SAngler 2.1.71 manual

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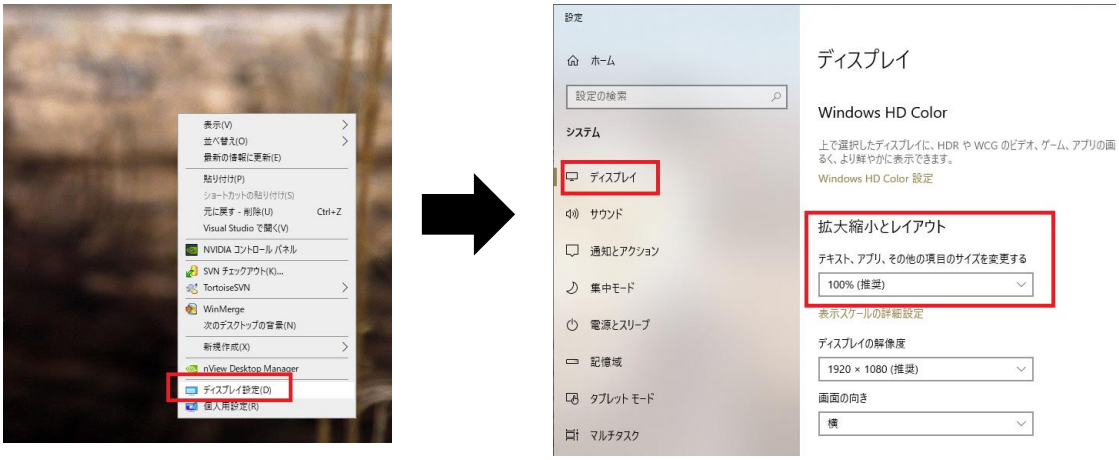
Contents

Introduction

① This manual corresponds to version 2.1.71 (February 16, 2024). Please note that the operation may change as the version goes up. Please refer to the latest manual.

② If the SAngler display is corrupted and buttons and other objects are hidden and not clickable, changing the display settings may fix the problem. In Windows 10 and 11, right-click on the desktop, go to "Display Settings," and under "Scale and Layout (change text, app, and other item sizes)," change the display scale to "100%. In most cases, the settings marked (recommended) are fine.



1. before use

① The program is only compatible with Windows. The current recommended operating environment is Windows 10 and 11, 64 bit. It also works in a Mac virtual environment.

② The program is available as a single compressed file. Please download and unzip it to your preferred location in your HD.

③ When the compressed file is extracted, the following file is generated.

folder	[system]	Location where system logs are output, which can be changed in ConfigSetting.
	[autorg_kek]	The folder containing the autorg_kek group of programs.
	[emb-python]	embeddable python
	[py]	A folder containing Python script files.
	[CormapMaker-XX]	CormapMaker(XX is the version)
EXE, DLL	clsImgAggrPrj.dll	DLLs used in each EXE.
	RemoteTrace.dll	DLL for remote control.

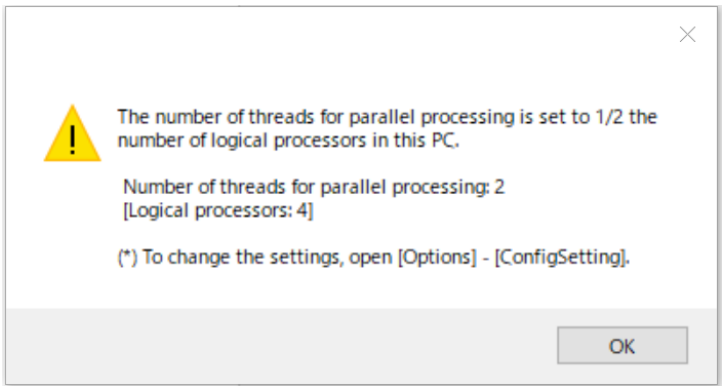
	Python.Runtime.dll	DLL that connects Windows applications to Python.
	SAngler.exe	SAngler body.
	ConfigCustom.exe	EXE for configuration file management and editing.
	AnalysisTool.exe	SAngler Analysis EXE.
	AzimuthalIntensityHistogram.exe	Circumferential data intensity histogram EXE.
	PointPickViewer.exe	PointPick Graph Viewer EXE.
Configuration File	system.xml	Basic settings used by SAngler, such as system log retention periods and parallel processing settings, are stored.
	facility.xml	Facility information to be used by SAngler, such as facility name and counter file information to be used, can be set by ConfigCustom.exe.
	detector.xml	Detector information used by SAngler, such as detector name, image extensions that the detector can handle, image size and pixel count, etc. Can be set using ConfigCustom.exe.
	calibrant.xml	The standard sample information used by SAngler is set in the【Calibration】tab, including the name of the standard sample used, surface spacing, and order. These can be set using ConfigCustom.exe.
	config.xml	Some of the previous conditions are saved.
	az_config.xml	Configuration file to be loaded at startup by AzimuthalIntensityHistogram.exe. Without this file, AzimuthalIntensityHistogram.exe cannot start.
	Ana_system.xml	The settings used in AnalysisTool, such as the conditions for Guinier analysis, are saved.
Other	NIST_GC_data.txt	SRM3600 (NIST) reference data used in the [ABS_GC] tab.
	LICENSE.txt	Python.NET License File

2. how to use

① Check basic software operation settings

i. Double-click "SAngler(.exe)" to start it.

※The following message box appears at startup



The number of threads for parallel processing is set to 1/2 the number of logical processors in this PC.

Number of threads for parallel processing: … The value that is set automatically is displayed here.

[Logical processors: …] The total number of logical processors in the PC is displayed here.

When performing circumferential averaging of image data into one-dimensional data, processing can be performed in a PC multi-threaded environment to analyze a large number of files at high speed. The number of multi-threads is automatically set to 1/2 the total number of logical processors in the installed PC at initial startup. If you wish to change the settings, please go to [Options] - [ConfigSetting]. (See ② ConfigSetting for details.)

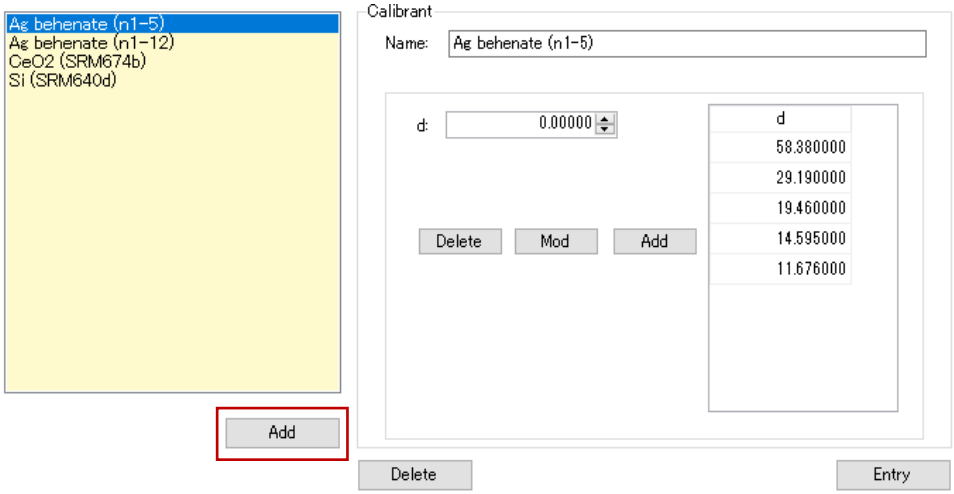
ii. ConfigSetting settings

See "② ConfigSetting".

iii. Next, run [Option]-[ConfigCustom]. Here, there is a [Facitily] tab to register the counter file specifications necessary to normalize the measured scattering intensity with the incident (integral) intensity, a [Detector] tab to set the available detector information, and a [Calibrant] tab to register information such as silver behenate for calibration. First, we will explain how

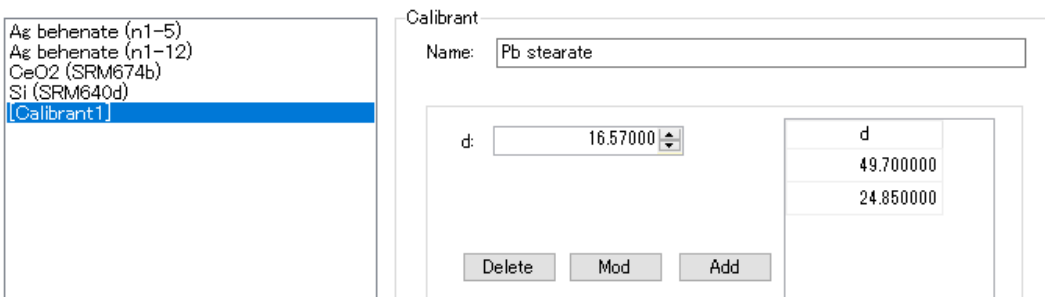
to register a new standard sample on the【Calibrant】tab.

iv. iv. When moving to the [Calibrant] tab, four patterns of three types are registered by default: "Ag behenate (n1-5)", "Ag behenate (n1-12)", "CeO2 (SRM674b) (cerium oxide, ceria)", and "Si (SRM640d)". The following three types of four patterns are registered. SRMs (Standard Reference Materials) are calibration standards supplied (sold) by NIST (National Institute of Standards and Technology).

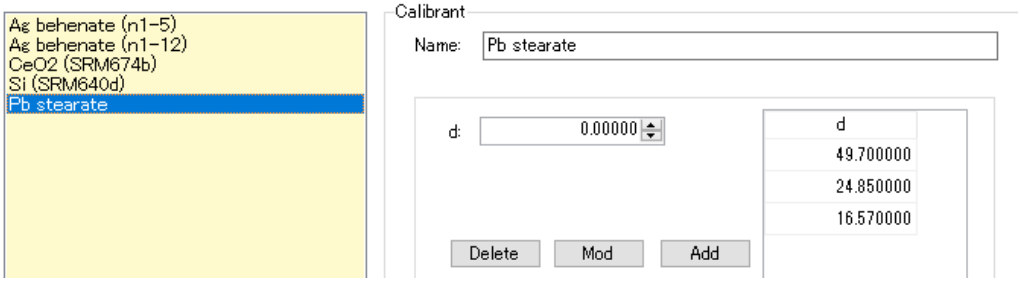


If you click on Ag behenate (n1-5) as a test, the table on the right shows the first to fifth order values based on the areal spacing d: 58.38 Å. If data from another sample, such as lead stearate, is to be used for Calibration, it must be registered anew. To add a new one, click [Add] (red frame in iv figure) in the lower left corner.

v. v. A new entry named "Calibrant1" will be added. Edit the sample name [Name] in the [Calibrant] column on the right, enter a value in [d], and click [Add] to put the value in the table on the right. Continue to complete the calibration table by sequentially entering the order values needed for the analysis. To delete a value, select it and click [Delete]; to modify a value, select it, change the value displayed in [d], and click [Mod].

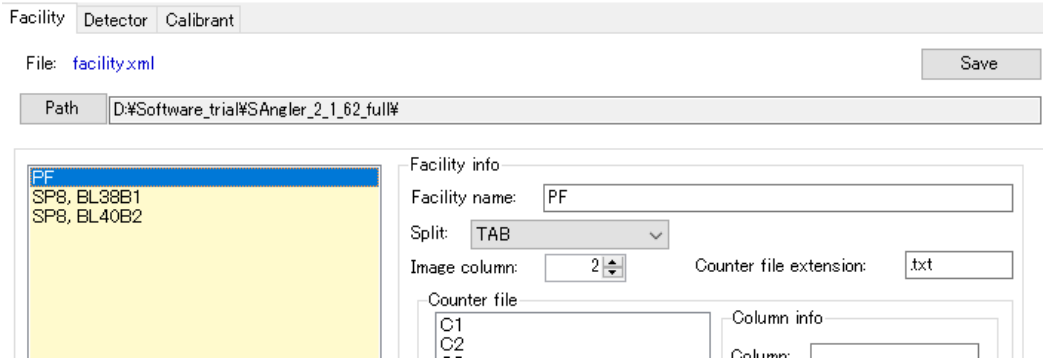


vi. When you have finished entering the calibration table, click [Entry] in the lower right corner. The calibration sample you just entered will then be newly added.

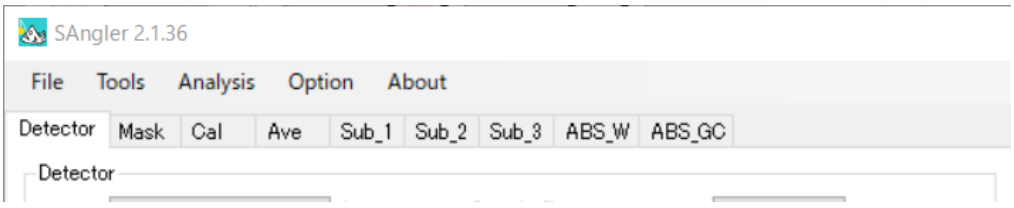


vii. Click "Save" in the upper right corner when you have completed the addition process. The saved file overwrites "calibrant.xml" in the same folder. When finished, close the window with an "x" in the upper right corner. The information newly registered here will become effective when "Load" is performed in the【Calibration】tab.

viii. In the【Facility】tab, the counter file specifications required to normalize the scattering intensity by the incident X-ray intensity, etc. are set for the PF beamlines and BL38B1 and BL40B2 of SPring-8.



ix. In the [Detector] tab, settings are made with respect to the supported detectors. Currently, SAngler supports PILATUS series (tif and cbf files) and R-AXIS series file formats. The same type of detector can be supported by a new setting here.



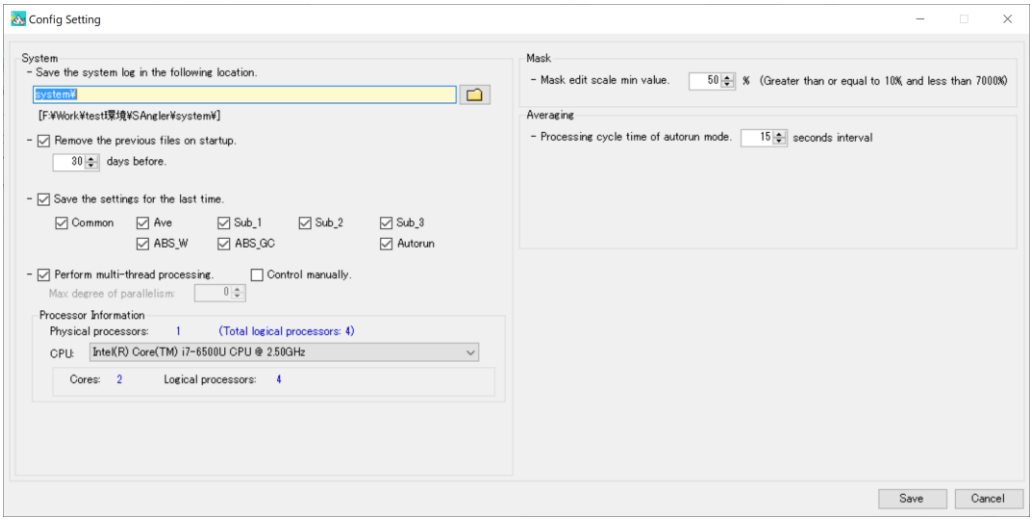
x. SAngler's main window has seven tabs. You can process the data in order by going from

[Detector], [Mask], [Cal], [Ave], (ABS_W or ABS_GC), [Sub_1] or [Sub_2] or [Sub_3]. In addition, since version 2.1.25, the【Analysis】tab, which enables the creation of log plots, Guinier plots, etc., has been made independent as a separate program. (Start from [Analysis] - [SAnglerAnalysis])

On the other hand, the [ABS_W] and [ABS_GC] tabs allow you to use the scattering intensities of water and Glassy Carbon (based on NIST SRM3600) to obtain a conversion factor (CF=Conversion Factor) for converting the scattering intensity (counts) of the measured sample to absolute scattering intensity (cm-1). For this purpose, there are menus in the [Sub_2] and [Sub_3] tabs and the [ABS] tab to determine the transmittance using the (integral) intensity (I0) of the incident X-rays and the (integral) intensity (I1) of the X-rays transmitted through the sample. In addition, there is always a Dark level in the value of the integrated intensity of the incident X-rays. Therefore, when using those values to normalize the scattering intensity, the Dark level must always be subtracted. Such functions are also implemented in the [Ave], [Sub_2], [Sub_3], and [ABS] tabs.

② ConfigSetting settings

ConfigSetting allows you to configure settings related to SAngler behavior, such as settings when SAngler starts and stops, interactions with other EXEs, and settings during analysis.



System	- Save the system log in the following location.	Location where system logs are output. Default value is "system¥".
	- Remove the previous files on startup.	Automatic system log deletion period. The default value is 30 days. Prior to that time, system logs will be deleted.
	- Save the settings for the last time.	Set which information to save when saving the previous analysis condition. Check the checkboxes for the items you wish to save.
	- Perform multi-thread processing.	Check the checkbox for parallel processing. To manually set processing thread control, check the [Control manually.] checkbox and enter the number of threads If a number greater than the total number of logical processors is set, a warning message will be displayed. ※Larger values can also be set. The items below will display information about your current PC, so please use them as a reference for your settings. Physical processors: Number of physical

Mask	- Mask edit scale min value.	processors Total logical processors: Total number of logical processors Cores: Number of cores Logical processors: Number of logical processors Sets the minimum image reduction value on the MaskEdit screen. The default value is 50%.Set the value between 10 and 7000.
Averaging	- Processing cycle time of autorun mode.	Analysis cycle during Autorun processing

i. Execute [Option] - [ConfigSetting] from the menu at the upper left of the window.

ii. In the [System] field, specify the folder where the system logs will be savedSAngler checks the date at startup and creates a system log file.system log files are maintained by date. If the system is running across dates, it is recorded in the system log file written first. The system log file is initially set to the "system" folder in the SAngler folder. To change, click to specify.

iii. system log files increase by date. Checking the [Remove the previous files on startup.] checkbox will check at startup and automatically delete system log files that have been in existence for the specified number of days. By default, log files are set to be deleted after 30 days.

iv. The "Save the setting for the last time." checkbox allows the user to specify which setting should be saved when saving the previous setting.

Common: Common Information.
・Facility information, counter file information, detector information, and Conversion Factor information,File Type

Ave: Information about the circumferential averaging process on the [Ave] tab.
・Mask information, wavelength, camera length, beam center, tilt, image size, and output information,Standardization information

Sub_1: Information on Sub_1 processing.
・Input information, output information, file information to be processed

Sub_2: Information on Sub_2 processing.
・Output information, φ value, Psv value

Sub_3: Information on Sub_3 processing.

・Output information, counter file, and file information to be processed

ABS_W: Information on ABS_W processing.

・Water file information

ABS_GC: Information on ABS_GC processing.

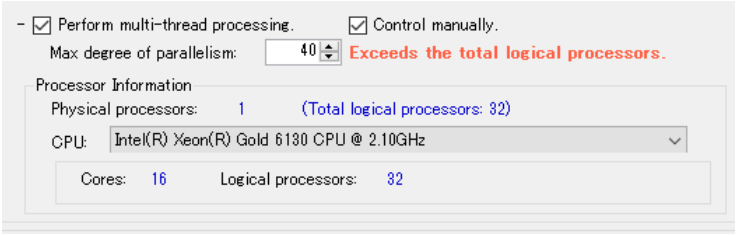
・GC File Information

Autorun: Information on processing circumferential averaging in Autorun mode on the [Ave] tab.

・Autorun Processing mode, pickup Q value, output information, counter file, Prefix Information

v. The [Perform multi-thread processing] checkbox determines whether parallel processing is used or not.
Since circumferential averaging processes a large number of files, parallel processing is implemented for higher speed.
Check the box to perform parallel processing. At that time, select whether the thread limit for parallel processing will be set by the CPU or manually.
To set manually, check the [Control manually] checkbox and set the maximum number of threads.
The maximum number of threads depends on the specs of the PC, other tasks other than SAngler, etc. The current PC information is shown at the bottom of the screen. Please refer to this information to set the maximum number of threads.

※ If you set a value greater than the number of logical processors, a warning message will appear, but it can be processed. However, this is not recommended since it will overload the PC.



vi. In [Averaging], when using the automatic folder monitoring function (Autorun) with circumferential averaging, the default setting is that the process is executed every 15 seconds, but please change the time appropriately according to the speed of measurement and processing.な Note that circumferential averaging without parallel processing takes 1 second per image for PILATUS 2M size.

vii. When settings are complete, click "Save" to close. The dialog "The setting changes will take

effect after you restart SAngler. The setting changes will take effect after you restart SAngler.

③ Detector settings

Select the type and model of detector used and the image data format. The data format is fixed to the one set here for processing from the【Mask】tab onward.

i. Select the name of the detector in Name and the model (size) in Model.

ii. In [File type], select the format (extension) of the image data: tif (32bit Tiff) or cbf (crystallography binary format) for PILATUS, or stl or osc for R-AXIS.

iii. Click "Set" to fix the value as the default value for processing. If you want to change them during subsequent processing, click [Set] again on the【Detector】tab.

iv. You are done. Go to the【Mask】tab.

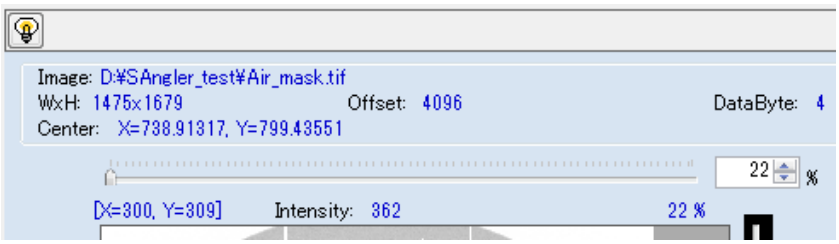
④ Create Mask file

PILATUS achieves a large area by arranging 100K basic modules in a mosaic-like pattern. For this reason, a GAP of 3 to 5 mm exists between modules. By masking and processing this GAP, it is possible to perform the same analysis as for seamless data. In addition, some pixels are bad (bad pixel) and need to be masked, such as the shadow of a beam stopper. In SAngler, mask files are easy to create.

i. First, load the exposed image to create a Mask file. It is recommended that relatively long exposures of air scattering and Glassy Carbon data be obtained without a sample for mask file preparation, but it is not required. If not available, load one suitable image. [Under "Image file:", select an image from a folder. You can also directly input (copy-paste) the folder structure (string) or specify the file directly with Drag & Drop.

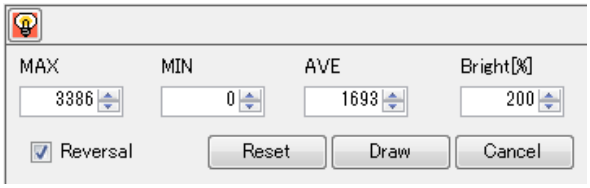
ii. After selecting an image, click "Draw.

iii. Data is displayed on the right side of the window. The top of the image shows information about the file, the number of pixels, and the currently set beam center. When you bring the mouse cursor over the image, the coordinates and intensity of the pixel are clearly shown in the upper left corner of the image ([X=300, Y=309], Intensity: 362 in the following state). Image enlargement and reduction can be controlled by scrolling the mouse, but can also be changed by using the slider bar at the top of the image or by editing the magnification value directly. A line profile centered on that point is also displayed on the right side and bottom of the image.



iv.  mark to adjust the contrast and brightness of the image. [MAX] represents the maximum count value in that image and [MIN] represents the minimum value (at or above zero). [AVE] literally represents the average value, but as this value is decreased, the display becomes darker, i.e., weak scattering is visible, and as it is increased, the display becomes lighter. [Brightness] adjusts the brightness of the display. Unchecking [Reversal] will invert the

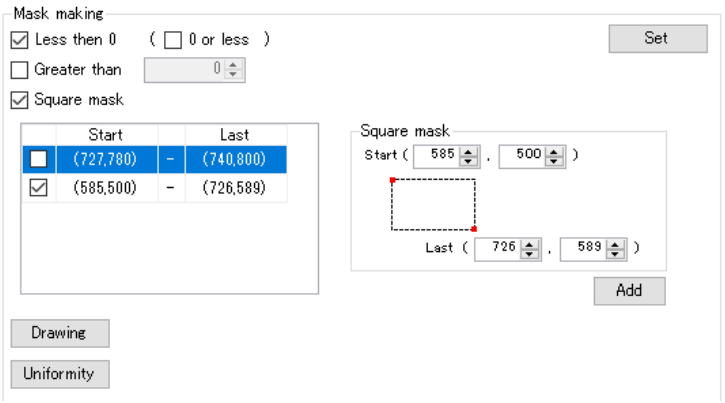
display to black and white. After changing the values, click "Draw" to change the display.



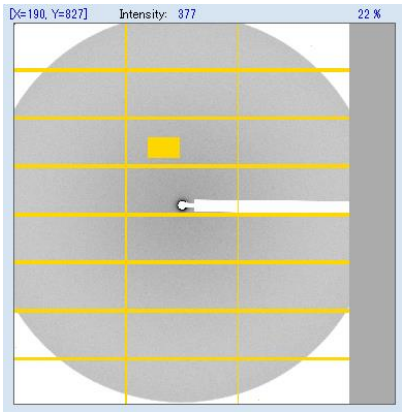
v. Select the mask conditions in the【Mask making】column. [Less than 0] allows negative values to be masked automatically. PILATUS GAP and Bad pixel are set to be output with a value of -1 and -2, respectively, so if you wish to mask these, check the "Less than 0" checkbox. Also check (0 or less) if the value of 0 is also included. The masked area is displayed in yellow.

※Bad pixel is output as "-2" if it has been previously set, but may be unset if newly generated. If you find such pixel, you may be able to mask it automatically if you also check 0 or less.

vi. Contrary to [Less than], [Greater than] masks pixels that are larger than the set value. Some of the newly generated bad pixels are hot pixels (always output very large values) instead of dead pixels (always zero values). This function is used to mask such pixel. If you set a value slightly smaller than the count value of the pixel you found, you can mask that pixel reliably.



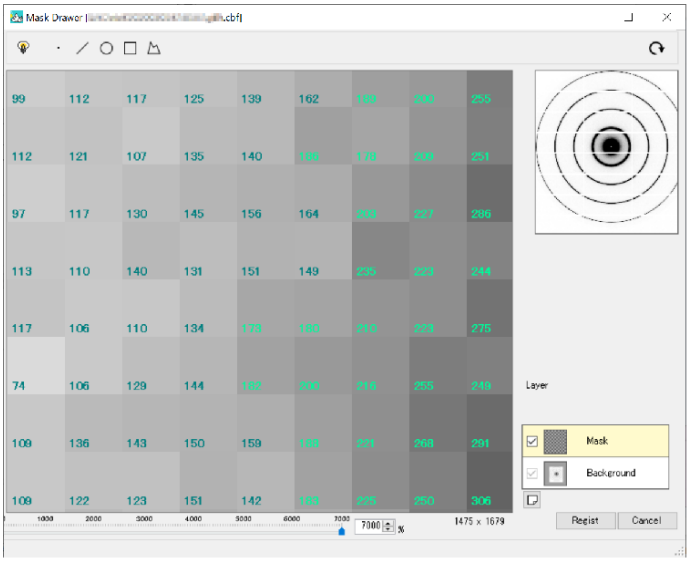
vii. [Square mask] allows you to mask a range of specified squares. As shown on the screen, specify the upper left (Start) and lower right (Last) pixels of the rectangle. If you want to specify only 1 pixel, specify the same coordinates for Start and Last. Once entered, click "Add. The information you entered will be moved to the left column. If checked, it will be applied; if unchecked, it will not. Click [Set] to confirm the input and set it as a mask area.



In the left figure, the rectangular mask near the center is the area of the test entered in (vi). It is erased in (viii) (5) below.

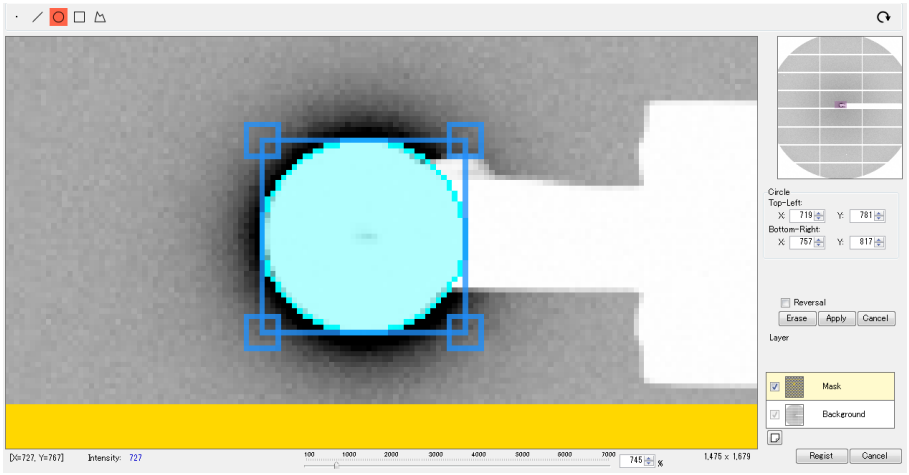
viii. To create a round or polygonal (polygon) mask, click Drawing. Click to open a new Mask drawer window. By drawing the area to be masked on the image data in the window, masks of various shapes can be created. The image is displayed in full size, but you can change the display area by dragging while left-clicking the mouse, and enlarge it by scrolling. The functions can be summarized as follows

- You can draw a range of points, lines, circles, rectangles, and polygons and mask the area.
- Draw a circle, rectangle, or polygonal area and check [Reversal] to invert the masked area (mask areas other than the drawn area).
- You can change the magnification displayed by operating the slider bar shown at the bottom or by directly specifying a numerical value. (from 50 to 7000%)
- When viewed at maximum magnification, the intensity of each cell is displayed.

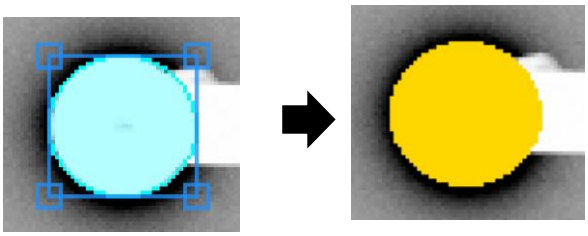


Below are the steps for creating a mask; GAPs, bad pixels, etc. can be masked separately, so here we will try to mask the shadow of the beam stopper.

(1) First, zoom in around the center of the beam by scrolling the mouse to mask the round shadow. Click the ◯ in the upper left corner of the window to draw over the data.

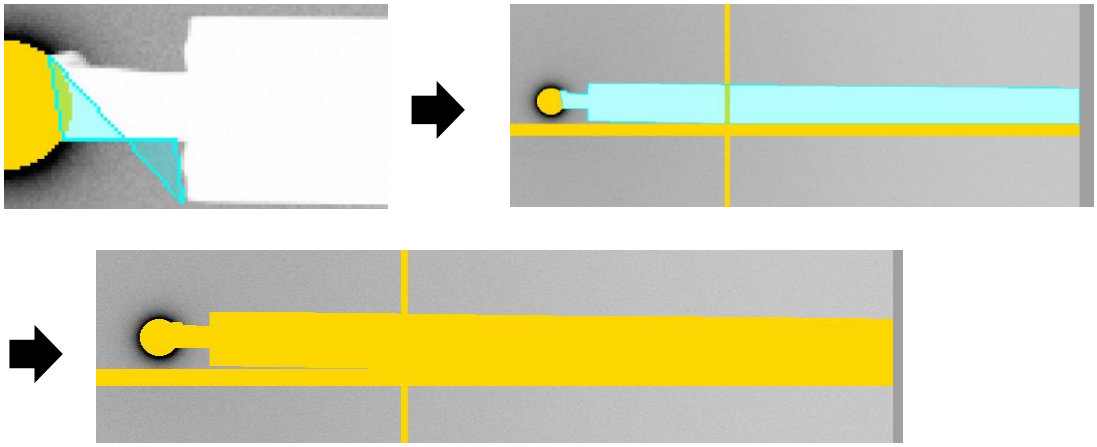


(2) The four corners of the rectangle circumscribed by the circle can be moved by clicking on them. By moving these corners, you can fine-tune the size and shape of the circle. You can also use the [Circle] menu on the right side of the window to change the Top - Left and Bottom - Right coordinates by using the arrow keys (if you enter the values directly, press [Enter] to apply them). Press "Apply" when finished. The mask area will turn yellow and be applied.

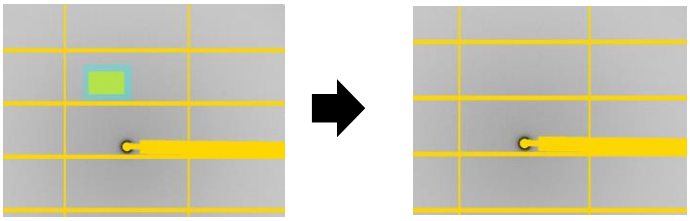


When completed, click the red background ◯ mark again to exit the drawing mode and move the image data.

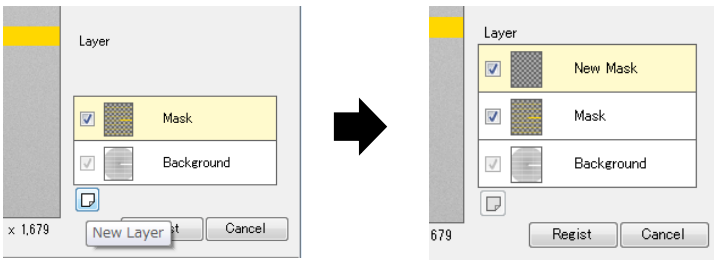
(3) Next, the beam stopper's handle is masked with a polygonal shape. Click on the polygon symbol, then click on each pixel that corresponds to a vertex of the polygon in turn. When the image is enlarged, the root side of the stopper handle is not in the display range. There is a sub-window of image data in the upper right corner of the window, the display area is shown in purple. While drawing a mask, you can change the display range by dragging and moving this purple display range. When completed, click "Apply" to confirm.



