



APEX/PROTEUM3

Converting frames to Bruker format

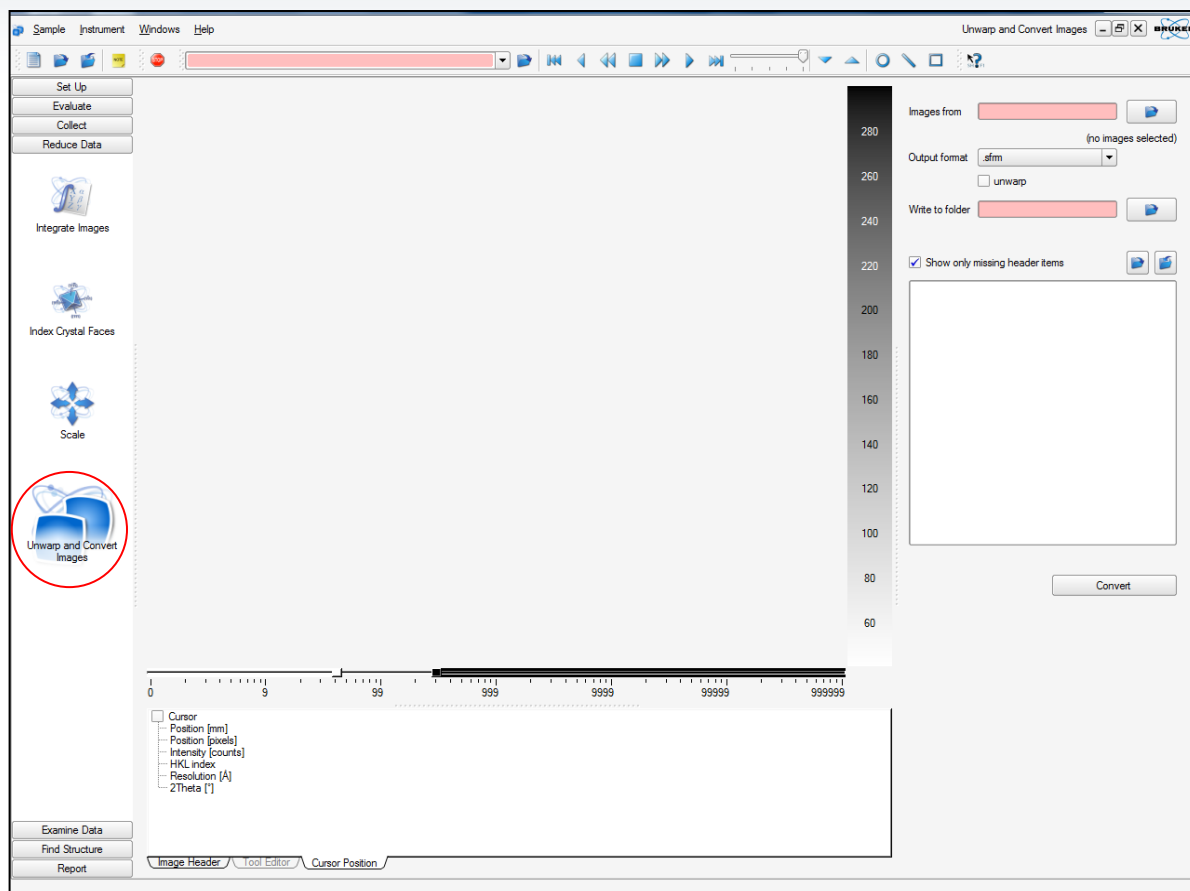
- Mar (Rayonix)
 - Image plate
 - CCD
- ADSC
- Dectris
 - Pilatus
 - Eiger

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Converting frames to Bruker format



- Click on the “Unwarp and convert images” icon from the “Reduce Data” menu
- This will bring up the conversion window
- In older versions of PROTEUM, the plugin was in the instrument menu



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Converting frames to Bruker format



Fill in the following parameters and then click the "Convert" button to convert the frames

- **Images from:** select the image files to convert
- **Output format:** select the .sfrm format
- **Unwarp:** this box should be unchecked
- **Write to folder:** select a output folder
- **Header input:**
 - Unchecking the missing header box will display all the header parameters
 - Read in the appropriate .hdr file using the icon circled
 - At this point the only things you might have to change are the beam center and detector offset

