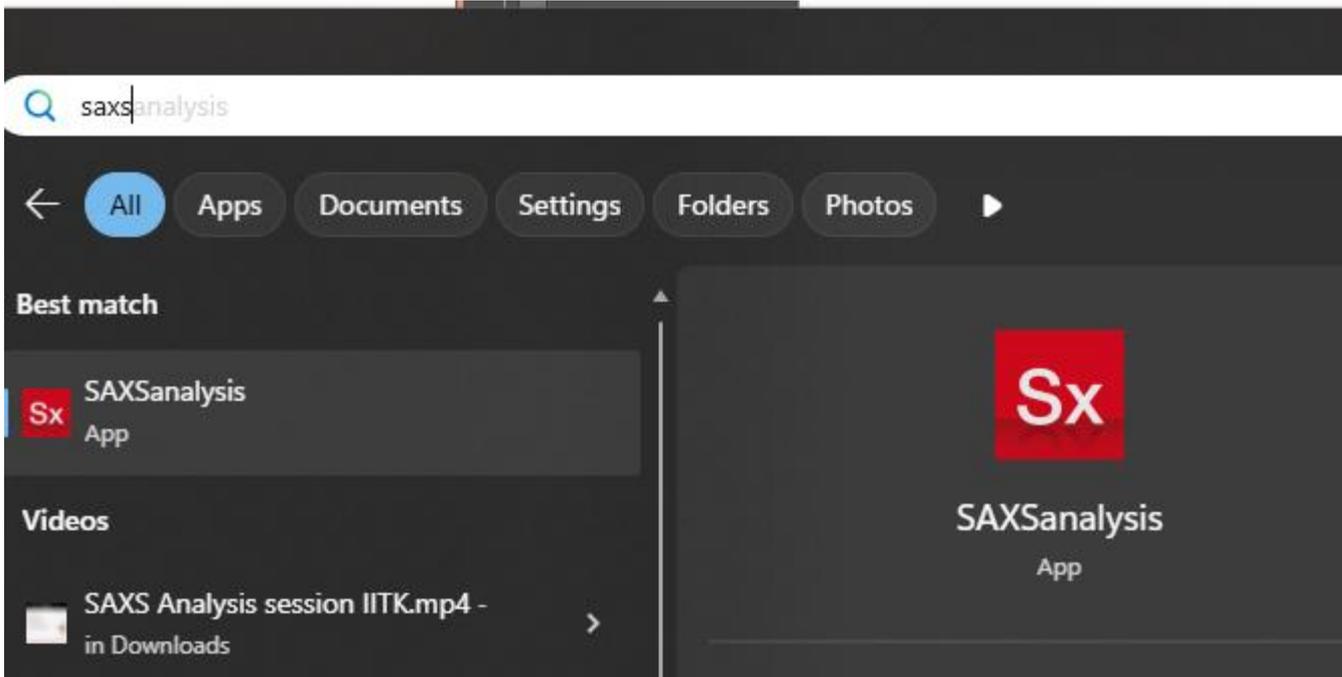


SAXSAnalysis Guide



SAXSAnalysis is for doing pre-data processing, data merge, data export and selective analysis

Please choose how to start

+ Start session

Start a new session by adding your experimental data files

[Add files](#)

📁 Open session

Open a session file saved on your computer

[Open session](#)

⬇️ Import SAXSanalysis package

Import and extract a session and data files contained in a SAXSanalysis package

[Import Package](#)

📄 Start empty session

Start a new empty session

[Start empty session](#)

📄 Open Analysis Mode

NEW

Analysis Mode

[Open analysis mode](#)

This mode one can do quick data reduction and analysis (particle size distribution, specific surface area, concentration)

Start session or load previous session/package using these options

This the start screen of SAXSAanlysis

Please choose how to start

+ Start session

Start a new session by adding your experimental data files

[Add files](#)

📁 Open session

Open a session file saved on your computer

[Open session](#)

⬇️ Import SAXSanalysis package

Import and extract a session and data files contained in a SAXSanalysis package

[Import Package](#)

📄 Start empty session

Start a new empty session

[Start empty session](#)

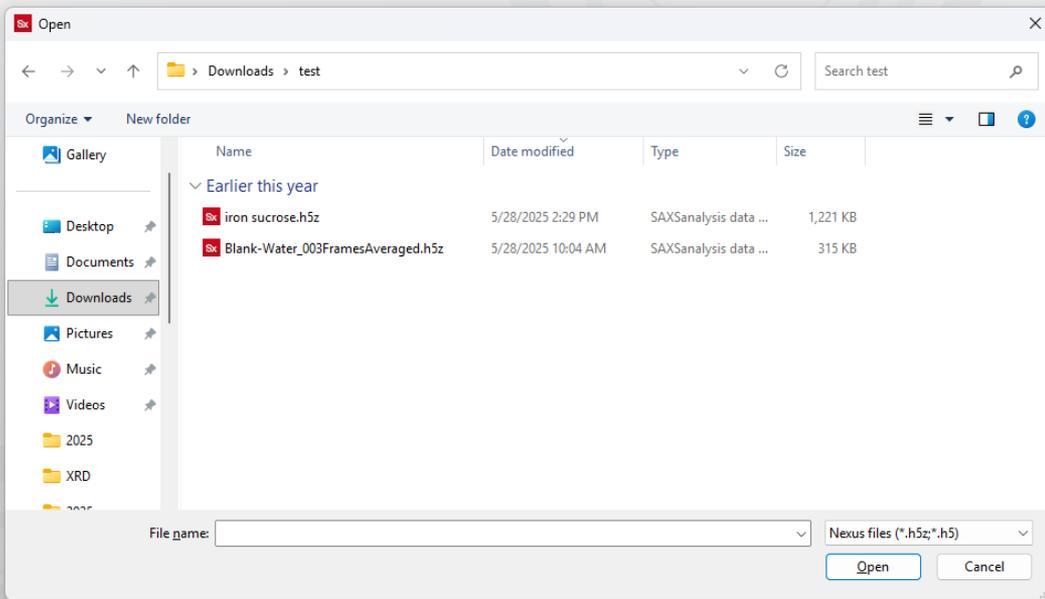
📄 Open Analysis Mode

NEW

Analysis Mode

[Open analysis mode](#)

Start new session by clicking “Add files”



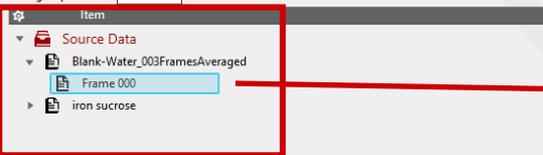
Pop-up opens and browse to the file location to add them. Select files and click open

art empty session

new empty session

empty session

Processing memory: 3.0 GB
Data group: all



Configuration Figures Data groups

Frame 000

File name Blank-Water_003FramesAveraged/000
Path C:\Users\komaljain\Downloads\test\Blank-Water_003FramesAveraged.nsz
Data type AnalysisData2D
Value $z = f(x,y) [x[-0.0370431763031929..0.0401318236968071]; y[-0.0193841320815436..0.0604158679184564]] = 1096951$
Units Detector Counts I [cts]
X units ScatteringDistance sD [m]
Y units ScatteringDistance sD [m]

