Reduction and Analysis graphic user interface (RAGui)

Shun Yu

Goal: development and simple graphic user interface, which can reduce the scattering data in hdf5 format, offer multiple plotting options and perform simple line profile analysis

Available Functions:
- Easy loading and viewing raw data in hdf5
- Data reduction with multiple function selection
- Saving reduction data in hdf5
- Fast 1D plot with multiple choice:
  - Single plot within one hdf5
  - Compare single line profile from different hdf5
  - Waterfall plot within one hdf5
- Fast 2D plot of the "cake" cut and profile change as a function of frame number

Under development:
- Multicomponent fitting
- Plotting as a function of meta data, e.g. motor position and time stamp

1. Define raw data path, saving path, and basic GUI operation

2. Tab menu to selection between Raw data viewing and 1D profile plotting
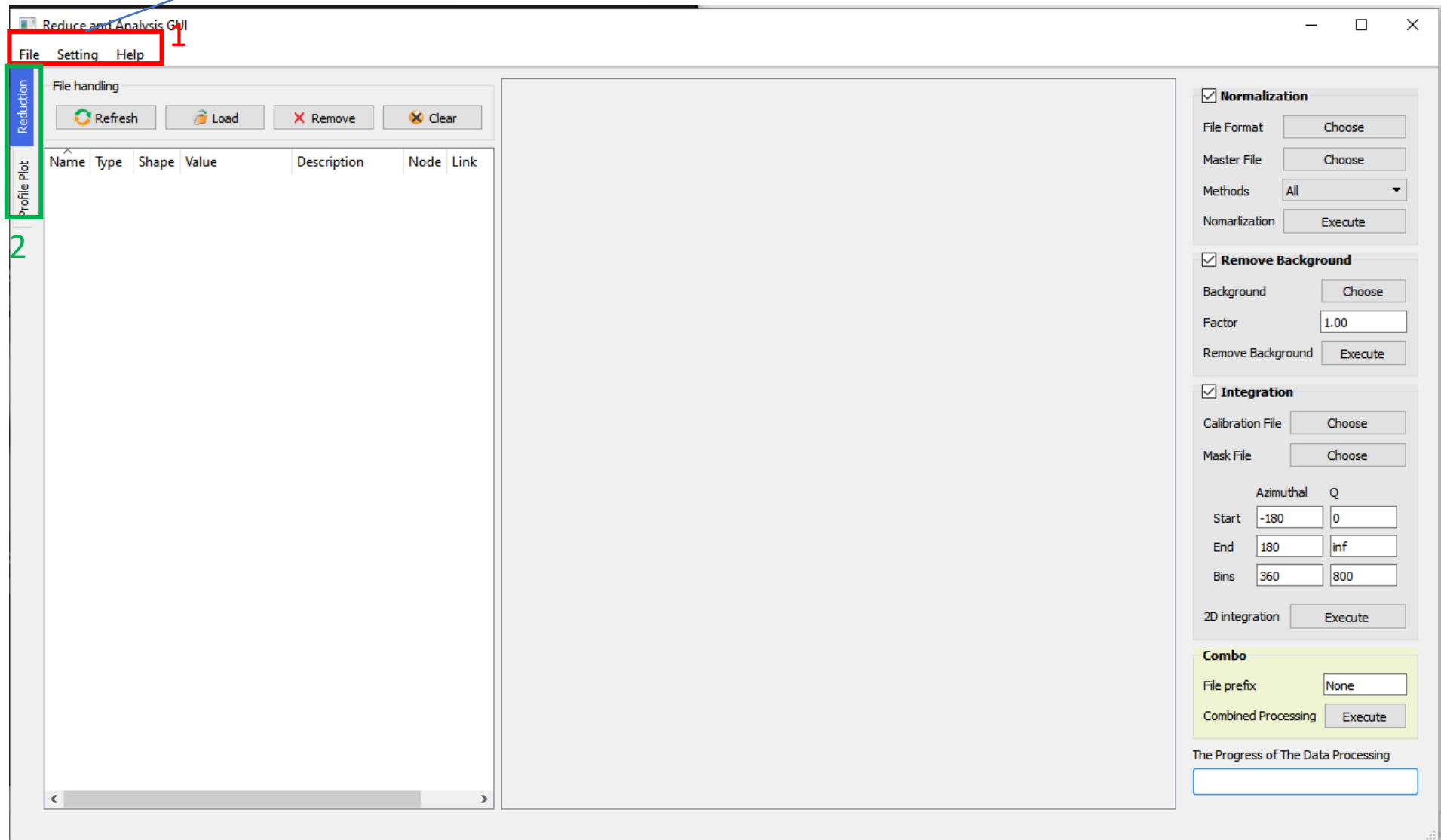
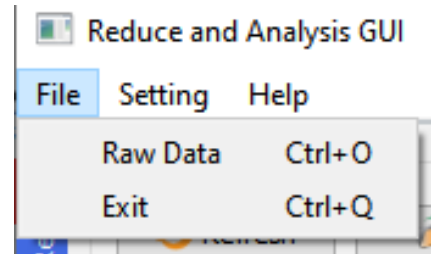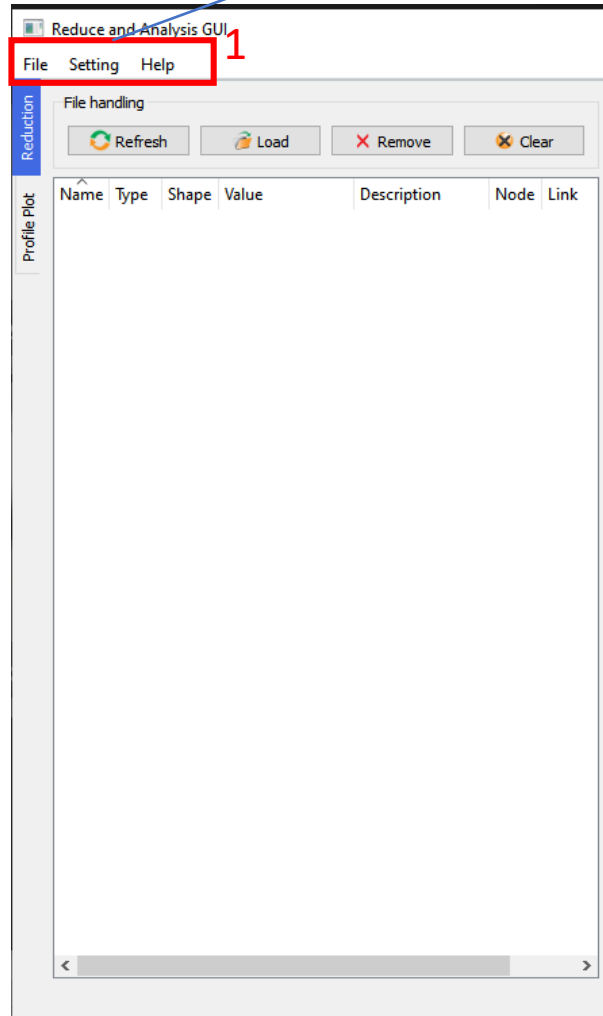# 1. Define raw data path, saving path, and basic GUI operation