The screenshot shows a software window for converting frames. At the top, there are fields for "Images from" (C:\frames\guest\JK) and "Write to folder" (C:\frames\guest\JK), both with folder selection icons. Below these is "Output format" set to ".sfrm" and an unchecked "unwarp" checkbox. A "Show only missing header items" checkbox is also present, with a circled folder icon next to it. The main area is a table of header parameters:

<input checked="" type="checkbox"/>	Detector ID	PILATUS-GMF
<input type="checkbox"/>	Detector circular?	No
<input checked="" type="checkbox"/>	Horizontal tiles	1
<input checked="" type="checkbox"/>	Vertical tiles	1
<input type="checkbox"/>	Pixel width [mm]	0.172
<input type="checkbox"/>	Pixel height [mm]	0.172
<input type="checkbox"/>	Horizontal beam center	3.27
	Unit	millimeters
	Origin	center
	Direction	right
<input type="checkbox"/>	Vertical beam center	3.10
	Unit	millimeters
	Origin	center
	Direction	up
	Beam tilt [°]	0.00
	Detector pitch angle [°]	0.00
<input checked="" type="checkbox"/>	Detector roll angle [°]	-90.00
	Detector yaw angle [°]	0.00
	Baseline offset	0

At the bottom right, there is a "Convert" button.

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Header files



The header file contains all the relevant information for the data frame and can be updated for a particular experimental setup

- The parameter is fixed when it is updated by clicking on the current value (for example "Detector ID") and inputting the new value
- The checked box indicates a saved parameter
- After all the changes are made, the hardware file can be saved by clicking the circled icon
- This file can be used for every data set collected with this experimental setup
- For beamline data, the detector roll defines the orientation of the spindle and is not always in the header. It will either be 0, 90, 180 or 270. For example, if the spindle is horizontal as with Dectris setups, the roll would be either 90 or 270 (-90). The best way to determine the correct value is to try and index a few degrees of data not just one frame

The screenshot shows a software interface for configuring header files. It includes several input fields and checkboxes:

- Images from:** C:\frames\guest\training (with a folder selection icon)
- Output format:** .sfm (with a dropdown arrow)
- Write to folder:** C:\frames\guest\training (with a folder selection icon)
- Show only missing header items:** (checkbox, circled in red)

Below these are several parameter settings, each with a checkbox and a value:

<input checked="" type="checkbox"/>	Detector ID	pilatus6m
<input type="checkbox"/>	Detector circular?	No
<input type="checkbox"/>	Horizontal tiles	5
<input type="checkbox"/>	Vertical tiles	12
<input type="checkbox"/>	Pixel width [mm]	0.1720
<input type="checkbox"/>	Pixel height [mm]	0.1720
<input type="checkbox"/>	Horizontal beam center	0.09
Unit		millimeters
Origin		center
Direction		right
<input type="checkbox"/>	Vertical beam center	-0.09
Unit		millimeters
Origin		center
Direction		up
Beam tilt [°]		0.00
Detector pitch angle [°]		0.00
<input checked="" type="checkbox"/>	Detector roll angle [°]	90.00
Detector yaw angle [°]		0.00
Baseline offset		0
<input type="checkbox"/>	Overflow	496476
Electrons/ADU		1.00
Electrons/photon		1.00
Phosphor efficiency		1.00

At the bottom right, there is a "Convert" button.

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Header files



- For the header files you need to fill in the information for the detector characteristics
 - Electrons/ADU
 - Electrons/photon
 - Phosphor efficiency
 - Read noise
- Update the Monochromator for beam polarization
 - Goniometer vertical 2T=90.00 Roll=90
 - Goniometer horizontal 2T=90.00 Roll=0
- Update Start and End positions if necessary
 - Set the geometry
 - Bruker (Eulerian)
 - Bruker (Kappa)
 - Nonius (Eulerian)
 - Nonius (Kappa)
 - Horizontal
 - Mar DTB

