RAMAN DATA PROCESSING V6
QUICK MANUAL

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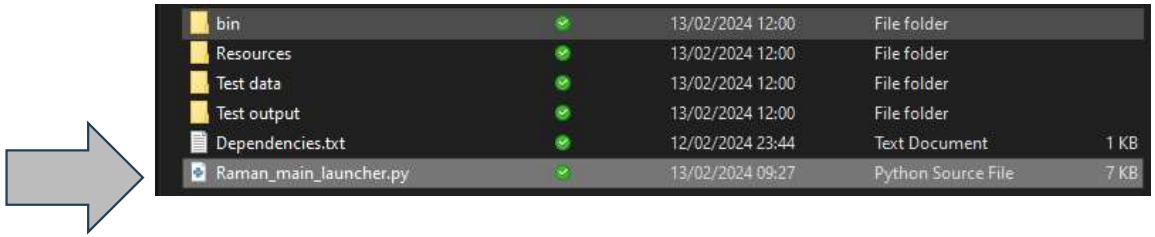
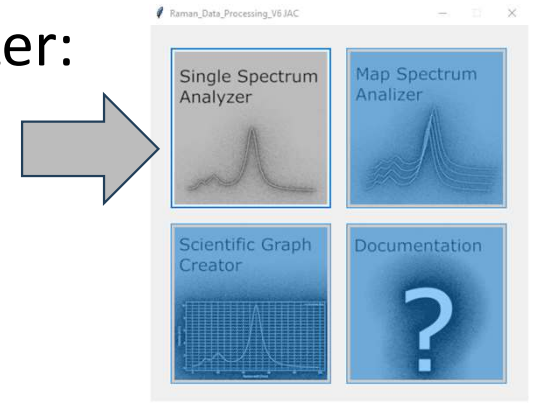
1. Install python >= 3.8.18
2. Install the following libraries:
   - **Multiprocessing**
   - **Tendo**
   - **sys**
   - **os**
   - **csv**
   - **re**
   - **pillow>=10.2.0**
   - **numpy>=1.24.4**
   - **matplotlib>=3.7.4**
   - **numexpr>=2.8.6**
   - **scipy>=1.10.1**
   - **lmfit>=1.2.2**
   - **tkinter>=8.6**

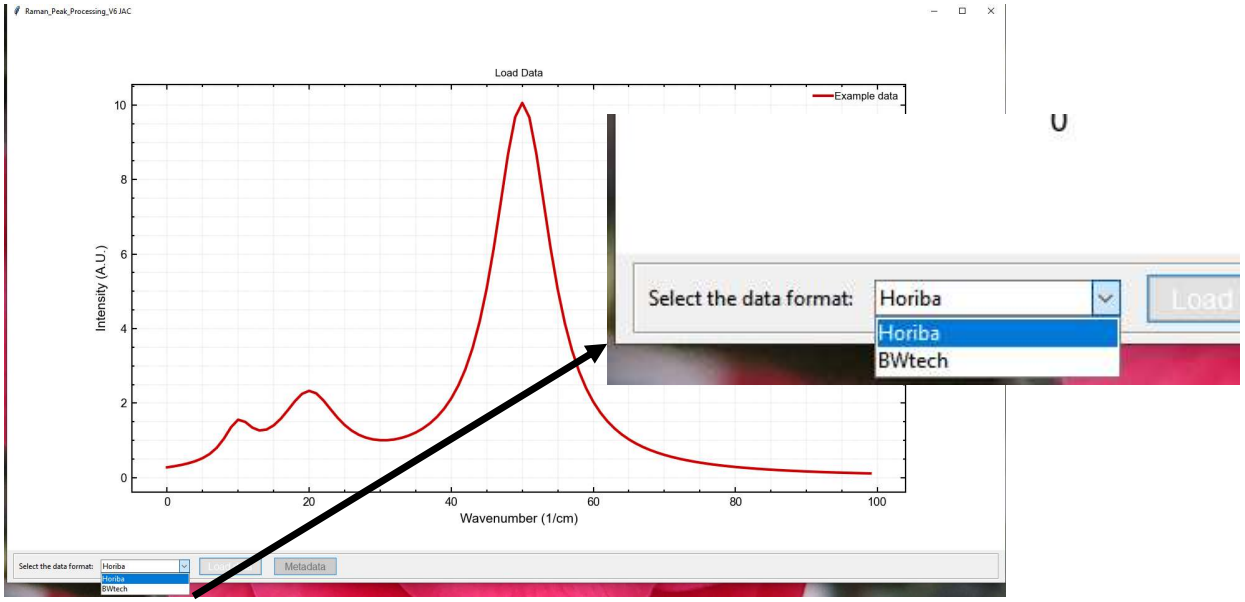
- Currently the software works for individual spectra taken in Horiba YobinYvon and B&WTech spectrometers.
- Data must be saved as .txt files.
- Run the main launcher:



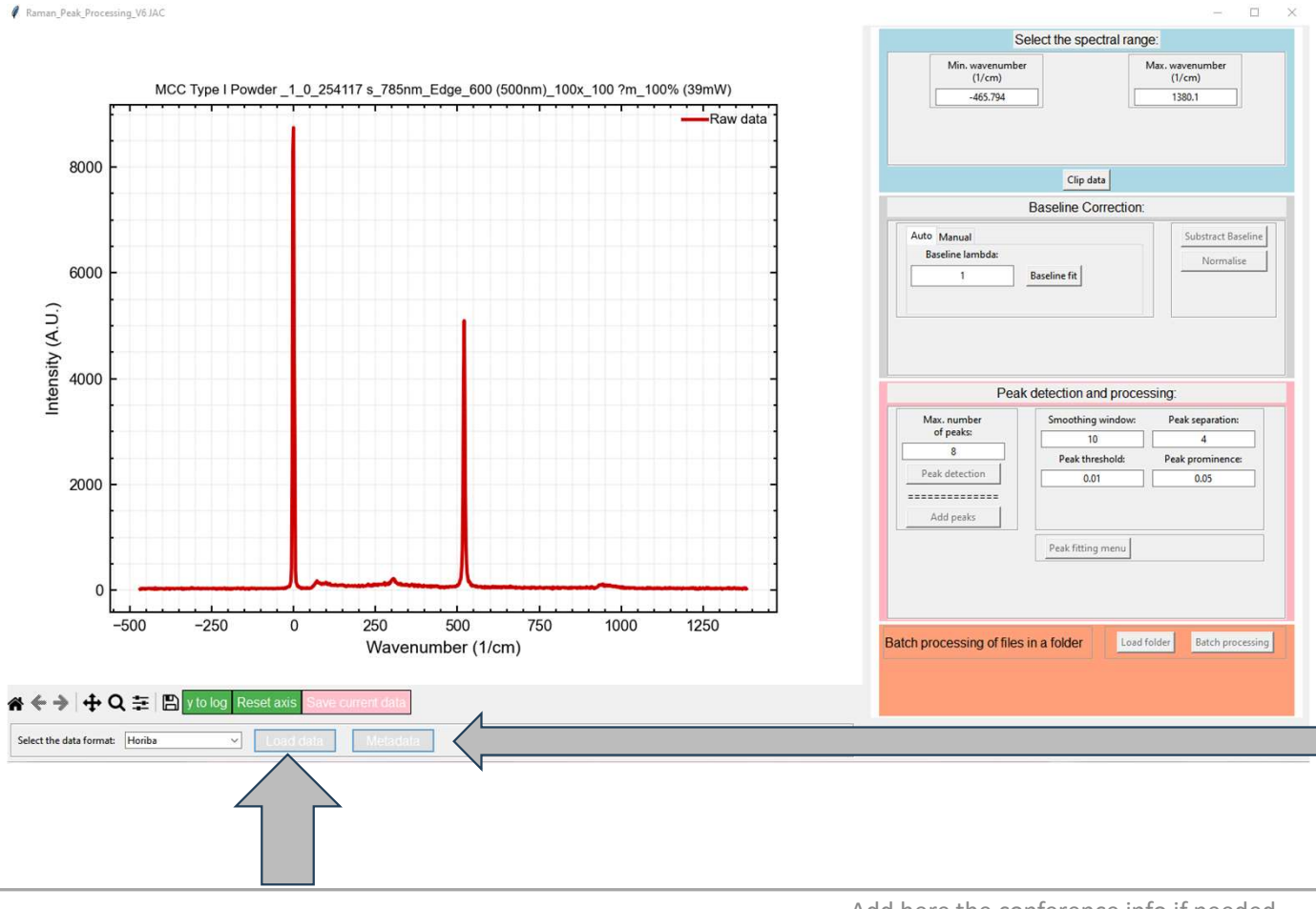
- Select the Single Spectrum Analyzer:



- Select the file format:



