatic routine (7-a)



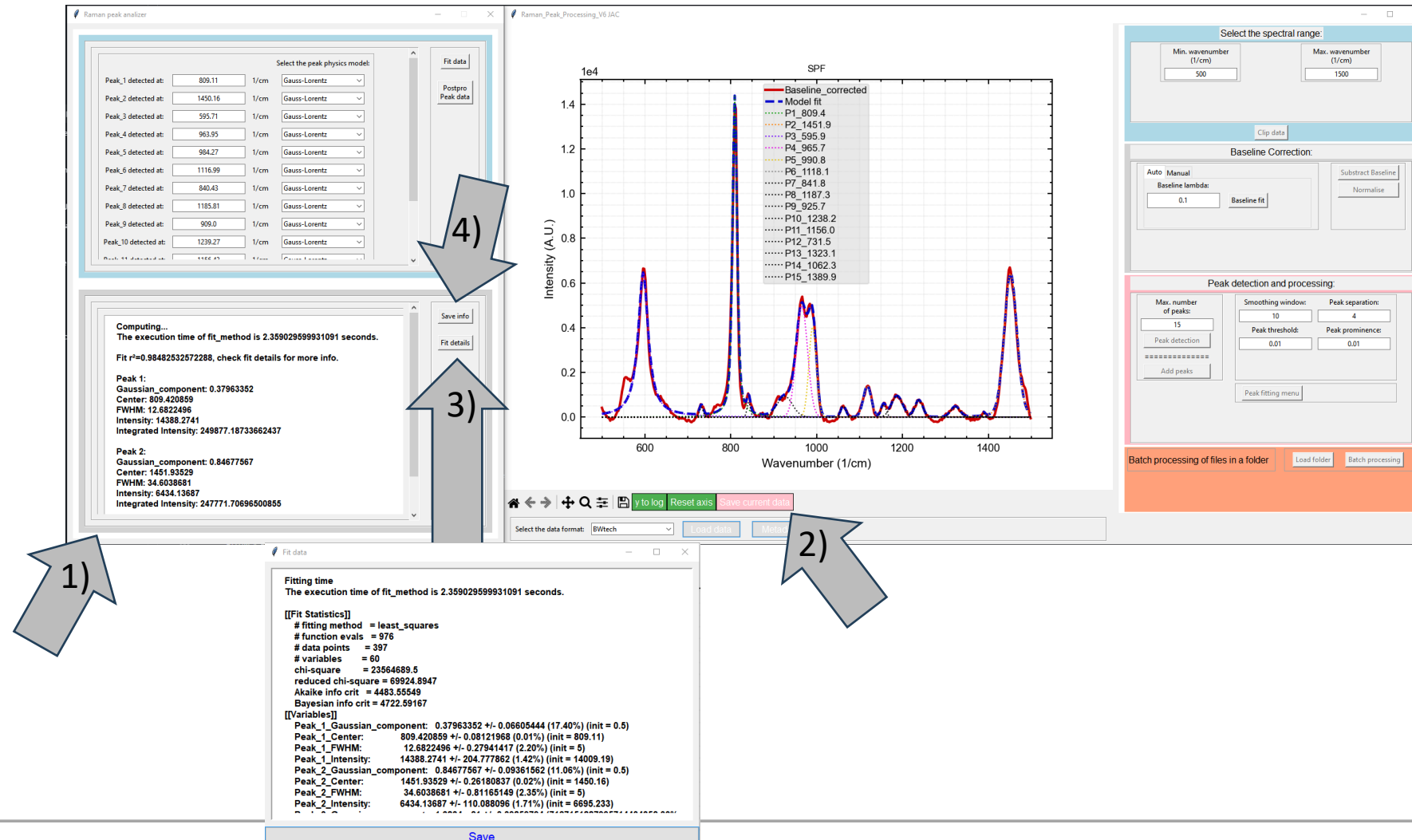
• Peak fitting:

- Select peak fitting menu 1).
- Finetune the position of detected peak if needed 2).
- Select the individual model for each peak.
- By default, it uses a Gauss-Lorentz approach (pseudo-Voigt) with a FWHM estimated following Kielkopf approach (0.02% error)*
- Full Voigt and Voigt Fano (Fano-Full) can be used as well.

