
DAWN: RIXS Image Processing Software at I21

User Manual and Tutorial

I21 RIXS Beamline | [Diamond Light Source](#)

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START-UP

What is DAWN?



DAWN is an open-source software ([licence](#)) for the visualization and processing of scientific data. Although specifically developed for data from synchrotron-based techniques, many of the features of DAWN are useful in other fields. DAWN loads data from many common formats (text files, tiffs, hdf5...), as well as those specific to x-ray techniques (NeXus, EDF, MAR...).

Accessing DAWN from your own machine:

Visit the website <https://dawnsci.org/>, download and install the software matching your operating system. Installation instructions are provided on the website.

Accessing DAWN from a linux machine at Diamond:

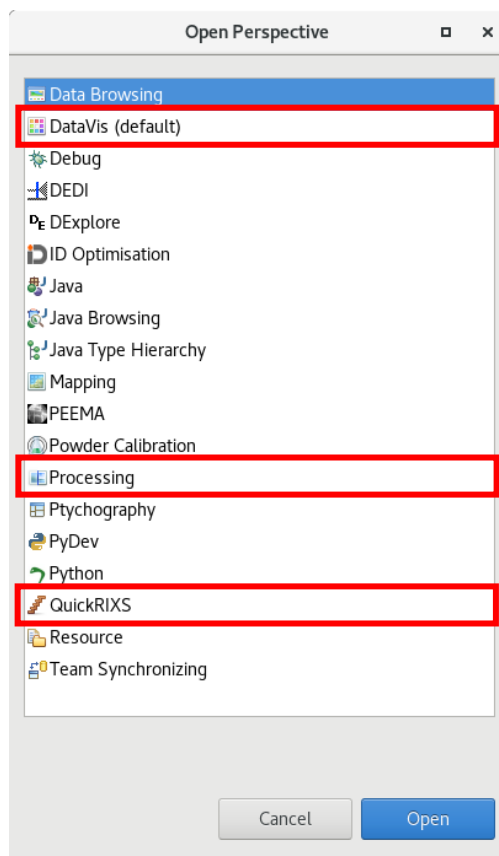
Open a terminal >> Type `'module load dawn/rixs'` ↵ >> `'dawn'` ↵

START-UP

DAWN Perspectives

DAWN perspectives: DAWN is designed for different applications and has different perspectives for different purposes.

A perspective can be opened by clicking on the *Open Perspective* button in the box.



For RIXS data analysis, we need to open following three perspectives:

1. DataVis: for visualizing the processed data and exporting them into data files

2. Processing: for post-processing raw RIXS data obtained from the experiment

3. QuickRIXS: to quickly plot the carbon tape images and check the resolution (Mostly, users do not need to use this perspective, once the beamline resolution is optimized for certain resonance edge by beamline staffs)

START-UP

DAWN Perspectives

Processing: This is where you will choose the kind of operations you want to do on the files in the *Data Slice View* panel.

Model: This is where you will put the parameters related to the operations you chose in the *Processing* panel

File Viewer or Project Explorer:
Navigating the scan files

Data Slice View: This is where you will drag the files you want to process from the *Data Slice View* or *Project Explorer*.

Output: When you click on a process in the *Processing* panel, you will see here the results of the processing done on the files selected in *Data Slice View* Panel

Input: When you click on a file in the panel above, you will see here the image it contains

The screenshot shows the DAWN software interface with the following panels and components:

- Project Explorer:** Displays a tree view of scan files under the path `/dls/i21/data/2023/mm33194-1`. A file filter and wildcard dropdown are present.
- Data Slice View:** A large empty panel for displaying data slices.
- Processing:** A list of processing operations including "Image background subtraction - Fitted to a PDF", "RIXS image reduction", and "RIXS elastic line reduction".
- Model:** A table for defining parameters for the selected process. The table has columns for "Name" and "Value".
- Input:** A panel showing a grid for visualizing the input image of a selected file.
- Output:** A large grid area for displaying the results of the processing.

Red arrows from the text boxes point to the following locations:

- From the "Processing" text box to the Processing panel.
- From the "Model" text box to the Model panel.
- From the "File Viewer or Project Explorer" text box to the Project Explorer panel.
- From the "Data Slice View" text box to the Data Slice View panel.
- From the "Output" text box to the Output grid.
- From the "Input" text box to the Input panel.

START-UP

Before Start: Required Information

Prerequisites:

Ask your local contact to provide:

1. **Energy dispersion value (eV/pixel):** For converting the CCD pixels to energy units in eV.
2. **Slope correction value:** For correcting the tilt of the image on the CCD detector.
3. **Dark image file number:** For subtracting the background signal that appears on the detector. The dark image file **must** have the same acquisition time as the RIXS image file.
4. **RIXS image file number** and an elastic spectrum collected immediately after it.

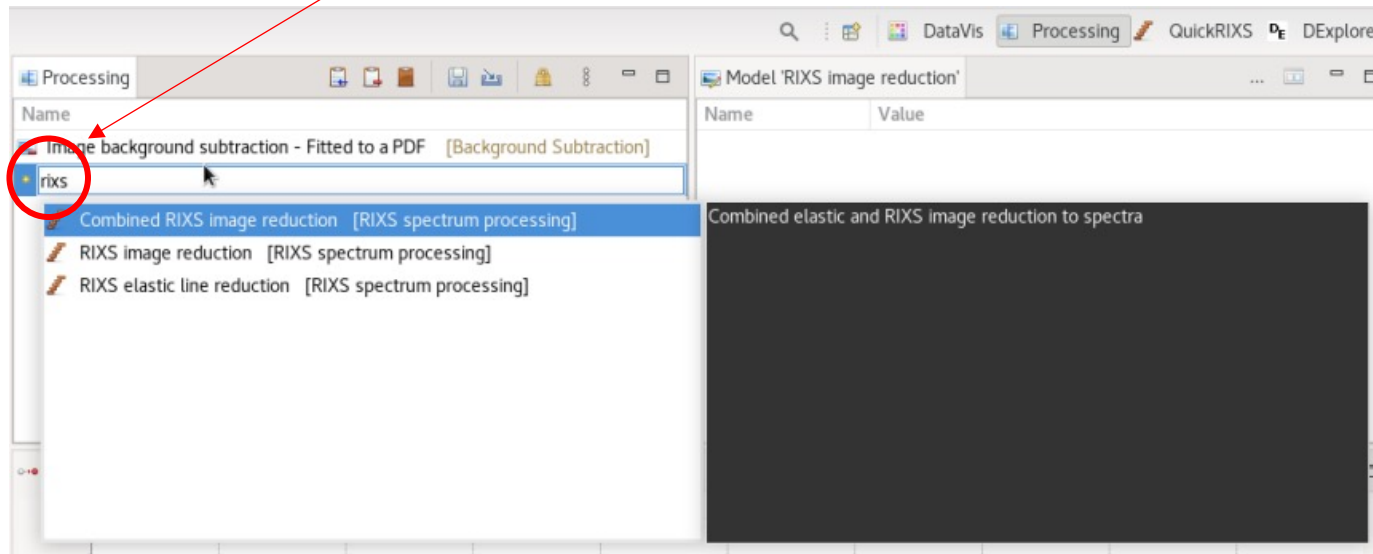
START-UP

Before Start: List of Operation Required for RIXS Image Processing

Operations:

In *Processing* panel, we call Operations to process the raw data loaded in the *Data Slice View* panel step-by-step. The list of operations required for RIXS image processing is summarized on the right side. Please note that the processing takes place from top to bottom operations. Thus, it is important to load the operation following the right sequence.

How to load Operations: (1) Click the empty line. (2) Drop-down list appears. (3) Choose the Operation you want to load (or type the keyword)



List of operations for RIXS:

1. Image background subtraction

This operation is to subtract dark background image from the raw RIXS detector image.

2-1. RIXS image reduction

When you want to process the data without measuring the carbon tape image, we can load this operation.

2-2. Combined RIXS image reduction

When you want to process the data with carbon tape image (for adjusting the zero energy loss position to the elastic line), we can load this operation instead of 2-1.

+ RIXS elastic line reduction

(This operation is mostly used by beamline staff to measure the dispersion and slope)

START-UP

Before Start: List of Operation Required for RIXS Image Processing

Combined RIXS Image Reduction Operation is generally employed to process the raw RIXS images obtained by the detector. In this operation, we need to provide a file number of carbon-tape RIXS image to find the exact position of elastic peak and to align the RIXS spectra from sample. To this end, we can either collect a carbon tape image for each RIXS scan (“NEXT_SCAN” or “PREVIOUS_SCAN” mode) or share the same carbon tape image for all RIXS scan datasets (“SAME_SCAN” mode)

TIPS:

- (1) If the elastic peak of your RIXS data from sample is too weak so not easily located, it is recommended to measure the carbon tape to precisely determine the position of the elastic peak -> Use **Combined RIXS Image Reduction**
- (2) If you take a dataset in which the position of elastic peak slightly varies data by data (e. g. energy-dependent map), it is recommended to take a carbon tape image for every RIXS data -> Use **Combined RIXS Image Reduction**

RIXS Image Reduction Operation is employed when the users want to skip the measurement of carbon tape RIXS image (partly to save measurement time).

TIPS:

If the elastic peak of your RIXS data from the sample is easily identifiable, you do not have to measure the carbon tape for every single RIXS scan. This will significantly save your measurement time -> Use **RIXS Image Reduction**

This manual demonstrates how to process your RIXS data by using **RIXS Image Reduction** (page 9-23). The procedure for Combined RIXS Image Reduction is also very similar, so please read this manual carefully in any cases. A short guide on **Combined RIXS Image Reduction** will be also provided on page 24.

DATA LOADING

Loading Your Data Files: File Viewer

1. Choose the beamtime folder
(Folder name: beamtime session number)

2. Select the files to analyze
You can select multiple files with "Shift" and "Ctrl" button

The screenshot displays the DAWN software interface. The File Explorer on the left shows a folder structure with 'NdNiO2' selected. The File Viewer shows a list of files with 11 files selected. The Processing window shows a table with one entry: 'Image background subtraction - Fitted to a PDF [Background Subtraction]'. The Images Monitor plot shows a grid with X and Y axes ranging from 0 to 100.

Name	Value
Image background subtraction - Fitted to a PDF [Background Subtraction]	

Name	Size	Type
i21-291505.nxs	182.9 KiB	No
i21-291504.nxs	182.9 KiB	No
i21-291503.nxs	182.9 KiB	No
i21-291502.nxs	182.9 KiB	No
i21-291501.nxs	182.9 KiB	No
i21-291500.nxs	182.9 KiB	No
i21-291499.nxs	182.9 KiB	No
i21-291498.nxs	182.9 KiB	No
i21-291497.nxs	182.9 KiB	No
i21-291496.nxs	182.9 KiB	No
i21-291495.nxs	182.9 KiB	No
i21-291494.nxs	182.9 KiB	No
i21-291493.nxs	182.9 KiB	No
i21-291492.nxs	182.9 KiB	No
i21-291491.nxs	182.9 KiB	No
i21-291490.nxs	182.9 KiB	No

DATA LOADING

Loading Your Data Files: Move Data Files to Data Slice View

The screenshot shows the DAWN software interface with the following components:

- Project Explorer:** Shows the file structure under `/dls/i21/data/2023/cm3391`. The folder `cm33913-3` is expanded, showing subfolders like `NdNiO2`, `RbFeS2`, `processing`, `spool`, `tmp`, and `xml`.
- File Viewer:** Shows the contents of the selected folder `/dls/i21/data/2023/cm33913-2/NdNiO2`. A list of files is displayed, including `i21-291505.nxs` through `i21-291491.nxs`. The file `i21-291501.nxs` is selected.
- Data Slice View:** A central area where data files are loaded. A red box with the text **3. Drag and drop the files on Data Slice View** and an arrow points to this area.
- Processing:** Shows a list of processing tasks, including `Image background subtraction - Fitted to a PDF [Background Subtraction]`.
- Images Monitor:** A panel at the bottom right showing a grid of image slices. The current slice of data is indicated as `[- - - -]`. The X-Axis is labeled from 0 to 100.

DATA LOADING

Loading Your Data Files: Data Slice View

DAWN_snapshot - /home/lok75131/DAWN_snapshot - DAWN Science

File Tools Window Help

Project Explorer File Viewer x

/dls/i21/data/2023/cm33913

All Folders

- workspace
- BFO
- LSMO_Taiwan
- NdNiO2
- RbFeS2
- processing
- spool
- tmp
- xml
- cm33913-3

Contents of '/dls/i21/data/2023/cm33913-2/NdNiO2'

File Filter Wildcard

Name	Size	Type
i21-291505.nxs	182.9 KiB	No
i21-291504.nxs	182.9 KiB	No
i21-291503.nxs	182.9 KiB	No
i21-291502.nxs	182.9 KiB	No
i21-291501.nxs	182.9 KiB	No
i21-291500.nxs	182.9 KiB	No
i21-291499.nxs	182.9 KiB	No
i21-291498.nxs	182.9 KiB	No
i21-291497.nxs	182.9 KiB	No
i21-291496.nxs	182.9 KiB	No
i21-291495.nxs	182.9 KiB	No
i21-291494.nxs	182.9 KiB	No
i21-291493.nxs	182.9 KiB	No
i21-291492.nxs	182.9 KiB	No
i21-291491.nxs	182.9 KiB	No
i21-291480.nxs	200.8 KiB	No

11 object(s) selected 2,060,322 bytes

Data Slice View

Set up data for processing
Select dataset, axes, whether to process as images [2D] or lines [1D] and which dimensions of the array are the data dimensions

Select dataset: /entry/andor/data [2, 2048, 2048]

Line [1D] Image [2D]

Dimension	Display	Start:Stop:Step	Axis
0 [2]		:	/entry/andor/ds
1 [2048]	Y	:	indices
2 [2048]	X	:	indices

data[0,:,:]

Current s

Input

100 80 60 40 20 0

0 20 40 60 80 100

0 10 20 30 40 50 60 70 80 90 100

Cancel Finish

4. This pop-up window appears
Please check the raw RIXS detector image on the right side, whether it shows proper RIXS image

DATA LOADING

Loading Your Data Files: Check RIXS Image in Input Panel

The screenshot shows the DAWN software interface with the following components:

- Project Explorer:** Shows a file tree with folders like .workspace, BFO, LSMO_Taiwan, NdNiO2, RbFeS2, processing, spool, tmp, xml, and cm33913-3.
- Data Slice View:** Lists data files from i21-291501.nxs to i21-291491.nxs. A red arrow points to this panel with the instruction: "5. This pop-up window appears. Check all datafiles are properly loaded in Data Slice View panel".
- Processing:** Shows a list of processing steps, including "Image background subtraction - Fitted to a PDF [Background Subtraction]".
- Output:** Shows an "Images Monitor" plot with a grid and axes labeled 0 to 100. A red arrow points to the plot with the instruction: "6. Check the raw RIXS detector image. Check the raw RIXS detector image of each data files".
- Input Panel:** Shows a heatmap of the raw RIXS detector image with a color scale from 300 to 500. A red arrow points to this panel with the instruction: "If the data file contains more than 1 image frame, you can check different frames by clicking the backward/forward buttons".