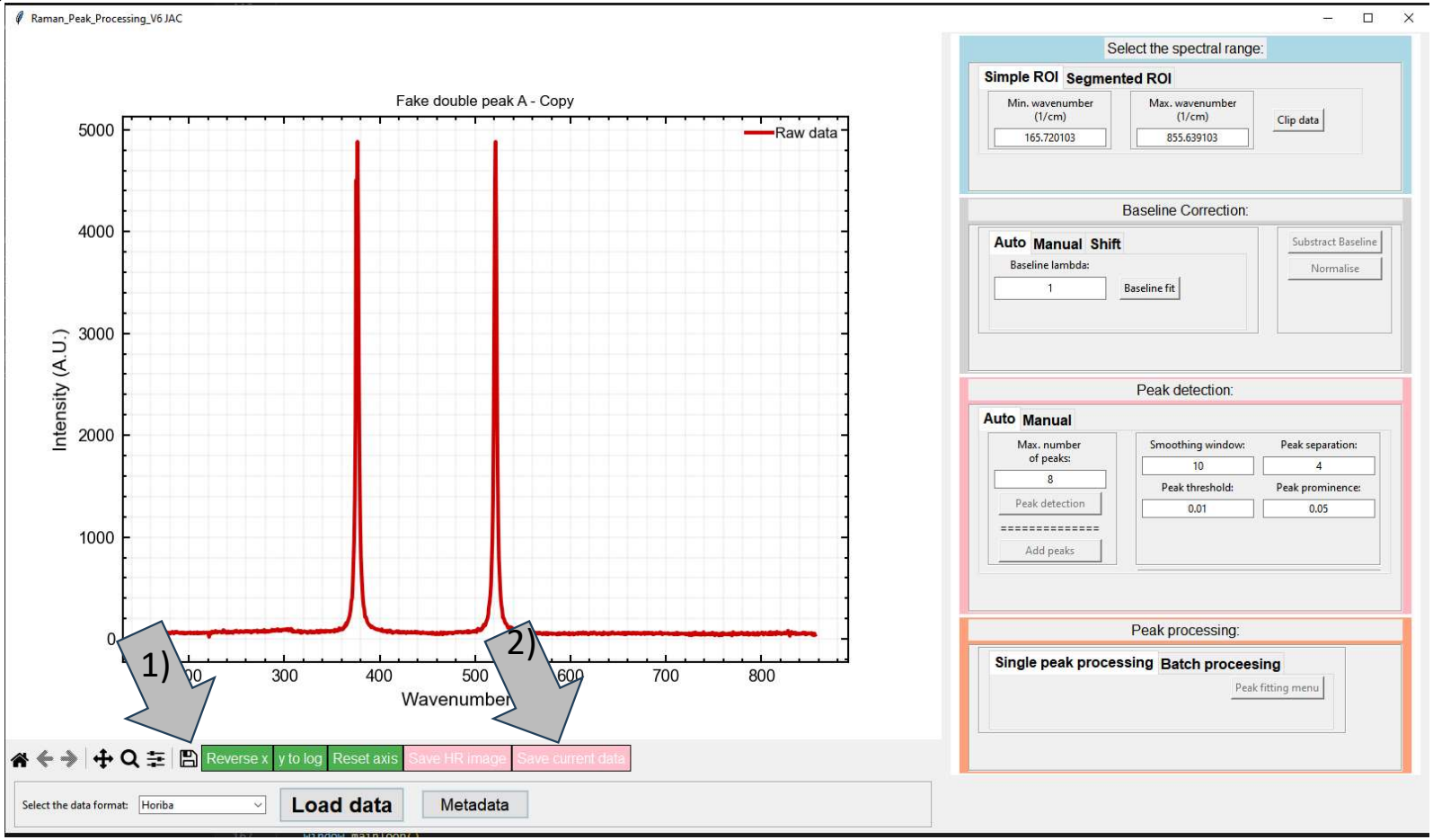
- Load data:



Retrieve metadata:

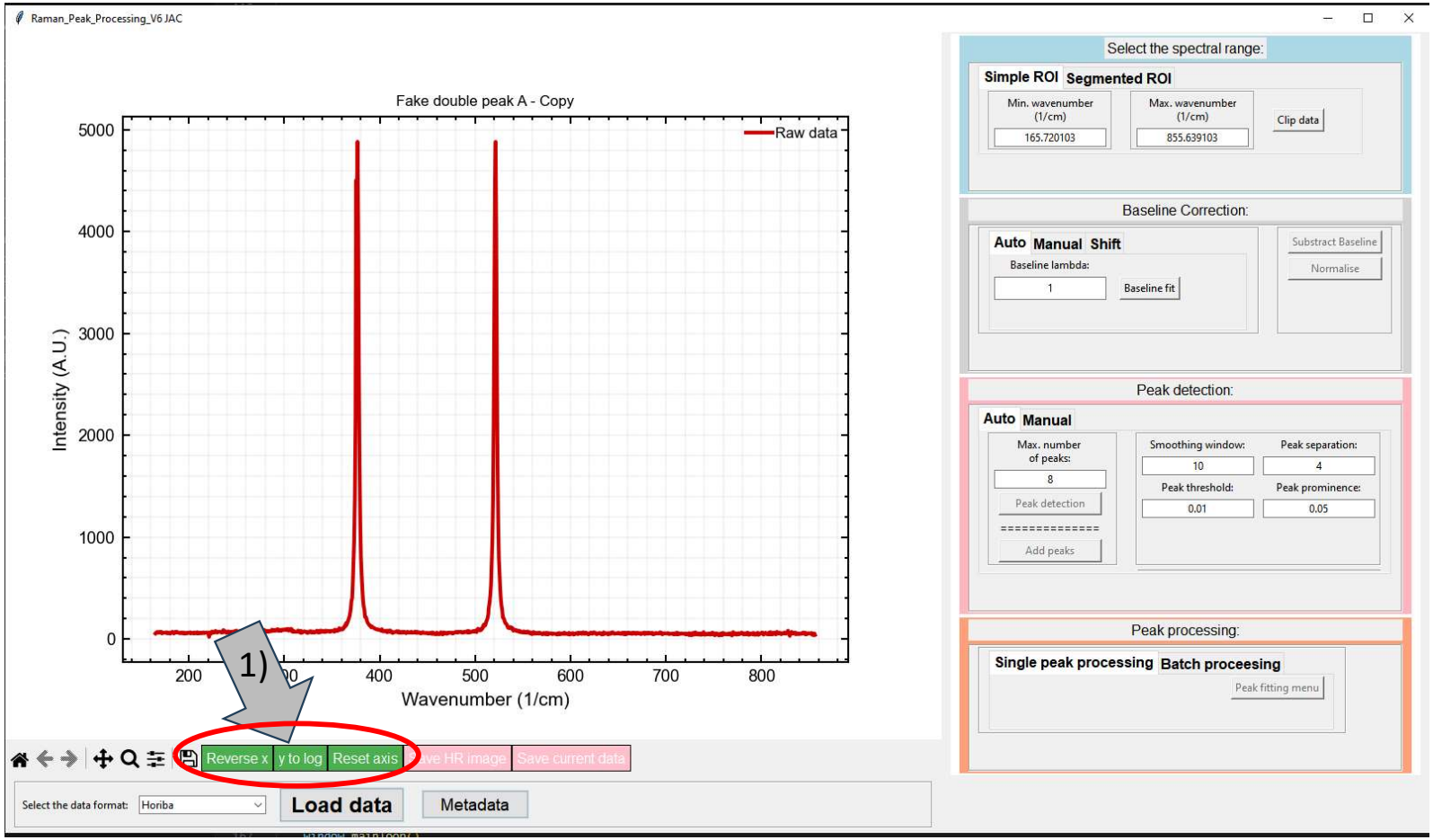
Step 4-b

- 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)