Data properties

Property	Value
averaged_frames	3 [-]
CountTime	600 [s]
DataEntity	Detector Counts I [cts]
Detector	Eiger R 1M
DetectorHeight	-0.01938413
DetectorPixelMask	Mask2D
DetectorPixelSize	[7.5E-05 [Variance=0]; 7.5E-05 [Variance=0]]
DetectorTransformation	x_translation < height < meridional_angle < distance
DetectorXTranslation	-0.03704318
file_name	Blank-Water_003FramesAveraged
flux_entering_sample	2310218 [cts]
flux_exiting_sample	620507.2 [cts]
FrameIndex	0
FrameOriginName	Blank-Water_003FramesAveraged
IsLineCollimation	False
IsSAXS	True
IsWAXS	False
NexusDataProvider	AntonPaar.Mc.Nexus.NexusReader
sample_composition	
sample_concentration	0 [kg/m ³]
sample_name	Blank-Water
sample_skeleton_density	0 [kg/m ³]
sample_temperature	293.1671 [K]
sample_thickness	0 [m]
sample_y	-1.206118E-07 [m]
SAXS/WAXS merge	False
sdd	0.826652 [m]
shutter	1 [-]
time	1801.822 [s]
total_intensity	61368.67 [cts]
transmittance	0.2685925 [-]
transmittance_variance	4.387543E-07 [-]
Wavelength	0.15418 [nm]
XAxisEntity	ScatteringDistance sD [m]

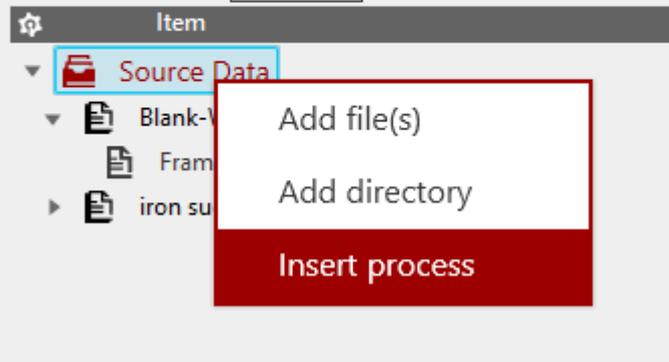
On clicking file one can see measurement parameters under “configuration” tab

All data can be seen under source data. One should add files under source data which needs to be processed/analyzed.

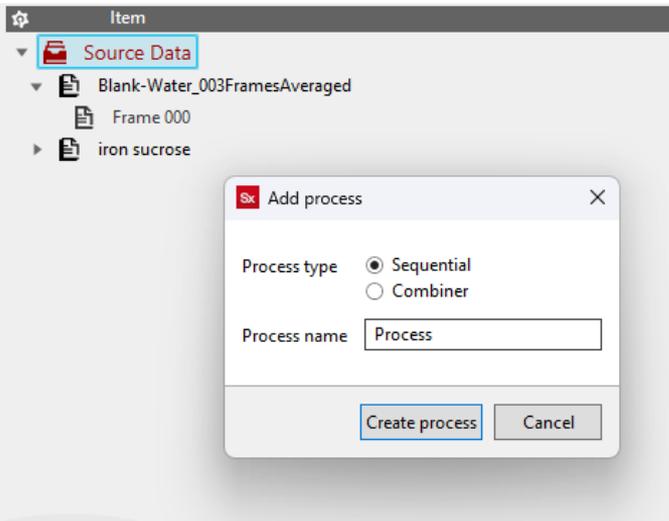
Calculate 

Processing memory: 3.0 GB ▾

Data group: all ▾



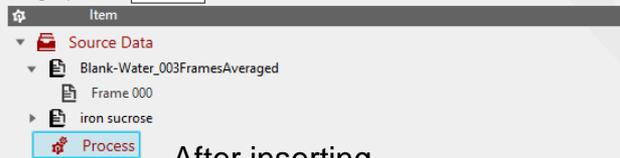
Right click we see options to add files or entire directory/folder and insert process. All operations are done under process



Clicking process pop-up for type of process shows.

- Sequential: This process contains tools/operation for all data preprocessing, data export and analysis
- Combiner: this process contains tools for data merger and combine

Here: create sequential process. One can rename the process

Processing memory: 3.0 GB
Data group: all

After inserting process. Do left click. One see window on left.

Configuration Figures Data groups

Process



Remove

Click on "Select" and below pop-up comes for files selection

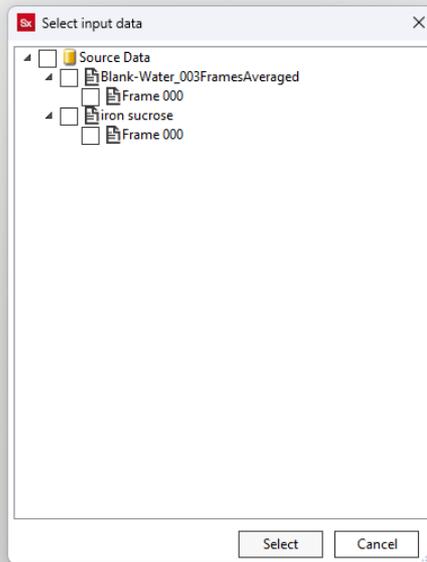
Selected Inputs Data group

Add group(s) to process Process

Group: No groups available

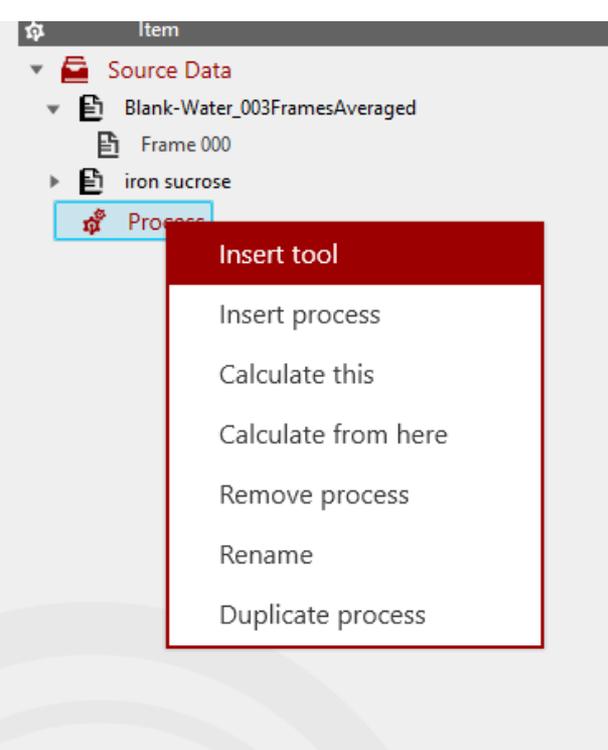
Pre process: From process input (optional): Add group input

Selected Inputs



Select the files on which operations need to be done checking the boxes next to file names.