(4) If you want to erase the created mask, draw the mask area indicated in yellow in the same way and [Erase]. For example, to erase the rectangle mask created test at (vii), click on the square in the upper left corner of the window and create a rectangle to cover the area to be erased. You can then click on "Erase" on the right side of the window to erase it.



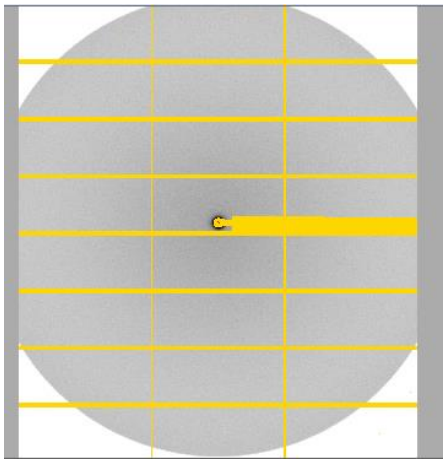
(5) On the other hand, when erasing a mask area once created, the mask area that you do not want to erase may be erased together. For example, in the figure above, the



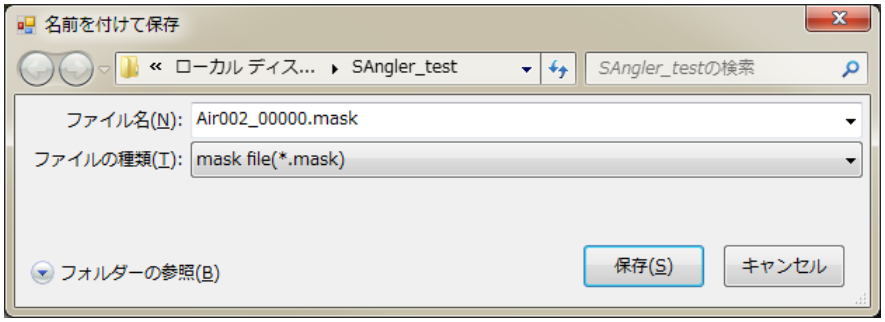
masked area of the GAP set in the grid overlaps the masked area of the beam stopper, so erasing only the beam stopper area would be a rather difficult task. Currently, this Mask Drawer allows you to add one Layer, so you can set up the next mask area to be added in a separate layer without changing the previous working state. To add a layer, click the Add New Layer button. [A "New Mask" will be added, where you can create a new mask area. Unchecking the box also allows you to exclude newly created mask areas from application.

(6) When all the work is completed, click "Register" and all the layer layers you have just created will be integrated.

ix. When you are done, click "Set" to apply the settings on the image, which will be displayed in yellow.



x. When settings are complete, click "Save" to save the Mask file. The file extension is automatically "mask". When saved, the display changes from yellow to green, and the saved Mask file is automatically applied in future processing. Even if you close the software once or process it on a different PC, you can load a previously saved mask file and process it under the same conditions.



⑤ Uniformity function

※(Note) To use this function, it is recommended to calibrate the camera length and beam center position in the【Calibration】tab first and save the "Cal file". Therefore, save the basic mask file in the "④ Create Mask File" operation, perform "⑥ Calibration of Beam Center and Camera Length (Calibration)" first to create a cal file, and then return to the [Mask] tab to perform it again.

In addition, in order to use this function, the image data must be properly masked in advance for areas that are not used for analysis. For example, please mask appropriately the grid GAP of the PILATUS detector, the dead pixel already set by the system, the shadow of the beam stopper, and the area outside the vacuum flange (i.e., outside the measurement range) seen on the wide-angle side.

It is relatively easy to mask Dead Pixels and Hot Pixels so that they are excluded from the processing, but it is not easy to detect abnormal Pixels that are always outputting slightly larger or smaller values than the surrounding pixels. This function finds such pixels during circumferential averaging and adds them to the mask. In circumferential averaging, the average value is obtained from a number of pixel values equidistant from the beam center, which should fall within a certain so-called noise level. On the other hand, if there were anomalous pixels, it is assumed that the value is fluctuating above that noise level. Therefore, a Threshold is set for the average value, and pixels with large fluctuations are found and added to the mask. As a result, it has the effect of suppressing fluctuations (suppressing errors) in the value during circumferential averaging.

※To determine whether a pixel is normal or abnormal, the average value of the points on the same circumference is calculated, and the difference (deviation) between the average value and each point is divided by the standard deviation, and the “Threshold” set for the value A is used as the basis for the judgment using the following relationship.

$$A = \{(\text{Pixel value}) - (\text{average value})\} \ / \ \text{standard deviation}$$

$$A \leqq \text{Threshold} \quad : \text{normal}$$

$$A > \text{Threshold} \quad : \text{abnormal}$$

i. Clicking the [Uniformity] button with a standard sample loaded, such as Air Scattering or Glassy Carbon, will launch a separate program "Azimuthal Intensity Histogram.exe".
※The configuration file "az_config.xml" is read at startup. If it fails to load, it will not start.

ii. If a mask file is specified in SAngler, it is automatically entered as the [Mask:] initial value.

iii. Specify image data (e.g. Glassy Carbon or air scattering data) in [Image:]. Multiple files of the same sample (condition) measured under the same conditions can be specified at a time. If multiple files are specified, analysis will be performed on the integral data (since the judgment of abnormality is clearer for the integral data, we recommend reading multiple files under the same conditions).

iv. Specify a Calibration file (cal file) in [cal:] to automatically set the analysis conditions (circumferential average conditions). If no cal file is available, please enter it manually.

v. Enter the [Threshold] and click the [Start] button (default value is 3.0). (This can be changed from [Options] - [Setting]). When the calculation is completed, the result is displayed. If Threshold is smaller than 3.0, the condition becomes more severe, and the number of pixels judged as abnormal increases.

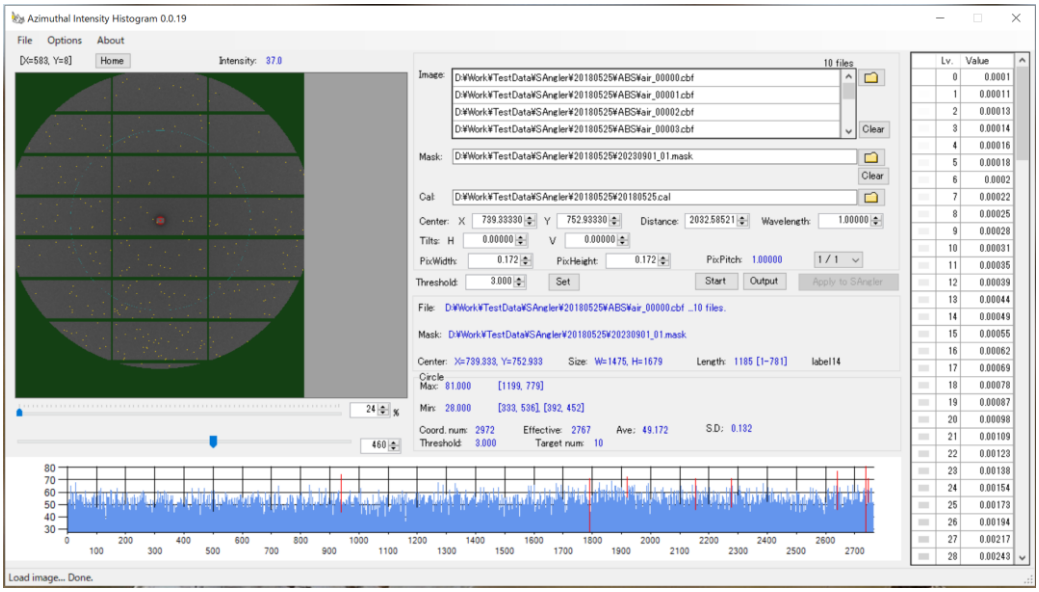
vi. To change only Threshold, edit the value and click the "Set" button.
※Difference between [Start] and [Set].
The [Start] button calculates the coordinates on the circumference based on the analysis conditions entered, then creates histogram data, and judges normality/abnormality, which takes time.
⇒To change the image file used, analysis conditions, or mask file and redo the analysis, click "Start".
The [Set] button uses the coordinate data on the circumference and the histogram data as the result of the previous run, and only judges normal/abnormal.
⇒To change only the Threshold value and redo the normal/abnormal judgment, click "Set".

vii. The left side of the window shows the loaded image data (or the data after integration in the case of multiple files). The dark green ■ area indicates a pre-loaded Mask area. Scaling of the image data can be changed by scrolling the mouse or by using the slider (in %) below the image (maximum 7000%, minimum varies with the system, adjusted to show the entire image). You can also left-drag to move the image. The beam center is indicated by a red

cross, whereas the light green ■ circle indicates the circumference equidistant from the beam center. The position of the circumference can be changed with the slider on the lower side. The number shown on the right side indicates, in essence, how many data points are in the data. The yellow pixels in the image data are the pixels judged to be abnormal based on Threshold.

viii. The graph at the bottom of the window is a 1D plot of the data on each circumference. The number of points on the x-axis varies depending on the number of points that make up the circumference. The value of each pixel is represented by a bar graph. As shown in the figure below, the points that exceed the Threshold are indicated in red, and these are the pixels indicated in yellow on the image data in the upper left. The【Circle】column above the bar graph shows a summary of the data on this circumference. In it, [Target num] represents the number of pixels that exceed the Threshold.

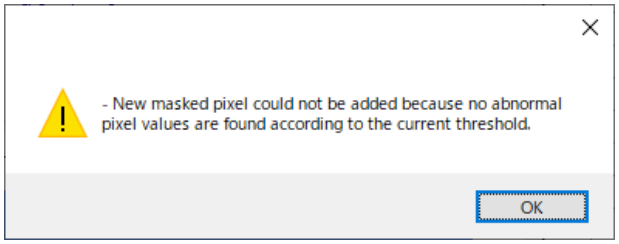
ix. Change the Threshold and consider the area to be Masked, checking the status of the data shown in ix. vii. and viii.



Circle	Circumference information. Maximum and minimum values, mean, standard deviation, and threshold values of points on the circumference, actual number of points on the circumference, number of valid points, and number of points that hit the threshold.
Image on software	They are colored according to the color table on the right. Points that hit the threshold are displayed in yellow.
Upper track bar	Image Scale
Lower track bar	circumference

histogram	Graph the intensity counterclockwise from the point on the circumference that hits zero degrees. Locations where thresholds are hit are shown in red.

x. If normal/abnormal judgment can be effectively performed by the set Threshold, abnormal pixels can be output as new mask data. [Click the "Output" button and you will be asked "Save mask data? Select "Yes. If none of the newly masked coordinates are present, a warning message is displayed.

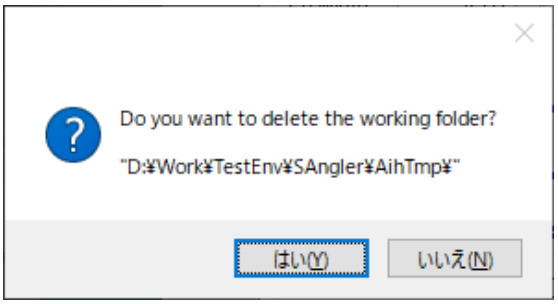


xi. To overwrite the existing mask file, click "Save" without changing the file name. To create a new mask file, enter a new file name and save the file.

xii. When the save is complete, a message box will appear asking "Do you want to update to the latest Information?" and confirming that the mask should be updated to the latest data. Select "Yes" to update, or "No" to continue processing. The update will take some time.

xiii. When a mask file is updated (overwritten) or a new mask file is created, the "Apply to SAngler" button next to the "Start" button will be enabled. If you want SAngler to load the latest mask file as well, click the "Apply to SAngler" button. A confirmation dialog box will appear.

xiv. The process is now complete. To exit, click [File] - [Close] or [x] in the upper right corner of the window. Note that if you try to exit without saving the new mask information, SAngler will display a confirmation message asking if you want to reflect the latest mask information. [Select "Yes" and you will be taken to the save screen. You will then be asked if you want to delete the working folder with "Do you want to delete the working folder ? and you will be



asked if you want to delete the working folder. Basically, you can delete it, but if you encounter errors in the process, etc., please leave it and contact the software developer. When the Window is closed, the latest mask file is loaded into SAngler.

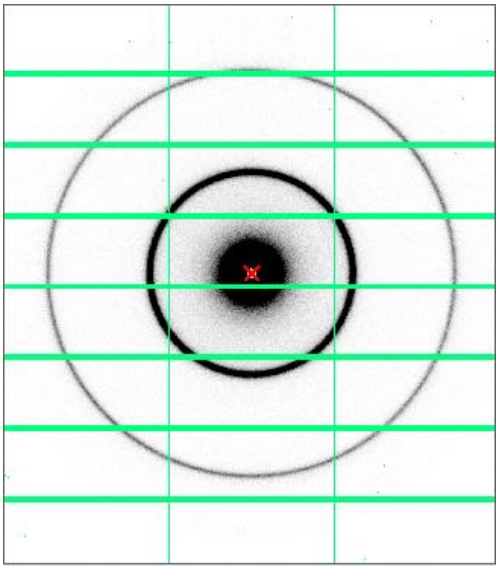
xv. If you do not want to apply the updated mask file to SAngler, do not press [Apply to SAngler] and exit the Window. A dialog box will appear asking if you wish to update. Select [No].

⑥ Calibration of beam center and camera length

Beam center and camera length are calibrated using powder diffraction data of silver behenate.

i. In the [Setting] column, check that the file you just created is set in the [Mask file:] field.（(To set up a previously saved file, click this to load the file. It can also be specified directly with Drag&Drop).

ii. In the [Image file:] field, select the image file that will be used for Calibration.



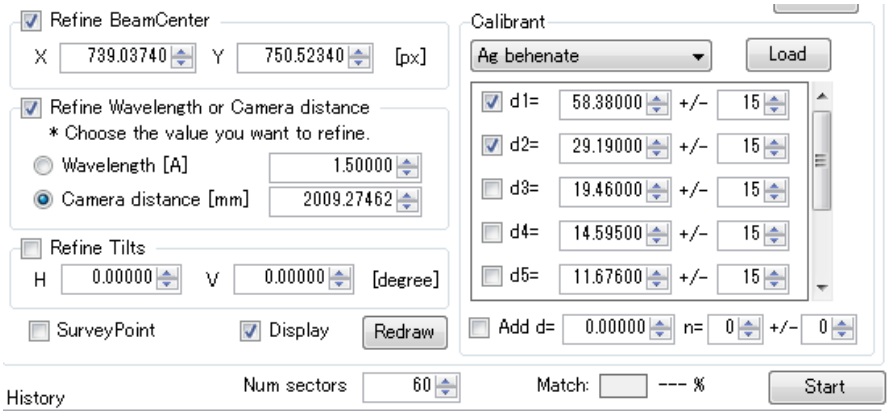
iii. Once selected, click "Draw" to display the file.

iv. If the display is too dim to see, click on the lamp mark and set [AVE] to 500 and [Bright] to 200 so that the ring pattern is visible.

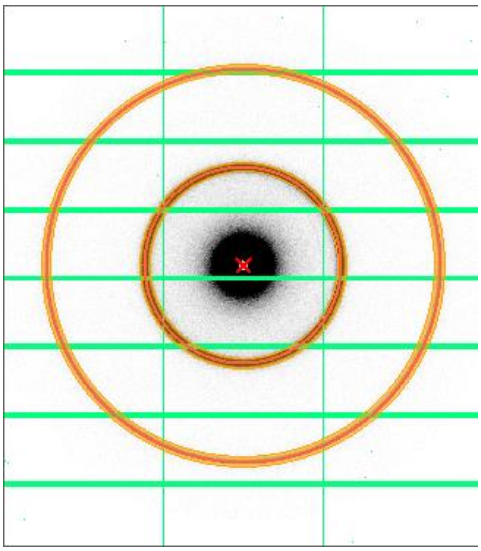
v. Check [Refine BeamCenter] and enter the approximate center coordinates. It is marked with a red × on the image. If it is in a completely different location, bring the mouse cursor near the beam center. Its coordinates will appear in the upper left corner of the image. Enter that value.
If the diffraction data used is wide-angle and there is no beam center in the image, the beam center can be set outside the image. (However, the margin is limited to 500px in both width and height.)

vi. Check [Refine Wavelength or Camera distance]. Since calibration of the measurement wavelength and camera length is performed exclusively, check either one and enter an approximate value.

vii. [Refine Tilts] corrects for detector tilt relative to the beam optical axis, where H is the angle



in the horizontal plane (detector is pivoting left or right) and V is the angle in the vertical plane (detector is leaning back or jawing). Note that the setting is set at a level that is not affected by normal small-angle scattering, so there is no need to calibrate it. If you wish to calibrate, check the box.



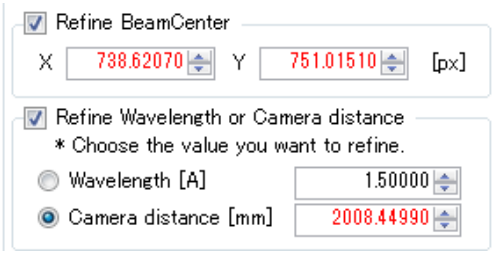
In the [Calibrant] column, select the parameter to be used from the pull-down menu. In the [Ag behenate (n1-5)] field, parameters up to the 5th order are entered. Here, d3 through d5 are erased and only d1 and d2 are used, since the loaded image only shows up to the second order ring. On the other hand, if the initially registered calibration standards are set separately from [Option] - [ConfigCustom], clicking [Load] will update the information in the pro-down menu.

viii. Check [Display] to display the Prediction based on the initial values. Edit the initial values so

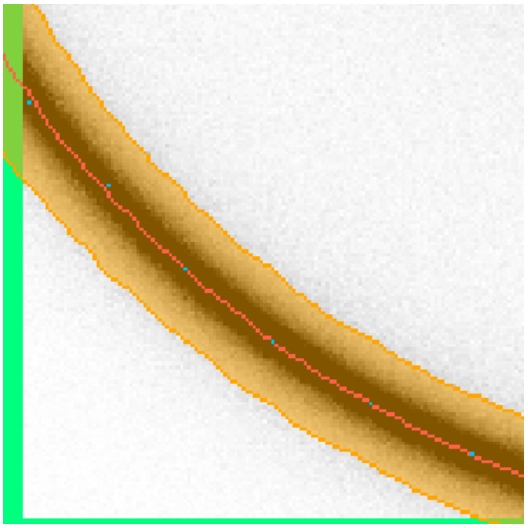
that the Prediction ring matches the actual ring. Press the [Redraw] button to recalculate the Prediction.

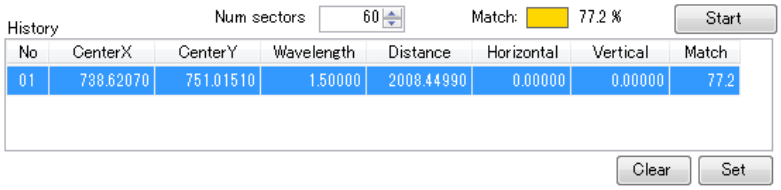
ix. [Num sectors] specifies how many divisions of the full 360-degree circumference of the ring pattern will be processed when Calibration is executed. The default setting is 360 (i.e., every 1 degree is processed).

x. When ready, click "Start. A dialog box will appear. Click "Yes" to execute. The calculation will be completed immediately and the calibrated value will be displayed in red.

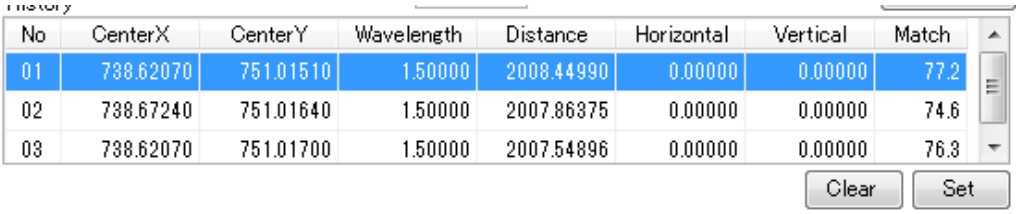


xi. A history of the calculation results is recorded as a table. The degree of agreement between the ring of each measured order and the Prediction ring obtained as a result of the calibration is indicated by [Match]. Specifically, each ring is divided into the number specified by [Num sectors], and the number of matches at that location.
For example, if [Num sectors] is set to 60, the ring positions are compared at 6 degree intervals. If you want to confirm the measured position on the ring in the data, check the [Survey Point] checkbox and the pixels will be displayed in light blue on the image data as shown below (it may take some time to render).





xii. Match is green ■ when more than 80% match, yellow ■ when 50-79% match, and red ■ when less than 50% match. Basically, the calculation is repeated until it appears green. The final step is complete when the value no longer fluctuates much. On the other hand, repeated calculations may be worse in the opposite direction. In that case, you can return to the value at that time by selecting the value (row) you want to return in the history table and clicking "Set" or double-clicking that row with the left mouse button. [Click "Clear" to delete the entire history. On the other hand, there may be cases, such as when the ring pattern does not exceed 80% no matter how many times you try, but the cause is simply poor S/N of the ring pattern in most cases. In other words, it is due to "insufficient exposure time". If it does not work, try extending the exposure time again and re-measuring.



xiii. When Calibration is finished, click "Save" to save the results. The file extension will automatically be "cal".Even if you close the software once or process it on a different PC, you can load a previously saved cal file and process it under the same conditions.

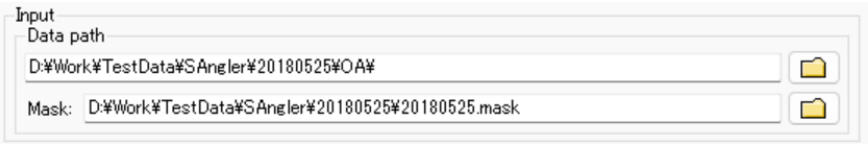
xi. This completes the Calibration process. Go to the【Ave】tab.

⑦ Circumferential average (Average)

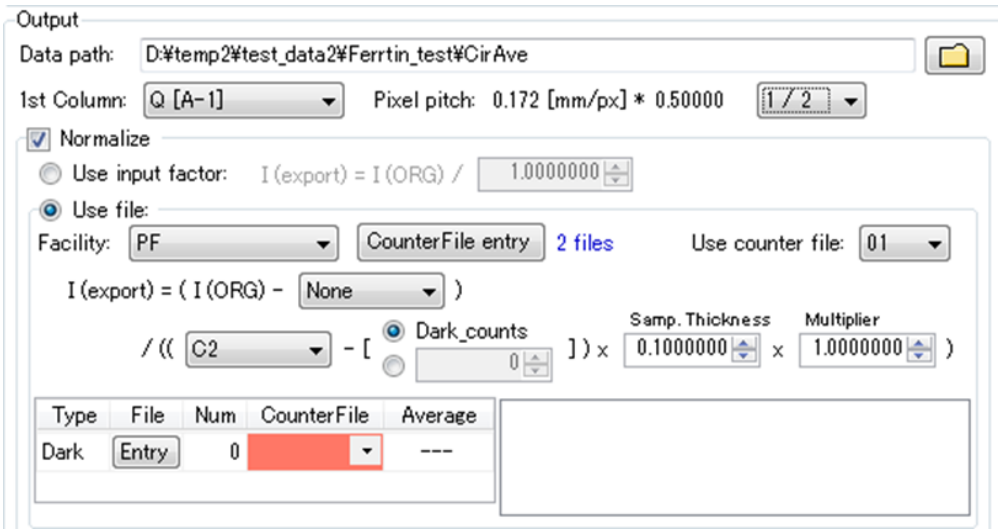
Based on the calibration results, circumferential averaging is performed. In circumferential averaging, there are basically two modes.

（1）To specify the measured data in order and process them

i. In the [Input] section, under [Data path], click the folder symbol to specify the folder where the image data is stored. This field can also be edited directly.



ii. For PILATUS data, make sure the MASK file you just created is selected. To load a previously processed MASK file, click on the folder symbol to specify it. Direct editing and Drag&Drop of target files are also possible.



iii. Next, set the [Output] item. iii. Specify the folder to output the circumferential averaged file in the [Data Path:] field. As with [Input], press the folder symbol, edit it directly, or set it up with Drag&Drop.

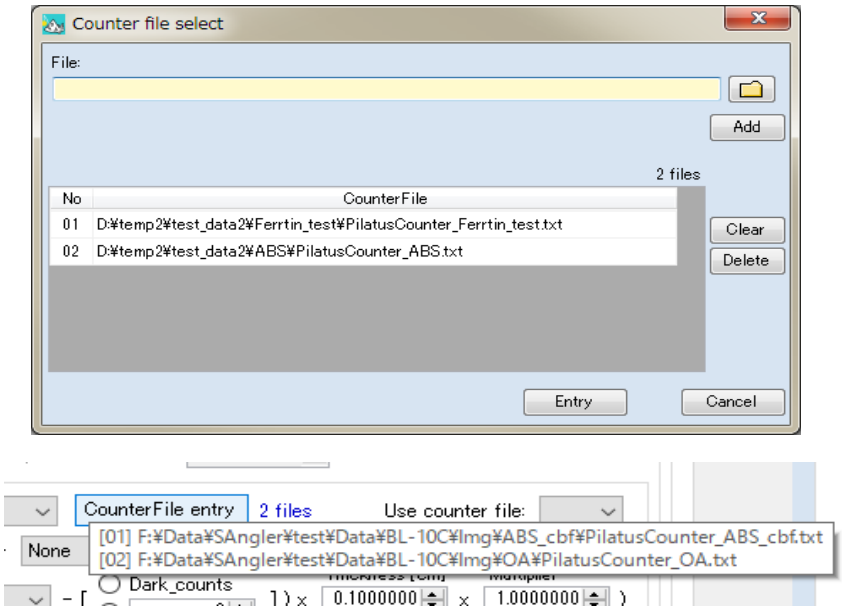
iv. Specify in which unit the horizontal axis（1st Column）of the data should be output.
Q (=4πsinθ/λ) [Å^{-1}]、Q [nm^{-1}]、S (=2sinθ/λ) [Å^{-1}]、S [nm^{-1}]、d [Å]、d [nm]、2θ [degree]、
r [mm]（Distance from beam center）

v. [Pixel pitch] allows you to change the spacing of the horizontal axis data. PILATUS pixel size is 0.172 x 0.172 mm, so data is output at 0.172 mm intervals (0.1 mm for R-AXIS). Here the data can be divided based on pixel size and set to output more finely spaced data. The default is "1/1," and if "1/2," "1/4," or "1/5" is selected, data will be output at that pitch. On the other hand, you can increase the number of measurement points, but if you make them too fine, the S/N will deteriorate. Check the output data and select the appropriate number of divisions (in BioSAXS, the default of 1/1 is acceptable in principle).

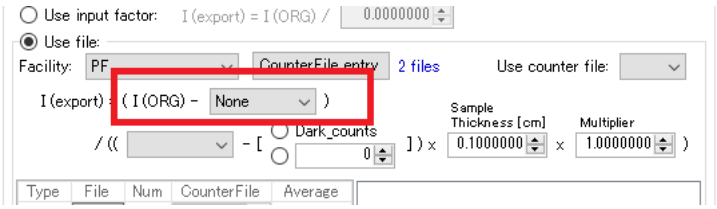
vi. Check [Normalize] to normalize the scattering intensity by the incident X-ray intensity, etc. To normalize the scattered intensity by a specific value, enter a value in the "Use input factor" field.

vii. To normalize using values such as (integral) intensity of incident X-rays, specify and read a log file of counter values in which intensity values are output separately from the image data. First, select [Facility], which corresponds to the counter file format for PF and SPring-8 BL38B1 and 40B2.

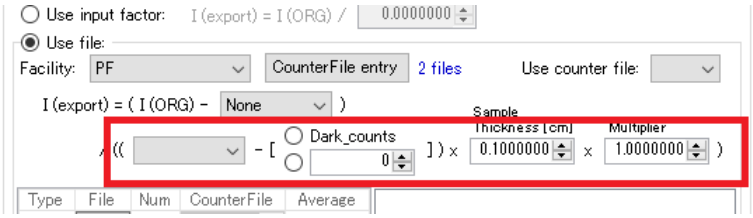
viii. Next, under "Counter File entry," set the counter file to be used. Click to open the [Counter file select] dialog box. Click on the folder symbol  to select the counter file, then press the [Add] button to move to the list column at the bottom of the dialog. This completes the selection. It is also possible to Drag&Drop a file into this field, in which case the selection will be completed immediately. On the other hand, if there are multiple counter files corresponding to the data you want to make one-dimensional, you can specify multiple counter files. For example, if the counter file corresponding to the actual data you want to process is different from the counter file corresponding to the dark level you measured before the experiment described in (xiv), you will have to read each of those files. Counter files are numbered in the order in which they are read, so later settings are specified by this number. In this manual, "01" is the counter file corresponding to the actual data and "02" is the counter file when the dark level is measured. Note that when the mouse cursor is hovered over the "Counter File entry" button, information on the registered counter files will pop up for 30 seconds. When settings are complete, click "Entry" to close.



ix. At [Use counter file:], select the counter file corresponding to the data to be converted to 1D. (viii) allows multiple counter files to be set up, but specifies what number among them.この In the manual, "01" is the counter file corresponding to the actual data, so select "01" from the pull-down menu.

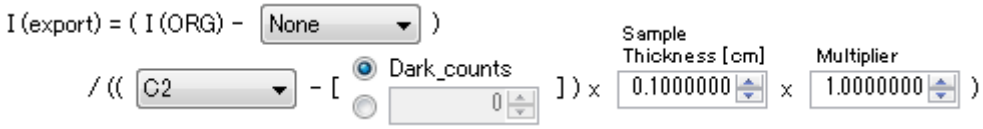


x. Next, the formula for performing circumferential averaging with actual normalization is given. Enter each field of that formula as you select it. First, the upper side of the equation (the so-called molecular side) sets whether the dark level of the detector is subtracted when the scattering intensity is circumferentially averaged. PILATUS does not have a dark level and does not need to be subtracted. Therefore, it remains [None]. On the other hand, R-AXIS has a dark level, so if you want to pre-measure and pull a dark image, select [I(Dark)]. Note that when measuring the R-AXIS dark image, it is recommended that you measure the same exposure time as the actual data (although this is not always necessary, it makes processing in SAngler easier). The R-AXIS dark image is not necessarily the same time as the actual data. On the other hand, the image file in which the dark level is actually measured is set in (xiii).



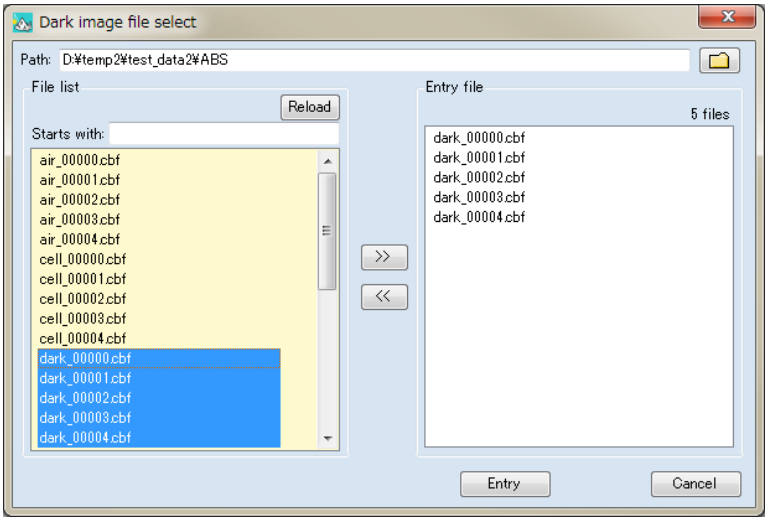
xi. Next, set the lower side of the equation (the so-called denominator side). First, select which channel values recorded in the counter file should be used for normalization. For PF, C2 is the value of the integrated intensity of incident X-rays measured in the microion chamber before the sample, and C4 is the value of the integrated intensity of transmitted X-rays measured by the Si PIN photodiode embedded in the direct beam stopper after the sample. Similarly, in BL38B1 at SPring-8, MIC up is incident intensity and BS is transmission intensity, and in 40B2, C3 is incident intensity and C4 is transmission intensity (please check with the person in charge to be sure).

xii. For PF and BL38B1, a dark level (dark count) exists in the value of this counter. In other words, the value is not zero if measured even in the absence of X-rays. This is because the measurement equipment is set up and used in such a way to ensure the linearity of data even in low count regions (please check with the person in charge for the status of each facility and beamline). Therefore, to normalize by the value of the channel specified in (xi), the dark count for that channel must be subtracted. Therefore, set up the system so that "the dark image is measured with the beamline shutter closed and with the same exposure time as the actual data, and the dark count value is used in the calculation. To do so, select [Dark_counts]. If you want to subtract a specific value as a dark count, toggle the radio button and enter the value there.

