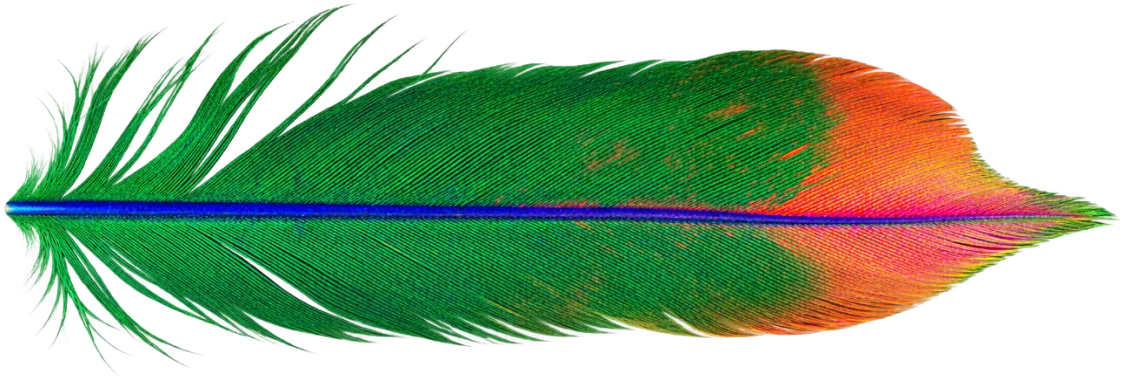
User Manual

BioXAS – Imaging



Canadian Light Source Inc.
44 Innovation Boulevard
University of Saskatchewan
Saskatoon, Saskatchewan Canada

Authors: Mangaljit Singh and Viorica (Ibi) Bondici

Last Updated: October 21, 2026

FACILITY CONTACTS

From any CLS phone, you must dial '9' to access an external line. For CLS internal numbers (starting with 306-657-), you only need to dial the 4-digit extension.

07ID-1 beamline	306-657-**3625**
Floor Coordinator	306-657-**3639**
HSE Department	306-657-**3663**
Reception Desk	306-657-**3500**
User Services Office	306-657-**3700**

44 Innovation Blvd.
Saskatoon, SK S7N 2V3

EMERGENCY NUMBERS

Fire Department	**911**
Ambulance	**911**
Campus Security	9-306-966-5555
Poison Control	9-1-866-454-1212

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BEAMLINE CONTACTS

Viorica (Ibi) Bondici **(306) 657-3707**
ibi.bondici@lightsource.ca

Mangaljit Singh **(306) 657-3584**
mangaljit.singh@lightsource.ca

Ozra Mohammadi **(306) 657-3694**
ozra.mohammadi@lightsource.ca

Amanda Quirk **(306) 657-3755**
amanda.quirk@lightsource.ca

Zachary Arthur **(306) 657-3708**
zachary.arthur@lightsource.ca

This content is managed by the User Services Office, in cooperation with CLSI HSE and Beamline Staff.

For assistance, call the Floor Coordinator at 306-657-3639.

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USER CODE OF CONDUCT

HEALTH & SAFETY

When accessing the CLS, users must comply with all CLS policies and procedures, and heed and comply with the directions of CLS staff, including beamline staff and Floor Coordinators.

Occupational injuries, unsafe conditions or practices, and damage to property must be reported to CLS staff.

ALCOHOL & DRUG USE

Use of alcohol, cannabis, illegal drugs, or impairing substances is prohibited while at the CLS.

CODE COMPLIANCE

All users of the CLS must acknowledge and agree to the terms of their institution's agreement to access the facility.

Scan to read the full CLS User Code of Conduct

COMPLIANCE WITH LAWS

All activities at the CLS must comply with applicable laws, rules and regulations of the Province of Saskatchewan and the laws of Canada.

RESPECT & DIVERSITY

Respectful behaviour is required and expected of staff and users alike.

Harassment, discrimination, or any form of disrespectful behaviour is not tolerated.

We value diversity and hold everyone to the standard that all interactions be conducted with kindness, professionalism, and mutual respect.

WORKPLACE VIOLENCE

Anyone acting in a violent, threatening, or intimidating manner may be removed from CLS property, and all reported incidents will be investigated.

BEAMLINE STAFF AVAILABILITY

The CLS aims to provide excellent user support while preserving a healthy work-life balance for beamline staff.

Monday - Friday **9am - 5pm** Excluding Weekends and Statutory Holidays	Beamline staff are either on-site, or available remotely on short notice.
Monday - Friday **5pm - 10pm** Weekends and Statutory Holidays **10am - 10pm**	You may contact Beamline staff by email, but a response is not guaranteed.
Monday - Friday **10pm - 8am** Weekends and Statutory Holidays **10pm - 10am**	Beamline staff are not expected to respond, unless arranged ahead of time.

Beamline Staff Responsibilities

- ✓ Set up the beamline
- ✓ Help with paperwork and training at the start of the experiment
- ✓ Train new user groups to operate the beamline

User Group Responsibilities

- ✓ Ensure there are enough qualified individuals to run the experiment
- ✓ Cooperate with requests from CLS staff
- ✓ Comply with the User Code of Conduct

Additional support may be available by prior agreement between users and beamline staff. If significant assistance with experimental planning, data acquisition and interpretation is required, users are normally expected to treat beamline staff as collaborators, with appropriate recognition given (e.g. co-authorship). Where practical, additional assistance should be solicited ahead of the user's experiment.

FC | Floor Coordinator

FCs are on-site 24 hours a day during beamtime. Call any time! They are your best source of beam-related information, but may not have the expertise in specific beamline operations to resolve more technical problems.

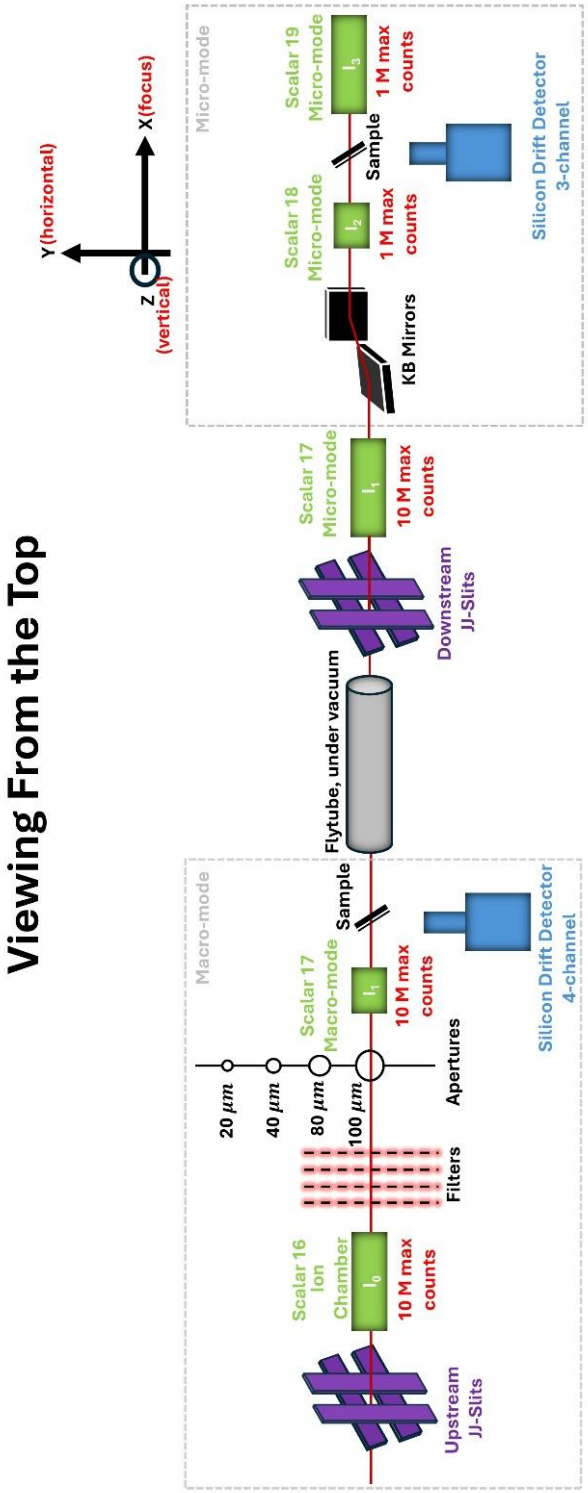
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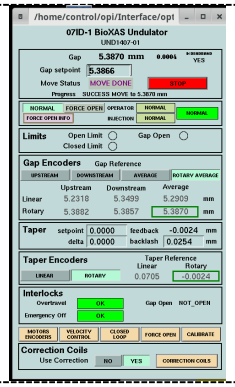
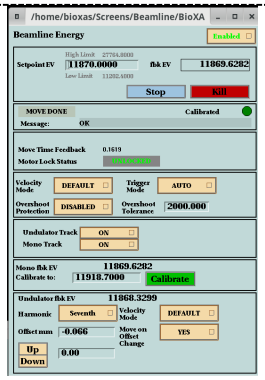
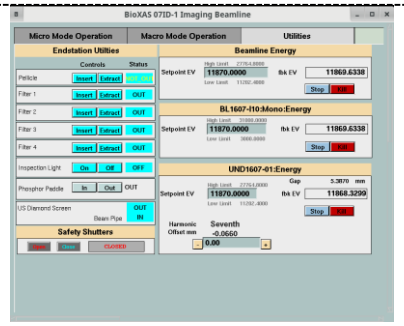
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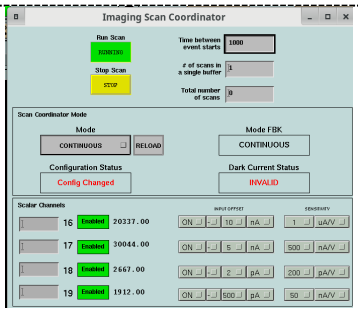
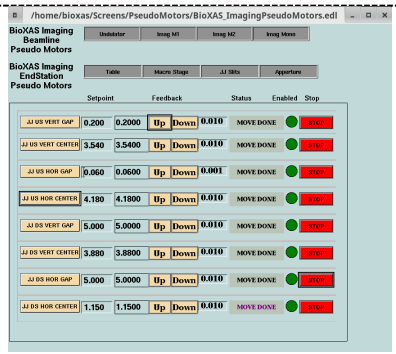
1. Schematic of the setup



Schematic of the setup at the BioXAS Imaging beamline endstation

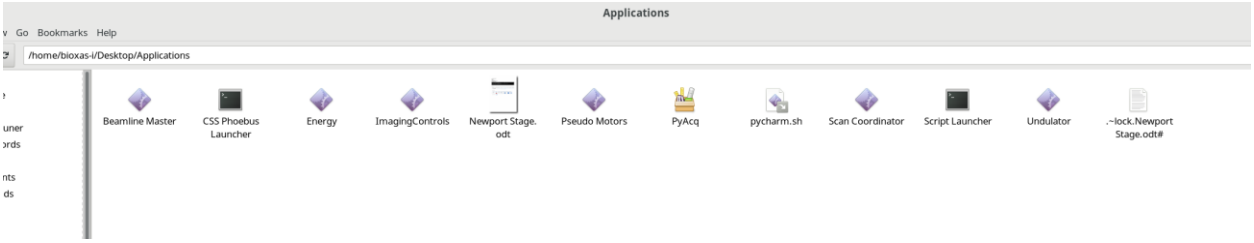
2. Important Applications

Undulator	Beamline Energy	ImagingControls
		

Scan Coordinator	Pseudo Motors	PyAcq
		

Channel 16 – 10 million max counts
Channel 17 – 10 million max counts
Channel 18 – 1 million max counts
Channel 19 – 1 million max counts

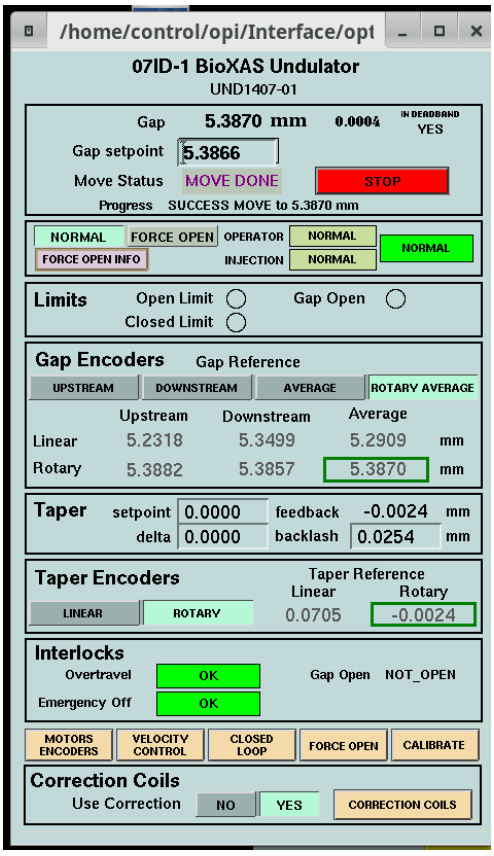
Shortcuts to all these applications are in the **‘Applications’** folder on the Desktop.



The names of these applications will be referenced throughout the remainder of this document.

2.1 Application: Undulator

This application displays the gap between the magnets of the BioXAS-Imaging beamline's insertion device in the storage ring. The insertion device used by the beamline is an undulator.



The undulator gap determines the magnetic field generated between the magnets. The magnetic field, in turn, determines the energy of the X-ray photons produced by the insertion device. Therefore, the undulator gap is directly related to the beamline's X-ray energy. For a given beamline energy, the undulator is set to the corresponding gap required to produce the desired photon energy.

Users must never change the undulator gap.

The maximum undulator gap is approximately 29 mm. At this position, the undulator is considered fully open and produces essentially no useful X-ray beam for the beamline.