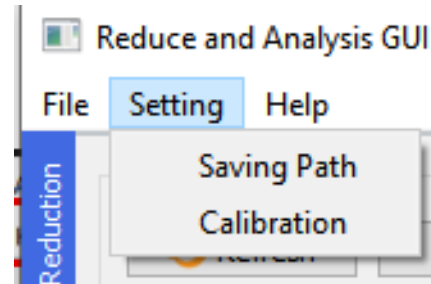- "Raw Data": Define the raw data path
- "Exit": quit GUI

- "Saving Path": Define the saving data
- "Calibration": call "pyFAI-calib2" Calibration GUI

- "Help wiki" :Open browser for User Manuel
- "About": introduction of the GUI

Default path:
Raw Data → "./test data"
Saving Data → "./processed data"
Feel free to change the path
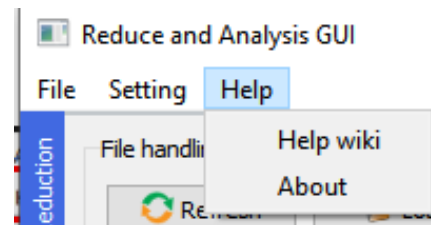
Mask and Poni file could be created from this GUI

Reduce and Analysis GUI

File   Setting   Help

1

File handling
- Refresh
- Load
- Remove
- Clear

Reduction

Profile Plot

Name Type Shape Value   Description   Node Link

2

3

4

☑ **Normalization**
File Format   Choose
Master File   Choose
Methods   All
Nomarlization   Execute

☑ **Remove Background**
Background   Choose
Factor   1.00
Remove Background   Execute

☑ **Integration**
Calibration File   Choose
Mask File   Choose

	Azimuthal	Q
Start	-180	0
End	180	inf
Bins	360	800

2D integration   Execute

Combo
File prefix   None
Combined Processing   Execute

5

The Progress of The Data Processing

6

1. Raw data File handling
   - Refresh: user defined quick reload from Raw data folder (define in GUI Menu "File") and show in file in Panel 2
   - Load: open pop up window to load any hdf5 from any accessible folder and show in file in Panel 2
   - Remove: user selected single file or multiple file in Panel 2 (occasionally Exception warning pop up, but does not influence the use once warning is acknowledged)
   - Clear: remove all listed file from Panel 2

