

Introduction to ADLER:
Advanced Data Loading, Evaluation and Reduction software
for the PEAXIS instrument at Helmholtz Zentrum Berlin

Version 2.1
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PEAXIS Data Files



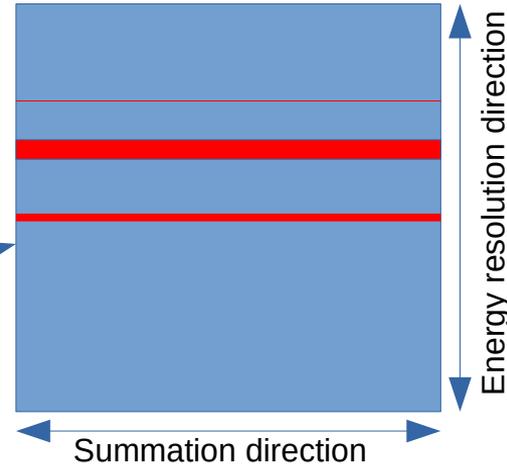
2048x2048
pixels

A single measurement

Detector Image (2D array)
SIF format, binary

Data Header file
.dat extension, text format

Parameter log
.xas extension, text format



Nominal values of photon energy, sample position, instrument parameters...

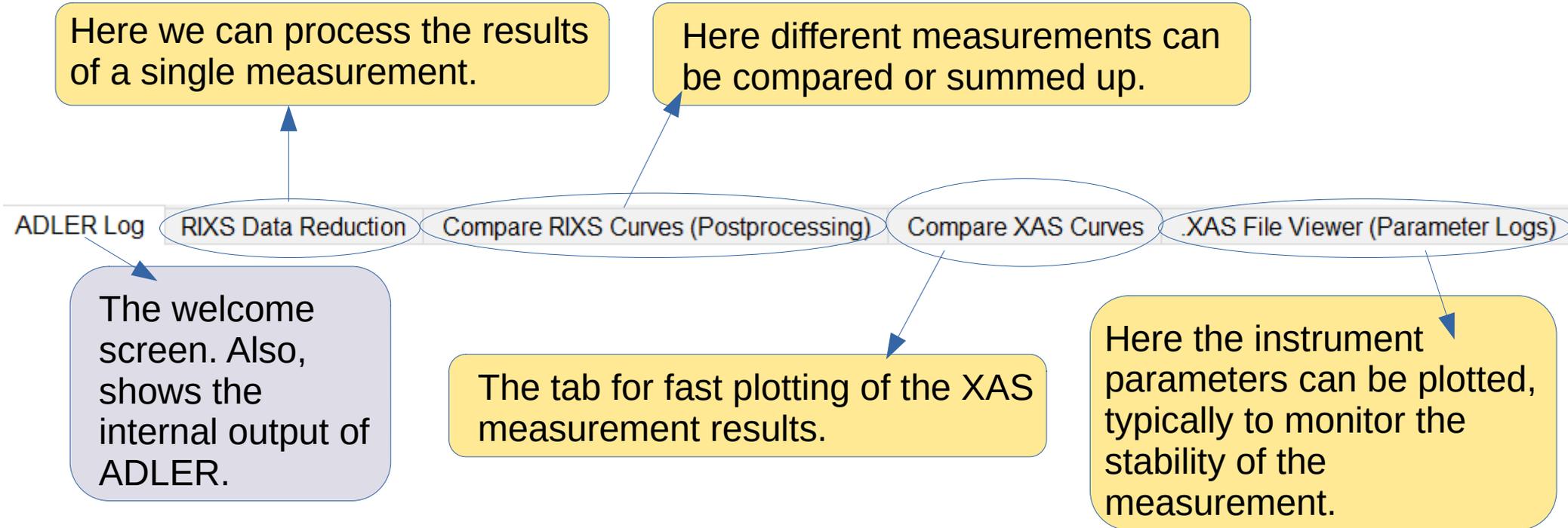
Real parameter values logged as a function of time, every N seconds.

... ADLER reads them all.

Work flow in ADLER

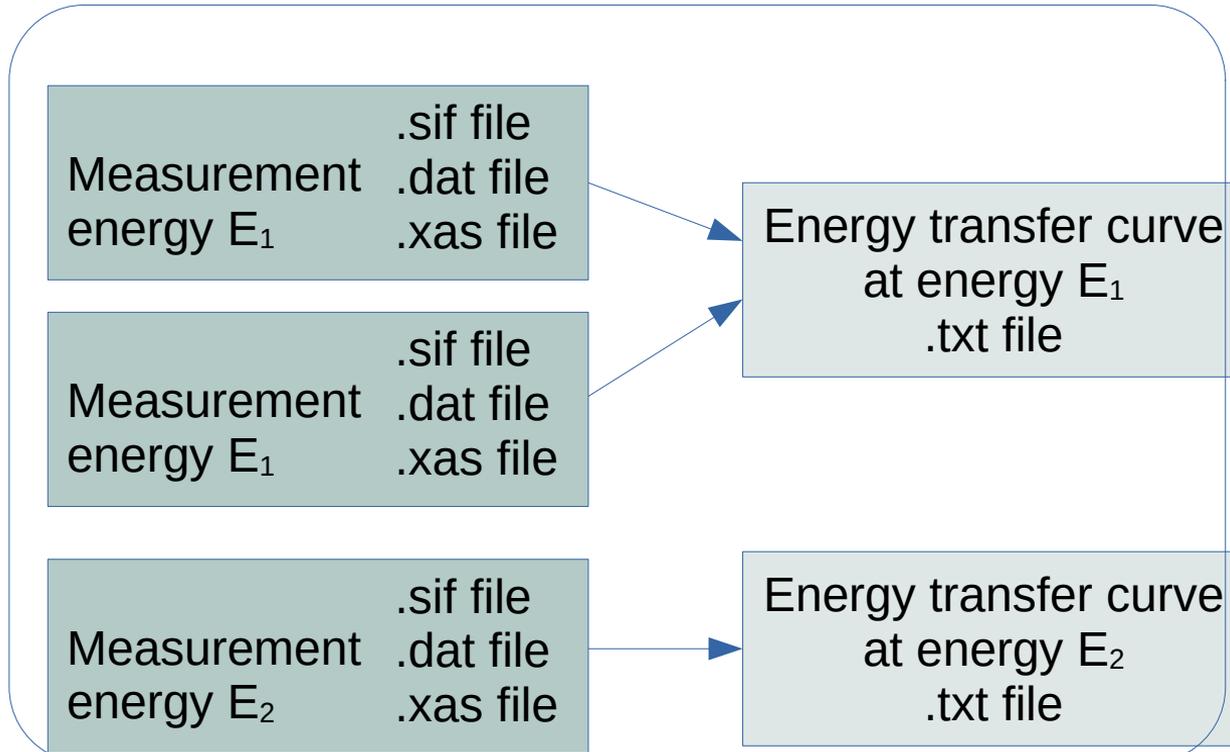


The interface is divided into tabs. These are intended for everyday use:

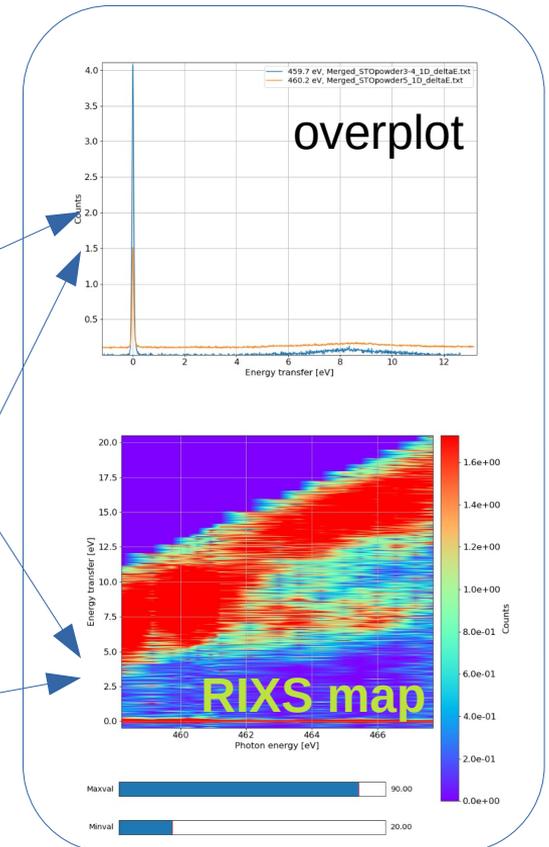




“RIXS data reduction” tab



“Compare RIXS curves” tab



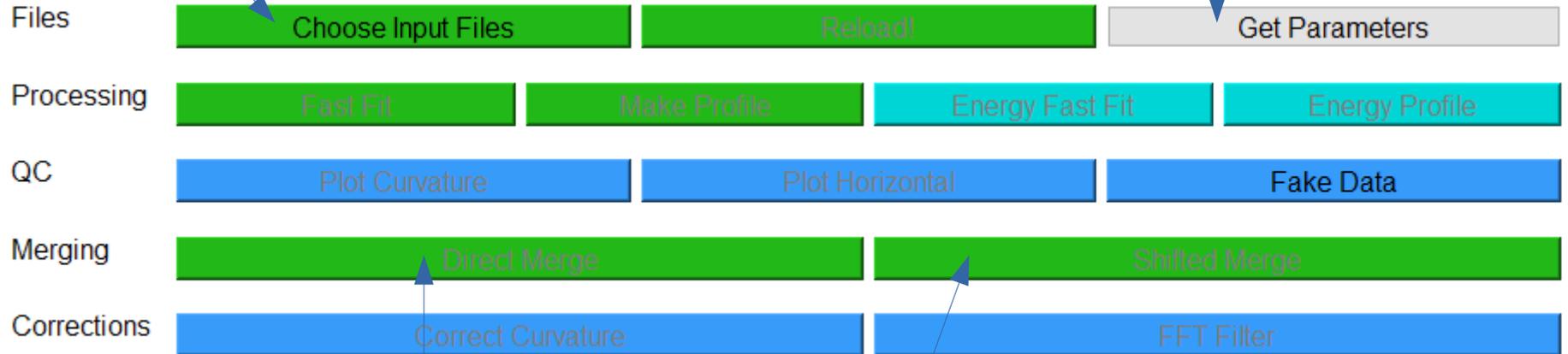
Working with the RIXS Data Reduction tab



Typical data reduction procedure:

Step 1: Load some SIF files.

Step 0: load parameters from another ADLER output file.



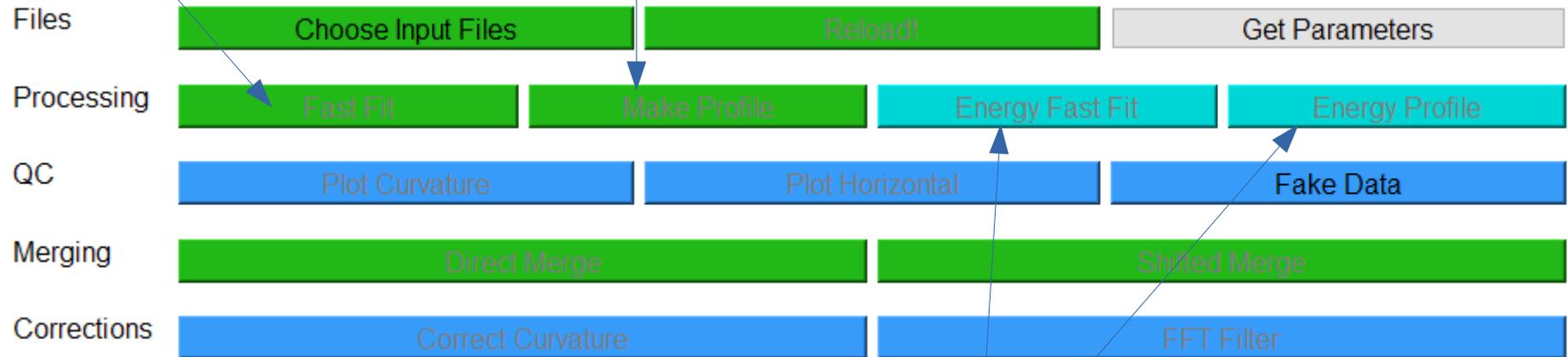
Step 1a: Choose how to merge the SIF files (if you picked more than one).



Typical data reduction procedure:

Step 2: Convert the 2D data array to a 1D profile using automatic parameters.

Step 3: Adjust parameters, create a better profile.



Step 4: Convert the data to energy transfer units.

Secret move!

If your energy calibration is defined, and you set elastic line limits to be outside of range, the Energy Profile button will output a text file of your spectrum with the **x-axis in the absolute energy units** (instead of energy transfer).