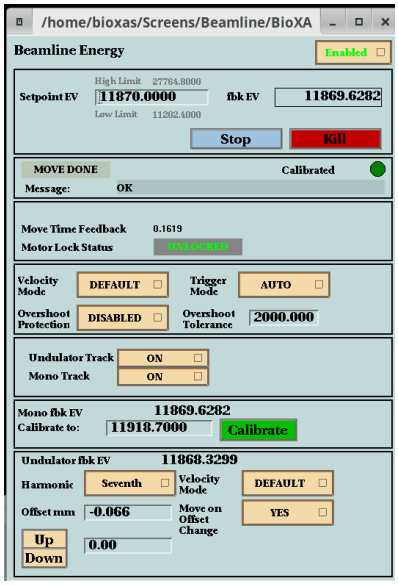
During normal BioXAS-Imaging operation, the undulator gap for most used beamline energies is typically in the range of approximately 5 - 7 mm. The exact gap depends on the selected X-ray energy.

The undulator gap may be opened by the Control Room to approximately 29 mm following a beam trip recovery. Before the storage ring is re-injected with beam as part of the beam-trip recovery procedure, the Control Room will fully open the undulator gap. Once beam has been successfully restored, the undulator is returned to the appropriate gap corresponding to the required beamline energy.

Users should not attempt to manually adjust or change the undulator gap, including during or after a beam trip. Any required adjustment is performed by the Control Room as part of the normal beamline operating and beam-trip recovery procedures.

For further information on beam-trip recovery and the procedure for restoring beamline operation, refer to **Section - 11** of this User Manual.

2.2 Application: Beamline Energy



This application displays the X-ray photon energy currently selected for the beamline. The displayed energy corresponds to the energy of the X-ray beam being used for the experiment.

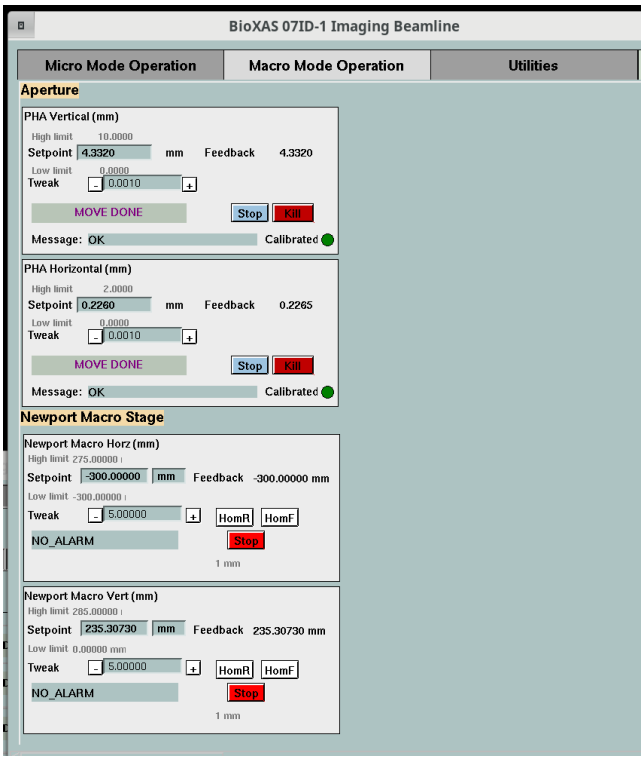
Users may need to change the beamline energy after completing an XAS acquisition, especially when returning back to XRF imaging after completing the XAS. More detailed information is provided in **Section - 5, 6, and 9** of this User Manual.

2.3 Application: Imaging Controls

This application has three subsections: Macro Mode Operation, Micro Mode Operation, and Utilities.

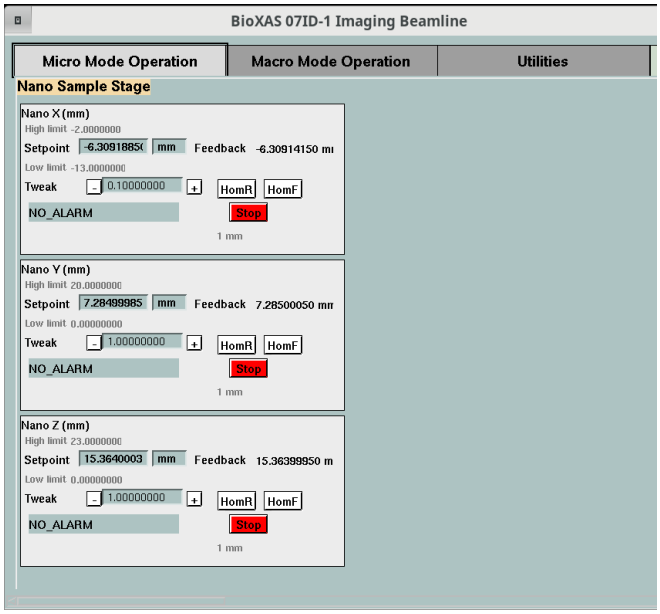
2.3.1. Macro-Mode Operation

The Macro-Mode Operation subsection allows users to control the position of the pinholes/apertures used to define the beam size. It also provides control of the sample position in the vertical and horizontal directions.



2.3.2. Micro-Mode Operation

The Micro Mode Operation subsection allows users to control the sample stage position in the vertical and horizontal directions, as well as the sample translation along the beam path. These controls allow users to position the sample within the focused X-ray beam produced by the focusing optics.

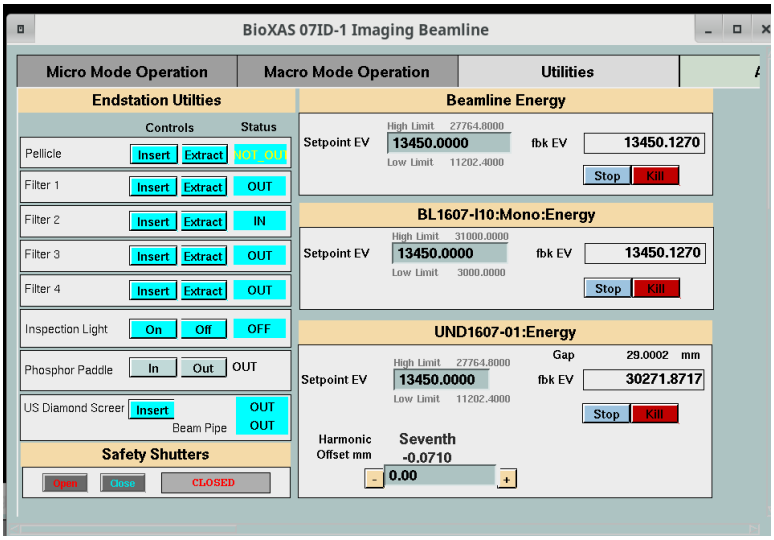


The focusing optics consist of a pair of Kirkpatrick–Baez (KB) mirrors, which focus the X-ray beam to the small beam size required for micro-mode setup. The sample can be translated along the beam path to position it at the location of the smallest focused beam, corresponding to the appropriate focal position of the KB mirrors.

A schematic of the BioXAS-Imaging beamline endstation is provided in Section - 1 of this User Manual.

2.3.3. Utilities

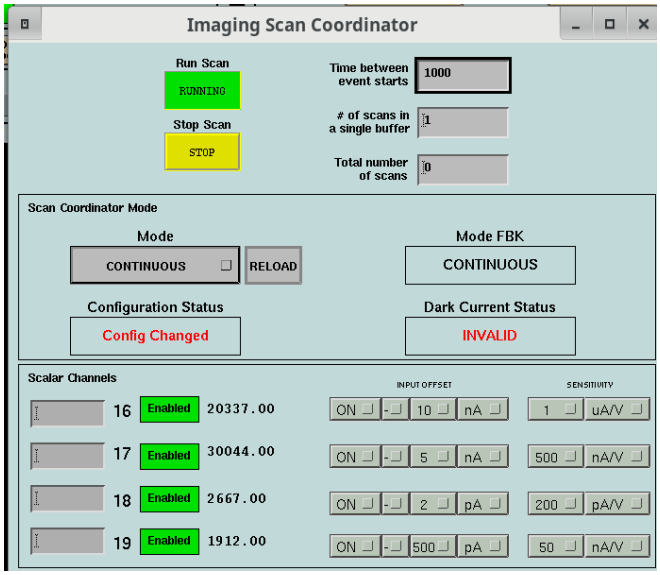
The Utilities subsection allows users to insert or remove filters from the X-ray beam path when beam attenuation is required. Filters may be used, for example, when working with samples containing high concentrations of elements, where attenuation of the incident beam may be necessary to prevent excessive detector counts. The upstream filter slot is labelled Filter 1, and four filter slots are available.



The Utilities subsection also provides control of the safety shutter, which can be opened or closed to allow or block the X-ray beam from entering the experimental hutch.

2.4 Application: Scan Coordinator

The Scan Coordinator application displays the ion chambers used at the BioXAS-Imaging beamline to monitor and measure the X-ray beam intensity (flux) at different locations along the beam path.



There are four ion chambers located within the experimental hutch.

See the schematic of the BioXAS-Imaging beamline endstation in **Section - 1** of this User Manual.

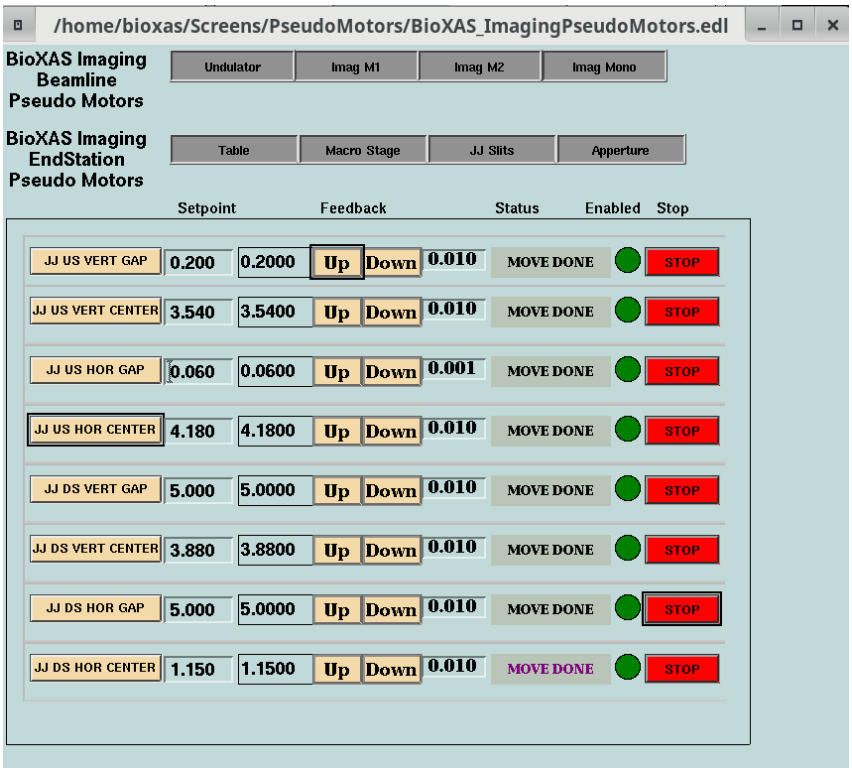
Under the Imaging Scan Coordinator:

- **Scalar Channel 16 - Ion Chamber I_0:**
  Monitors the intensity of the X-ray beam after the Upstream JJ slits.
- **Scalar Channel 17 - Ion Chamber I_1:**
  Monitors the intensity of the X-ray beam at the sample during Macro-mode operation and is used to normalize data collected during Macro-mode measurements. It is important to note that the physical location of I1 differs in Micro-mode. In Micro-mode, I1 is positioned further downstream, immediately upstream of the KB micro-focusing mirrors, and therefore measures the beam intensity before the beam is focused by the KB mirrors.
- **Scalar Channel 18 - Ion Chamber I_2:**
  Monitors the intensity of the focused X-ray beam immediately upstream of the sample during Micro-mode operation. The I2 signal represents the incident intensity at the sample position and is used to normalize data collected during Micro-mode measurements.
- **Scalar Channel 19 - Ion Chamber I_3:**
  Monitors the intensity of the X-ray beam downstream of the sample during Micro-mode operation. The I3 signal therefore represents the transmitted beam intensity after the X-rays have passed through the sample.

2.5 Application: Pseudo Motors

This application contains multiple sections; however, the only section relevant to users is the **JJ Slits** section. This section allows users to adjust the gap and position of both the upstream and downstream JJ slits.

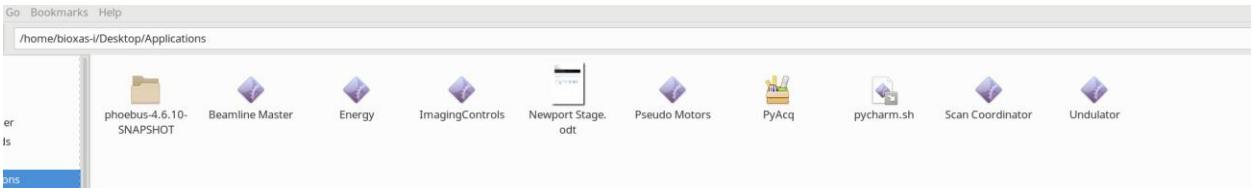
Users performing XAS measurements will need to adjust the JJ slit gaps according to the requirements of the measurement. The appropriate slit settings and procedures for XAS measurements are described in the upcoming sections of this User Manual.

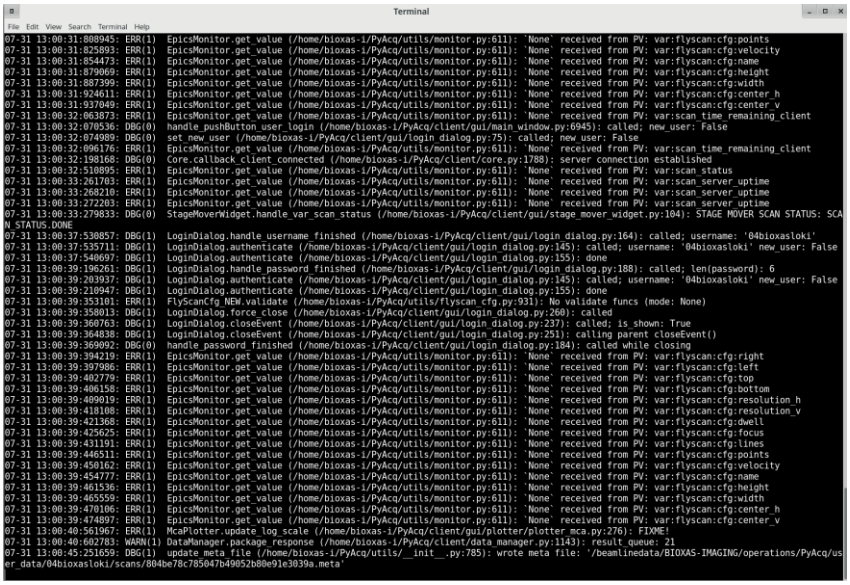


3. Starting the PyAcq Client

3.1 Launch PyAcq

Go to the Applications folder on the Desktop and double-click the PyAcq icon. The action will open a terminal window and the PyAcq client.