Baseline offset	0
<input type="checkbox"/> Overflow	496476
Electrons/ADU	1.00
Electrons/photon	1.00
Phosphor efficiency	1.00
Read noise [electrons]	0.00
<input type="checkbox"/> Wavelength [Å]	0.97539
Monochromator 2Theta [°]	0.00
Monochromator roll [°]	0.00
<input type="checkbox"/> Exposure time [s]	0.20
<input type="checkbox"/> Number of exposures	1
<input type="checkbox"/> Start position	Nonius (Eulerian) ▼
Distance [mm]	400.0000
2Theta [°]	0.0000
Omega [°]	0.0000
Phi [°]	10.0000
Chi [°]	0.0000
<input type="checkbox"/> End position	Nonius (Eulerian) ▼
Distance [mm]	400.0000
2Theta [°]	0.0000
Omega [°]	0.0000
Phi [°]	11.0000
Chi [°]	0.0000
<input type="checkbox"/> Distance offset [mm]	0.0000

Pilatus 6M

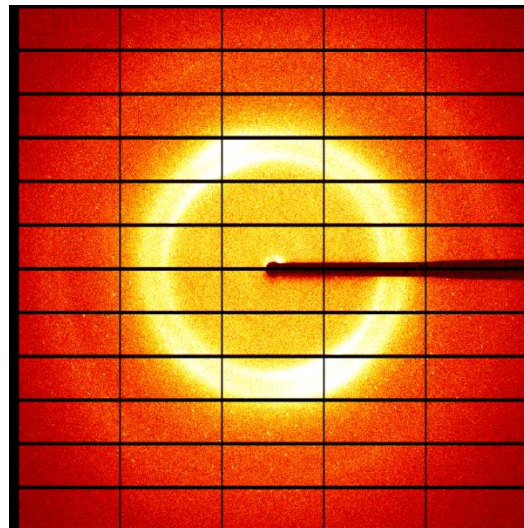
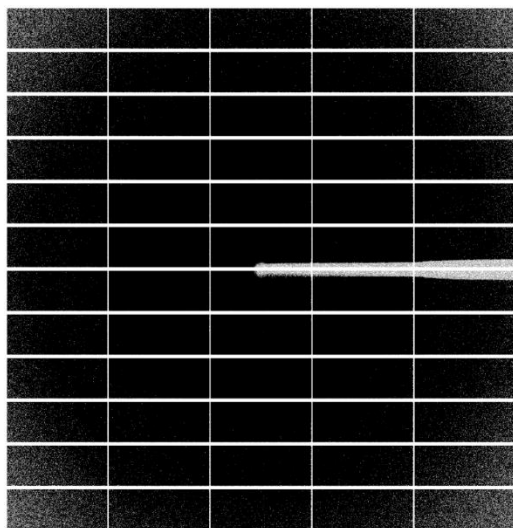
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Making an Active Pixel Mask



For the detectors with sensor gaps, you will want to create a mask to remove both the gaps and beamstop shadow from the image. If the goniometer is a fixed spindle, the beamstop is usually placed along the rotation axis and the shadow may not need to be removed since it's in the Lorentz region

- Load a converted frame into PROTEUM/APEX Viewer
- First adjust the contrast, if needed, so that it's easier to see the gaps. The colored background sets the gaps to black by default which is the color needed for generating a mask



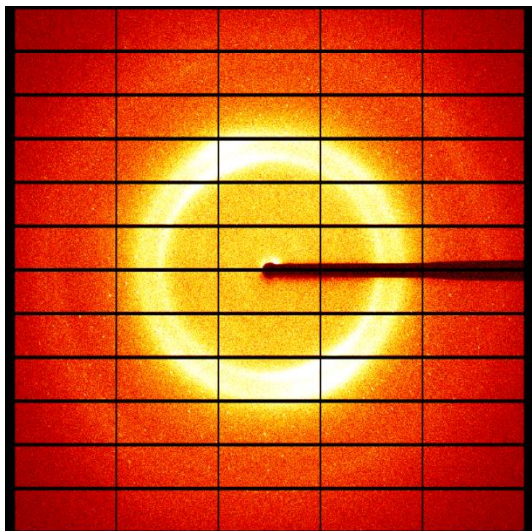
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Making an Active Pixel Mask

- Use a graphics program convert the *active areas to white* and the *inactive areas to black* and save a PNG file adjusting the image size to match actual frame size

In a cmd window type:

- Bnrun c:\bn\src\misc\imagesum.pyc *filename*.png to *mask._am*
 - You must run imagesum from the same folder as the PNG file
- This will convert the PNG file to a mask file in sfrm format
- The *filename_xa_01_0001.sfrm* convention can also be used as output