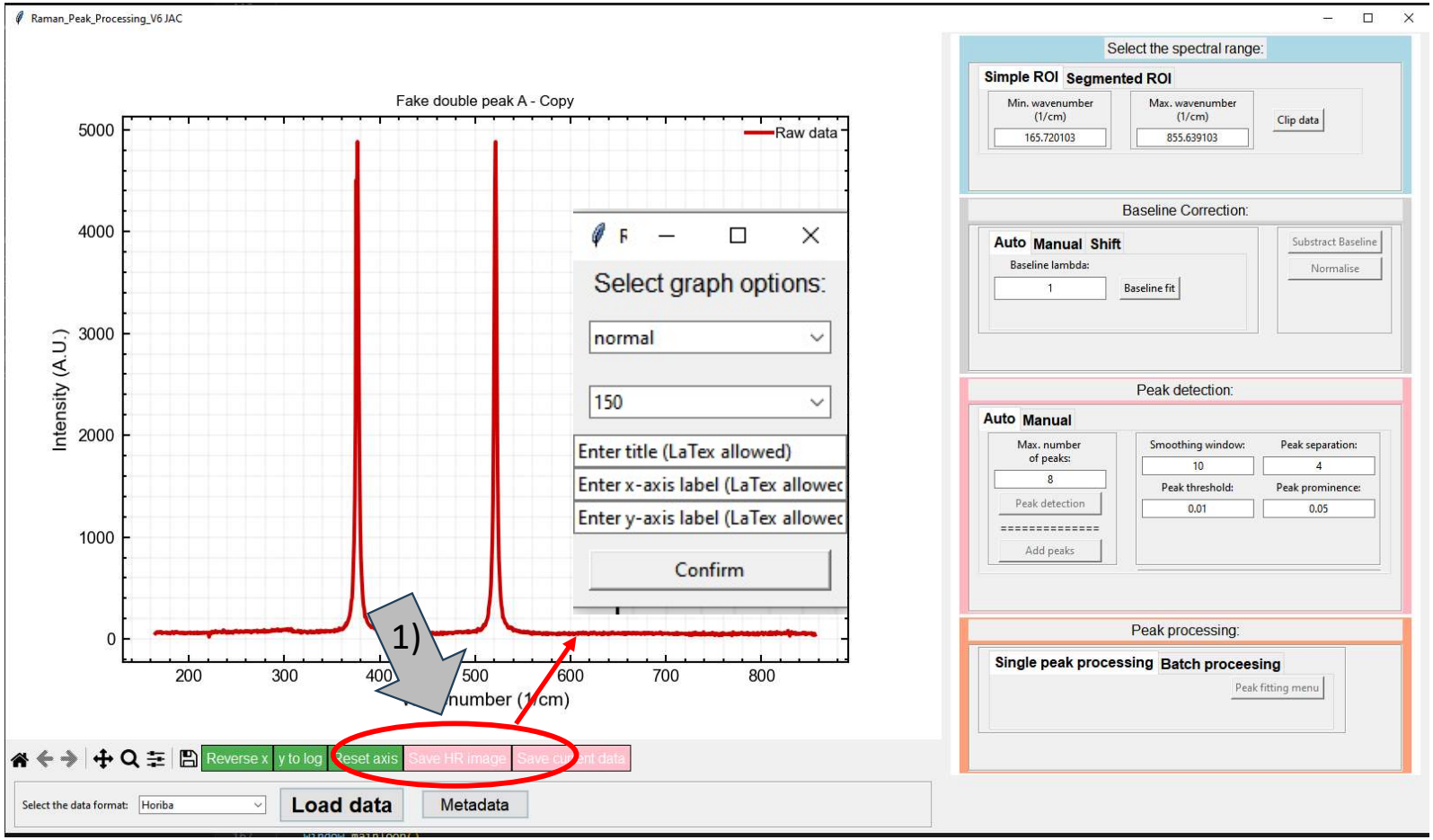
Step 4-c

- The data can be plotted in reverse order (for IR for example). Also the intensity can be plotted in Log scale.



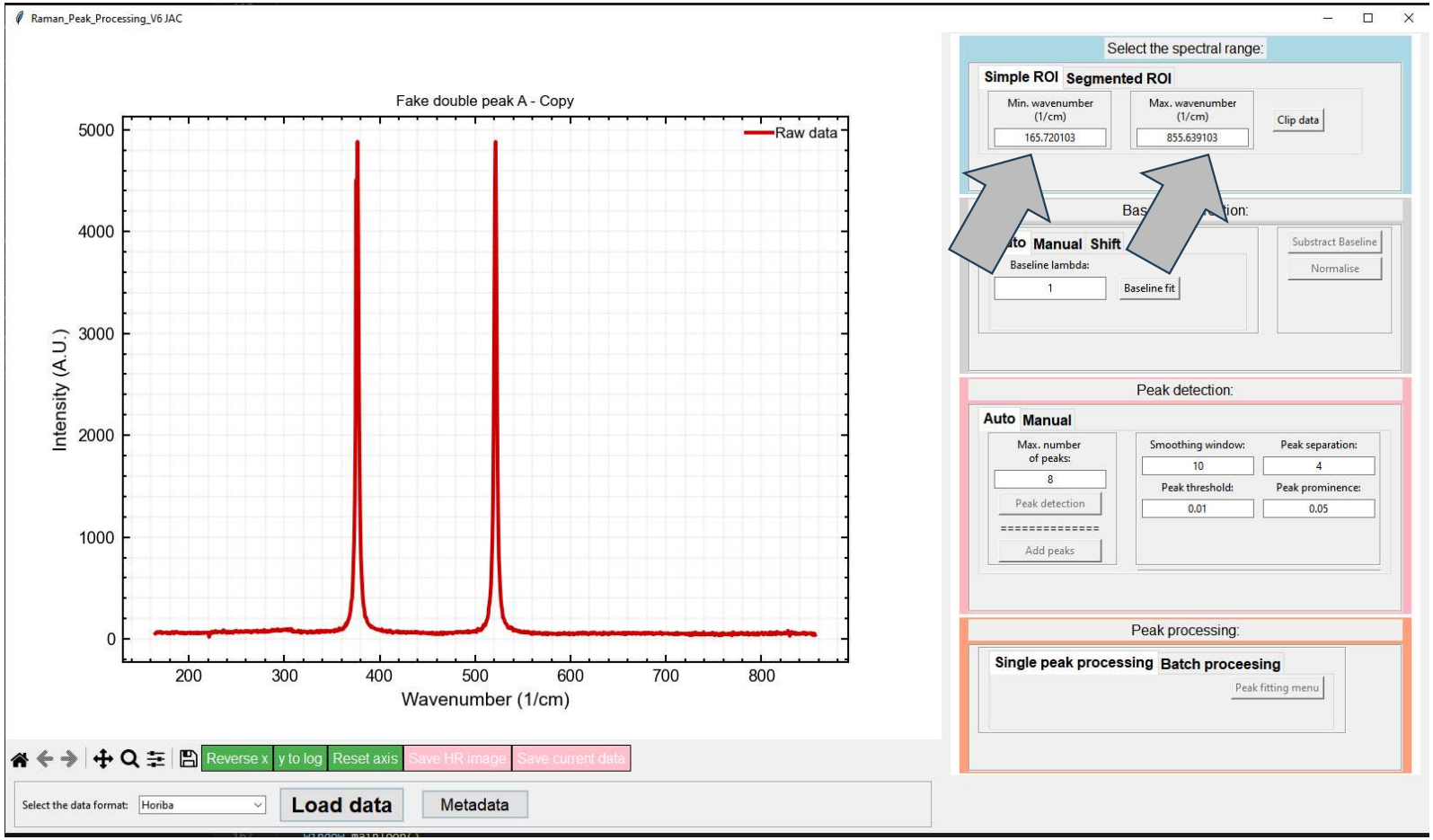
Step 4-d

- The graphs of the window can be exported as publication ready graphs.
- Title and axis labels can be modified using LaTex syntaxis.
- The size of the image and the DPI can also be adjusted.



Step 5

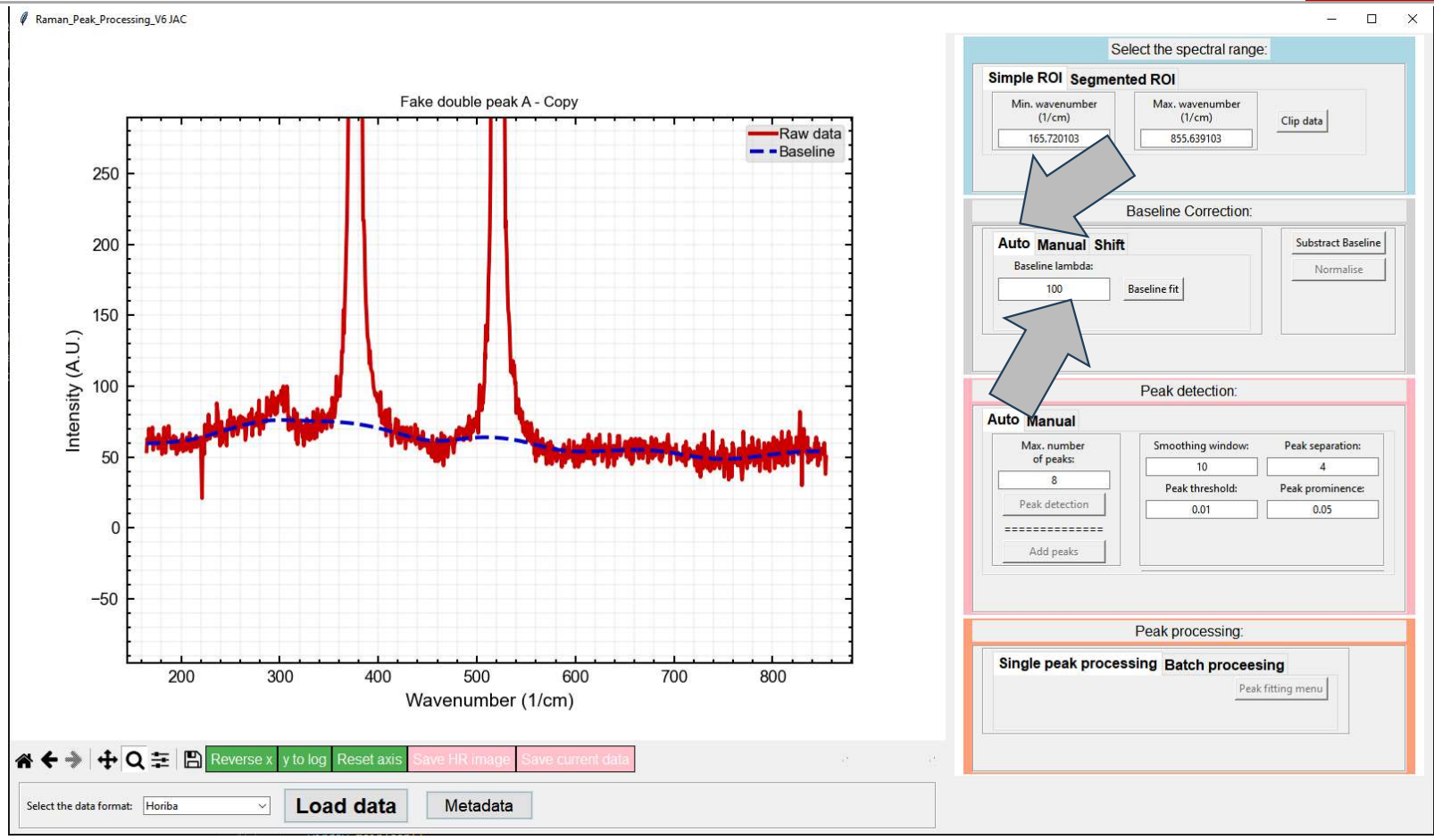
- Select the region of interest for the analysis.