The screenshot displays the ADLER software interface. At the top right, the text "U7D" is visible next to a stick figure icon. The interface is divided into several sections:

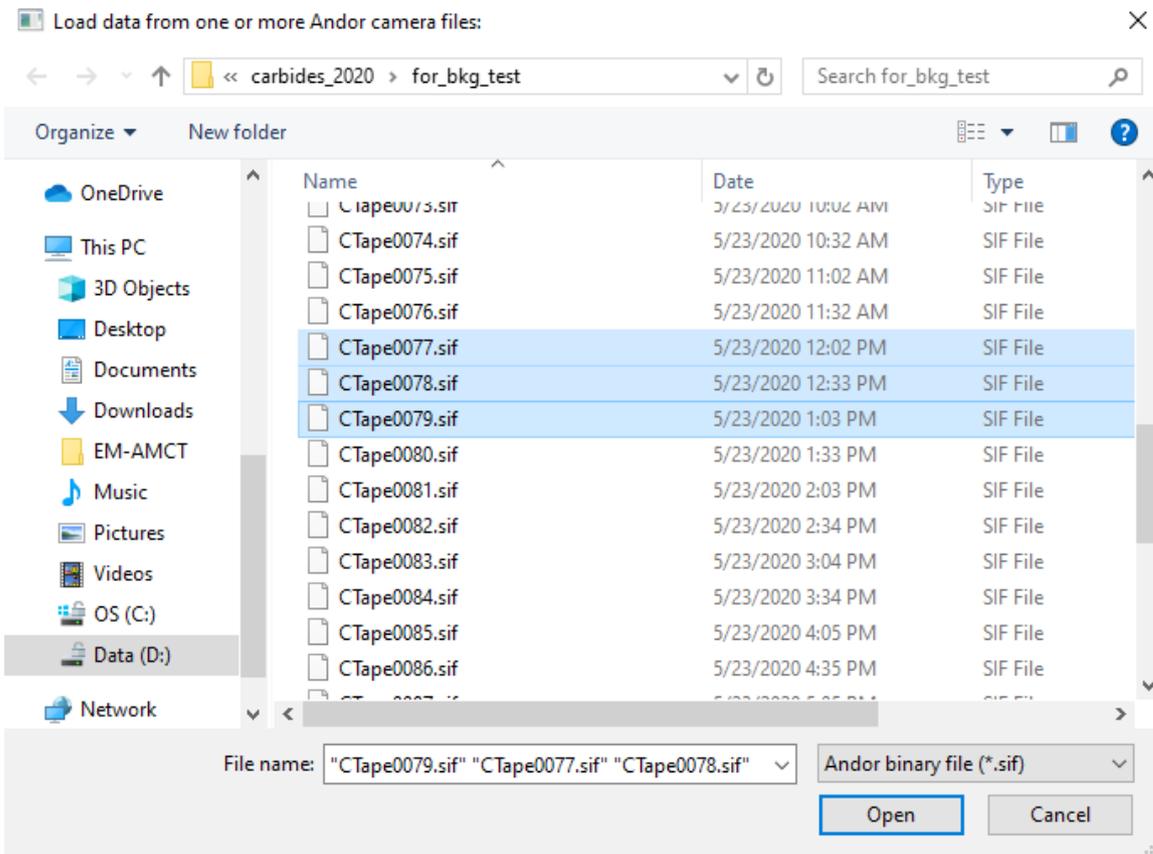
- Elastic Line** (highlighted with a dashed orange box):
 - Elastic line limits: Two input boxes containing "-1" and "-1", followed by the unit "pixel".
 - Detection limit for BKG: An input box containing "55.0", followed by the unit "percentile".
 - Curvature segment size: An input box containing "16", followed by the unit "pixel".
- Energy Calibration** (highlighted with a dashed orange box):
 - Energy calibration pair 1: Two input boxes containing "1073.96" and "458.05", followed by the unit "pixel, eV".
 - Energy calibration pair 2: Two input boxes containing "575.936" and "465.8", followed by the unit "pixel, eV".

Below the parameter settings is a workflow menu with the following categories and buttons:

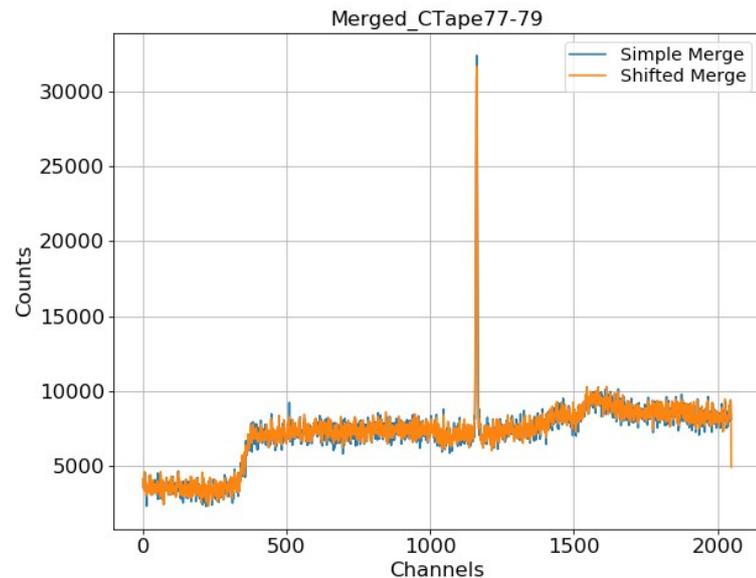
- Files**: Choose Input Files (green), Reload! (green), Get Parameters (grey).
- Processing**: Fast Fit (green), Make Profile (green), Energy Fast Fit (cyan), Energy Profile (cyan).
- QC**: Plot Curvature (blue), Plot Horizontal (blue), Fake Data (blue).
- Merging**: Direct Merge (green), Shifted Merge (green).
- Corrections**: Correct Curvature (blue), FFT Filter (blue).

A dashed orange box highlights the "Energy Fast Fit" and "Energy Profile" buttons in the Processing row. A blue arrow points from the stick figure icon in the top right corner to the "Energy Profile" button.

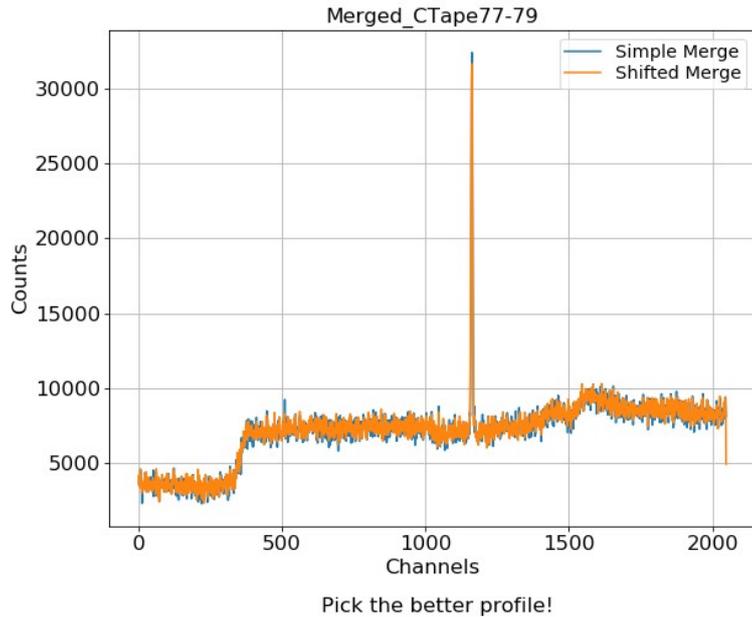
File loading



One or more files can be marked for loading.



