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Manual of Red2D

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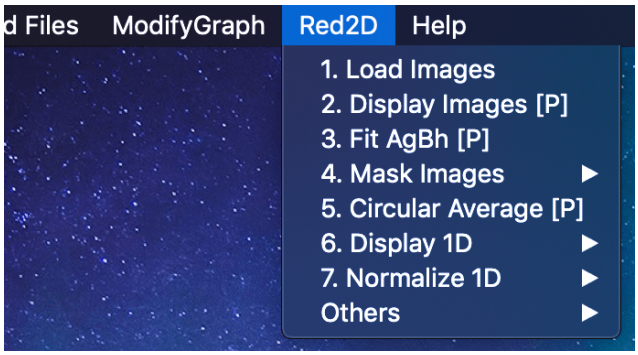
This is a small package for Igor Pro to convert 2D scattering data to 1D profiles of scattering intensity vs scattering vector or scattering angle. The function of this package is limited for simple data reduction, suitable for light users. I have reduced the several 2D images using "Red2D" and "Nika" by Dr. Jan Ilavsky, and confirmed the good consistence of the data reduced between these packages.

It will be nice if you acknowledge me in your publications.

Example: The SAXS/WAXS/SANS data reduction is performed by using a reduction package Red2D (https://github.com/hurxl/Red2D) on a data analysis software Igor Pro.

How to install

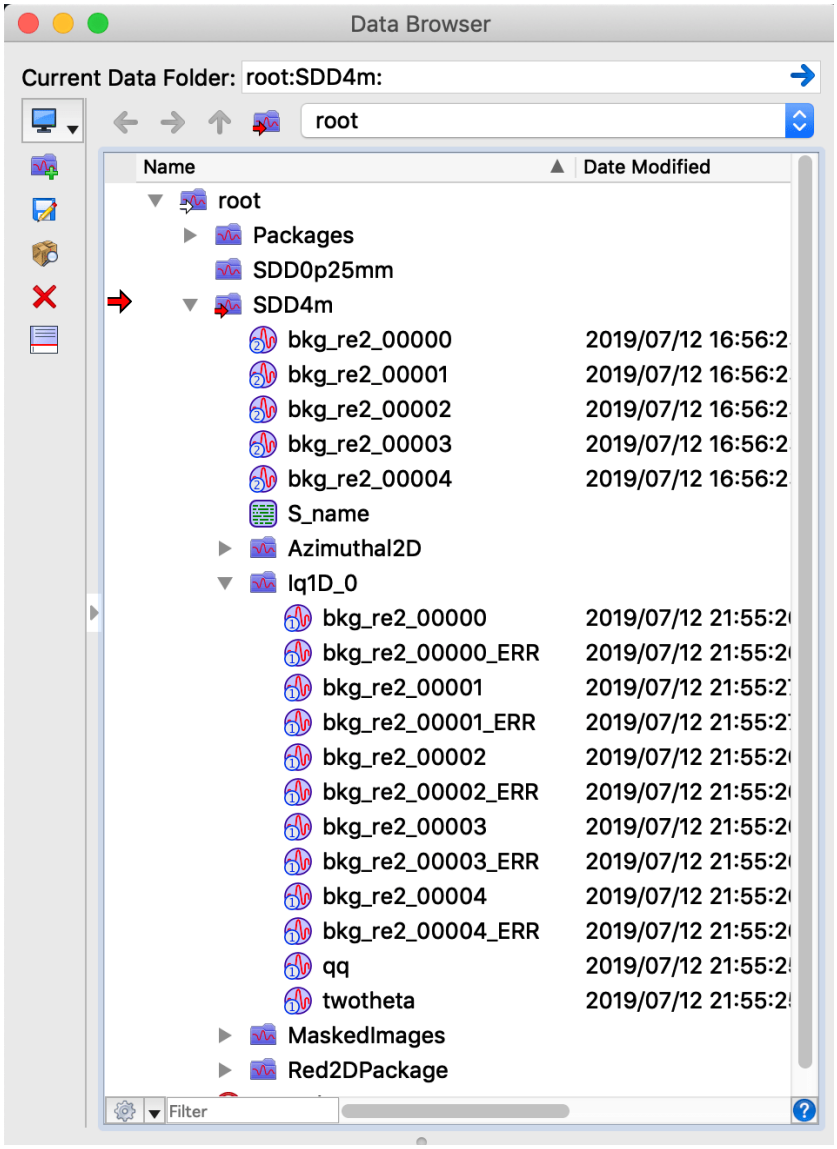
- Download the package from GitHub and unzip the file https://github.com/hurxl/Red2D/blob/master/README.md
- Move the unzipped folder into your local WaveMetrics folder:
  Documents » Wavemetrics » Igor Pro 8 User Files » Igor Procedures
- Launch Igor Pro application and you will see a "Red2D" tab.