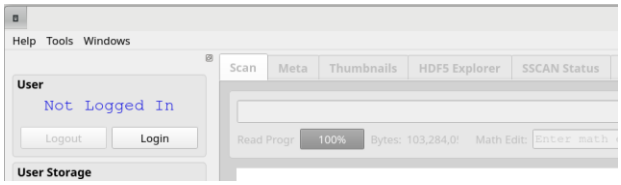




Do not close the terminal. The terminal may be minimized instead.

3.2 Log In

Click Login in the top-left corner of the PyAcq window.



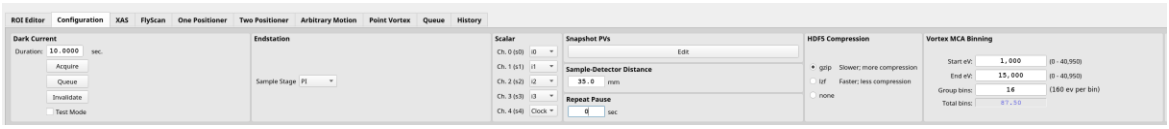
3.3 Enter Login Credentials

A new window requesting the username and password will open.

- In the Username field, enter your project number.
- In the Password field, enter the password provided by BioXAS staff.

3.4 Configure PyAcq

Under the Configuration tab, perform the following:



- Select the correct stage.
    - For micro-mode, select PI.
    - For macro-mode, select Newport.

Beamline staff should have already selected the correct stage for the beamtime. Restarting the PyAcq software should not change this setting.

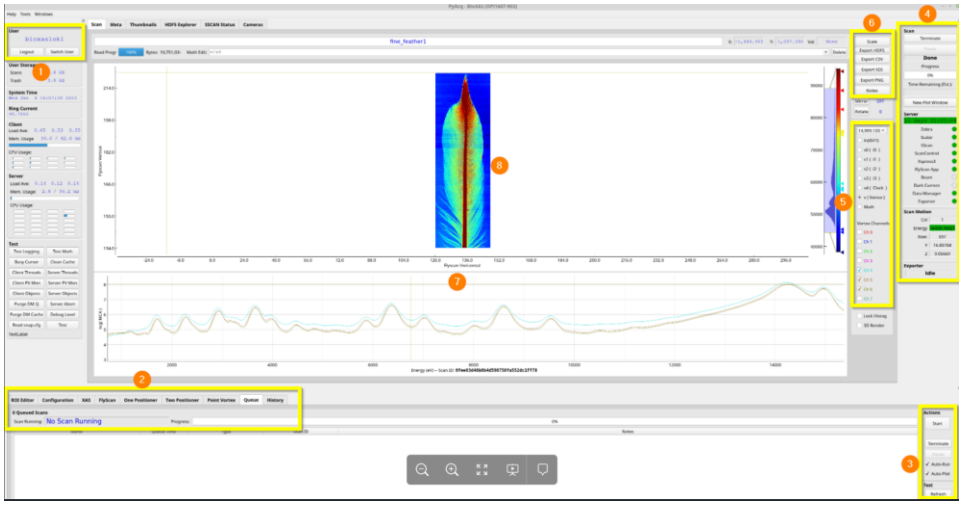
- Enter the sample-to-detector distance as 35 mm.
- Set the Vortex MCA Binning value:
    - Enter a value that is at least 1500 eV higher than the beamline energy.
    - For example, for a beamline energy of 13,500 eV, the recommended value is 15,000 eV. This setting is required after every PyAcq restart because the software always loads its default value of 10,280 eV.

Note: Restarting PyAcq will not interrupt the running scan. However, scans that are waiting in the queue can be lost.

4. Features of PyAcq Client

Beamline data are collected using a multi-threaded, Python-based data acquisition software package consisting of a standalone graphical user interface (GUI) and a Scanner application. The GUI and Scanner can operate independently.

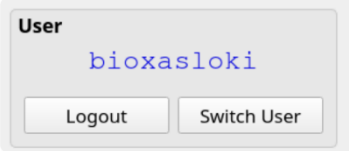
This page is intended to familiarize users with the layout and basic functions of the software, including the purpose of the various tabs. Screenshots of the key software tabs are numbered and briefly described below.



Important Features of Data Collection Software:

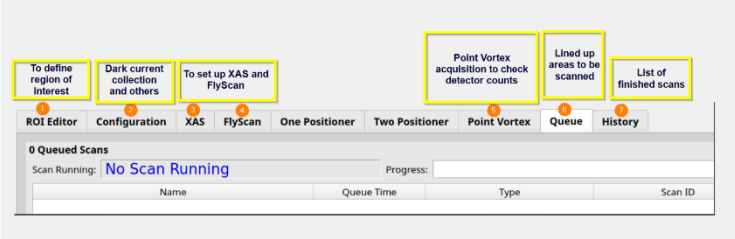
4.1 User Account

A user account is created for each project that has been awarded beamtime through the peer-review process. Beamline staff will create the account before the experiment. Once the account has been set up, users can log in using their project number (case-sensitive) and password.



4.2 Tabs for Different Data Collection Methods

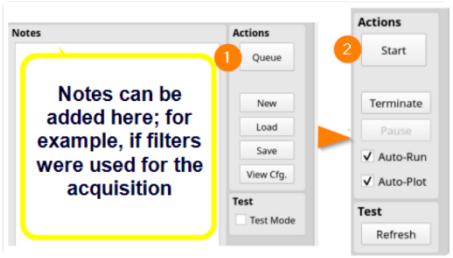
The software provides separate tabs for different data collection methods. Select the appropriate tab based on the type of experiment you wish to perform.



4.3 Starting Data Acquisition

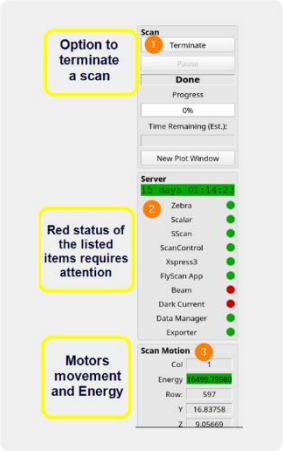
When a scan is ready to begin, navigate to Actions, located in the lower-right corner of the GUI, and select the Queue tab. This opens the queue panel.

If Auto-Run is enabled, the scan or data acquisition will start automatically. Otherwise, click Start to begin the scan manually.



4.4 Terminating a Scan and Monitoring Status

The software allows users to terminate an ongoing scan and monitor its progress. If a scan is terminated, the scan data completed up to that point will be saved.

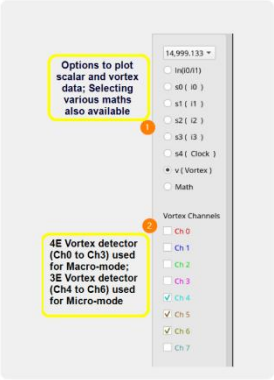


Monitoring the status of the beamline hardware and software components is essential. Any component indicated by a red status indicator requires attention before data collection can proceed. For example, if the Dark Current status is red, a dark current measurement must be collected before starting the experiment.

The Scan Motion section (shown in the screenshot below) is particularly useful during data collection. Changing Y and Z values indicate the horizontal and vertical movement of the sample stage, respectively. Monitoring these values can help diagnose why a scan has stalled or is not progressing as expected.

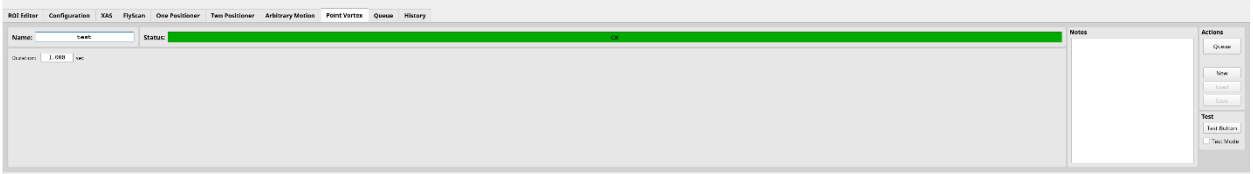
4.5 Plotting Scalar or Vortex Data

This panel allows users to display either Scalar (Ion Chamber) data or Vortex detector data for a scan. Several mathematical operations are available for viewing X-ray Absorption Spectroscopy (XAS) spectra and normalized X-ray Fluorescence (XRF) scans. To display the correct data, ensure that the appropriate detector channels are selected.



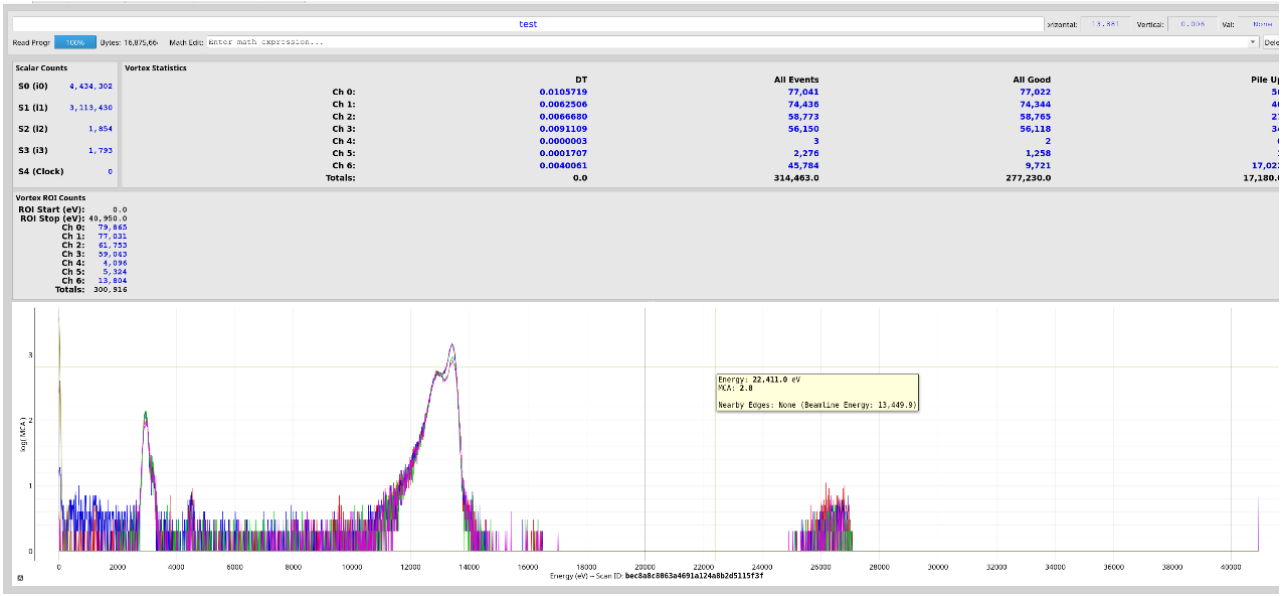
4.6 Taking a Point Vortex Acquisition

Go to the Point Vortex tab, enter an appropriate name for the acquisition, and click Queue to add the point vortex acquisition to the queue.



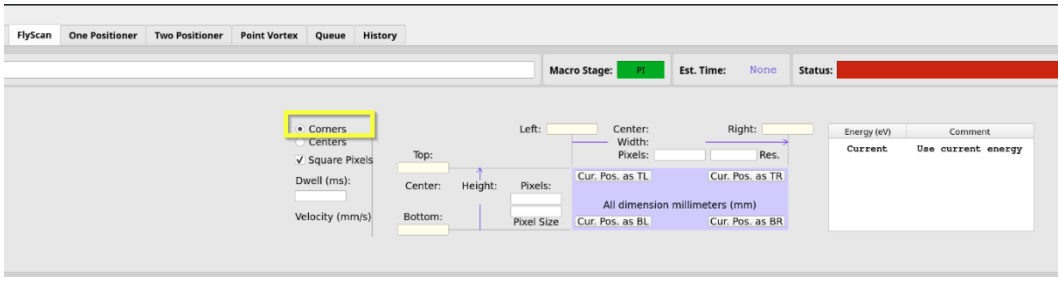
Ch 0, Ch 1, Ch 2, and Ch 3 indicate the counts recorded by the 4-channel Vortex detector used in the macro-mode setup.

Ch 4, Ch 5, and Ch 6 indicate the counts recorded by the 3-channel Vortex detector used in the micro-mode setup.



4.7 Setting up an XRF Scan

4.7.1. Using Corners

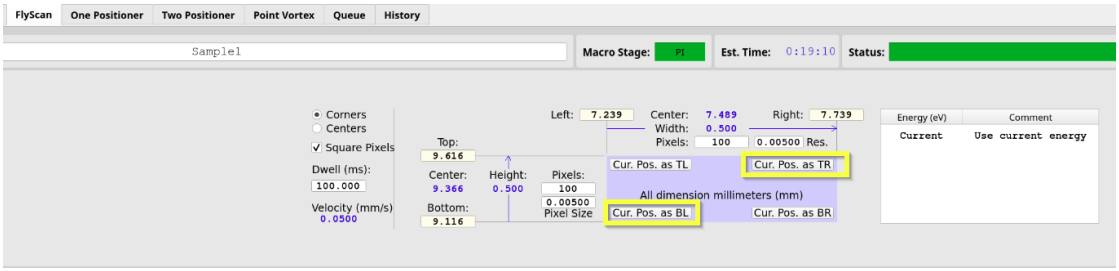


- Select the coordinates of the area of interest by moving the stage and positioning the marked beam on two diagonally opposite corners, one at a time.