Pick the better profile!



If more than one file was chosen for loading, the 2D data arrays will be **summed up** into a single 2D image.

To compensate for a possible shift of position, a “**shifted merge**” option is available, where the 2D arrays are offset along the vertical direction to minimise the differences between images.

In the ideal case, both merging methods will produce the same results, and “direct merging” can be used.

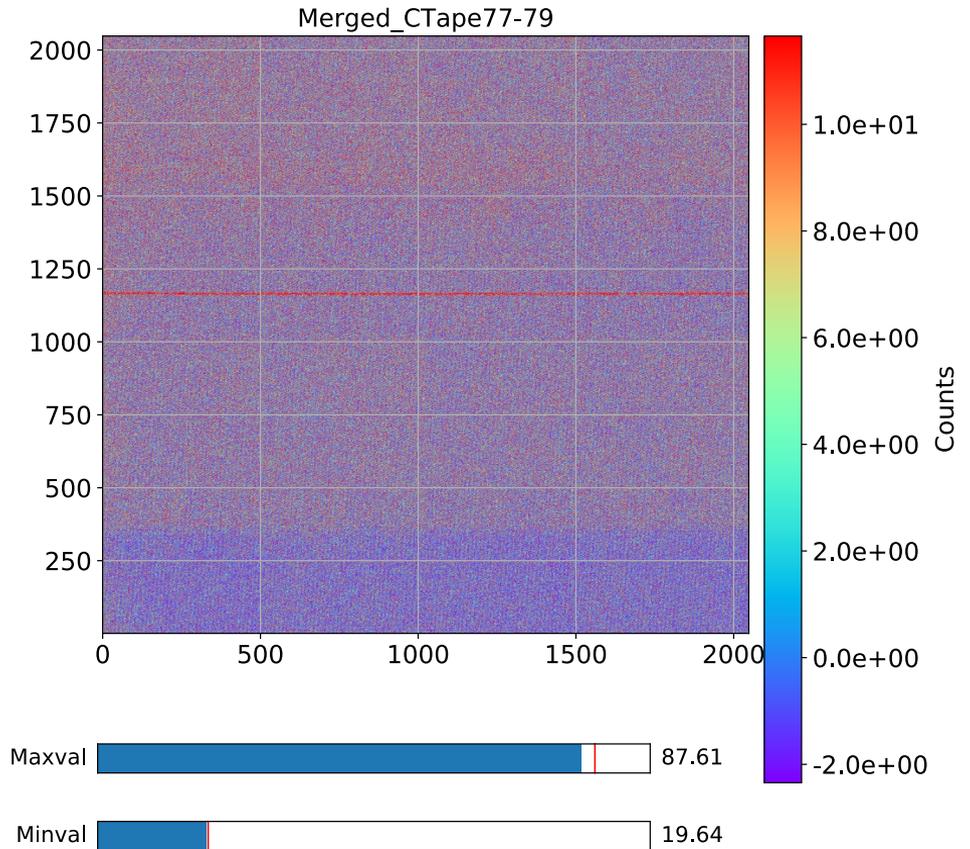
Please keep in mind that you can also process each file separately, and then merge them into a single curve in the Post-processing tab.



Once the files have been combined, you will see the 2D array of the detector data.

Normally, all you want to do now is to sum up the pixels along the horizontal direction, and convert the pixel positions along the vertical direction into energy units.

Additionally, the fitting of the elastic line with a Gaussian function will provide information on the instrument resolution.





Normally, there should be no need to change the file loading parameters. If you do want to change them anyway, a quick description is given here.

To narrow down the detector are that is summed up into the profile, you can change these limits. Detector cutoff 100-1950 will remove a 100 pixels on the left side, and 98 pixels on the right.

File Loading			
Detector cutoff	<input type="text" value="0"/>	<input type="text" value="2048"/>	pixel
Background per pixel	<input type="text" value="960.78154"/>		counts
Time-dependent background	<input type="text" value="1.0"/>		fraction
Cosmic ray correction factor	<input type="text" value="3.0"/>		StdDev

Cosmic rays appear locally in narrow regions of the detector. To remove them, we calculate the **mean value M** and **standard deviation S** of each row of pixels. Then, every individual pixel with a value more than $n \times S$ away from **M** is replaced with **M**. The **n** factor can be adjusted here; the lower the **n**, the more pixels will be discarded.



Normally, there should be no need to change the file loading parameters. If you do want to change them anyway, a quick description is given here.

The detector has a constant base line of the background. The number given here will be subtracted from every single pixel.

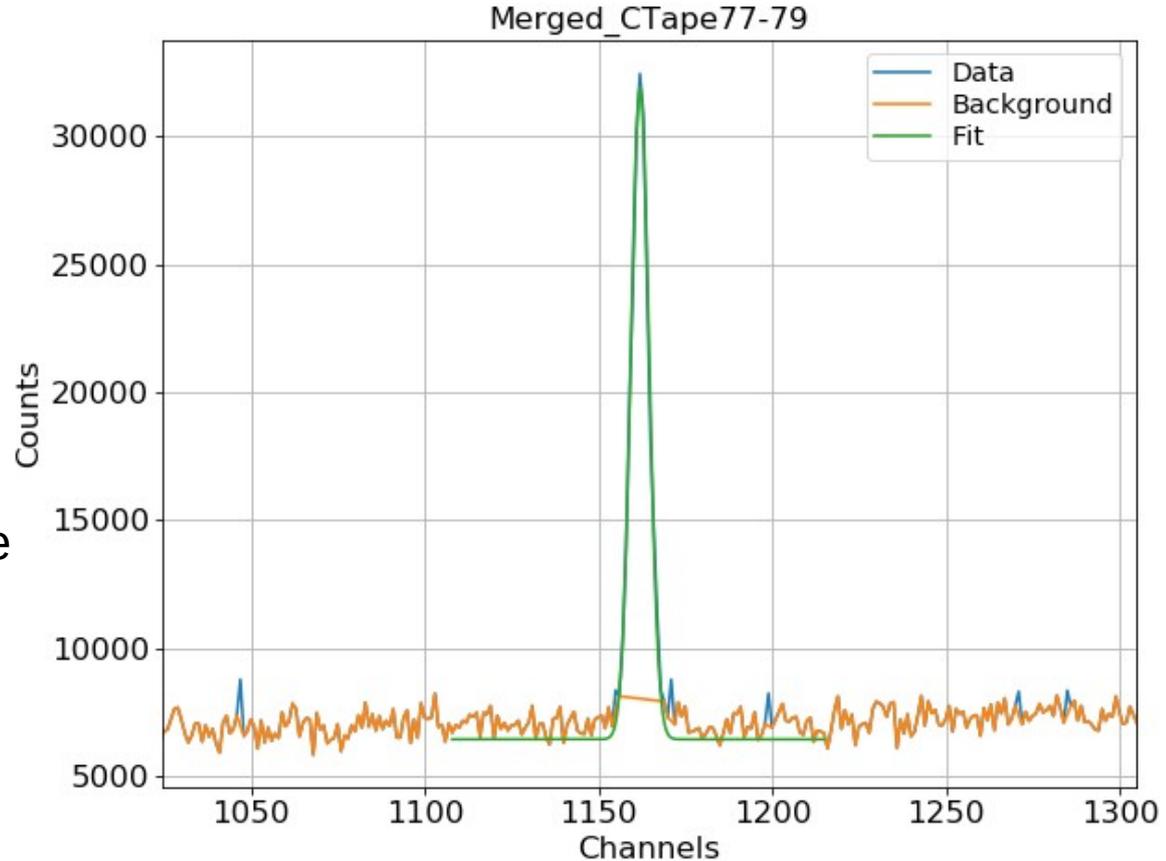
File Loading			
Detector cutoff	<input type="text" value="0"/>	<input type="text" value="2048"/>	pixel
Background per pixel	<input type="text" value="960.78154"/>		counts
Time-dependent background	<input type="text" value="1.0"/>		fraction
Cosmic ray correction factor	<input type="text" value="3.0"/>		StdDev