How to use

Common tips:

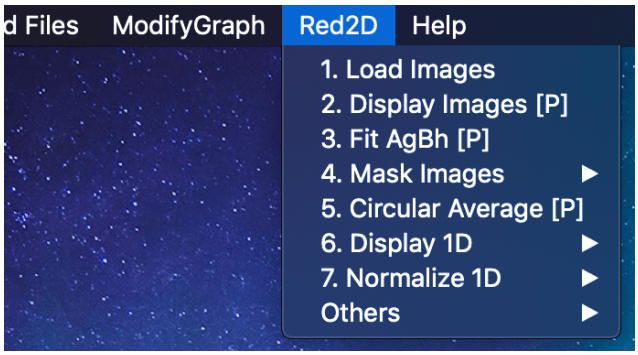
1) Use data browser (Command + B) to organize your data.
2) Make different datafolders for different configurations (SDD, beam center, etc.).
3) Set datafolder to where the target data exist. The data in child folder will not be used.
   a) e.g. display images, mask image, circular average → set datafolder to where the images exist (e.g. SDD2m).
   b) Display 1D, normalization 1D → set datafolder to where1D data exist (Iq1D…).



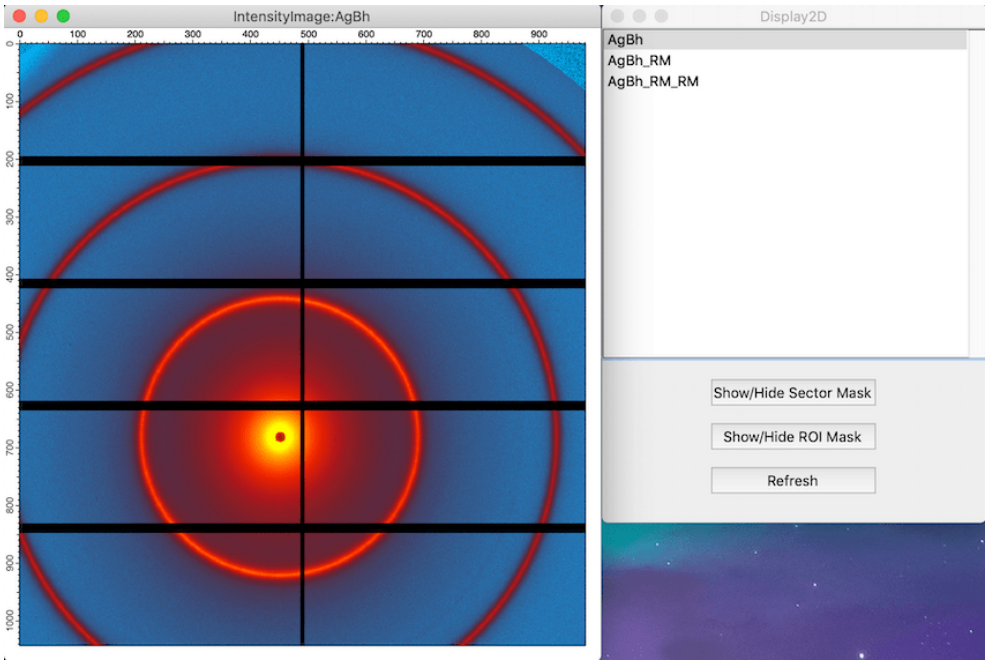
1. Click "Load Images" and select all the images you want to load.

Tips:

1) The files are loaded in the order as you selected.
2) Image name rule: 1. starts from alphabet, 2. no space, 3. no symbol except underscore. 4. Concerning Igor Pro before version 8, make sure the file names shorter than 32 characters.