Step 6-a

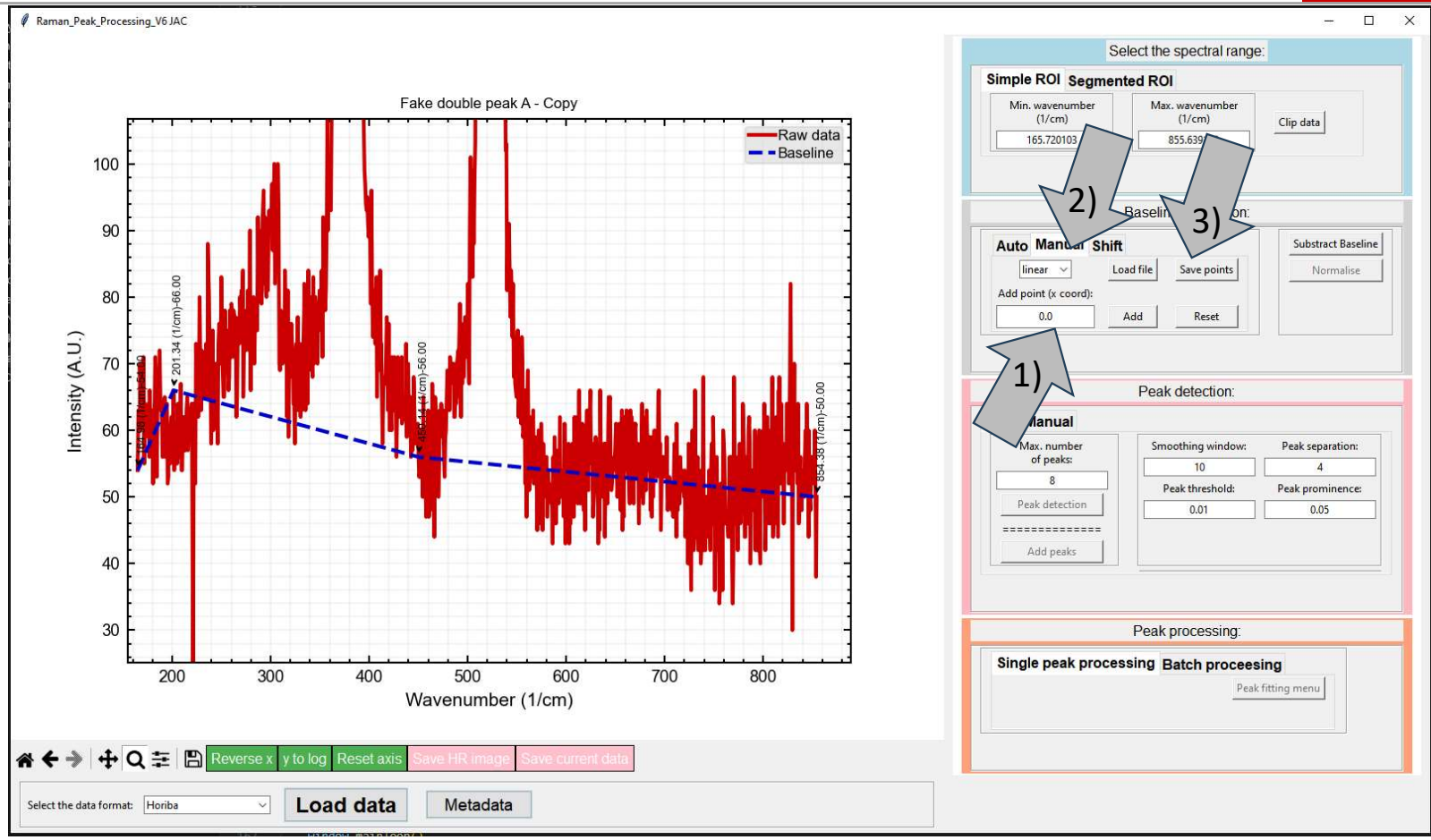
- Remove baseline:
  - Auto:
    - Uses the asymmetrically reweighted penalized least squares (arPLS) baseline correction on the given spectrum.* Adjust lambda (0-1e6), closer to 1 less sensitive to peak, higher values more sensitive to peaks
    - Subtract baseline.
    - Normalise the data to the highest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



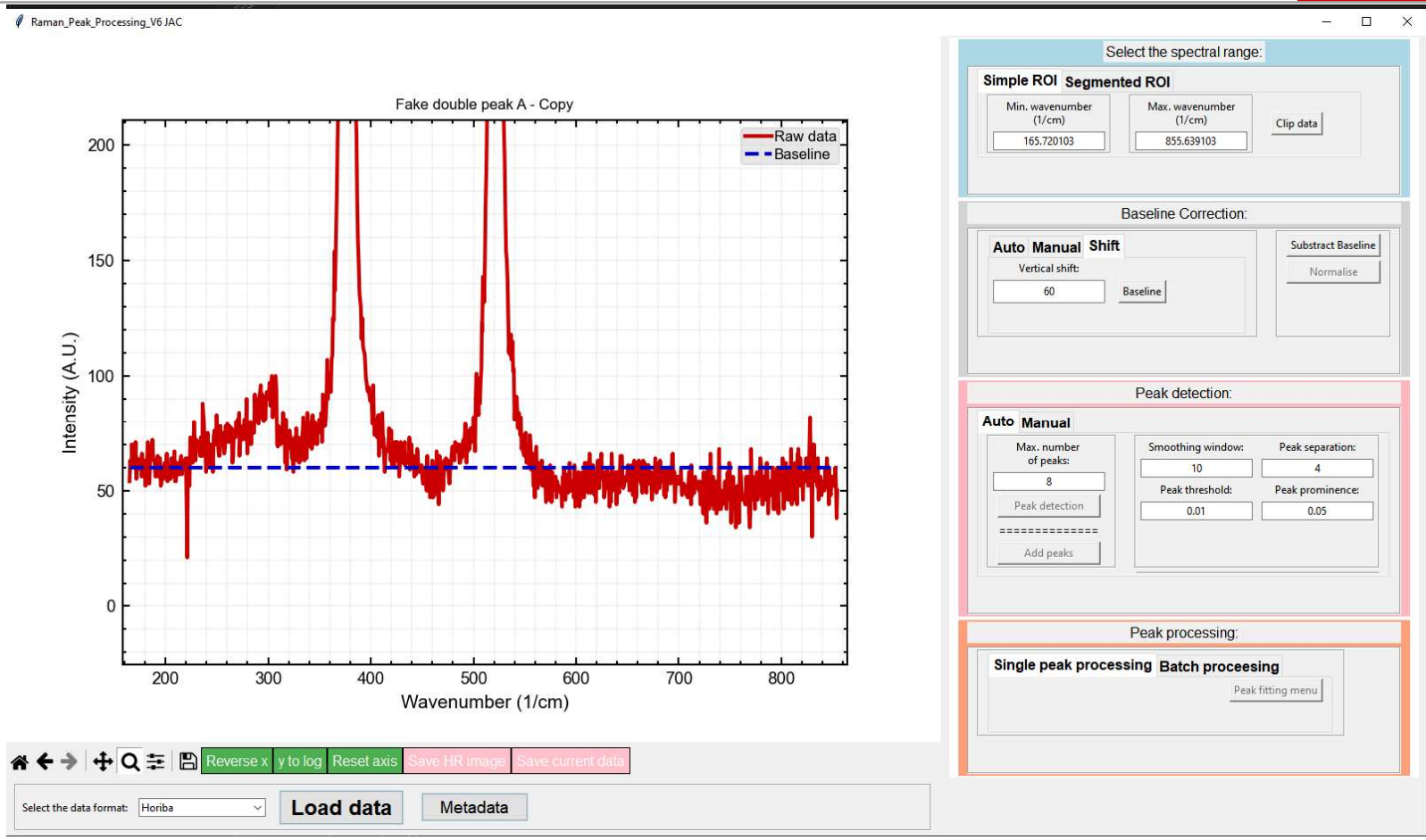
Step 6-b

- 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.