2. hdf5 tree view:
Visualized all the structure inside readable hdf5

3. Data view window:
Default silx viewer's data viewing window with multiple choice of showing the data

4. Reduction Panel:
Three checkable Groupbox: *Process, Remove Background* and *Integration*
- *Process: Normalization function (Selection include: transmission (I_t), flux (I_0), exposure time(Δt) and all of them)*
- *Remove Background: select background in **hdf5 (cosaxs format)** and calculate the **average** over all the detector image as the background with user defined scaling factor of the background. Removing background is done by **Subtracting** background from selected single or multiple file in Panel 2*
- *selected single or multiple files Integration: azimuthal integration of all detector images in selected single or multiple from Panel 2.*
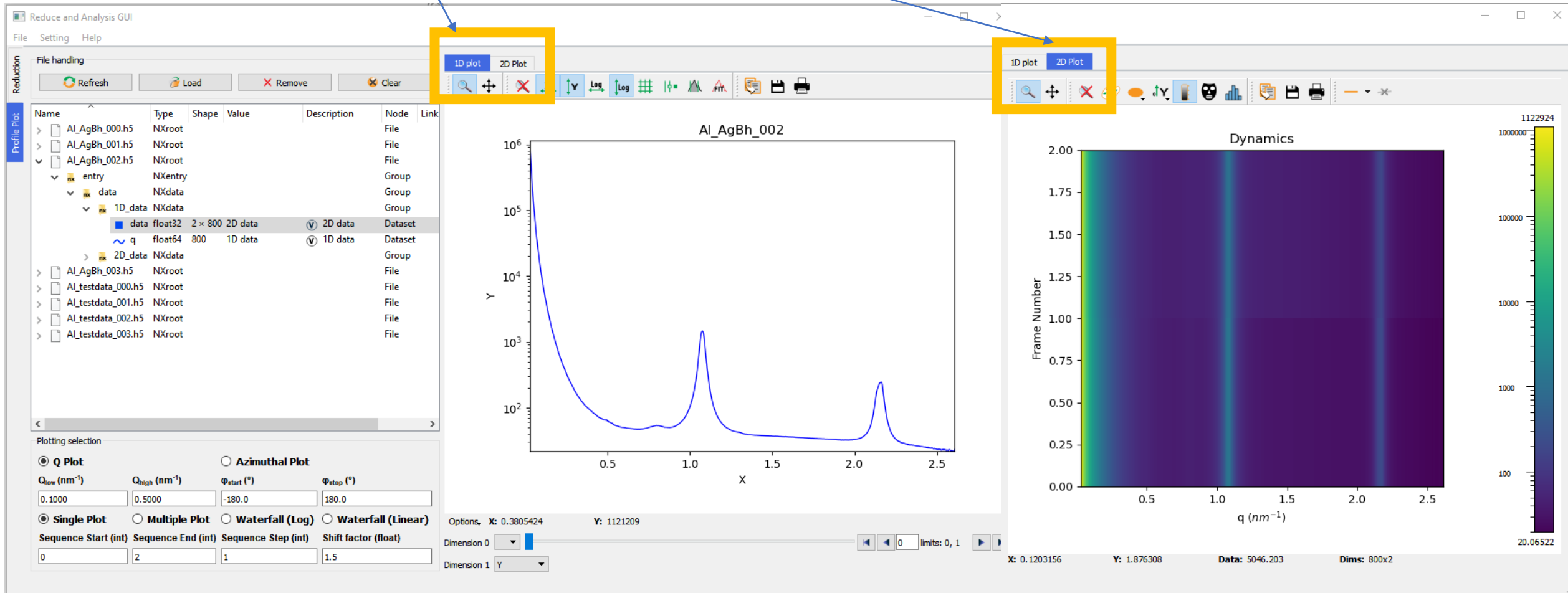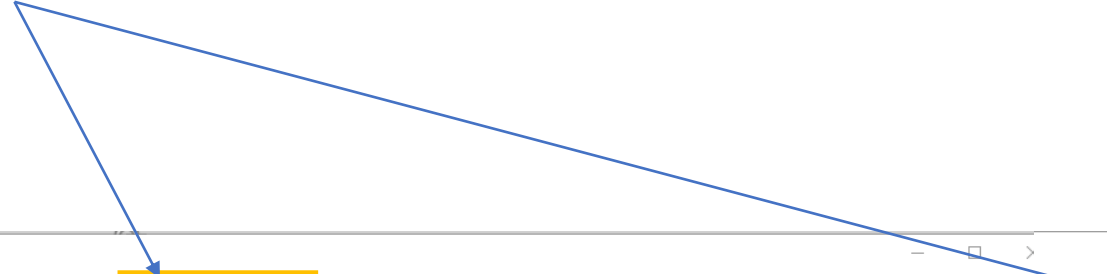
5. Combo processing
Combined Reduction to perform all Checked Groupbox functions **in Panel 4 in one click.**
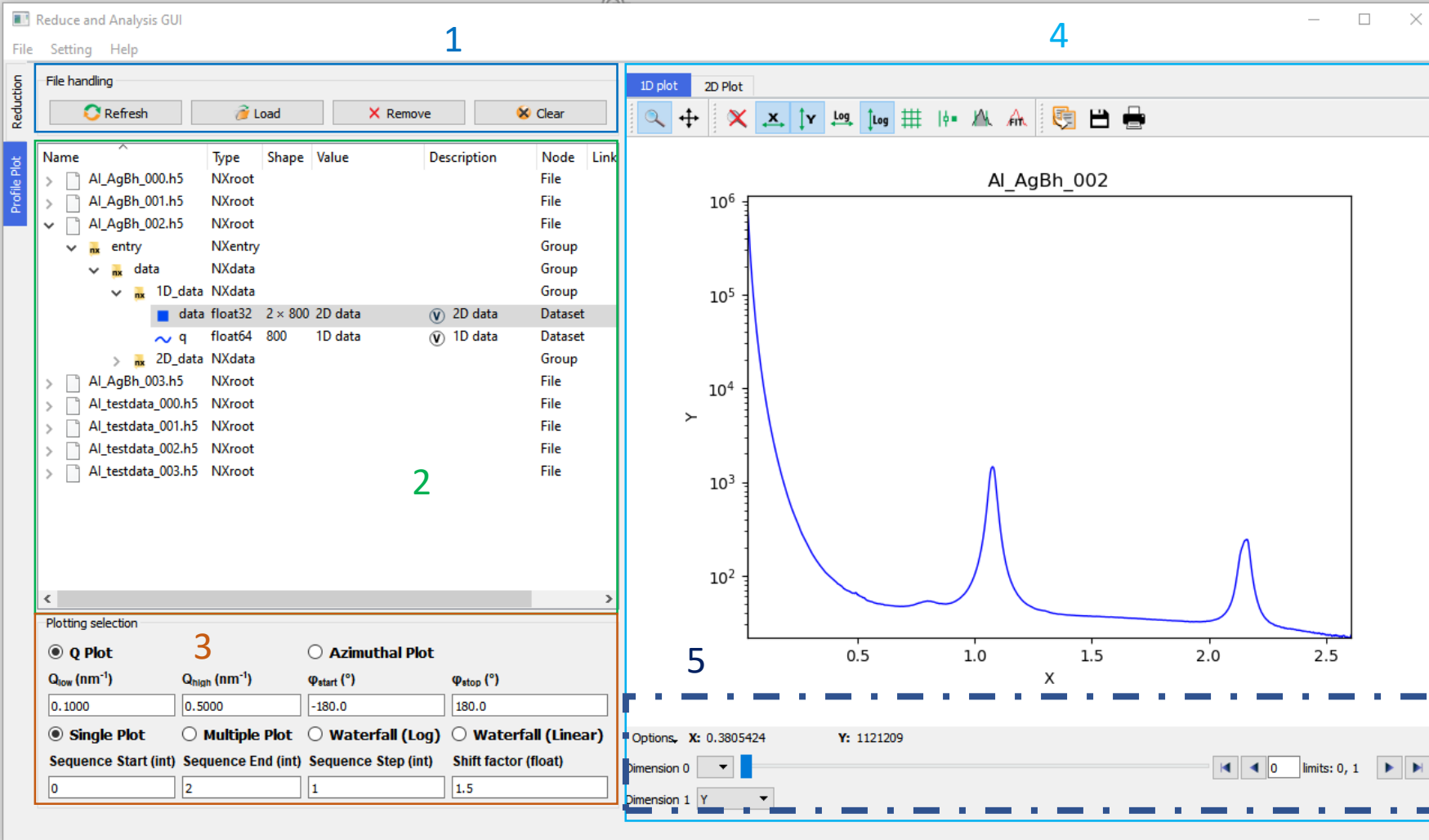(Working but not implemented at CoSAXS yet)

6. ProgressBar
It shows the progress of actions in *Panel 4* and **5** for each file (despite multiple files are selected)

Select between 1D and 2D plot

2. hdf5 tree view:
Visualized all the structure inside readable hdf5

3. 1D profile plotting selection
- Selected between *Q plot* and *Azimuthal plot*

Q_{low} and Q_{high} is for lower and upper limit of Q to do the intensity summation for Azimuthal plot

- Plot mode: *single, multiple and waterfall*

Single: 1D plot with slider menu in one hdf5

*Multiple: 1D plots **with limited slider menu (only latest opened file)** from multiple hdf5 file*