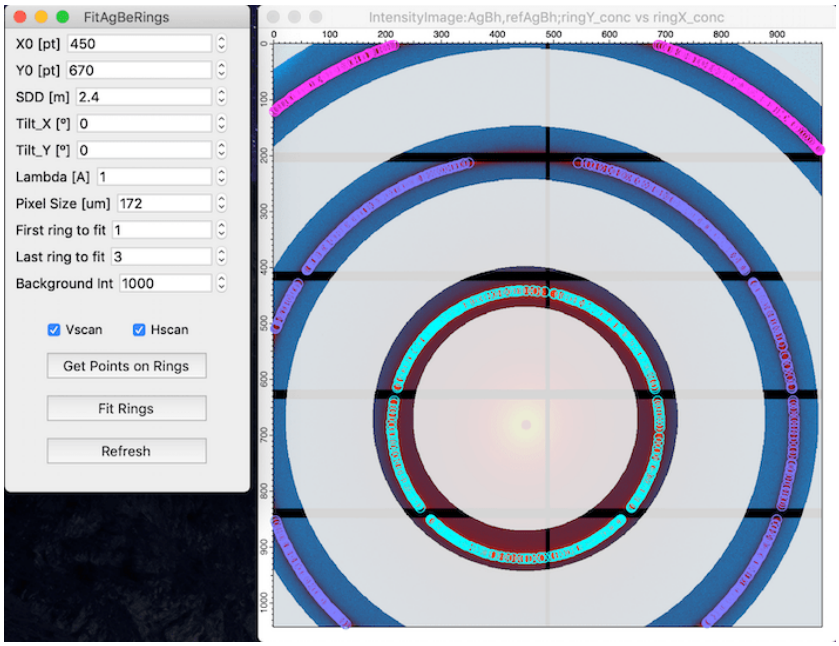
2. Use "Display Images" to show 2D images.

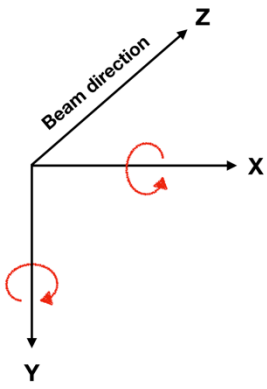


Tips:

1) Set datafolder to where the images exist.
2) Click "Refresh" button to refresh the list of images.
   - If sector mask or ROI mask is generated, you can show and hide the masks.