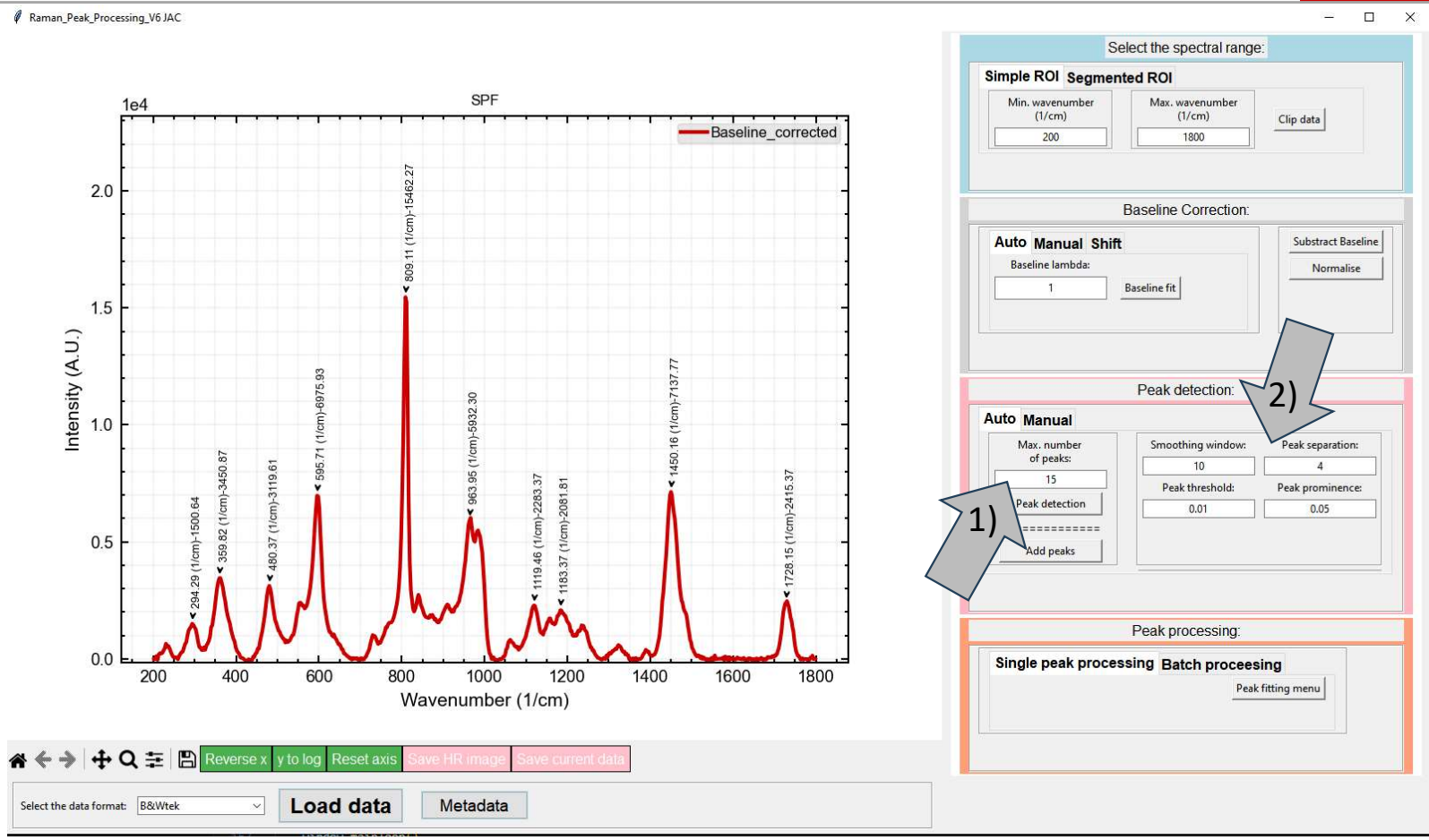
Step 6-c

- Remove baseline:
  - Shift:
    - A constant shift is subtracted from the range of interest.

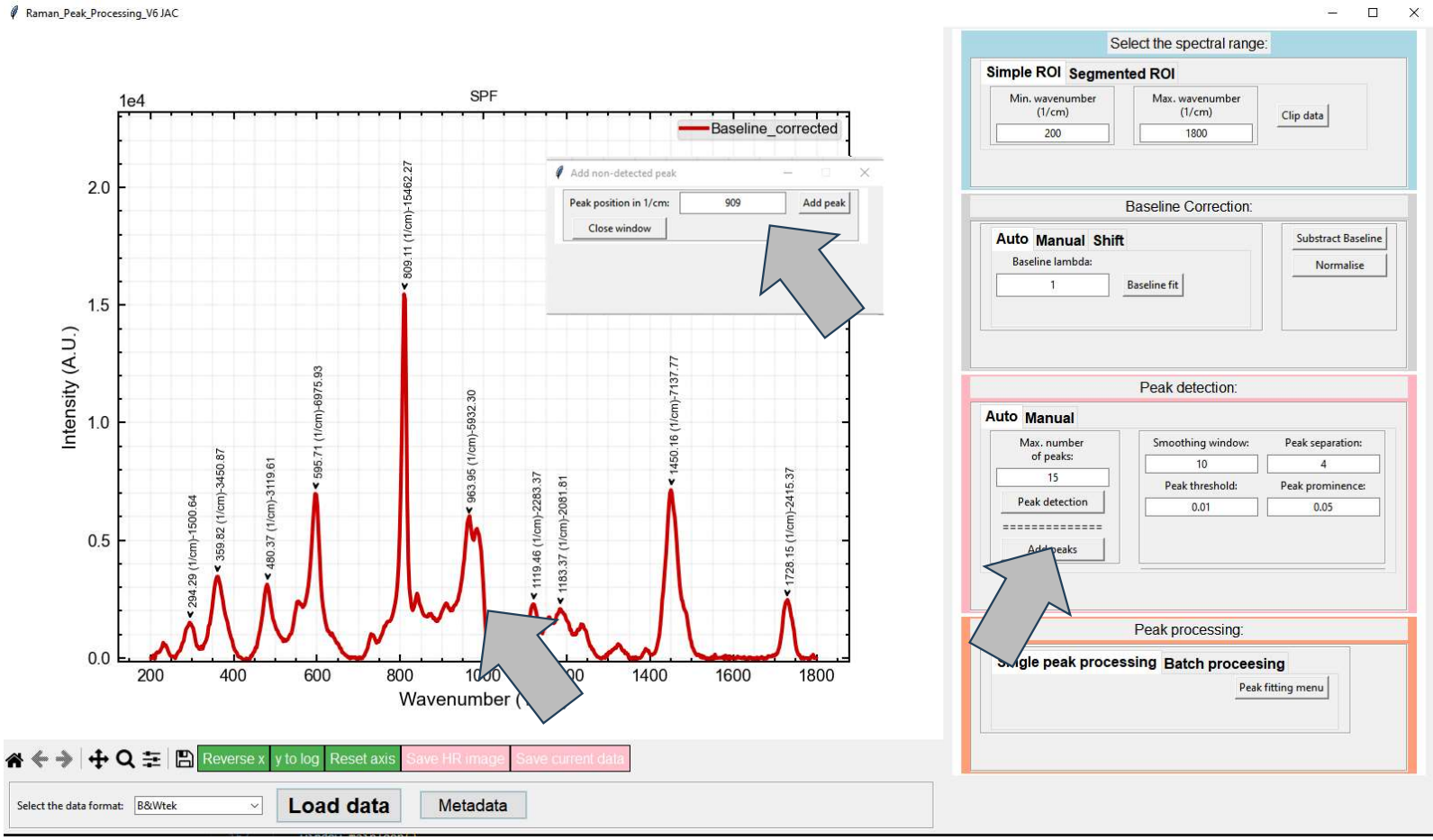


Step 7-a

- 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 3pixels to detect contiguous peaks.
      - Peak Threshold: Ratio from minimum peak heigh to max peak heigh to be detected.
      - Peak prominence: Parameter to be more or less sensitive to shoulders.

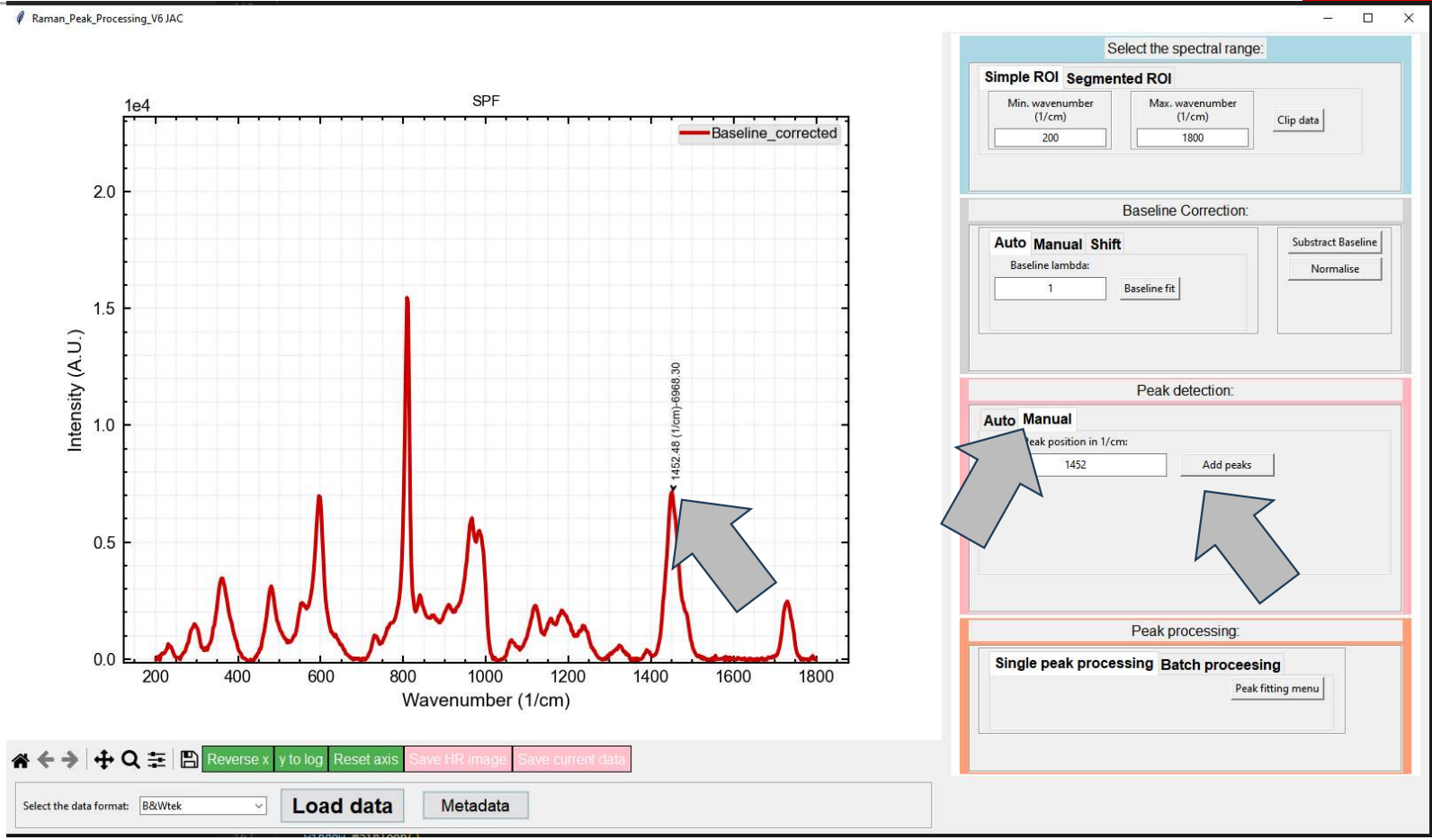


- Peak detection:
  - Auto:
    - Manual:
      - Automatic Peaks can be added if the automatic routine cannot find them by introducing their wavenumber.
      - This is a combination of the automatic routine (7-a) and only works for the single spectrum processing. The batch processing only works with automatic detection limits or the full manual routine.