Waterfall: 1D plots in waterfall format within one hdf5 with user defined start, stop, sequence step and plotting gap.
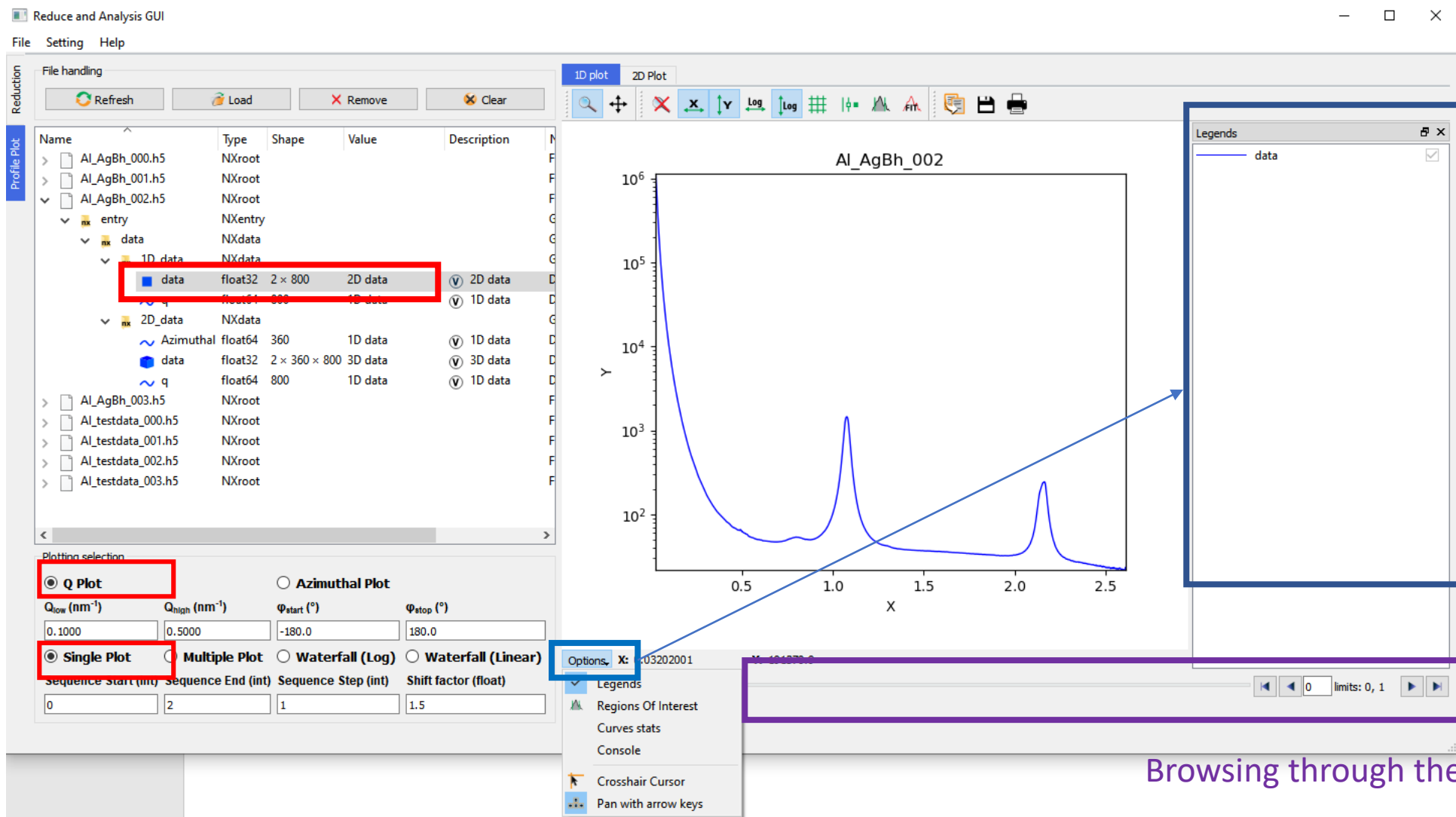
4. Data view window:
Default 1D profile window with multiple choice defined in Panel 3
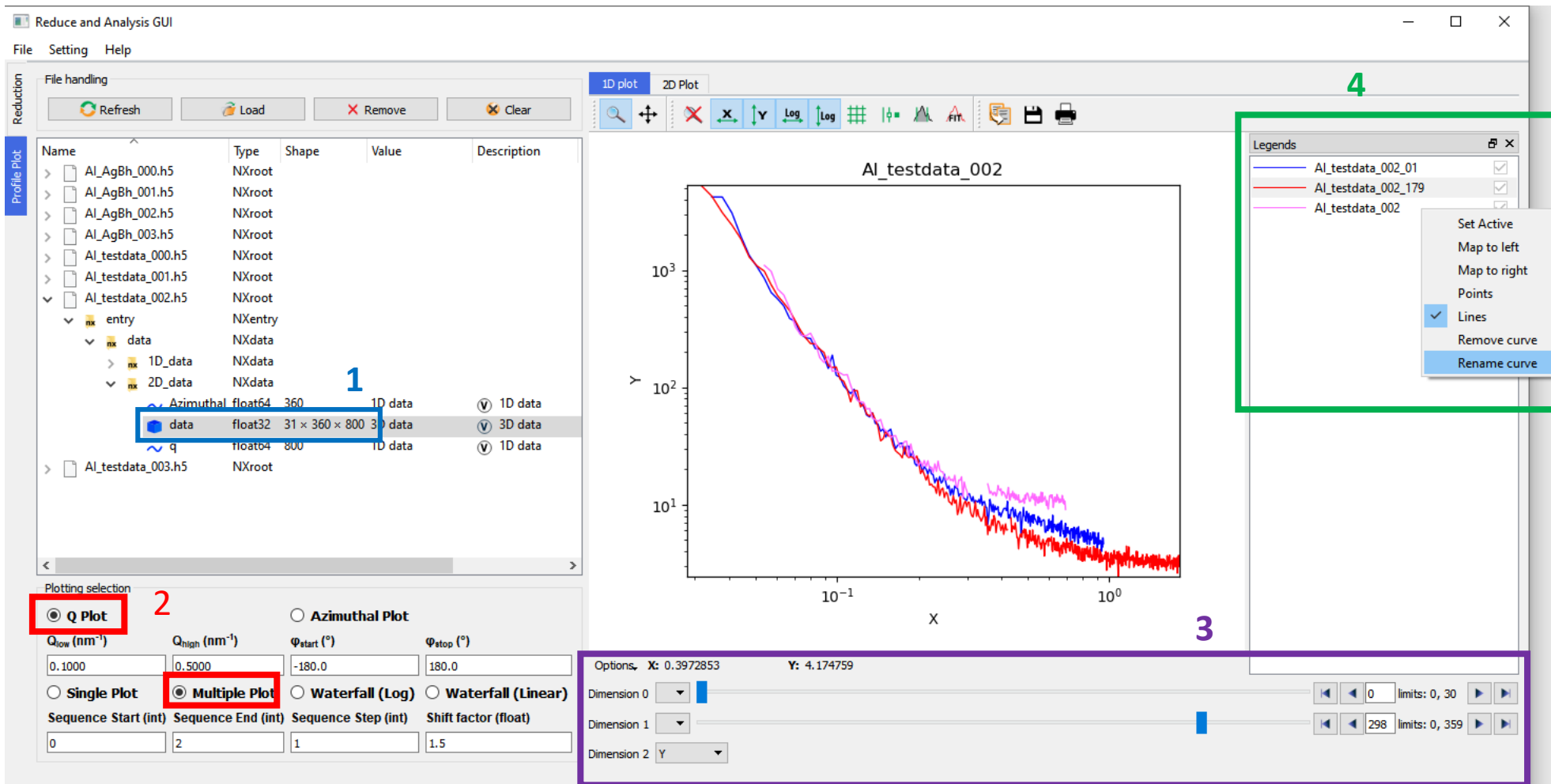
5. Slider menu
Use to cut through the 3D data file in **single plot mode** and through **the latest opened file in multiple file.**