The detector has a weak, time-dependent background of dark current. This has been measured and can be subtracted from the data, scaled by the “time-dependent background” factor. Factor 0 means no subtraction, factor 1 means correct subtraction (and other values, although possible, are difficult to justify...)



It is important to determine the position of the elastic line correctly, as it will define the position of the 0 eV energy transfer value once you convert to the energy scale.

If you use “Fast Fit”, ADLER will try to guess the elastic line position. It will pick the pixel with the highest counts as the elastic line position, or, if energy calibration is provided, it will calculate the position based on the photon energy.



FWHM = 6.091 +/- 0.119
centre = 1162.011 +/- 0.051
area = 164993.107 +/- 4275.511



You can specify by hand the lower and upper limits of detector pixel range where ADLER will look for the elastic line. These will **only** be used if you press “Make Profile” or “Make Energy Profile”.

Elastic Line			
Elastic line limits	<input type="text" value="0"/>	<input type="text" value="2048"/>	pixel
Detection limit for BKG	<input type="text" value="75.0"/>		percentile
Curvature segment size	<input type="text" value="16"/>		pixel
Energy Calibration			
Energy calibration pair 1	<input type="text" value="-1.0"/>	<input type="text" value="-1.0"/>	pixel, eV
Energy calibration pair 2	<input type="text" value="-1.0"/>	<input type="text" value="-1.0"/>	pixel, eV

The background used in the fitting procedure is **constant** and determined by this parameter. ADLER will take all the points within the Nth percentile, and take their mean value as the background value. This is necessary, as inelastic features are commonly present next to the elastic line and would interfere with the fitting of the background.

Elastic line fitting parameters



To calibrate the energy scale of the instrument, two measurements at different photo energy are needed, where the elastic line is clearly visible. After fitting the elastic line positions in both of them, you can input the elastic line position on the detector (in pixels) and the corresponding photon energy (in eV). Then every pixel on the detector can be assigned an energy value using a linear function.

Elastic Line			
Elastic line limits	<input type="text" value="0"/>	<input type="text" value="2048"/>	pixel
Detection limit for BKG	<input type="text" value="75.0"/>		percentile
Curvature segment size	<input type="text" value="16"/>		pixel
Energy Calibration			
Energy calibration pair 1	<input type="text" value="-1.0"/>	<input type="text" value="-1.0"/>	pixel, eV
Energy calibration pair 2	<input type="text" value="-1.0"/>	<input type="text" value="-1.0"/>	pixel, eV

You can create an energy profile out of your data only after you have input a valid energy calibration.

Data correction parameters



You are not likely to ever use the parameters shown here, but they are documented for completeness.

If you are worried about a periodic/stripy pattern on the detector, you can try to filter it out by applying Fourier transforms to the data. You are welcome to try it out for fun, but the risk of removing something important from the data is high.

The elastic line is not perfectly horizontal on the detector. You can fit the curvature with a quadratic polynomial and shift all the detector pixels to correct for the curvature. The improvement to the resolution is usually minimal.

If you do not need high resolution, you can reduce the number of pixels, and at the same time the overall noise in the data.

Corrections				
Curvature Correction	<input type="text" value="-100.0"/>	<input type="text" value="-100.0"/>	<input type="text" value="-100.0"/>	N/A
Removed FFT region	<input type="text" value="-1000000000.0"/>	<input type="text" value="-1000000000.0"/>		N/A
Reduction factor	<input type="text" value="1.0"/>			N/A

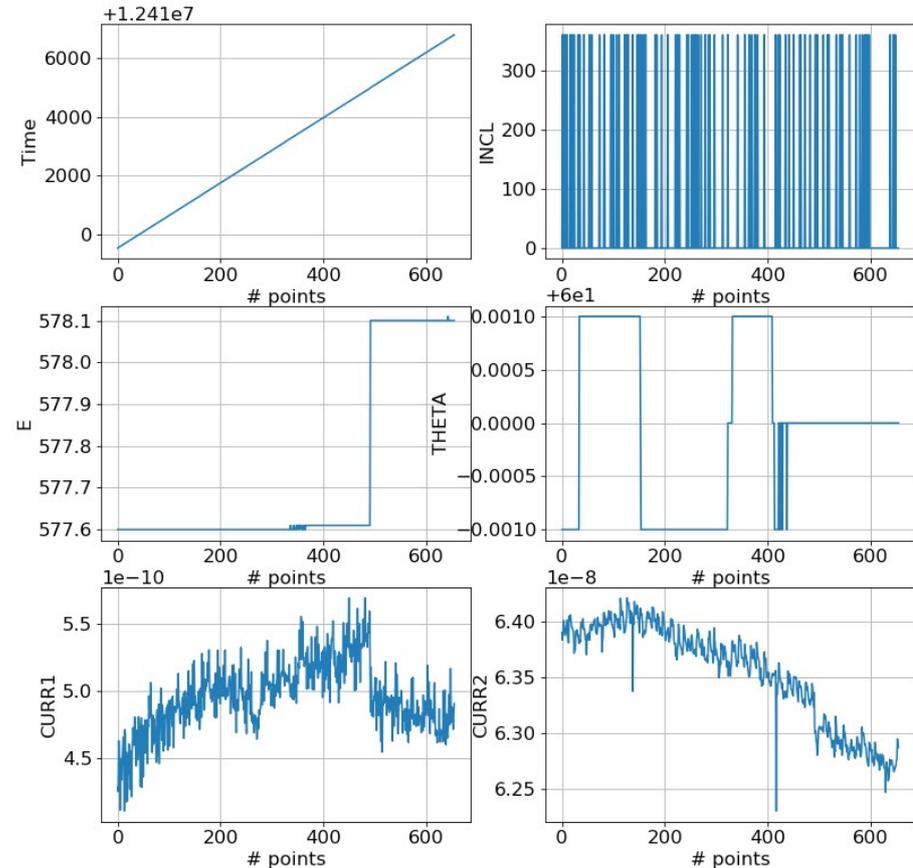
Monitor the stability of parameters in Variable Viewer.