  For example, first, move the stage to the **bottom-left corner** of the desired area. Under the **FlyScan** tab, click **Cur. Pos. as BL**. The coordinates of this stage position will be automatically updated in the software.

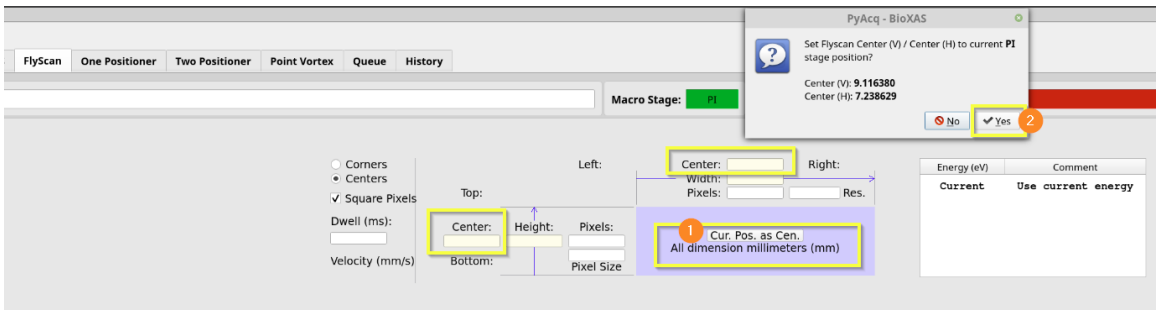
  Next, move the stage to the **top-right corner** of the desired area and click **Cur. Pos. as TR** again.

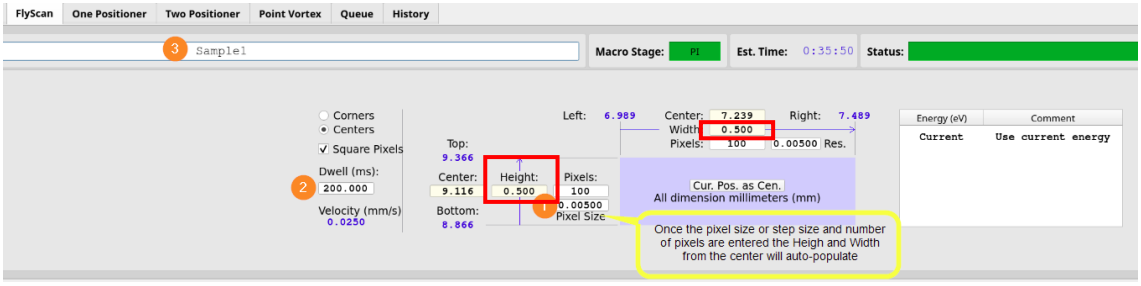
- Enter step size and dwell time to fully define the scan.
- Give an appropriate name to the scan. It is recommended to include dwell time and step size in the scan name, *e.g.*, scan1_fine_100msecDwell_5umStep.



4.7.2. Using Center

- An area can also be selected by positioning the stage at the **center of the area of interest.** To do so, click **Cur. Pos. as Cen** to use the current stage position as the center of the scan area. The Center (V, H) coordinates will then be automatically populated.

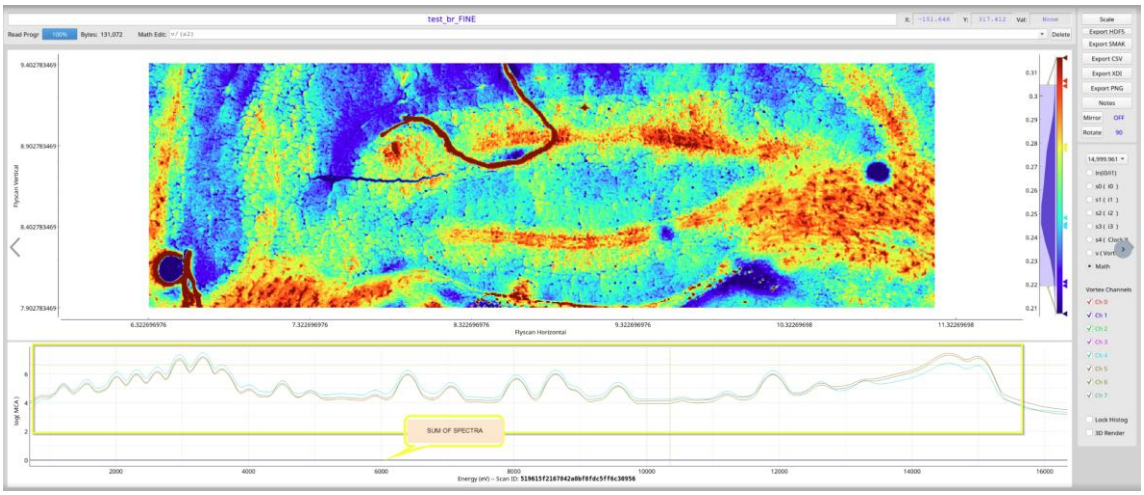




- Specify the scan dimensions in the horizontal and vertical directions by entering the desired distance in **mm.**

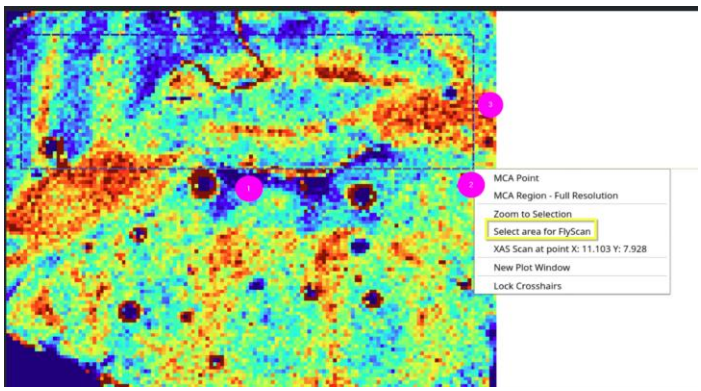
4.8 Sum of Spectra

- The summed fluorescence spectrum from all the pixels is displayed at the bottom of the XRF image.
- The three different coloured line graphs represent the different channels of the Vortex detector.

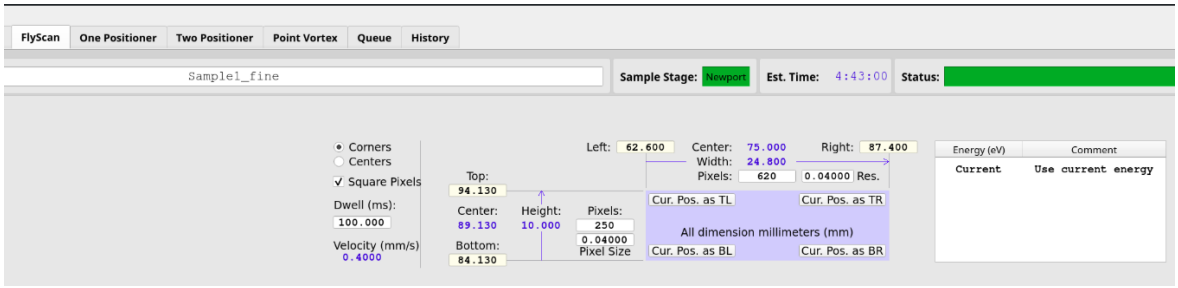


4.9 Fine Scan Setup Using a Coarse Scan

- A coarse scan is a low-resolution scan that is performed by choosing a step size larger than the beam size. For example, using 5 um beam in micro-mode, the recommended step size for the coarse scan is 20 um. In macro mode using 20 um beam, the recommended step size for a coarse scan is 200 um.
- A fine scan can then be set up using an existing coarse scan. In the **History** tab, select the coarse scan of interest, then draw a rectangle around the area of interest by right-clicking and dragging the mouse.



- Right-click anywhere outside the rectangle and select **Select Area for FlyScan**.
- The motor coordinates will be automatically populated under FlyScan tab. Update the name, dwell time, and step size as required for the fine scan.

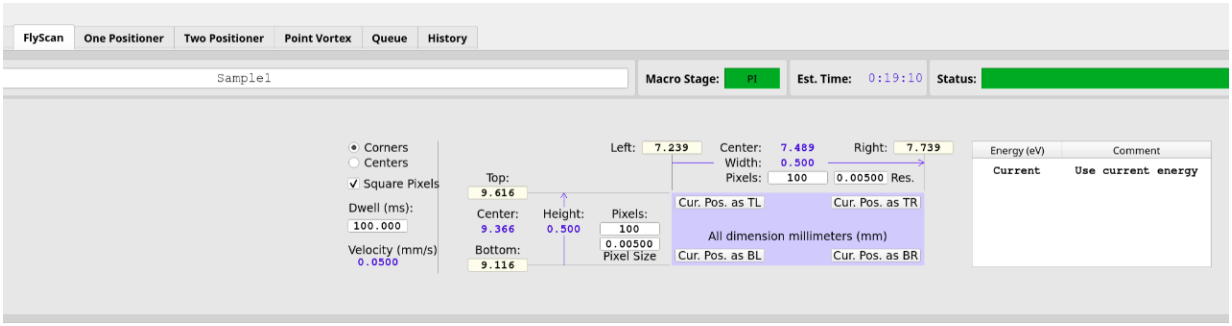


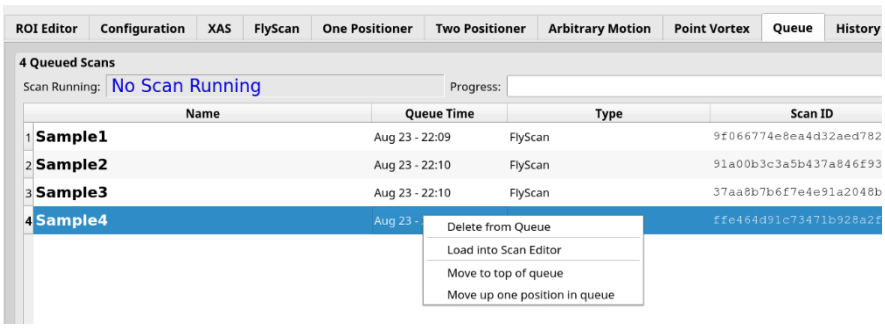
- To remove the rectangle, right-click anywhere on the image and select **MCA**. This will display the MCA spectrum from a single pixel.
- To view the summed spectrum without the rectangle, right-click again and select **MCA All**.

4.10 Setting Up Multiple Scan Queues

- Before setting up multiple scans in a queue, deselect Autorun to prevent the scan from starting automatically when the first area is selected.

- Select a coarse scan from the history tab. On the coarse scan, draw a rectangle around the desired area, right-click, and select **Select Area for FlyScan**. This will automatically fill all the scan coordinates in the **FlyScan** tab.



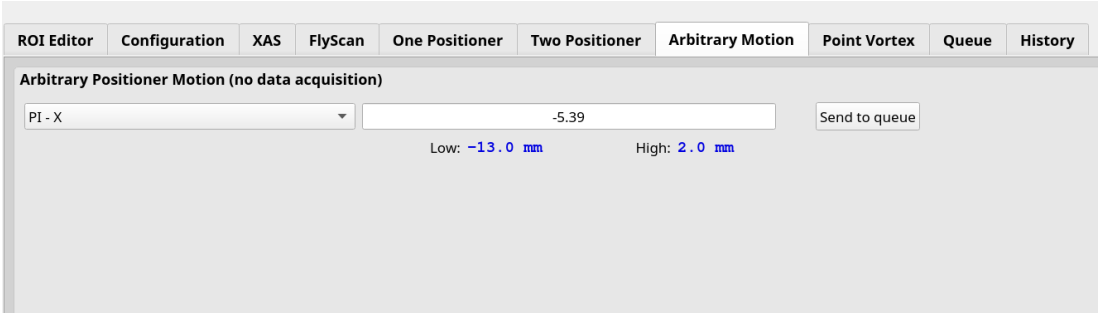


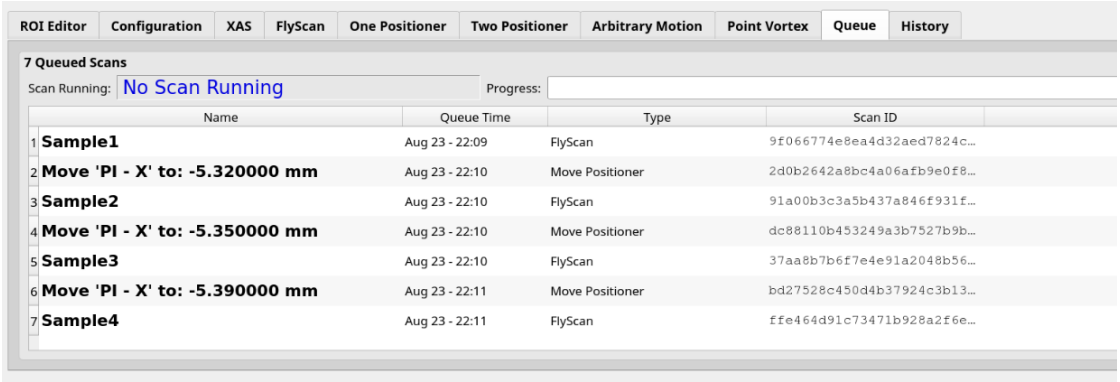
- Click the **Queue** button under **Actions** to add the scan to the queue.
- Draw additional rectangles over the coarse scan and add them to the queue as required.
- Make sure **Autorun** remains deselected while setting up and editing the queue.
- Right-click on a scan to change its position in the queue or remove it from the queue.
- Once the queue is ready, select **Autorun** to begin executing the queued scans.

4.11 Queue Sample Focal Positions

In Micro-mode, the sample must remain in the focal plane of the Keyence microscope to ensure that the sample is positioned at the beam focus. However, multiple samples mounted on the same frame may lie at different focal planes. Therefore, when queuing scans for multiple samples, it is important to also queue the sample position in the **X direction** (see the schematic in **Section - 1**).