Initial PNG file

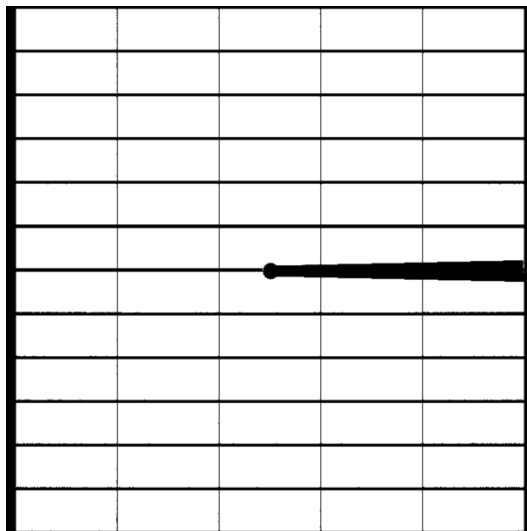
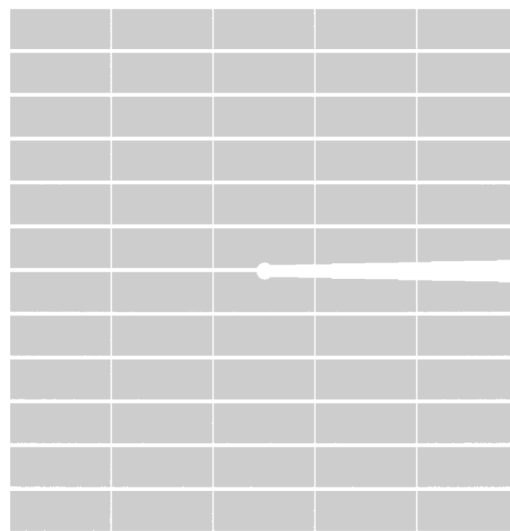


Image with updated colors



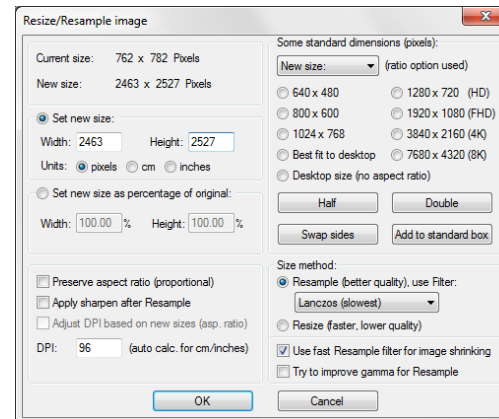
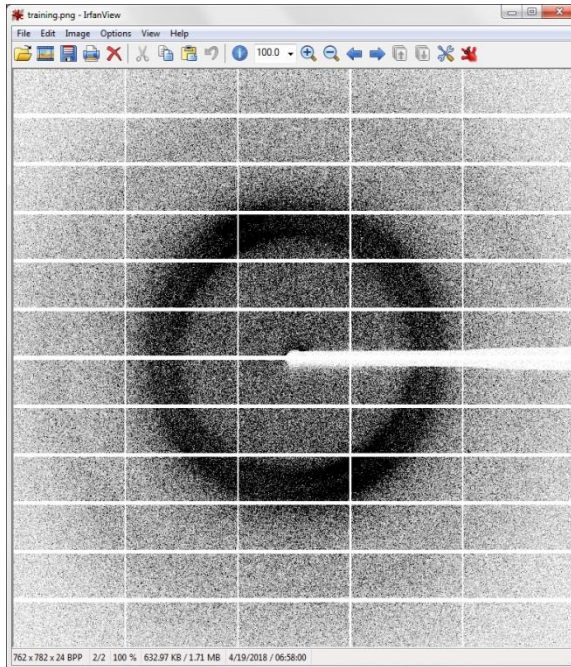
Final mask

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Making an Active Pixel Mask



- Use a graphics program convert the active areas to white and the inactive areas to black and save a PNG file adjusting the image size to match actual frame size
- Typical Pilatus 6M image is 2463 x 2527 but the png file outputted from PROTEUM will be much smaller so you need to change the image resolution of the png file to match that of the actual image otherwise you will get an error in SAINT



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Reading an Active Pixel Mask



If the standard mask filename conversion is not used, you will have to read in the Pre-existing mask

- Under Integration options
 - Select more options
 - Click on "Use Pre-existing static mask"
 - Browse for the mask file