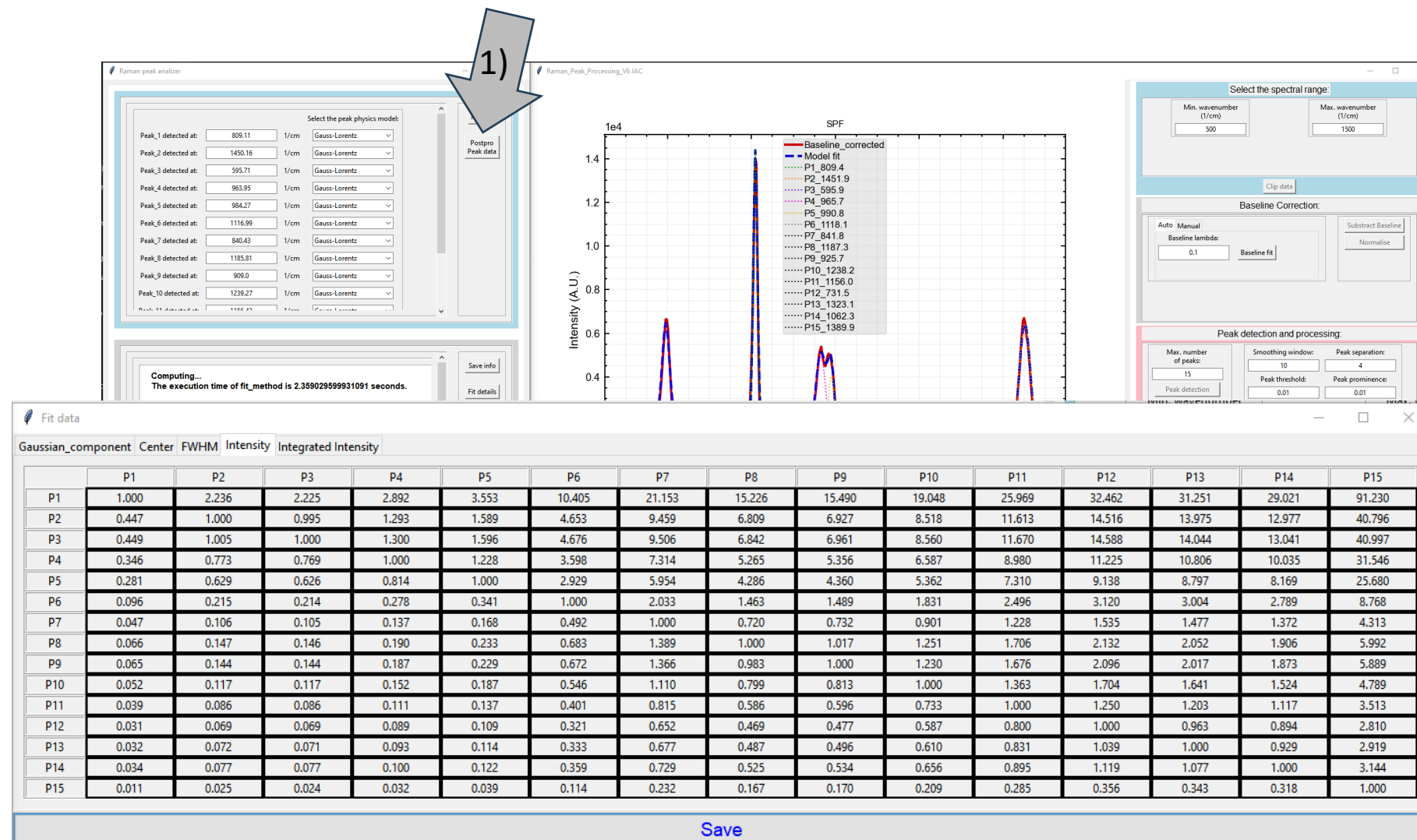


* John F. Kielkopf (1973), "New approximation to the Voigt function with applications to spectral-line profile analysis", *Journal of the Optical Society of America*, **63** (8): 987,