BACKGROUND SUBTRACTION

Dark Image Background Subtraction

2. Click "Image background subtraction" operation

3. Click "Show all fields"

1. Check all operations are properly loaded
We need "Image background subtraction" and "RIXS image reduction" (or "Combined RIXS image reduction")

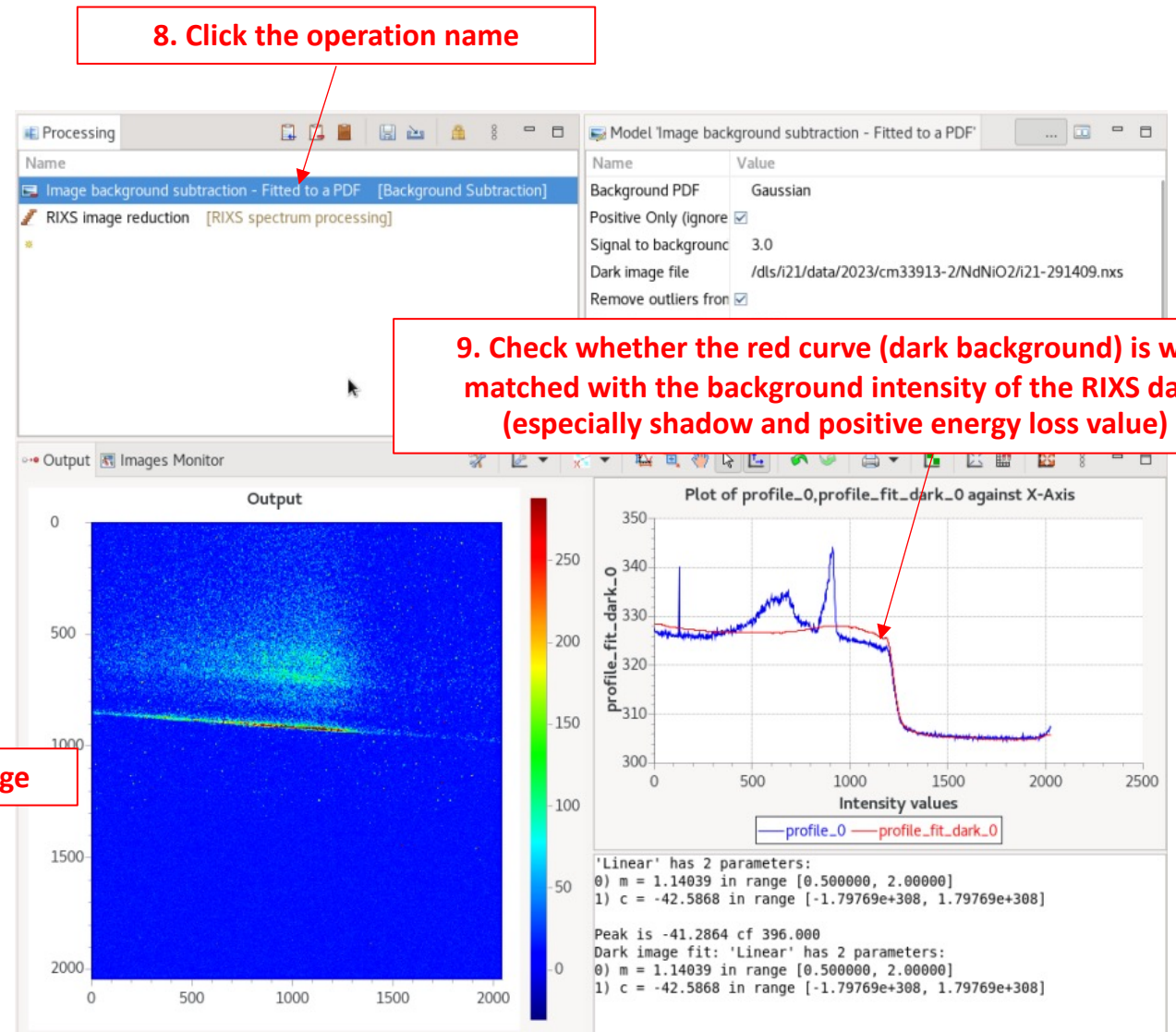
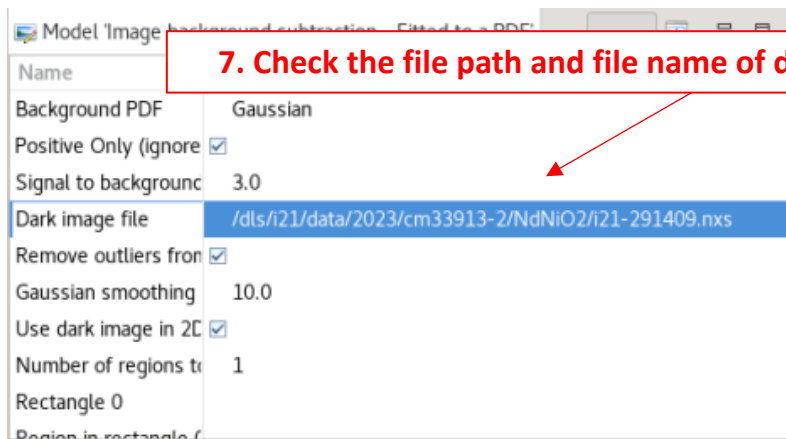
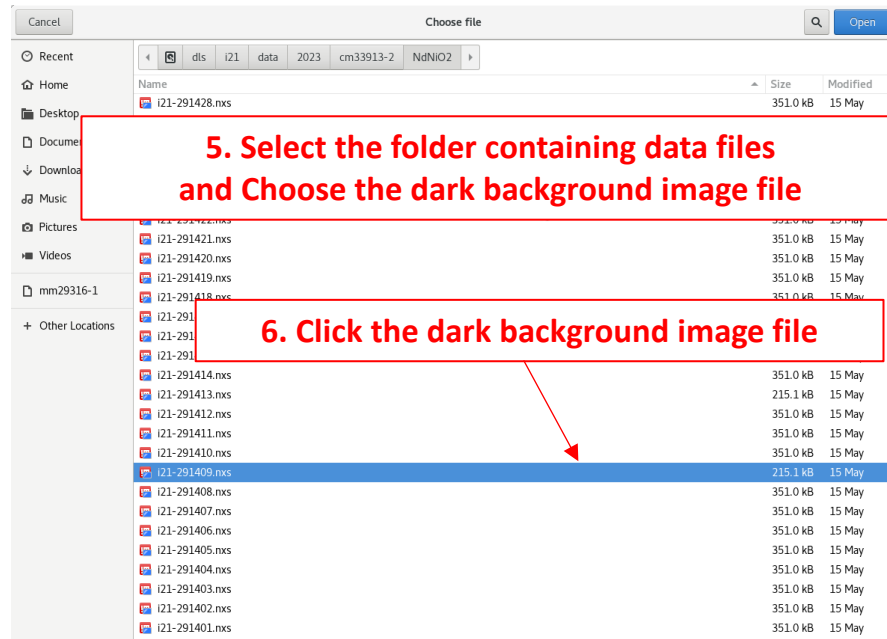
The screenshot displays the DAWN software interface with several key components:

- Project Explorer:** Lists folders like .workspace, BFO, LSMO_Taiwan, and NdNiO2.
- Data Slice View:** Shows a list of .nxs files (e.g., i21-291501.nxs to i21-291495.nxs).
- Processing Panel:** Contains operations such as 'Image background subtraction - Fitted to a PDF' and 'RIXS image reduction'. A red arrow points to the 'Image background subtraction' operation.
- Model Configuration Window:** Titled 'Model Image background subtraction - Fitted to a PDF', it shows parameters for a Gaussian background fit. A red arrow points to the 'Show all fields' button. A 'Browse to an external file' button is also highlighted with a red arrow.
- Plots:** A 2D heatmap shows 'data[0,...]' with a color scale from 300 to 600. A line plot shows 'Log10 of Background fit' vs 'Intensity values' with a legend for 'Log10 of Histogram counts' and 'Log10 of Background fit'. Text below the plot indicates: 'Peak is 114841 cf 112560', 'Fitted PDF in 322:433: residual = 3.04953e+08', and 'Gaussian' has 3 parameters: 0) posn = 322.500 in range [322.500, 325.000], 1) fwhm = 25.0616 in range [1.00000, 43.8026], 2) area = 3.06364e+06 in range [112560, 4.93043e+06]. Threshold = 353.