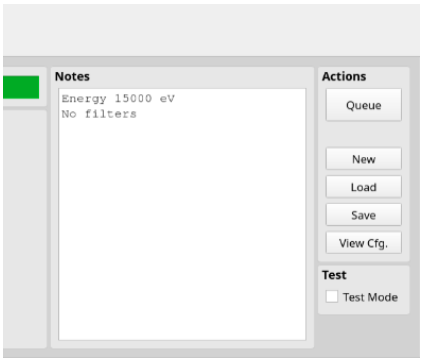
To do this, go to the **Arbitrary Position** tab in PyAcq, select **PI-X** from the drop-down menu, enter the **X coordinate** at which the sample is in the focal plane of the Keyence microscope, and click **Send to Queue**.





In the above example, **Sample 1** is already in focus and is the first scan sent to the queue. For **Sample 2**, the focal plane is at **X = −5.32 mm**. Similarly, the focal planes for **Sample 3** and **Sample 4** are at **X = −5.35 mm** and **X = −5.93 mm**, respectively.

4.12 Saving Configuration file for a Scan



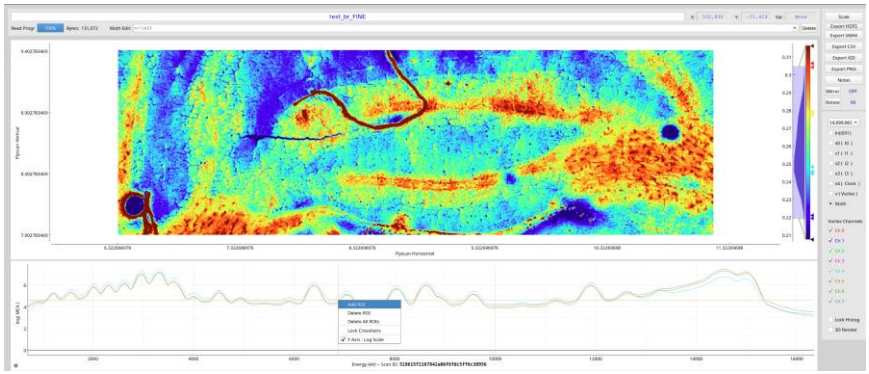
It is recommended to save the coordinates for each scan by selecting **Save** under **Actions**. This will save the scan configuration to a config file. To retrieve the coordinates for a specific scan, click **Load** and select the corresponding config file.

Saving a config file for each scan is important in case PyAcq crashes, which can result in the loss of all scans in the queue. Having a configuration file saved for each scan allows the scan parameters and coordinates to be restored and used to create a new queue.

Note: The scan that is currently running will not be lost if PyAcq crashes.

4.13 Viewing XRF Images Using ROIs

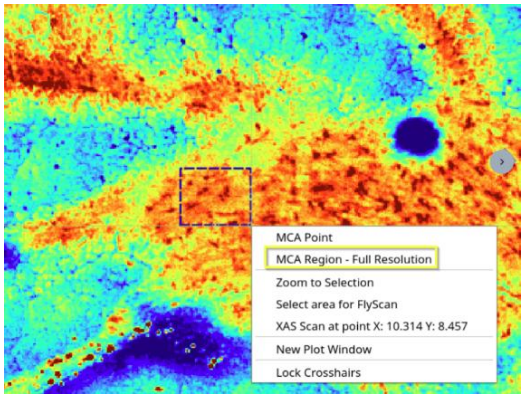
An XRF image of an element of interest can be generated by setting a spectral Region of Interest (ROI).



To set an ROI, right-click on the fluorescence spectrum, select **Add ROI**, and position the highlighted region over the emission peak of interest.

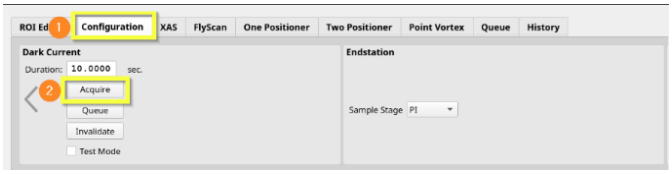
Hovering the mouse over an emission peak may provide suggestions for the elements that could be present in the sample.

4.14 MCA/Fluorescence Spectrum of a Region or a Single Pixel



- An MCA spectrum can be extracted from a defined region after or during data acquisition.
- To do so, hold right click and drag to draw a region of interest over the XRF map. Then right-click anywhere outside the region and select **MCA Region – Full Resolution**.
- An MCA spectrum can be extracted from a single pixel by right-clicking on a pixel and selecting **MCA Point**.

4.15 Dark Current Measurement



- Whenever the ion chamber sensitivity is changed, it is important to collect a new dark current measurement. This is indicated by the blinking red LED in the **PyAcq** acquisition software. To collect the dark current, close the Safety Shutter. Then, under the **Configuration** tab in PyAcq, select **Acquire.**
- A successful dark current measurement should turn the dark current status LED in PyAcq from red to green.

4.16 Acquire an XAS scan using PyAcq

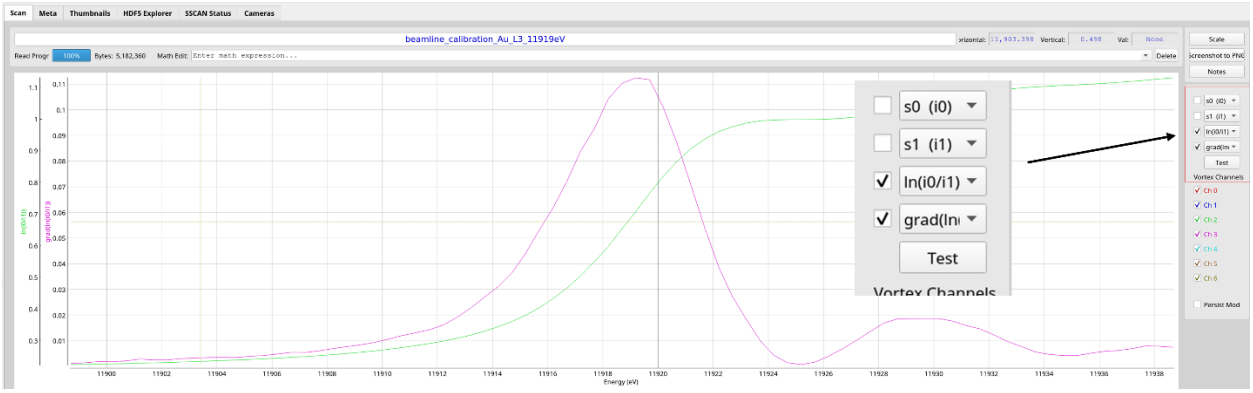
XAS scans require beam flux optimization for a given sample concentration. See Section 5 and 6 for procedure on XAS in transmission mode, and Section 9 and 10 for those in fluorescence mode. The example below is an XAS scan in transmission mode with flux optimized.

Under the XAS tab in PyAcq, select the desired element from the 'Element' drop-down menu.



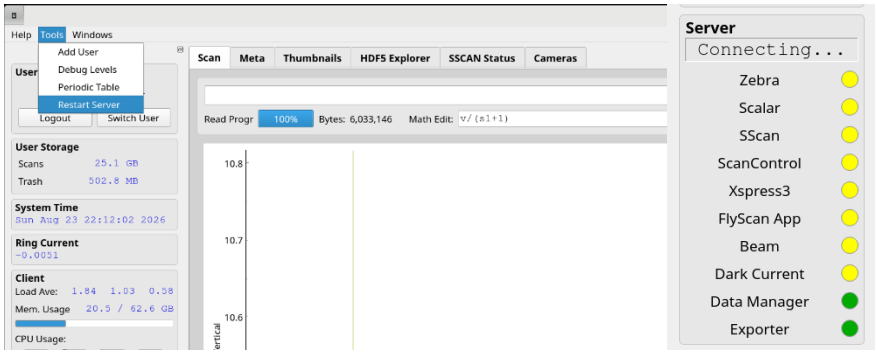
The XAS scan is divided into different energy regions, and each box allows you to specify the pre-edge and post-edge boundaries for that region. Pre and post energy region boundaries can be added or removed as required by right clicking in the box. Enter the appropriate energy step size and dwell time for each region. See the example below for the Gold L3 edge.

Press Queue to add the XAS scan to the queue and run it with the specified parameters. To view the XAS spectrum, select ln(I0/I1) and grad(ln(I0/I1)), as shown below. The first peak in grad(ln(I0/I1)), which is called the **first-derivate of the gradient function**, represented by the red curve in the example below corresponds to the L3 absorption edge of Gold.



4.17 Restart PyAcq Server

In certain situations, it may be necessary to restart the PyAcq server, for example, when scans do not start or a scan becomes stalled, as indicated by no motion in the **Scan Motion** window (**see Section - 4.4**). To restart the server, in PyAcq, go to **Tools → Restart Server**.



- During the restart, some of the status LEDs may turn yellow momentarily. These LEDs will turn green again once the server restart is complete.
- Do not restart the server while a scan is in progress. Before restarting the server, make sure **Auto-run** is not selected if there are scans waiting in the queue, and terminate any scan currently in progress before restarting the server.
- After restarting the server, the previously acquired dark current will no longer be valid. This will be indicated by the **Dark Current** status LED turning red. Acquire a new dark current once the server restart is complete (see **Section - 4.15**).

5. Transmission XAS for a Standard in Macro-mode setup

Note: This section assumes that the user is familiar with the interfaces of relevant beamline control applications and the features of PyAcq. Refer to **Section: 2** of this user manual for a brief introduction to the different beamline control applications and **Section: 4** for a detailed description of PyAcq features.

1. Place the standard in the filter slot

Place standard in one of the filter slots. The upstream slot is labelled Filter 1 in the **ImagingControls** app. There are four slots available. Identify which filter slot was used to place the standard. Make sure the standard is at its place but not yet inserted in the beam path.

2. Record the Sensitivity Values

Take a picture of Sensitivity values on the **Scan Coordinator** app. You will be changing some of these values and these need to be reverted to the original values after the XAS is complete.

3. Extract all the attenuators from the Beam Path

Using controls in the **ImagingControls** app, make note of which attenuators/foils are in inserted state from the previous setup, and extract all the attenuators from the beam path.

4. Insert the Standard into the Beam Path

Using the controls in the **ImagingControls** app, insert the standard into the beam path.

5. Record the JJ Slit Settings

From the **Pseudo Motors** app, take a picture of all the JJ slit settings. These settings must be restored after completing the XAS scan.

6. Set the JJ Slit Gaps

To illuminate the standard with full beam, set the JJ slit gaps as follows:

- Upstream vertical: 5 mm; Upstream horizontal: 5 mm
- Downstream vertical: 0 mm; Downstream horizontal: 0 mm

7. Remove the Vertical Aperture from the Beam Path

Take a picture of the aperture coordinates from **ImagingControls** app. Change the vertical aperture position to **1.0** to remove it from the beam path.

8. Set Beamline Energy to the Pre-Edge

In the **Beamline Energy** app, note the energy used for XRF mapping, and change it to approximately 20 eV below the absorption edge (pre-edge).

WARNING: Be very careful when entering the beamline energy. Enter the intended value first, carefully verify that the entered value is correct, and then press Enter to send the command to change the beamline energy. For example, for the Bismuth L3 edge at 13,418.6 eV, enter a beamline energy of 13,400 eV.

9. Send the Beam into the Hutch

Send beam in the hutch and make sure Mode on the **Scan Coordinator** app is 'Continuous'.

10. Adjust the Sensitivities

With **Scan Coordinator** app set to 'Continuous' mode, check counts on Channel 16 and Channel 17. Adjust the sensitivity corresponding to each channel as required so that the counts on both Channel 16 and Channel 17 are between 4 and 7 million.

11. Acquire Dark Current if Sensitivities Were Changed

If the sensitivities were changed in the previous step, the Dark Current LED on the PyAcq client will turn red. In this case, acquire a dark current with Beam OFF. See instructions in **Section - 4.15.**

12. Verify PyAcq Status

Check and make sure that all status LEDs on the PyAcq client are green.

13. Acquire the XAS Scan

Follow instructions given in **Section - 4.16** to acquire an XAS scan using PyAcq.

14. Extract the Standard from the Beam Path

If you have another standard, remove the previous standard and replace it with the next one. Follow Steps 7–13 to perform the XAS measurement for the next standard and repeat the same procedure for all other standards you may have.

In the **ImagingControls** app, make sure the next standard remains inserted in the beam path.

15. Restore the Vertical Aperture Position

When all standards are completed, restore vertical aperture to the position noted in Step 9.

16. Restore the Beamline Energy

In the **Beamline Energy** app, enter the beamline energy that was previously used to acquire XRF images. The beamline energy will remain at the value where the XAS scan completes.

Therefore, it is important to change the beamline energy back to the value previously used for the XRF imaging.

17. Restore the JJ Slit Settings

Revert all JJ slit values to the ones noted in Step 5.

18. Insert all the attenuators back into the Beam Path

Using **ImagingControls** app, reinsert the attenuators/foils that were noted in Step 3.

19. Restore the Sensitivity Values

Revert the sensitivity values to those noted in Step 2.

20. Acquire Dark Current After Restoring Sensitivities

Changing sensitivity again will cause the Dark Current LED to turn red.

Acquire another dark current with Beam OFF.

6. Transmission XAS for a Standard in Micro-mode setup

Note: This section assumes that the user is familiar with the interfaces of relevant beamline control applications and the features of PyAcq. Refer to **Section: 2** of this user manual for a brief introduction to the different beamline control applications and **Section: 4** for a detailed description of PyAcq features.

1. Place the standard in the filter slot

Place standard in one of the filter slots. The upstream slot is labelled Filter 1 in the **ImagingControls** app. There are four slots available. Identify which filter slot was used to place the standard. Make sure the standard is at its place but not yet inserted in the beam path.

2. Block the beam going into the KB mirrors

Place a thick aluminum foil before the KB mirrors to avoid sending the beam onto the mirrors.

3. Record the Sensitivity Values

Take a picture of Sensitivity values on the **Scan Coordinator** app. You will be changing some of these values and these need to be reverted to the original values after the XAS is complete.