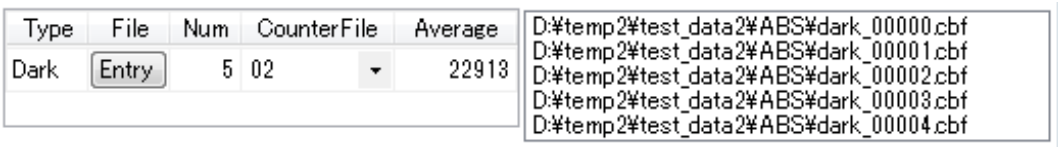


xiii. If [Dark_counts] is set, the table below specifies the actual dark images and the corresponding counter file numbers. [Clicking "Entry" opens a dialog to select a measured dark image. Press or directly edit the folder symbol to specify the folder with dark images in [Path:]. With the folder entered in the Path field, click Reload, and all image data in that folder will be displayed on the left side. Select multiple dark images at the same time (or a single image). For example, you can select multiple images by holding down the [ctrl] key and clicking multiple images, or simply click and drag multiple images with the mouse. [Starts with:] is a filter function that allows you to display only specific data sets by entering a string

of characters at the beginning of the filename that excludes other files. You can then press [ctrl + A] to select all of them. Clicking the right arrow [>>] moves the file to the right and confirms it. You can also delete the list from the Entry side by selecting the list on the [Entry file] side and pressing the [Enter] key or the [Delete] key, or by pressing the left arrow [<<] button. When you have completed your work, click "Entry" to close the dialog.

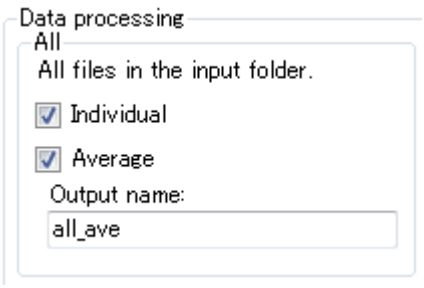


xiv. Specify the counter file corresponding to this dark image.（Since we have already set this up in (viii), here we select "02" from the pull-down menu (if unselected, this field will be displayed in "red"). (In the unselected state, this field is displayed in "red". The Average column of the table displays the average dark counts corresponding to the dark images you have set, and the right side of the table displays a list of the selected dark images. Note that the dark count is also an integral value, so it changes in proportion to the exposure time. Therefore, it is safe to measure with the same exposure time as the actual measurement data. Also, if the detector is PILATUS, it is better to measure multiple samples and use the average of the measurements, as is the case with sample measurements, since it is likely that measurements will be made by repeating short-time exposures and integrating (averaging) the results later.



xv. Finally, enter the sample thickness [Sample Thickness (cm)]. The unit is cm, and the default is 0.1 cm (1 mm). The solution cell manufactured by Unisok Corporation, which is used as standard in PF, has a thickness of 1.25 mm (0.125 cm), so please be careful to use the right one. Also, if you want to divide the scattering intensity by a specific value, enter a value in [Multiplier]. If you do not need it, you can leave it at "1". This completes the condition setting

for normalization.



xvi. Then, in the "Data processing" section, select the range of files to be processed. SAngler can process multiple files at once, but there are two main ways to specify this:【All】and【Range selection】.

(1) For【All】

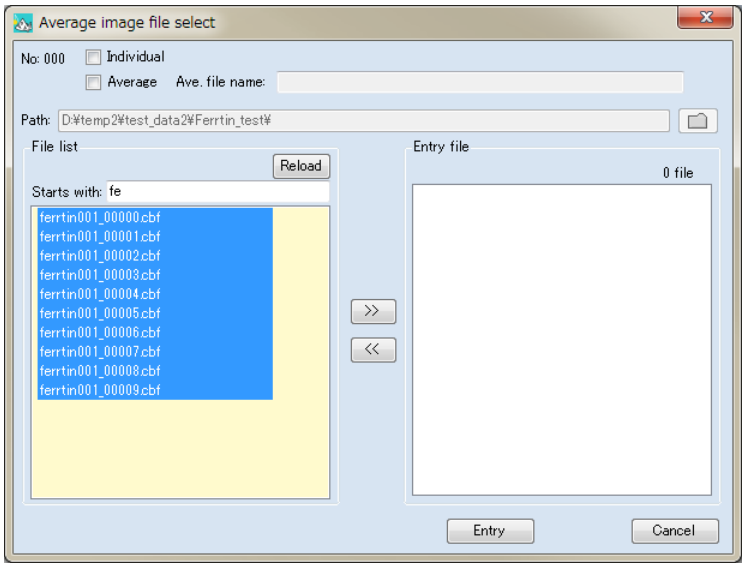
All image data in the previously specified [Input Data Path] folder will be processed at once. [Individual] averages all the image data in a folder individually around the circumference of each image. The output file name is the same as the image file name, only the extension is "dat". [Average] specifies the file name to average all images in this folder (the dat extension is automatically attached). You can run both Individual and Average, or only the one you select.

(2) For【Range selection】

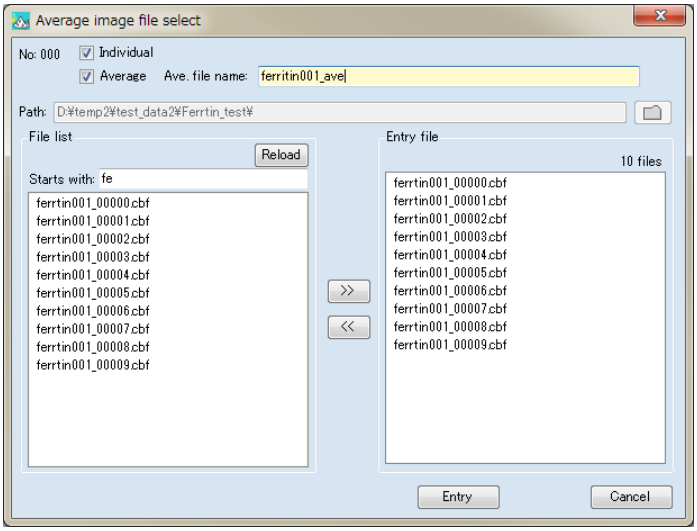
Specify the range of data to be processed in the [Input Data Path] folder. For example, you can specify a range of background data and a range of sample data to be processed separately.

A) Click [Add]. A separate window will open. The [File list] shows the current folder and the files in the folder.

B) Select multiple files to be loaded at the same time (or one file). You can also hold down the [ctrl] key and click to select multiple images, or simply click and drag with the mouse to select multiple images. [Starts with:] is a filter function that allows you to display only specific data sets by entering a string of characters at the beginning of the filename that excludes other files. You can then press [ctrl + A] to select all of them.

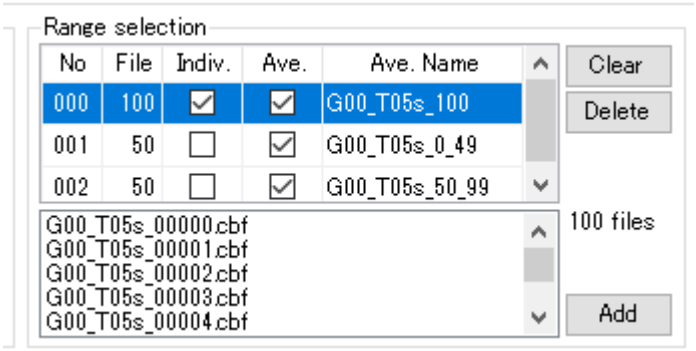


C) Click the right arrow [>>] to confirm the selected data. The file will then move to the right. Repeat the same operation for other files if necessary. Select whether you want to perform a circumferential average for each selected file individually (Individual), collectively (Average), or both. For [Individual], the file name remains the same and the file extension is dat. For [Average], enter the name of the file after averaging (the extension dat will be added automatically). When finished, click [Entry] to close the window.



D) In the [Range selection] field, the job you just set is entered. Click to display the list of files to be processed. If you wish to process other data sets simultaneously, repeat (A) ~ (C). Each job performs independent processing, so if different jobs specify different processing for the same image data, the instructions are executed without interference.

(Example) For a data set of 100 sheets named G00_T05s_00000.cbf ~ G00_T05s_00099.cbf



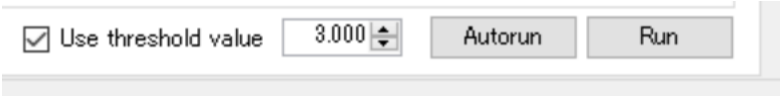
(Job1) Perform circumferential averaging of the 100 sheets by Individual and Average.

(Job2) Perform Average only for the first 50 sheets from 00000 to 00049.

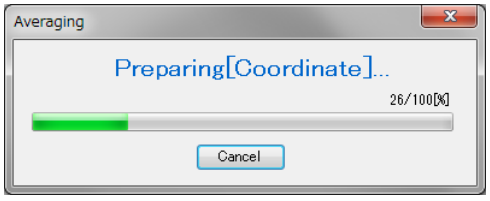
(Job3) Execute Average only for the second 50 sheets in the second half from 00050 to 00099.

Since 3 jobs are executed, 103 dat files will be output.

xvii. The [Mask] tab has a function "Uniformity" to pre-mask abnormal pixels found during circumferential averaging. However, this function cannot handle cases such as when a zinger (a spike-like peak caused by the detection of cosmic rays during measurement, etc.) is observed. Similar to the Uniformity function, this【Ave】tab has a function to determine the pixel values to be excluded from the circumferential average based on the Threshold value (threshold value) when the actual data is averaged circumferentially. If the [Use threshold] checkbox is checked and a threshold value is set, an abnormality judgment is made at any time during analysis, and the results reflecting this judgment are output. For example, it is possible to exclude aberrant values that occur suddenly, such as pixels (Zinger) where cosmic rays, etc., have been detected. The default value is set to 3.0. When the Uniformity function of [Mask] is used, the Threshold value set at that time is automatically included, but it can be changed to another value. On the other hand, the time required for circumferential averaging is longer, since the average value data is created once for each image data before the abnormality judgment process is performed. Therefore, since Ver. 2.1.34, parallel processing can be performed utilizing the multi-threaded environment during circumferential averaging.



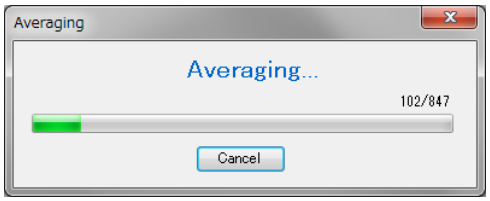
xviii. When you have completed the entry, click the "Run" button to execute. Only when SAngler is started and done for the first time, the "Preparing [Coordinate]..." dialog will appear first. This is done to speed up the circumferential averaging process and is not displayed after the second time. However, if Calibration is redone, it will be performed again.



xix. When "Preparing..." is completed, circumferential averaging begins (from the second time, circumferential averaging begins immediately). With PILATUS3 2M and multithreading off, it takes about 1 second per image if the pixel pitch is left at the default (the finer the pixel pitch, the longer it will take). The time required is about 1 second per image if the pixel pitch is left at the default setting. When averaging multiple sheets, the number of sheets will vary depending on the number of sheets. If a multi-threaded environment is applied (3. ②Config Setting), the processing speed will vary depending on the environment. Individual processing" takes priority over "Average processing" for multiple jobs entered. For example, for the three jobs 000, 001, and 002 shown in (xvi.) (2) D), all Individual processing is performed first, followed by Average processing for each job after completion.

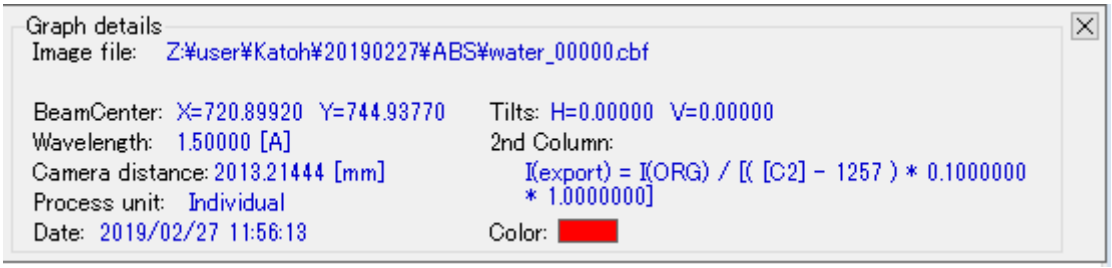
(e.g.) (xvi.) In the case of diagram (2) D), the following order of processing is used.

1. 00000～0009 Individual
2. Average of 00000～0009
3. Average of 00000～00049
4. Average of 00050～00099

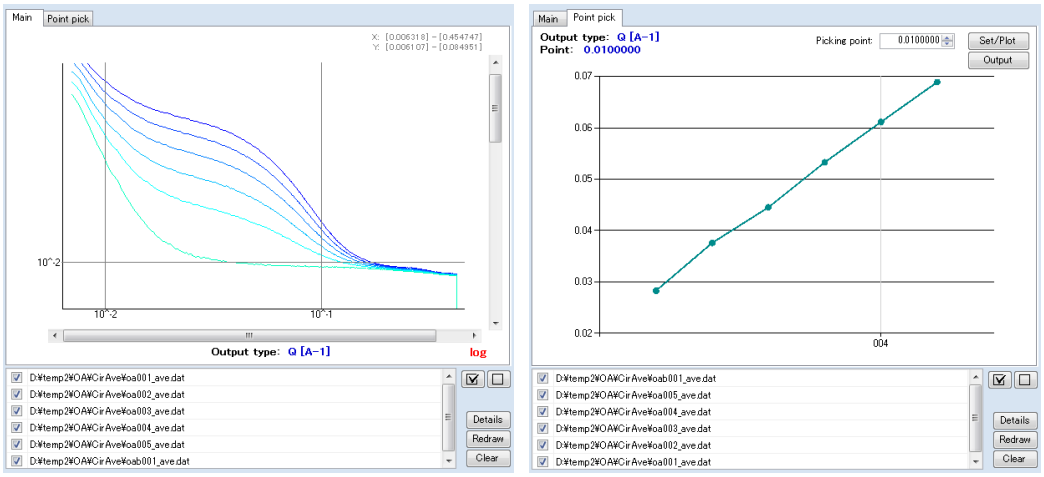


xx. When all processing is complete, the graph will be displayed in a double-log plot. The graph can be zoomed in and out by scrolling the mouse or by left-clicking and dragging the desired area. You can select which graphs to display by checking or unchecking the checkboxes below and clicking "Redraw. [Clear] will erase all the data. Drag&Drop a dat file into the columns of this table to display the graph. [Clicking on "Details" will show data header

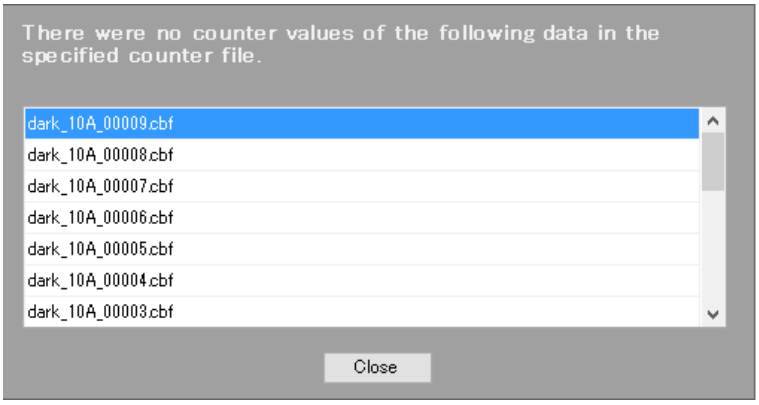
information at the top of the SAngler window.



xxi. The graph window has two displays. One is the【Main】tab, which shows the entire scattering curve. Another【Point pick】tab allows you to plot the vertical axis values (scatter intensity) against a specific horizontal axis value of the data being read. For example, to display a plot of scattering intensity for Q [Å-1]=0.01, enter 0.01 in the [Picking point:] field and click [Set/Plot]. By plotting the change in scattering intensity near the small angle, the presence or absence of effects due to radiation damage can be confirmed. It is also possible to output the data from this plot. Click [Output] to save the data as text data.



xxii. If the counter file specified to normalize the scattering intensity is incorrect, the circumferential averaging process may end quickly. Specifically, this is the case when the counter file specified in viii and ix is incorrectly numbered, the count value of the image data to be processed does not exist in that file in the first place, or the counter file was forgotten to be changed when the folder where the data is stored was changed. If this is the case, re-specify the correct file or number.



※Derivation of standard errors

I. Circumferential averaging of data from N pixels at distance r from the beam center.

II. The average x_m of the N data x_1, x_2, …, x_N is as follows.

$$x_m = \frac{1}{N}\sum_{i=1}^{N} x_i$$

III. The variance V with respect to the mean x_m is as follows.

$$\mathrm{V} = \frac{1}{N}\sum_{i=1}^{N} (x_i - x_m)^2$$

IV. since the square root of variance V is the Standard Deviation SD (Standard Deviation),

$$\mathrm{SD} = \sqrt{V}$$

V. The Standard Error SE (Standard Error) is the following relation by the error propagation law. This value is output.

$$\mathrm{SE} = \frac{SD}{\sqrt{N}}$$

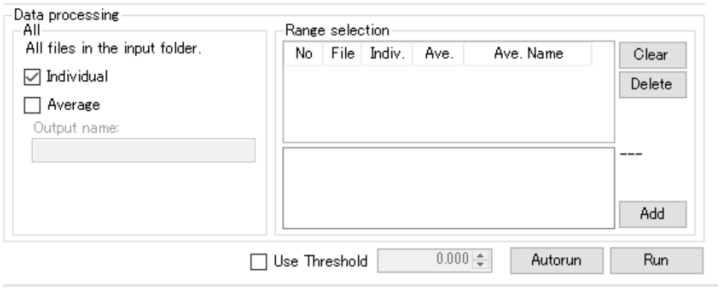
※When performing circumferential averaging by averaging multiple images, all images to be averaged are first integrated before the circumferential averaging process is performed.

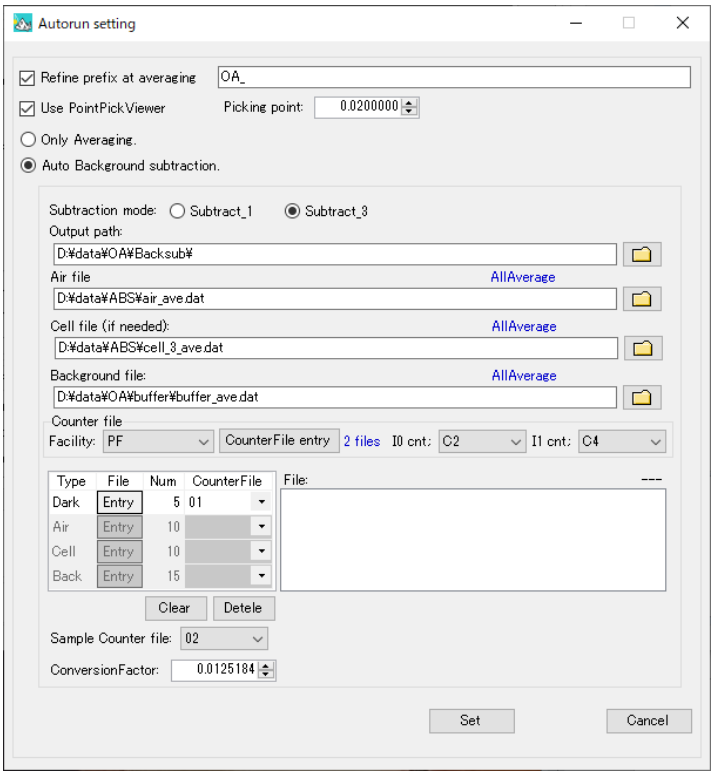
（2） When monitoring a specified folder and automatically performing circumscription averaging (Autorun) of updated image data (background subtraction can also be performed automatically at the same time)

It can monitor the folder where image data is created and automatically perform circumferential average [Average] and background subtraction [Sub_1 or 3] processing. The results can be plotted as matrix data in three dimensions, or displayed and created as a one-dimensional plot of the change in value of a specified X coordinate (PointPickViewer.exe).

i. First, as a preliminary preparation, perform steps (i) through (xv) in (1) to set up the system.

ii. Autorun processing is basically on an individual file basis. Under [Data processing] - [All], check [Individual] and click [Autorun]. The Autorun setting window opens.





iii. In (i), the data storage folder to be monitored is specified. If there are multiple data sets in a folder and you wish to analyze only files that contain a specific string in the file name, check [Refine prefix at averaging] and enter the target string.

iv. Check "Use Point Pick Viewer" if you want to display the processing results automatically during Autorun. If you want to pick up a specific X-coordinate value, enter the value of that X-coordinate in the Picking Point. For example, for Q(Å-1), we usually put in a value such as 0.02.

v. Select the processing method.

- Perform circumferential averaging only … Select "Only Averaging".
- Select "Auto Background subtraction" to automatically perform Background subtraction after circumferential averaging as well.

vi. If Auto Background subtraction is checked, select subtraction mode.

- Sub_1 processing after circumferential averaging … Select [Subtract_1].
- Sub_3 processing after circumferential averaging … Select [Subtract_3].

For details on Subtraction mode, see (10) to (12) (Subtraction of Background 1 to 3) in the latter section.

A. if [Subtract_1] is selected.

B. In [Output path], specify the folder where the data will be output after the Background is subtracted. Click on a folder symbol  to specify it, or edit directly in the blank box.

C. Specify the Background file (dat file) to be used. You can specify files by clicking on the folder symbol  , by editing directly in the blank box, or even by Drag&Drop a dat file into the blank box. Background files must be circumferentially averaged and one-dimensional in advance.

vii. if [Subtract_3] is selected.

A. In the [Output path] field, specify the folder where the data will be output after the Background is subtracted. Click on a folder symbol  to specify it, or edit directly in the blank box.

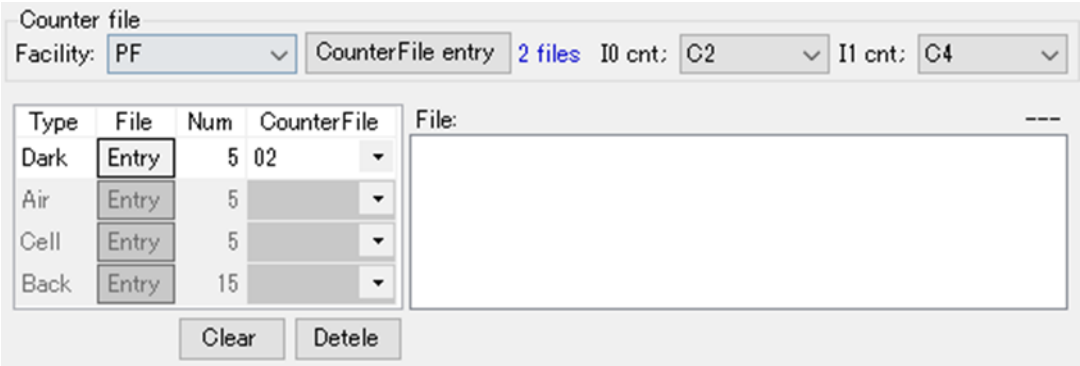
B. If you have previously performed the "absolute scattering intensity (cm-1) conversion of scattering intensity (counts)" using water or Glassy Carbon as described in ⑬ABS_W and ⑭ABS_GC, the [Air file:], [Cell file (if needed):] specified during that process file is

entered. If not performed, specify air scattering data (Air file) and sample cell data (cell only data without sample, Cell file) (both are dat files). You can specify files by clicking on the folder symbol, by editing directly in the blank box, or even by Drag&Drop a dat file into the blank box. Since it is a dat file, it must be circumferentially averaged and made 1-dimensional in advance.

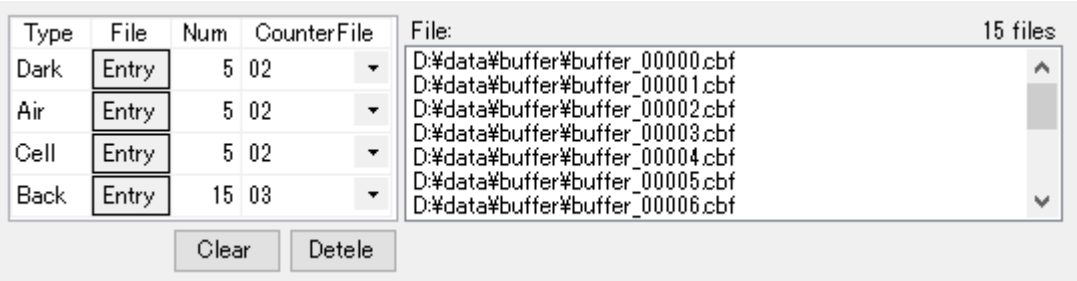
C. Specify the Background file (dat file) to be used. You can specify files by clicking on the folder symbol, by editing directly in the blank box, or even by Drag&Drop a dat file into the blank box. Background files must be circumferentially averaged and one-dimensional in advance.

viii. In [Counter file], the counter file information set earlier in the [Ave] tab is loaded. I0 cnt specifies the channel of incident X-ray (integral) intensity measured before the sample and I1 cnt specifies the channel of transmitted X-ray (integral) intensity measured after the sample. For PF, C2 is the incident intensity and C4 is the transmitted intensity. In BL38B1 at SPring-8, MIC up is the incident intensity and BS is the transmission intensity; in 40B2, C3 is the incident intensity and C4 is the transmission intensity (check with the person in charge to be sure).

ix. For each Air, Cell, and Background file, " Individual " is displayed in the column if the file has been processed individually, or " All Average " if the file is averaged from multiple pieces of data. On the other hand, if the file was processed with Ver. 2.0.7 or earlier, the integral intensity (counter value) of the beam being exposed is not recorded in the header of the file, so it is necessary to read the counter file to be used separately from the dat file and specify the data corresponding to Air, Cell, Background The data corresponding to Air, Cell, and Background must be specified. ⑦ **Circumferential Average (Average) (1) Set the corresponding files and counter files for Air, Cell, and Background by referring to the Dark file designation method described in (xiii.) in the case of processing measured data by specifying them in order.**



●When using files processed with Ver. 2.1.0 or later, the counter value information used in the circumferential averaging process is recorded in the header of the dat file, so when the Air, Cell, and Background dat files are read, the counter information table is shaded gray and no input is required. The counter information table will be shaded gray and no input is required.



●If you use a file prior to Ver. 2.0.7, you need to specify the counter value information to be used again, as in the case of Dark.

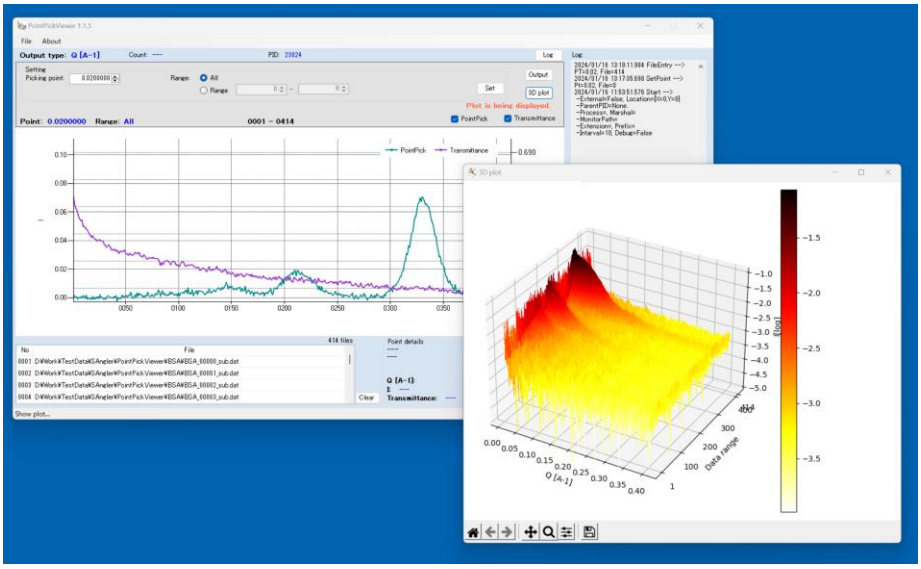
x. In [Sample Counter file], set the counter file number of the sample counter file specified in [Counter File entry]. The counter file number set in the Ave tab is displayed as the initial value. Please change it according to your conditions.

xi. [Conversion Factor (conversion value for normalization to absolute scattering intensity)] is explained in **⑬ABS_W and ⑭ABS_GC.** If you run the program first, the values should be automatically loaded here. If not, check the value and enter it manually, or leave it at 1.0000000 if it is not necessary.

xii. Click "Set" to display a dialog box to confirm the condition.

When [Use Point Pick Viewer] is checked, the Point Pick Viewer will be started and the automatic processing will proceed at the time interval set in (vii.) of **②Config Setting.**

⑧ PointPickViewer



By reading a set of continuous scattering curve data (dat) and specifying the X-coordinate to be picked up, changes in scattering intensity and X-ray transmission by the sample (*) are plotted simultaneously in one dimension. It also displays a 3D plot of the entire scattering curve data set loaded by pressing the [3D Plot] button in a separate window.

※ Depending on the dat file loaded, transmittance changes may not be plotted.

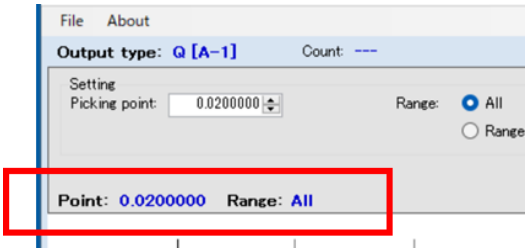
【Point Pick plot】

Load the dat file and set the X coordinate you want to pick up in the [Picking point] column to display the graph.

[PickingPoint]: Enter the X coordinate value you wish to pick up.

[Range]: You can specify the range of data to be displayed. Select "All" to display all dat data read, or "Range" to specify a range, and enter a numerical value.
If only the start position is set and the end position is entered as 0, the display will start from the start position to the end.

[Set]: Press the button to draw a PointPick graph based on the set PickingPoints and display range. The currently set PickingPoints and ranges are displayed at the top of the Plot.



[PointPick][Transmittance]:

For Dat files that have been averaged only, only PointPick will be displayed; for Dat files with background subtracted, both PointPick and Transmittance graphs will be displayed. This check box allows the user to toggle between showing and hiding.

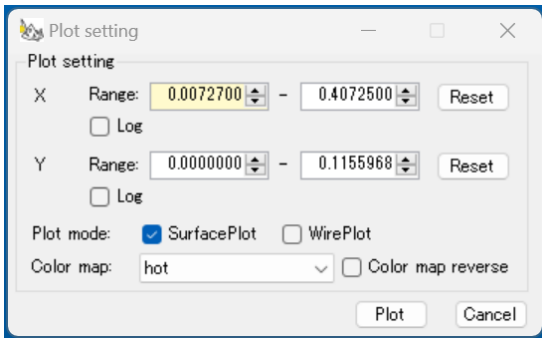
Note that when the PointPick and Transmittance graphs are displayed, the left side of the Y-axis (scattering intensity: I) and the right side of the Y-axis (X-ray transmittance by the sample (Transmittance)) are on different scales.

[Point details]:

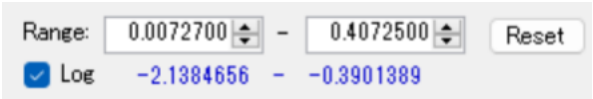
Click on each point in the plot to select that point. Detailed information about the selected point is displayed in [Point details:] in the lower right corner of the plot.

【3D plot】

With the dat file loaded, click the "3D Plot" button to display the settings dialog. When pressing the “Plot” button after setting them, the 3D plot window will appear. You make settings for each axis (The 3D plot uses Matplotlib in Python.).



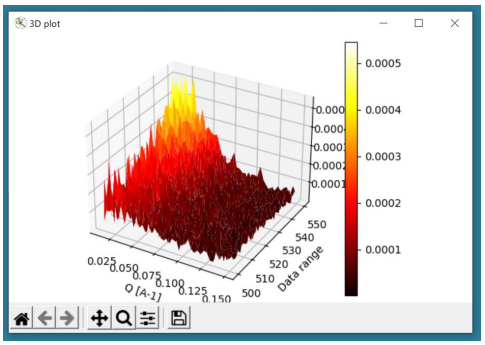
[Range]: You can specify the display area. The initially displayed values are the minimum and maximum values of the data in the dat file specified by PointPick. If you want to display the log, check the Log checkbox, and the logged range will be displayed below.



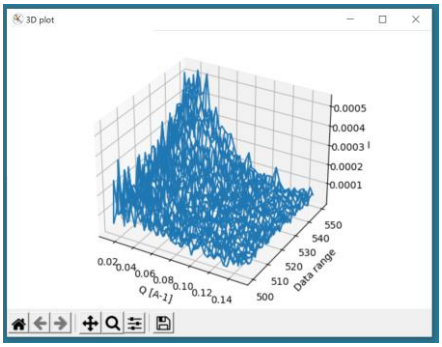
The display area is limited. In this 3D plot, **if there is a negative value in the Y-axis data, that data point will not be read (treated as Nan).** Therefore, in the case of linear plot, the Y-axis is basically a display range above zero. On the other hand, in the case of Log plot, zero is also not allowed. If a value below zero is entered, pressing the [Plot] button will result in an error; in Log plot, the text color will warn the user when the value is entered.

If you want to return to the original full range after specifying any range, press the "Reset" button.