The screenshot shows the Bruker software interface with the 'Integration Options' dialog box open. The dialog is titled 'Integration Options' and contains several sections:

- Model Profiles:** Includes checkboxes for 'Enable LS Profile Fitting' (checked) and 'Blend Profiles from All Detector Regions'. It also has input fields for 'Intensity/Sigma Lower Limit for Model Profile Update' (10.000), 'Fraction of Model Profile Maximum for Simple Sum Mask' (0.050), 'Intensity/Sigma Upper Limit for LS Model Profile Fit' (8.000), 'Lower Resolution Limit for LS Model Profile Fit [Å]' (9999.000), and 'Profile XYZ Half-Widths' (4, 4, 4).
- Active Mask:** Has three radio button options: 'Generate Mask' (unselected), 'Use Pre-Existing Static Mask' (selected), and 'Use Pre-Existing Dynamic Masks' (unselected). The 'Active Mask File' is set to 'C:\frames\guest\JK\mask_am'. There is also a 'Fractional Lower Limit of Average Intensity' field set to 0.000.
- Algorithm:** Has two radio button options: 'Use Narrow Frame Algorithm' (selected) and 'Use Wide Frame Algorithm' (unselected).
- Monte Carlo Simulation:** Includes a 'Number of Monte Carlo Simulations' field set to 0.
- Image Timeout:** Includes a checkbox for 'Wait for Images During Data Collection' which is checked.
- Background Update:** Includes a 'Background Update Scaling Factor' field set to 1.000.
- Image Queue:** Includes an 'Active Image Queue Half-Width [Images]' field set to 7.
- Beam Monitor:** Includes checkboxes for 'Enable Beam Monitor Normalization' and 'Normalize each Run Separately', both unselected.
- Twin Overlap Determination:** Includes fields for 'Minimum Common Volume [%]' (4.000), 'Separation Factor' (1.000), and 'Maximum Range' (1.300).
- Modulated Structure Integration:** Includes a 'Maximum Satellite Index' field set to 1.
- Output / Diagnostic Files:** Includes checkboxes for 'Generate Diagnostic Plot Files', 'Keep Temporary Files', 'Append Listing Files', and 'Hide Log Window', all unselected. It also has fields for 'Verbosity of Listing File' (2) and 'Snapshot Output Frequency [Images]' (100).

The background window shows a table with columns 'Starting Image Filename', 'Images', and 'Output Filename'. The first row contains the values 'C:\frames\guest\JK\cy31_01_0001.sfm', '30', and 'C:\frames\guest\jk\work\cy31_01.raw'. The 'Integration Options' dialog is positioned over this table.

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Updating the Beam Center



Sometimes the beam center is not correctly stamped in the frame header. To change this:

- Activate the rectangle tool and zoom in the image to view the beamstop shadow.
- Using the circle tool, drag the circle down until it's very small with the left mouse button. This will show the position of the beam center based on the values in the frame header.
- Click the manual button for the corrections. The boxes for the X and Y offset will become active.

PROTEUM2 v2015.9-RC7 - User: (guest) - Sample: s8 - Temporary license (64 days remaining)

Sample Instrument Windows Help

C:\frames\guest\8\8.0001

Set Up
Screen

Screen Crystal

Determine Unit Cell

View Reciprocal Lattice

View Images

Cursor: Position [mm] 9.32
Position [pixels] 1142
Intensity [counts] 187
HKL index -0.74
Resolution [Å] 4.11
2Theta [°] 13.68

Image Header Tool Editor

Determine Unit Cell

Reflections: Group 0: 284 reflections

Go to Image: C:\frames\guest\8\8.0001

Min. I/sigma(I): 10.00

Resolution [Å]: 9999.00 - 0.92

Reflections must be isolated
 Reflections must span images
 Reflections must be whole

284 Reflections selected for indexing

Store: a=19.11Å, α=90.00°, V=2595Å³
b=5.89Å, β=107.88°, Monoclinic P
c=24.25Å, γ=90.00°

Corrections: From store From last harvest Manual

Distance [mm]: 0.00 Pitch [°]: 0.00
X Beam Center [mm]: 0.30 Roll [°]: -90.00
Y Beam Center [mm]: 0.18 Yaw [°]: 0.00

Methods: Difference Vectors
 Fast Fourier Transform
 Least Squares

Index... Cancel

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Updating the Beam Center



- Enter new values for the offsets, as you do the circle will move.
- When the circle is where you think the beam is, continue with indexing. The new values for the offsets will be used.
- You can update the beam center in the frame headers by inputting the new values in "Unwarp and Convert" and converting the frames again.