Note: Files added under source will only be shown. Make sure that all required files are already added under source data.



Sort the tools by using options in the box

To check the details on tools please refer to SAXSAnalysis manual.

Here: Select “Absolute intensity” tool and click “Create tool” to add the tool.

This tool is used to normalize scattering with respect to transmission.

Right click on process to add required “Tool” to carry out desired operations

On clicking “Tools” pop-up on right will open.

Processing memory: 3.0 GB
Data group: all

Item

- Source Data
 - Blank-Water_003FramesAveraged
 - Frame 000
 - iron sucrose
- Process
 - Absolute Intensity**

Select the Absolute tool

Configuration Figures Data groups

Absolute Intensity

Mandatory user provided values:

Sample thickness cm

Fallback values (when no data is provided by the sample):*

Intensity hitting the sample (phi) counts (*from sample "flux_entering_sample")

Transmission coefficient % (*from sample "transmission")

Mandatory values provided by the sample:

Frame count time - s (from sample "CountTime")

Here insert sample thickness and click apply.

Note: tool picks transmission data automatically from the file. For that please be sure the while doing the measurement transmission data was collected.

Item

- Source Data
 - Blank-Water_003FramesAveraged
 - Frame 000
 - iron sucrose
- Process
 - Absolute Intensity

- Insert tool
- Calculate this**
- Calculate from here
- Remove tool
- Rename

Right click on tool and click “calculate this”. This will do the tool operation.

Or

Click “calculate” at the bottom to calculate all tools in the tree

Or

Click “calculate from here” at the bottom to calculate all tools in the tree from the selected tools onwards

Processing memory: 3.0 GB
Data group: all

Item

- Source Data
 - Blank-Water_003FramesAveraged
 - Frame 000
 - iron sucrose
 - Process
 - Absolute Intensity

Data type: Any 1D 2D

Tool category: Any Preprocessing Analysis DataExport Advanced

- Absolute Intensity
- Align To Beam 2D
- Beamline Parameter Fit 1D
- Beamline Parameter Fit 2D
- Beamline Parameter Fit Applier
- Binning 1D
- Binning 2D
- Clip Axis 1D
- Data Reduction 2D
- Desmear 1D
- Export ASCII
- Export ATSAS
- Export Born Again
- Export Nexus
- Export PDH
- Fitting
- Formula 1D
- Formula 2D
- Guinier
- Masking 1D
- Masking 2D
- Molecular Weight
- Plugin (beta)
- Porod
- Porod Volume
- Prepare Length Profile 1D
- Prepare Width Profile 1D
- Q Transformation
- Range Parameters 1D
- Range parameters 2D
- Remove masked & NaN values 1D
- Resampling 1D
- Rotate 2D
- Run External Command
- Specific Surface
- Standard Operations 1D
- Standard Operations 2D
- XRDynamic 500 background subtraction
- Zero Point By Click 1D
- Zero Point By Click 2D
- Zero Point By Moments 1D
- Zero Point By Moments 2D**

Tool name: Zero Point By Moments 2D

Create tool Cancel

Right click on “Absolute intensity” tool to add “Zero point by Moments 2D” tool.
This tool is used to correct the x-axis position with respect to primary beam

Processing memory: 3.0 GB
Data group: all

Item

- Source Data
 - Blank-Water_003FramesAveraged
 - Frame 000
 - iron sucrose
- Process
 - Absolute Intensity
 - Zero Point By Moments 2D

Select the tool to configure it.

Zoom near the primary beam by pressing left click and dragging the mouse cursor while keeping the left click pressed.