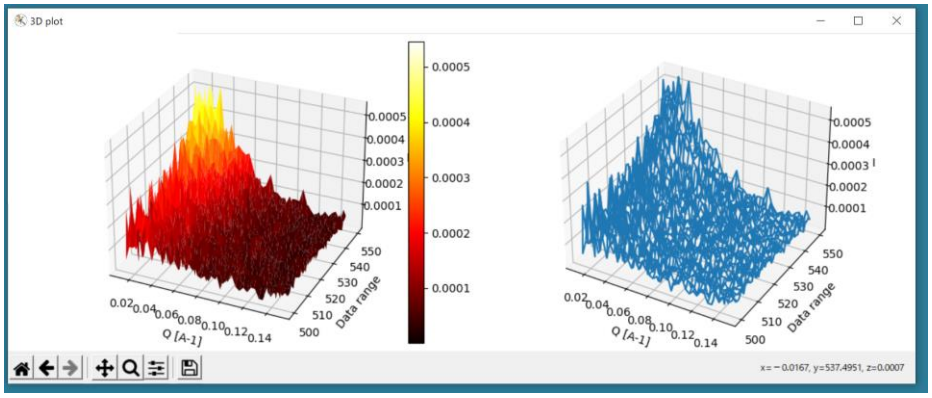
[Plot mode]: The 3D Plot can display two types of graphs: "Surface Plot" and "Wire Plot". Check the checkboxes for the graphs you wish to display. If both are checked, they can be displayed at the same time.



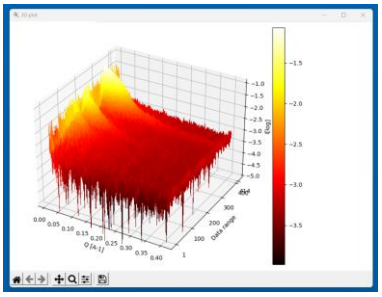
Surface plot



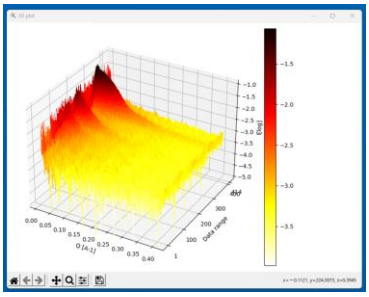
Wire plot



[Color map]: You may specify it from any colormap registered in Matplotlib. The default setting is "hot". If you want to change it, select it from the combo box. If you want to reverse the colormap, check "Color map reverse".



Color map: hot



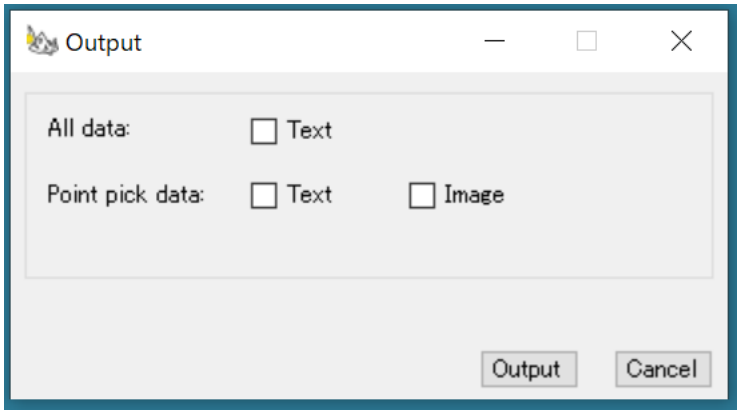
Color map: hot [reverse]

The plot window plots the state of **the data at the time it was read**; if the dat data is read again, or the data is updated during folder monitoring, etc., close the 3D Plot window and press the [3D Plot] button again to display the 3D Plot window again.

【Output】

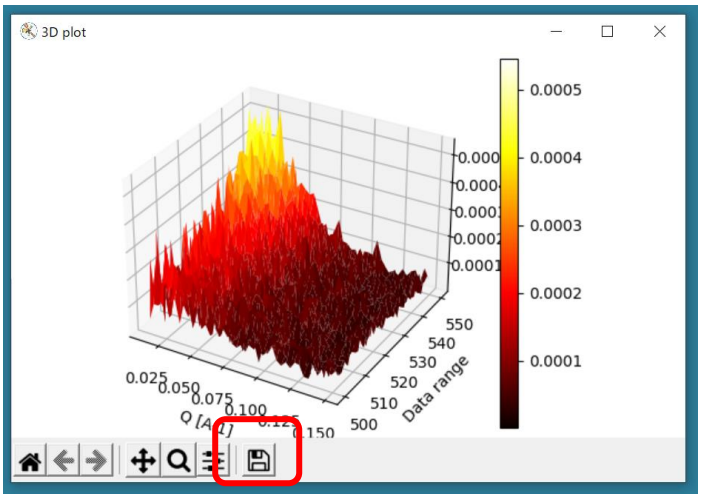
All data, PointPick graph text data (dat), and PointPick graph images can be output.

Press the [Output] button or select the menu [File]-[Output] to display the output dialog box.



[All data]: To output all read data as a single file, check the [Text] checkbox under [All data].
[Point pick data]: To output only PointPick graphs, check the [Text] checkbox for text output and the [Image] checkbox for image output.
[Output]: After setting the output conditions, press the [Output] button.

※If PickkingPoint is not specified after reading dat data, only all data can be output.
※To output the 3D plot image, press the Save button in the 3D plot window.

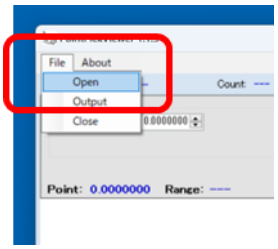


●Point Pick Viewer can also be started independently of SAngler.

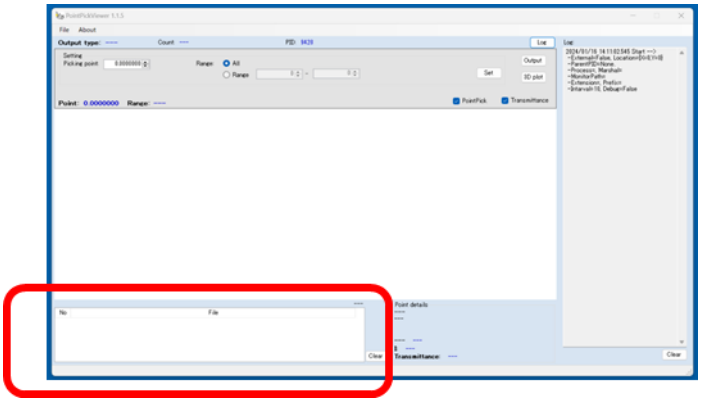
【Normal startup time】

i. Select SAngler's menu [Tools] - [PointPickViewer] to start.
(It can also be started by double-clicking PointPickViewer.exe directly.)

ii. Drag&Drop the dat file you want to display to the table section in the lower left of the window, or select the dat file in the dialog box displayed by the menu [File]-[Open] to load the dat data. A list of loaded files is displayed in the list at the bottom. The file is read in as an "append". Clicking the [Clear] button clears the loaded data. If a file has been added by mistake, press the "Clear" button once to reset the file, and then add the file again.



or



[File] – [Open]

Drag & Drop to this area.

Enter the value of the X coordinate you wish to display in the [Picking Point] field, set the [Range] if necessary, and click the [Set] button to display the graph below. For Dat files that have been averaged only, only PointPick will be displayed; for Dat files with background subtracted, both PointPick and Transmittance graphs will be displayed. (You can also switch between the two.)

iii. Once the dat data has been loaded, the 3D plot can be drawn. Click the [3D Plot] button, set the X and Y axis display range, plot type (Linear or Log), and color map in the dialog box, and click the [Plot] button to display the 3D plot.

iv. All data read can be output as text data, or if PickkingPoint is set, PointPick graph images and text data can be output. Output can be done by clicking on the [Output] button or the menu item [File]-[Output]. To output a 3D plot image, use the Save button in the 3D Plot window.

v. To exit, press Form × or Menu [File]-[Close]. An output confirmation message is displayed at the end of the process. If a previous output was made, its file name will be displayed together. (When exiting, if the 3D plot window is open, you will not be able to exit. Please close the 3D plot window before exiting PointPickViewer.)

【When monitoring folders】

i. When "PickingPoint" is specified in the [Autorun] process in the [Ave] tab and the Autorun process is started, PointPickViewer will start in the folder monitoring mode. SAngler proceeds with automatic processing at set intervals, so dat files are loaded and automatically drawn in accordance with progress.

ii. When loading dat files, operations that do not interfere with data loading, such as setting PickkingPoint, can be performed. No other operations can be performed while the screen is being drawn. Only [PickingPoint] can be changed except when loading.

iii. When the monitoring mode is terminated in SAngler, the monitoring is also terminated in PointPickViewer. If monitoring is started again by SAngler, PointPickViewer will also resume monitoring.

※ Once the linkage with SAngler is disconnected, it behaves the same as a normal startup. To link with SAngler again, close PointPickViewer once and start it from SAngler.

※Header of output file (circumferential average only)

（1）For Individual processing

```
# Date: 2020/05/20 15:21:41
# SAngler Version: 2.1.36
# Type: ImgAverage
# BeamCenter X: 720.89920/ Y: 744.93770
# Wavelength: 1.50000
# Camera distance: 2013.21444
# PixPitch: 0.172 * 0.50000
# Tilts H: 0.00000/ V: 0.00000
# Image: D:¥data¥sample¥sample_00000.cbf
# Unit: Individual
# Counter file: D:¥data¥sample¥PilatusCounter_sample.txt
# Ch: [C1]6548045.000     [C2]271137.000   [C3]0.000          [C4]326187.000   [C5]0.000
          [C6]0.000          [C7]0.000          [C8]0.000
##
# 1st. Column: Q [A-1]
# 2nd. Column: I(export) = I(ORG) / [( [C2] - 1257 ) * 0.1000000 * 1.0000000]
# 3rd. Column: SE I(export) = SE I(ORG) / [( [C2] - 1257 ) * 0.1000000 * 1.0000000]
# SE = Standard error.
# Dark File: 5 files
# - D:¥data¥ABS¥dark_00000.cbf
# - D:¥data¥ABS¥dark_00001.cbf
# - D:¥data¥ABS¥dark_00002.cbf
# - D:¥data¥ABS¥dark_00003.cbf
# - D:¥data¥ABS¥dark_00004.cbf
# DarkCh: [C1]7711436.000          [C2]1257.000     [C3]0.000          [C4]1056.800
          [C5]0.000          [C6]0.000          [C7]0.000          [C8]0.000
# DarkCounts(Average): 1257.000
# SampleThickness[cm]: 0.1000000
# Multiplier: 1.0000000
# Threshold: None.
##
## Version: VERSION 1.5, CBFlib v0.7.8 - PILATUS detectors
## Detector: PILATUS3 2M, S/N 24-0116
## Measurement Date: 2019-02-27T22:38:38.005
## PixelSize: 172e-6 m x 172e-6 m
```

Silicon sensor, thickness 0.000320 m
Exposure Time: 20.0000000 s
Exposure Period: 20.0100000 s
Tau: 0 s
Count CutOff: 1061219
Threshold Setting: 4132 eV
Gain Setting: autog (vrf = 1.000)
N Excluded Pixels: 207
Excluded Pixels: badpix_mask.tif
Flat Field: FF_p24-0116_E8265_T4132_vrf_m0p100.tif
Trim File: p24-0116_E8265_T4132.bin
Ratecorr Lut Directory: ContinuousStandard_v1.1
##
Number of DATA: 1545
0.00483126178742133 0.00471187718391302 5.81627082733806E-05
0.00501019722061095 0.00436550658493805 0.000123891946896222
0.00518913263322968 0.00398326188821211 0.000125698913737578
: : :

（2）For Average processing (average processing of multiple files)
Date: 2020/05/20 16:49:32
SAngler Version: 2.1.36
Type: ImgAverage
BeamCenter X: 720.89920/ Y: 744.93770
Wavelength: 1.50000
Camera distance: 2013.21444
PixPitch: 0.172 * 0.50000
Tilts H: 0.00000/ V: 0.00000
Image: D:¥data¥sample¥sample_00000.cbf
Image: D:¥data¥sample¥sample_00001.cbf
Image: D:¥data¥sample¥sample_00002.cbf
Image: D:¥data¥sample¥sample_00003.cbf
Image: D:¥data¥sample¥sample_00004.cbf
Image: D:¥data¥sample¥sample_00005.cbf
Image: D:¥data¥sample¥sample_00006.cbf
Image: D:¥data¥sample¥sample_00007.cbf
Image: D:¥data¥sample¥sample_00008.cbf
Image: D:¥data¥sample¥sample_00009.cbf

Unit: AllAverage
Counter file: D:¥data¥sample¥PilatusCounter_sample.txt
Ch: [C1]6541457.500 [C2]270717.900 [C3]0.000 [C4]325850.600 [C5]0.000
[C6]0.000 [C7]0.000 [C8]0.000
##
1st. Column: Q [A-1]
2nd. Column: I(export) = I(ORG) / [([C2] - 1257) * 0.1000000 * 1.0000000]
3rd. Column: SE I(export) = SE I(ORG) / [([C2] - 1257) * 0.1000000 * 1.0000000]
SE = Standard error.
Dark File: 5 files
- D:¥data¥ABS¥dark_00000.cbf
- D:¥data¥ABS¥dark_00001.cbf
- D:¥data¥ABS¥dark_00002.cbf
- D:¥data¥ABS¥dark_00003.cbf
- D:¥data¥ABS¥dark_00004.cbf
DarkCh: [C1]7711436.000 [C2]1257.000 [C3]0.000 [C4]1056.800
[C5]0.000 [C6]0.000 [C7]0.000 [C8]0.000
DarkCounts(Average): 1257.000
SampleThickness[cm]: 0.1000000
Multiplier: 1.0000000
Threshold: 0.400
##
Version: VERSION 1.5, CBFlib v0.7.8 - PILATUS detectors
Detector: PILATUS3 2M, S/N 24-0116
Measurement Date: 2019-02-27T22:38:38.005
PixelSize: 172e-6 m x 172e-6 m
Silicon sensor, thickness 0.000320 m
Exposure Time: 20.0000000 s
Exposure Period: 20.0100000 s
Tau: 0 s
Count CutOff: 1061219
Threshold Setting: 4132 eV
Gain Setting: autog (vrf = 1.000)
N Excluded Pixels: 207
Excluded Pixels: badpix_mask.tif
Flat Field: FF_p24-0116_E8265_T4132_vrf_m0p100.tif
Trim File: p24-0116_E8265_T4132.bin
Ratecorr Lut Directory: ContinuousStandard_v1.1

##
Number of DATA: 1545

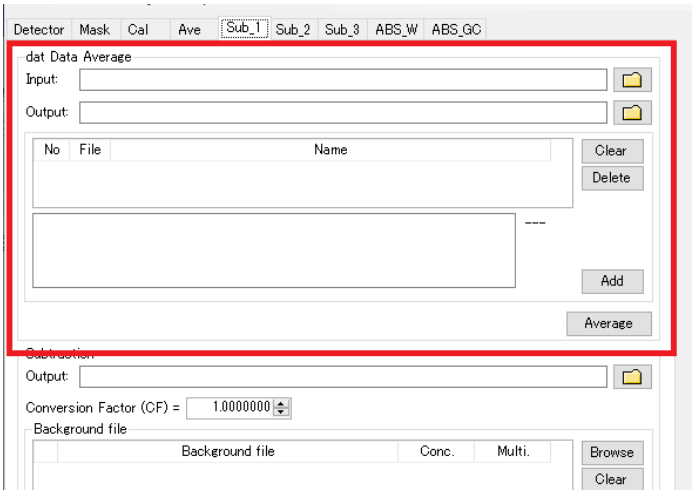
0.00735588299689442	0.0192514741809156	0.00209853198579806
0.00776454270765224	0.0180931033805649	0.000952245234077713
0.00817320234450698	0.0138984048003198	0.000594581681742784
:	:	:

Date	Data output date
SAnger Version	SAngler Version
Type	Output Data Type
BeamCenter	Beam Center
Wavelength	wavelength
Camera distance	Camera length
PixPitch	Pixel pitch
Tilts H: / V:	slope (of a linear function)
Image	image file
Unit	Single Analysis/Additional Analysis
Counter file	counter file
Ch	Counter value [by Ch] (individual: single value/ total: average value)
1st. Column	1st column data
2nd. Column	2nd column data
3rd. Column	3rd column data
Dark File	dark file
DarcCh	Dark counter average [by Ch].
DarkCounts(Average)	Dark Counter Average
SampleThickness	Sample Thickness
Multiplier	multiplier
Threshold	Threshold
##	Header data for image data
Number of Data	Number of rows of data

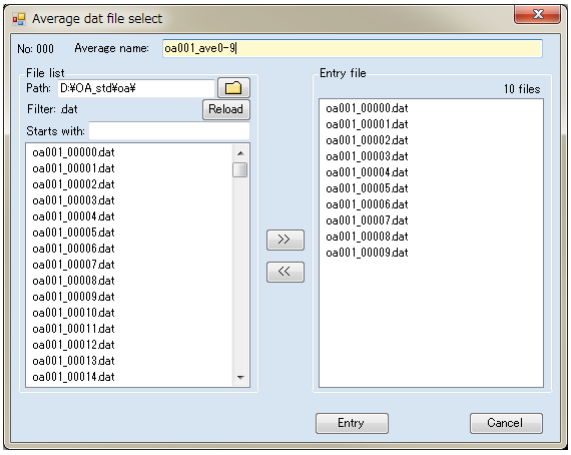
The output data contains three columns of data: the first column contains the specified abscissa (Q (Å-1), etc.), the second column contains the scattering intensity I, and the third column contains the standard error of the scattering intensity σI. If normalization of scattering intensity is specified, the values in the second and third columns are the normalized values.

⑨ Average of dat file after circumferential averaging (DatAverage)

The [Sub_1] tab provides "Tools for averaging dat files after circumferential averaging" in the upper row and "Tools for subtracting background" in the lower row. First, let us discuss the averaging of dat files.



i. [Input:] is automatically populated with the [Output] folder specified in Averaging. If you start here, click on the folder symbol to specify the folder where the dat files are stored. This field can also be edited directly.



ii. In [Output:], specify the folder to which the averaged files will be output. Press the folder symbol or edit it directly (copy-paste if it is the same as Input).

iii. Click "Add" to specify the dat file to be averaged as in the previous section on Averaging. After entering the output averaged file name, click "Entry" to close.

iv. If you want to average yet another set of data, click [Add] to add more.

v. When you are finished, click on "Average. An averaged file is output and a graph is displayed. In the output file, the header clearly indicates which file was used for averaging, and the values of the horizontal axis, such as Q, the scattering intensity I, and the standard error of the scattering intensity σI are output. Standard errors are recalculated according to the error propagation rule.

※Error after dat file averaging

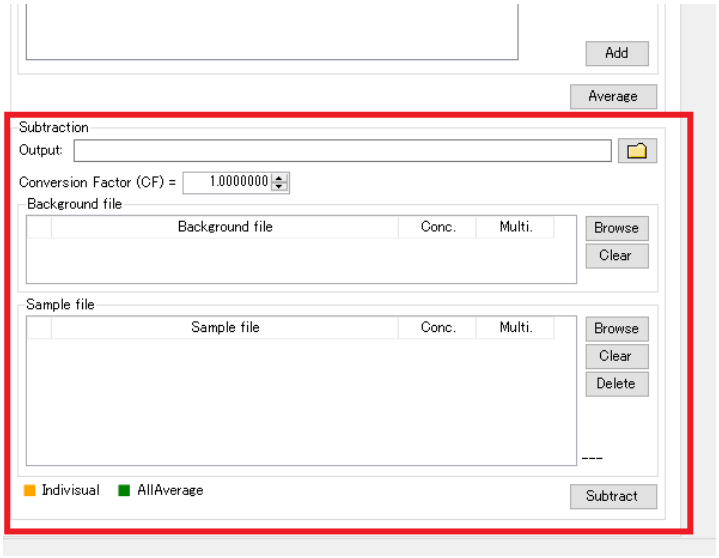
N data $x_1 \pm \sigma_1$, $x_2 \pm \sigma_2$ ..., with errors σ The average value $x_m \pm \sigma_m$ of $x_N \pm \sigma_N$ is obtained according to the error propagation rule by the following equation.

$$x_m \pm \sigma_m = \frac{\sum_{i=1}^{N} x_N}{N} \pm \frac{\sqrt{\sum_{i=1}^{N} \sigma_N^2}}{N}$$

※When averaging images on the [Ave] tab, all images are first added together before processing. Therefore, the output results are different from the method of averaging individual images after circumferential averaging because the calculation method is different.

⑩ Background subtraction 1 (Sub_1)

Subtraction of Background data from Sample data. Sub_2] tab has been added since Ver. 2.0.0, and [Sub_3] since Ver. 2.0.7. The [Sub_1] tab simply subtracts the Background scattering intensity from the Sample scattering intensity. The [Sub_2] tab allows you to subtract the scattering intensity of the Background from the Sample based on the X-ray transmission of the scatterer, excluding the scattering intensity of the empty sample cell, and also taking into account the excluded volume effect of sample concentration. In the [Sub_3] tab, it is possible to perform the calculation for a large number of data at once (perform Background subtraction considering only transparency), where the term Φ for the excluded volume effect is set to 1 for [Sub_2]. First, the function of [Sub_1] is explained.



i. Specify a folder to output the calculation results in [Output:] on the lower side of the [Sub_1] tab. Click on a folder symbol to select it or edit it directly.

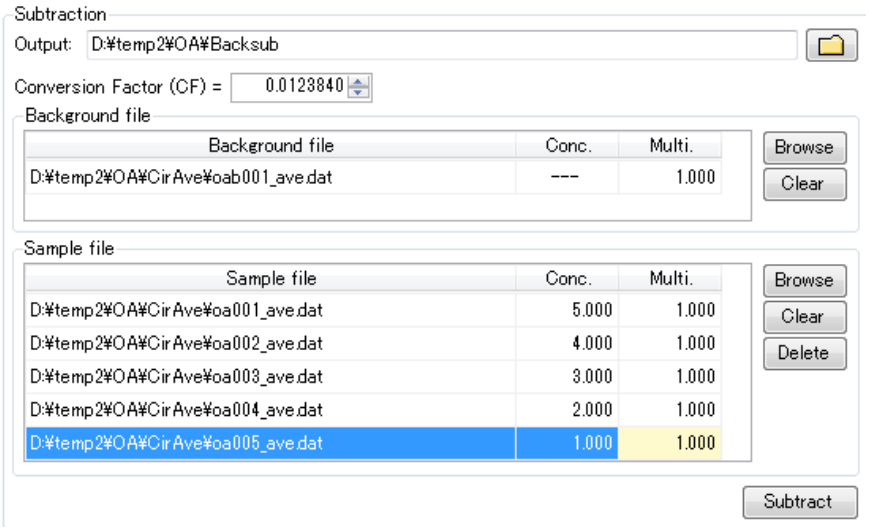
The [Conversion Factor (CF)] is the factor used to convert the scattering intensity into units of absolute scattering intensity. The method to obtain the CF value is explained in "⑬ **ABS_W**" and "⑭ **ABS_BC**".

ii. In the [Background file] field, specify the file to be used as the background. You can click [Browse] to specify a file, or you can Drag&Drop a file into this field. There is only one Background file to be entered.

iii. Specify the file to which you want to apply the Background in the "[Sample file]" field. You can enter as many as you like at once (there is basically no limit). Click [Browse] to specify files. To

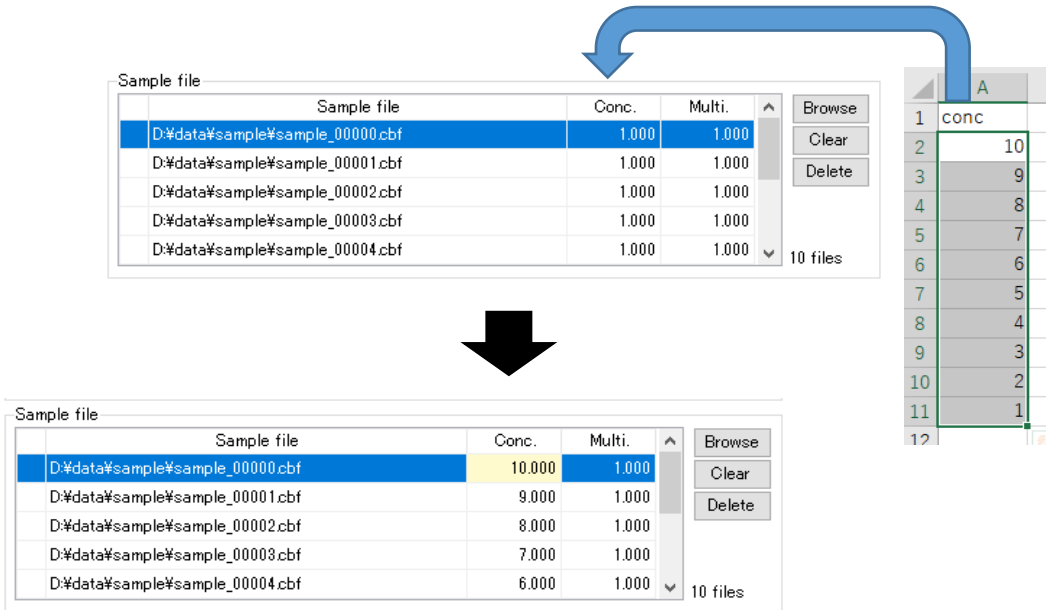
specify multiple files, hold down the ctrl or shift key while clicking to select them. It is also possible to Drag&Drop files into this field. Select and Drop multiple files at once. In [Option] - [ConfigSetting], the default number of files that can be processed at one time is set to 300 (can be changed).

iv. If you enter a value in the [Multi.] field for both Background and Sample, you can multiply the scattering intensity by that value. Usually it is 1.000. In the Sample section, you can also enter the "Conc. (sample concentration)". The concentration values are recorded in the header of the output file and are automatically read in during later analysis.

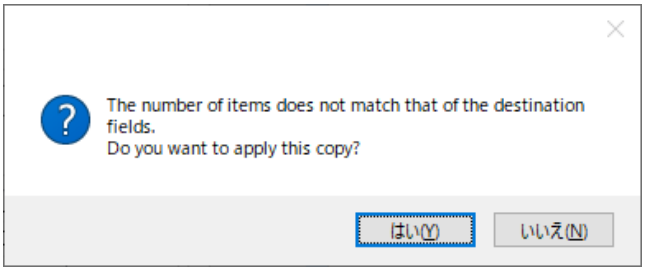


v. If you are reading multiple data as shown above, you can set the density values one line at a time, or you can copy them as table data from Excel or other source and paste them into this column.

vi.



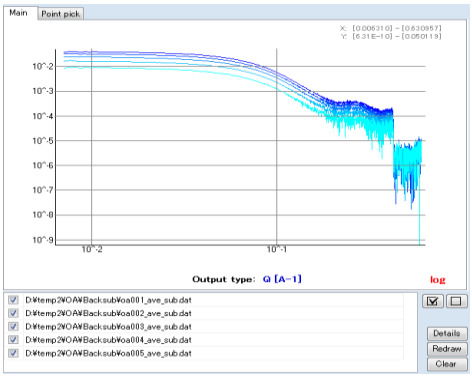
(e.g.) If you want to read 10 files and enter each concentration, you can prepare the data in Excel with the concentrations in a single column and copy-paste it as tabular data into the [Conc.] column of SAngler. However, only one column at a time can be copied. If the number of data to be copied is greater than the number of data displayed in the list, a confirmation message will be displayed.

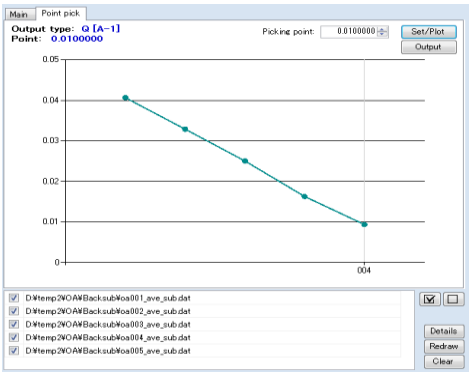


vii. The formula used in Sub_1 is clearly shown in the upper right corner of the window.

viii. When ready, click [Subtract]. A file is output and the graph is displayed as a double-log plot. The graph can be enlarged or reduced by scrolling the mouse, or by left-clicking and dragging to specify the area to be enlarged. You can select which graphs to display by checking or unchecking the checkboxes below and clicking [Redraw]. [Clear] will erase all the data. Clicking on [Details] will show data header information at the top of the SAngler window. Drag&Drop a dat file into this field to display the graph.

ix. The graph window has two displays. One is the【Main】tab, which shows the entire scattering curve. Another【Point pick】tab allows you to plot the vertical axis values (scatter intensity) against a specific horizontal axis value of the data being read. For example, to display a plot of scattering intensity for Q[Å-1]=0.01, enter 0.01 in the [Picking point:] field and click [Set/Plot]. By plotting the change in scattering intensity near the small angle, the presence or absence of effects due to radiation damage can be confirmed. It is also possible to output the data from this plot. Click [Output] to save the data as text data.





※Derivation of error in Sub_1

If the error on the Sample side is σ_A and the error on the Background side is σ_B, the error σ_m when subtracted according to the Sub_1 formula is obtained by the following formula according to the error propagation law.

$$\sigma_m = \sqrt{(\sigma_A \times multi._{sample})^2 + (\sigma_B \times multi._{Background})^2}$$

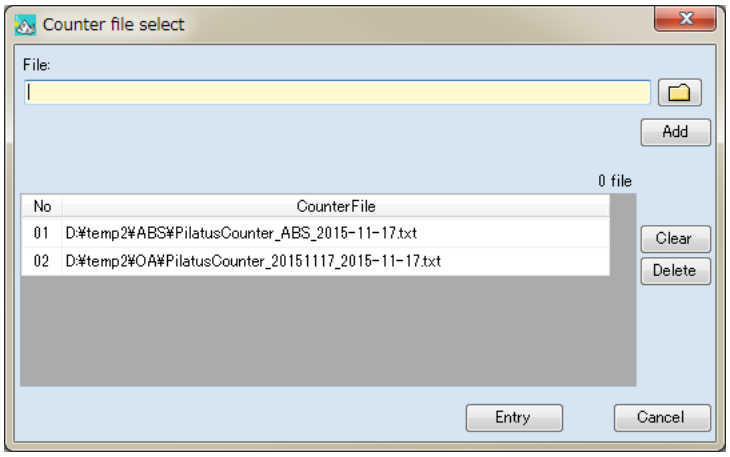
⑪ Subtraction of Background2 (Sub_2)

The [Sub_2] tab allows you to calculate the scattering intensity of an empty sample cell, the X-ray transmittance of an empty cell - Background - Sample measurement, as well as the sample concentration-dependent excluded volume effect.

i. In [Output:], specify the folder to which the calculation results will be output. Click on a folder symbol to select it or edit it directly.

ii. Next, select "Facility" to specify the counter file specifications in order to set up the counter file needed for the transmittance calculation (basically, the settings on the [Ave] tab are taken over as they are, so there is no need to change them if the process proceeds with the same settings). Corresponds to the counter file format of PF and SPring-8 BL38B1 and 40B2.

iii. Next, in "CounterFile entry," set the counter file to be used (basically, the settings in the【Ave】tab are taken over as they are, so there is no need to change them if you wish to proceed with the process using the same settings). Click to open the Counter file select dialog box. Click on the folder symbol to select the counter file, then press the Add button to move to the list column at the bottom of the dialog. This completes the selection. It is also possible to Drag&Drop a file into this field, in which case the selection will be completed immediately. On the other hand, if there are multiple counter files to be used, multiple counter files can be specified. For example, if the counter files corresponding to Dark, Air, and Cell are different from those corresponding to Background and Sample, they should be loaded separately. Counter files are numbered in the order in which they are read, so specify each of these numbers in the (ix) setting. When settings are complete, click on "Entry" to close.



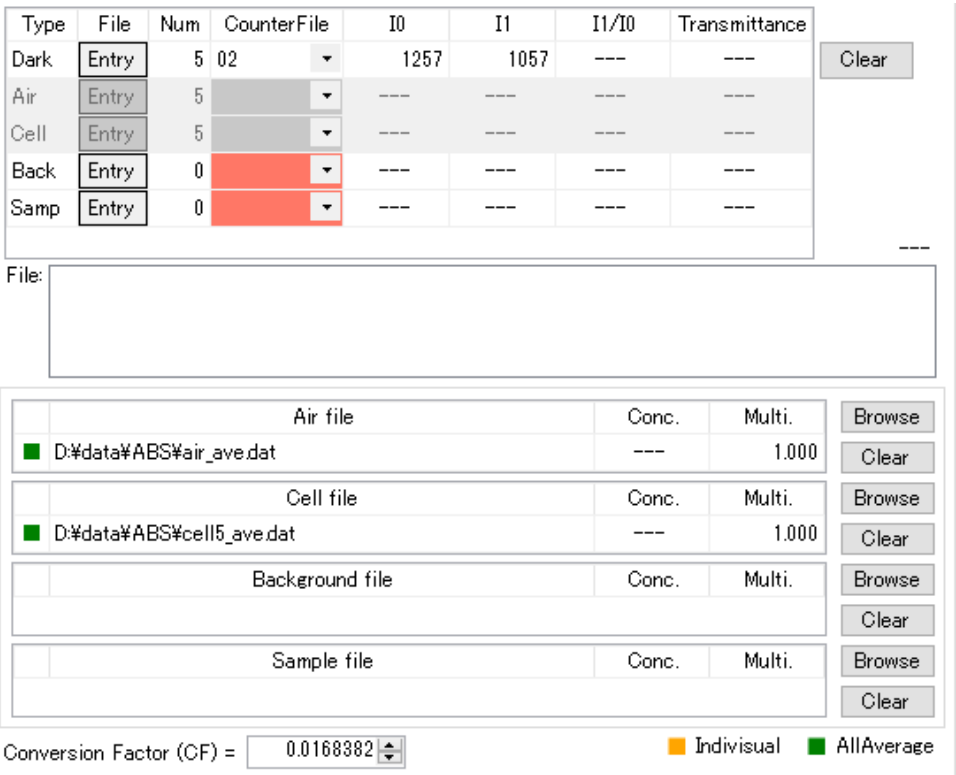
iv. [I0 cnt:] is the channel of incident X-ray (integral) intensity before the sample and [I1 cnt:] is the channel of transmitted X-ray (integral) intensity after the sample. In PF, C2 is injection and C4

is transmission; in BL38B1 at SPring-8, MIC up is injection and BS is transmission; in 40B2, C3 is injection and C4 is transmission (check with the person in charge to be sure).