3. Fit standard to get beam center and SDD

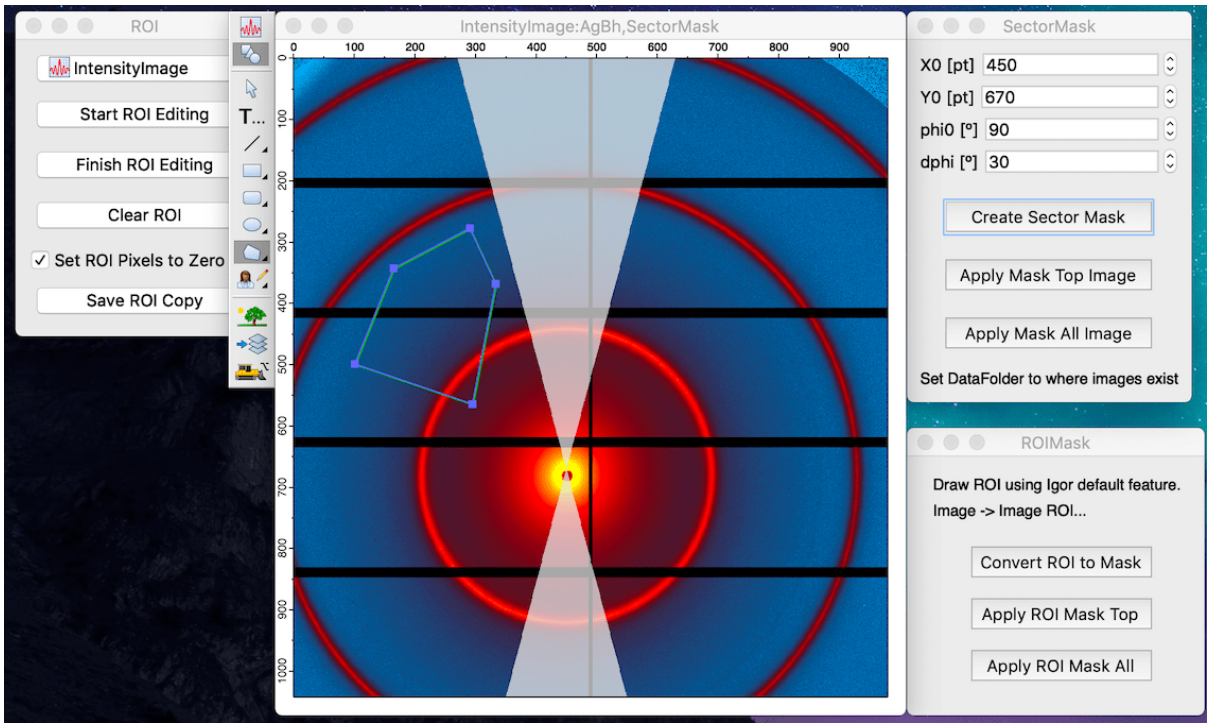




Tips:

1) Fill all the parameters. X0, Y0 and SDD are fit parameters. All the other parameters are independent variables and must be precise.
2) A white mask will appear based on the parameters you set.
   a) Only the non-masked pixels will be used to estimate beam center and SDD.
   b) Generally, fitting one ring is good enough.
3) Set background intensity to remove the noise and click “Get Points on Rings”.
   a) Colorful points appear on the rings.
   b) If the points are not on the rings, change the background intensity then click “Get Points on Rings” again. You can also try to check/uncheck Vscan (vertical peak scan) and Hscan (horizontal peak scan).
4) Click “Fit Rings” to do the fit.
   a) The fit result appears in the command window. X0, Y0 and SDD will be stored as global variables in a datafolder “Red2Dpacakge”.
5) Use tilt-X and tilt-Y to correct tilt angles of detector plane. We use right-hand coordinates and right-handed screws rule for tilt direction.

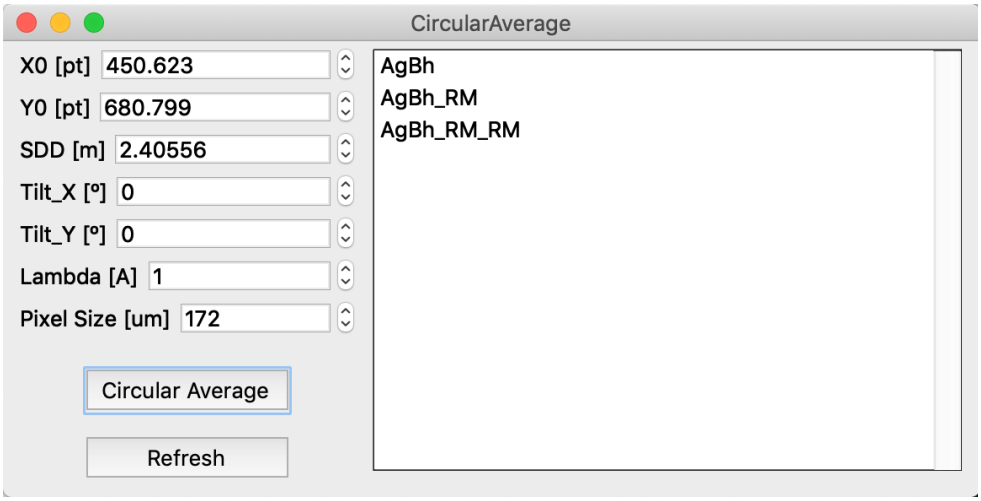
4. Create and apply sector and ROI mask [optional]



Tips:

1) Fill beam center position (X0, Y0) and fill the angle (phi0) and the range (dphi).
2) "Create Sector Mask" generates a sector mask.
3) "Apply Mask" creates masked images. The masked image will be saved in a separate datafolder. The original image will not be changed.
4) To use ROI mask, you need draw a ROI first by select "Image" ≫"Image ROI…" in the Igor menu bar. Then click convert ROI to Mask.
5) You can apply mask to the masked image.
6) The panel space (value = −1) will be automatically removed when performing circular average. You do not have make a mask for the panel space.