Every time you load one or more SIF files, the corresponding .xas files are read as well and the data points are sorted based on their individual time stamps.

You can plot the values and verify if the instrument and sample were always in the state you expected.

Please note that you can also **load the .xas files directly** in this tab, without loading the corresponding SIF files.



Monitor the stability of parameters in Variable Viewer.



You can choose which data set will be used as the X axis for plotting. Many of the parameters are pretty much guaranteed to form a flat line in the plot, so plotting them as a function of step number or time is usually a good way to start.

Plotting

Plot 1D Plot Grid

Data Handling

Clear List Load Logs Directly

	1	2	3	4	5	6
1	Name	Length	Xlimits	Plot it?	Set as X	Set as Y
2	Step	656	1.0,164.0	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
3	Time	656	12409550.0,124...	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
4	XPOS	656	2.9755,2.9755	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
5	YPOS	656	5.1931,5.1931	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
6	ZPOS	656	-29.496,-29.496	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
7	INCL	656	0.0,360.0	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
8	ROT	656	-3.5,-3.5	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
9	ZDIR	656	30.1,30.1	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
10	E	656	577.6,578.11	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
11	THETA	656	59.999,60.001	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
12	CURR1	656	4....	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

Plotting

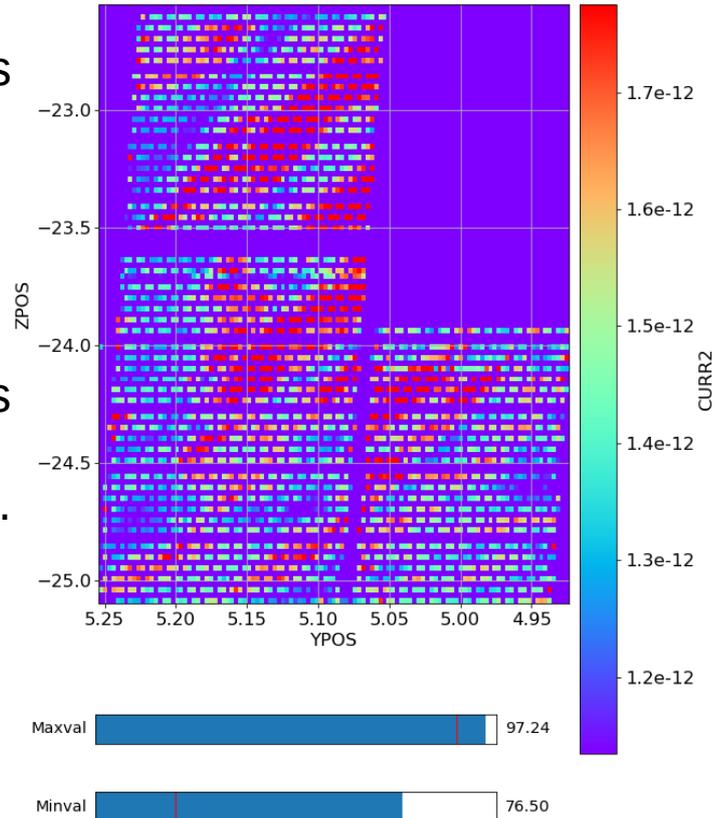
Multiplet offset maximum rel. intensity

Legend position N/A

Monitor the stability of parameters in Variable Viewer.



If you are using the continuous motion feature of PEAXIS, your sample will be moving all the time during the RIXS measurement. You may be interested in setting the sample position parameters as X and Y axes, and plotting other parameters on a 2D grid. Only one parameter can be plotted this way at a time.



In this example, the homogeneity of the sample can be mapped by plotting the recorded sample current as a function of the sample position.

Compare the measurements using the “Compare RIXS curves” tab



Every time you create a 1D plot out of a 2D array in ADLER, the resulting profile is saved to a text file.

You can load these profiles later in order to compare them.



Compare the measurements using the “Compare RIXS curves” tab



It is not possible to compare profiles that have different units on the X axis.

Having said that, a stubborn user is allowed to edit the “Xunits” field manually and force ADLER to create such a plot anyway.

	1	2	3	4	5	6	7	8	9
	Filename	Ei (eV)	Xlimits	Xunits	Use it?	FWHM	+/- dFWHM	Int.	+/- dInt.
2	Merged_CTape...	577.6	1.0,2048.0	Detector ...	<input checked="" type="checkbox"/>				
3	Merged_CTape...	578.1033	1.0,2048.0	Detector ...	<input checked="" type="checkbox"/>				
4	Merged_CTape...	578.8	1.0,2048.0	Detector ...	<input checked="" type="checkbox"/>				

Compare the measurements using the “Compare RIXS curves” tab



These parameters can be used to cut off the ends of the plotted curves, and to re-bin the curves to reduce the number of points plotted.

The fitting parameters work the same as in the main tab.

You can override some of the Matplotlib plotting parameters here.

Please see the next slides for some examples.