1. **Reduced File handling**
   - Refresh: user defined quick reload from Raw data folder (define in GUI Menu "File") and show in file in Panel 2
   - Load: open pop up window to load any hdf5 from any accessible folder and show in file in Panel 2
   - Remove: user selected single file or multiple file in Panel 2 (occasionally Exception warning pop up, but does not influence the use once warning is acknowledged)
   - Clear: remove all listed file from Panel 2

Q-I 1D plot

Browsing through the frames of 1D

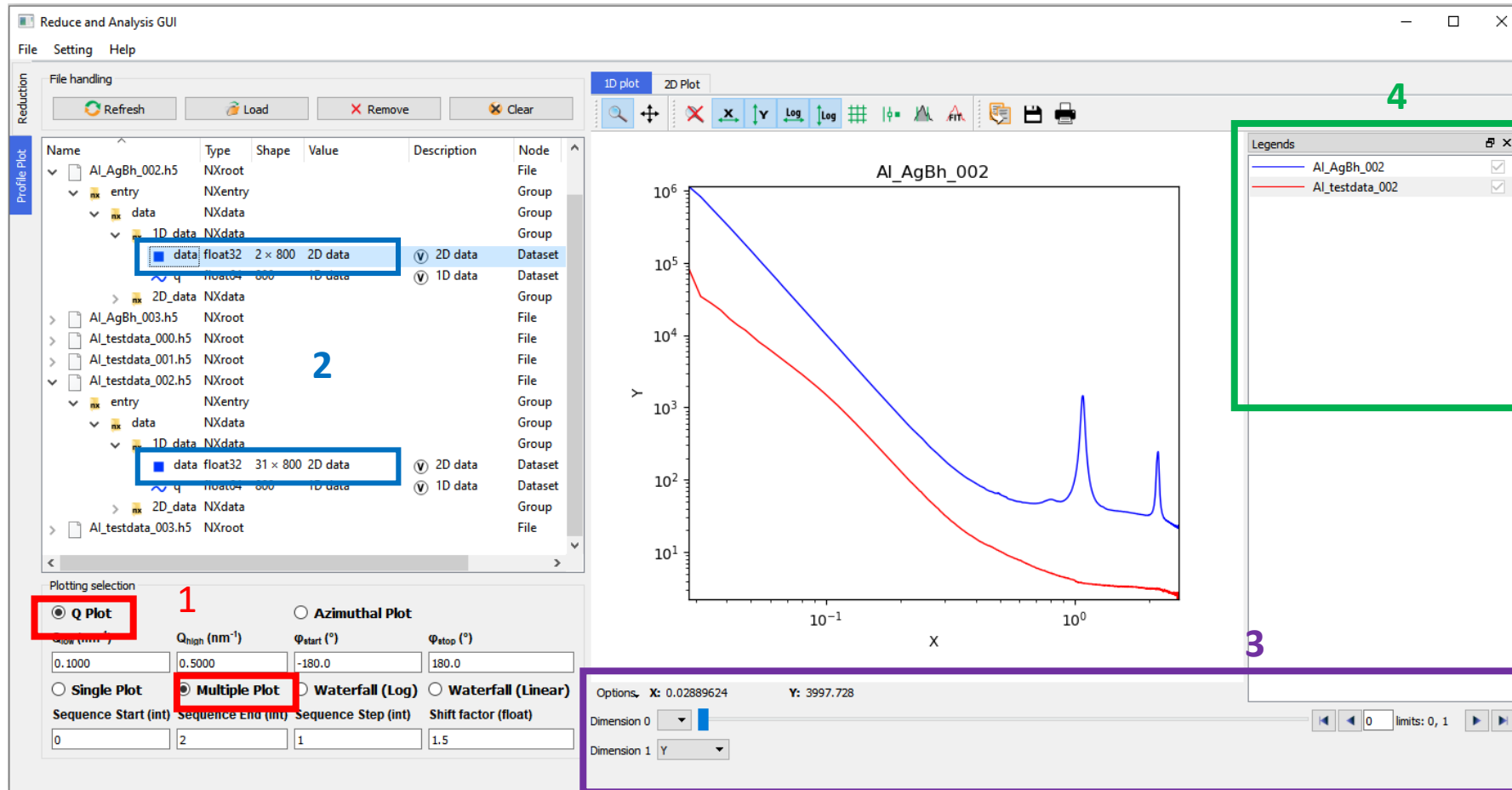# Q-I multiple Plots in a single file

Step:
1. Select the a single hdf5 file
2. Select the plotting mode