The screenshot displays the PROTEUM2 v2015.9-RC7 software interface. The main window shows a diffraction pattern with a central spot labeled '222.45'. A red circle is positioned at the center of the pattern. The interface includes a menu bar (Sample, Instrument, Windows, Help), a toolbar, and a sidebar with buttons for 'Set Up', 'Screen', 'Screen Crystal', 'Determine Unit Cell', 'View Reciprocal Lattice', and 'View Images'. The right-hand side contains a control panel with various settings for reflections, resolution, and corrections. A pop-up window titled 'Corrections' is overlaid on the bottom right, showing the following settings:

Corrections:	<input type="radio"/> From store	<input type="radio"/> From last harvest	<input checked="" type="radio"/> Manual
Distance [mm]:	<input type="text" value="0"/>	Pitch [°]:	<input type="text" value="0.00"/>
X Beam Center [mm]:	<input type="text" value="1.03"/>	Roll [°]:	<input type="text" value="-90.00"/>
Y Beam Center [mm]:	<input type="text" value="-0.34"/>	Yaw [°]:	<input type="text" value="0.00"/>

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Photon Counting Detectors



- If the diffraction is not particularly strong, there are a couple of options to minimize harvesting bogus reflections from the active area/gap boundary
 - Add the line "scalebeforeharvest=0" to the c:\bn-config.py (windows), /usr/local/lib/bn-config.py (Linux) file. It can go anyway in this file. This will slow things down a bit during harvesting
 - Check the "smooth images" box in the "Harvest spots" window
 - Check the "Save reflections that only span images" box in the "Harvest spots" window
 - Remove the bad reflections with RLATT

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Writing out CBF frames during experiment



You can automatically write out CBF frames along with sfrm frames during data collection by setting the AutoCBF flag in the BIS configuration file.

- Shutdown BIS
- Edit the [BrukerAXS.Server.BIS.exe.config](#) found in the `c:\Program files (x86)\Bruker AXS\DIFFRAC.MEASUREMENT CENTER.V6` folder
- Search for CBF in the file, set the CBF flag to "True" and save the file:

```
<!-- Automatically convert Bruker frame files to CBF frame files -->
```

```
<!-- Default False: Only create Bruker Frame Files -->
```

```
<setting name="CBF" serializeAs="String">
```

```
<value>False</value>
```

```
</setting>
```

```
<!-- Automatically convert Bruker frame files to CBF frame files -->
```

```
<!-- Default False: Only create Bruker Frame Files -->
```

```
<setting name="CBF" serializeAs="String">
```

```
<value>True</value>
```

```
</setting>
```