4. Click "Browse to an external file"

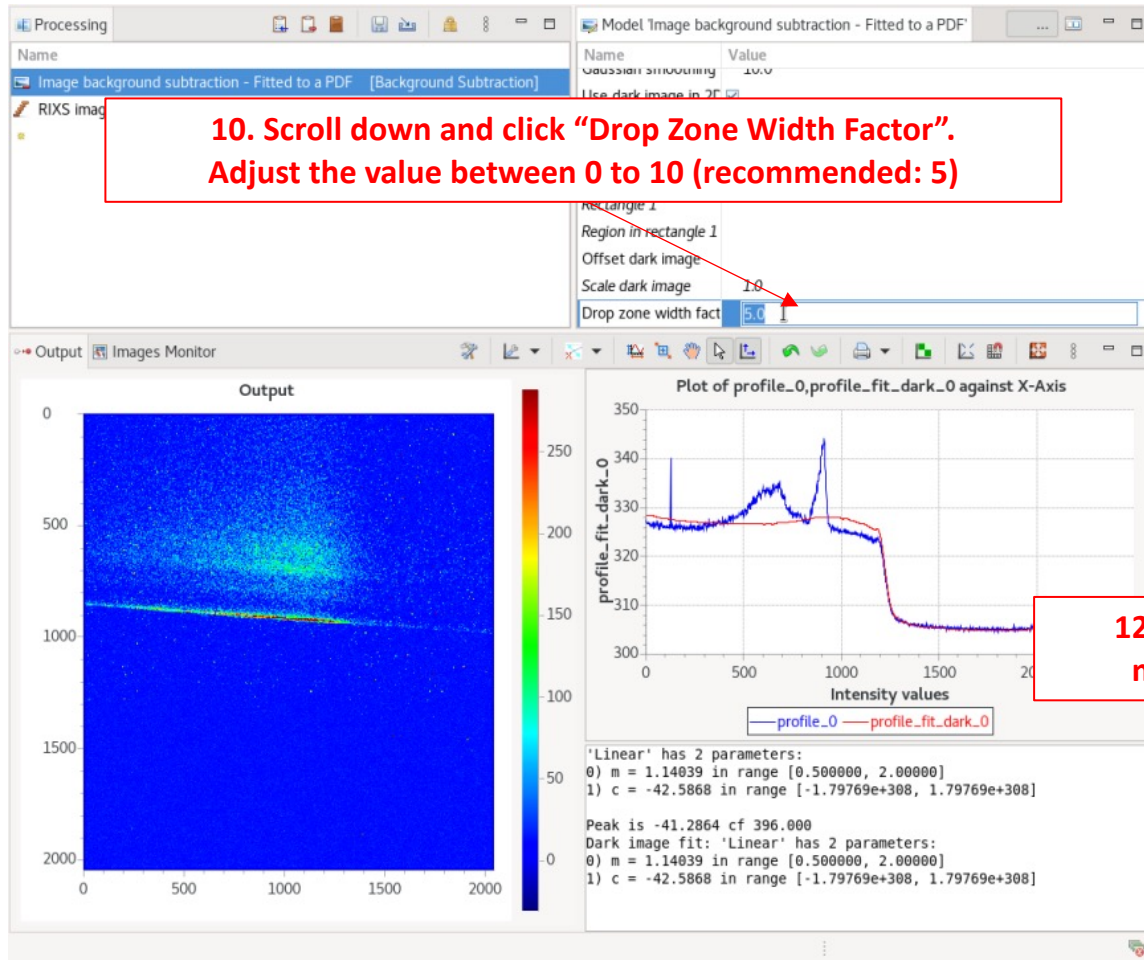
BACKGROUND SUBTRACTION

Dark Image Background Subtraction

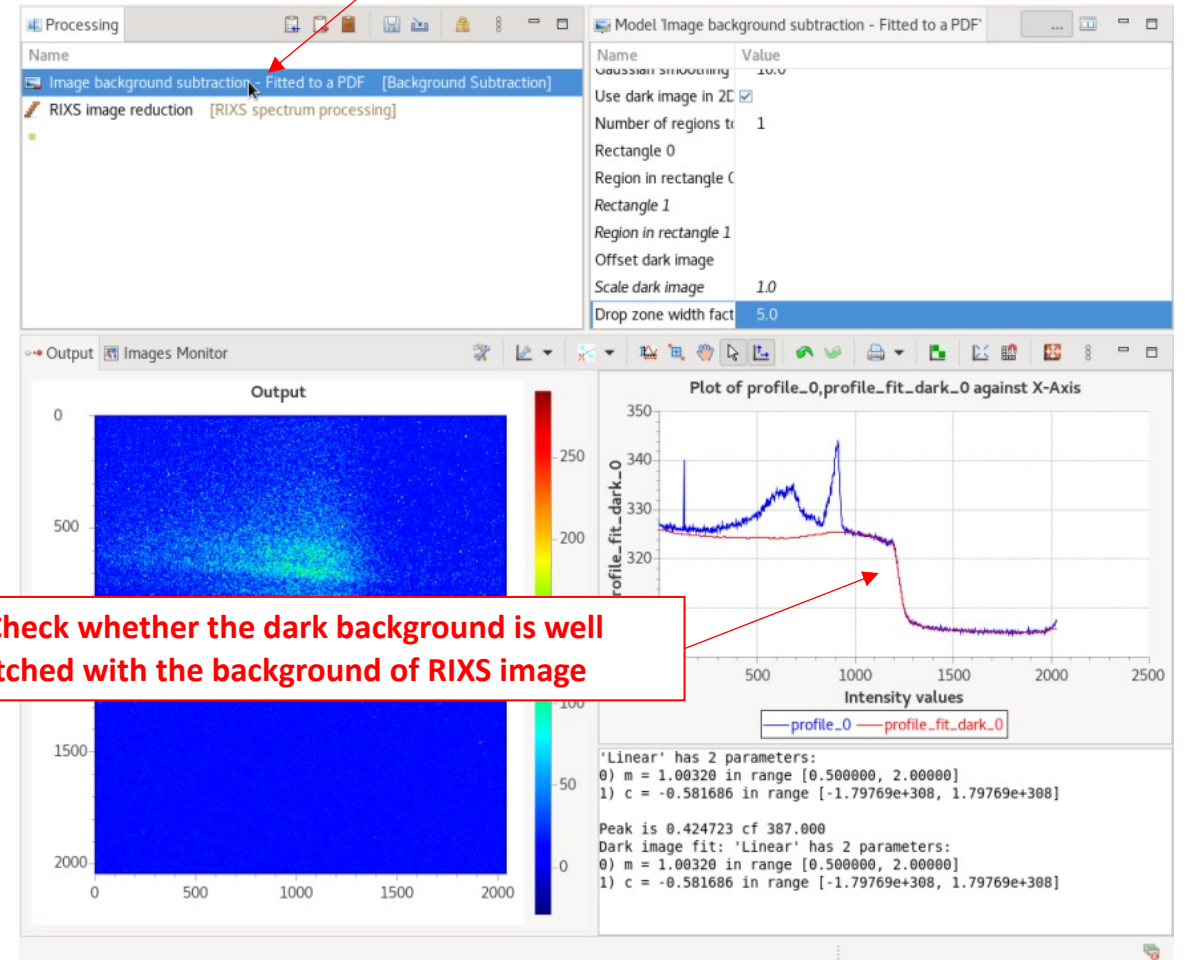


BACKGROUND SUBTRACTION

Dark Image Background Subtraction



11. Click the name of operation one more time

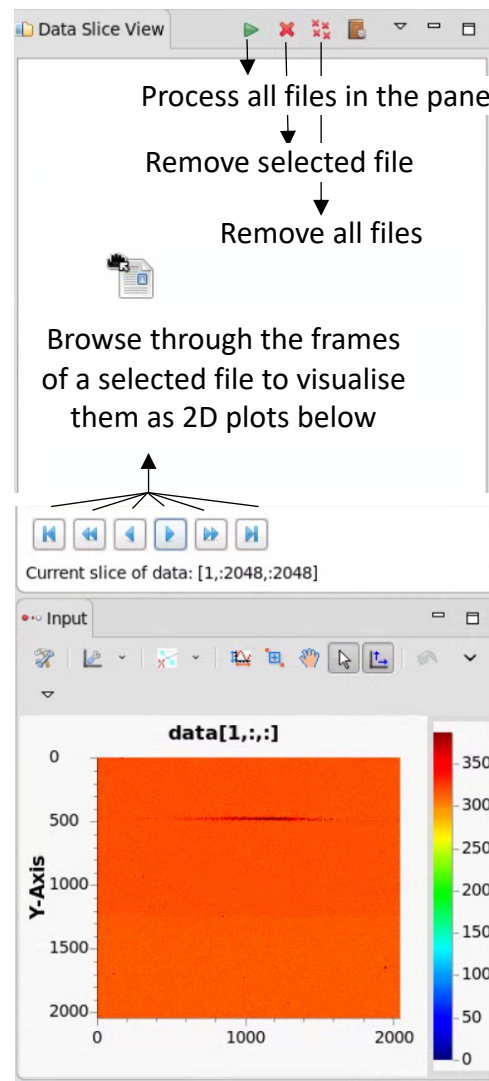
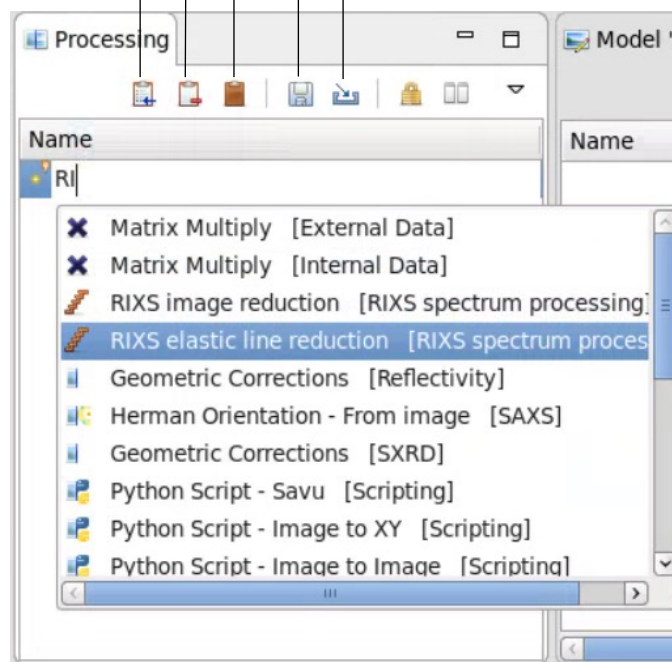


12. Check whether the dark background is well matched with the background of RIXS image

RIXS IMAGE PROCESSING

RIXS Image Processing: Dispersion and Slope Correction

- Load a saved list of operations with model parameters
- Save the list of operations along with model parameter
- Remove all operations
- Remove selected operation
- Insert operation



RIXS IMAGE PROCESSING

RIXS Image Processing: Dispersion and Slope Correction

1. Load and Click "RIXS image reduction" operation

2. Click "Show All Fields" to expand the model list

TIP: if you tick the "Cutoff enable" box, you can subtract the contamination from gamma ray

The screenshot shows the DAWN software interface with the following components:

- Project Explorer:** Shows the file structure for the project, including folders like `.workspace`, `BFO`, `LSMO_Taiwan`, `NdNiO2`, `RbFeS2`, `processing`, `spool`, `tmp`, `xml`, and `cm33913-3`.
- Data Slice View:** Displays a list of data files (e.g., `i21-291501.nxs` to `i21-291538.nxs`) and a small plot of `data[0,:]`.
- Processing Panel:** Shows the 'Model RIXS image reduction' operation selected. The 'Cutoff enable' checkbox is checked. Other parameters include 'Cutoff for pixels' (5.0) and 'Cutoff window size' (1).
- Output/Plot of profile:** Displays two plots: 'Output' (a 2D intensity map) and 'Plot of profile' (a line graph showing intensity values vs. intensity). The plot shows a peak at approximately 800 intensity units, with a fit line overlaid.

RIXS IMAGE PROCESSING

RIXS Image Processing: Dispersion and Slope Correction

3. Click "Elastic Line Fit File Option". Choose "Manual_Override"



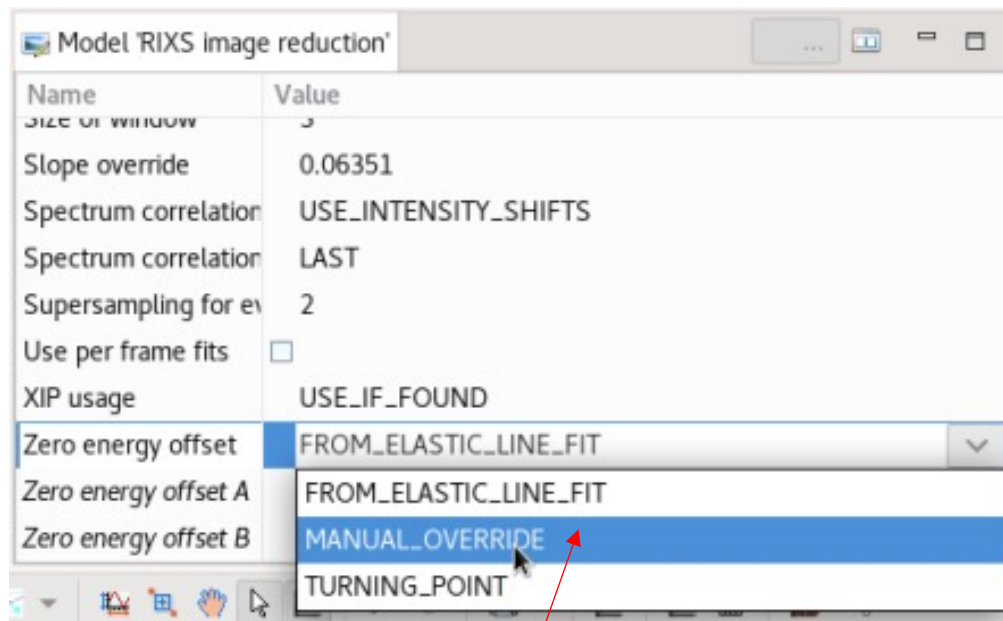
4. Click and type in the energy dispersion value provided by beamline staff in the "Energy dispersion at" slot



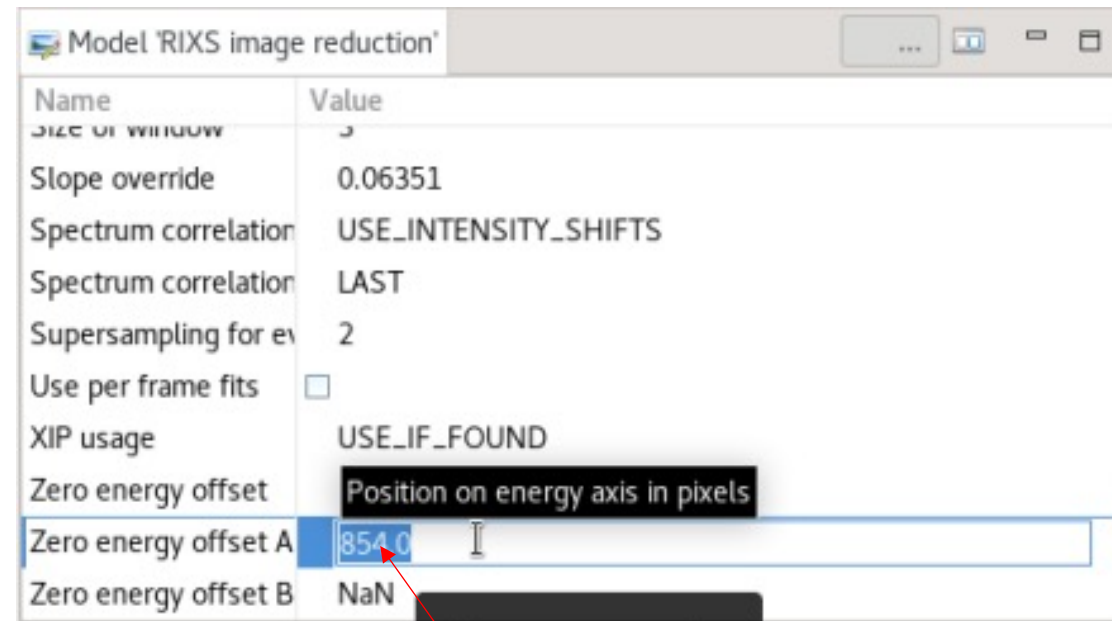
5. Click and type in the slope value provided by beamline staff in the "Slope Override" slot.

RIXS IMAGE PROCESSING

RIXS Image Processing: Offsetting the Elastic Peak



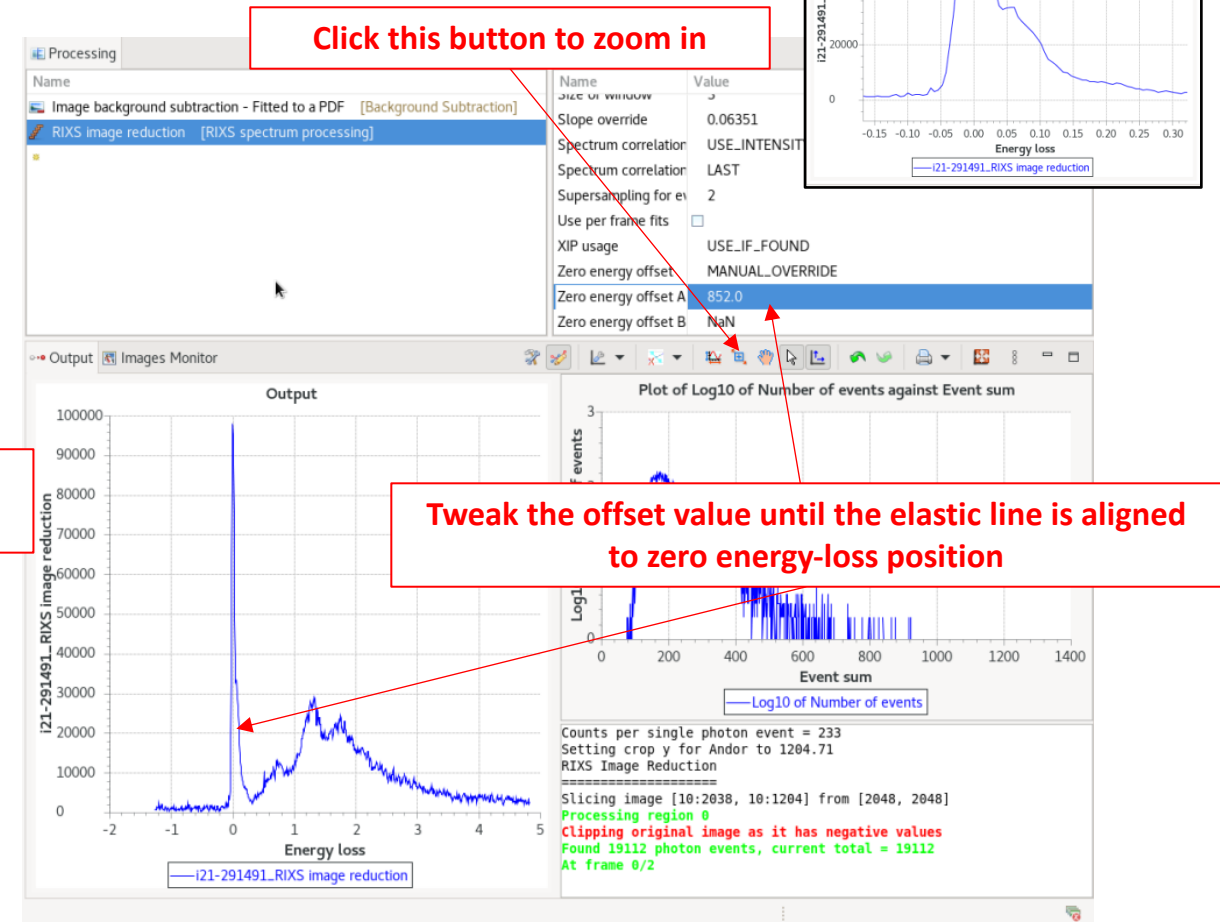
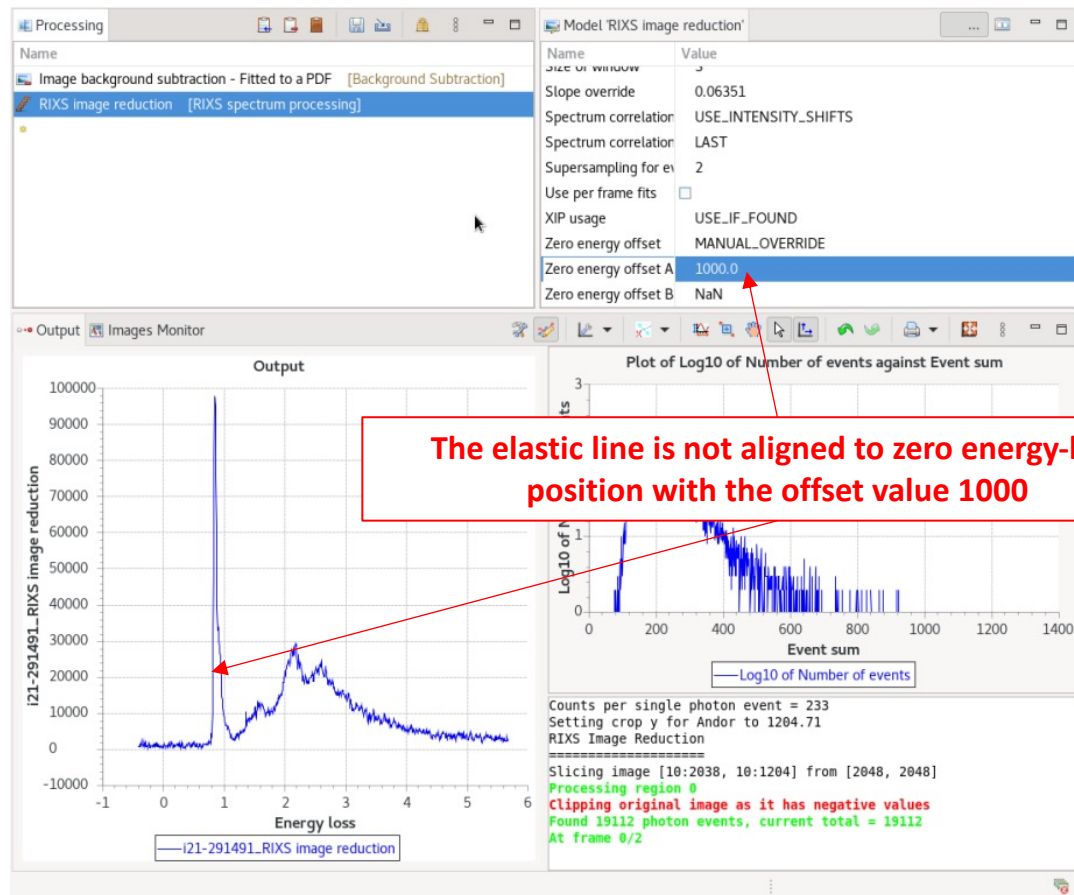
6. Click the drop box in "Zero Energy Offset" and Choose "MANUAL_OVERRIDE"
(Since we do not have RIXS image for the carbon tape)



7. Type in the pixel value where the elastic peak is located
Need to be tweaked until the elastic peak is precisely aligned

RIXS IMAGE PROCESSING

RIXS Image Processing: Offsetting the Elastic Peak



RIXS IMAGE PROCESSING

RIXS Image Processing: Creating Processed Files

The screenshot displays the DAWN software interface with the following components:

- Project Explorer:** Shows the file structure for the project, including folders like `.workspace`, `BFO`, `LSMO_Taiwan`, `NdNiO2`, `RbFeS2`, `processing`, `spool`, `tmp`, `xml`, and `cm33913-3`.
- Data Slice View:** Lists data files such as `i21-291501.nxs` through `i21-291538.nxs`. A red arrow points to `i21-291498.nxs`, which is highlighted in blue.
- Processing Panel:** Shows the current processing step: `RIXS image reduction [RIXS spectrum processing]`.
- Model 'RIXS image reduction':** Displays parameters like `Slope override` (0.06351), `Spectrum correlation` (USE_INTENSITY_SHIFTS), and `Supersampling for ev` (2).
- Output Window:** Contains a log of the processing steps, including:
 - Counts per single photon event = 233
 - Setting crop y for Andor to 1204.71
 - RIXS Image Reduction
 - Slicing image [10:2038, 10:1204] from [2048, 2048]
 - Processing region 0
 - Clipping original image as it has negative values
 - Found 16628 photon events, current total = 16628
 - At frame 0/2
- Plots:**
 - Heatmap:** `data[0,:,:]` showing intensity distribution.
 - Line Plot:** `i21-291498_RIXS image reduction` showing `Log10 of Number of events` vs `Energy loss`.
 - Histogram:** `Log10 of Number of events` vs `Event sum`.