5. Circular Average [Panel]



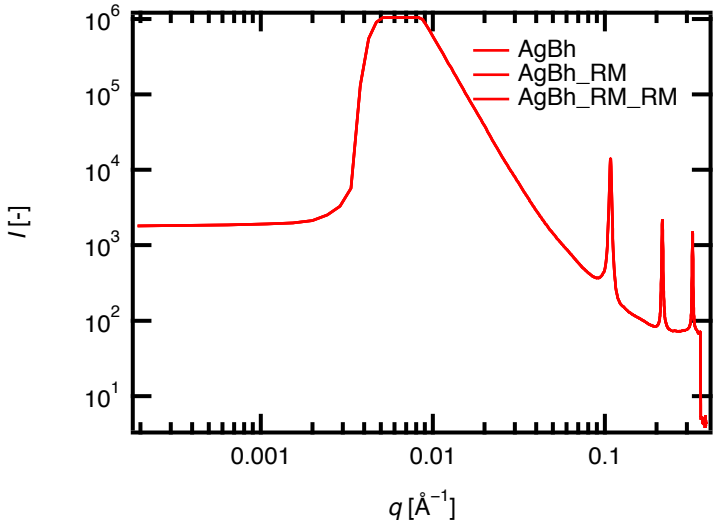
Tips:

1) Click refresh to update the image list and parameters when you changed the images or moved to other data folder.
2) Fill all the values then clicking circular average.
3) A new datafolder named "Iq1D", which contains the reduced 1D data, will appear after the circular average.
4) Use tilt_X and tilt_Y to correct the tilted angle of detector plane if necessary. See "3. **Fit standard to get beam center and SDD**" for detail.
5) Other notes
   a) Negative pixels will be automatically removed. You do not need to make a mask for panel spaces, where the intensity is generally -1.
   b) Intensity in 1D profile is the intensity per pixel.
   c) The error of intensity of each pixel is calculated based on Poisson probability distribution ($e = I^{0.5}$) and then averaged for multiple pixels using error propagation equations ($e = (e_1^2 + e_2^2 + \ldots)^{0.5} = (I_1 + I_2 + \ldots)$).
   d) Relative pixel area difference, which depends on scattering angle, is properly corrected based on B. R. Pauw, Everything SAXS: small-angle scattering pattern collection and correction. J Phys Condens Matter. 25, 383201 (2013).

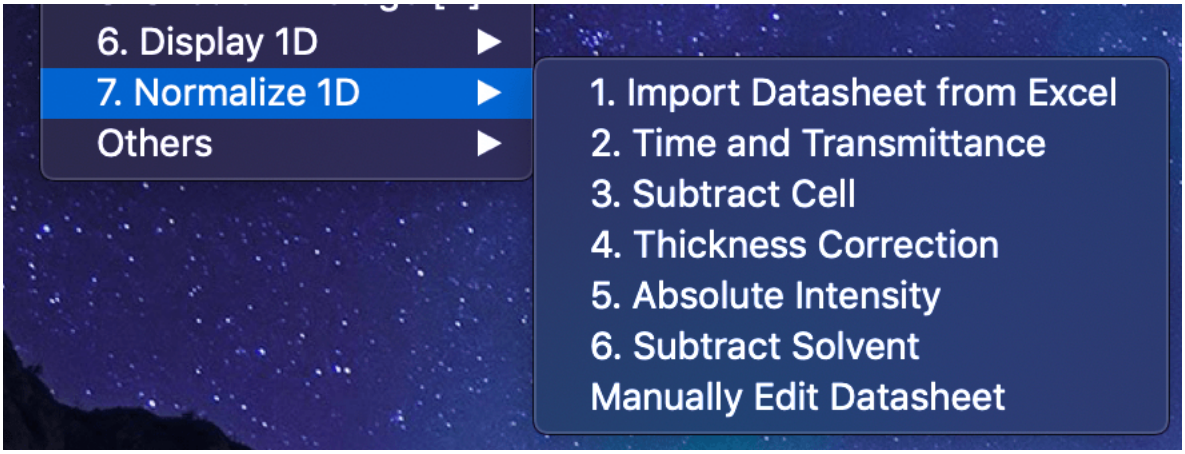
6. Click Display 1D and append 1D to show 1D data in a graph.