4. Extract all the attenuators from the Beam Path

Using controls in the **ImagingControls** app, make note of which attenuators/foils are in inserted state from the previous setup, and extract all the attenuators from the beam path.

5. Insert the Standard into the Beam Path

Using the controls in the **ImagingControls** app, insert the standard into the beam path.

6. Record the JJ Slit Settings

From the **Pseudo Motors** app, take a picture of all the JJ slit settings because you will have to revert back to these settings after completing the XAS scan.

7. Set the JJ Slit Gaps

To illuminate the standard with full beam, set the upstream vertical, upstream horizontal, downstream vertical, and downstream horizontal JJ slit gaps to 5 mm each.

8. Set Beamline Energy to the Pre-Edge: In the **Beamline Energy** app, note the energy used for XRF mapping, and change it to approximately 20 eV below the absorption edge (pre-edge).

WARNING: Be very careful when entering the beamline energy. Enter the intended value first, carefully verify that the entered value is correct, and then press Enter to send the command to change the beamline energy.

For example, for the Bismuth L3 edge at 13,418.6 eV, enter a beamline energy of 13,400 eV.

9. Send the Beam into the Hutch

Keep the thick aluminum foil in place from Step 2 and send the beam in the hutch and make sure the Mode on **Scan Coordinator** app is Continuous.

10. Adjust the Sensitivities

With **Scan Coordinator** app set to 'Continuous' mode, check counts on Channel 16 and Channel 17. Adjust the sensitivity corresponding to each channel as required so that the counts on both Channel 16 and Channel 17 are between 4 and 7 million.

11. Acquire Dark Current if Sensitivities Were Changed

If sensitivities were changed in the previous step, the dark current LED will turn red on the PyAcq client. In this case, take a dark current acquisition with Beam OFF. See instructions in **Section - 4.15.**

12. Verify PyAcq Status

Check and make sure all the LEDs on the PyAcq client are green.

13. Acquire the XAS Scan

Follow instructions given in **Section - 4.16** to acquire an XAS scan using PyAcq.

14. Extract the Standard from the Beam Path

If you have another standard, remove the previous standard and replace it with the next one. Follow Steps 8 - 13 to perform the XAS measurement for the next standard and repeat the same procedure for all other standards you may have.

In the **ImagingControls** app, make sure the next standard remains inserted in the beam path.

15. Restore the Beamline Energy

When all standards are completed, in the **Beamline Energy** app, enter energy that was previously used for XRF imaging. The energy will remain at a value where XAS scan is completed. It is important to change the energy back to the value previously used for imaging.

16. Restore the JJ Slit Settings

Revert all JJ slit values to those noted in Step 6.

17. Insert all the attenuators back into the Beam Path

Using the controls in the **ImagingControls** app, reinsert the attenuators/foils that were recorded in Step 4 and restore them to their previous positions.

18. Restore the Sensitivity Values

Revert the sensitivity values to those noted in Step 3.

19. Acquire Dark Current After Restoring Sensitivities

Take dark current acquisition with Beam OFF If sensitivities are changed in the previous step.

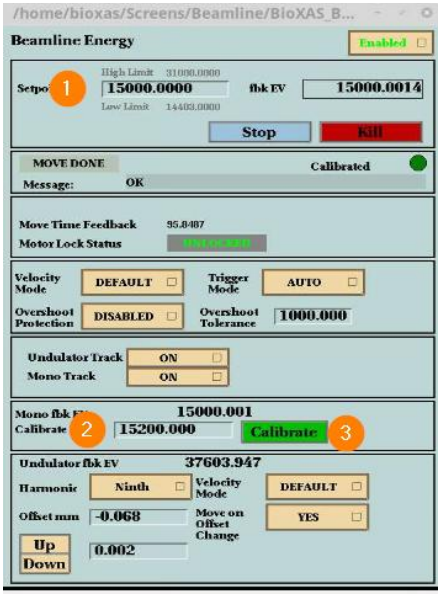
20. Remove the Thick Aluminum Foil

Remove the thick aluminum foil placed in front of the KB mirrors.

7. Beamline Energy Calibration

Note: This section assumes that the user is familiar with the interfaces of relevant beamline control applications and the features of PyAcq. Refer to **Section: 2** of this user manual for a brief introduction to the different beamline control applications and **Section: 4** for a detailed description of PyAcq features.

- Perform an XAS scan for a suitable foil in the transmission mode:
  - Follow instructions given in **Section - 5** if you are working in macro-mode.
  - Follow instructions given in **Section - 6** if you are working in micro-mode.
- Note down the energy corresponding to the first derivate in the XAS spectrum. See **Section - 4.16**.
- No need to proceed if the first derivative energy is same as the tabulated absorption edge value for the foil. This implies that beamline energy is already well calibrated. In **Beamline Energy** app, set the beamline energy to the one used for XRF imaging and proceed with your experiment.



- If the energy corresponding to the first derivate differs from the tabulated absorption edge value, proceed with the following steps:
  1. Enter the first derivative energy value as the **Beamline Energy setpoint** and press Enter. Press Enter again to make sure the **fbk EV** value is as close as possible to the **setpoint** value.
  2. Enter the tabulated absorption energy value of the foil as the **Mono fbk Calibration** and press enter.
  3. Press **Calibrate** button to calibrate the beamline energy.

8. X-Ray Beam Flux Optimization for the Sample

Note: This section assumes that the user is familiar with the interfaces of relevant beamline control applications and the features of PyAcq. Refer to **Section: 2** of this user manual for a brief introduction to the different beamline control applications and **Section: 4** for a detailed description of PyAcq features.

1. Check the Beamline Energy

To ensure that all elements of interest in your sample are excited by the incident X-Ray beam, check the **Beamline Energy** app to make sure the beamline energy is set to the value intended for XRF imaging. If the displayed energy is different from the intended value, set it to the correct energy before starting the XRF imaging measurement. This is important because a previous XAS measurement may leave the beamline energy set to the value corresponding to the last data point of the previous XAS scan, which may differ from the energy intended for XRF imaging.

2. For macro mode only: Maximize X-Ray Flux going through the aperture

Select Continuous mode in the **Scan Coordinator** application.

To maximize the X-ray flux passing through the aperture, use the **ImagingControls** app to fine-tune the vertical and horizontal position of the aperture. While making these adjustments, monitor Scalar Channel 17 in the **Scan Coordinator** app. Adjust the aperture position in small increments in both the vertical and horizontal directions until the maximum count rate is observed in Channel 17. This indicates that the aperture is optimally aligned with the X-ray beam and allows the maximum available beam flux to pass through the aperture.

3. For micro mode only: Bring Sample into the Focal Plane of the Keyence Microscope

Using the **ImagingControls** app, move the X-stage in small steps until the sample is brought into focus.

4. Take a single Point Vortex Measurement on the Sample

Move the stage using **Imaging Controls** app to bring the beam at an appropriate location where you think the sample has high concentration. Take a point vortex acquisition using **PyAcq** to check counts each channel sees for the vortex detector. Instructions are given in **Section - 4.6.**

5. Optimize the Vortex Detector Counts

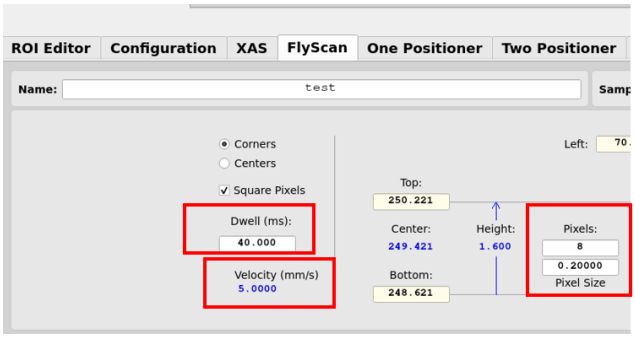
If concentrations in the sample are high, it is possible that the vortex detector can be saturated. To avoid saturation, each channel should have a maximum of **1 million counts**.

If higher counts are observed, attenuate the beam intensity by inserting a filter in the beam path using **ImagingControls** app and take another point vortex measurement until each channel is having close to one million or below counts. You can use multiple filter combinations. Do not reduce the vortex counts too low. 1 million is a sweet high spot.

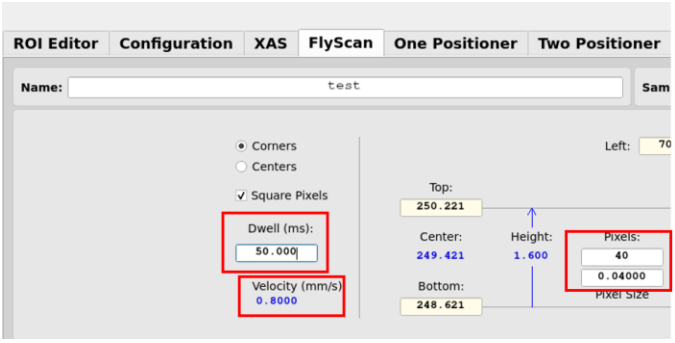
6. Perform a Coarse Scan

Acquire a coarse scan. Discuss with beamline staff the recommended parameters for a coarse scan. The usual recommended parameters are:

- **Macro-mode:** Step size of 200 microns (0.2 value to be entered in PyAcq, units in mm) and a dwell time of 40 msec for high concentrations (a velocity of 5 mm/sec). For low concentration samples, use a 200-micron step size and 100 msec or higher dwell time to acquire enough signal from the sample. Do not exceed **10 mm/sec** of velocity.



- **Micro-mode:** Step size of 40 microns (0.04 value to be entered in PyAcq, units in mm) and a dwell time of 50 msec for high concentrations (a velocity of 0.8 mm/sec). For low concentration samples, use a 40-micron step size and 100 msec or higher dwell time to acquire enough signal from the sample. Do not exceed **1.0 mm/sec** of velocity.



7. Identify a Hot Pixel

After coarse scan completion, remove all the ROIs from the fluorescence spectrum, increase the contrast using the colorbar, and identify a hot pixel.

8. Move the Stage to the Hot Pixel:

Right-click on hot pixel and move the stage to this point.

9. Perform another Point Vortex Measurement

Take another point vortex acquisition to check counts each vortex channel sees.

10. Optimize again the Vortex Detector Counts

Repeat the instructions in Step 5.

11. Check the Ion Chamber Counts

With beam ON, put **Scan Coordinator** app in Continuous mode.

- **For macro-mode**: Check counts in the ion chamber just upstream of sample indicated by channel 17. Installing filters in the beam path in the previous steps will reduce the counts in the channel. Channel 17 saturates at 10 million counts. Change the sensitivity to go somewhere in the middle of 10 million. Any value between 3 and 7 million is good.
- **For micro-mode**: Check counts in the ion chamber just upstream of sample indicated by channel 18. Installing filters in the beam path in the previous steps will reduce the counts in the channel. Channel 18 saturates at 1 million counts. Change the sensitivity to go somewhere in the middle of 1 million. Any value between 300k and 700k is good.

12. Acquire Dark Current

Changing the sensitivity in the above step will turn the dark current LED red. Therefore, do another dark current acquisition with BEAM OFF. See instructions in **Section - 4.15.**

With these settings, the setup is ready to perform XRF imaging without saturating the detectors**.**

9. Point-XAS Measurement in Micro-mode setup

Note: This section assumes that the user is familiar with the interfaces of relevant beamline control applications and the features of PyAcq. Refer to **Section: 2** of this user manual for a brief introduction to the different beamline control applications and **Section: 4** for a detailed description of PyAcq features.

1. Optimize X-Ray Beam Flux for the Sample

Follow instruction in **Section - 8** of this user manual.

2. Perform a Fine Scan

With X-Ray Beam Flux optimized for the sample, identify a region of interest in the coarse scan ran during the beam flux optimization procedure and draw a rectangle to do a fine scan out of it. Discuss with beamline staff the recommended parameters for a fine scan. For high concentration samples the usual recommendation is using a 5-micron (0.005 value to be entered in PyAcq, units in mm) step size and 50 msec dwell time.

For low concentration samples, use a 5-micron step size and 100 msec or higher dwell time to acquire enough signal from the sample.

3. Select a Pixel for Point-XAS:

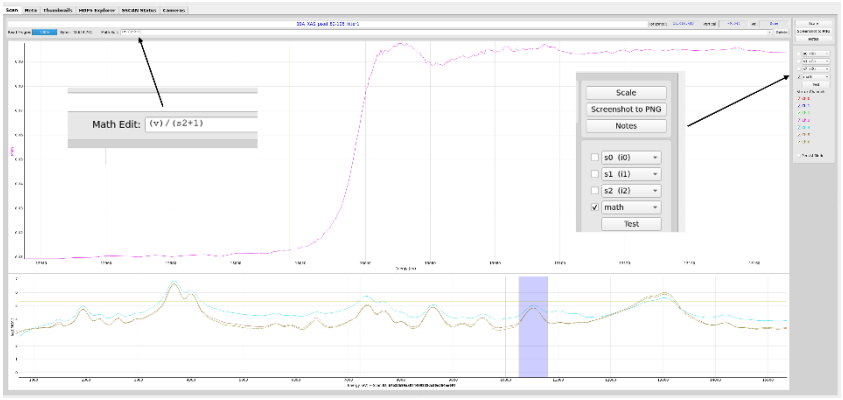
Identify a pixel of interest from the fine scan. Then right-click on the pixel and click on 'Select XAS at point' to perform point-XAS. Follow instructions given in **Section – 4.16** to set up the XAS scan.

4. Perform an Additional Fine Scan if Required

If the fine scan was done sometime ago, the beam might drift a few microns away from the previous position. This might result in not targeting the intended pixel of interest using the previous fine scan. To avoid this situation, you can perform another very small fine scan from the previously acquired big fine scan to target with confidence the pixel of interest. This small scan should+*09.5 not take more than a few minutes.

5. Visualize the Point-XAS Spectrum

In the **PyAcq** client, drop an appropriate ROI over the fluorescence spectrum, and use the equation **(v)/(s2+1)** to visualize the point-XAS spectrum. To avoid getting errors due to a mistake in writing the equation, make sure 'Math' option is not selected in PyAcq while writing the equation. Write the equation first and then select 'Math' option.