Callout Box:

Click other data files to confirm all the images on Data Slice View have been properly processed
 * Offset value for one specific data file may not apply to all data files equally well, so please do not bother offsetting too much at this moment. We can align it on DataVis

RIXS IMAGE PROCESSING

RIXS Image Processing: Creating Processed Files

1. Click the "Process All Files" icon

The interface shows a file explorer on the left with folders like 'workspace', 'BFO', 'LSMO_Taiwan', 'NdNiO2', 'RbFeS2', 'processing', 'spool', 'tmp', and 'xml'. The 'Data Slice View' window displays a list of files such as i21-291501.nxs, i21-291500.nxs, i21-291499.nxs, i21-291498.nxs, i21-291497.nxs, i21-291496.nxs, i21-291495.nxs, i21-291494.nxs, i21-291491.nxs, i21-291540.nxs, i21-291539.nxs, and i21-291538.nxs. The 'Current slice of data' is [0.:2048.:2048]. Below the file list is an 'Input' section and a heatmap visualization of 'data[0,:,:]' with axes from 0 to 2000 and a color scale from -300 to 500.

2. Click the "Select an external folder" button and find the suitable folder path. Do not use the parent folder. You can use "processing" subfolder to save the data

2. Select one of the data saving options. We recommend to select "Link Original Data (No data copied)" and press "OK"

The interface shows a 'Processing' window with a 'Model RIXS image reduction' section. A 'Please select a directory' dialog box is open, showing the folder path '/dls/i21/data/2023/cm33913-2/processing/202306191'. The dialog box has options: 'Automatically load data to DataVis perspective', 'Processed data only', 'Link original data (no data copied)', and 'Process data into copy of original'. The 'Link original data (no data copied)' option is selected. The 'OK' button is highlighted. The background shows a plot of 'Log10 of Number of events' against 'Event sum' and an 'Energy loss' plot.

*** List of data-saving options**

Link original data (no data copied):

Process data into copy of original:

RIXS IMAGE PROCESSING

RIXS Image Processing: Creating Processed Files

The screenshot displays the DAWN Science software interface. The main window shows a list of data files in the Data Slice View, with the current slice of data being processed. A red box highlights the text "Data is being processed frame by frame".

The Progress Information dialog box shows the following details:

- Processing
- i21-291497.nxs [0.:2048.:2048] Image background subtraction - Fitted to a PDF
- Cancel

The main window also displays a plot of the Log10 of Number of events against Event sum, and a plot of the Log10 of Number of events against Energy loss. The plot of Log10 of Number of events against Energy loss shows a peak at approximately 1.5 eV.

The Processing window shows the following parameters:

Name	Value
Slope override	0.06351
Spectrum correlation	USE_INTENSITY_SHIFTS
Spectrum correlation	LAST
Supersampling for ev	2
Use per frame fits	<input type="checkbox"/>
XIP usage	USE_IF_FOUND
Zero energy offset	MANUAL_OVERRIDE
Zero energy offset A	852.0
Zero energy offset B	NaN

The console output shows the following information:

```

Counts per single photon event = 233
Setting crop y for Andor to 1204.71
RIXS Image Reduction
=====
Slicing image [10:2038, 10:1204] from [2048, 2048]
Processing region 0
Clipping original image as it has negative values
Found 16628 photon events, current total = 16628
At frame 0/2
  
```

RIXS IMAGE PROCESSING

Combined RIXS Image Processing:

1. Select Combined RIXS image reduction operation

2. We have to choose an option for "Elastic line scan".

Model 'Combined RIXS image reduction'

Name	Value
Elastic line cutoff for	5.0
Elastic line cutoff win	1
Elastic line scan	NEXT_SCAN
Elastic line scan file	
Energy calibration file	
Energy direction	SLOW
Energy dispersion at	NaN
Fallback value for co	74
Ignore linked elastic	<input type="checkbox"/>
Normalization database	/entru/m4r-1/m4r-1

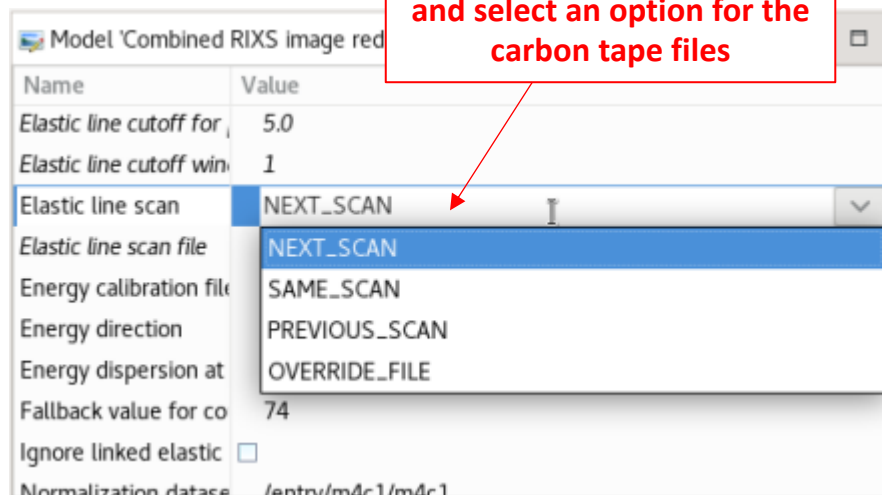
Output Images Monitor

X-Axis

X-Axis

RIXS IMAGE PROCESSING

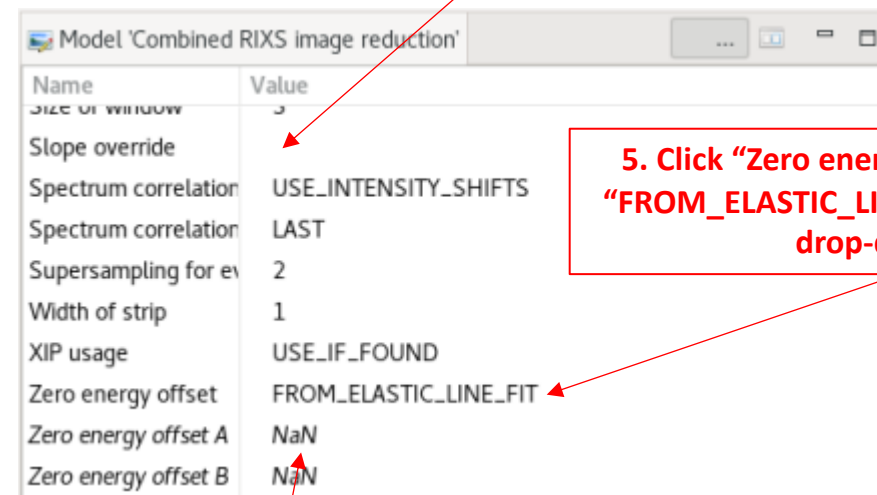
Combined RIXS Image Processing:

**1. NEXT_SCAN (or PREVIOUS_SCAN):**

DAWN recognizes the nxs file with filename +1 (or -1) as carbon tape image of the specific RIXS data file. In this case, you can load only RIXS data files on the *Data Slice View* panel.

2. SAME_SCAN:

The same carbon tape image will be commonly applied to all RIXS data files. You can provide the file name in "Elastic line scan file".

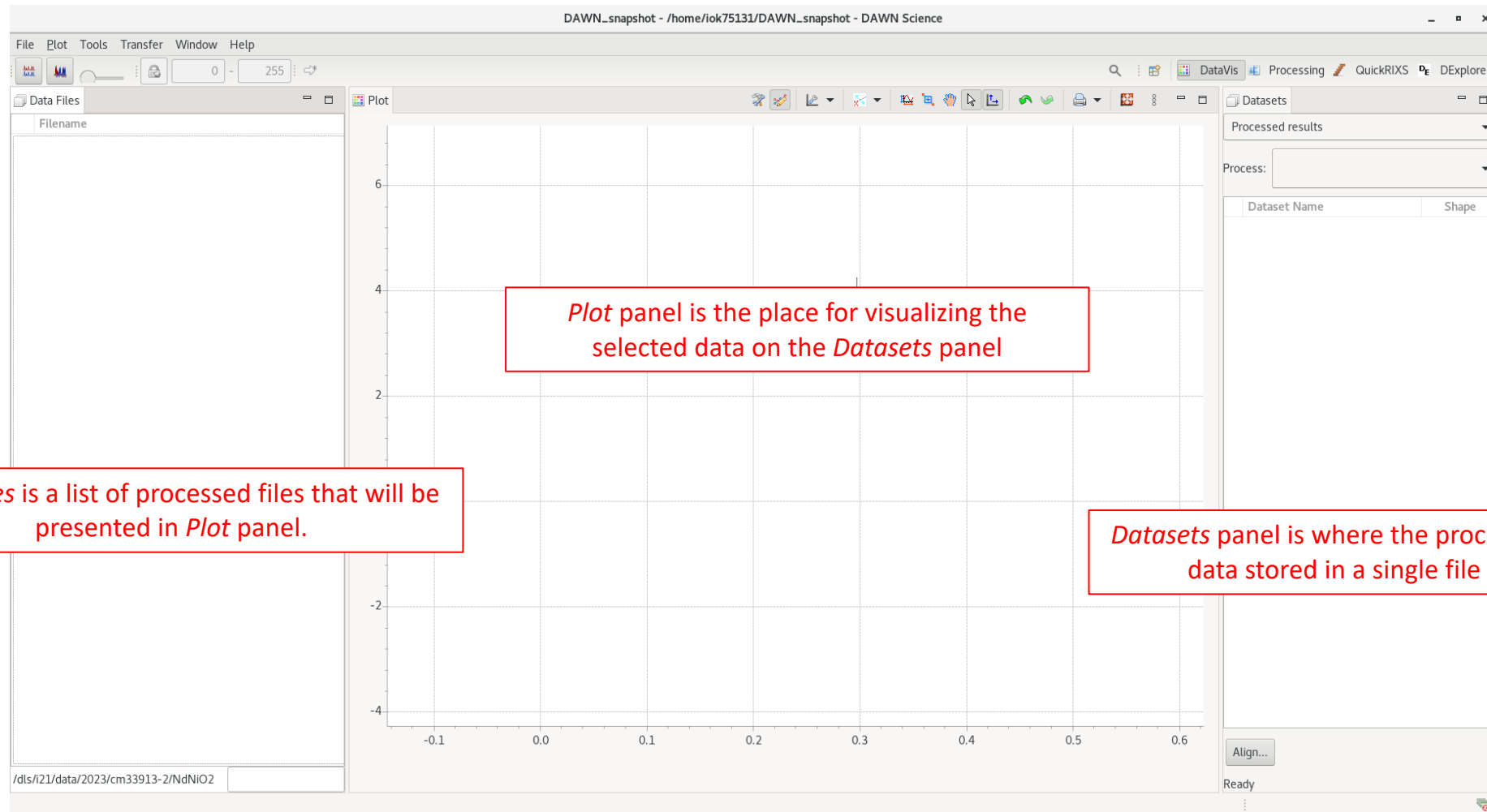


6. You do not have to provide any number here as the position of elastic peak is automatically adjusted

DATA VISUALIZATION

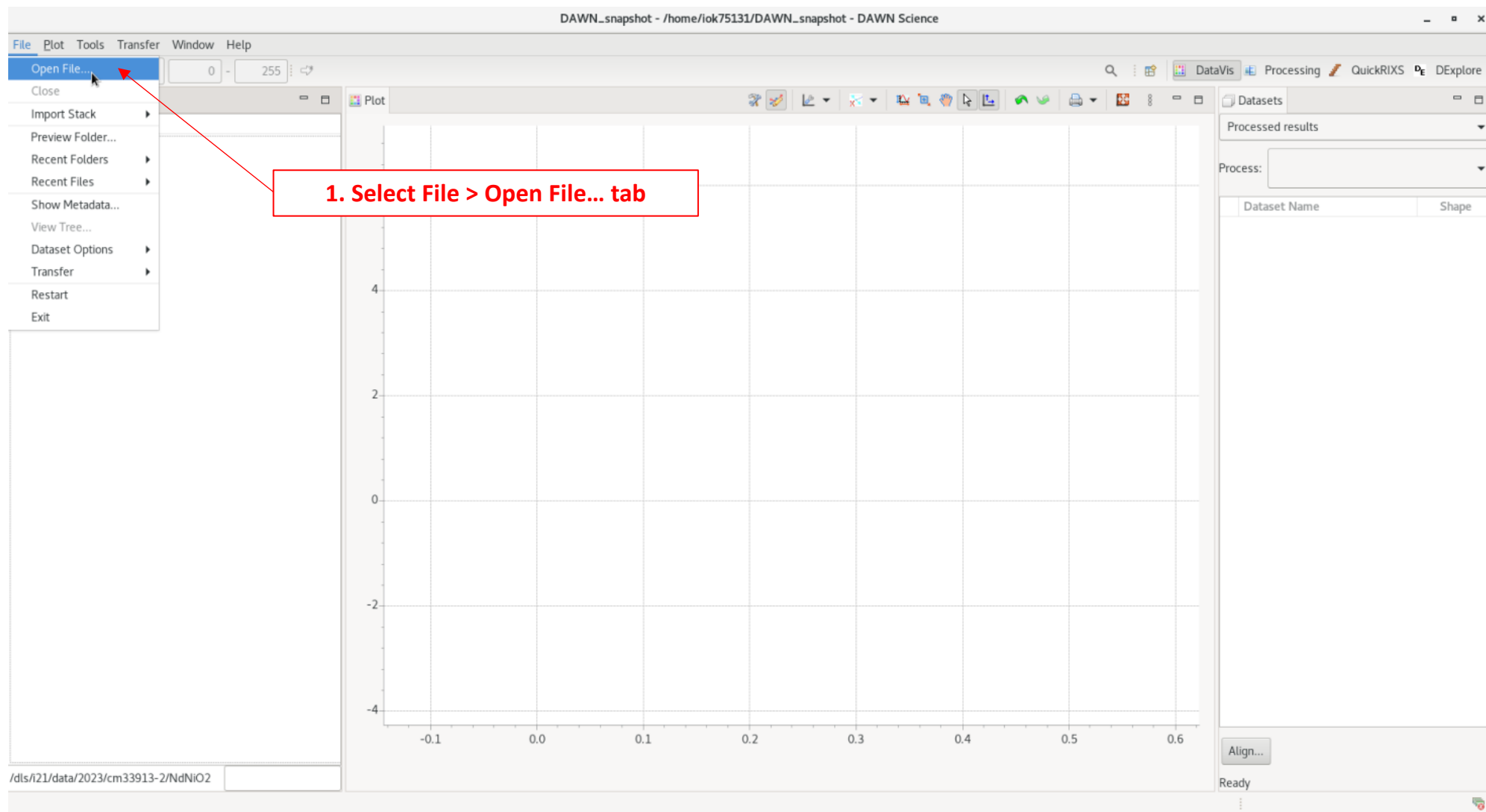
DataVis: Data Visualization Software

DataVis is a data visualization software tool implemented as a perspective of DAWN package. You can (1) check the processed data, (2) adjust misaligned RIXS spectra, and (3) export them into data file. You can click the button “DataVis” to open.