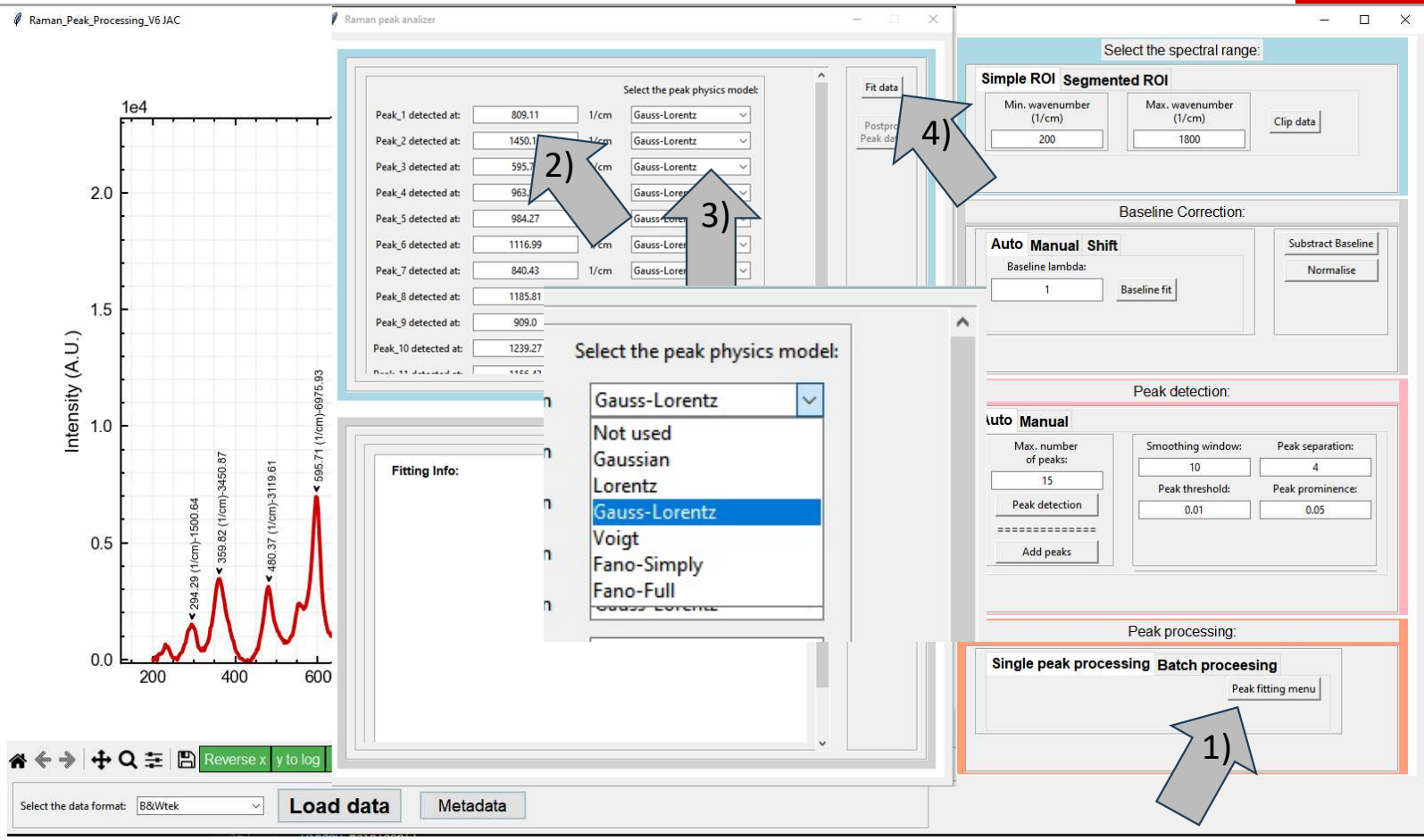
Step 7-c

- Peak detection:
  - Manual:
    - Peak positions can be specified manually.
    - This positions will also be remembered for the batch processing, but if new peaks appear the will be ignored or not detected.
    - Note that when swapping the tab from manual; to auto or auto to manual the previous peaks are erased.



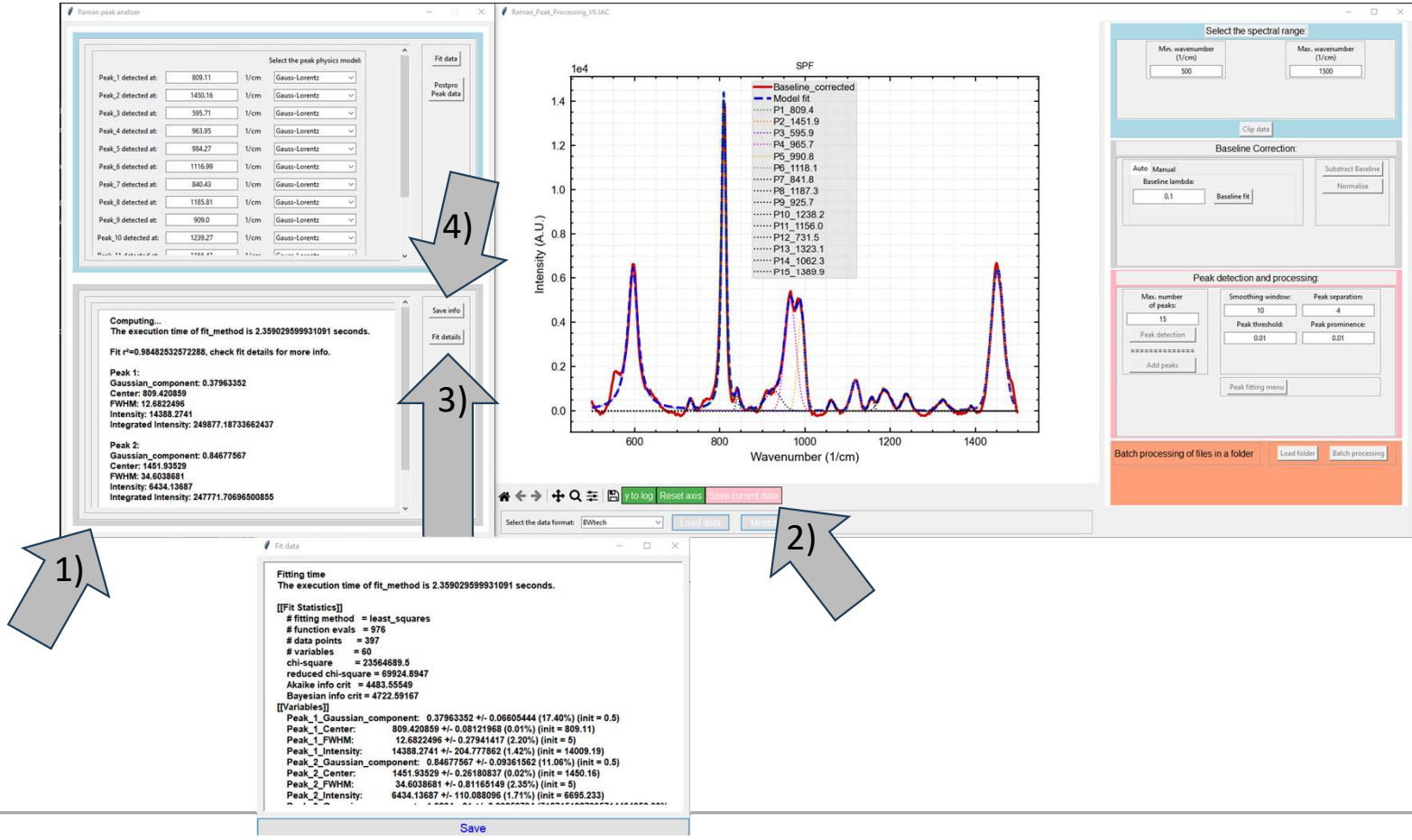
Step 8-a

- 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.