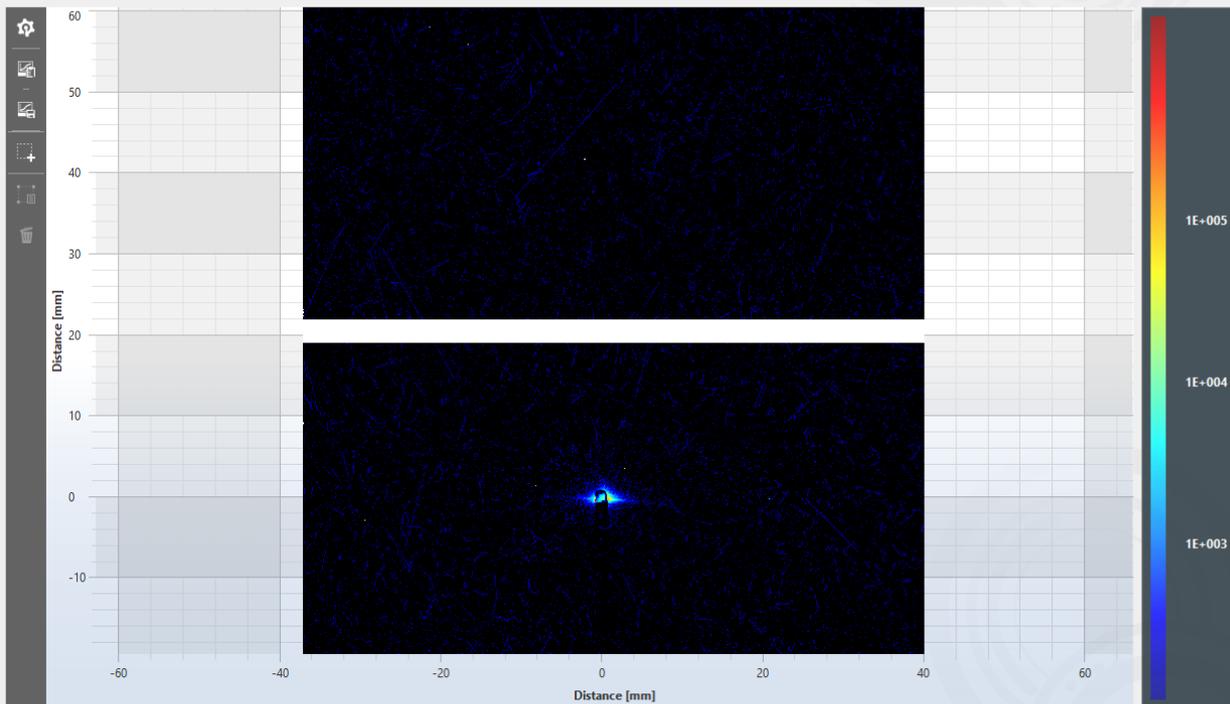
There are unsaved tools

Calculate 

Configuration Figures Data groups

Zero Point By Moments 2D

Select Dataset: Blank-Water_003FramesAveraged/000/Process/Absolute Intensity

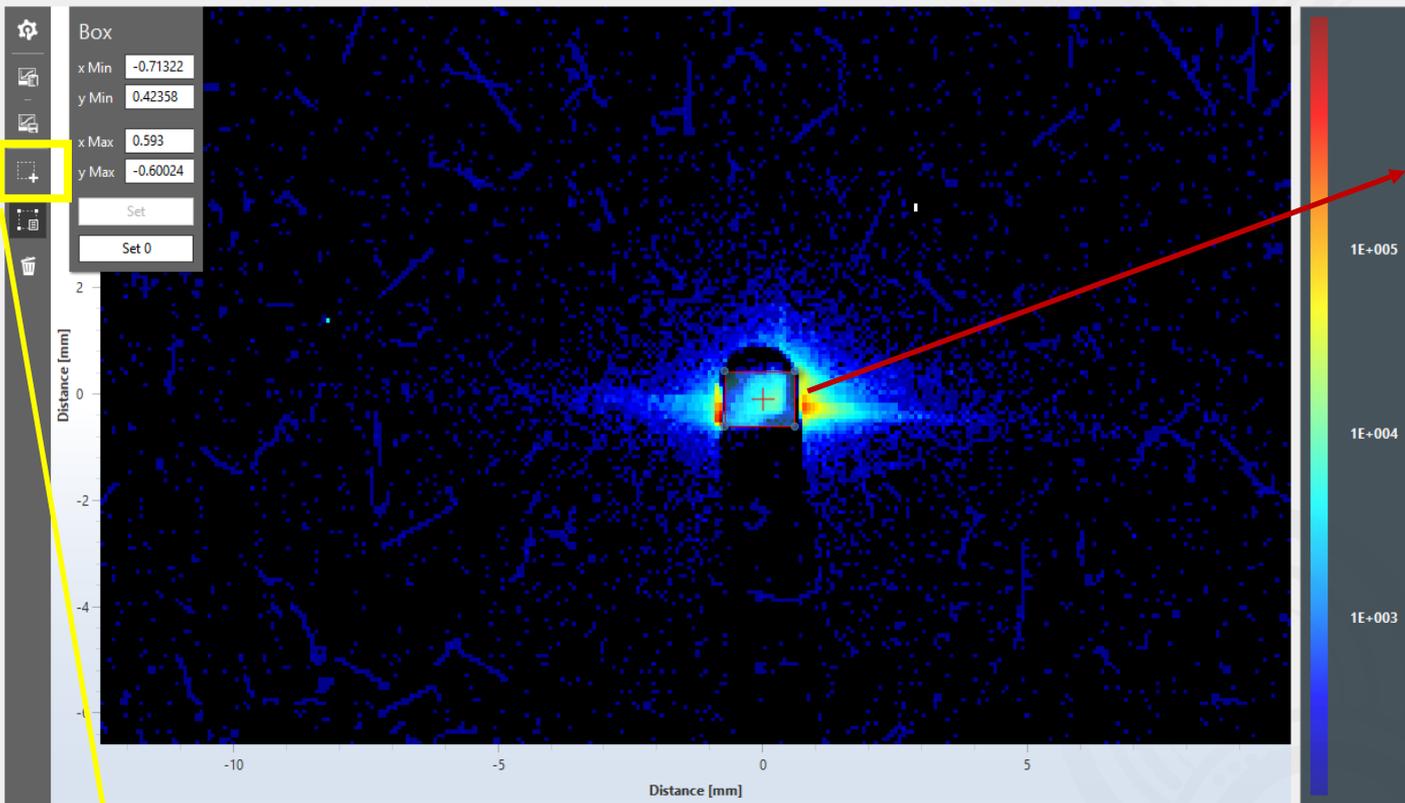


Recalculate

Apply

Cancel

Select Dataset Blank-Water_003FramesAveraged/000/Process/Absolute Intensity



Select the region of primary beam visible from semi-transparent Ni beamstop/primary beam.

To select press the left click and leave it. Then drag the mouse cursor. Red box shows area under selection. Press left click again to end the selection

Then click "Apply" to apply the settings/selection and then calculate the tool

Recalculate Select the area select tool by left clicking it

Apply

Cancel

Add tool

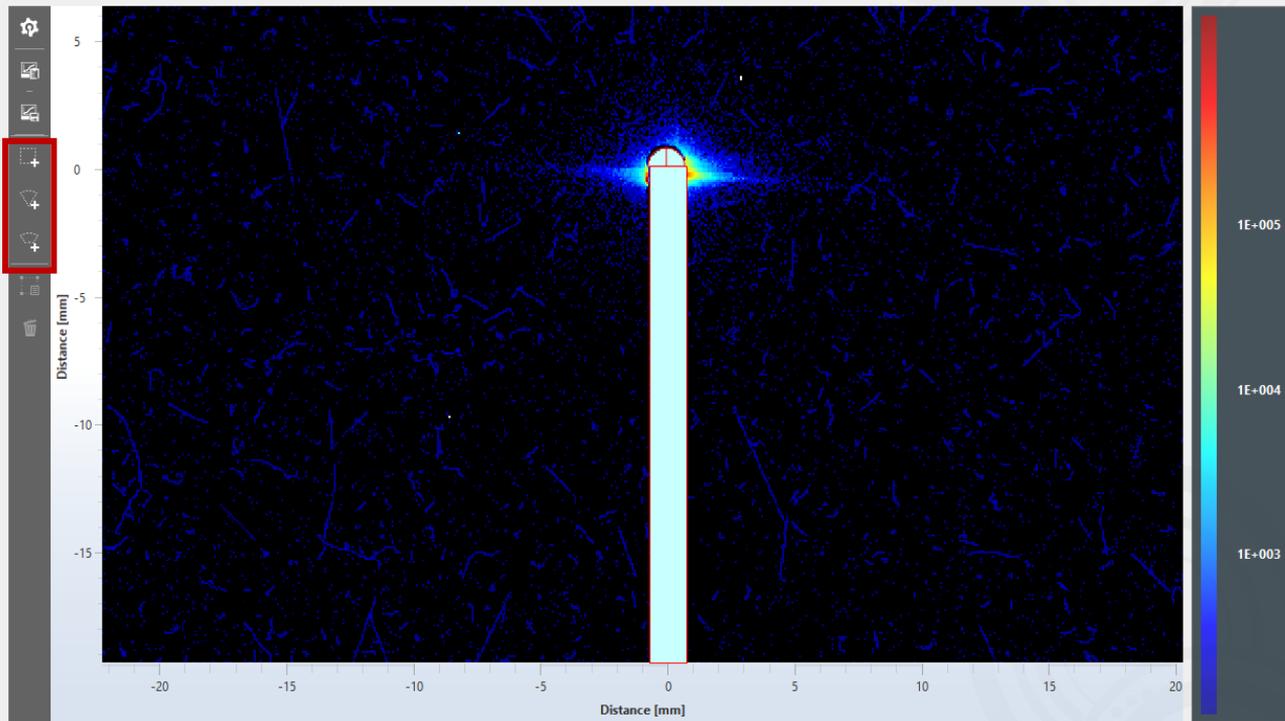
Data type
 Any 1D 2D

Tool category
 Any Preprocessing Analysis DataExport Advanced

- Absolute Intensity
- Align To Beam 2D
- Beamline Parameter Fit 1D
- Beamline Parameter Fit 2D
- Beamline Parameter Fit Applier
- Binning 1D
- Binning 2D
- Clip Axis 1D
- Data Reduction 2D
- Desmear 1D
- Export ASCII
- Export ATSAS
- Export Born Again
- Export Nexus
- Export PDH
- Fitting
- Formula 1D
- Formula 2D
- Guinier
- Masking 1D
- Masking 2D**
- Molecular Weight
- Plugin (beta)
- Porod
- Porod Volume
- Prepare Length Profile 1D
- Prepare Width Profile 1D
- Q Transformation
- Range Parameters 1D
- Range parameters 2D
- Remove masked & NaN values 1D
- Resampling 1D
- Rotate 2D
- Run External Command
- Specific Surface
- Standard Operations 1D
- Standard Operations 2D
- XRDynamic 500 background subtraction
- Zero Point By Click 1D
- Zero Point By Click 2D
- Zero Point By Moments 1D
- Zero Point By Moments 2D