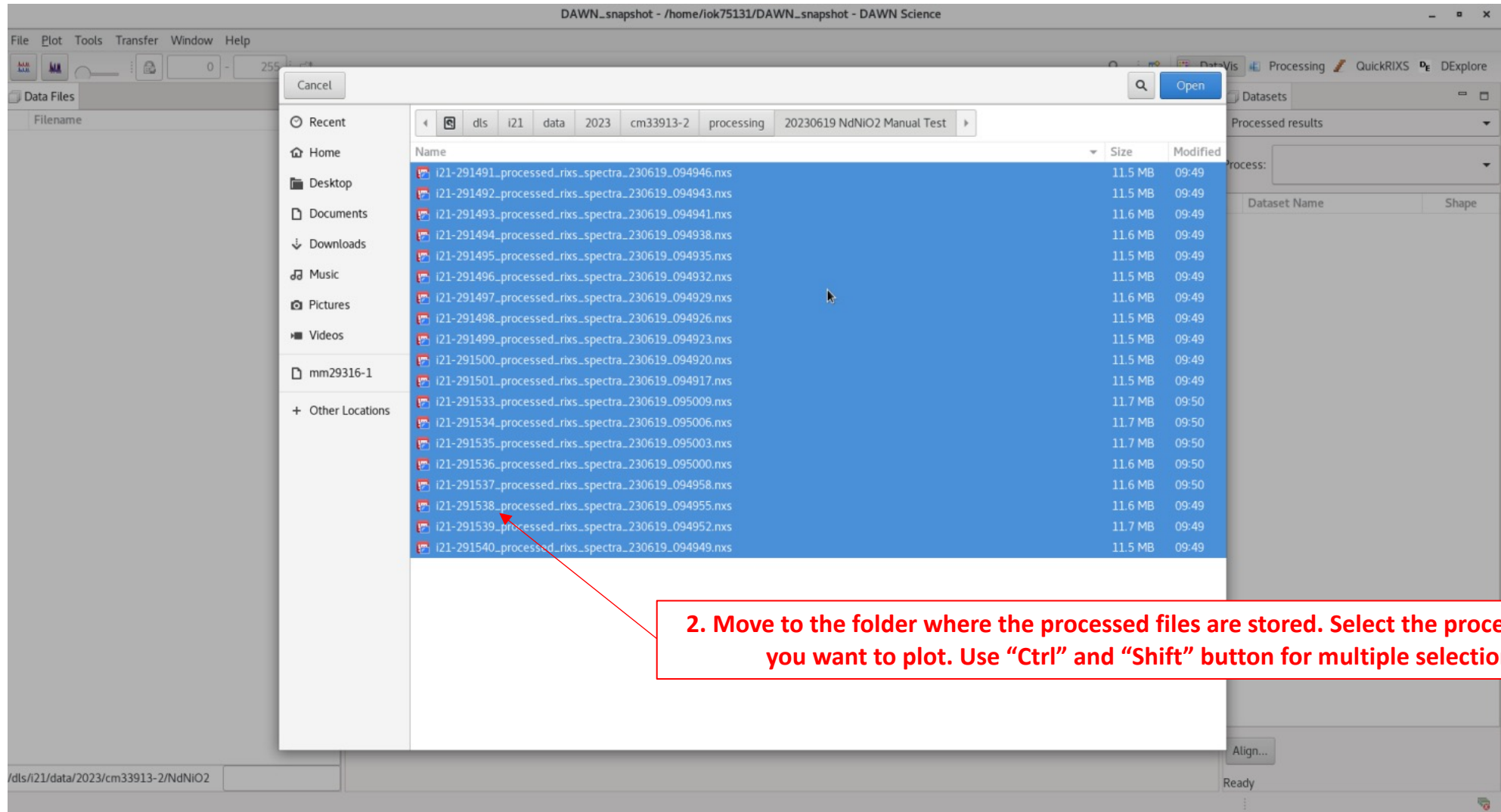
DATA VISUALIZATION

DataVis: Open Processed Files



DATA VISUALIZATION

DataVis: Open Processed Files



DATA VISUALIZATION

DataVis: Open Processed Files

The screenshot displays the DataVis software interface. The main window is titled "DAWN_snapshot - /home/iok75131/DAWN_snapshot - DAWN Science". The interface is divided into several panels:

- Data Files Panel:** Located on the left, it shows a list of files with the following filenames:
 - i21-291540_processed_rixs_spectra_230619_094949.nxs
 - i21-291539_processed_rixs_spectra_230619_094952.nxs
 - i21-291538_processed_rixs_spectra_230619_094955.nxs
 - i21-291537_processed_rixs_spectra_230619_094958.nxs
 - i21-291536_processed_rixs_spectra_230619_095000.nxs
 - i21-291535_processed_rixs_spectra_230619_095003.nxs
 - i21-291534_processed_rixs_spectra_230619_095006.nxs
 - i21-291533_processed_rixs_spectra_230619_095009.nxs
 - i21-291501_processed_rixs_spectra_230619_094917.nxs
 - i21-291500_processed_rixs_spectra_230619_094920.nxs
 - i21-291499_processed_rixs_spectra_230619_094923.nxs
 - i21-291498_processed_rixs_spectra_230619_094926.nxs
 - i21-291497_processed_rixs_spectra_230619_094929.nxs
 - i21-291496_processed_rixs_spectra_230619_094932.nxs
 - i21-291495_processed_rixs_spectra_230619_094935.nxs
 - i21-291494_processed_rixs_spectra_230619_094938.nxs
 - i21-291493_processed_rixs_spectra_230619_094941.nxs
 - i21-291492_processed_rixs_spectra_230619_094943.nxs
 - i21-291491_processed_rixs_spectra_230619_094946.nxs
- Plot Panel:** The central area shows a plot with a grid. The Y-axis ranges from 0 to 100, and the X-axis ranges from 0 to 100. A crosshair is positioned at the coordinates [66.4927, 76.7263].
- Datasets Panel:** Located on the right, it shows a tree structure of datasets. The selected dataset is "/processed/result/data" with a shape of [2, 1065]. Other datasets include "/processed/result/ds" [2], "/processed/summary/0-Image bac" [552, 2028], and various "/processed/summary/1-RIXS imag" datasets with different shapes.

Two red callout boxes provide instructions:

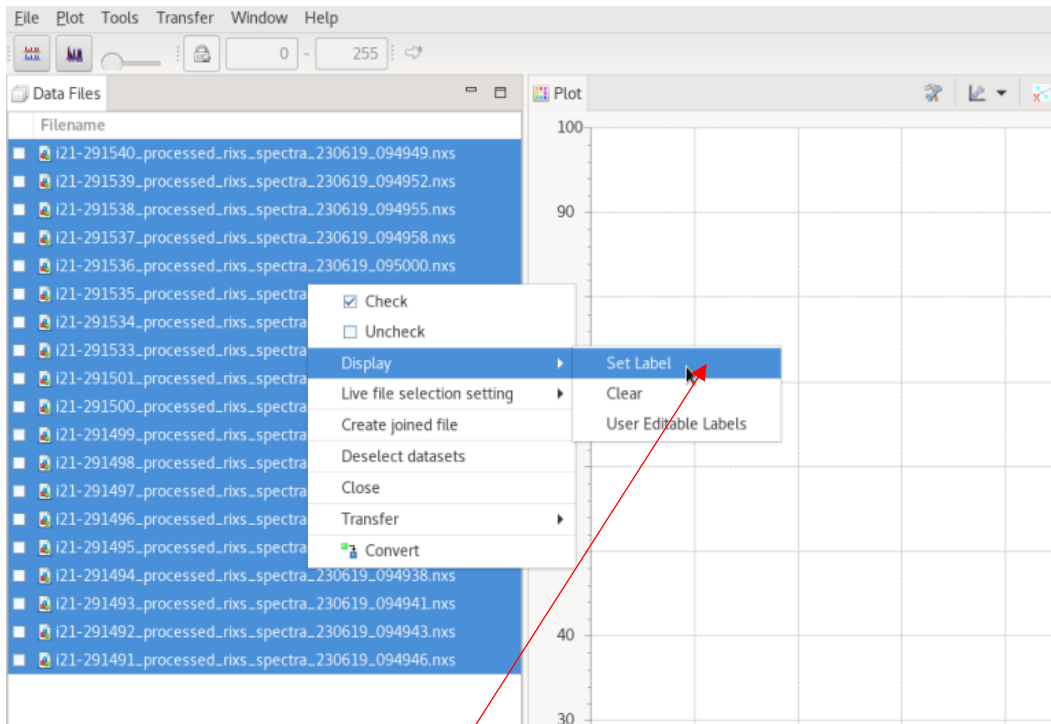
3. Data Files are loaded on *Data Files* panel.
4. On the *Datasets* panel, all lists of processed and raw data stored in a tree structure are shown

The status bar at the bottom shows the path "/dls/i21/data/2023/c...9 NdNIO2 Manual Test" and the system status "Ready". The Python path is also visible: "Sync System PYTHONPATH: (15%)".

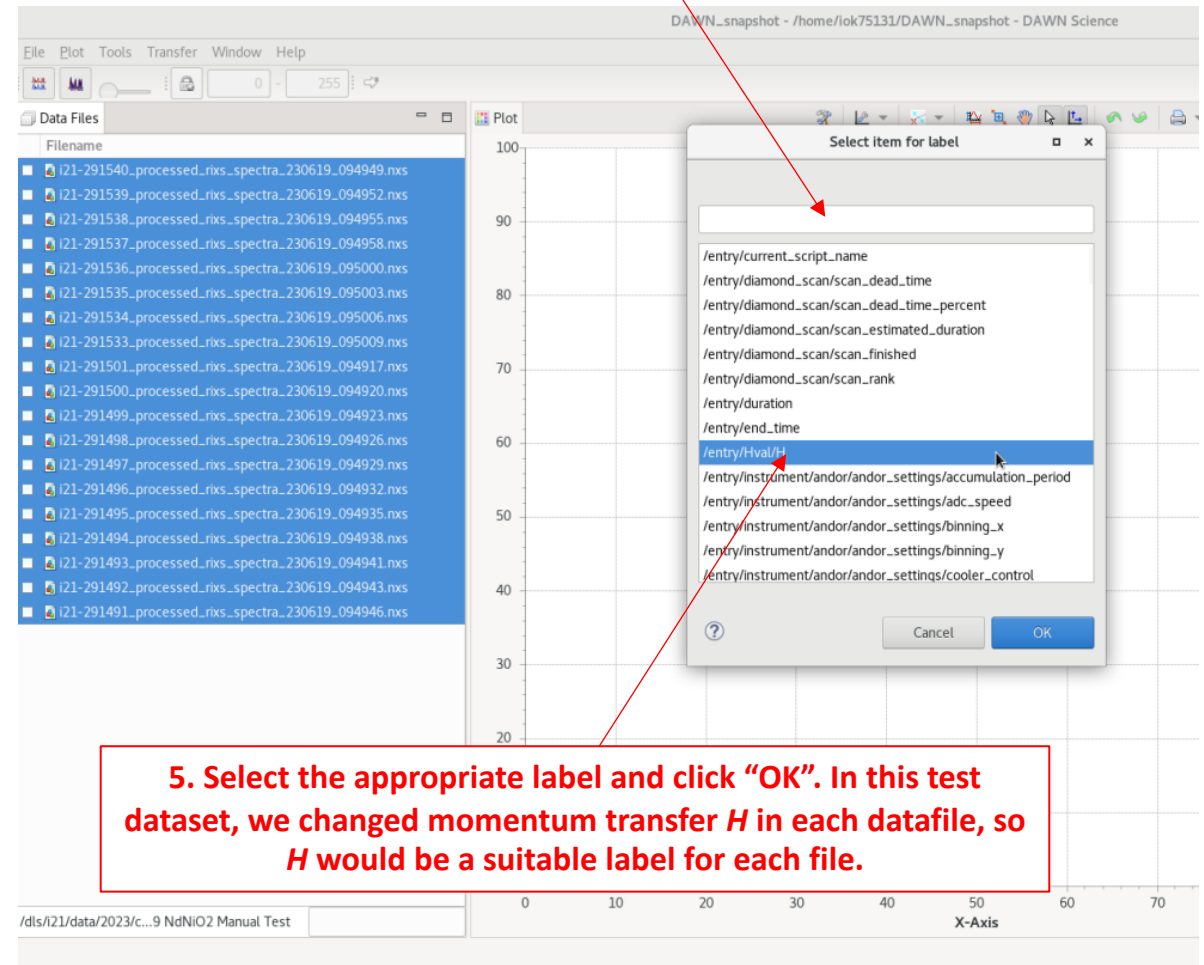
DATA VISUALIZATION

DataVis: Plot RIXS Spectra

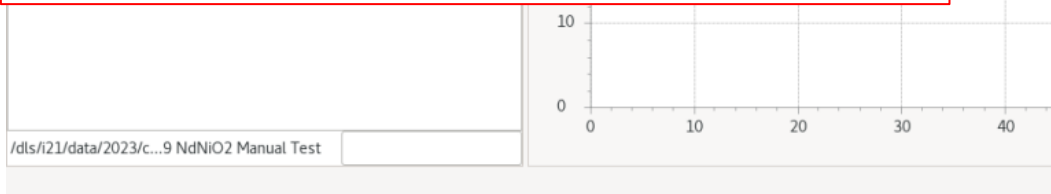
Tip: You can also type in keywords here. For example, H for /entry/Hval/H or energy for /entry/instrument/pgm/energy



4. Select all files to plot and right click the mouse and choose Display > Set Label. This is for labelling each file to sort them with an order (e. g. energy or Q)

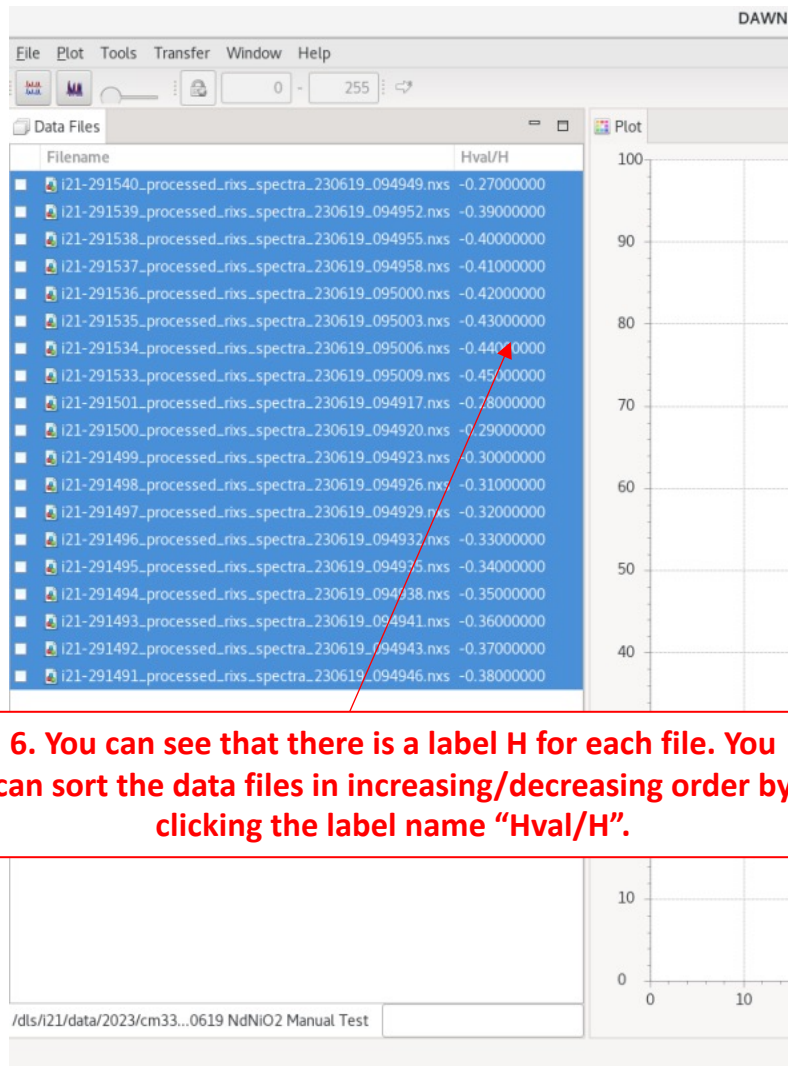


5. Select the appropriate label and click "OK". In this test dataset, we changed momentum transfer H in each datafile, so H would be a suitable label for each file.