Tips:

1) Set the datafolder to where the 1D data exist then click display or append 1D.



7. Normalize 1D data



	A	B	C	D	E	F	G	H	I
1	imageName	SampleName		Time_s	Thick_cm	SDD	Comment0		Trans
2	AgBh	t		4	7	5	10		1
3									
4	AgBh_RM_R	ttt		6	9	5	bb		0.9
5	AgBh_Rm	tt		5	8	5	aa		0.4

Datasheet_Table:Datasheet.Id

R0 Label

Row	Datasheet.I		Datasheet[][0].	Datasheet[][1].	Datasheet[][2].	Datasheet[][3].	Datasheet[][4].	Datasheet[][5].	Datasheet[][6].	Datasheet[][7].
	x	y	ImageName	Time_s	Trans	Thick_cm	Comment0	Comment1	Comment2	Comment3
0			AgBh	4	1	7	10			
1			AgBh_RM	5	0.4	8	aa			
2			AgBh_RM_RM	6	0.9	9	bb			
3										

Tips:

1) Set the datafolder to where the 1D data exist.
2) Create a datasheet with Excel and import that using “Import Datasheet from Excel”.
   a) A template excel sheet is included in the zip file that you downloaded.
   b) The first row in excel sheet is the header. Only the header named with “ImageName”, “Time_s”, “Trans”, “Thick_cm” and “Comment0-3” will be imported.
   c) “ImageName” that does not exist in the datafolder of Igor will not be imported.
   d) “Trans”, “Tims_s” and “Thcik_cm” must be filled. If you want to skip a normalization of any data, type 1 into the corresponding cell.
3) You can manually fill the datasheet if you want. If you need to delete the datasheet, go to the Red2Dpackage datafolder and delete a textwave named “datasheet”.
4) After you filled the datasheet, you can normalize the 1D data. If you understand what the normalizations do, you do not have to follow the index order in front of each normalization.
5) Note for absolute intensity correction:
   (i) Load calibration curve of glassy carbon by using “Others” ≫ “Load GC calibration curve”. The original data is downloaded from https://www-s.nist.gov/srmors/view_detail.cfm?srm=3600
   (ii) Compare the intensity ratio of [your data]/[Calibration curve] at a proper q value.
   (iii) Click “Absolute Intensity” and type the intensity ratio value.

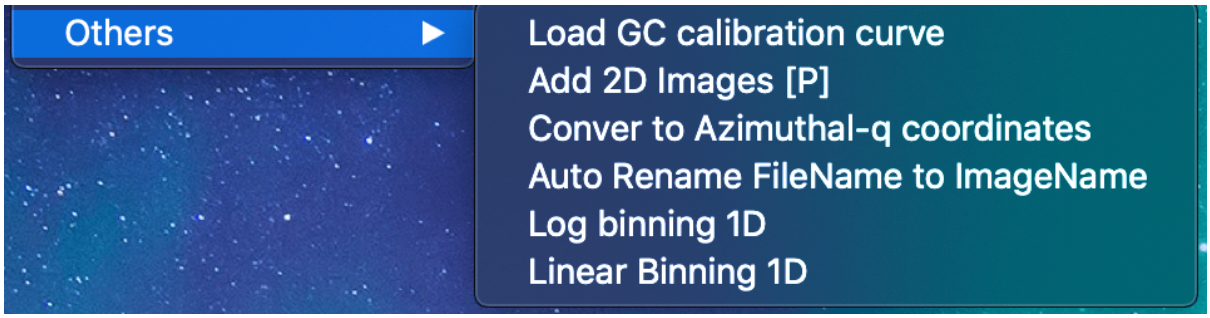
Appendix

Red2Dpackage folder

This datafolder will be automatically created in a directory where your images are stored. This datafolder stores global values, strings and waves used in background process. You can edit these values by yourself when necessary.

Others

You can find several useful functions in “others”.