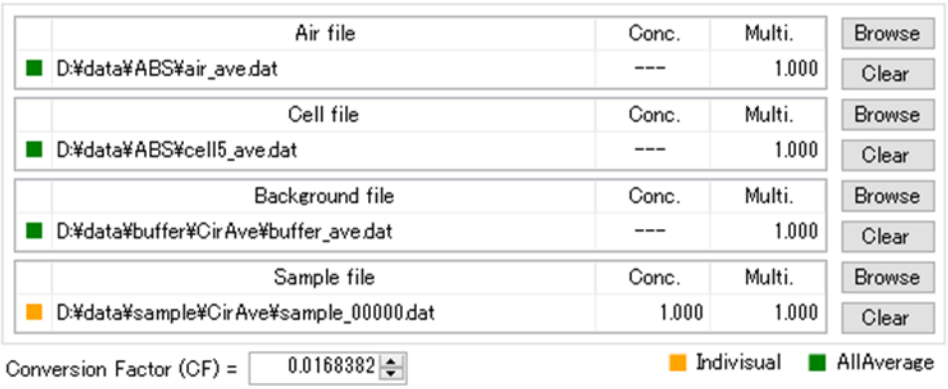
v. Next, set up the measurement data for Dark, Air, Cell, Background, and Sample to be used for processing, and the counter files needed to calculate transmittance. The processing procedure differs between Ver. 2.0.7 or earlier and Ver. 2.1.0 or later.

- When using files processed after Ver 2.1.0

A. In the table section, only Dark reflects the settings made in the [Ave] tab. Air and below are not used. Below that, move on to the columns for specifying Air, Cell, Background, and Sample data. If you have previously performed the "absolute scattering intensity (cm-1) conversion of scattering intensity (counts)" using water or Glassy Carbon as described in **⑬ABS_W and ⑭ABS_GC**, the files specified during that process are entered in the [Air file] and [Cell file] fields. If not performed or if you want to change the file used, specify the data for air scattering (Air file) and the data for sample cells (cell only data without sample, Cell file) (both are dat files). Click "Browse" to specify the file or Drag&Drop the dat file into the blank box. Since it is a dat file, it must be circumferentially averaged and made 1-dimensional in advance.



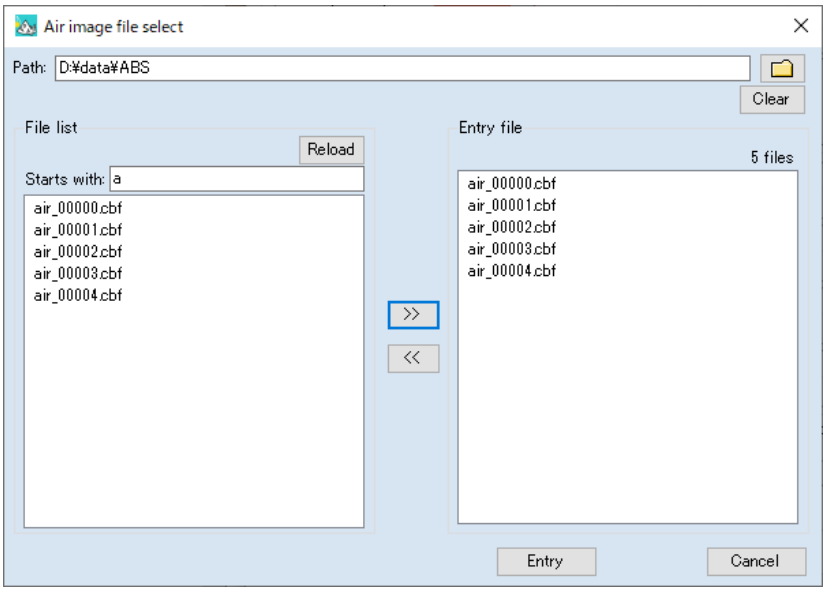
B. Specify the Background and Sample files (dat files) to be used. [Click "Browse" to specify the file or Drag&Drop the dat file into a blank box. Both specify a single dat file that has been pre-circumferentially averaged and made 1-dimensional. For both Background and Sample, enter a value in the "Multi." field to multiply the scattering intensity by that value. Usually it is 1.000. Also, the Sample person can enter [Conc. (sample concentration)]. The concentration values are recorded in the header of the output file and are automatically read in during later analysis. When the four files have been properly loaded, the portion from Air to Samp in the table above will be grayed out, indicating invalidity. This column also determines whether these dat files are files in which a single image data is processed individually (Individual: yellow) or averaged over multiple image data (All Average: green).



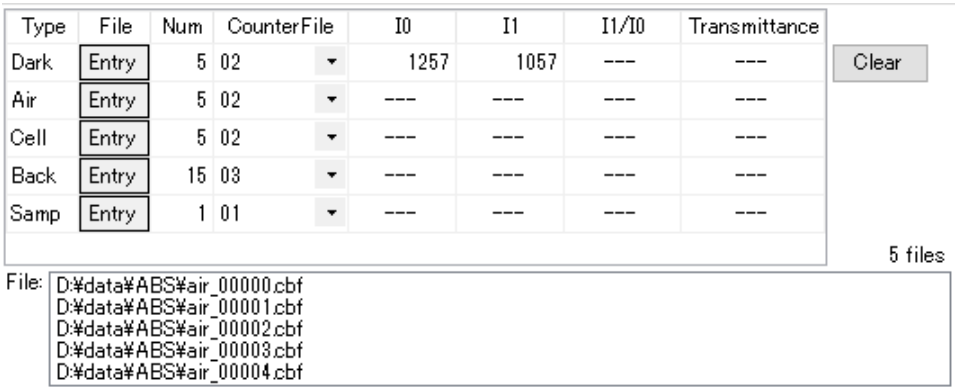
C. Move on to vi.

- When using circumferential averaging files processed before Ver. 2.0.7

A. In order to calculate the transmittance, the following table shows the data for Dark, Air, Cell, Background, and Sample. Dark is set in the [Ave] tab, but if you want to change it, edit it as follows. Clicking "Entry" on each item opens a dialog box for selecting the image data file. Specify the folder where the data is located in [Path:]. Press the folder symbol  or edit it directly (or copy-paste). Clicking the reload symbol  will display a list of image data in the folder, and select multiple copies of the corresponding file at the same time (or a single copy). You can also hold down the [ctrl] key and click to select multiple images, or simply click and drag with the mouse to select multiple images. [Starts with:] is a filter function that allows you to display only specific data sets by entering a string of characters at the beginning of the filename that excludes other files. You can then press [ctrl + A] to select all of them. Clicking the right arrow  moves the file to the right and confirms it. When finished, click "Entry" to close the dialog. Repeat each of these operations.



B. After completing the image data selection, in the "CounterFile" field, select what number of each of the counter files set in (iii) should be used. Move the mouse cursor over the [CounterFile entry] button and the registered counter files will be displayed in a pop-up window. This column is displayed in red before setting, but returns to white when a number is selected. If multiple image data are set for each item, the counter value will also show the average value, but the calculation differs between Dark and others. For Dark, it simply shows the average of the dark counts for [I0] and [I1]. On the other hand, for Air~Sample, only the average value of [I1/I0] is shown. See the last section of this section ⑪ **Background subtraction 2 (Sub_2)** for details of the formula. Click the "Clear" button to clear all settings in this table.



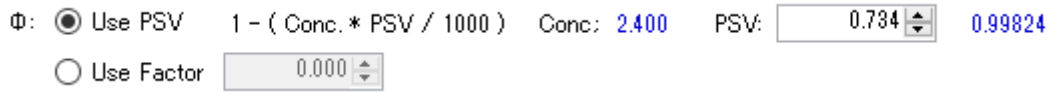
C. Specify the Air, Cell, Background, and Sample files (dat files) to be used. Click "Browse" to specify the file or Drag&Drop the dat file into the blank box. Both files specify a single dat file that has been pre-circumferentially averaged and made 1-dimensional. In the case of a dat file obtained by averaging multiple files, in table B, if you specify the

multiple data used for that averaging, the average value will be used for the transmittance. Enter a value in the [Multi.] field to multiply each scattering intensity by that value. Normally, the value is 1.000. Also, the Sample person can enter [Conc. (sample concentration)]. The concentration values are recorded in the header of the output file and are automatically read in during later analysis. When using files processed before Ver. 2.0.7, Individual and All Average are not determined.

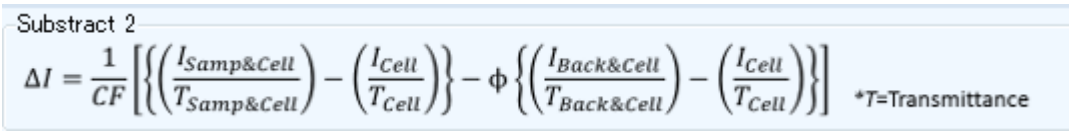
D. Move on to vi.

vi. [Conversion Factor (conversion value to normalize to absolute scattering intensity)] is explained in **⑬ABS_W and ⑭ABS_GC.** If you run it first, the values should be automatically loaded here. If it is not loaded, check the value and enter it manually, or leave it at 1.0000000 if no setting is required.

vii. set the [Factor] (here assumed to be Φ) to account for the exclusion volume effect. Once the Partial Specific Volume (PSV) value is entered, the Φ value is calculated according to the formula using the Conc. (concentration) value set in the [Sample file] field. The PSV value defaults to 0.734, a value often used in the analysis of protein solution samples, but can be freely changed. If 1.000 is acceptable, or if you wish to use a separately obtained value, switch the radio button to "Use Factor" and enter the value.



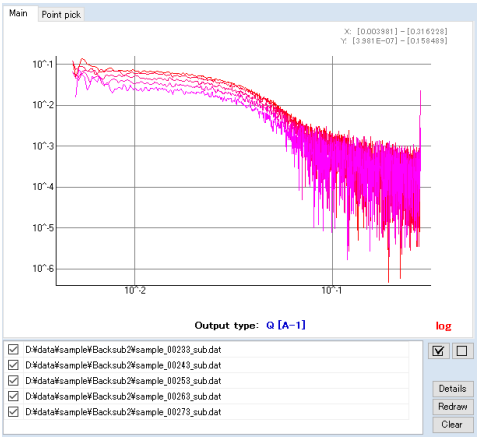
viii. Note that the formula used in Sub_2 is clearly indicated in the upper right corner of the window.

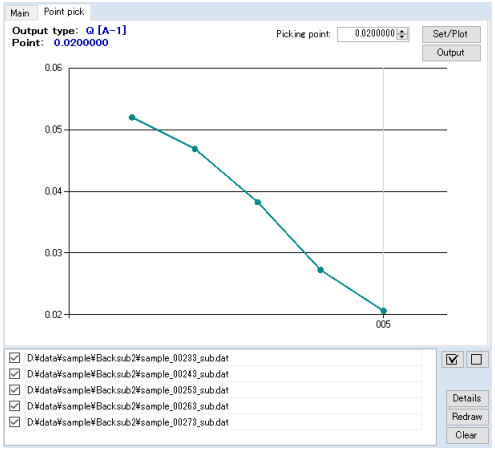


ix. When everything is ready, click "Subtract. A file is output and the graph is displayed as a double-log plot. The graph can be enlarged or reduced by scrolling the mouse, or by left-clicking and dragging to specify the area to be enlarged. You can select which graphs to display by checking or unchecking the checkboxes below and clicking "Redraw". "Clear" will erase all the data. Clicking on "Details" will show data header information at the top of the SAngler window. Drag&Drop a dat file into this field to display the graph.

x. The graph window has two displays. One is the【Main】tab, which shows the entire scattering curve. Another【Point pick】tab allows you to plot the vertical axis values (scatter intensity) against a specific horizontal axis value of the data being read. For example, to display a plot of

scattering intensity for Q[Å-1]=0.01, enter 0.01 in the [Picking point:] field and click [Set/Plot]. Plotting the change in scattering intensity near the small angle allows us to see if there are any effects due to radiation damage. Note that it is also possible to output the data from this plot. Click [Output] to save the data as text data.





※Calculation method of X-ray transmittance (common to Sub_2 and Sub_3)

No.	Image
Dark	j
Air	k
Cell	l
Back	m
Samp	n

$$I_{0\_Dark_{ave}} = \frac{\sum_{i=1}^{j}(I_{0\_Dark})_j}{j}\ ,\quad I_{1\_Dark_{ave}} = \frac{\sum_{i=1}^{j}(I_{1\_Dark})_j}{j}$$

$$T_{Samp\&Cell} = \frac{\left\{\frac{\sum_{i=1}^{n}\left[\frac{(I_{1\_Samp} - I_{1\_Dark_{ave}})}{(I_{0\_Samp} - I_{0\_Dark_{ave}})}\right]_n}{n}\right\}}{\left\{\frac{\sum_{i=1}^{k}\left[\frac{(I_{1\_Air} - I_{1\_Dark_{ave}})}{(I_{0\_Air} - I_{0\_Dark_{ave}})}\right]_k}{k}\right\}}$$

$$T_{Cell} = \frac{\left\{\frac{\sum_{i=1}^{l}\left[\frac{(I_{1\_Cell} - I_{1\_Dark_{ave}})}{(I_{0\_Cell} - I_{0\_Dark_{ave}})}\right]_l}{l}\right\}}{\left\{\frac{\sum_{i=1}^{k}\left[\frac{(I_{1\_Air} - I_{1\_Dark_{ave}})}{(I_{0\_Air} - I_{0\_Dark_{ave}})}\right]_k}{k}\right\}}$$

$$T_{Back\&Cell} = \frac{\left\{\frac{\sum_{i=1}^{m}\left[\frac{(I_{1\_Back} - I_{1\_Dark_{ave}})}{(I_{0\_Back} - I_{0\_Dark_{ave}})}\right]_m}{m}\right\}}{\left\{\frac{\sum_{i=1}^{k}\left[\frac{(I_{1\_Air} - I_{1\_Dark_{ave}})}{(I_{0\_Air} - I_{0\_Dark_{ave}})}\right]_k}{k}\right\}}$$

Since a dark count exists for each channel, the ratio of incident intensity to transmitted intensity is determined for each piece of data and averaged while subtracting the dark value, and finally the transmittance is calculated for a cell (sample) with nothing in it (Air). If there is no cell, i.e., the X-rays hit a bare sample, the calculation can be performed as Air=Cell or Air=Cell=Background.

※Calculation of error in Sub_2

∗ Multi=M

$$\Delta I = \underbrace{\left[\left(\frac{I_{Samp} \times M_{samp}}{T_{Samp}}\right) - \left(\frac{I_{Cell} \times M_{Cell}}{T_{Cell}}\right)\right]}_{A} - \phi \underbrace{\left[\left(\frac{I_{Back} \times M_{Back}}{T_{Back}}\right) - \left(\frac{I_{Cell} \times M_{Cell}}{T_{Cell}}\right)\right]}_{B} = A - \phi B$$

for the two terms A and B, respectively, as well as the error calculation for Sub_1,

$$\sigma_A = \sqrt{\left(\frac{\sigma I_{Samp} \times M_{samp}}{T_{Samp}}\right)^2 + \left(\frac{\sigma I_{Cell} \times M_{Cell}}{T_{Cell}}\right)^2} \quad \sigma_B = \sqrt{\left(\frac{\sigma I_{Back} \times M_{Back}}{T_{Back}}\right)^2 + \left(\frac{\sigma I_{Cell} \times M_{Cell}}{T_{Cell}}\right)^2}$$

is considered to be Thus, the final calculated error σm is,

$$\begin{aligned}
\Delta\sigma I &= \sqrt{(\sigma_A)^2 + (\phi\sigma_B)^2} \\
&= \sqrt{\left\{\left[\left(\frac{\sigma I_{Samp} \times M_{samp}}{T_{Samp}}\right)^2 + \left(\frac{\sigma I_{Cell} \times M_{Cell}}{T_{Cell}}\right)^2\right]^{1/2}\right\}^2 + \left\{\phi \times \left[\left(\frac{\sigma I_{Back} \times M_{Back}}{T_{Back}}\right)^2 + \left(\frac{\sigma I_{Cell} \times M_{Cell}}{T_{Cell}}\right)^2\right]^{1/2}\right\}^2} \\
&= \sqrt{\left(\frac{\sigma I_{Samp} \times M_{samp}}{T_{Samp}}\right)^2 + \left(\frac{\sigma I_{Cell} \times M_{Cell}}{T_{Cell}}\right)^2 + \phi^2 \times \left[\left(\frac{\sigma I_{Back} \times M_{Back}}{T_{Back}}\right)^2 + \left(\frac{\sigma I_{Cell} \times M_{Cell}}{T_{Cell}}\right)^2\right]} \\
&= \left[\left(\frac{\sigma I_{Samp} \times M_{Samp}}{T_{Samp}}\right)^2 + \phi^2\left(\frac{\sigma I_{Back} \times M_{Back}}{T_{Back}}\right)^2 + (1+\phi^2)\left(\frac{\sigma I_{Cell} \times M_{Cell}}{T_{Cell}}\right)^2\right]^{1/2}
\end{aligned}$$

⑫ Subtracting Background3（Sub_3）

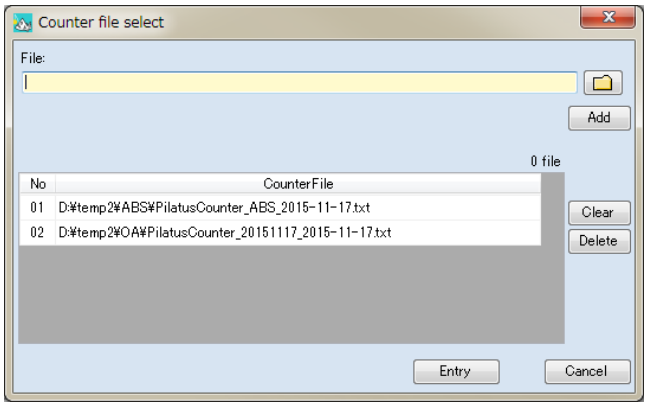
In Sub_3, calculations can be performed for a number of files, taking into account the x-ray transmission in the empty cell, Background, and Sample measurements, while subtracting the scattering intensity of the empty sample cell (the calculation is based on the excluded volume effect of sample concentration as 1 in Sub_2). The calculation is performed for a large number of files.

※ The basic setup method is the same as Sub_2, except that the term Φ for the excluded volume effect is not set and a large number of Sample data can be loaded at once.

i. In [Output:], specify the folder to which the calculation results will be output. Click on a folder symbol to select it or edit it directly.

ii. Next, select "Facility" to specify the counter file specifications in order to set up the counter file needed for the transmittance calculation (basically, the settings on the [Ave] tab are taken over as they are, so there is no need to change them if the process proceeds with the same settings). Corresponds to the counter file format of PF and SPring-8 BL38B1 and 40B2.

iii. Next, in "CounterFile entry," set the counter file to be used (basically, the settings in the【Ave】tab are taken over as they are, so there is no need to change them if you wish to proceed with the process using the same settings). Click to open the Counter file select dialog box. Click on the folder symbol to select the counter file, then press the Add button to move to the list column at the bottom of the dialog. This completes the selection. It is also possible to Drag&Drop a file into this field, in which case the selection will be completed immediately. On the other hand, if there are multiple counter files to be used, multiple counter files can be specified. For example, if the counter files corresponding to Dark, Air, and Cell are different from those corresponding to Background and Sample, they should be loaded separately. Counter files are numbered in the order in which they are read, so the setting in (ix) specifies each of these numbers. When settings are complete, click on "Entry" to close.



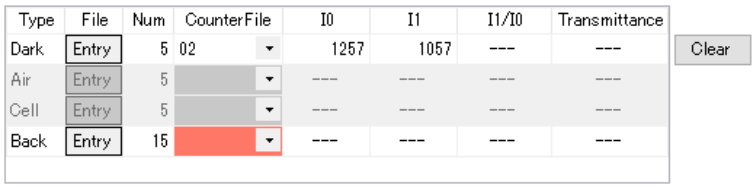
iv. [I0 cnt:] is the channel of incident X-ray (integral) intensity before the sample and [I1 cnt:] is the

channel of transmitted X-ray (integral) intensity after the sample. In PF, C2 is injection and C4 is transmission; in BL38B1 at SPring-8, MIC up is injection and BS is transmission; in 40B2, C3 is injection and C4 is transmission (please check with the person in charge to be sure).

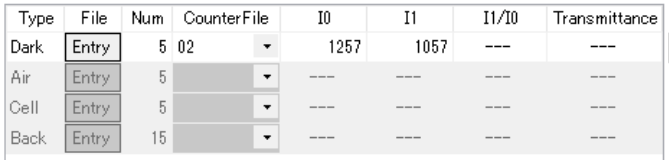
v. Next, set up the measurement data for Dark, Air, Cell, Background, and Sample to be used for processing, and the counter files needed to calculate transmittance. The processing procedure differs between Ver. 2.0.7 or earlier and Ver. 2.1.0 or later.

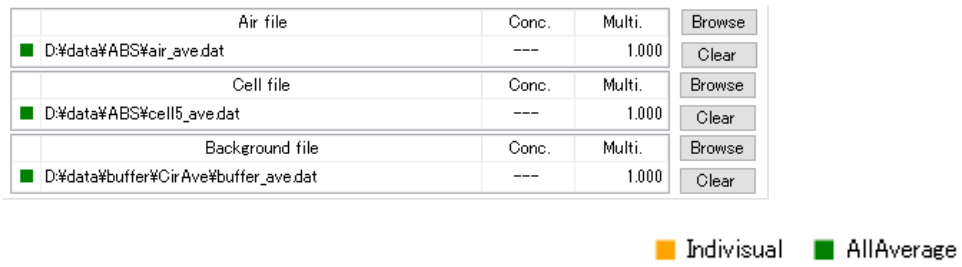
- When using files processed after Ver 2.1.0

A. In the table section, only Dark reflects the settings made in the [Ave] tab; Air and below are not used. Below that, move on to the columns for specifying Air, Cell, Background, and Sample data. If you have previously performed the "absolute scattering intensity (counts) to absolute scattering intensity (cm-1) conversion" using water or Glassy Carbon as described in "⑬ **ABS_W**" and "⑭ **ABS_GC**", the files specified during that process are entered in the [Air file] and [Cell file] fields. If not performed or if you want to change the file used, specify the data for air scattering (Air file) and the data for sample cells (cell only data without sample, Cell file) (both are dat files). Click [Browse] to specify a file or Drag&Drop a dat file into a blank box.



B. Specify the Background file (dat file) to be used. [Click "Browse" to specify the file, or Drag&Drop the dat file into a blank box. Specify one dat file that has been pre-circumferentially averaged to 1D. Enter a value in the [Multi.] field to multiply the scattering intensity by that value. Normally, this value is 1.000.



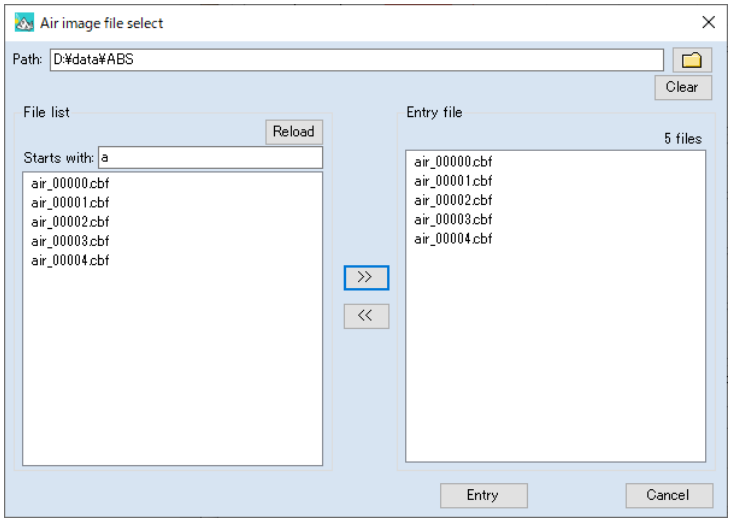


C. When the four files are properly loaded, the Air to Back portion of the table above will be grayed out indicating invalidity. This column also determines whether these dat files are files in which a single image data is processed individually (Individual: yellow) or averaged over multiple image data (All Average: green).

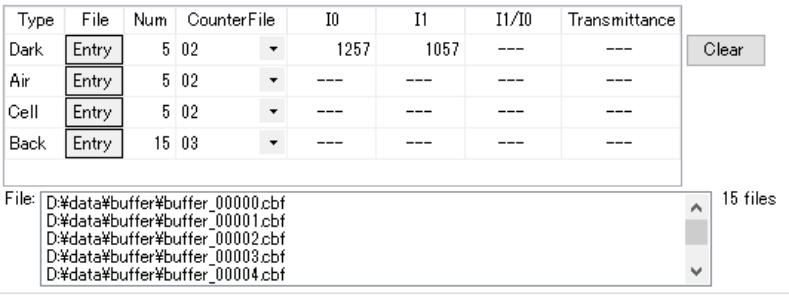
D. Move on to vi.

- When using circumferential averaging files processed before Ver. 2.0.7

A. In order to calculate transmittance, the following table shows the data from Dark, Air, Cell, and Background measurements. Dark is set in the [Ave] tab, but if you want to change it, edit it as follows. Clicking "Entry" on each item opens a dialog box for selecting the image data file. Specify the folder where the data is located in [Path:]. Press the folder symbol or edit it directly (or copy-paste). Clicking the reload button Reload will display a list of image data in the folder, and select multiple copies of the corresponding file at the same time (or a single copy). You can also hold down the [ctrl] key and click to select multiple images, or simply click and drag with the mouse to select multiple images. [Starts with:] is a filter function that allows you to display only specific data sets by entering a string of characters at the beginning of the filename that excludes other files. You can then press [ctrl + A] to select all of them. Clicking the right arrow moves the file to the right and confirms it. When finished, click "Entry" to close the dialog. Repeat each of these operations.



B. After completing the image data selection, in the "CounterFile" field, select what number of each of the counter files set in (iii) should be used. Move the mouse cursor over the [CounterFile entry] button and the registered counter files will be displayed in a pop-up window. This column is displayed in red before setting, but returns to white when a number is selected. If multiple image data are set for each item, the counter value will also show the average value, but the calculation differs between Dark and others. For Dark, it simply shows the average of the dark counts for [I0] and [I1]. On the other hand, for Air~Sample, only the average value of [I1/I0] is shown. See the last section of this section **(⑫ Background subtraction 3 (Sub_3))** for details of the formula. Click the [Clear] button to clear all settings in this table.

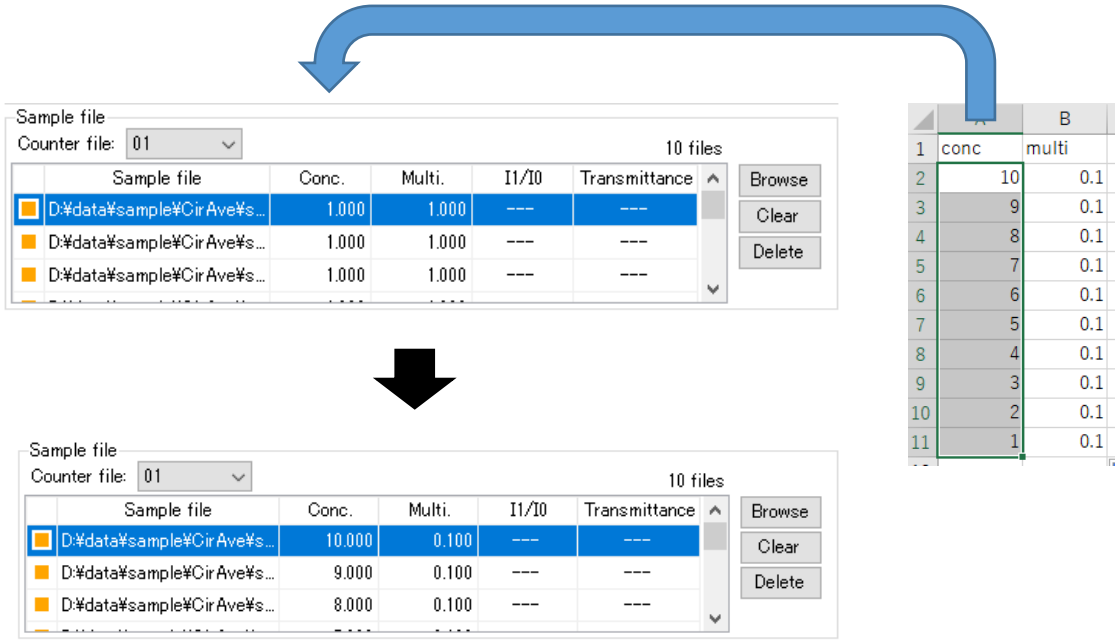


C. Specify the Air, Cell, and Background files (dat files) to be used. Click "Browse" to specify the file or Drag&Drop the dat file into the blank box. Both files specify a single dat file that has been pre-circumferentially averaged and made 1-dimensional. In the case of a dat file obtained by averaging multiple files, in table B, if you specify the multiple data used for that averaging, the average value will be used for the transmittance. Entering a value in the [Multi.] field multiplies each scattering intensity by that value. Usually it is 1.000. When using files processed before Ver. 2.0.7, Individual and All Average are not determined.

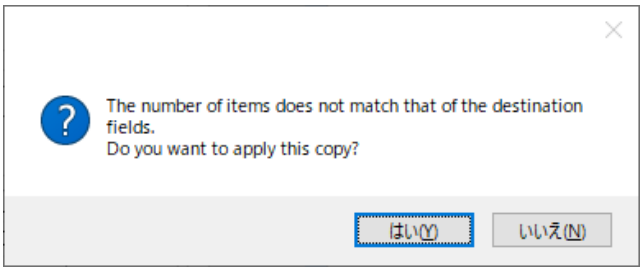
D. Move on to vi.

vi. Next, load the Sample file. You may enter any number of files at a time in the [Sample file] field (there is basically no limit). Click [Browse] to specify files. To specify multiple files, hold down the ctrl or shift key while clicking to select them. You can also Drag&Drop files into this field. Select and Drop multiple files at once. Also, use [Counter file] to set the number of the file in which the Sample value is recorded out of the counter file set in [CounterFile entry] in iii.

vii. Enter a value in the [Multi.] field to multiply the scattering intensity by that value. Normally, the value is 1.000. Also, the Sample person can enter [Conc. (sample concentration)]. The concentration values are recorded in the header of the output file and are automatically read in during later analysis. The values for [Multi.] and [Conc.] can be set one row at a time, or if multiple data are being read, they can be copied as tabular data from Excel or other sources and pasted into this column.

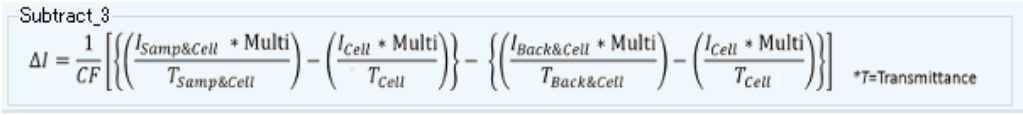


(e.g.) If you want to read 10 files and input Conc and Multi, you can prepare data in Excel with Conc and Multi in a single column, and copy-paste it as tabular data into SAngler's Conc and Multi columns. However, only one column at a time can be copied. If the number of data to be copied is greater than the number of data displayed in the list, a confirmation message will be displayed.



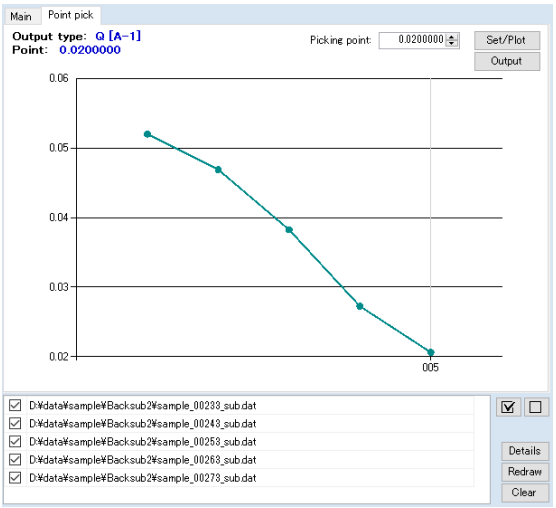
viii. [Conversion Factor (conversion value for normalization to absolute scattering intensity)] is explained in ⑬ **ABS_W** and ⑭ **ABS_GC**. If you run it first, the value should be automatically loaded here. If not, check the value and enter it manually, or leave it at 1.0000000 if no setting is needed.