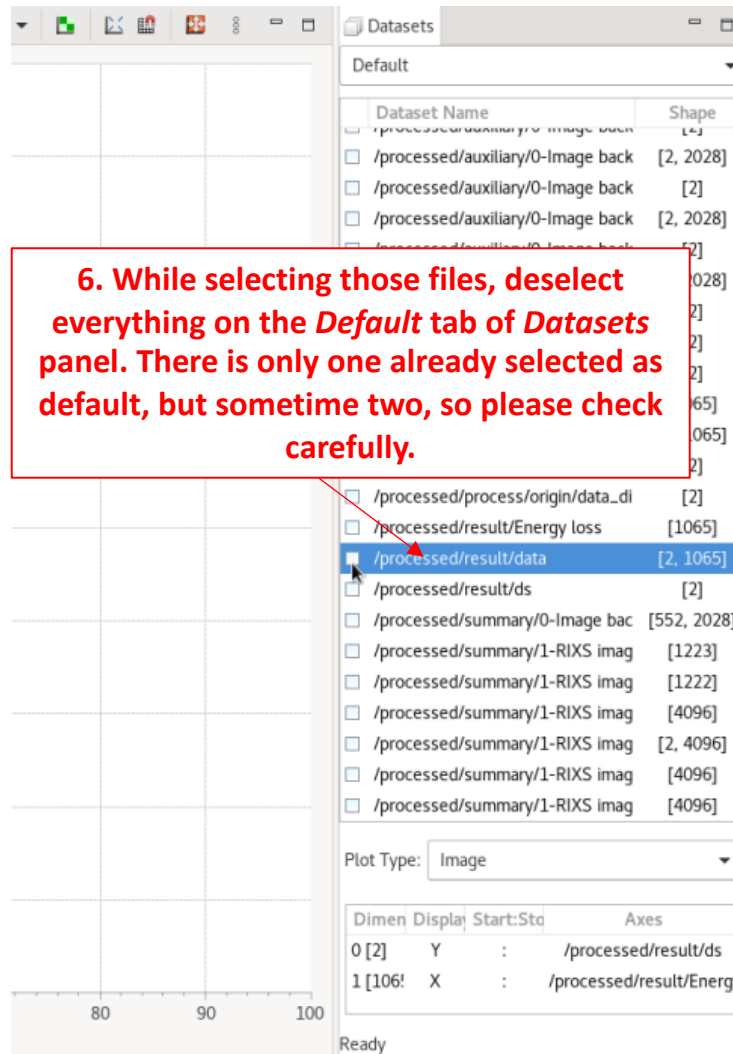


DATA VISUALIZATION

DataVis: Plot RIXS Spectra

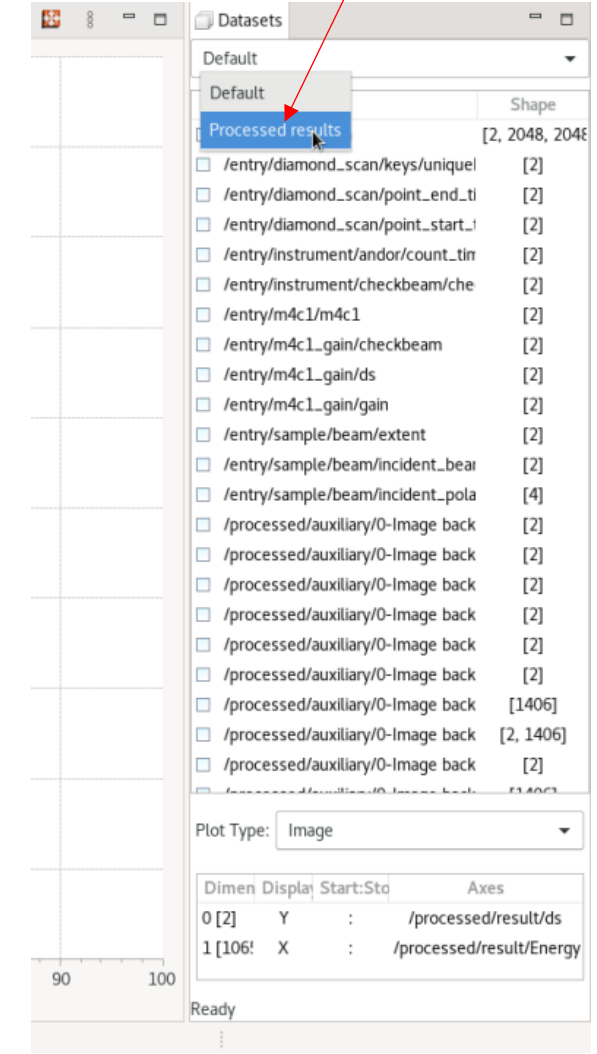


6. You can see that there is a label H for each file. You can sort the data files in increasing/decreasing order by clicking the label name "Hval/H".



6. While selecting those files, deselect everything on the *Default* tab of *Datasets* panel. There is only one already selected as default, but sometime two, so please check carefully.

7. Click the radio box "Default" and change it to "Processed results".



DATA VISUALIZATION

DataVis: Plot RIXS Spectra

9. Select "normalized_correlated_spectrum_0"

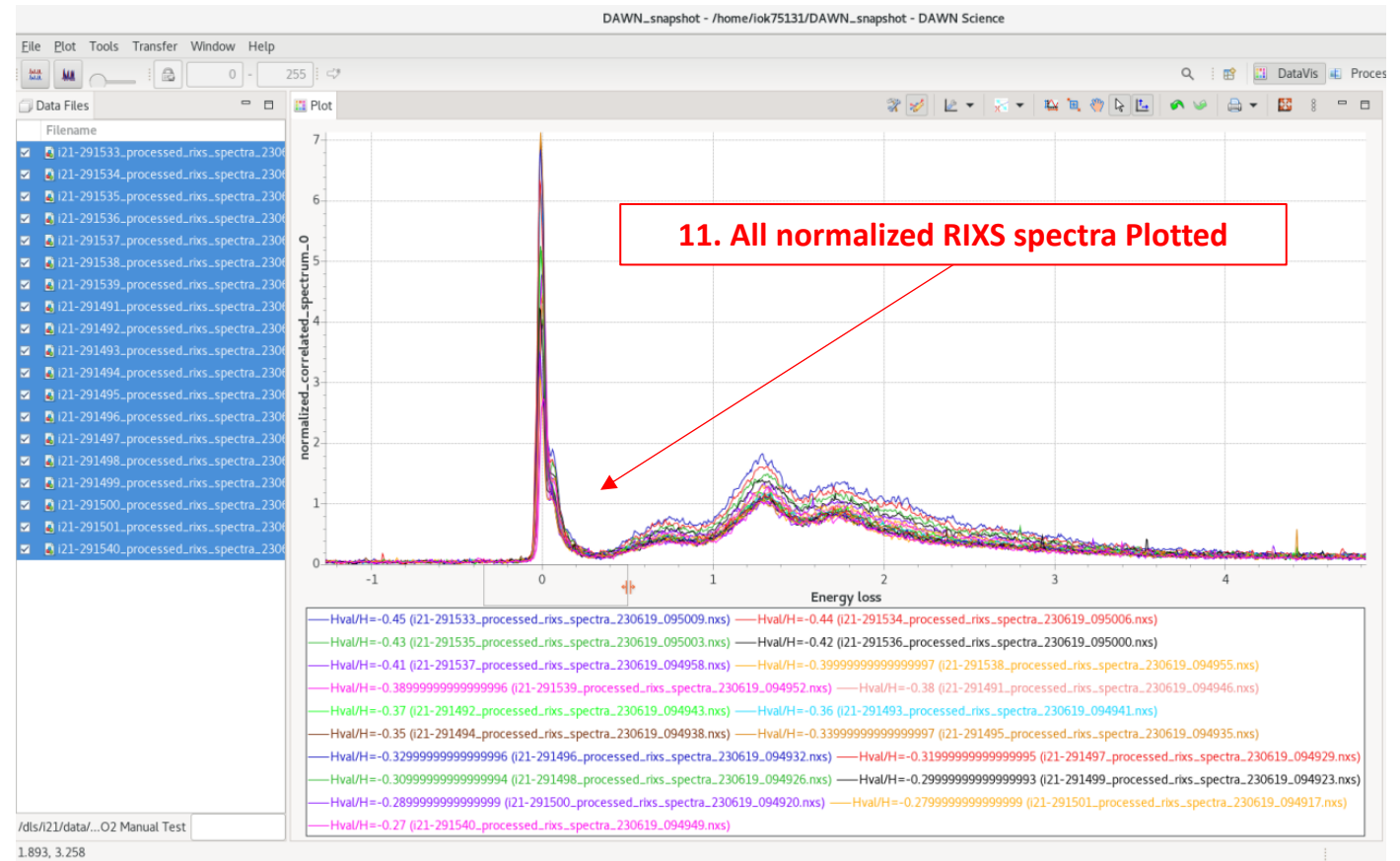
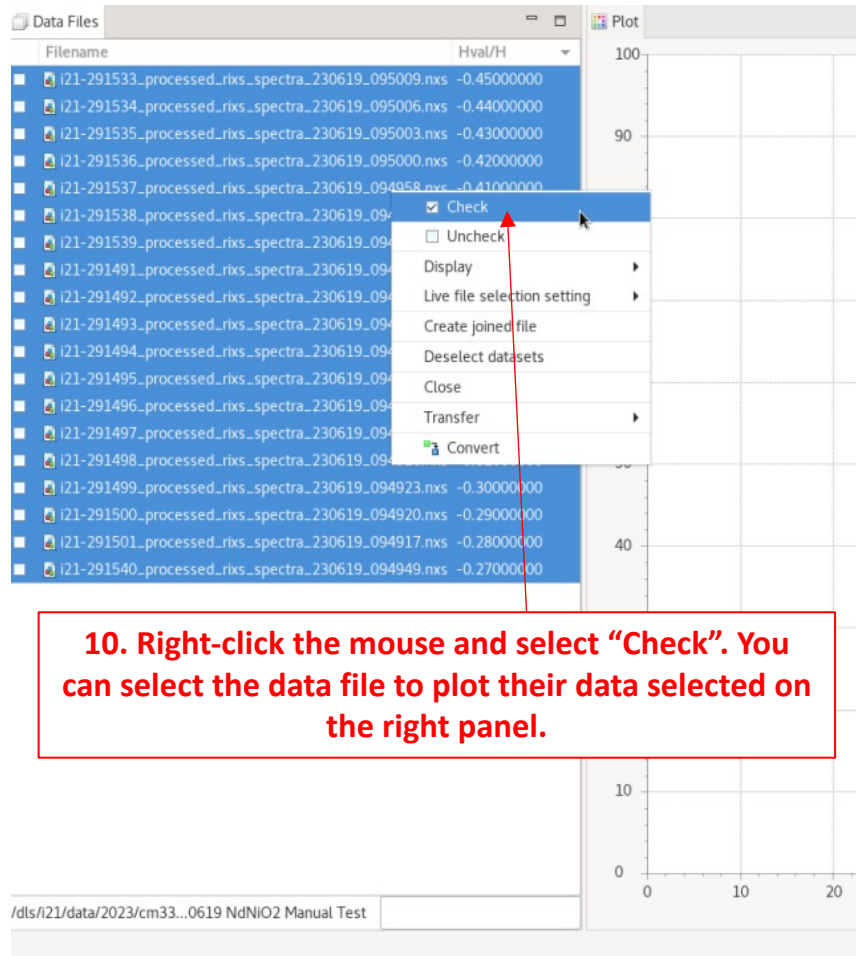
Dataset Name	Shape
<input type="checkbox"/> spectrum_0	[2, 1065]
<input type="checkbox"/> Log10 of Number of events	[1222]
<input type="checkbox"/> correlated_multiple_photon_spectr	[2, 4096]
<input type="checkbox"/> correlated_multiple_photon_spectr	[4096]
<input type="checkbox"/> correlated_shift_0	[2]
<input type="checkbox"/> correlated_single_photon_spectra	[2, 4096]
<input type="checkbox"/> correlated_single_photon_spectru	[4096]
<input type="checkbox"/> correlated_spectrum_0	[2, 1065]
<input type="checkbox"/> correlated_spectrum_0	[1065]
<input type="checkbox"/> counts_per_photon	[1]
<input type="checkbox"/> drain_current	[1]
<input type="checkbox"/> line_0_c	[1]
<input type="checkbox"/> line_1_m	[1]
<input type="checkbox"/> multiple_photon_count_0	[2]
<input type="checkbox"/> multiple_photon_minimum	[1]
<input type="checkbox"/> multiple_photon_spectra_0	[2, 4096]
<input type="checkbox"/> multiple_photon_spectrum_0	[4096]
<input checked="" type="checkbox"/> normalized_correlated_spectrum_0	[1065]
<input type="checkbox"/> photon_counts_0	[2]
<input type="checkbox"/> photon_positions_0	[28030]
<input type="checkbox"/> photon_values_0	[28030]
<input type="checkbox"/> single_events_fraction_0	[2]

* List of processed data

- **spectrum_0** : all individual RIXS spectra from each frame
- **correlated_spectrum_0**: a single RIXS spectra for each file that all individual RIXS spectra are correlated (this means, aligned and averaged)
- **normalization**: incident photon flux (m4c1)
- **normalized_correlated_spectrum_0**: correlated RIXS spectrum, normalized to the incident photon flux