Tool name

Insert the “Masking 2D” tool to mask the primary beam signal and beamstop to remove unwanted beam signal



Annotation(s)

Mask [M]

Unmask [U]

Threshold

Min 0 Max 1E+100

Mask Threshold

Reset Threshold

Unmask All

 Dynamically apply threshold to data

Use appropriate area selection tools (in red box) to select the area. Then click 'Mask' (in yellow box) to mask the desired area.

Note: Do this one selection at a time.

Then calculate the tool

Sx Add tool ×

Data type

Any 1D 2D

Tool category

Any Preprocessing Analysis DataExport Advanced

- Absolute Intensity
- Align To Beam 2D
- Beamline Parameter Fit 2D
- Beamline Parameter Fit Applier
- Binning 2D
- Data Reduction 2D
- Export ASCII
- Export Born Again
- Export Nexus
- Formula 2D
- Masking 2D
- Q Transformation**
- Range parameters 2D
- Rotate 2D
- Run External Command
- Standard Operations 2D
- Zero Point By Click 2D
- Zero Point By Moments 2D

Tool name

Insert “Q transformation” tool to change the axis of data from “distance (mm)” to “q-space”

Processing memory: 3.0 GB ▾

Data group: all ▾

Item

- Source Data
 - Blank-Water_003FramesAveraged
 - Frame 000
 - iron sucrose
- Process
 - Absolute Intensity
 - Zero Point By Moments 2D
 - Masking 2D
 - Q Transformation

Configuration Figures Data groups

Q Transformation

Transformation Type

- Transmission
- Gisaxs

Select the transformation type as per data/measurement and calculate the tool.

Configure the calculation chain
Right click on elements for configuration options

Data type

Any 1D 2D

Tool category

Any Preprocessing Analysis DataExport Advanced

- Absolute Intensity
- Align To Beam 2D
- Beamline Parameter Fit 2D
- Beamline Parameter Fit Applier
- Binning 2D
- Data Reduction 2D**
- Export ASCII
- Export Born Again
- Export Nexus
- Formula 2D
- Masking 2D
- Q Transformation
- Range parameters 2D
- Rotate 2D
- Run External Command
- Standard Operations 2D
- Zero Point By Click 2D
- Zero Point By Moments 2D

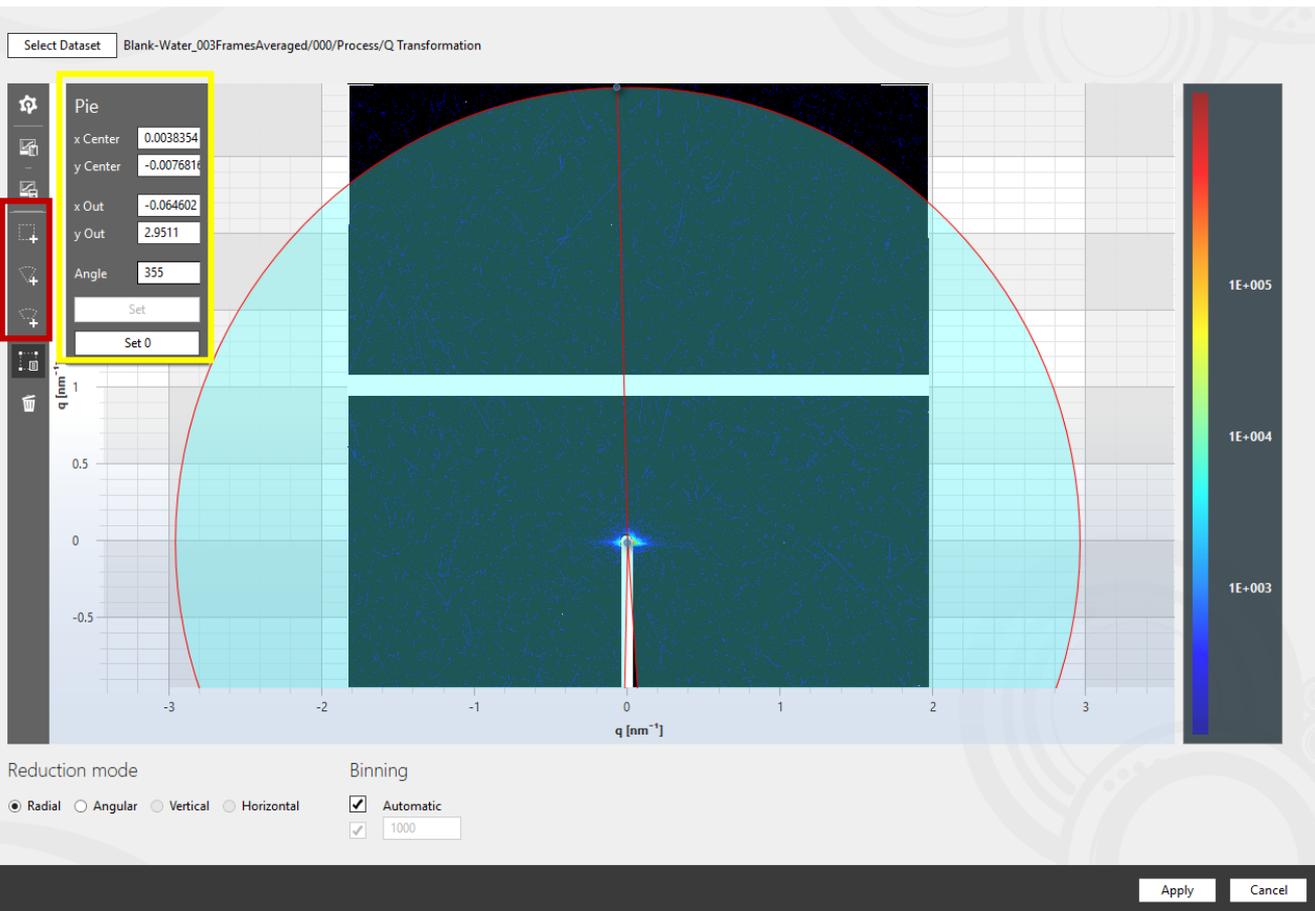
Insert the “Data reduction 2D” tool to reduce the 2D data to 1D data.