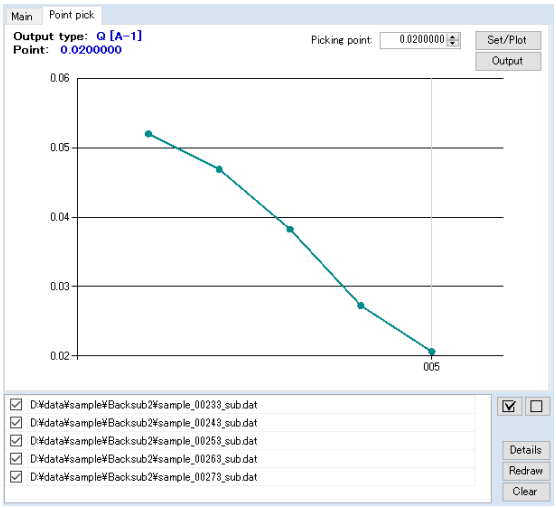
ix. The formula used in Sub_3 is clearly indicated in the upper right corner of the window.



x. When everything is ready, click "Subtract. The file will be output and the graph will be displayed as a double-log plot. The graph can be enlarged or reduced by scrolling the mouse, or by left-clicking and dragging to specify the area to be enlarged. You can select which graphs to display by checking or unchecking the checkboxes below and clicking "Redraw. "Clear" will erase all the data. Click [Details] to show the data header information at the top of the SAngler window. You can also drag & drop a dat file into this column to display a graph.

xi. The graph window has two views. One is the【Main】tab, which displays the entire scattering





curve. Another【Point pick】tab allows you to plot the vertical axis values (scatter intensity) against a specific horizontal axis value of the data being read. For example, to display a plot of scattering intensity for Q[Å-1]=0.01, enter 0.01 in the [Picking point:] field and click [Set/Plot]. By plotting the change in scattering intensity near the small angle, the presence or absence of effects due to radiation damage can be confirmed. Note that it is also possible to output the data from this plot. Click [Output] to save the data as text data.

※Calculation method of X-ray transmittance (common to Sub_2 and Sub_3)

No.	Image
Dark	j
Air	k
Cell	l
Back	m
Samp	n

$$I_{0\_Dark_{ave}} = \frac{\sum_{i=1}^{j}\left(I_{0\_Dark}\right)_j}{j}\ ,\quad I_{1\_Dark_{ave}} = \frac{\sum_{i=1}^{j}\left(I_{1\_Dark}\right)_j}{j}$$

$$T_{Samp\&Cell} = \frac{\left\{\frac{\sum_{i=1}^{n}\left[\frac{\left(I_{1\_Samp} - I_{1\_Dark_{ave}}\right)}{\left(I_{0\_Samp} - I_{0\_Dark_{ave}}\right)}\right]_n}{n}\right\}}{\left\{\frac{\sum_{i=1}^{k}\left[\frac{\left(I_{1\_Air} - I_{1\_Dark_{ave}}\right)}{\left(I_{0\_Air} - I_{0\_Dark_{ave}}\right)}\right]_k}{k}\right\}}$$

$$T_{Cell} = \frac{\left\{\frac{\sum_{i=1}^{l}\left[\frac{\left(I_{1\_Cell} - I_{1\_Dark_{ave}}\right)}{\left(I_{0\_Cell} - I_{0\_Dark_{ave}}\right)}\right]_l}{l}\right\}}{\left\{\frac{\sum_{i=1}^{k}\left[\frac{\left(I_{1\_Air} - I_{1\_Dark_{ave}}\right)}{\left(I_{0\_Air} - I_{0\_Dark_{ave}}\right)}\right]_k}{k}\right\}}$$

$$T_{Back\&Cell} = \frac{\left\{\frac{\sum_{i=1}^{m}\left[\frac{\left(I_{1\_Back} - I_{1\_Dark_{ave}}\right)}{\left(I_{0\_Back} - I_{0\_Dark_{ave}}\right)}\right]_m}{m}\right\}}{\left\{\frac{\sum_{i=1}^{k}\left[\frac{\left(I_{1\_Air} - I_{1\_Dark_{ave}}\right)}{\left(I_{0\_Air} - I_{0\_Dark_{ave}}\right)}\right]_k}{k}\right\}}$$

Since a dark count exists for each channel, the ratio of incident intensity to transmitted intensity is determined for each piece of data and averaged while subtracting the dark value, and finally the transmittance is calculated for a cell (sample) with nothing in it (Air). If there is no cell, i.e., the X-rays hit a bare sample, the calculation can be performed as Air=Cell or Air=Cell=Background.

※Calculation of error in Sub_3 (consider Φ=1 in Sub_2)

∗ Multi=M

$$\Delta I = \underbrace{\left[\left(\frac{I_{Samp} \times M_{samp}}{T_{Samp}}\right) - \left(\frac{I_{Cell} \times M_{Cell}}{T_{Cell}}\right)\right]}_{A} - \underbrace{\left[\left(\frac{I_{Back} \times M_{Back}}{T_{Back}}\right) - \left(\frac{I_{Cell} \times M_{Cell}}{T_{Cell}}\right)\right]}_{B} = A - B$$

for the two terms A and B, respectively, as well as the error calculation for Sub_1,

$$\sigma_A = \sqrt{\left(\frac{\sigma I_{Samp} \times M_{Samp}}{T_{Samp}}\right)^2 + \left(\frac{\sigma I_{Cell} \times M_{Cell}}{T_{Cell}}\right)^2} \qquad \sigma_B = \sqrt{\left(\frac{\sigma I_{Back} \times M_{Back}}{T_{Back}}\right)^2 + \left(\frac{\sigma I_{Cell} \times M_{Cell}}{T_{Cell}}\right)^2}$$

is considered to be Thus, the final calculated error σm is,

$$\sigma_m = \sqrt{(\sigma_A)^2 + (\sigma_B)^2}$$

$$= \sqrt{\left\{\left[\left(\frac{\sigma I_{Samp} \times M_{Samp}}{T_{Samp}}\right)^2 + \left(\frac{\sigma I_{Cell} \times M_{Cell}}{T_{Cell}}\right)^2\right]^{1/2}\right\}^2 + \left\{\left[\left(\frac{\sigma I_{Back} \times M_{Back}}{T_{Back}}\right)^2 + \left(\frac{\sigma I_{Cell} \times M_{Cell}}{T_{Cell}}\right)^2\right]^{1/2}\right\}^2}$$

$$= \sqrt{\left(\frac{\sigma I_{Samp} \times M_{Samp}}{T_{Samp}}\right)^2 + \left(\frac{\sigma I_{Cell} \times M_{Cell}}{T_{Cell}}\right)^2 + \left(\frac{\sigma I_{Back} \times M_{Back}}{T_{Back}}\right)^2 + \left(\frac{\sigma I_{Cell} \times M_{Cell}}{T_{Cell}}\right)^2}$$

$$= \left[\left(\frac{\sigma I_{Samp} \times M_{Samp}}{T_{Samp}}\right)^2 + \left(\frac{\sigma I_{Back} \times M_{Back}}{T_{Back}}\right)^2 + 2\left(\frac{\sigma I_{Cell} \times M_{Cell}}{T_{Cell}}\right)^2\right]^{1/2}$$

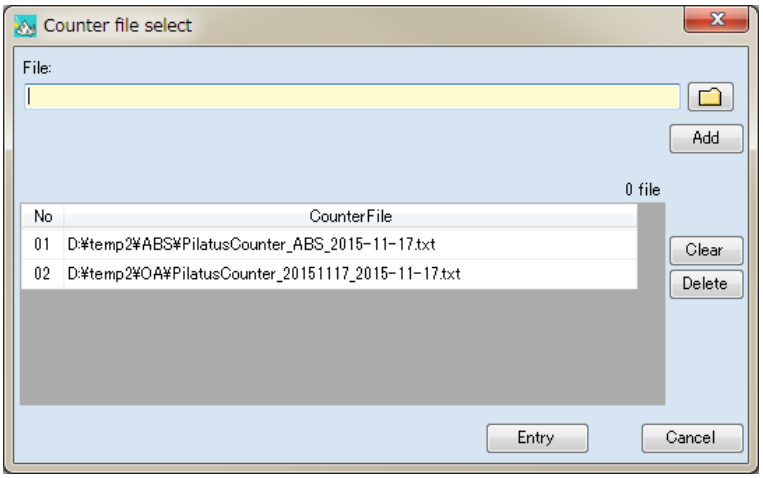
⑬ Convert units of scattering intensity to absolute scattering intensity using water (ABS_W)

The [ABS_W] tab allows you to perform an analysis to determine the Conversion Factor (CF) required to convert the units of scattering intensity of a sample to absolute scattering intensity (cm-1) using the scattering intensity of water (counts).

i. Before the calculations on this tab, convert the scattering intensity data measured for Air, Empty Cells, and Water to 1D by following the procedure in "**⑦ Circumferential Average (Average)**". It is a good idea to average the results of multiple measurements. This file is specified in (v). **If you want to process from【CirAve】to【ABS_W】consecutively, skip steps (ii) and (iii) and move on to step (iv).**

ii. To calculate the transmittance, set the count values, etc. for Dark, Air, Cell, and Water measurements, respectively. First, select Facility, which corresponds to the counter file format of PF and SPring-8 BL38B1 and 40B2.

iii. Next, under "CounterFile entry," set the counter file to be used. Click to open the [Counter file select] dialog box. Click on the folder symbol to select the counter file, then press the [Add] button to move to the list column at the bottom of the dialog. This completes the selection. It is also possible to Drag&Drop a file into this field, in which case the selection will be completed immediately. On the other hand, if there are multiple counter files to be used, multiple counter files can be specified. For example, if the counter files for Dark, Air, and Cell are different from the counter file for Water, then each of those files should be loaded. Counter files are numbered in the order in which they are read, so each counter file setting specifies this number. When settings are complete, click on "Entry" to close.



iv. [[I0 cnt:]] is the channel of incident X-ray (integral) intensity before the sample and [I1 cnt:] is the channel of transmitted X-ray (integral) intensity after the sample. In PF, C2 is injection and C4 is transmission; in BL38B1 at SPring-8, MIC up is injection and BS is transmission; in 40B2, C3 is injection and C4 is transmission (please check with the person in charge to be sure).

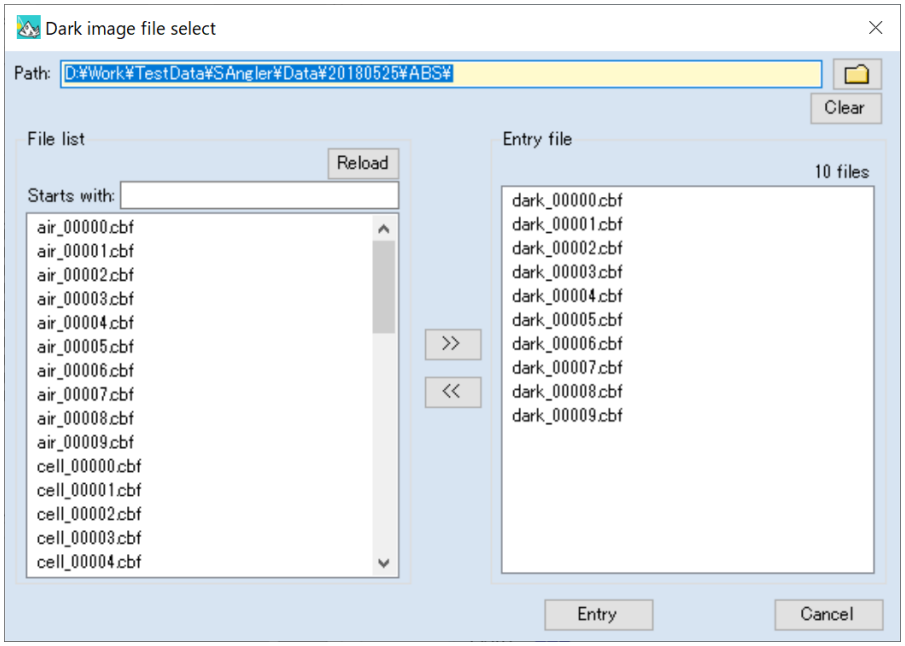
v. Next, set up the Dark, Air, Cell, and Water measurement data to be used for processing and the counter files needed to calculate transmittance. The processing procedure differs between Ver. 2.0.7 or earlier and Ver. 2.1.0 or later.

※You cannot use a dat file after averaging the data using "⑨ Average of dat file after circumferential averaging (DatAverage)".

- When using files processed in Ver 2.1.0 or later **(* However, if you have already set up the Dark file on the [CirAve] tab first, start with step B, as it has already been set up)**.

A. In the table section, only Dark is set. Clicking on "Entry" opens a dialog box for selecting an image data file. Specify the folder where the data is located in [Path:]. Press the folder symbol  or edit it directly (or copy-paste). Clicking the reload button 

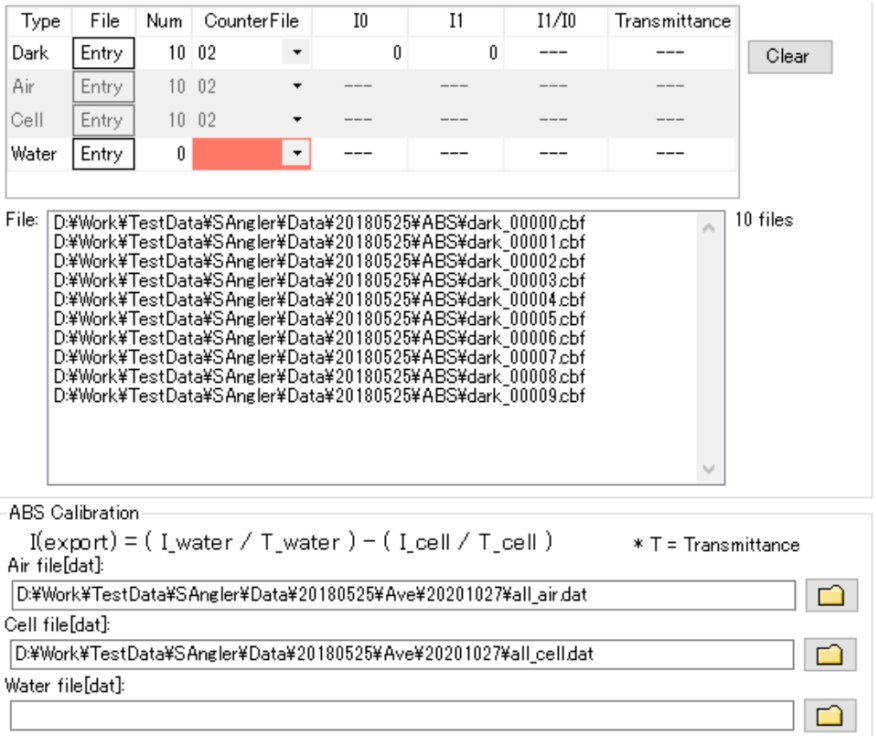
will display a list of image data in the folder, and select multiple copies of the corresponding file at the same time (or a single copy). You can also hold down the [ctrl] key and click to select multiple images, or simply click and drag with the mouse to select multiple images. [Starts with:] is a filter function that allows you to display only specific data sets by entering a string of characters at the beginning of the filename that excludes other files. You can then press [ctrl + A] to select all of them. Clicking the right arrow  moves the file to the right and confirms it. When finished, click [Entry] to close the dialog; do not use Air or below.



B. Use the lower left column to specify the Air, Cell, and Water data. Settings made here will also be reflected in the [Air file] and [Cell file] in the [Ave] and [Sub] tabs. If not performed or if you want to change the file used, specify the air scattering data (Air file), sample cell data (cell only data without sample, Cell file), and water scattering data (Water file) (both are dat files).

C. Click [Browse] to specify a file or Drag&Drop a dat file into a blank box.

D.

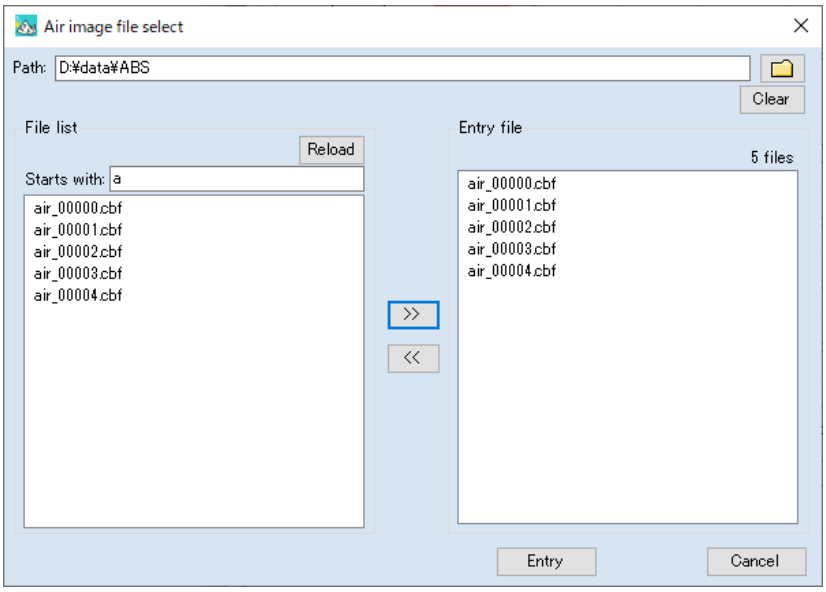


E. When the three files are properly loaded, the File and CounterFile in the table above will be set automatically and the Air to Water section will be grayed out indicating invalidity.

F. Move on to vi.

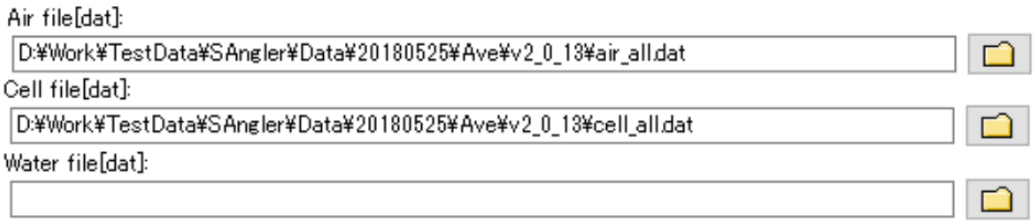
- When using circumferential averaging files processed before Ver. 2.0.7

A. In the following table, specify the respective data measured for Dark, Air, Cell, and Water. Clicking "Entry" on each item opens a dialog box for selecting the image data file. Specify the folder where the data is located in [Path:]. Press the folder symbol or edit it directly (or copy-paste). Clicking the reload button Reload will display a list of image data in the folder, and select multiple copies of the corresponding file at the same time (or a single copy). You can also hold down the [ctrl] key and click to select multiple images, or simply click and drag with the mouse to select multiple images. [Starts with:] is a filter function that allows you to display only specific data sets by entering a string of characters at the beginning of the filename that excludes other files. You can then press [ctrl + A] to select all of them. Clicking the right arrow » moves the file to the right and confirms it. When finished, click "Entry" to close the dialog. Repeat each of these operations.



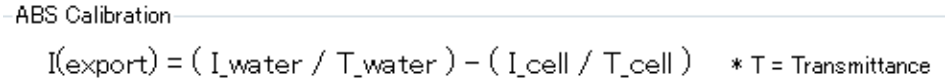
B. After completing the image data selection, in the [CounterFile] field, select what number of each of the counter files set in (iii) is to be used. Move the mouse cursor over the [CounterFile entry] button and the registered counter files will be displayed in a pop-up window. This column is displayed in red before setting, but returns to white when a number is selected. After the final calculation, if multiple image data are set for each item, the average of the counter values is shown here, but the calculations are different for Dark and others. For Dark, it simply shows the average of the dark counts for [I0] and [I1]. On the other hand, for Air to Water, only the average value of [I1/I0] is shown. The method of calculating transmittance is basically the same as in "⑪ **Subtract Background 2 (Sub_2)**", so please refer to the end of "⑪ **Subtract Background 2 (Sub_2)**" for details of the formula.

C. Specify the pre-determined one-dimensional Air, Cell, and Water data in each [Air file [dat]:], [Cell file [dat]:], and [Water file [dat]:]. Click on the folder symbol to specify the file or Drag&Drop the dat file into the blank box.

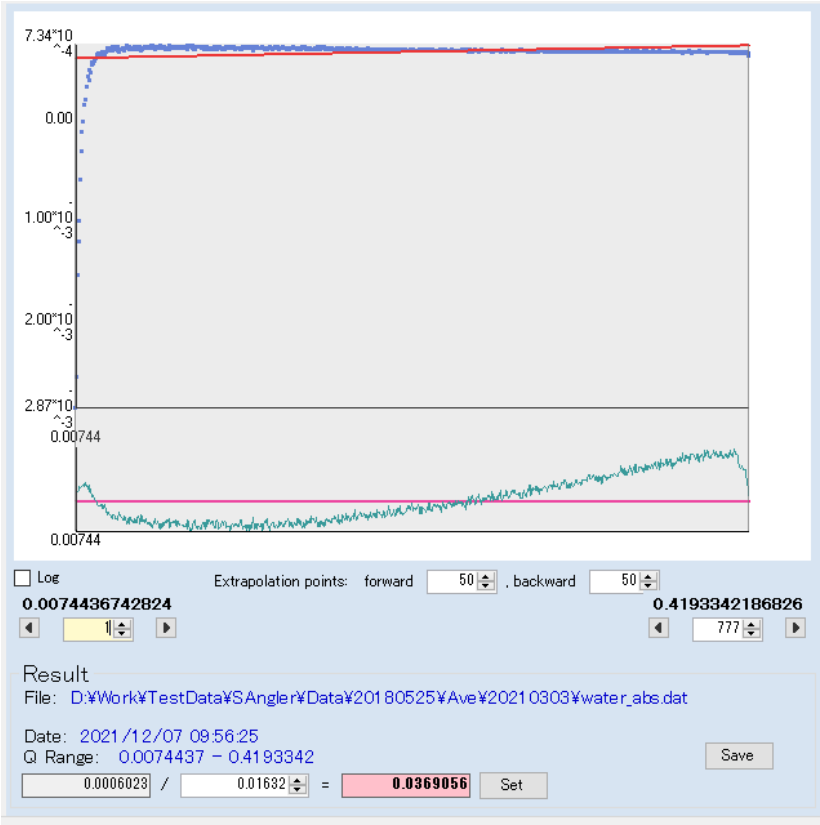


D. Moving on to vi.

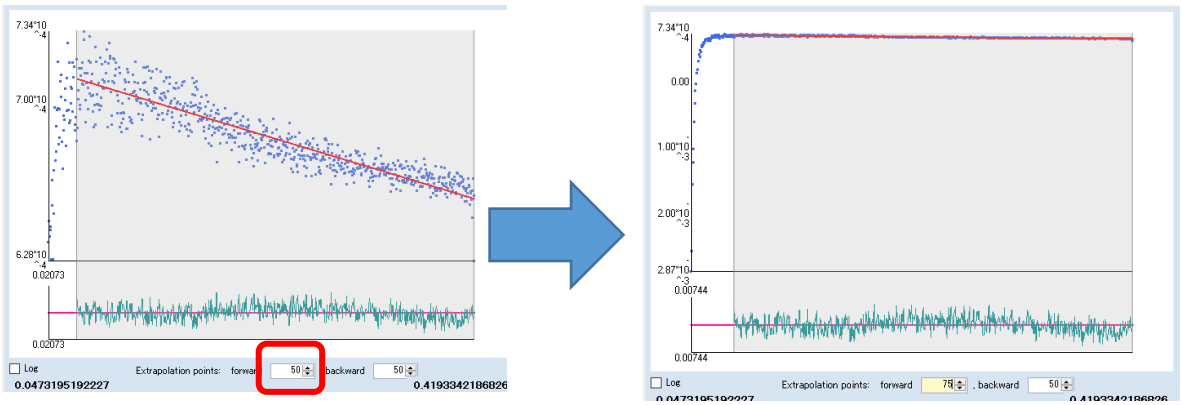
vi. The formula for determining the scattering intensity of water is shown in [ABS Calibration].



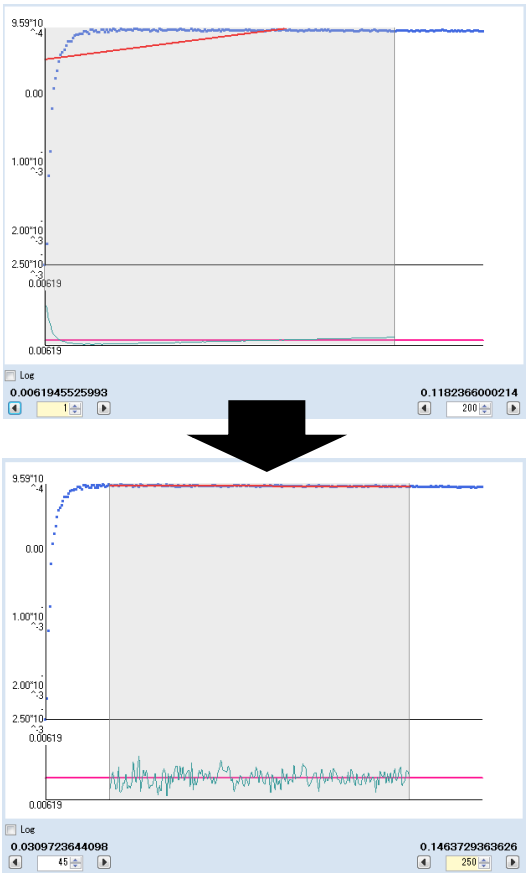
vii. When everything is ready, click Run. The file is output and plotted with blue dots on the right side of the window. The file is output to the same folder [Output path:] where the Water data was read, and is named with "_abs" added to the name of the dat file that was read (in the above example, "water_ave_abs.dat").The horizontal axis of the graph is the unit system specified by Averaging, and the vertical axis is the scattering intensity. The small-angle region of this data is approximated by a straight line, the approximate straight line being indicated by the red line. The lower plot shows the difference from the approximate straight line. The plot of the difference is used to manually approximate the straight line.



viii. The graph shows the entire startup area. The actual abscissa values and data range used for linear approximation are displayed at the lower right and lower left of the graph, and the ← → keys are used to change the linear approximation range (the graph display range is also automatically linked). The out-of-range display area is set to 50 points forward and 50 points backward at startup. If you want to display a wider area than the set range, change the value.



ix. For the linear approximation, the high-angle side uses a unit system of Q (Å-1) from around 0.1 to 0.15. Conversely, the low angle side shows changes such as a drop as shown in the above figure, so this area is adjusted so that it can be excluded while viewing the difference plot. The vertical axis can also be displayed in Log.

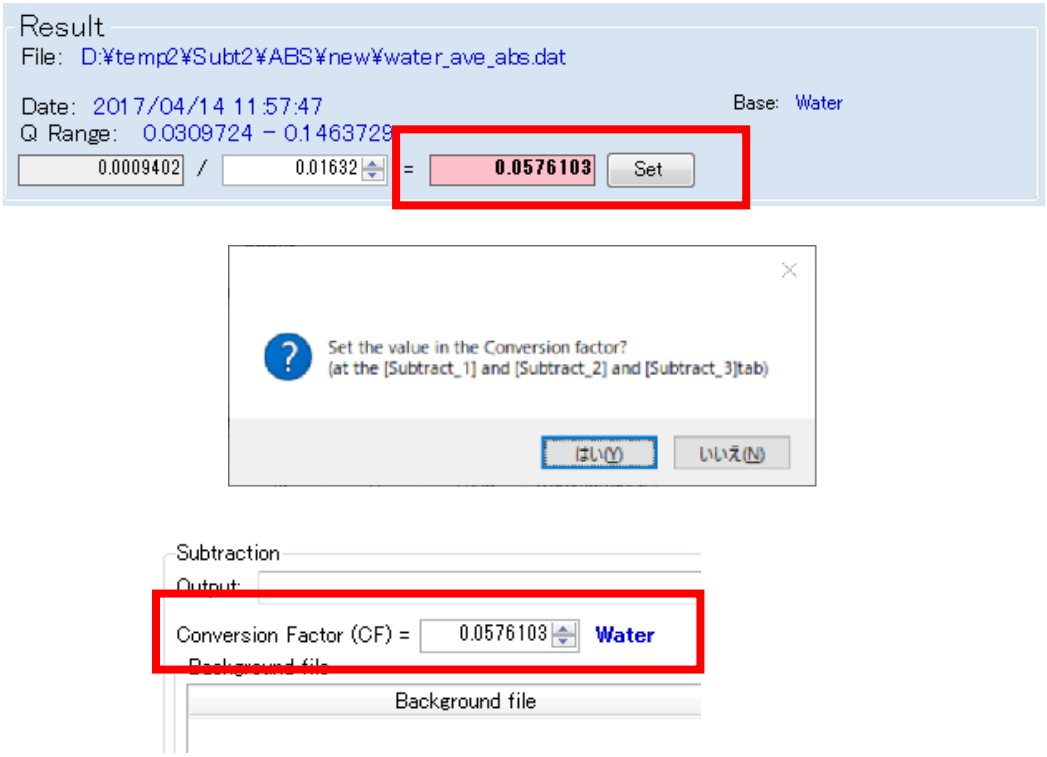


x. The linear approximation is complete when the residual plot is even with the reference line of zero (pink). The value of the Y-intercept of this approximate line is the measured water scattering intensity (counts). The absolute scattering intensity of water at 20°C (293 K) is 0.01632 cm-1 (references are given at the end of this section). Therefore, the conversion factor CF when measured at 20°C can be obtained by dividing the measured water scattering intensity by 0.01632.

※Starting with version 2.1.59, the difference formula has been changed to the following formula

Difference value = (Measured value - Approximate value) / Error

xi. In the [Result] column, the automatically calculated results are displayed. The value of the Y-intercept is automatically loaded as determined from the linear approximation, with a default value of 0.01632 cm-1 indicated (can be changed). To use this value as CF, click Set. A confirmation dialog box will appear, and if you press [Yes], the values will be copied to the CF columns of Subtract_1, Subtract_2, and Subtract_3, indicating that this value is the value obtained from Water. This completes the process.



xii. Note that if the sample concentration is accurate, the molecular weight can be expressed in terms of the absolute scattering intensity by the following equation

MW（kDa） = 1500×I(0) [cm^{-1}] / c [mg/ml]

(Example) A protein with a molecular weight of 36 kDa was measured at a concentration of 9.4 mg/ml, and the absolute scattering obtained from water with the SAngler

The analysis was performed using the CF value to the intensity obtained from water by SAngler.

Results of Guinier analysis：R_g = 33.3 [Å]、I(0)/c＝ 0.02267 [cm^{-1}・ml/mg]

MW（kDa） = 1500×0.02267 = 34 kDa

xiii. References are listed below.

Orthaber, D., Bergmann, A. and Glatter, O. SAXS experiments on absolute scale with Kratky systems using water as a secondary standard. *J. Appl. Cryst.* **33**, 218–225 (2000).

In addition, the following documents may also be helpful.

Fan, L., Degen, M., Bendle, S., Grupido, N. and Ilavsky, J. The Absolute Calibration of a Small-Angle Scattering Instrument with a Laboratory X-ray Source. J*. Phys.: Conf. Ser.* **247**, 012005 (2010).

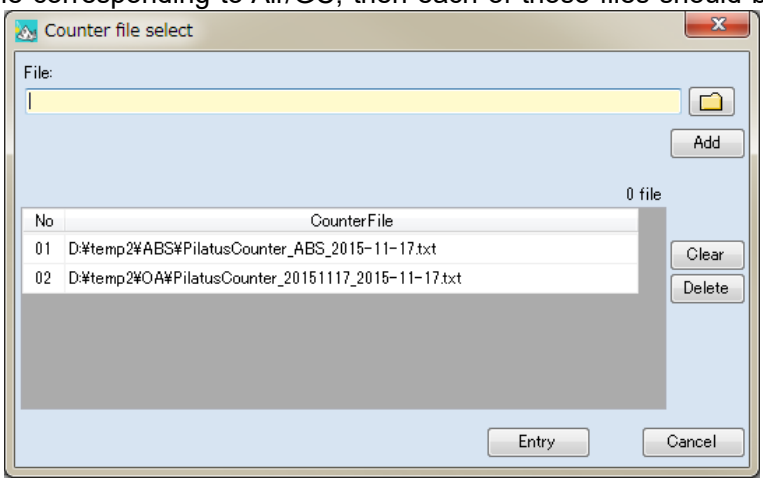
⑭ Convert units of scattering intensity to absolute scattering intensity using Glassy Carbon (ABS_GC)

In the [ABS_GC] tab, you can use the scattering intensity (counts) of Glassy Carbon to obtain the Conversion Factor (CF) necessary to convert the units of scattering intensity of the sample to absolute scattering intensity (cm-1). Note that SRM3600, which is sold by NIST as a calibration sample for absolute intensity conversion, will be used.
https://www-s.nist.gov/srmors/view_detail.cfm?srm=3600
The following procedure follows the steps described in the "Certificate" section of the above website. The reference data can be downloaded from the "Data and Information Files," and SAngler has included this reference data within.

i. Before the calculations in this tab, convert the scattering intensity data measured for Air (Air) and Glassy Carbon (GC) to 1D by following the procedure in "**⑦ Circumferential Average (Average)**". It is a good idea to average the results of multiple measurements. Specify this file with (v). **When processing from【CirAve】to【ABS_GC】consecutively, skip steps (ii) and (iii) and move on to step (iv).**

ii. For the calculation of transmittance, we will set the count values, etc. for Dark, Air, and GC measurements, respectively. First, select Facility, which corresponds to the counter file format for PF and SPring-8 BL38B1 and 40B2.

iii. Next, in [CounterFile entry], set the counter file to be used. Click to open the [Counter file select] dialog box. Click on the folder symbol to select the counter file, then press the [Add] button to move to the list column at the bottom of the dialog. This completes the selection. It is also possible to Drag&Drop a file into this field, in which case the selection will be completed immediately. On the other hand, if there are multiple counter files to be used, multiple counter files can be specified. For example, if the counter file corresponding to Dark is different from the counter file corresponding to Air/GC, then each of those files should be loaded. Counter



files are numbered in the order in which they are read, so specify each of these numbers in the counter file settings. When settings are complete, click "Entry" to close.