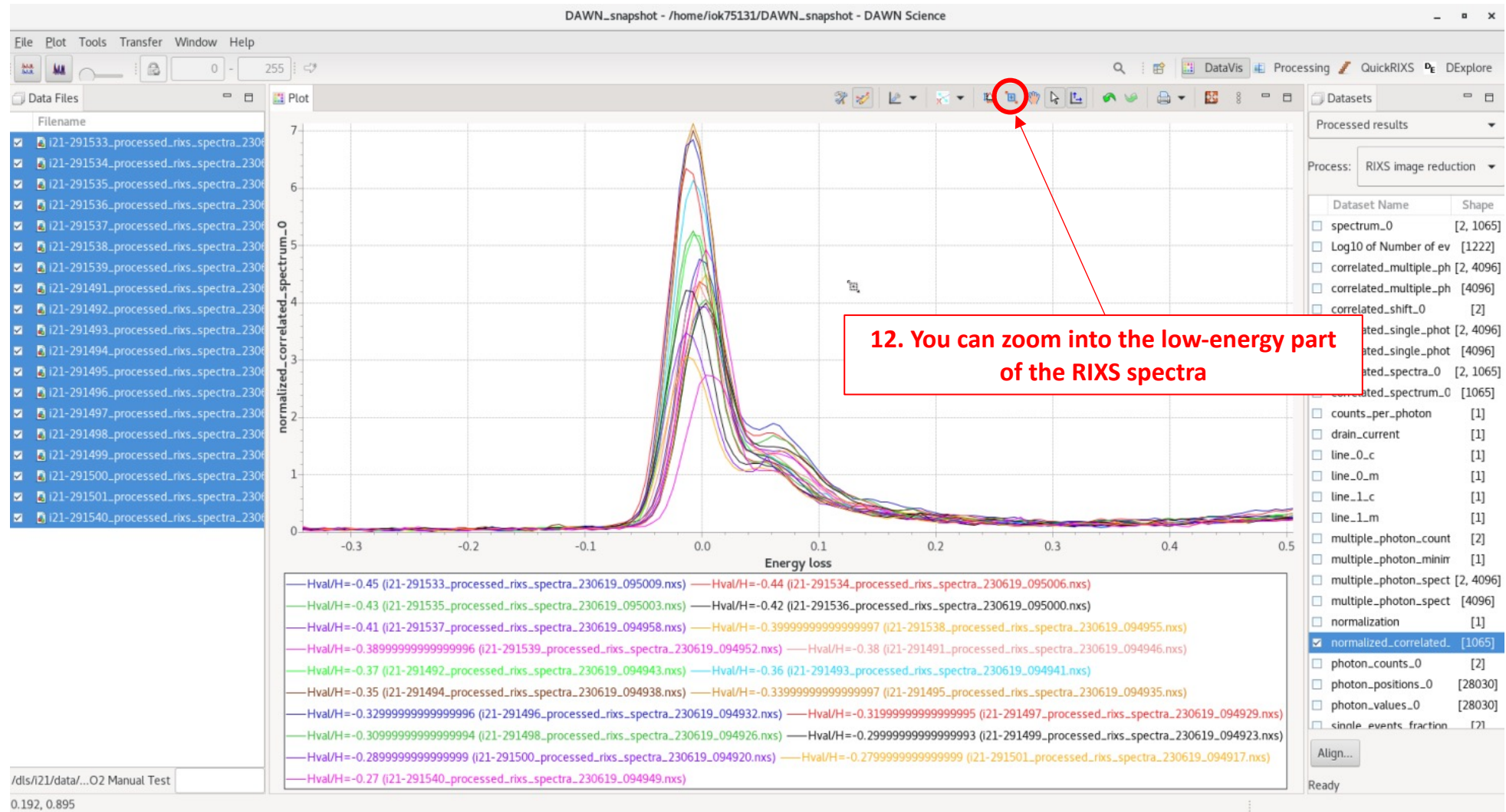
DATA VISUALIZATION

DataVis: Plot RIXS Spectra



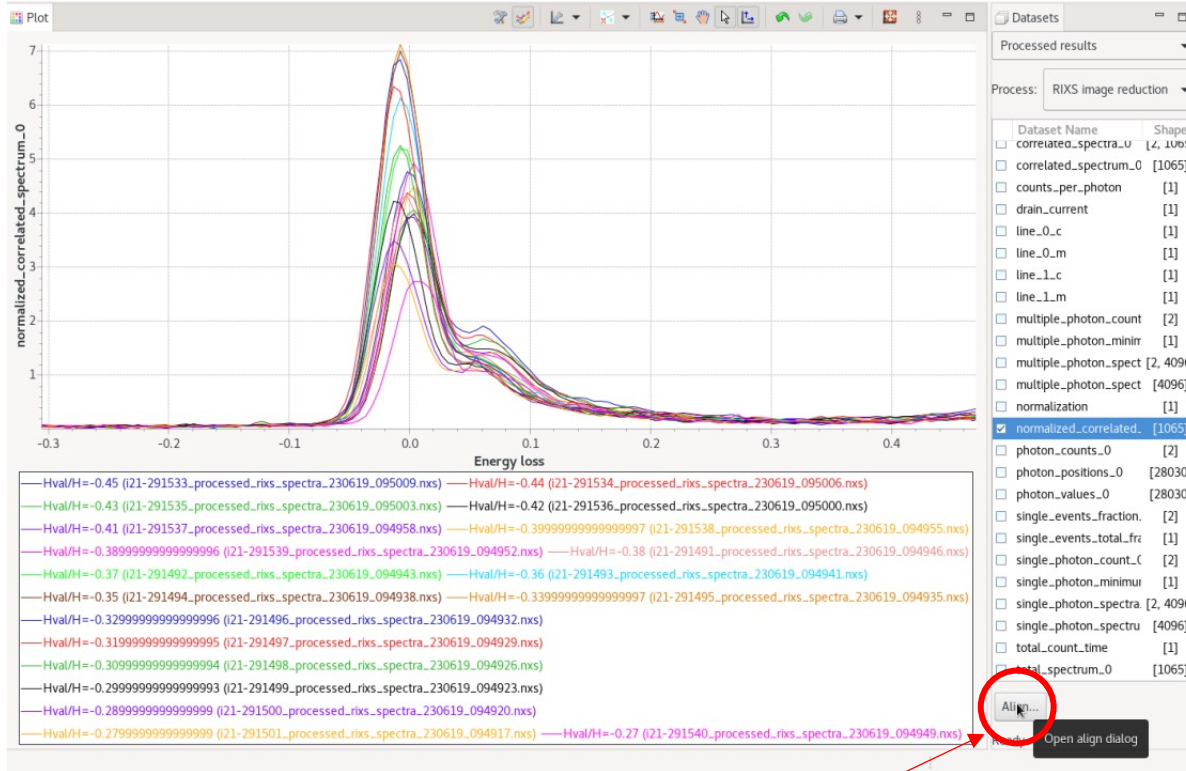
DATA VISUALIZATION

DataVis: Plot RIXS Spectra

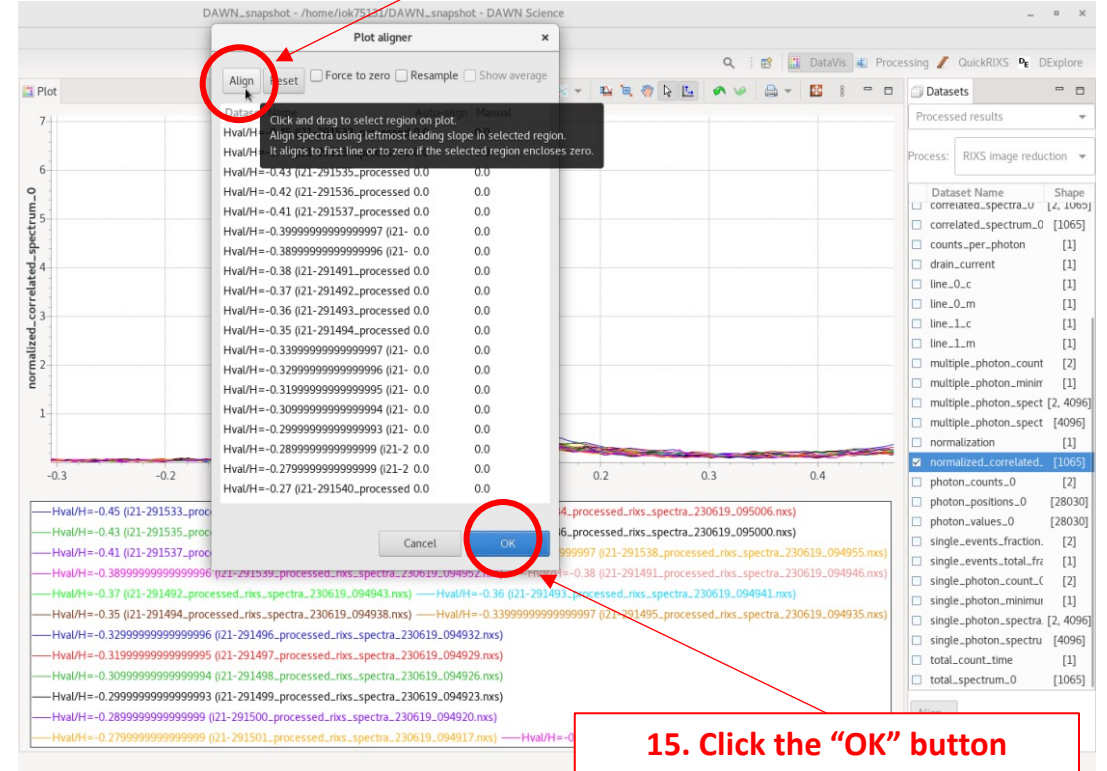


DATA VISUALIZATION

DataVis: Align the Elastic Peak



13. Click the "Align" button

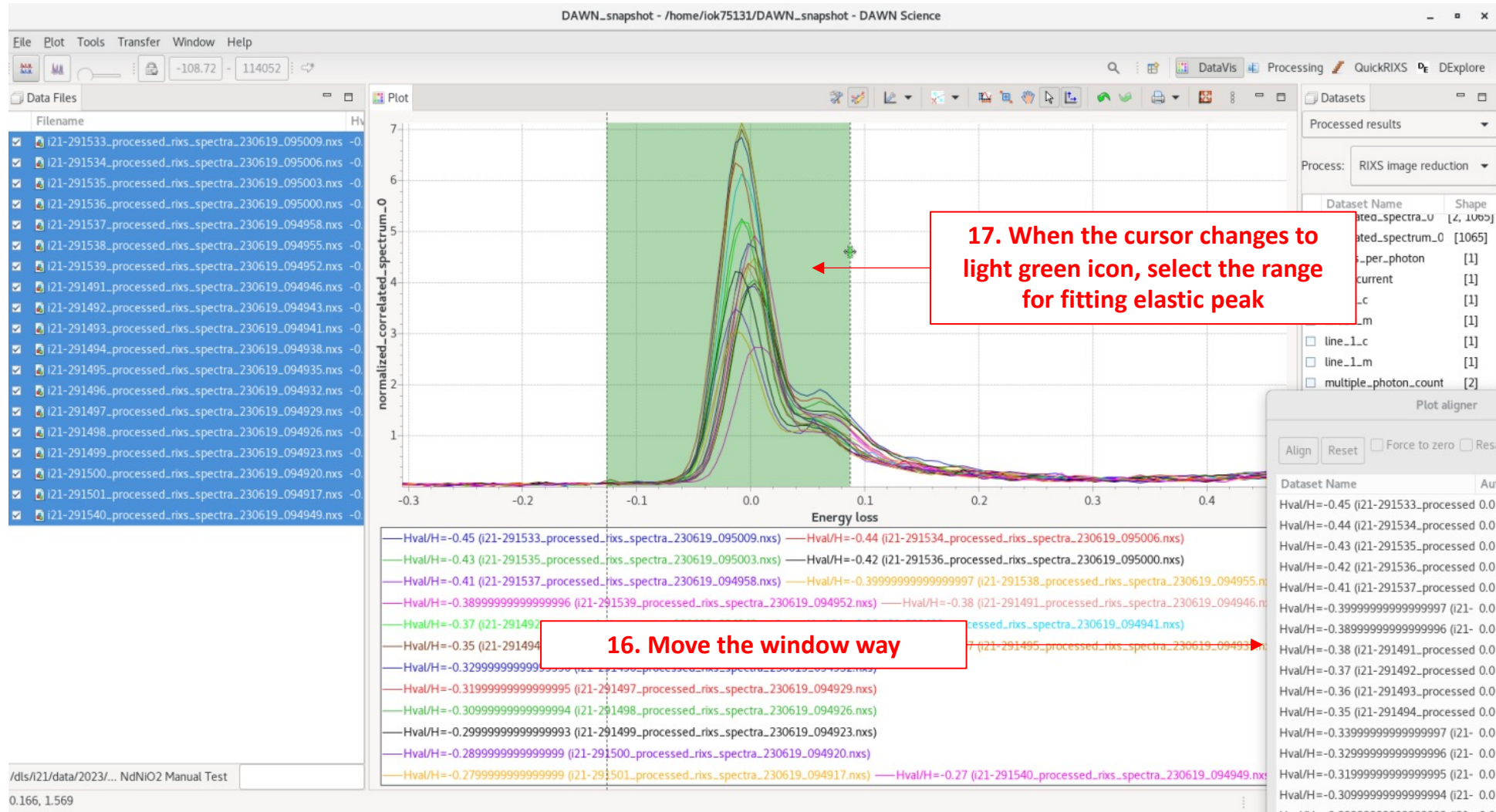


14. Click the "Align" button

15. Click the "OK" button

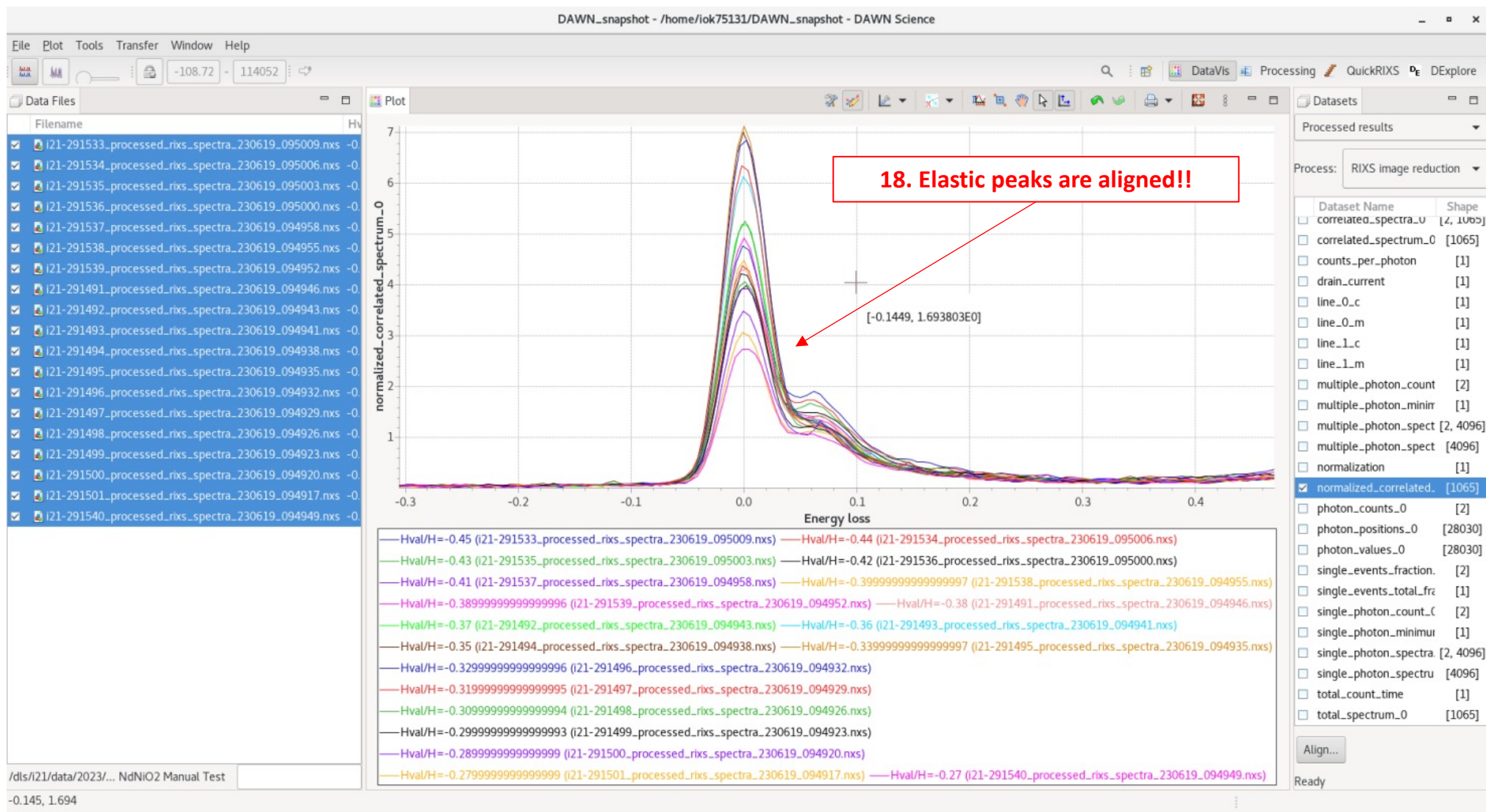
DATA VISUALIZATION

DataVis: Align the Elastic Peak



DATA VISUALIZATION

DataVis: Align the Elastic Peak



DATA VISUALIZATION

DataVis: Export the RIXS Spectra into Data Files

19. Click on the little arrow beside the printer

The screenshot displays the DAWN Science software interface. The main window shows a plot of normalized correlated spectra versus energy loss. The plot contains multiple overlapping curves, each representing a different scattering angle (Hval/H). The y-axis is labeled 'normalized_correlated_spectrum_0' and ranges from 0 to 7. The x-axis is labeled 'Energy loss' and ranges from -0.3 to 0.4. A legend at the bottom of the plot lists the Hval/H values for each curve, such as -0.45, -0.44, -0.43, etc., down to -0.27.