Tool name

Data Reduction 2D

Create tool

Cancel



Configure 'Data reduction 2D tool':

Select the data area to be reduced to using "area selection" tools (in red box).

Further, change selection area size by using options in yellow box.

Click "Apply and calculate the tool"

▼  Data Reduction 2D

 Blank-Water_003FramesAveraged/000

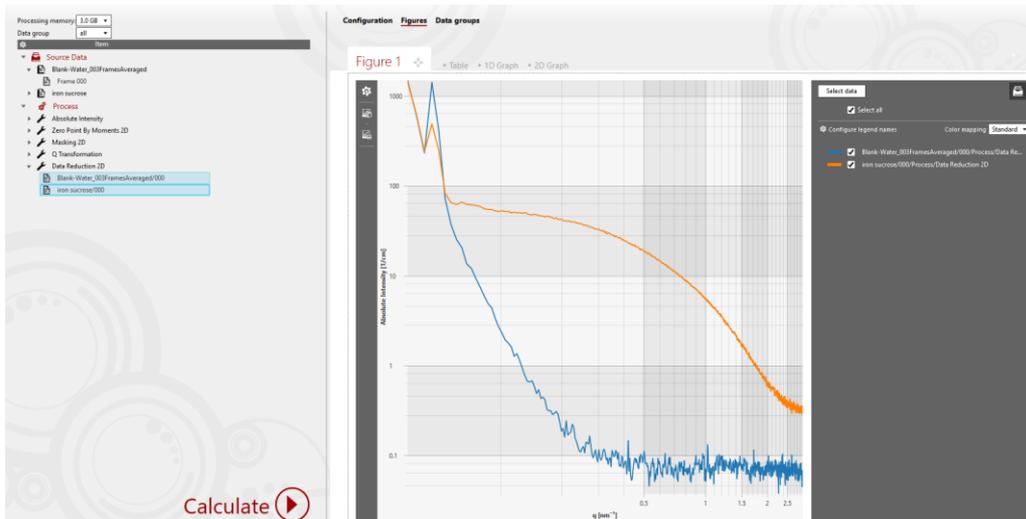
 iron sucrose/000

Show in new figure

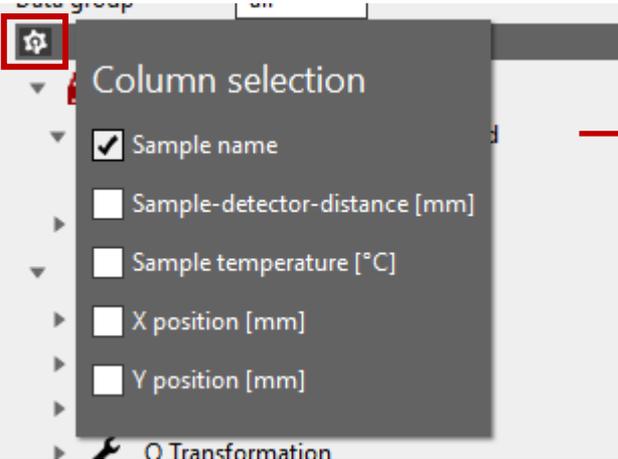
Remove frame from process

Show in Qt Primus

See the processed data/file after each tool. Select the file to view the right click and click on “show in new figure”



Left screenshot shows reduced data from 2D to 1D



To show sample name, SDD, etc; click on small setting button (red box) and select the desired parameters.

Click on setting button again to collapse the column selection.

To show legend in graph area; click on setting button (yellow box).
Select the location of legend from drop down menu (green box)