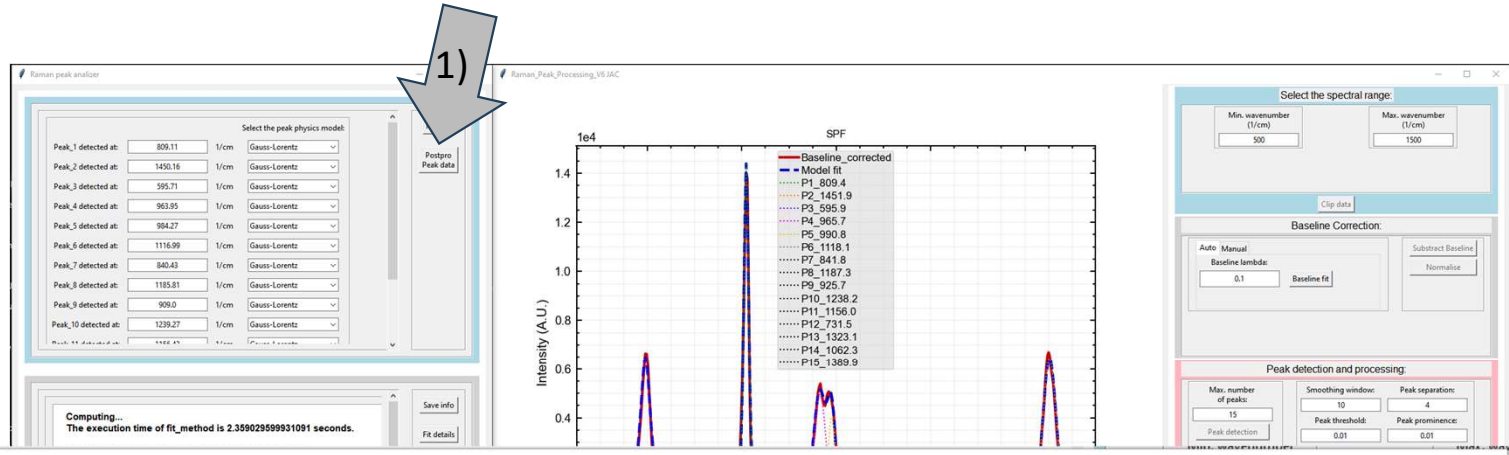


* John F. Kielkopf (1973), "New approximation to the Voigt function with applications to spectral-line profile analysis", *Journal of the Optical Society of America*, **63** (8): 987,

- 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)



Fit data

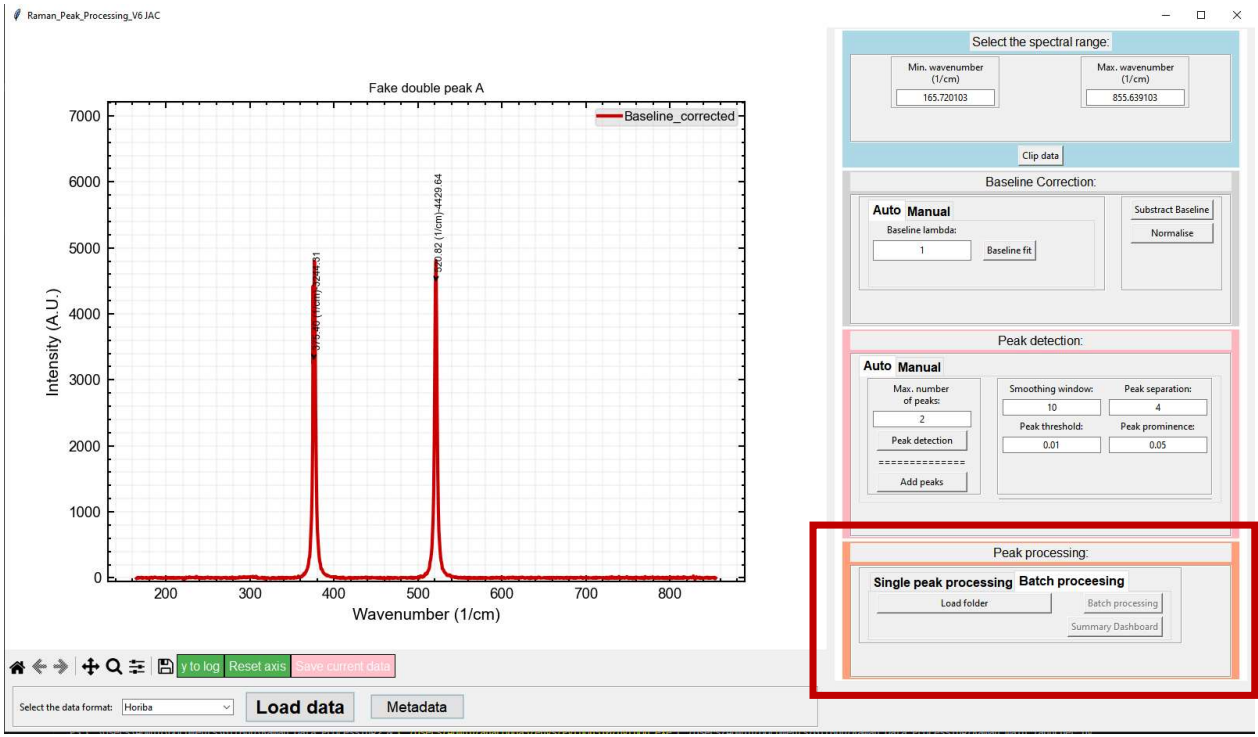
Gaussian_component | Center | FWHM | Intensity | Integrated Intensity

	P1	P2	P3	P4	P5	P6	P7	P8	P9	P10	P11	P12	P13	P14	P15
P1	1.000	2.236	2.225	2.892	3.553	10.405	21.153	15.226	15.490	19.048	25.969	32.462	31.251	29.021	91.230
P2	0.447	1.000	0.995	1.293	1.589	4.653	9.459	6.809	6.927	8.518	11.613	14.516	13.975	12.977	40.796
P3	0.449	1.005	1.000	1.300	1.596	4.676	9.506	6.842	6.961	8.560	11.670	14.588	14.044	13.041	40.997
P4	0.346	0.773	0.769	1.000	1.228	3.598	7.314	5.265	5.356	6.587	8.980	11.225	10.806	10.035	31.546
P5	0.281	0.629	0.626	0.814	1.000	2.929	5.954	4.286	4.360	5.362	7.310	9.138	8.797	8.169	25.680
P6	0.096	0.215	0.214	0.278	0.341	1.000	2.033	1.463	1.489	1.831	2.496	3.120	3.004	2.789	8.768
P7	0.047	0.106	0.105	0.137	0.168	0.492	1.000	0.720	0.732	0.901	1.228	1.535	1.477	1.372	4.313
P8	0.066	0.147	0.146	0.190	0.233	0.683	1.389	1.000	1.017	1.251	1.706	2.132	2.052	1.906	5.992
P9	0.065	0.144	0.144	0.187	0.229	0.672	1.366	0.983	1.000	1.230	1.676	2.096	2.017	1.873	5.889
P10	0.052	0.117	0.117	0.152	0.187	0.546	1.110	0.799	0.813	1.000	1.363	1.704	1.641	1.524	4.789
P11	0.039	0.086	0.086	0.111	0.137	0.401	0.815	0.586	0.596	0.733	1.000	1.250	1.203	1.117	3.513
P12	0.031	0.069	0.069	0.089	0.109	0.321	0.652	0.469	0.477	0.587	0.800	1.000	0.963	0.894	2.810
P13	0.032	0.072	0.071	0.093	0.114	0.333	0.677	0.487	0.496	0.610	0.831	1.039	1.000	0.929	2.919
P14	0.034	0.077	0.077	0.100	0.122	0.359	0.729	0.525	0.534	0.656	0.895	1.119	1.077	1.000	3.144
P15	0.011	0.025	0.024	0.032	0.039	0.114	0.232	0.167	0.170	0.209	0.285	0.356	0.343	0.318	1.000