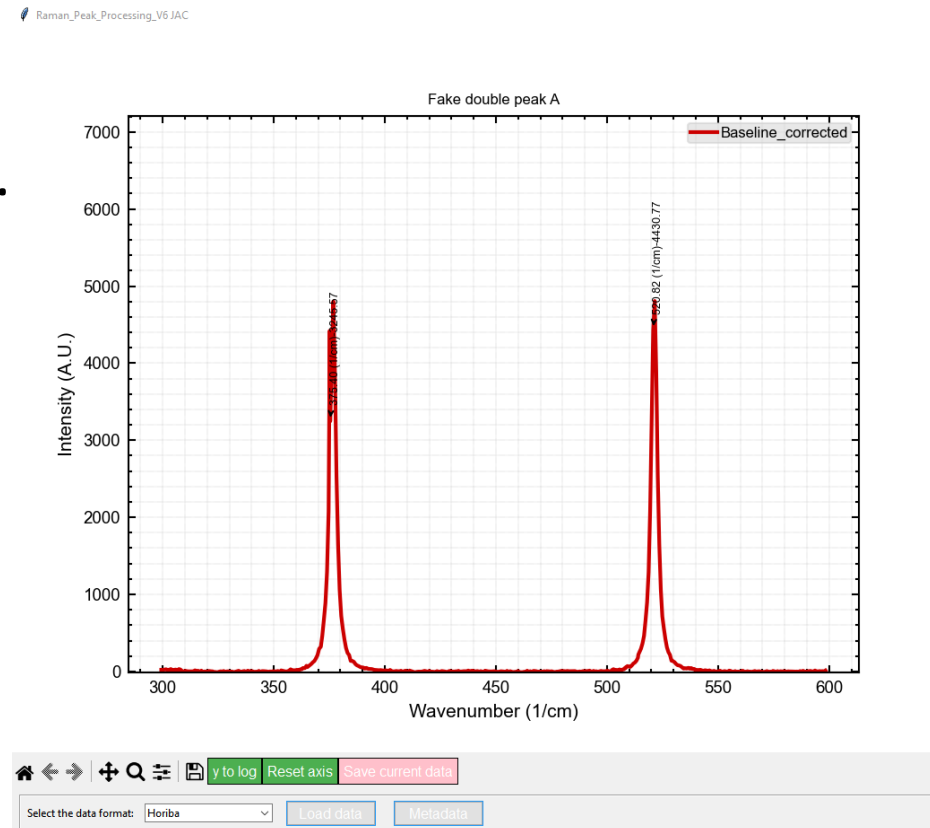
- Peak fitting:
 - Review the fit data summary 1).
 - The resultant fit is shown in the main window.
 - Fitted peak positions are shown in the legend from higher intensity to lower intensity.
 - All data displayed in the figure can be saved as a .csv file 2).
 - Complete fitting details, including cross-correlations can be retrieved and saved 3)
 - Summary report can be saved as .txt 4)



- Peak fitting:
 - Postprocessed correlations between all parameters can be calculated and saved 1)



1. Save all the raw data files to be processed in a common folder.
2. Open 1 data file and follow steps 3-7b.
3. This fixes the following conditions to analyse all files in the folder.
 1. Data range
 2. Baseline type and properties
 3. Max peak detected and parameters to detect a peak.
 4. All peaks fitted with the default pseudo-Voigt default function.



Select the spectral range:

Min. wavenumber (1/cm): 300

Max. wavenumber (1/cm): 600

Clip data

Baseline Correction:

Auto Manual

Baseline lambda: 1

Baseline fit

Subtract Baseline

Normalise

Peak detection and processing:

Max. number of peaks: 8

Peak detection

Smoothing window: 10

Peak threshold: 0.01

Peak separation: 4

Peak prominence: 0.05

Add peaks

Peak fitting menu

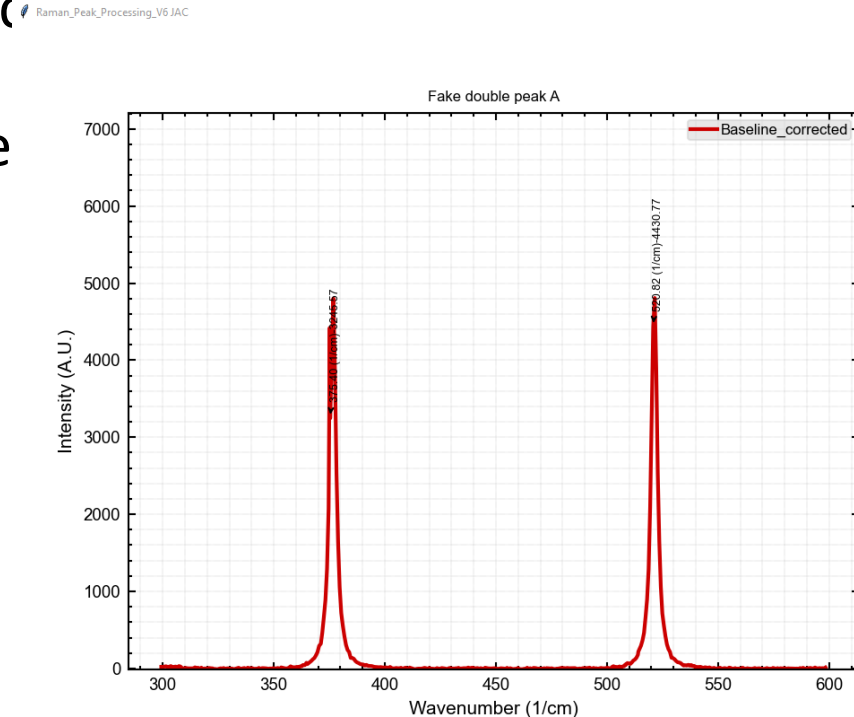
Batch processing of files in a folder

Load folder

Batch processing

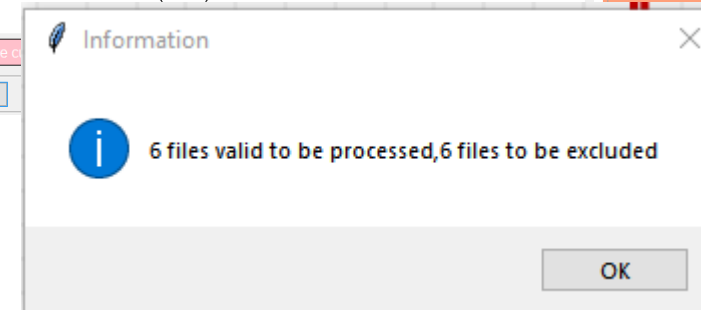


4. When the parameters are selected, click on “Load folder” button 1). This will scan for valid .txt data files in the folder
5. Click on “Batch processing” to analyse all files in folder 2).



Select the data format: Horiba

Load data



Select the spectral range:

Min. wavenumber (1/cm): 300

Max. wavenumber (1/cm): 600

Clip data

Baseline Correction:

Auto Manual

Baseline lambda: 1

Baseline fit

Subtract Baseline

Normalise

Peak detection and processing:

Max. number of peaks: 8

Peak detection

Add peaks

Smoothing window: 10

Peak threshold: 0.01

Peak separation: 4

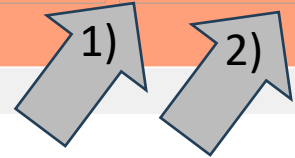
Peak prominence: 0.05

Peak fitting menu

Batch processing of files in a folder

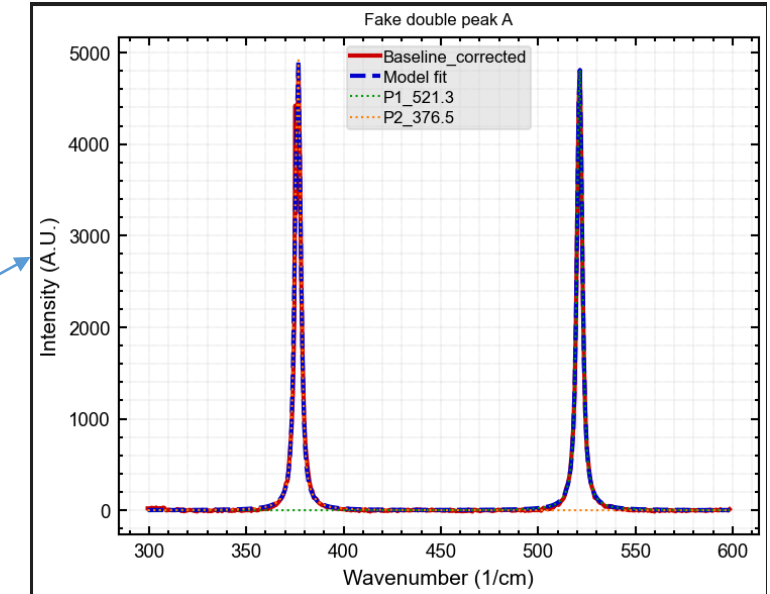
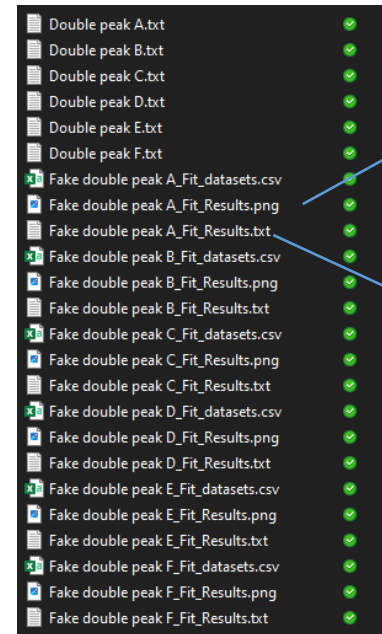
Load folder

Batch processing



6. Review the data that has been saved in the processed folder. It will include:

1. An image file for each processed file
2. A csv file with all the data shown in the image.
3. A txt file with all the information of the fitting.



```
File Edit Format View Help
[1: ('Gaussian_component': 0.1776099, 'Center': 521.328679, 'FWHM': 3.29246185, 'Intensity': 4863.99684, 'Integrated Intensity': 23525.90483965668)
2: ('Gaussian_component': 0.33634011, 'Center': 376.500209, 'FWHM': 3.53976256, 'Intensity': 5065.59305, 'Integrated Intensity': 24928.370991332755)]

Fit Report:
[[Fit Statistics]]
# fitting method = least_squares
# function evals = 72
# data points = 429
# variables = 8
chi-square = 1589251.18
reduced chi-square = 3774.86323
Akaike info crit = 3541.22880
Bayesian info crit = 3579.72045

[[Variables]]
Peak_1_Gaussian_component: 0.17760990 +/- 0.04196682 (23.63%) (init = 0.5)
Peak_1_Center: 521.328679 +/- 0.01483816 (0.003%) (init = 520.8221)
Peak_1_FWHM: 3.29246185 +/- 0.05576401 (1.69%) (init = 5)
Peak_1_Intensity: 4863.99684 +/- 40.5387230 (1.00%) (init = 4430.77)
Peak_2_Gaussian_component: 0.33634011 +/- 0.03824014 (11.37%) (init = 0.5)
Peak_2_Center: 376.500209 +/- 0.01414932 (0.003%) (init = 375.4021)
Peak_2_FWHM: 3.53976256 +/- 0.05065559 (1.43%) (init = 5)
Peak_2_Intensity: 5065.59305 +/- 60.2519989 (1.19%) (init = 3245.569)

[[Correlations]] (unreported correlations are < 0.100)
C(Peak_2_FWHM, Peak_2_Intensity) = -0.8272
C(Peak_1_FWHM, Peak_1_Intensity) = -0.7455
C(Peak_2_Gaussian_component, Peak_1_FWHM) = -0.6792
C(Peak_2_Gaussian_component, Peak_2_FWHM) = -0.6817
C(Peak_2_Gaussian_component, Peak_2_Intensity) = -0.4947
C(Peak_1_Gaussian_component, Peak_1_Intensity) = -0.4246
C(Peak_2_Center, Peak_2_FWHM) = -0.2167
C(Peak_2_Gaussian_component, Peak_2_Center) = -0.1696
C(Peak_2_Center, Peak_2_Intensity) = -0.1558

Postprocessed ratios between peak parameters:
Gaussian_component:
P1, P2
1.000, 0.528
1.094, 1.000

Center:
P1, P2
1.000, 1.385
0.722, 1.000

FWHM:
P1, P2
1.000, 1.385
0.722, 1.000
```