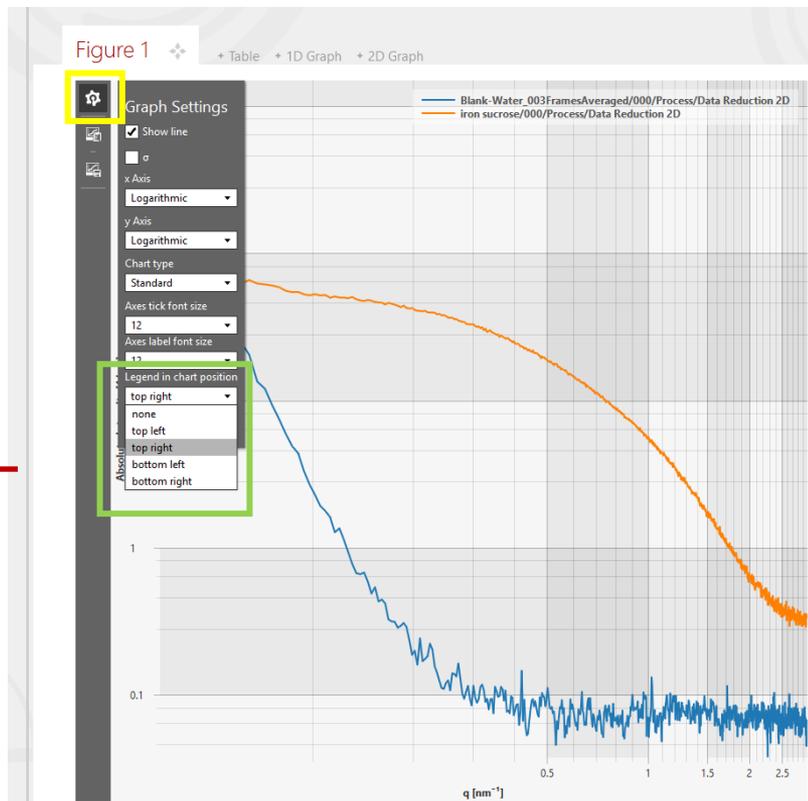
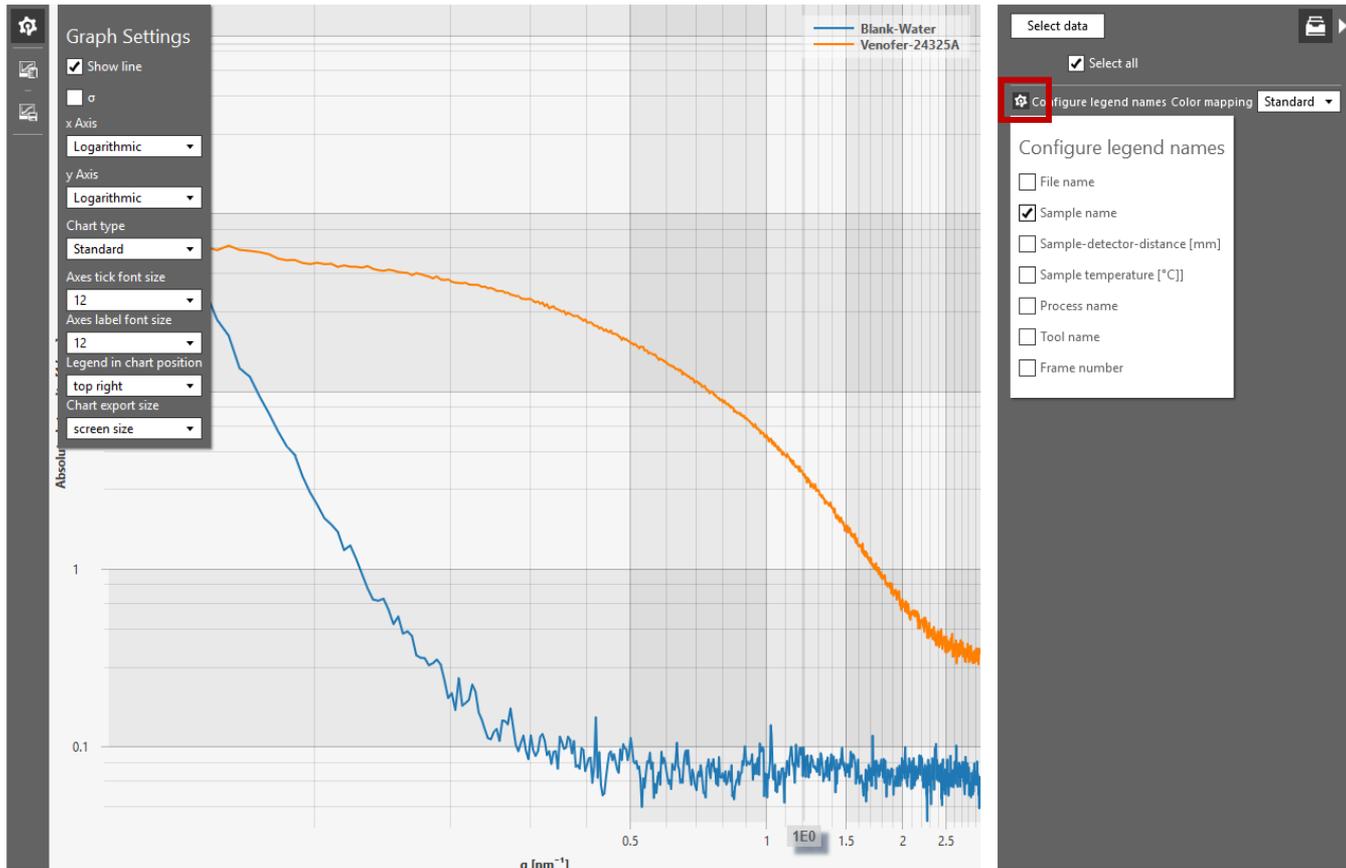
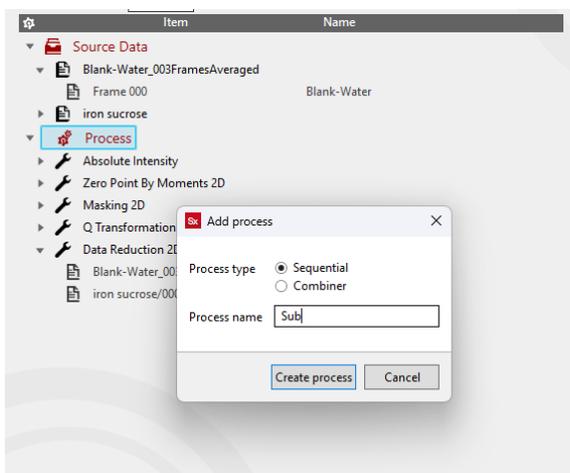


Figure 1 + Table + 1D Graph + 2D Graph



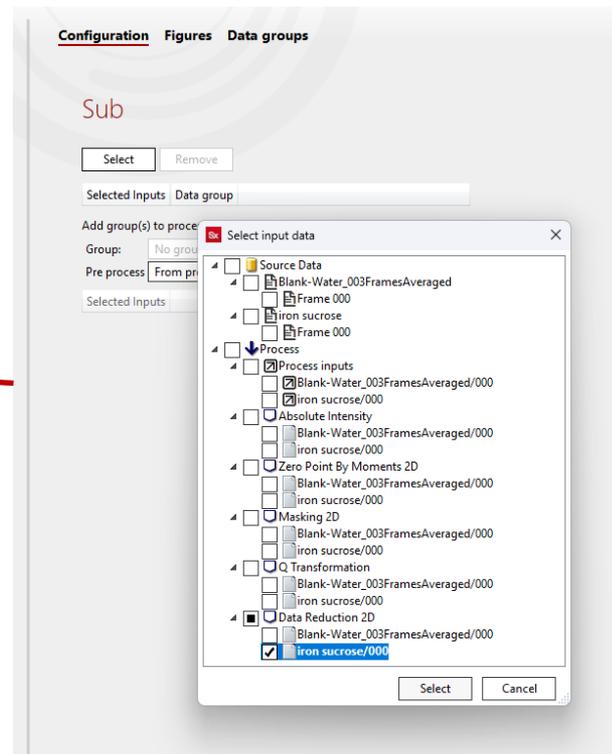
To configure legend name; click on small setting button (red box) and select desired options.

Click on setting button again to collapse the menu



Add another process to do background data subtraction from the sample data.

Right click on process added earlier and insert another sequential process



Here, Add only the sample data file

Add tool [X]

Data type
 Any 1D 2D

Tool category
 Any Preprocessing Analysis DataExport Advanced

- Absolute Intensity
- Beamline Parameter Fit 1D
- Beamline Parameter Fit Applier
- Binning 1D
- Clip Axis 1D
- Desmear 1D
- Export ASCII
- Export ATLAS
- Export Nexus
- Export PDH
- Fitting
- Formula 1D
- Guinier
- Masking 1D
- Molecular Weight
- Porod
- Porod Volume
- Prepare Length Profile 1D
- Prepare Width Profile 1D
- Q Transformation
- Range Parameters 1D
- Remove masked & NaN values 1D
- Resampling 1D
- Run External Command
- Specific Surface
- Standard Operations 1D**
- XRDynamic 500 background subtraction
- Zero Point By Click 1D
- Zero Point By Moments 1D

Tool name

Add “Standard operations 1D” tool for background subtraction

Normalize intensity by

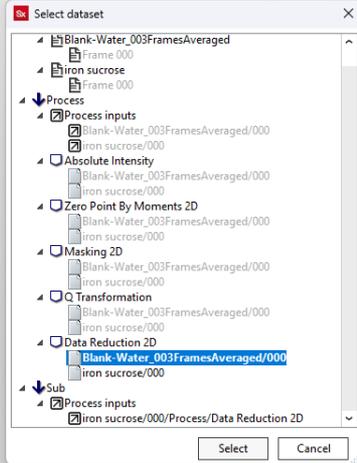
- Maximum intensity
- Mean intensity
- Area
- Transmittance
- Exposure time

Subtract intensity

- Mean intensity
- Porod background intensity
- Reference background

Set x axis zero point to

- x @ maximum intensity
- x @ minimum intensity
- x @ center of gravity



Configure “Standard operations 1D” tool

- Select “Reference background” option under “Subtract intensity”
- Click “Select reference”. This will open dataset selection option.
- “Select dataset” window → Select the reduced reference/background file and click select.