Save

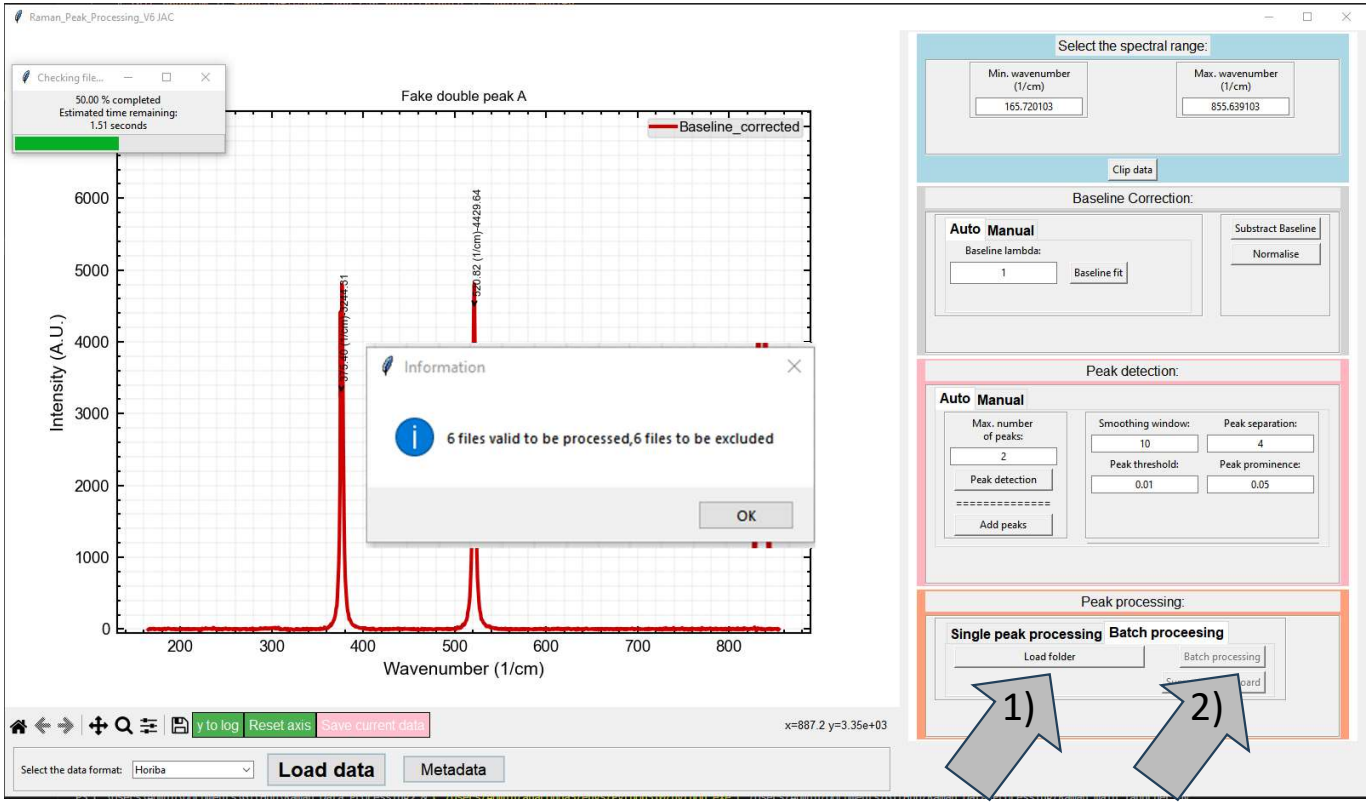
Batch processing

1. Save all the raw data files to be processed in . a common folder.
2. Open one data file and follow steps 3 to 7.
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.



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).



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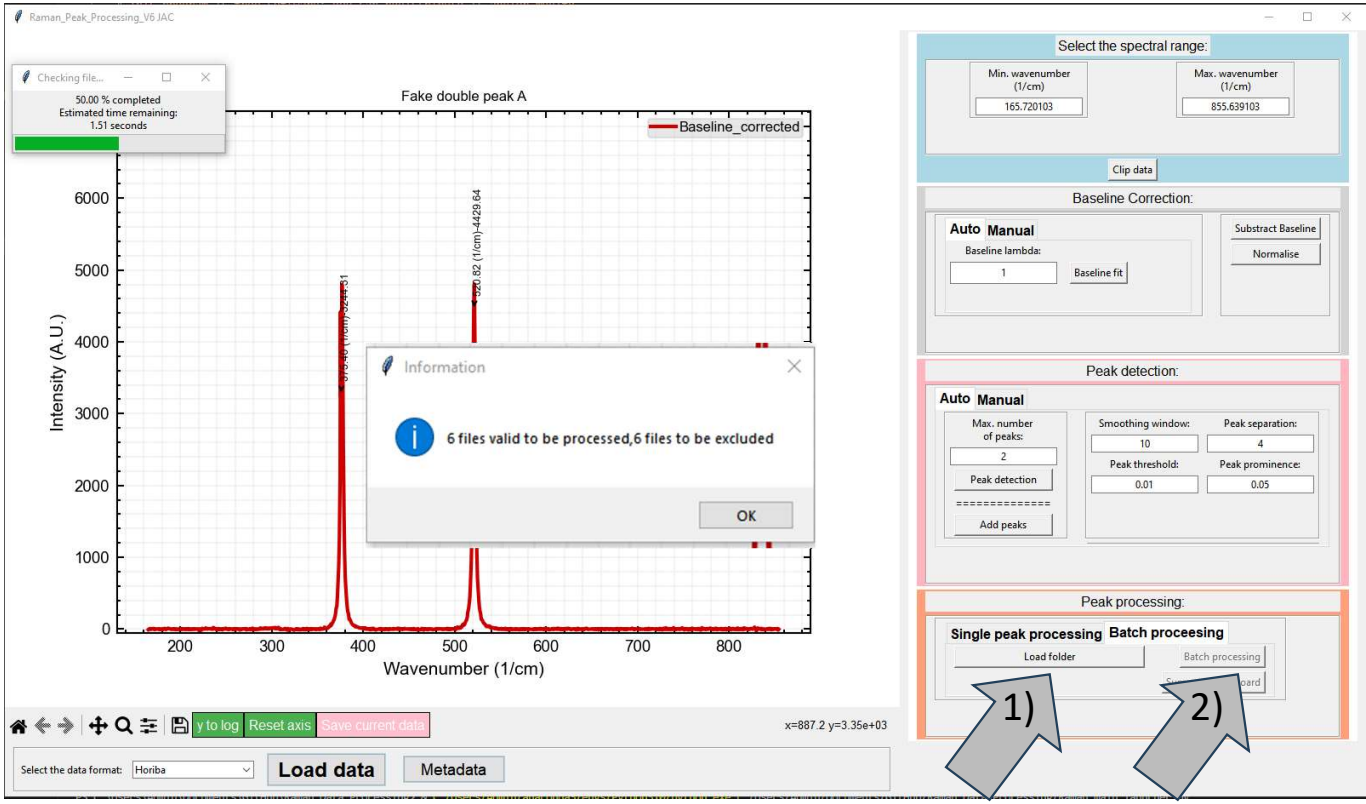
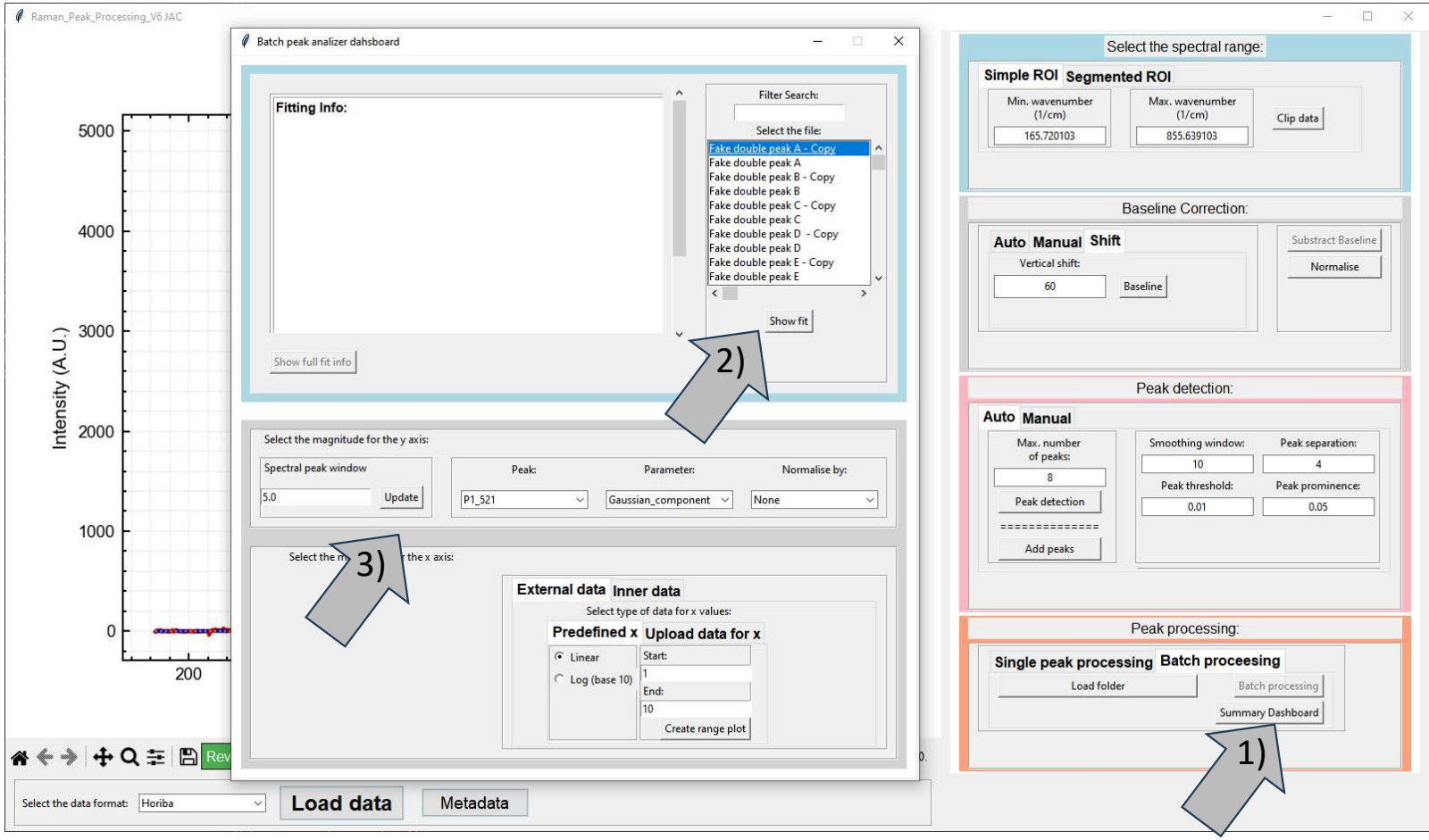


Batch processing

4. A dashboard panel will appear that allow to retrieve the fit for each file in the folder (2)
5. Data for each parameter in the folder can be also explored using the bottom dashboard (3).



Batch processing

4. Select the minimum separation between peaks (1)
5. Select the peak you want to analyse (2)
6. Select the parameter you want to extract for all files in the folder (3). You can normalise that value by the same value of a different peak if needed (4)
7. Select against what you want to plot the results. Can be a predefined equispaced sequence or a file containing the values for the X.