File Loading

Spectrum cutoff pixel

Reduction factor N/A

Elastic Line

Elastic line limits pixel

Detection limit for BKG percentile

Plotting

Mutliplot offset maximum rel. intensity

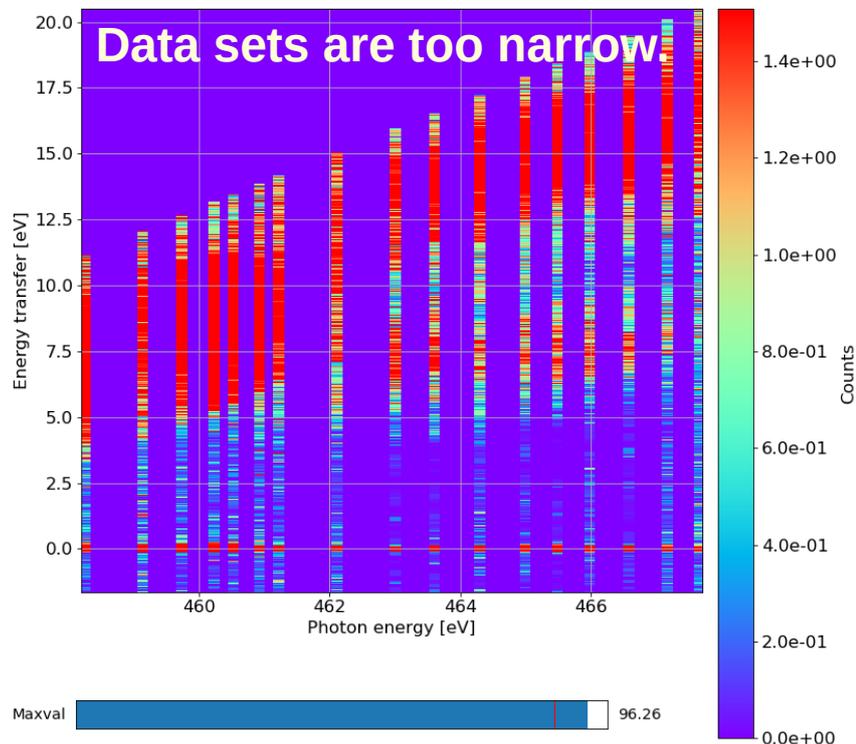
Legend position N/A

RixsMap Smearing meV

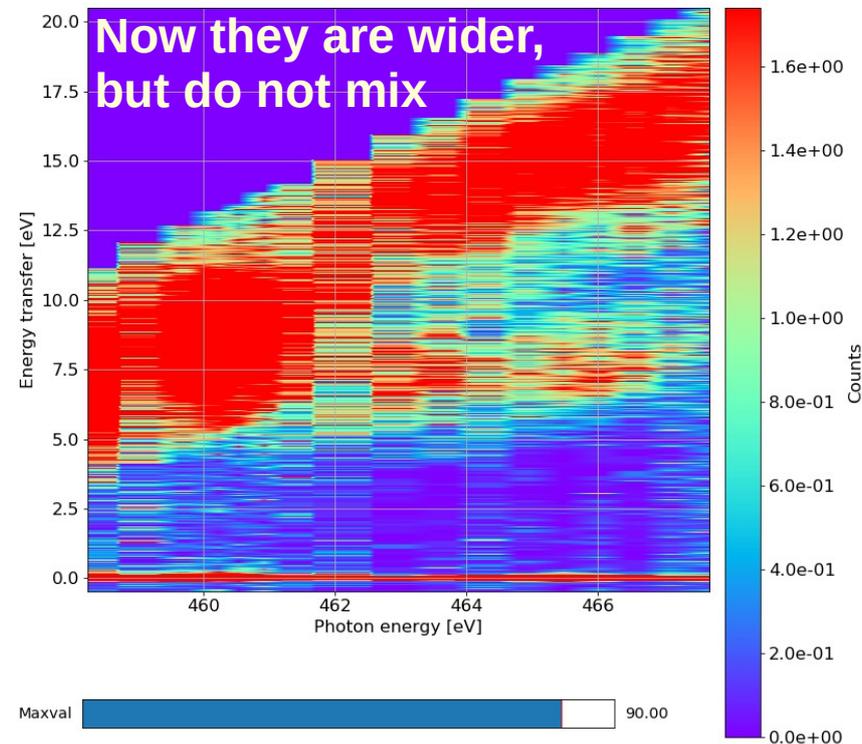
Plot a RIXS map using the “Compare RIXS curves” tab



Smearing = 0.1 eV



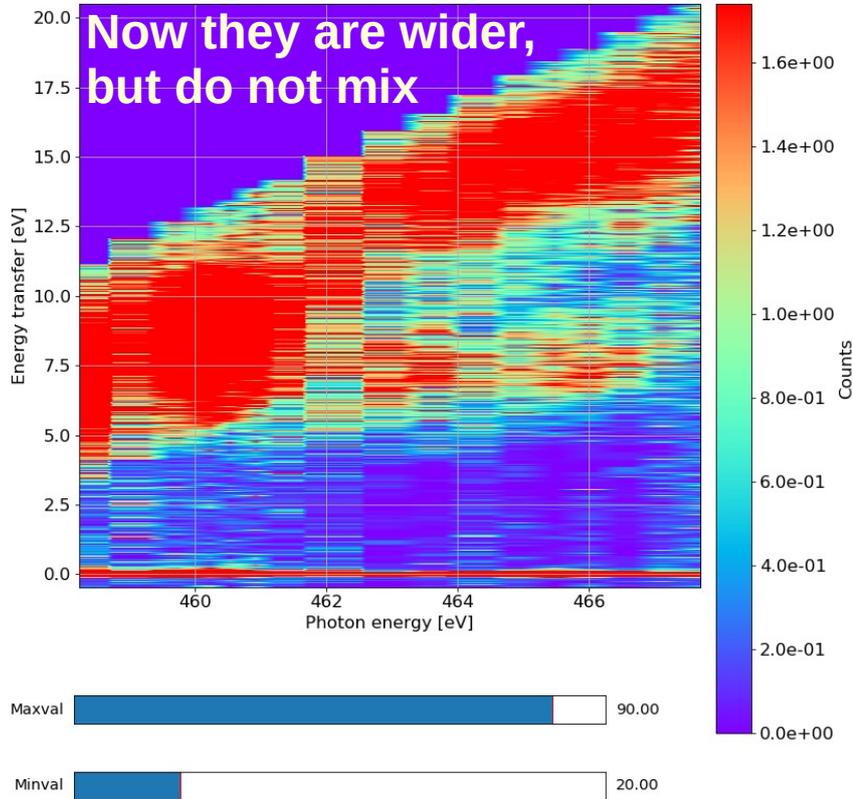
Smearing = 0.5 eV



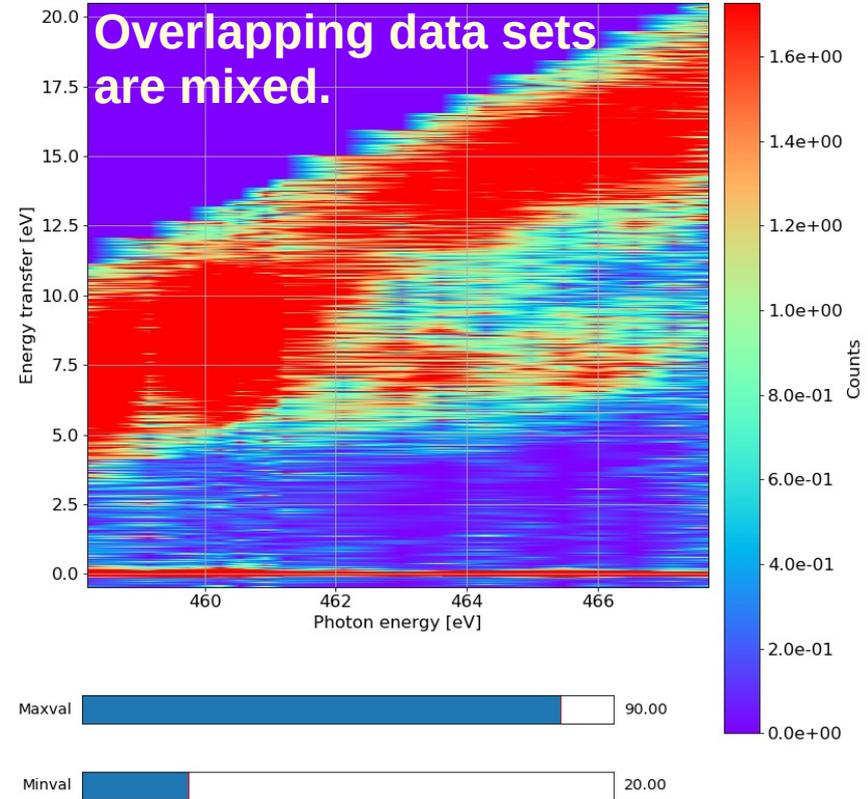
Plot a RIXS map using the “Compare RIXS curves” tab