3. Scroll to the number to be plotted
4. Change legend *by **right clicking the mouse** and choosing* **"Rename curve"** *before scrolling to the next curve in panel 3*
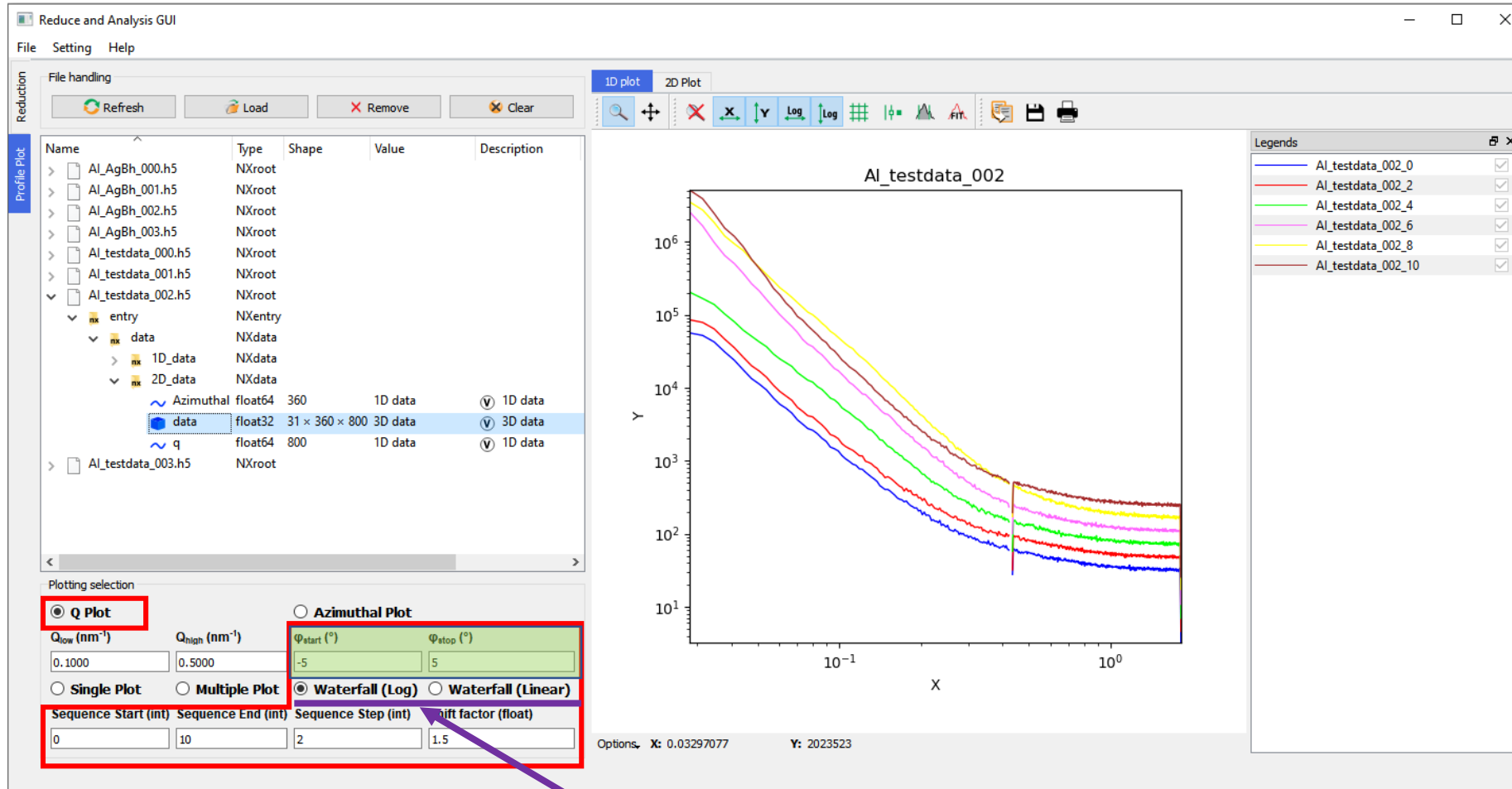
Q-I multiple Plots from multiple files

Step:

1. Select the plotting mode

2. Select the multiple hdf5 files one by one

3. For each file, scroll to the curve number to be plotted

4. If **multiple curves** from **one hdf5** will be plotted, then legends need to be modified for those curves. Otherwise, no need to change legend between hdf5.
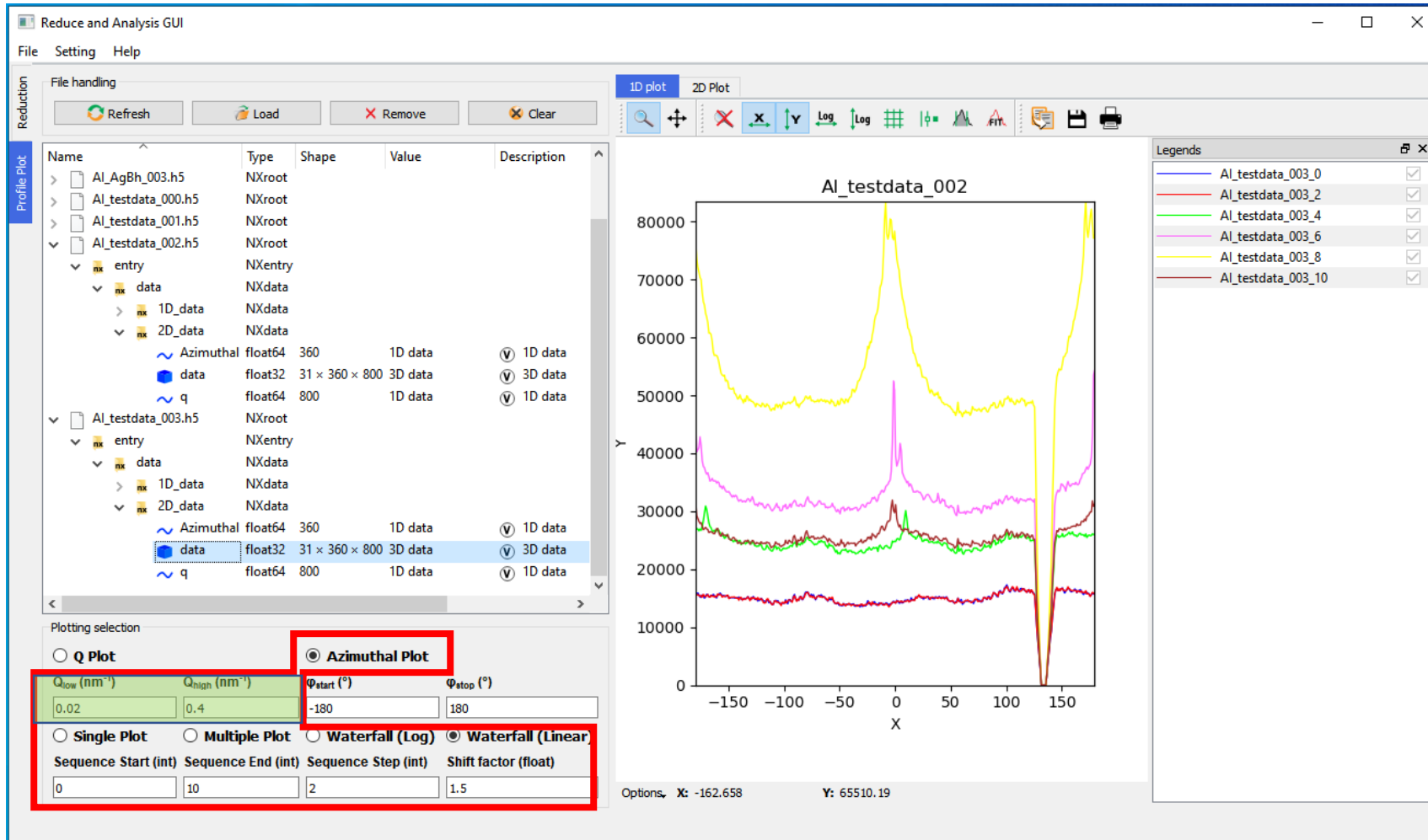
Q-I Waterfall plot from a single file