6. Optimize Filters for Different Concentration Regions

If your sample has varying concentrations with very high and very low concentration regions, and you want to do point-XAS on these different regions, you will have to optimize the detector counts and hence the filter insertion choices separately for different concentration regions. The filter selection for the high concentration region might completely attenuate the signal coming from the low concentration region, resulting in very noisy or no XAS data at all.

10. Point-XAS Measurement in Macro-mode setup

Note: This section assumes that the user is familiar with the interfaces of relevant beamline control applications and the features of PyAcq. Refer to **Section: 2** of this user manual for a brief introduction to the different beamline control applications and **Section: 4** for a detailed description of PyAcq features.

1. Optimization X-Ray Beam Flux for the Sample: Follow instruction in **Section - 8.**

2. Perform a Fine Scan

With X-Ray Beam Flux optimized for the sample, identify a region of interest in the coarse scan ran during the beam flux optimization procedure and draw a rectangle to do a fine scan out of it. Discuss with beamline staff the recommended parameters for a fine scan.

For high concentration samples, the usual recommendation is using same step size as aperture/beam size (*e.g.,* 40-micron step size with 40-micron beam, 0.04 value to be entered in PyAcq, units in mm) and a dwell time of 50 msec. For low concentration samples, use a 40-micron step size and 100 msec or higher dwell time to acquire enough signal from the sample.

3. Select a Pixel for Point-XAS:

From the fine scan, right-click on a pixel of interest and click on 'Select XAS at point' to set up a point-XAS. See instruction under **Section - 4.16**

4. Visualize the Point-XAS Spectrum

In the **PyAcq** client, use the equation **(v)/(s1+1)** and follow instructions in step 5 under the **Section – 9** to visualize the point-XAS spectrum from the element of interest.

Do not forget to insert an ROI over the fluorescence spectrum.

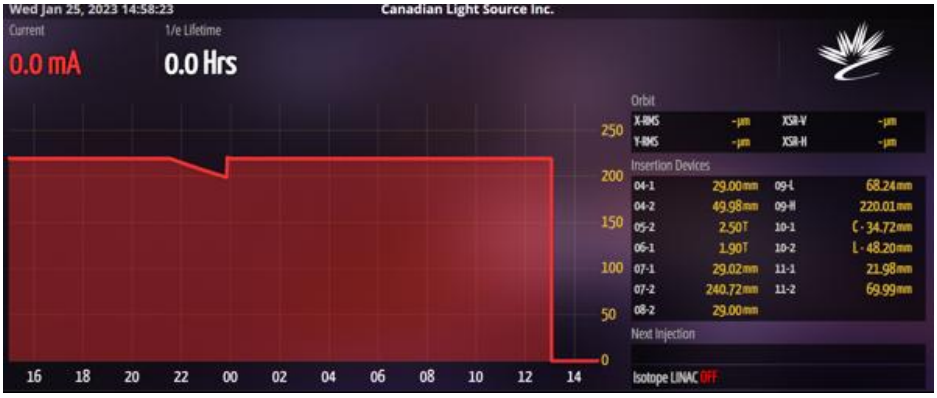
5. Optimize Filters for Different Concentration Regions

If your sample has varying concentrations with very high and very low concentration regions, and you want to do point-XAS on these different regions, you will have to optimize the detector counts and hence the filter insertion choices separately for different concentration regions.

The filter selection for the high concentration region might completely attenuate the signal coming from the low concentration region, resulting in very noisy or no XAS data at all.

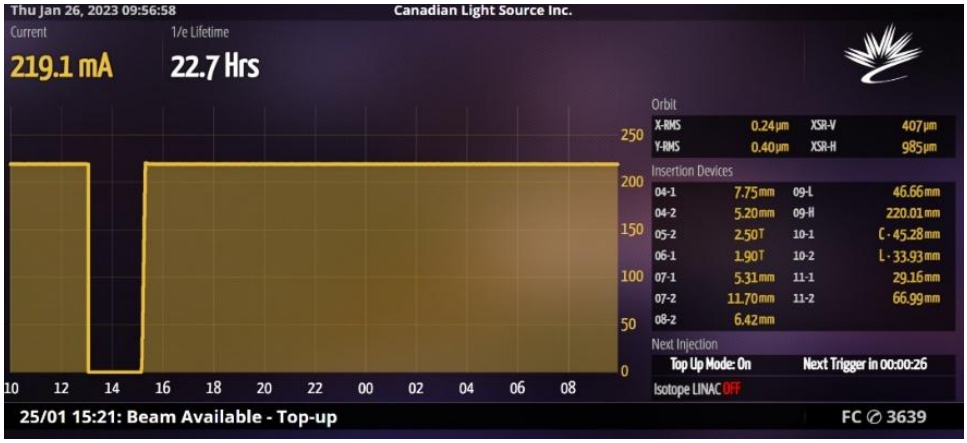
11. Beam Trip

The status of storage ring is available at public webpage https://mstatus.lightsource.ca/ or on a dedicated display at the beamline. The beam in Top-up mode is displayed as a straight line at a current of 219.4 mA beam current. However, the beam sometimes can be in Decay mode at < 219.4 mA. But it is still a usable beam for data collection. In some cases, there is a beam trip, which would be displayed as a red plot showing 0 mA beam current. Beam trip implies that there is no beam available to the whole facility.



A red plot showing 0 mA beam current. BioXAS-Imaging Undulator (07-1) ID open with a gap value 29.02 mm

BioXAS-Imaging Undulator is 07-01 its status is either fully open with gap 29.02 mm or it is a smaller gap value corresponding to and specific beamline Energy. More details in **Section - 2.1.**



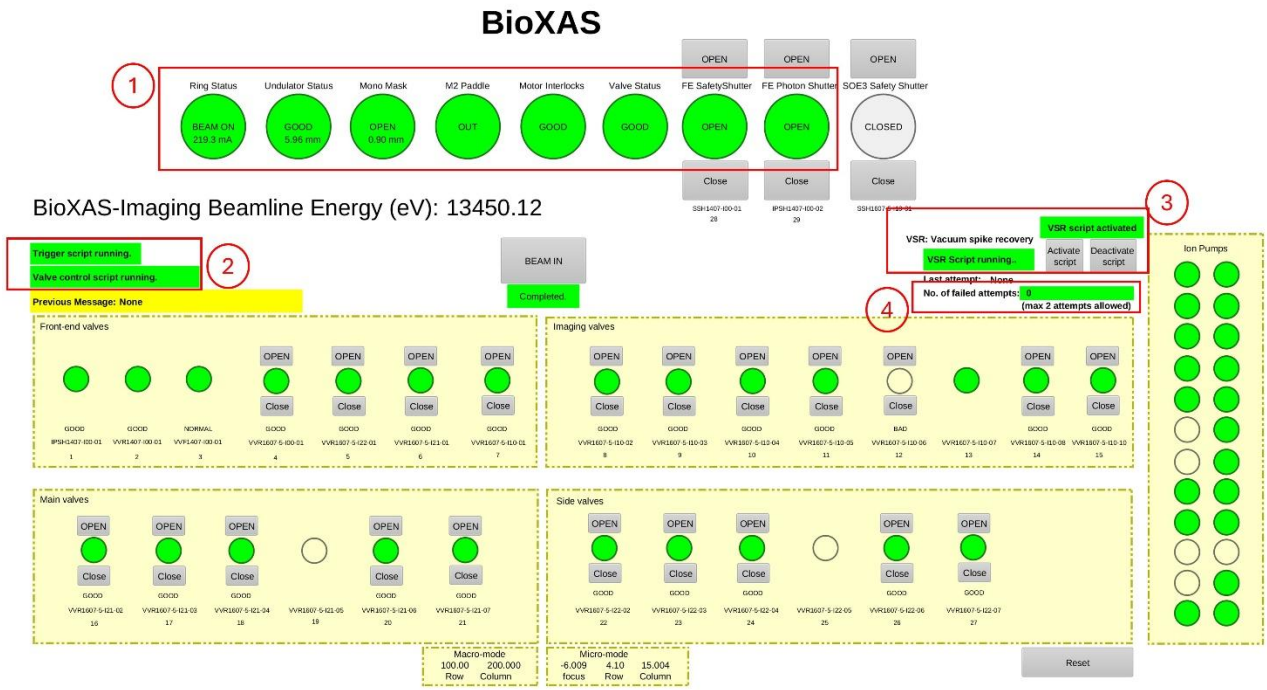
Top-up mode with 07-1 ID closed at a gap value of 5.31 mm

11.1 Beam Recovery Procedure After a Beam Trip

In case of a beam trip, immediately take the following actions:

- If multiple scans are queued in PyAcq, uncheck Auto-Run to prevent the scans from being executed in the absence of beam.
- Once Auto-Run is unchecked, terminate the current scan. Scan completed until then will be saved.
- Although not necessary, it is recommended to close the safety shutter using the **ImagingControls** app.

The following CSS Phoebus screen should be open on one of the displays. The status of the various beamline recovery scripts is indicated in the labelled Boxes 2 and 3.



CSS Phoebus Screen

Once the beam is available post beam-trip recovery, the beamline recovery scripts should automatically take all the necessary actions to make the beamline ready to send the beam in the hutch.

Beamline Status Checks

Review the statuses on the CSS Phoebus screen. Use the following table to determine the expected status and the appropriate action.

Status / Box	Normal condition	If RED	Required action
Ring Status	Green	Beam is not currently available in the storage ring.	No action is required. Wait until the Ring Status turns green.
Undulator Status	Green	The undulator is still open.	The Control Room will close the undulator once beam is available. It should turn green within 10 minutes after the Ring Status turns green. If it does not, contact beamline staff or Floor Coordinator.
Mono Mask	Green	Indicates a problem with the Mono Mask.	Contact beamline staff or Floor coordinator. The Mono Mask should remain green regardless of whether beam is available or not.
Motor Interlocks	Green	Indicates a motor interlock issue.	Contact beamline staff or Floor Coordinator.
Beamline Ready	Green	Beamline is not ready.	It should turn green within 10 minutes after the Ring Status and Undulator Status turn green. If it does not, contact beamline staff or Floor Coordinator.
2. Script Status	Green	The script is not running.	Contact beamline staff. This status should always be green.
3. Script Status	Green	The script is not running.	Contact beamline staff. This status should always be green.
FE Safety Shutter	Green	May be red during beam recovery.	It should turn green within 10 minutes after the Ring Status and Undulator Status turn green. If it does not, contact beamline staff or Floor Coordinator.
FE Photon Shutter	Green	May be red during beam recovery.	It should turn green within 10 minutes after the Ring Status

			and Undulator Status turn green. If it does not, contact beamline staff or Floor coordinator.
4. Script Failure Status	Green	The script has failed more than two times.	After Ring Status and Undulator Status are green, the Beam IN button may be used to manually perform beamline recovery. If recovery is unsuccessful, contact beamline staff.
SOE3 Safety Shutter	As required	—	This is the shutter used to send the beam into the hutch. Open or close it as required by the experiment using **ImagingControls** app.

Beam Recovery Procedure

Step 1: Wait for the storage ring. If the Ring Status is red, beam is not yet available in the storage ring. No action is required. Wait until the Ring Status turns green.

Step 2: Confirm the Undulator Status. Once the Ring Status turns green, the Control Room will close the undulator. The Undulator Status should turn green within 10 minutes.

Step 3: Escalate if the undulator remains open. If the Undulator Status remains red more than 10 minutes after the Ring Status turns green, contact the Floor coordinator.

Step 4: Allow automatic beamline recovery. Once both the Ring Status and Undulator Status are green, allow the background scripts to perform the beamline recovery.

Step 5: Allow up to 10 minutes for the scripts. The FE Safety Shutter and FE Photon Shutter may be red during recovery. The background scripts should return these statuses to green within 10 minutes after the Ring Status and Undulator Status are green.

Step 6: Check the script statuses. Boxes 2 and 3 should remain green. If either is red, contact beamline staff. If Box 4 is red, the script has failed more than two times and wouldn't be executed again.

Step 7: Perform manual recovery if required. If Box 4 is red, press the Beam IN button to manually perform beamline recovery. Do not press Beam IN unless both the Ring Status and Undulator Status are green.

Step 8: Escalate if recovery is unsuccessful. If automatic or manual recovery does not successfully restore the required statuses, contact beamline staff or Floor coordinator.

Quick Decision Guide

Condition	Action
Ring red	Wait — no action required.
Ring green + Undulator red	Wait for Control Room to close the undulator. Contact beamline staff or Floor coordinator if not green within 10 minutes.
Mono Mask red	Contact beamline staff or Floor Coordinator.
Motor Interlocks red	Contact beamline staff or Floor Coordinator.
Beamline Ready red	Contact beamline staff or Floor Coordinator.
Box 2 or Box 3 red	In the applications folder on Desktop, double click 'Script Launcher' app to run the necessary scripts. Contact beamline staff or Floor Coordinator if problem persists.
Box 4 red	Only after Ring and Undulator are green, press Beam IN for manual recovery if required.
FE Safety Shutter / FE Photon Shutter red during recovery	Allow up to 10 minutes after Ring and Undulator are green for scripts to recover them.
SOE3 Safety Shutter	Open/close as required to send the beam into the hutch.

11.2 Macro Mode: Flux Recovery After a Beam Trip

Note: This section assumes that the user is familiar with the interfaces of relevant beamline control applications and the features of PyAcq. Refer to **Section: 2** of this user manual for a brief introduction to the different beamline control applications and **Section: 4** for a detailed description of PyAcq features.

After a beam trip and subsequent beam recovery, the beamline optics may still be cold. As the optics warm up, the beam position can gradually drift back toward its previous position. Therefore, the beam path may initially be slightly misaligned. In Macro Mode, the beam passes through apertures/pinholes before reaching the sample. Since the beam position has shifted following a beam trip, the beam will no longer pass fully through the apertures/pinholes. This results in reduced beam flux and will be observed as a lower count rate in Channel 17 on **ScanCoordinator** app, the ion chamber located upstream of the sample.

The time required for the optics to warm up and for the beam flux to recover depends on how long the beam was absent due to beam trip. For example, a beam trip lasting approximately 30 minutes may require about an hour for the flux to recover to 70% of its pre-trip value. A beam trip lasting one hour or longer may require several hours for the flux to recover.