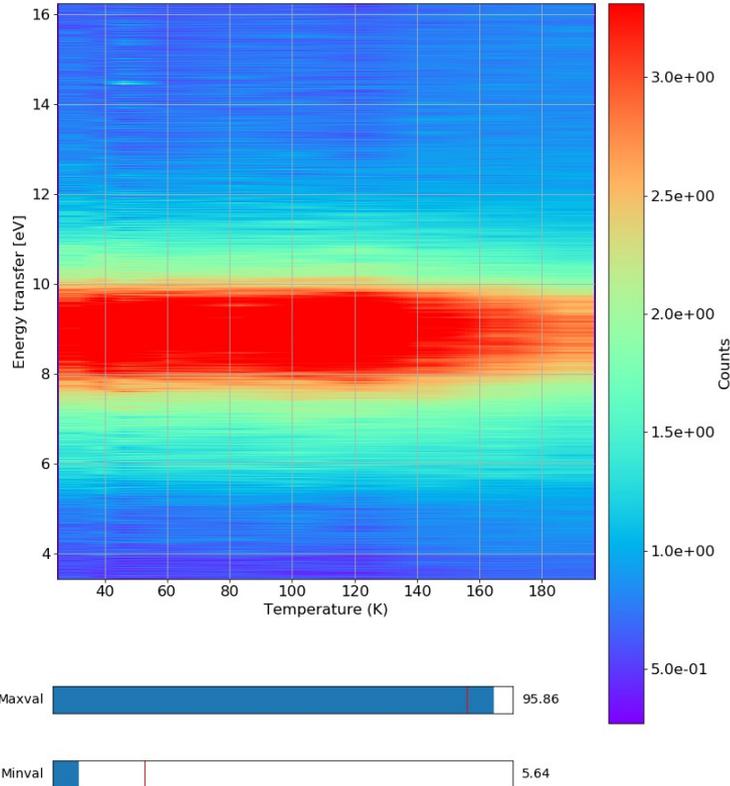
Smearing = 0.5 eV



Smearing = 2.0 eV



Plot a RIXS map against another parameter.



	2	3	4	5	6	7	8	9	10
1	Ei (eV)	Xlimits	Xunits	Temperature (K)	2 theta (deg)	Q (1/Å)	Use it?	FWHM	+/- dFWHM
2	460.5	-13.89,17.97	Energy transfer ...	23.84	60.056	0.23	<input checked="" type="checkbox"/>		
3	460.5	-13.89,17.96	Energy transfer ...	31.63	60.058	0.23	<input checked="" type="checkbox"/>		
4	460.5	-13.9,17.96	Energy transfer ...	39.61	60.058	0.23	<input checked="" type="checkbox"/>		
5	460.5	-13.89,17.96	Energy transfer ...	55.03	60.058	0.23	<input checked="" type="checkbox"/>		
6	460.5	-13.9,17.96	Energy transfer ...	79.81	60.058	0.23	<input checked="" type="checkbox"/>		
7	460.5	-13.9,17.96	Energy transfer ...	99.67	60.058	0.23	<input checked="" type="checkbox"/>		

RIXS map X axis: Temperature (K)

File Loading

Spectrum cutoff pixel

Reduction factor N/A

Elastic Line

Elastic line limits pixel

Detection limit for BKG percentile

Filter cutoff points

Plotting

Multiplet offset maximum rel. intensity

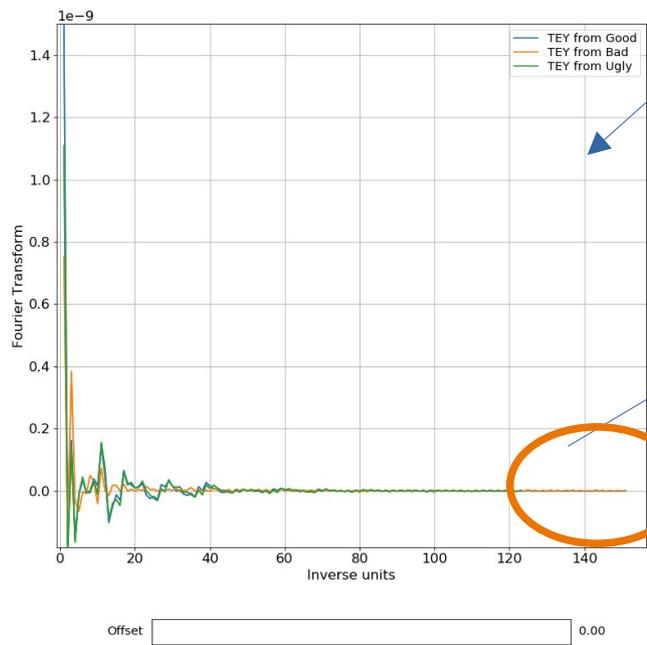
Legend position N/A

RixsMap Smearing x-axis unit

A RIXS map can be created also with other variables on the x axis.

Other features of ADLER:

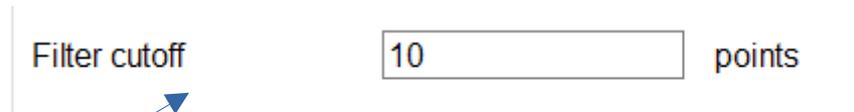
Removal of high-frequency noise from 1D curves, both for RIXS and XAS data.



1. Calculate the Fourier transform of the curves.



4. Apply the filter.



3. Decide how many points of the spectrum (starting from the end) should be set to 0.

2. Check for strong signal at the end of the spectrum (the high-frequency range)



Most users already have their favourite way of processing data, and they can fine-tune the parameters of their software to their liking.

Once your experiment is over, you are welcome to apply the best statistical methods to your data and spend all the time you want making sure that the results have the best quality possible.

However, while the experiment is still running, you may not have the time to do all this, and for this reason we provide a tool that performs only a limited number of operations on the data files, in a short time. This way you can get an overview of the results and adjust the measurement plan as necessary.

The goal of ADLER is not to be perfect, but to be convenient.