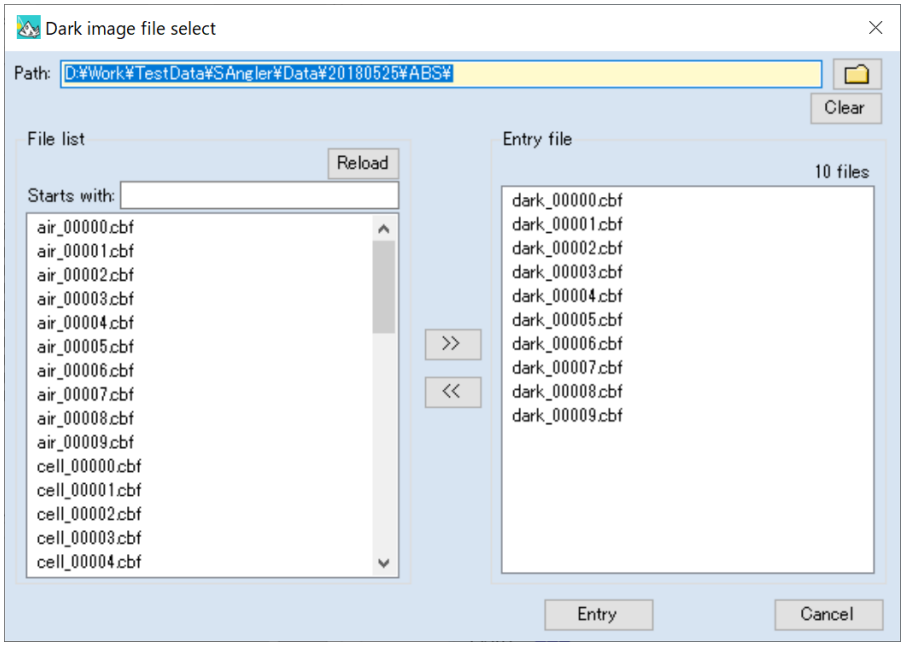
iv. iv. [[I0 cnt:]] is the channel of injected X-ray (integral) intensity before the sample and [I1 cnt:] is the channel of transmitted X-ray (integral) intensity after the sample. In PF, C2 is injection and C4 is transmission; in BL38B1 at SPring-8, MIC up is injection and BS is transmission; in 40B2, C3 is injection and C4 is transmission (please check with the person in charge to be sure).

v. Next, set up the Dark, Air, and GC measurement data to be used for processing and the counter files needed to calculate transmittance. The processing procedure differs between Ver. 2.0.7 or earlier and Ver. 2.1.0 or later.

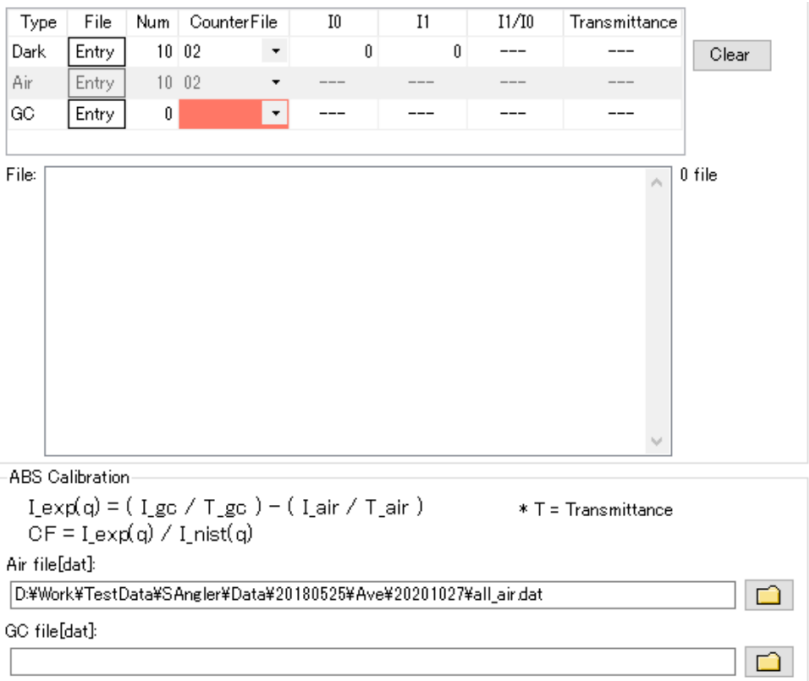
※You cannot use a dat file after averaging the data using "⑨ Average of dat file after circumferential averaging (DatAverage)".

- When using files processed in Ver 2.1.0 or later **(* However, if you have already set up the Dark file on the [CirAve] tab first, start with step B, as it has already been set up)**.

  A. In the table section, only Dark is set. Click [Entry] to open a dialog box to select the image data file. Specify the folder where the data is located in [Path:]. Press the folder symbol  or edit it directly (or copy-paste). Reload button  to display a list of image data in the folder, and select multiple copies of the corresponding file at the same time (or a single copy). You can also hold down the [ctrl] key and click to select multiple images, or simply click and drag with the mouse to select multiple images. [Starts with:] is a filter function that allows you to display only specific data sets by entering a string of characters at the beginning of the filename that excludes other files. You can then press [ctrl + A] to select all of them. Clicking the right arrow  moves the file to the right and confirms it. When finished, click [Entry] to close the dialog; do not use Air or below.



B. Use the lower left column to specify Air and GC data. If Air is set here, it will also be reflected in the [Air file] on the [Ave] and [Sub] tabs. If not performed or if you want to change the file used, specify the air scattering data (Air file) and the scattering intensity data (GC file) from Glassy Carbon (GC) measurements (both are dat files).
Click "Browse" to specify the file or Drag&Drop the dat file into the blank box. Since it is a dat file, it must be circumferentially averaged and made 1-dimensional in advance.

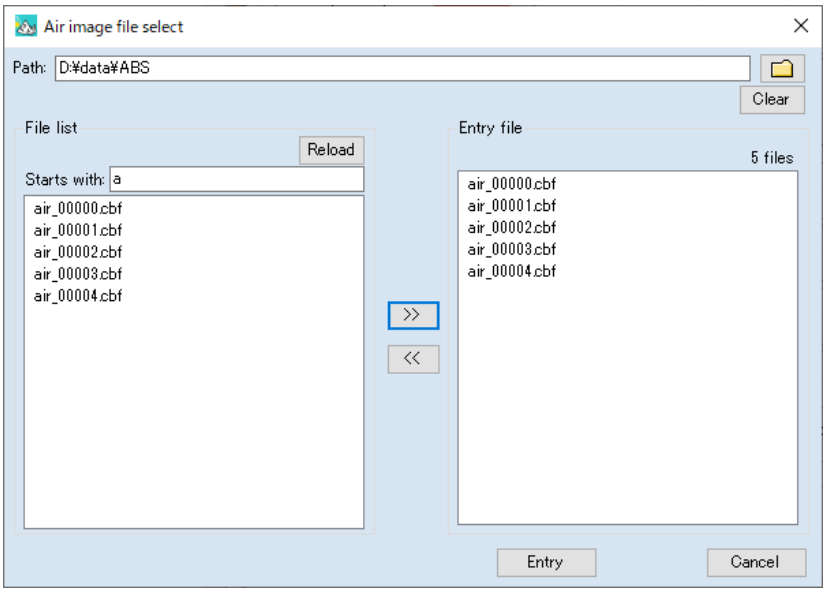


C. When the two files are properly read, the File and CounterFile in the table above will be set automatically, and the Air and GC portions will be grayed out indicating invalidity.

D. Moving on to vi.

- When using circumferential averaging files processed before Ver. 2.0.7

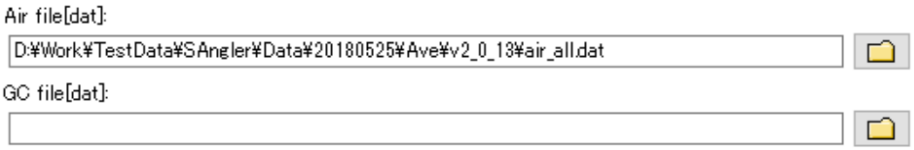
A. The following table specifies the respective data measured for Dark, Air, and GC. Clicking "Entry" on each item opens a dialog box for selecting the image data file. Specify the folder where the data is located in [Path:]. Press the folder symbol or edit it directly (or copy-paste). Clicking the reload button Reload will display a list of image data in the folder, and select multiple copies of the corresponding file at the same time (or a single copy). You can also hold down the [ctrl] key and click to select multiple images, or simply click and drag with the mouse to select multiple images. [Starts with:] is a filter function that allows you to display only specific data sets by entering a string of characters at the beginning of the filename that excludes other files. You can then press [ctrl + A] to select all of them. Clicking the right arrow >> moves the file to the right and confirms it. When finished, click "Entry" to close the dialog. Repeat each of these operations.



B. ｲ After completing the selection of the mage data, in the [CounterFile] field, select what file number from the counter files set in (iii), respectively, is to be used. Move the mouse cursor over the [CounterFile entry] button and the registered counter files will be displayed in a pop-up window. This column is displayed in red before setting, but returns

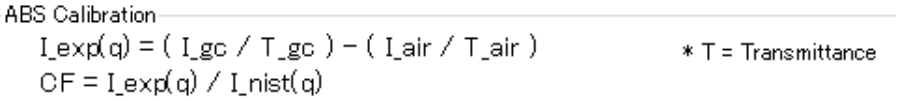
to white when a number is selected. After the final calculation, if multiple image data are set for each item, the average of the counter values is shown here, but the calculations are different for Dark and others. For Dark, it simply shows the average of the dark counts for [I0] and [I1]. On the other hand, for Air and GC, only the average value of [I1/I0] is shown. The method of calculating transmittance is basically the same as in "⑪ **Subtract Background 2 (Sub_2)**".。

C. Specify the Air and GC data that have been previously converted to 1D by [Air file [dat]:], [GC file [dat]:]. Click on the folder symbol to specify each file.

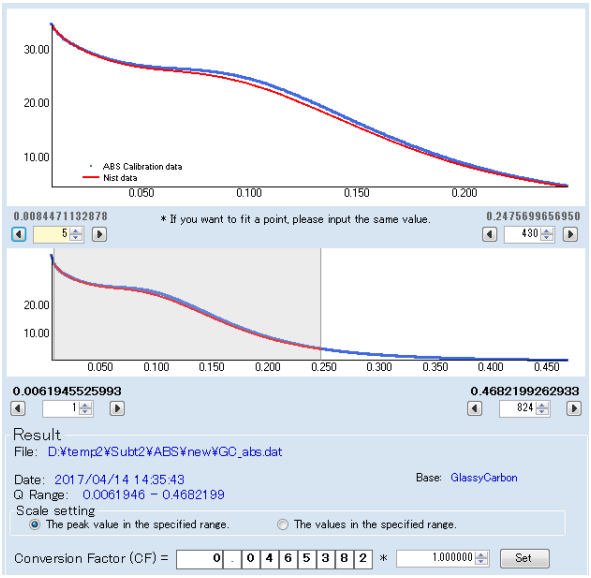


D. Move on to vi.

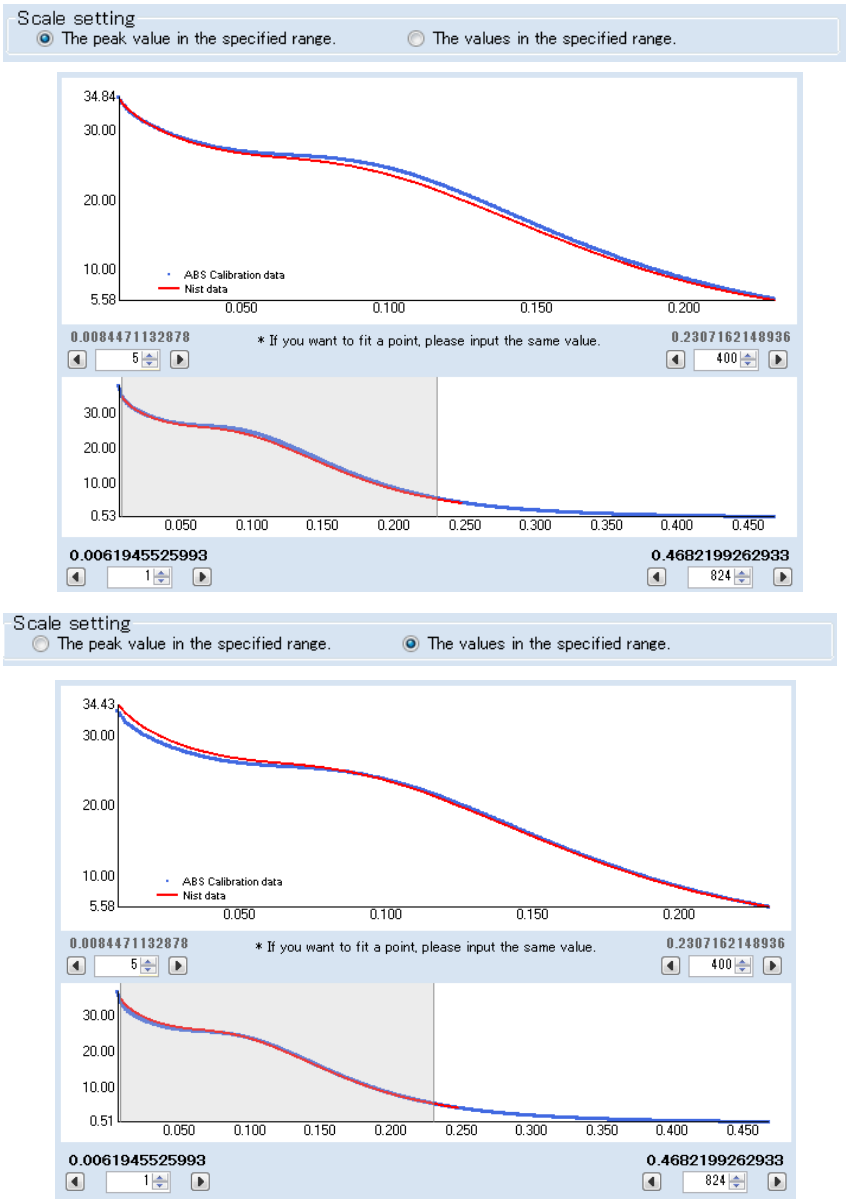
vi. The formula for determining the scattering intensity of Glassy Carbon is shown in [ABS Calibration]. The final step is to determine the factor CF for scaling the experimental scattering intensity against the reference data provided on the SRM3600 website.



vii. When everything is ready, click Run. The file is output and plotted with blue dots on the right side of the window. The file is output to the same folder [Output path:] where the GC data was read, and is named with "_abs" added to the name of the read dat file (in the above example, "GC_abs.dat").The horizontal axis of the graph is the unit system specified by Averaging, the vertical axis is the scattering intensity, and the reference data is indicated by a red dot. The upper plot shows the area used for scaling, while the lower plot shows the entire data.



viii. perform auto scaling based on the upper graph. The actual horizontal axis values used for scaling and the data range are displayed in the lower right and lower left of the graph, and the scaling range is changed by operating the ←→ keys. Two scaling patterns are available: "Scaling by the peak value in the specified range (The peak value in the specified range.)" or "Scaling by the average overlap of data in the specified range (The value in the specified range.)". The value in the specified range. Check the overlap of the plots and choose which one to use. The CF value resulting from the automatic scaling is displayed in the Result column.



ix. You can also make fine adjustments based on the results of the automatic scaling: left-click on each digit of the CF value and use the arrow keys to change the value of each digit, then adjust it while viewing the graph. You can return to the auto scaling values by changing the auto scaling range on the upper graph.

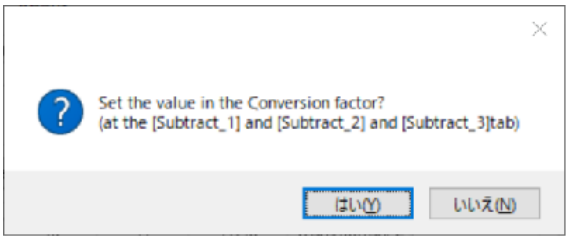
x. If you have measured SRM3600, this will determine the CF value. On the other hand, if the conversion factor is determined using separately purchased Glassy Carbon instead of SRM3600, it can be used if a correction factor between SRM3600 and that other Glassy Carbon

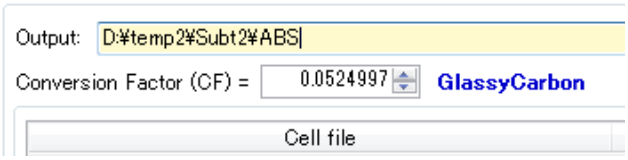
is determined in advance. Each Glassy Carbon is measured and the scattering intensity ratio to SRM3600 is determined. The CF converted to SRM3600 can be obtained by multiplying the measured values by the measured values.

※１）PF has Glassy Carbon made by BAS in a case at each beamline（http://www.bas.co.jp/1508.html#defaultTab14）. Each case describes the factor value needed to calculate the CF value, so enter that value as shown above.

※2）PF also has SRM3600 available, but due to its somewhat high cost, it is not available on the beamline. If you would like to standardize with your own Glassy Carbon, please ask our staff for the SRM3600, which we can loan you to obtain this strength ratio.

xi. Finally, if you want to use this value as CF, click Set. A confirmation dialog box will appear, and if you click Yes, the values will be copied to the Subtract_1, Subtract_2, and Subtract_3 CF columns, indicating that this value is the value obtained from Glassy Carbon. This completes the process.





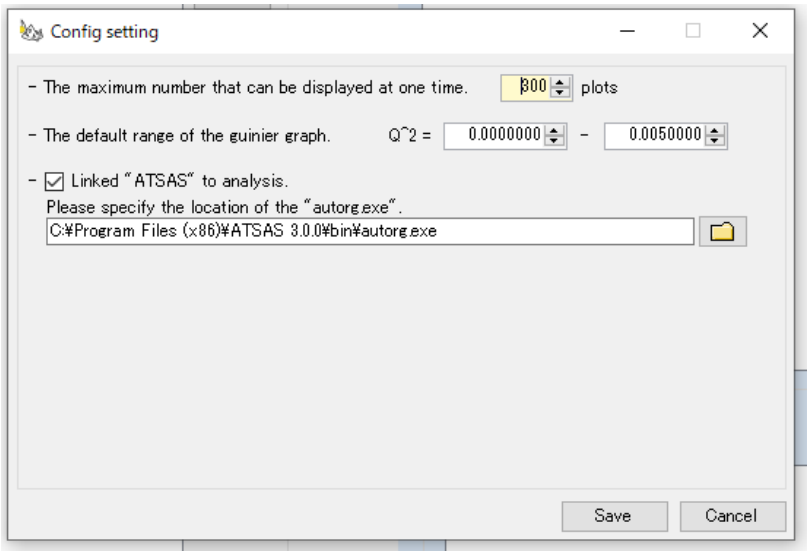
xii. References are listed below.

Zhang, F., Ilavsky, J., Long, G. G., Quintana, J. P. G., Allen, A. J. and Jemian, P. R. Glassy Carbon as an Absolute Intensity Calibration Standard for Small-Angle Scattering. *Metall. Mater. Trans. A* **41**, 1151–1158 (2009).

⑮ Analysis

The data obtained from the Average and Subtract processes are used to create graphs for analysis. Select the menu [Analysis] - [AnalysisTool] to start AnalysisTool.exe.

i. If this is the first time starting up, use ConfigSetting to configure various settings. Execute [Options] - [Config setting] from the window menu.

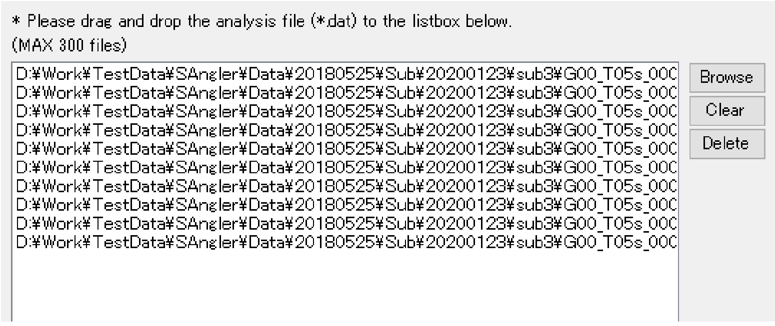


- The maximum number that can be display at one time.	Maximum data value that can be analyzed and displayed simultaneously. The default value is 300. If operation is unstable, try decreasing the value.
- The default range of the guinier graph.	Initial display range for Guinier analysis graphs.When creating a Guinier plot, the initial display range for the Q region (Å-1) is set. The default value is 0.000 to 0.005, but can be changed.
- Linked "ATSAS" to analysis.	Setting whether to use "ATSAS" in Analysis. The ATSAS autorg can be used for Guinier analysis, so its installation path is shown. ※

※ ATSAS must be installed separately by yourself; as of November 15, 2023, the latest version of ATSAS is 3.2.1. SAngler automatically recognizes and configures the folder where ATSAS is installed. If you want to use a previously installed previous version, etc., please change it manually. ATSAS is academically free, but there is a license fee for commercial use. For more information on ATSAS, please visit

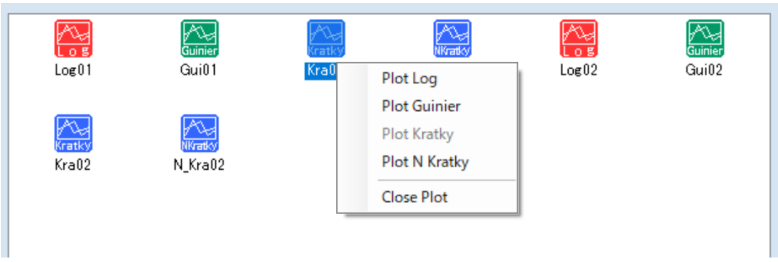
http://www.embl-hamburg.de/biosaxs/software.html

ii. First, load the data. Click [Browse] and a dialog box for selecting a file will appear. Select the file you wish to load. To specify multiple files, use the [ctrl] key or [shift] key to select them. You can also set up a file by Drag&Drop directly into this field. To set multiple files, select multiple files and Drop them (up to 300, can be changed in ConfigSetting).

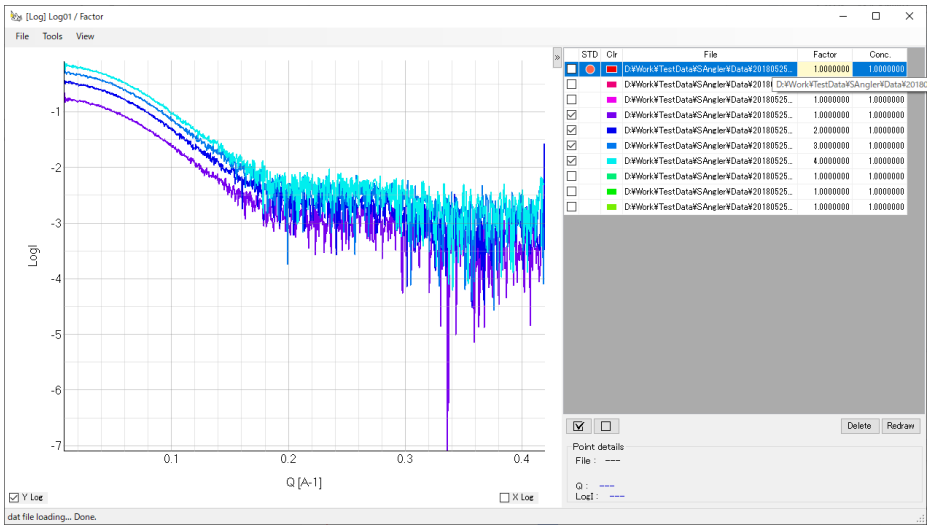


Currently, in AnalysisTool, you can create four types of plots: **"Log Plot (LogY)"** displaying the scattering intensity I on the Y-axis in a logarithmic scale, **"Guinier Plot"** where the X-axis is squared and the scattering intensity I on the Y-axis is shown in a natural logarithmic scale, **"Kratky Plot"** where the Y-axis scattering intensity I is multiplied by the squared values of the X-axis, and **"Normalized Kratky Plot =N Kratky"** which is based on Guinier analysis results, with the horizontal axis as R_g and the vertical axis as I(0) for normalization. By clicking each button, the graph will be displayed in a separate window in the order of the specified files. To change the list, press [Clear] to clear the list and load a new file.

iii. When a graph is displayed, it appears as an icon on the right side of the main window. By right-clicking on this icon, you can also close that graph or create a graph in a different format. Any number of graphs can be created in this manner. The following is a description of the functions in each Plot window in turn.

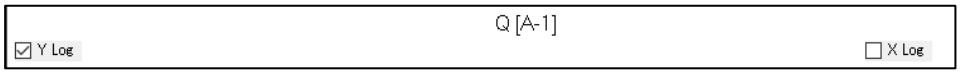


(1) LogY plot

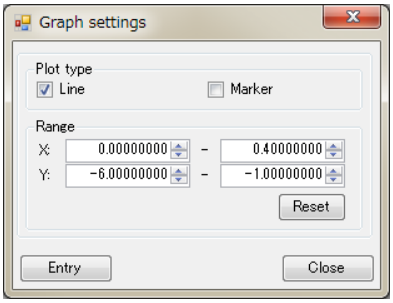


A) The newly opened graph window shows the graph on the left side and the file list on the right side. The leftmost checkbox in the list allows you to show/hide the graph. [Conc.] in the list is loaded with the concentration values entered during Subtraction. Enter a value in [Factor] to multiply by the Y-axis value. In addition, when standardization is performed, which will be explained later, the Factor of standardization is automatically displayed. In the graph, scrolling the mouse zooms in and out. You can also left-click to drag the display range to zoom in or out. Right-click to return to the original. If you want to add data to the graph, you can read it from [File] - [Input] in the File menu, or you can add it by Drag&Drop the data into the file list column on the right side of the window.

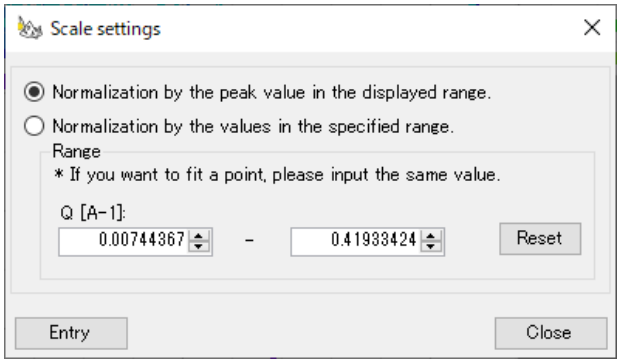
B) There is a check box at the bottom of the axis for switching the Log display. Check the box if necessary.

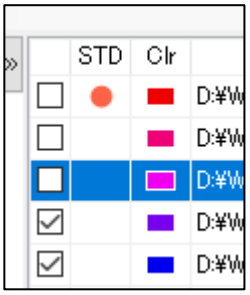


C) In the [View] - [Graph settings] file menu, set the graph plotting style, the display range of the X and Y axes, and other settings. After specifying the range, click [Entry].



D) [Tools] - [Normalization] allows you to normalize the Y-axis values. [Scale] normalizes using the Y-axis data for the specified X-axis range. [In [Concentration], normalize using the value of [Conc.]. **Normalization is performed on the basis of data marked ● in the file list as "STD".**





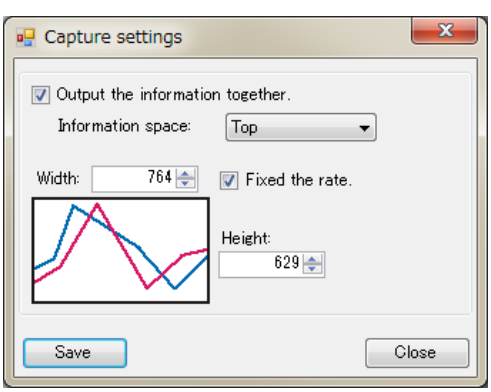
E) Select [Scale] to display a dialog box. Selecting [Normalization by the peak value in the displayed range] will normalize the graph by the value of the peak in the displayed range. Select [Normalization by the values in the specified range] to specify the area of the X-axis to be normalized and normalize it to fit the specified area. If you want to normalize on a specific X-axis point, enter the same value for the two blanks. Click [Entry] to execute. The same is true for [Concentration]. Execute [Reset] to return to the original state.

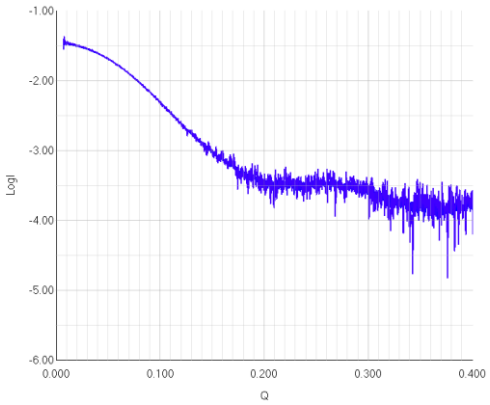
F) Data from the displayed graph can be output. Execute [File] - [Output] - [Output data file]. Set the output folder and check either [Individual] to output each data individually, [One file] to combine the data into one file, or both. For [One file], enter the name of the file to be saved. Click [Save] to output data. In the file, the X-axis values, the scattering intensity I, the standard error of scattering intensity σI, the X-axis values of the graph, the ordinary logarithm of the scattering intensity Log I, and the standard error of LogI σLogI are recorded in sequence. If normalization is performed, the normalized values are also output as LogI_norm and σLogI_norm.

※In the LogY plot, the output items change depending on the status of the Y-axis Log display switching check box.

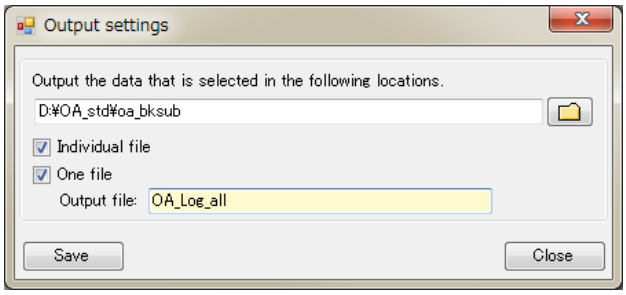
Log display： X、I、SigI、X1(X)、LogI、LogI_Sig

Linear display： X、I、SigI

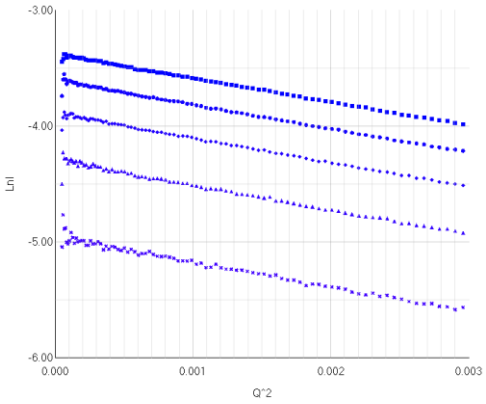




G) The displayed graph can also be output as an image (jpg, png, bmp). Execute [File] - [Output] - [Capture image]. In the dialog, check [Output the information together] if you want to save the file list together as an image. The [Fixed the rate] is checked by default so that the aspect ratio of the image is preserved. To save a larger image size, change the Width and Height (number of pixels). When settings are complete, click [Save]. Continue to specify the location to save the file, and the image file will be output.



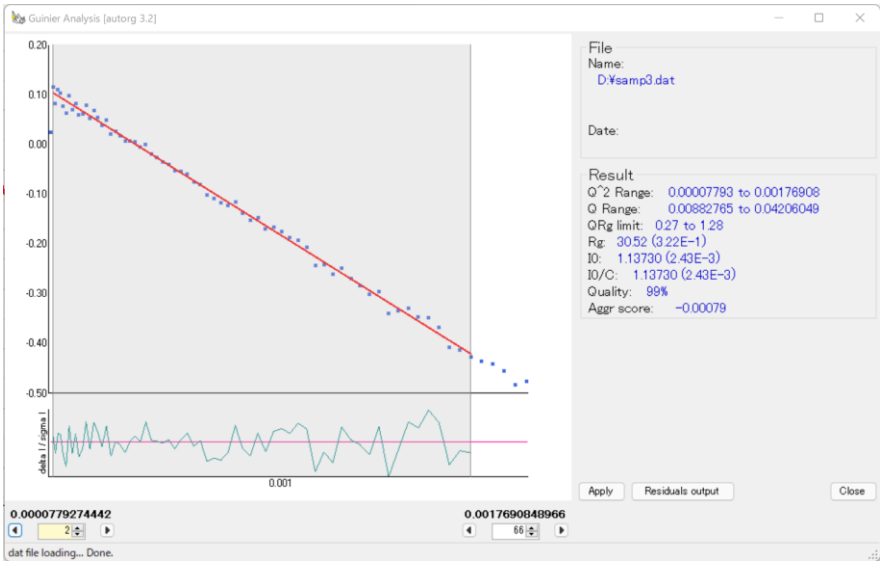
(2) Guinier plot



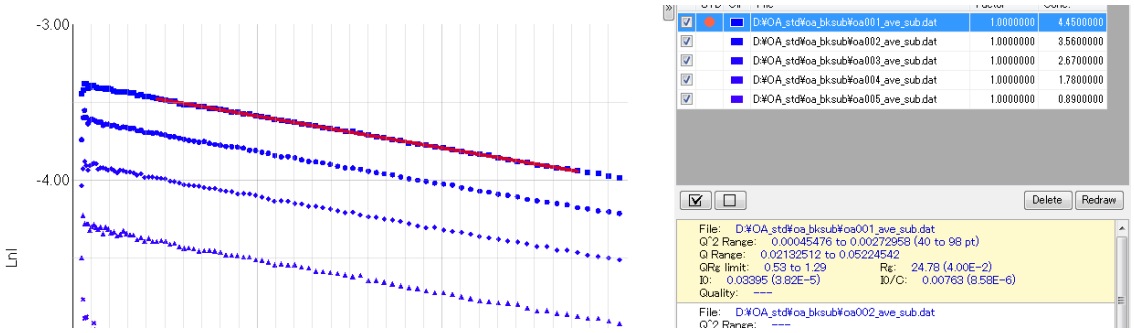
A) The basic functionality is the same as in Log plot, but Guinier implements a function for Guinier analysis (linear approximation). First, set the display range to enlarge the small corner area. In addition, since a linear approximation is performed, the "Marker" display style may be better.