A context menu is open over the plot area, showing options for saving, copying, printing, and exporting data. The option 'Export plot data to tif/dat/csv...' is highlighted. A red arrow points from the text '19. Click on the little arrow beside the printer' to the printer icon in the menu. Another red arrow points from the text '20. Select "Export Plot Data to tif/dat/csv"' to the highlighted menu item.

The 'Data Files' panel on the left lists various processed RIXS spectra files. The 'Datasets' panel on the right shows a list of data series, with 'normalized_correlated_' selected.

20. Select "Export Plot Data to tif/dat/csv"

DATA VISUALIZATION

DataVis: Export the RIXS Spectra into Data Files

21. Click the “Browse to an external file” button to open the pop-up for the file path

Export Data

Export plotted data to file

File: /home/iok75131/DAWN_rixs/DAWN Manual/

Overwrite file if it already exists

Format: dat csv

Number of files: single multiple

single x column

Buttons: Cancel, Finish

Background Plot: normalized_correlated_spectrum_0 vs energy (e.g., -0.3 to 0.4)

Left Panel (Data Files):

- File: i21-291533_processed_rixs_spectra_230619_095009.nxs
- File: i21-291534_processed_rixs_spectra_230619_095006.nxs
- File: i21-291535_processed_rixs_spectra_230619_095003.nxs
- File: i21-291536_processed_rixs_spectra_230619_095000.nxs
- File: i21-291537_processed_rixs_spectra_230619_094958.nxs
- File: i21-291538_processed_rixs_spectra_230619_094955.nxs
- File: i21-291539_processed_rixs_spectra_230619_094952.nxs
- File: i21-291491_processed_rixs_spectra_230619_094946.nxs
- File: i21-291492_processed_rixs_spectra_230619_094943.nxs
- File: i21-291493_processed_rixs_spectra_230619_094941.nxs
- File: i21-291494_processed_rixs_spectra_230619_094938.nxs
- File: i21-291495_processed_rixs_spectra_230619_094935.nxs
- File: i21-291496_processed_rixs_spectra_230619_094932.nxs
- File: i21-291497_processed_rixs_spectra_230619_094929.nxs
- File: i21-291498_processed_rixs_spectra_230619_094926.nxs
- File: i21-291499_processed_rixs_spectra_230619_094923.nxs
- File: i21-291500_processed_rixs_spectra_230619_094920.nxs
- File: i21-291501_processed_rixs_spectra_230619_094917.nxs
- File: i21-291540_processed_rixs_spectra_230619_094949.nxs

Right Panel (Process: RIXS image reduction):

- Dataset Name: correlated_spectrum_u [4, 1065]
- Dataset Name: correlated_spectrum_0 [1065]
- Dataset Name: counts_per_photon [1]
- Dataset Name: drain_current [1]
- Dataset Name: line_0_c [1]
- Dataset Name: line_0_m [1]
- Dataset Name: line_1_c [1]
- Dataset Name: line_1_m [1]
- Dataset Name: multiple_photon_count [2]
- Dataset Name: multiple_photon_minir [1]
- Dataset Name: multiple_photon_spect [2, 4096]
- Dataset Name: multiple_photon_spect [4096]
- Dataset Name: normalization [1]
- Dataset Name: normalized_correlated_ [1065]
- Dataset Name: photon_counts_0 [2]
- Dataset Name: photon_positions_0 [28030]
- Dataset Name: photon_values_0 [28030]
- Dataset Name: single_events_fraction [2]
- Dataset Name: single_events_total_frc [1]
- Dataset Name: single_photon_count_c [2]
- Dataset Name: single_photon_minimur [1]
- Dataset Name: single_photon_spectra [2, 4096]
- Dataset Name: single_photon_spectru [4096]
- Dataset Name: total_count_time [1]
- Dataset Name: total_spectrum_0 [1065]

Bottom Panel (Legend):

- Hval/H=-0.45 (i21-291533_processed_rixs_spectra_230619_095009.nxs)
- Hval/H=-0.44 (i21-291534_processed_rixs_spectra_230619_095006.nxs)
- Hval/H=-0.43 (i21-291535_processed_rixs_spectra_230619_095003.nxs)
- Hval/H=-0.42 (i21-291536_processed_rixs_spectra_230619_095000.nxs)
- Hval/H=-0.41 (i21-291537_processed_rixs_spectra_230619_094958.nxs)
- Hval/H=-0.39999999999999999 (i21-291538_processed_rixs_spectra_230619_094955.nxs)
- Hval/H=-0.38999999999999999 (i21-291539_processed_rixs_spectra_230619_094952.nxs)
- Hval/H=-0.38 (i21-291491_processed_rixs_spectra_230619_094946.nxs)
- Hval/H=-0.37 (i21-291492_processed_rixs_spectra_230619_094943.nxs)
- Hval/H=-0.36 (i21-291493_processed_rixs_spectra_230619_094941.nxs)
- Hval/H=-0.35 (i21-291494_processed_rixs_spectra_230619_094938.nxs)
- Hval/H=-0.33999999999999999 (i21-291495_processed_rixs_spectra_230619_094935.nxs)
- Hval/H=-0.32999999999999999 (i21-291496_processed_rixs_spectra_230619_094932.nxs)
- Hval/H=-0.31999999999999999 (i21-291497_processed_rixs_spectra_230619_094929.nxs)
- Hval/H=-0.30999999999999999 (i21-291498_processed_rixs_spectra_230619_094926.nxs)
- Hval/H=-0.29999999999999999 (i21-291499_processed_rixs_spectra_230619_094923.nxs)
- Hval/H=-0.28999999999999999 (i21-291500_processed_rixs_spectra_230619_094920.nxs)
- Hval/H=-0.27999999999999999 (i21-291501_processed_rixs_spectra_230619_094917.nxs)
- Hval/H=-0.27 (i21-291540_processed_rixs_spectra_230619_094949.nxs)

Bottom Left: /dls/i21/data/2023/... NdNiO2 Manual Test

Bottom Left: 0.354, 6.023

Bottom Right: Ready

DATA VISUALIZATION

DataVis: Export the RIXS Spectra into Data Files

22. Move to the folder where you want to save the data files, and write the filename. In the case that you create multiple files, the identifier “-##” (## is a numbering of data files) will be automatically added.

File Plot Tools Transfer Window Help

Name testRIXS_data Save

lok75131 DAWN_rixs DAWN Manual data

Cancel

Home Desktop Documents Downloads Music Pictures Videos mm29316-1 Other Locations

Filename

i21-291533_processed_rixs_spectra_230619

i21-291534_processed_rixs_spectra_230619

i21-291535_processed_rixs_spectra_230619

i21-291536_processed_rixs_spectra_230619

i21-291537_processed_rixs_spectra_230619

i21-291538_processed_rixs_spectra_230619

i21-291539_processed_rixs_spectra_230619

i21-291491_processed_rixs_spectra_230619

i21-291492_processed_rixs_spectra_230619

i21-291493_processed_rixs_spectra_230619

i21-291494_processed_rixs_spectra_230619

i21-291495_processed_rixs_spectra_230619

i21-291496_processed_rixs_spectra_230619

i21-291497_processed_rixs_spectra_230619

i21-291498_processed_rixs_spectra_230619

i21-291499_processed_rixs_spectra_230619

i21-291500_processed_rixs_spectra_230619

i21-291501_processed_rixs_spectra_230619

i21-291540_processed_rixs_spectra_230619

Processing QuickRIXS DExplore

Datasets

Processed results

Process: RIXS image reduction

set Name Shape

lated_spectra_u [4, 1065]

lated_spectrum_0 [1065]

ts_per_photon [1]

current [1]

line_0_c [1]

line_0_m [1]

line_1_c [1]

line_1_m [1]

multiple_photon_count [2]

multiple_photon_minir [1]

multiple_photon_spect [2, 4096]

multiple_photon_spect [4096]

normalization [1]

normalized_correlated_ [1065]

photon_counts_0 [2]

photon_positions_0 [28030]

photon_values_0 [28030]

single_events_fraction [2]

single_events_total_fr [1]

single_photon_count_c [2]

single_photon_minimur [1]

single_photon_spectra [2, 4096]

single_photon_spectru [4096]

total_count_time [1]

total_spectrum_0 [1065]

Align...

Ready

— Hval/H=-0.30999999999999994 (i21-291498_processed_rixs_spectra_230619_094926.nxs)

— Hval/H=-0.29999999999999993 (i21-291499_processed_rixs_spectra_230619_094923.nxs)

— Hval/H=-0.28999999999999999 (i21-291500_processed_rixs_spectra_230619_094920.nxs)

— Hval/H=-0.27999999999999999 (i21-291501_processed_rixs_spectra_230619_094917.nxs) — Hval/H=-0.27 (i21-291540_processed_rixs_spectra_230619_094949.nxs)

/dts/i21/data/2023/... NdNIO2 Manual Test

0.354, 6.023

DATA VISUALIZATION

DataVis: Export the RIXS Spectra into Data Files

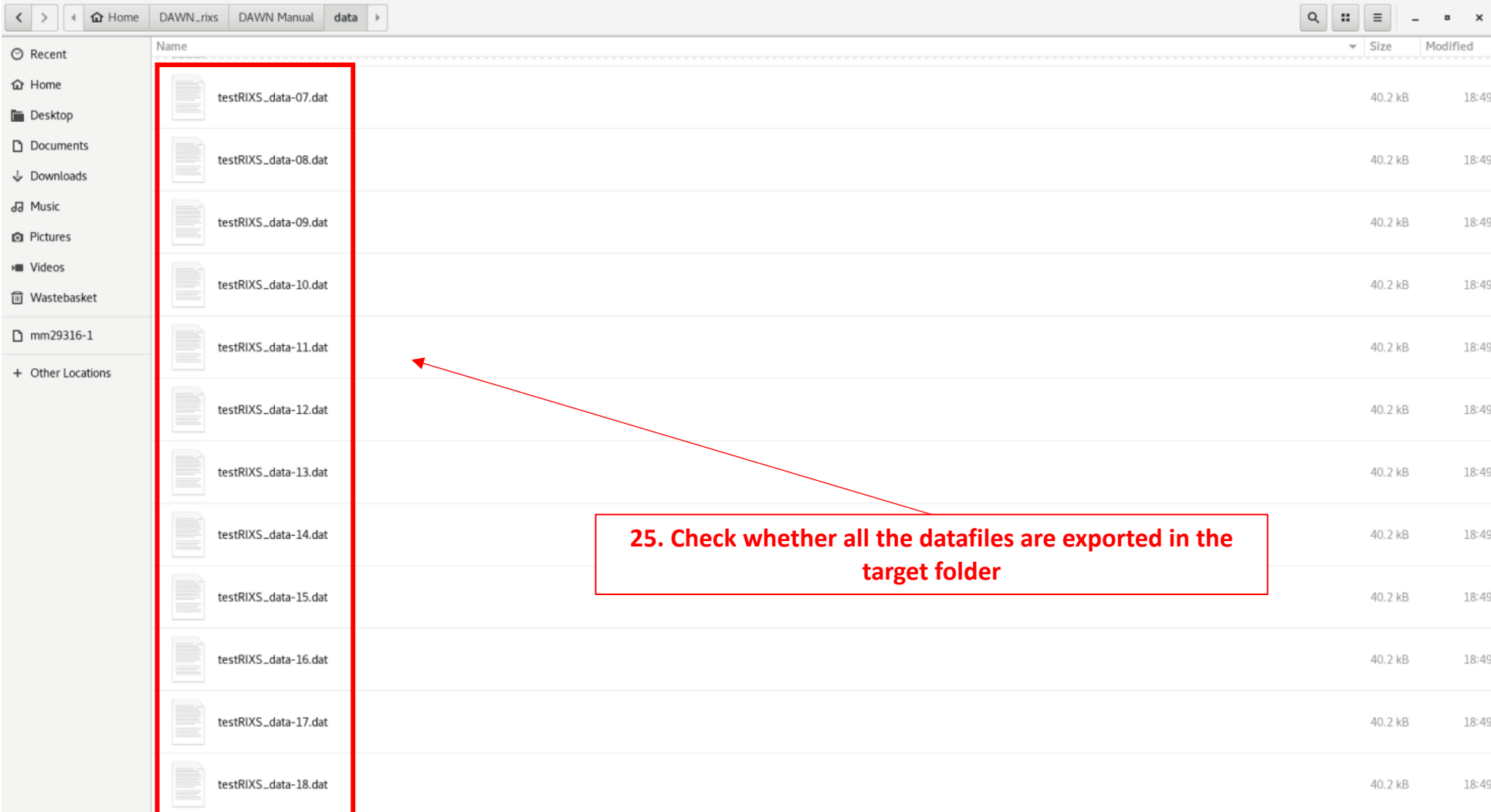
23. Select the file format

24-1. You can also choose "single" option. In this case, X (energy loss) and Y (RIXS Intensity) columns of all data files are stored in a single data file.

24. You can export the files as multiple files having XY columns or a single file as multiple XY column. In the case that you create multiple files, the identifier "-##" (## is a numbering of data files) will be automatically added.

DATA VISUALIZATION

DataVis: Export the RIXS Spectra into Data Files



The screenshot shows a file explorer window with the following table of files:

Name	Size	Modified
testRIXS_data-07.dat	40.2 kB	18:49
testRIXS_data-08.dat	40.2 kB	18:49
testRIXS_data-09.dat	40.2 kB	18:49
testRIXS_data-10.dat	40.2 kB	18:49
testRIXS_data-11.dat	40.2 kB	18:49
testRIXS_data-12.dat	40.2 kB	18:49
testRIXS_data-13.dat	40.2 kB	18:49
testRIXS_data-14.dat	40.2 kB	18:49
testRIXS_data-15.dat	40.2 kB	18:49
testRIXS_data-16.dat	40.2 kB	18:49
testRIXS_data-17.dat	40.2 kB	18:49
testRIXS_data-18.dat	40.2 kB	18:49

A red box highlights the first 10 files (testRIXS_data-07.dat to testRIXS_data-16.dat). A red arrow points from a red box containing the text "25. Check whether all the datafiles are exported in the target folder" to the 11th file (testRIXS_data-11.dat).

APPENDIX

Additional Information and Troubleshooting