For 2D "cake" input:
Green shadowed area is used to define the integrated azimuthal angle region

For 1D input:
Green shadowed area is **NOT** effective

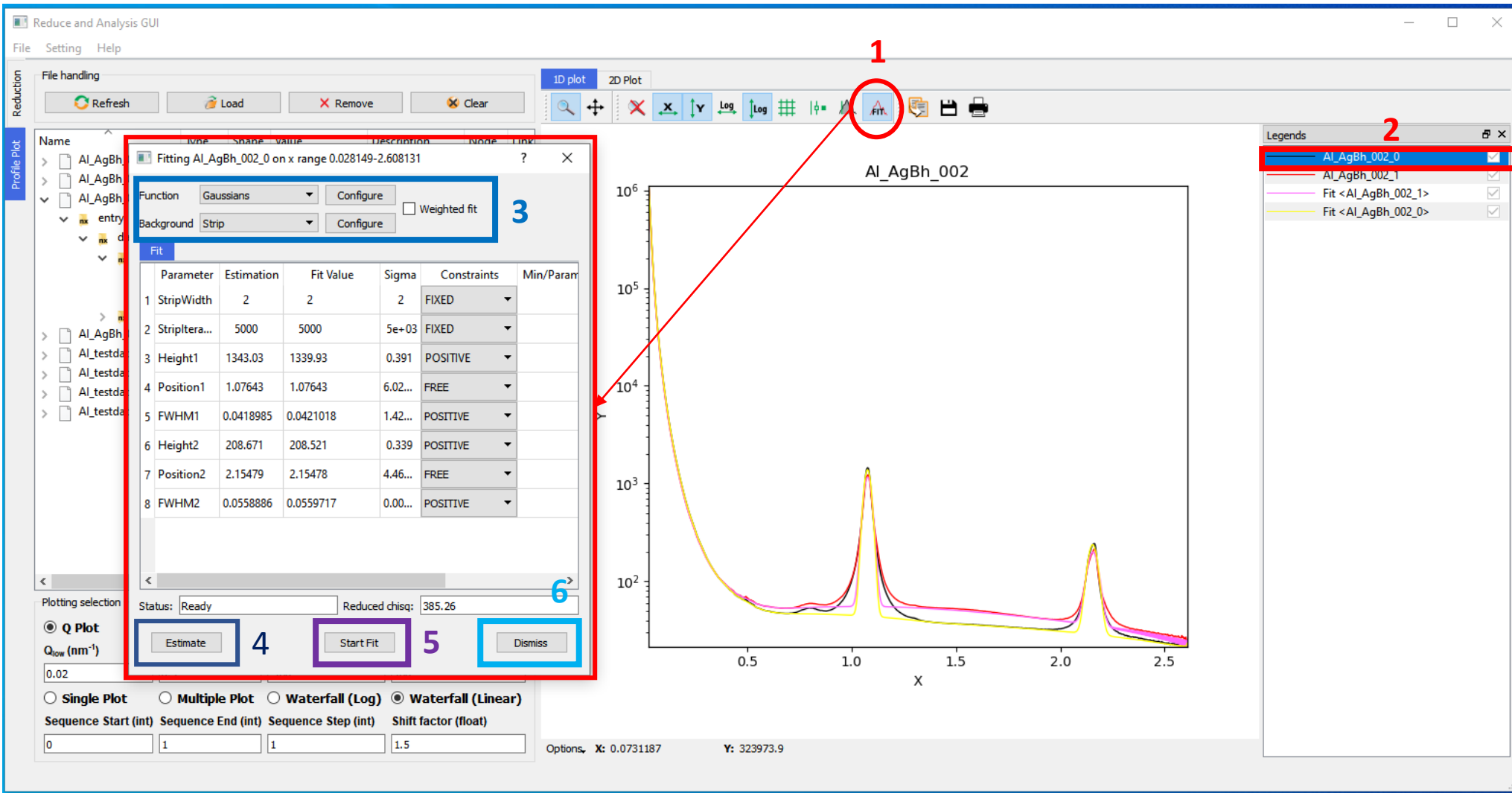Two modes are available in **log** scale and **linear** scale stacking

Azimuthal plot (only valid for 2D "cake" cut)

Shadowed area is used to define q range to be integrated for Azimuthal Intensity
The plotting modes (single, multiple, waterfall (log) and (linear)) are the same to Q-I plot