B) Perform a Guinier analysis. Select [Tools] - [Guinier Analysis] and you will see five menus: [Manual], [Auto (autorg)], [All auto (autorg)], [Auto (autorg_kek)] and [All auto (autorg_kek)]. The same menu appears when you select and right-click on data in the "File List" column.
Select [Manual] to open a separate window for manual linear approximation. Move the cursor at the start and end points of the linear approximation to adjust them.

※Starting with version 2.1.59, the calculation method for residuals has been changed as follows（Same as ATSAS.）
Residual = (Measured value - Approximate value) / Error



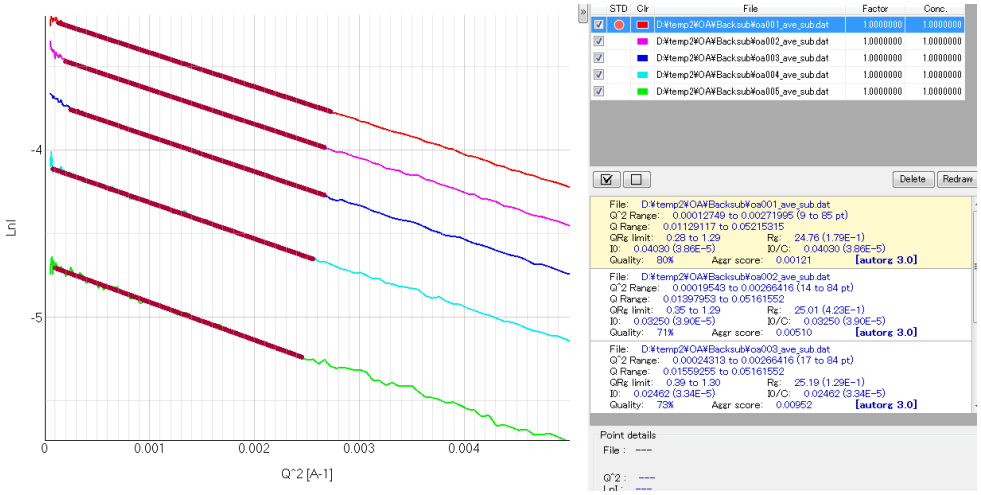
The range of Q x R_g (QR_g limit) is also displayed on the right side of the window, and the value of the residual between each data point and the approximate straight line is plotted at the bottom of the graph. Click [Residuals output] to save the residuals data as text data. When finished, click "Apply" to close, and the original



graph window will be drawn with a straight line and the resulting values.

C) In an environment where ATSAS is installed, it is possible to analyze using ATSAS autorg. When [Auto (autorg)] is executed, ATSAS autorg is run and the results are displayed in a separate window as in the manual analysis described earlier. If you are satisfied, click "Apply" to confirm. To modify, operate as in [Manual]. Note that when autorg is executed, a folder named "autorg_csv" is created in the same folder as the data, and the output results (csv files) of aurorg are automatically saved. In the csv file, the following results are output: file used, R_g, error of R_g, I(0), error of I(0), data points at the start and end of the linear approximation, Quality, and Aggregation score. Based on this output result, Angler calculates I(0)/C from I(0) and concentration, and the ranges of Q^2, Q, and Q x R_g from the start and end points of the linear approximation, and outputs them on SAngler.

D) You can also apply autorg to all data. Running [All auto (autorg)] will run autorg on all data in the file list and display the results.



E) You can also perform a Guinier analysis with the algorithm [autorg_kek] developed by PF as well as autorg in ATSAS. Please make your choice. The program used for the analysis is displayed in the results column.

F) Once the analysis is complete, the data and graph images can be output as well as LogY plots. When a straight line approximation is performed, the output data includes the X-axis value of the graph, the scattering intensity I, the standard error σI of the scattering intensity, the square value of the X-axis, the natural logarithm of the scattering intensity Ln I, the standard error σLnI of LnI, and the X and Y coordinates of the start and end points of the approximated line. Therefore, for example, if you create a Guinier plot using X squared and LnI on a graphing software such as Excel, add the data of the start and end points of this line, and connect the two points with a straight line, you can superimpose an approximate line on the experimental data in the same way as SAngler. It is also possible to output the results of a Guinier analysis as a Table. [File] - [Output] - [Output result data] will output information on each value of R_g, I(0), and I(0)/c, as well as the area of linear approximation (range of Q, Q^2, and QR_g

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	# Date: 201	5/06/24 21:04:48														
2	# Type: Guinier Result															
3	# No.	File														
4	# 001	D:¥OA_std¥oa_bksub¥oa001_ave_sub.dat														
5	# 002	D:¥OA_std¥oa_bksub¥oa002_ave_sub.dat														
6	# 003	D:¥OA_std¥oa_bksub¥oa003_ave_sub.dat														
7	# 004	D:¥OA_std¥oa_bksub¥oa004_ave_sub.dat														
8	# 005	D:¥OA_std¥oa_bksub¥oa005_ave_sub.dat														
9																
10	# No.	Q^2Start	Q^2Last	QStart	QLast	QRgLimitM	QRgLimitM	Conc	Rg	dRg	I0	dI0	I0/Conc	dI0/Conc	Quality	Aggregated
11	1	0.000711	0.002619	0.026656	0.051179	0.66	1.27	4.45	24.84	3.39E-01	0.03401	3.33E-05	0.00764	7.47E-06	0.53	0
12	2	0.00041	0.002565	0.020259	0.050646	0.51	1.27	3.56	25.02	4.60E-01	0.02712	2.87E-05	0.00762	8.06E-06	0.6	0
13	3	0.000526	0.002619	0.022924	0.051179	0.58	1.29	2.67	25.11	4.61E-01	0.02035	2.87E-05	0.00762	1.07E-05	0.58	0
14	4	0.000526	0.002674	0.022924	0.051712	0.58	1.3	1.78	25.23	8.74E-01	0.0136	3.00E-05	0.00764	1.68E-05	0.52	0
15	5	0.000368	0.002619	0.019193	0.051179	0.49	1.3	0.89	25.39	9.72E-01	0.00702	2.31E-05	0.00788	2.60E-05	0.55	0
16																

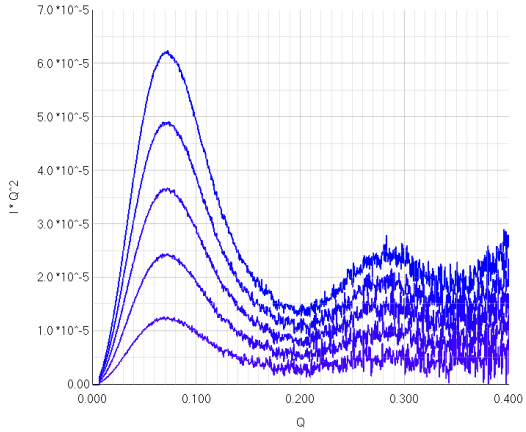
※1)

【Up to version 2.1.58】
The coordinates of the start and end points of the approximate straight line are the data sequence LineX and LineY on the output data. The first two points have values, which are the starting point and the end point, respectively. On the other hand, from the third point, both are "0 (zero)". This is done to allow software such as Igor pro to smoothly load the data at the same time as other data rows, and the zero has no meaning whatsoever. Erase after reading.
【Version 2.1.61 or later】
The coordinates of the start and end points of the approximate lines are recorded as LineX and LineY, but with a space between them below the other data columns in the output. When read by Igor pro, it is read in a separate block from the data column.

※2）Depending on the state of the data, "autorg" parsing may fail and no data may be output. There are some subtle results that make you wonder why this one is done and that one is not... In such cases, please use MANUAL to analyze the results.

(3) Kratky plot

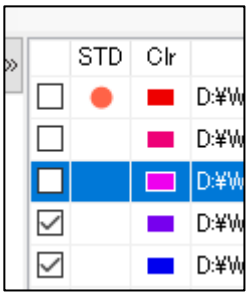
A) The Kratky plot is basically the same function as the LogY plot. The graph is shown



on the left and the file list on the right. The leftmost checkbox in the list allows you to show/hide the graph. In the list, [Conc.] is loaded with the concentration values entered during Subtraction. If you enter a value in [Factor], you can multiply it by the Y-axis value. When normalization is performed, the Factor of normalization is automatically displayed. The graph can be zoomed in and out by scrolling the mouse. Left-click to drag the display range, and the range will be enlarged and displayed. Right-click to return to the original range. If you want to add data to the graph, you can read it from [File] - [Input] in the File menu, or drag & drop it into the file list on the right side of the window.

B) In the File menu, click [View] - [Graph settings] to set the graph plotting style, the display range of the X and Y axes, and other settings. After specifying the range, click [Entry].

C) [Tools] - [Normalization] allows you to normalize the Y-axis values. [Scale] normalizes using the Y-axis data for the specified X-axis range. [Concentration] allows you to normalize using the values of [Conc.]. **Normalization is performed on the basis of data marked ● in the file list as "STD".**



D) Select [Scale] to display a dialog box. Select [Normalization by the peak value in the displayed range] to normalize by the peak values in the displayed range of the graph. [Select "Normalization by the values in the specified range" to specify the area of the X-axis to be normalized and normalize to fit that area. If you want to normalize by a specific X-axis point, enter the same values in the two blanks. Click

[Entry] to execute. The same goes for [Concentration]. Click [Reset] to return to the original.

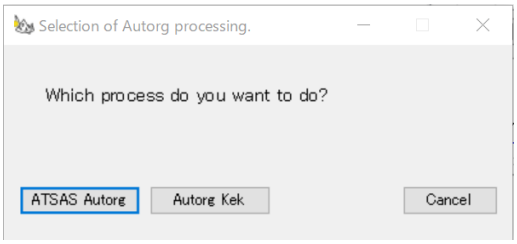
E) You can output the data of the displayed graph. Execute [File] - [Output] - [Output data file]. Set the output folder and check either [Individual] to output each data individually, [One file] to combine the data into one file, or both. For [One file], enter the name of the file to be saved. Click [Save] to output the data. In the file, the X-axis value, scattering intensity I, standard error of scattering intensity σI, X-axis value of the graph, I x Q^2 multiplied by the square of the scattering intensity I and X-axis value, and standard error of I x Q^2 σI x Q^2 are recorded in this order. If normalization is performed, the normalized values are also output as I×Q^2_norm and σI×Q^2_norm.

F) It is also possible to output the displayed graph as an image (jpg, png, bmp). Execute [File] - [Output] - [Capture image]. In the dialog, check [Output the information together] if you want to save the file list together as an image. The [Fixed the rate] is checked by default so that the aspect ratio of the image is preserved. To save a larger image size, change the Width and Height (number of pixels). When settings are complete, click [Save]. Continue to specify where to save the image, and the image file will be output.

(4) N Kratky（Normalized Kratky） plot

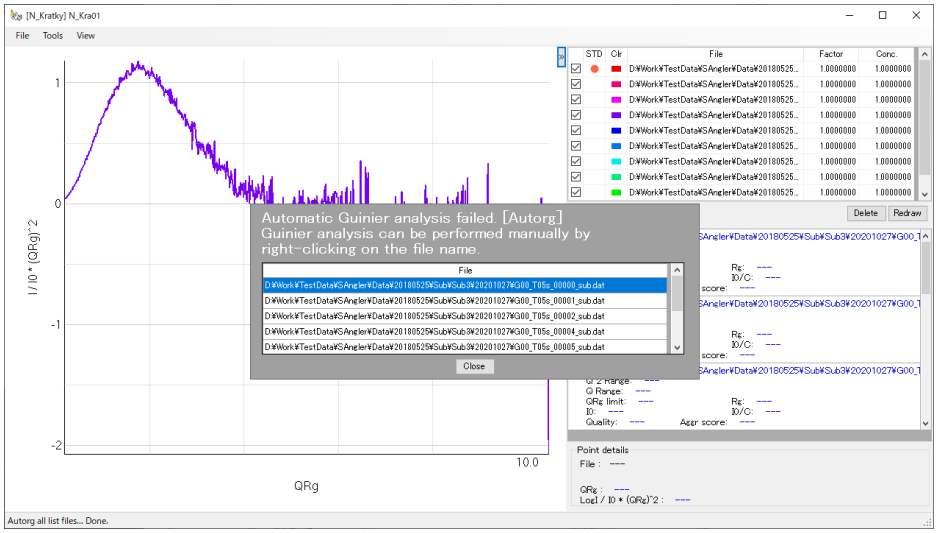
For a Kratky plot, it is nondimensionalized by multiplying the x-axis by Rg and the y-axis by Rg2 as well, and further normalized by dividing I(q) by I(0). Also called Dimmensionless Kratky plot.

A) Load the data first. Drag&Drop (or select the file from the [Browse] button) the file you want to load and click [N Kratky].



B) When loading is complete, a message box will appear as shown above. When multiple data are loaded, either ATSAS or KEK's autorg will be applied. If you wish to perform them separately, select one of them for now and perform the Guinier analysis separately later with reference to D, E, and F). If ATSAS is not installed, select "Autorg_kek".

C) If the automatic Guinier analysis fails, a list of failed files will be displayed. If the analysis proceeds without any problems, skip to G).



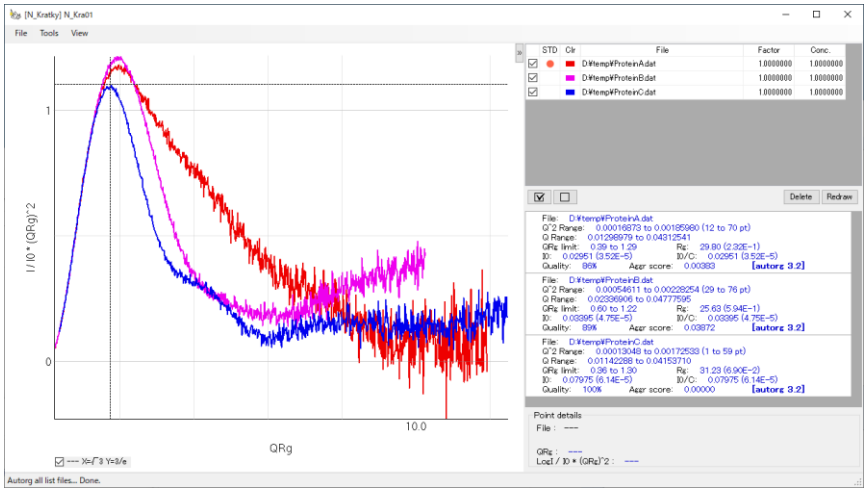
D) Select the data you want to analyze in the file list column on the right side of the graph window, and select [Tools] - [Guinier Analysis] to display five menus: [Manual],

[Auto(autorg)], [All auto(autorg)], [Auto(autorg_kek (autorg_kek)], and [All auto (autorg_kek)]. The same menu is also displayed when you select data and right-click in the file list column. If you select [Manual], a separate window for Guinier analysis will open, and you can move the cursor to adjust the start and end points of the linear approximation. The value of Q x R_g (QR_g limit) is also displayed on the right side of the window, and the approximate straight line and the residuals for each data point are plotted at the bottom of the graph for reference. When finished, click [Apply] to close, and the results of the Guinier analysis will be listed under the file list.

E) In an environment where ATSAS is installed, it is possible to analyze using ATSAS autorg. When [Auto (autorg)] is executed, ATSAS autorg is executed and the results are displayed in a separate window as in the manual analysis described earlier. If this is OK, click "Apply" to confirm. If you wish to modify the data, do so in the same way as in [Manual]. Note that when you run autorg, a folder named "autorg_csv" is created in the same folder as the data, and the aurorg output results (csv files) are automatically saved. In the csv file, the following results are output: file used, R_g, error of R_g, I(0), error of I(0), data points of start and end points of linear approximation, Quality, Aggregation score, etc. SAngler uses these output results to calculate I (0)/C from I(0) and concentration, and Q^2, Q, and Q x R_g from the start and end points of the linear approximation, and output them to SAngler.

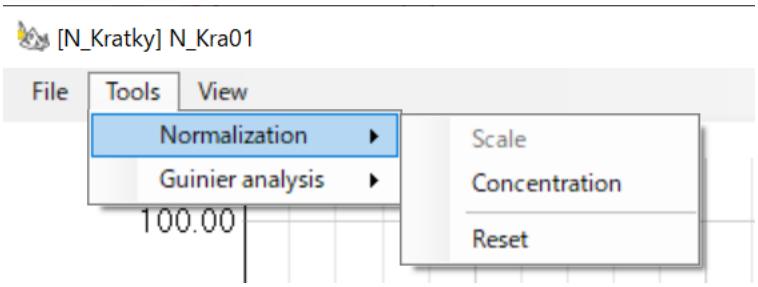
F) You can also run the Guinier analysis with the algorithm [autorg_kek] developed by PF as well as autorg in ATSAS. Please choose as you wish. The program used for the analysis will be displayed in the results column.

G) Once the Guinier analysis is complete, a Normalize Kratky Plot is drawn in the left-hand graph window using the obtained R_g and I(0) values. For an ideal spherical structure, $QR_g=\sqrt{3}$ and $I(Q)/I(0)(QR_g)^2=3/e$ will have a peak, so the line is drawn as a dotted line.



H) Once the analysis is complete, you can output data and graph images as well as Log plots. When a linear approximation is performed, the output data includes the value on the x-axis of the graph, the scattering intensity I, the standard error of the scattering intensity σI, QR_g multiplied by the value on the x-axis and R_g, $I/I(0)\times(QR_g)^2$, and its standard error $\sigma I/I(0)\times(QR_g)^2$. It is also possible to output the results of a Guinier analysis as a Table. [File] - [Output] - [Output result data] will output the values of R_g, I(0), and I(0)/C, as well as information on the linearly approximated region (range of Q, Q^2, and QR_g).

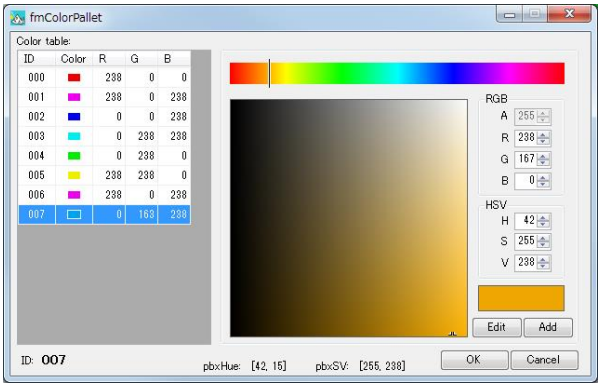
※ N Kratky plots cannot be normalized by Scale because each graph has a different R_g value.



※To change the color of a graph

The software automatically assigns colors to the graphs, but you can also change them manually by following the steps below.

(1) In the file list on the right side of each graph window, click [Clr], or Color column, of the data you want to change to open another window called [ColorPallet].



(2) The Color table used in the current graph is displayed on the left. If you want to replace the color in this table, click on the color (ID) and press [OK].

(3) If you want to add another color, adjust the color in the right palette and click "Add". Then the color will be added to the table on the left side. Select it in the same way as in (2) and click [OK].

(4) Click "OK" and you will be asked "Register Color table data?" Click "Yes".

(5) This will change the color.

iv. Information on Linear Approximation and Error

Supplementary information regarding the calculation of the linear approximation in the Guinier analysis and the calculation of the error for each value. All values are obtained according to the error propagation law. (We have also confirmed that the output results are the same as those of PRIMUS.

(5) For linear approximation

At data points (x_i, y_i), perform a regression analysis with a first order regression line y=A+Bx when y_i has error σ_i. Consider the weight ω_i of each data point according to the error.

$$\omega_i = \frac{1}{\sigma_i^2}$$

$$\Delta = \sum \omega_i \sum \omega_i x_i^2 - \left(\sum \omega_i x_i\right)^2$$

Defined as follows, the A and B values can be obtained by the following equations, respectively.

$$\mathrm{A} = \frac{1}{\Delta}\left(\sum \omega_i x_i^2 \sum \omega_i y_i - \sum \omega_i x_i \sum \omega_i x_i y_i\right)$$

$$\mathrm{B} = \frac{1}{\Delta}\left(\sum \omega_i \sum \omega_i x_i y_i - \sum \omega_i x_i \sum \omega_i y_i\right)$$

The errors σ_A and σ_B of the A and B values, respectively, are then expressed as follows.

$$\sigma_A = \sqrt{\frac{\sum \omega_i x_i^2}{\Delta}}$$

$$\sigma_B = \sqrt{\frac{\sum \omega_i}{\Delta}}$$

In the Guinier analysis, the expression for the Guinier approximation

$$\ln I(q) = \ln I(0) - \frac{R_g^2}{3} q^2$$

From Y intercept $\mathrm{A} = \ln I(0)$ to I(0), and slope $\mathrm{B} = -R_g^2/3$ to the value of R_g.

$$\mathrm{I}(0) = e^A$$

$$R_g = \sqrt{(3 \times |B|)}$$

The error of each is,

$$\sigma\mathrm{I}(0) = e^A \times \sigma_A$$

$$\sigma R_g = \frac{1}{2}(3 \times |B|)^{-\frac{1}{2}}(3 \times \sigma_B)$$

can be expressed.

(1) Error in the ordinary and natural logarithm of the scattering intensity I

The errors of LogI and LnI can be described from the error propagation law as follows.

$$\sigma \ln I = \frac{\sigma I}{I}$$

$$\sigma \log I = \frac{\sigma I}{(I \times \ln 10)}$$

(6) References, reference sites

The following textbooks and websites are used as references (sorry for Japanese)

・計測における誤差解析入門、John R. Taylor、林茂雄・馬場涼 訳、東京化学同人

・(例解)微分積分学演習、鈴木義也 他編著、共立出版株式会社

・産業技術総合研究所 計測標準部門 計量標準システム科 主任研究員 井原俊英様と
先端材料科 材料評価研究室 テクニカルスタッフ 新 重光様が開設されている
「化学標準物質の不確かさ」に関するページ
https://staff.aist.go.jp/t.ihara/

※This was very helpful. Thank you very much.

⑯ Cormap Maker

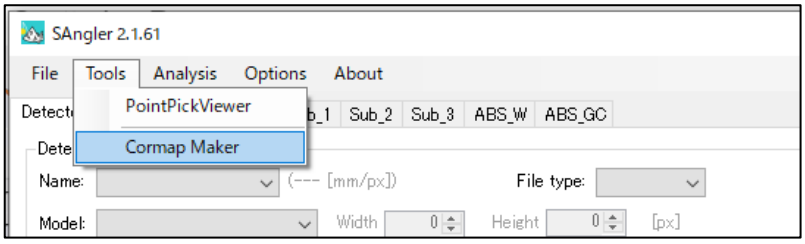
(Summary)

In modern SAXS measurements, multiple short-time exposures are measured (e.g., 10 1-second exposures are measured) using a fast-readout detector such as PILATUS (Dectris), and then the data are averaged to improve S/N for further analysis. Such a method is very effective for verifying the effects of radiation damage on the data, but it must be made clear that all data from multiple measurements must be considered identical in order to be averaged. SAngler has long implemented a function (Point Pick) in the right side graph section of the window that plots the Y value of a specified X-axis position in the CirAve and Sub tabs, allowing the evaluation of radiation damage based on the variability of values measured multiple times. Recently, a method to create a correlation map (Correlation map) between data points has been proposed to quantitatively evaluate data uniformity, such as the effect of radiation damage. Therefore, we have added a new tool to SAngler, Cormap Maker, which also creates Correlation maps. For more information on evaluation with the Correlation map, please refer to the following paper

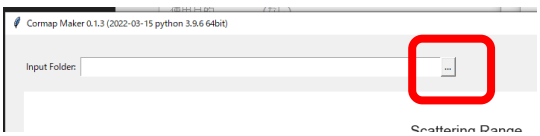
[1] Franke, D., Jeffries, C. M. and Svergun, D. I. Correlation Map, a goodness-of-fit test for one-dimensional X-ray scattering spectra. *Nature Methods* **12**, 419-422 (2015). doi:10.1038/nmeth.3358

[2] Brooks-Bartlett, J. C., Batters, R. A., Bury, C. S., Lowe, E. D., Ginn, H. M., Round, A. and Garman, E. F. Development of tools to automate quantitative analysis of radiation damage in SAXS experiments. *J. Synchrotron Rad.* **24**, 63-72 (2017). doi:10.1107/S1600577516015083.

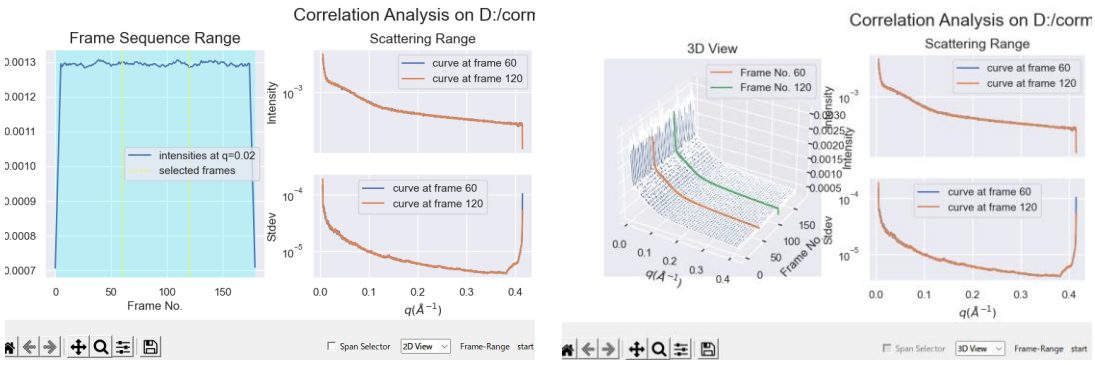
i. Select [Tools] - [Cormap Maker] from the upper left menu of the main window to launch it.



ii. In the [Input Folder:] field, specify the folder containing the dat files for which you want to calculate the map. Clicking the [...] button will display a folder selection dialog. You can also specify the target folder directly by Drag&Drop.



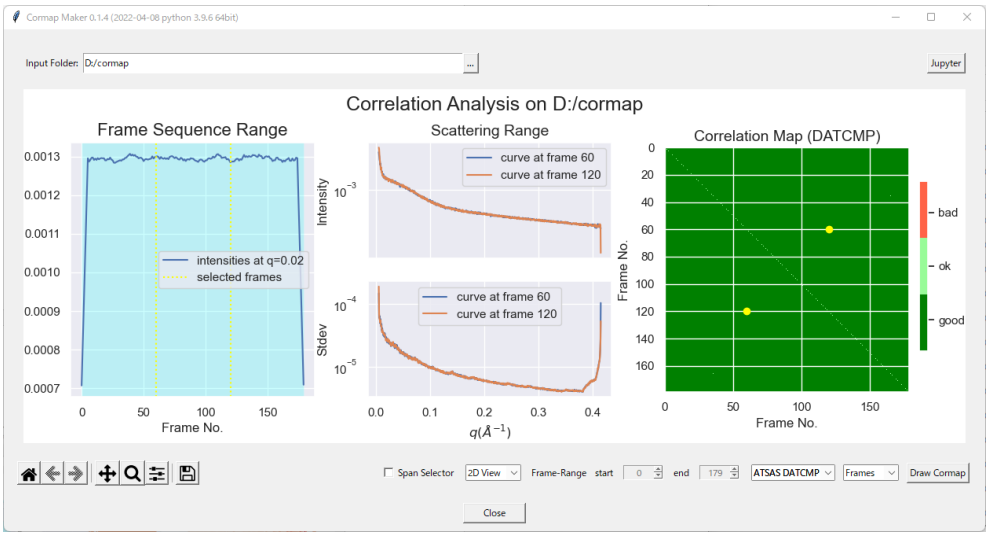
iii. The data in the specified folder will be reflected on the screen. The graph on the left shows the entire loaded data, but you can switch between "2D View (plotting values at specific X-axis locations)" or "3D View (matrix view of the entire data)" using the pull-down menu at the bottom of the window.



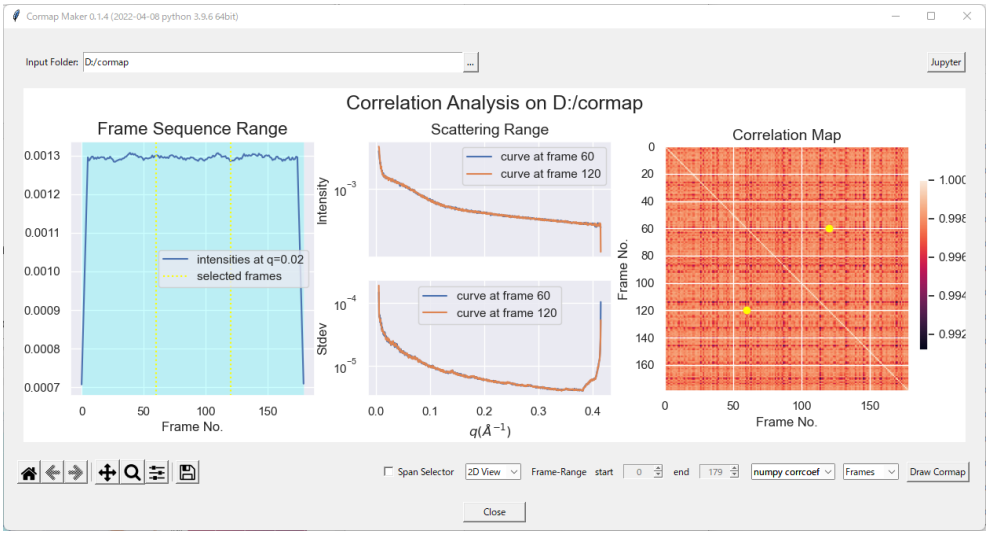
iv. Correlation maps can be created using two algorithms. One is DATCMP from ATSAS and the other is NumPy (numpy.corrcoef), a Python extension. Please select from the pull-down menu. Also, choose whether the Correlation Map should be created with "Frames (between data)" or "Angular (angle, Q, i.e., X coordinate)". In DATCMP, only "Frames" will be selected. After making these settings, press the "Draw Cormap" button.

v. Correlation map is displayed as follows.

A) Correlation map between frames (ATSAS DATCMP)



B) Correlation map between frames（numpy.corrcoef）



C) Correlation map（numpy.corrcoef）for angular

vi. To save the map as image data, click on the bottom left corner to save the map.

4. Reference

① Shimizu, N., Yatabe, K., Nagatani, Y., Saijyo, S., Kosuge, T. and Igarashi, N.
Software Development for Analysis of Small-angle X-ray Scattering Data.
AIP Conf. Proc., 1741, 050017 (2016).

② If autorg of ATSAS is used in the Guinier analysis or if a correlation map is created and used in DATCMP, please be sure to reference ATSAS as well. Please state, "One dimensionalization of the data and background subtraction were performed in SAngler, and Guinier analysis was performed in ATSAS autorg."

Petoukhov, M.V., Franke, D., Shkumatov, A.V., Tria, G., Kikhney, A.G., Gajda, M., Gorba, C., Mertens, H.D.T., Konarev, P.V. and Svergun, D.I. (2012) New developments in the ATSAS program package for small-angle scattering data analysis. *J. Appl. Cryst.* **45**, 342-350.

[latest]

Manalastas-Cantos, K., Konarev, P.V., Hajizadeh, N.R., Kikhney, A.G., Petoukhov, M.V., Molodenskiy, D.S., Panjkovich, A., Mertens, H.D.T., Gruzinov, A., Borges, C., Jeffries, C.M., Svergun, D.I., Franke, D. (2021) ATSAS 3.0: expanded functionality and new tools for small-angle scattering data analysis. *J. Appl. Cryst.* **54**, 343-355.

※ *After setting up ATSAS and Link, the message shown on the left will be displayed.

③ PointPickViewer uses the following system

- Python 3.9 (https://www.python.org/)
  Copyright (C) 2001-2020 Python Software Foundation; All Rights Reserved
- Python.NET (https://github.com/pythonnet/pythonnet)

5. Supplement

① The results of each stage of processing are checked against the results processed outside of SAngler using Igor, Excel, etc. to confirm that the calculations are in accordance with the specifications We also referred to PETRAIII, ATSAS (mainly PRIMUS and autorg) developed by Dr. D. I. Svergun and his group at EMBL, and Igor pro macro Nika developed by Dr. Jan Ilavsky at APS to ensure that the results are consistent with the output of each The results of the analysis were checked to be consistent with the output results of each of them.

「ATSAS software」
https://www.embl-hamburg.de/biosaxs/software.html
「"Nika" package of 2D -> 1D SAS data reduction macros for Igor Pro」
https://usaxs.xray.aps.anl.gov/software/nika