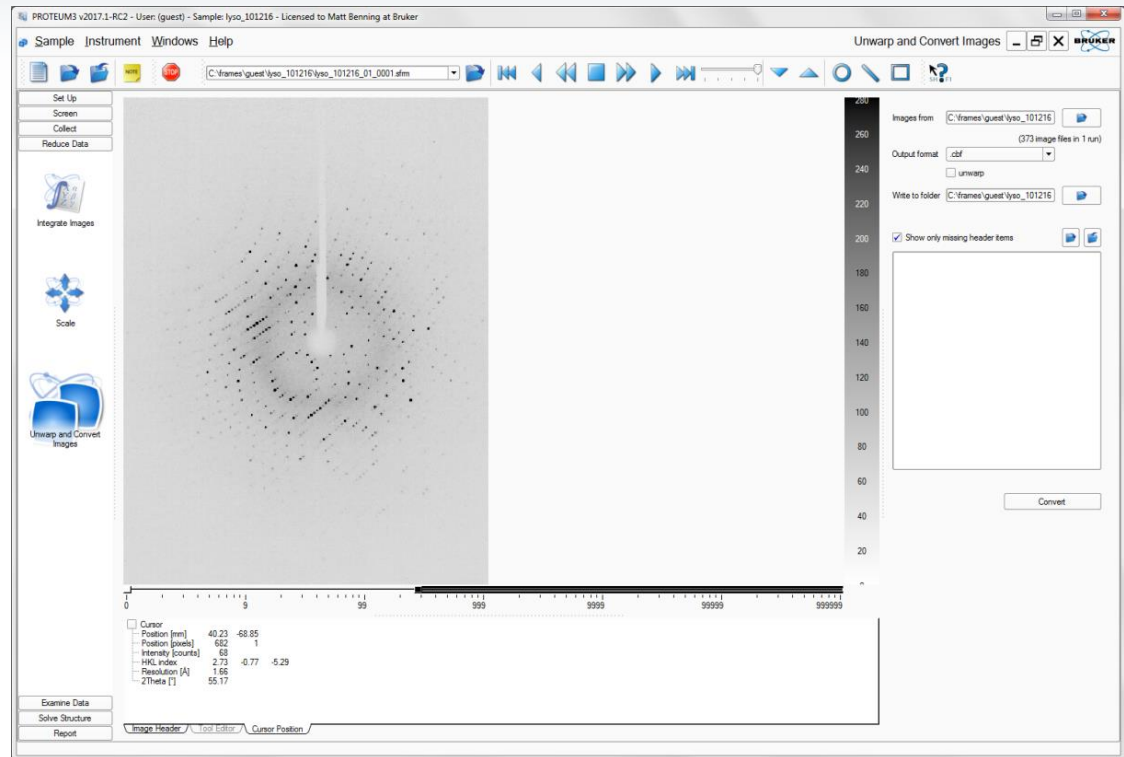
- Restart BIS

APEX/PROTEUM3 XDS, Convert sfrm images to cbf format



To use XDS to process Bruker images you first have to convert our sfrm format to CBF.

- Convert .sfrm images to CBF format using “Unwrap and Convert images” under the Reduce Data menu
- Assign the scans to convert in the “Images from” box using the browser button
- Select the “Output format” as CBF
- Leave the unwrap box unchecked
- Assign an output folder in the “Write to folder” box
- Click the Convert button



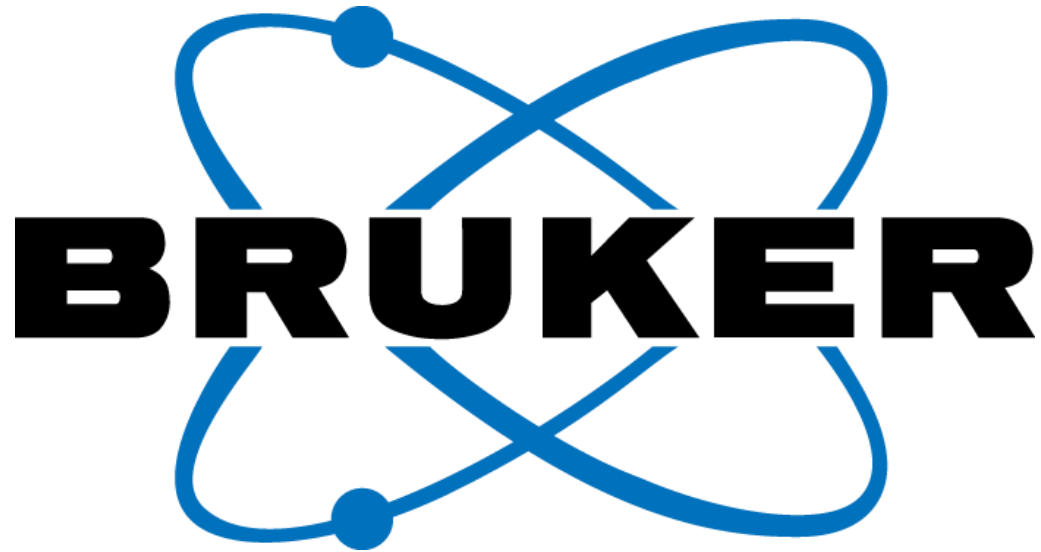
Cursor	
Position [mm]	40.23 -68.85
Position [pixels]	682 1
Intensity [counts]	68
HKL index	2.73 -0.77 -5.29
Resolution [Å]	1.66
2Theta [°]	55.17



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Using XDS for data reduction

- Run the `generate_xds.inp` script on each data run to create the XDS input files:
 - `generate_xds.inp "filename_01_????.cbf"`
- Run XDS and XSCALE as normal
- Note that the Y beam position is inverted
 - X=514, Y=510, Y will be 514 in the script



Innovation with Integrity