Simple fitting

1. Click on fit icon to activate the fitting panel.
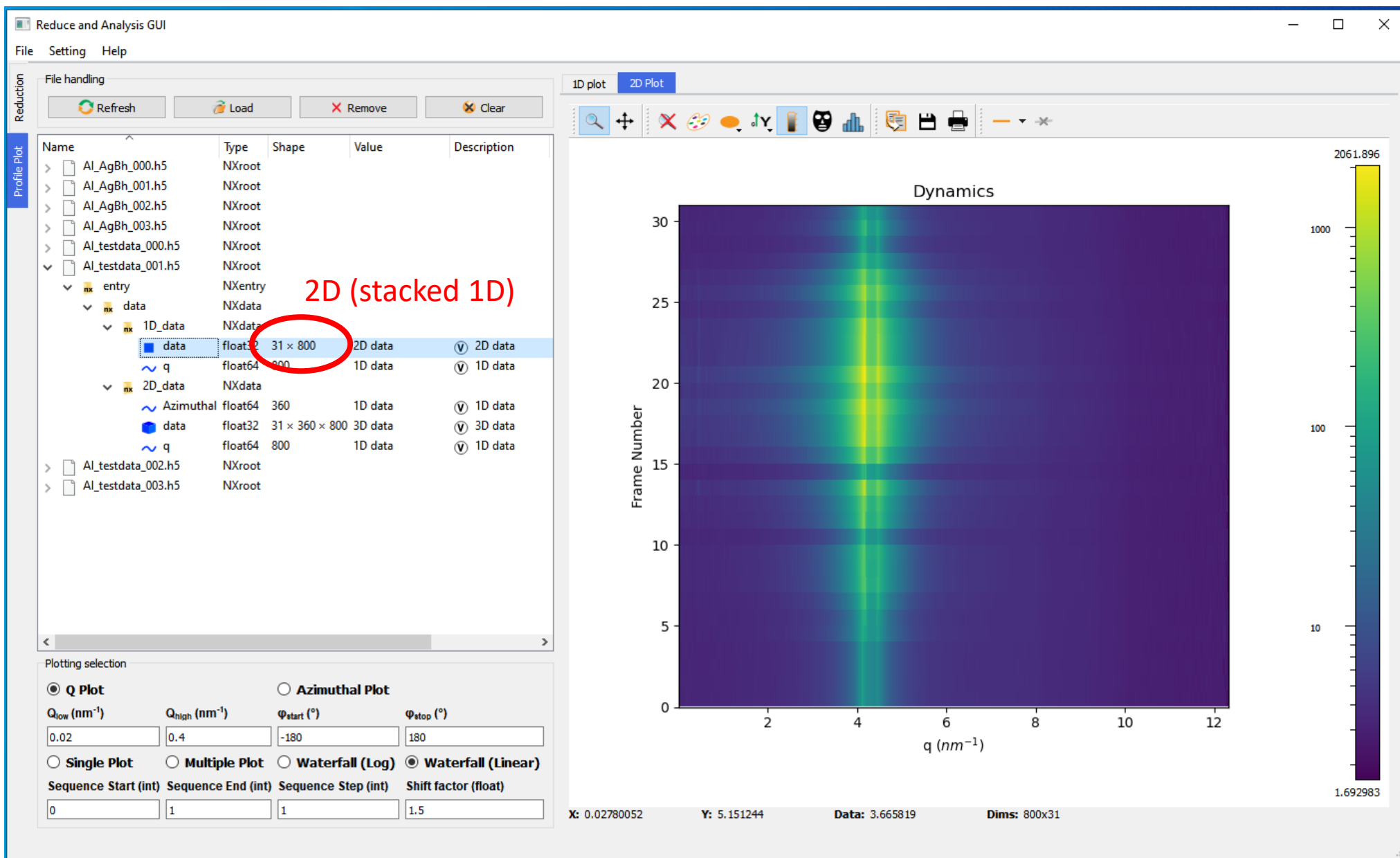2. Left click to activate the curve to be fitted
3. Select fitting function
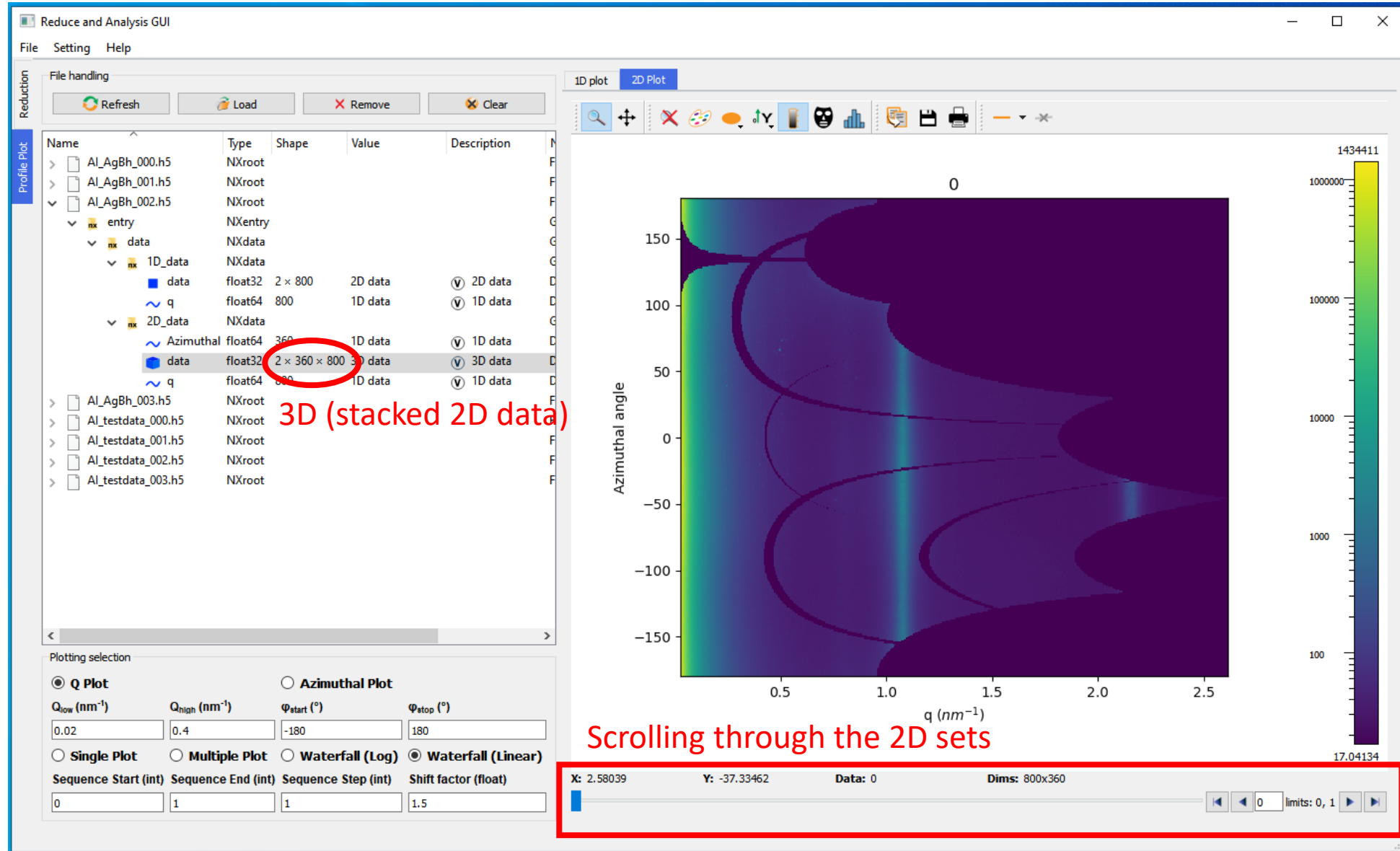4. Estimate (multiple peaks may be generated automatically)
5. Start fit. The fitting results will be automatically updated
6. Finishing fitting by click dismiss

Plot stacked 1D data into 2D image

Plot 3D data as stacked 2D ("cake" cut) image

Line cut in 2D plot

Choose the line profile style

Integration region (in pixels)

Define an horizontal line profile
Define a vertical line profile
Define a line profile
Define a directed line profile
Define a cross profile

Basic functions are the same as in 1D plot window, e.g. legend, fitting, saving data, etc.

Mouse dragging