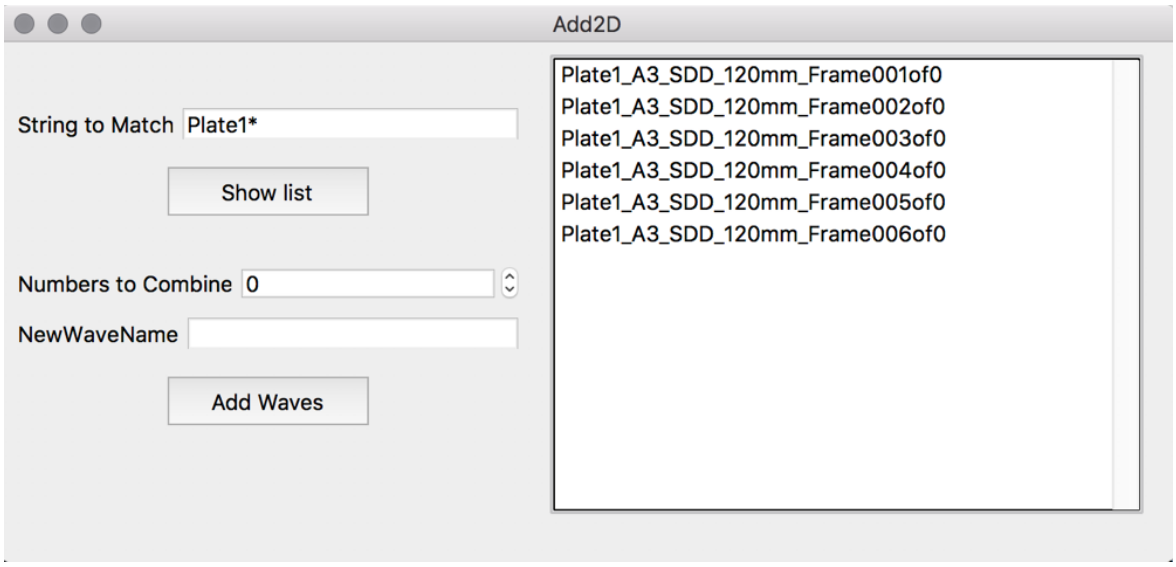


- Load GC calibration curve

The calibration curve of glassy carbon from NIST is included in this package. You can use this function to load the data.

- Add 2D Images

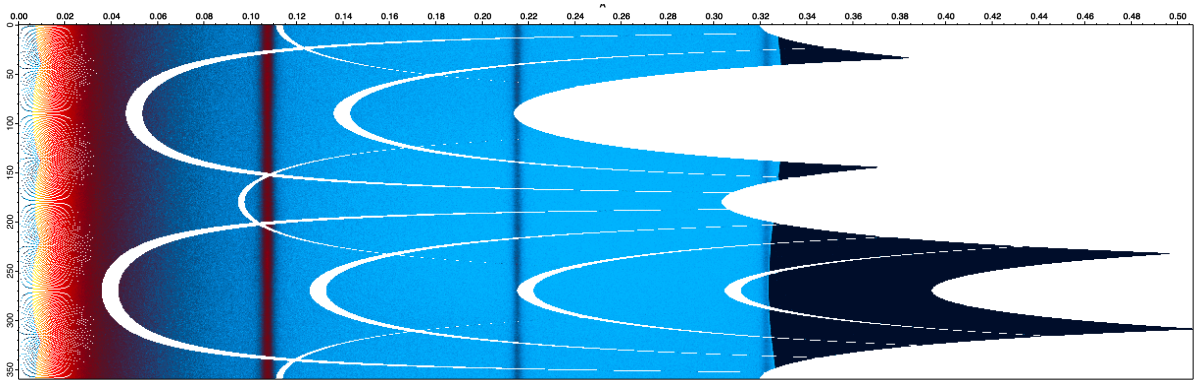
You can add multiple images into 1 image by using “Add 2D images”.



1) String to Match: type the common part of the image names. Use an asterisk (*) as a wildcard, e.g. "*abc*" matches "testabctest".
2) Numbers to Combine: type the number of images to combine. e.g. If you have 10 images and Numbers to Combine = 2, then 5 combined images will be generated.
3) NewWaveName: when multiple images generated, a sequential number will be added at the end of the names.
4) Data will be saved in a datafolder "Added".

- Convert to Azimuthal-q coordinates

You can convert normal X-Y Images to Azimuthal degree vs q images.



- Auto Rename File (beta)

Convert file name to imagename

- Log Binning 1D

Binning 1D data logarithmically. Very useful if your x-axis is log-spaced.