Show formula

Configuration Figures Data groups

Standard Operations 1D

Normalize intensity by

- Maximum intensity
- Mean intensity
- Area
- Transmittance
- Exposure time

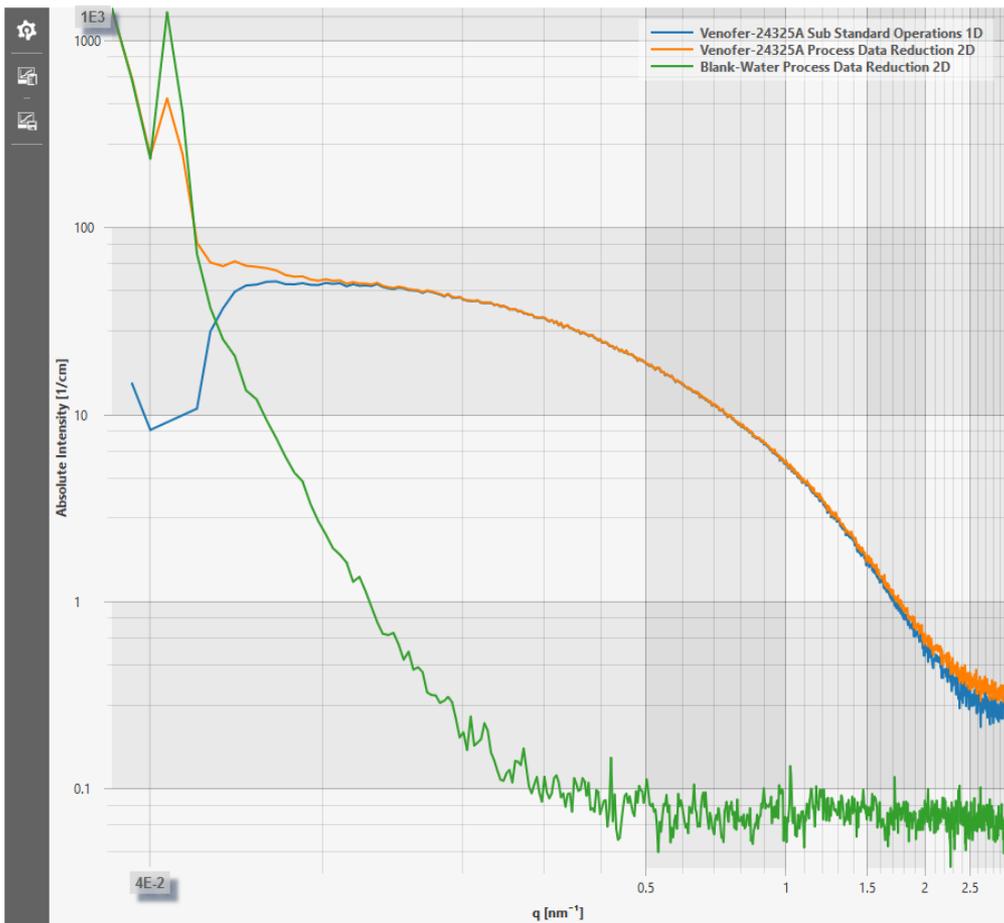
Subtract intensity

- Mean intensity
- Porod background intensity
- Reference background Blank-Water_003FramesAveraged/000/Process/Data Reduction 2D

Set x axis zero point to

- x @ maximum intensity
- x @ minimum intensity
- x @ center of gravity

Click “Apply” at the bottom right corner and calculate the tool.



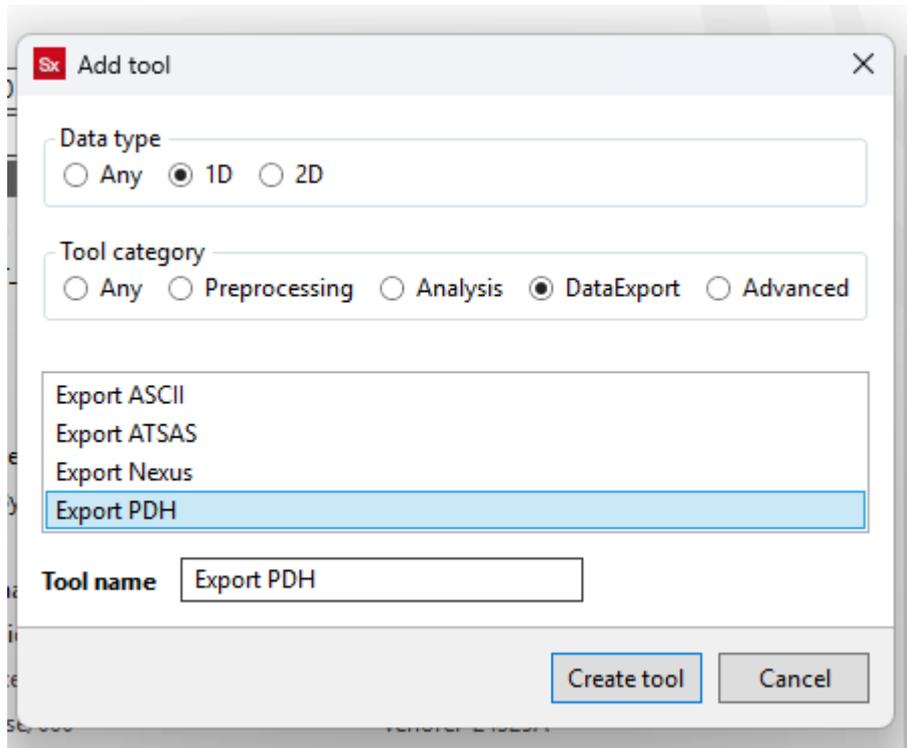
Select data 

Select all

Configure legend names Color mapping Standard

- Venerfer-24325A Sub Standard Operations 1D
- Venerfer-24325A Process Data Reduction 2D
- Blank-Water Process Data Reduction 2D

Figure shows sample data (orange), reference/background data (green) and background subtracted sample data (blue)



Add tool

Data type
 Any 1D 2D

Tool category
 Any Preprocessing Analysis DataExport Advanced

Export ASCII
Export ATSAS
Export Nexus
Export PDH

Tool name

Create tool Cancel

Data export:

To export the processed data insert data export tool.

- Right: the tool has been sorted as per dataexport.
- Select export options as per software where data to be used. In this case “ Export pdh” option is selected to export data in pdh format for use in PCG software.
- Click “create too”

Export PDH 

Output file name

Prefix

+

- No file name
 File name
 File name + frame
 Full file path

+

 Sample name

- Sample temperature [°C]
 Sample x position [mm]
 Sample y position [mm]
 Consecutive number

+

Postfix

Output path

 Overwrite existing files

Configure “data export” tool as per requirement and then click “Apply”

Calculate the tool to export the files.

This completes the data pre-processing process.