After the beam has returned, follow these steps before resuming data acquisition:

1. Send the beam into the hutch by opening the safety shutter using **ImagingControls** app.
2. In the **Scan Coordinator** app, select Continuous Mode.
3. Monitor the counts in Channel 17.
4. Compare the current Channel 17 count rate with the count rate recorded before the beam trip.
5. Allow the beamline optics to warm up. The beam position and flux will gradually return toward their pre-trip condition. General recommendation is to not resume data acquisition until the Channel 17 flux has recovered to at least 70% of the pre-beam-trip value.
6. If the Beamtime Is Ending Soon:
   If insufficient beamtime remains to wait for the optics to fully warm up and the flux to recover, users may proceed with data collection by fine-tuning the aperture position:

a. In the **ImagingControls** app, fine-tune the aperture position to align the aperture with the beam to maximize the Channel 17 count rate. Majority of the correction needs to be done in the vertical position of the aperture.
b. Once the maximum beam flux is obtained through the aperture, the scan may be started.
c. As the optics continue to warm up, the beam flux will decrease during the scan, which would result in a decrease in the fluorescence signal from the sample. However, this change can be normalized relative to the Channel 17 ion chamber signal. To do so, in PyAcq, use the equation (v)/(s1 + 1) and select Math Operation.

   WARNING: Do not change the mode to Continuous in the **Scan Coordinator** app while a scan is running. Doing so will compromise the current scan.

d. As the optics continue to warm up, the beam position will drift away from the aperture, resulting in a decrease in flux.
e. Wait for the current scan to complete and readjust the aperture position in **ImagingControls** to maximize counts in Channel 17.
f. Repeat the aperture adjustment as necessary for the remainder of the beamtime.

11.3 Micro Mode: Flux Recovery After a Beam Trip

Note: This section assumes that the user is familiar with the interfaces of relevant beamline control applications and the features of PyAcq. Refer to **Section: 2** of this user manual for a brief introduction to the different beamline control applications and **Section: 4** for a detailed description of PyAcq features.

After a beam trip and subsequent beam recovery, the beamline optics may still be cold. As the optics warm up, the beam position can gradually drift back toward its previous position. Therefore, the beam path may initially be slightly misaligned.

In Micro Mode, the beam passes through two sets of narrowly opened vertical and horizontal slits. If the beam position has shifted, the full beam flux will not pass through these slits, resulting in reduced flux at the sample. This will be observed as a lower count rate in Channel 18 on **Scan Coordinator** app, the ion chamber located immediately upstream of the sample.

The time required for the optics to warm up and for the beam flux to recover depends on how long the beam was absent due to beam trip. For example, a beam trip lasting approximately 30 minutes may require about an hour for the flux to recover to 70% of its pre-trip value. A beam trip lasting one hour or longer may require several hours for the flux to recover. After the beam has returned, follow these steps before resuming data acquisition:

1. Send the beam into the hutch by opening the safety shutter using **ImagingControls** app.
2. In the **Scan Coordinator** app, select Continuous Mode.
3. Monitor the counts in Channel 18.
4. Compare the current Channel 18 count rate with the count rate recorded before the beam trip.
5. Allow the beamline optics to warm up. The beam position and flux will gradually return toward their pre-trip condition.
6. Continue monitoring the Channel 18 counts as the beam recovers. Users can use the Channel 18 count rate and its recovery trend to determine when the beam has sufficiently flux for their experiment.
7. General recommendation is to not resume data acquisition until the Channel 18 flux has recovered to at least 70% of the pre-beam-trip value.
8. If you are at the end of your beamtime and want to scan your sample at low flux, you may proceed with the scan. The beam flux will increase during the scan, which would result

in an increase in the fluorescence signal from the sample. However, this change can be normalized relative to the Channel 18 ion chamber signal. In PyAcq, use the equation (v)/(s2 + 1) and select Math Operation.

WARNING: Do not change the mode to Continuous in the **Scan Coordinator** app while a scan is running. Doing so will compromise the scan.

12. BioXAS-Imaging Beamline Data Export Guide

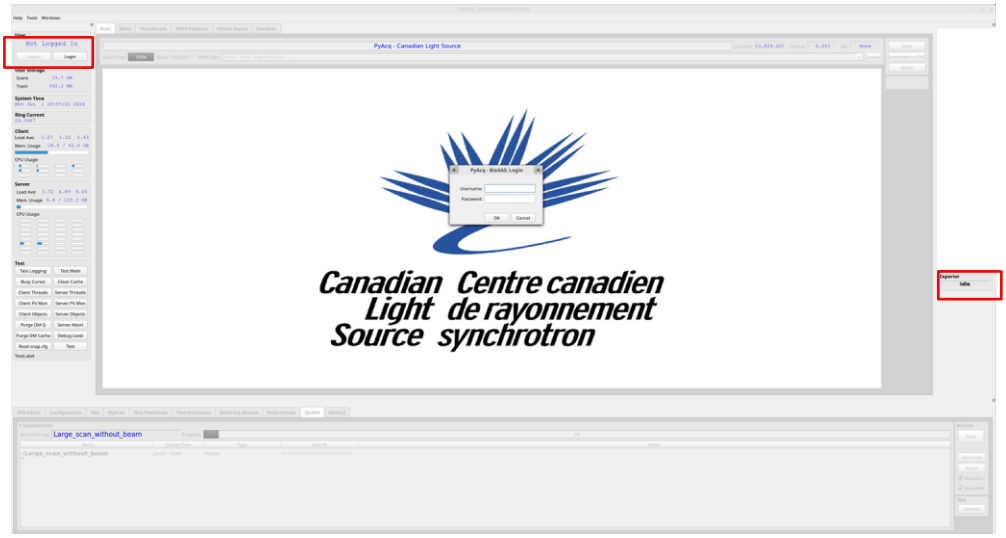
At the BioXAS-Imaging beamline, three types of data are collected:

1. 2D elemental distribution scans
2. XAS scans in transmission mode
3. XAS scans in fluorescence mode

If you are on-site, please ask the beamline staff for access to a designated computer. For remote access, separate instructions for connecting to the computer using NoMachine will be provided by the beamline staff.

Note: Please always coordinate with beamline staff before remotely connecting to any computer for data export.

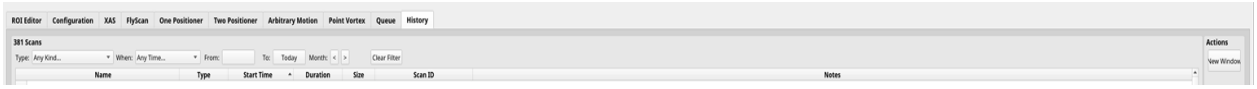
Once connected, the PyAcq client should be available on the connected computer. Click the **Login** button and enter your project name as the username (case-sensitive) and the password provided by the beamline staff.



This will open a PyAcq session displaying all previously recorded data associated with your project number from current and past beamtime sessions.

12.1 Exporting 2D Elemental Distribution Maps

The 2D scans are listed as **Flyscan** entries. In the **History** tab, select **Type: Flyscan** instead of **Type: Any Kind** to filter the list and display only 2D flyscans.

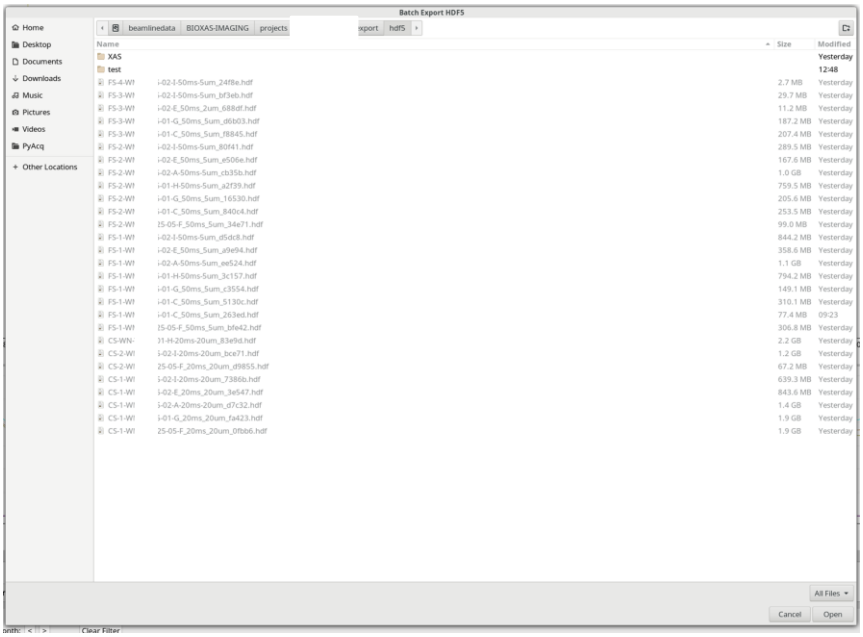


Select the scans you want to export. To select multiple scans, hold **Ctrl** and click each scan individually. Alternatively, click the first scan, hold **Shift**, and then click the last scan to select all scans in between.

Once the desired scans are selected, right-click and choose **Export HDF5**.



A new window will open, prompting you to confirm the location where the files should be exported. Export the files to the **hdf5** folder, or create a new subfolder within it if necessary.



Click **Open** to begin the export process.

The **Exporter** window will display the message **"Exporting..."**, indicating that the data export process has started. Once the export is complete, the status will change back to **"Idle"**.

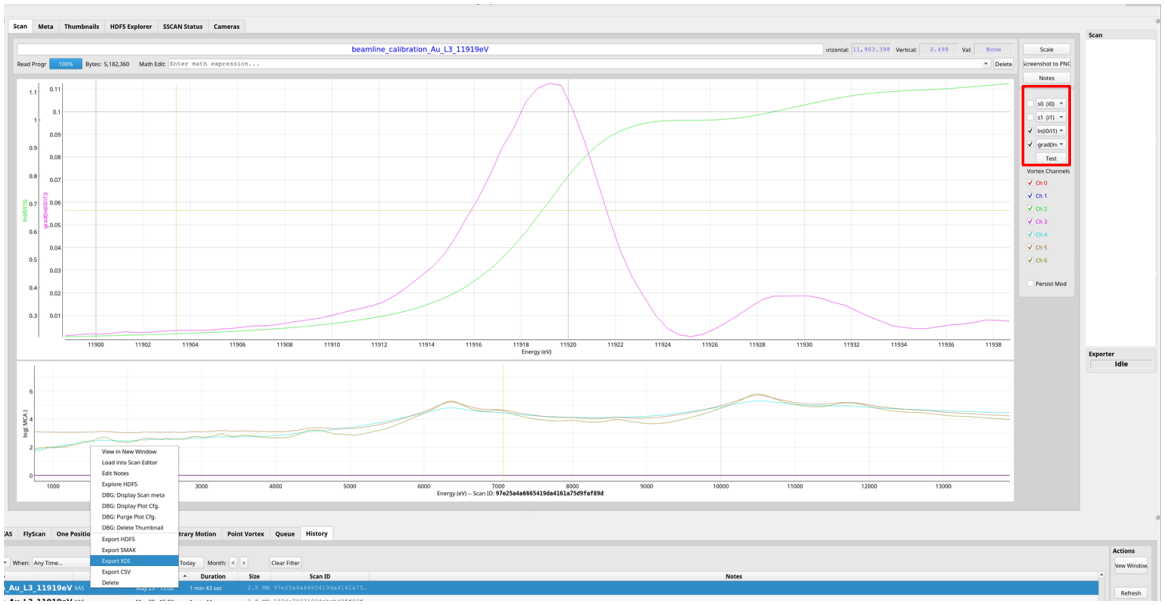


12.2 Exporting XAS Data Recorded in Transmission Mode

In the **History** tab, select **Type: XAS** instead of the default **Type: Any Kind** to filter the list and display only XAS data.

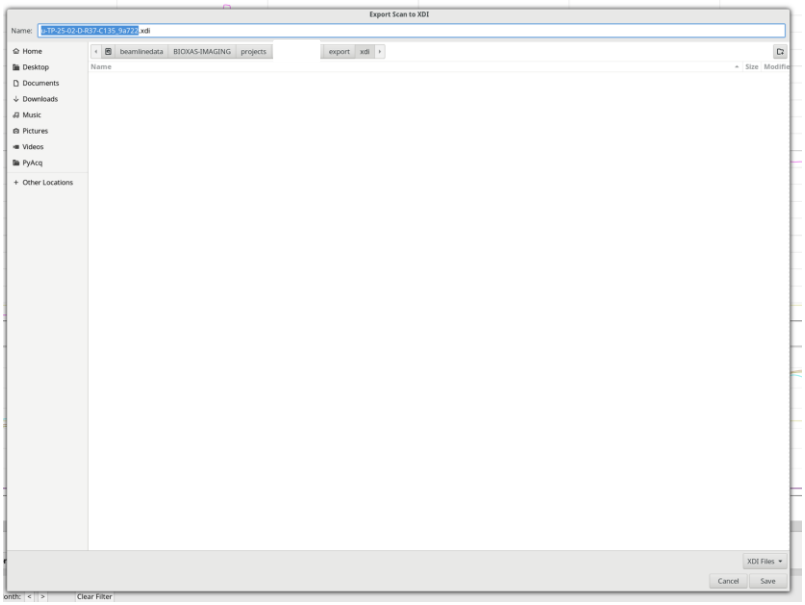


To obtain the correct view of your data, select the correct math operations, **ln(i0/i1)** and **grad(ln(i0/i1))**, in the corresponding tabs.
Note: The selection of a math operation has no effect on the exported data.



Right-click on the selected scan and choose **Export XDI** to export the XAS data. To export multiple scans, hold **Ctrl** and click each scan individually. Alternatively, click the first scan, hold **Shift**, and then click the last scan to select all scans in between. Once the desired scans are selected, right-click and choose **Export XDI** to export the XAS data.

A new window will pop up. Select the appropriate directory where you would like to export the data, and then proceed with the export.



The **Exporter** window will display the message **"Exporting..."**, indicating that the data export process has started. Once the export is complete, the status will return to **"Idle"**.

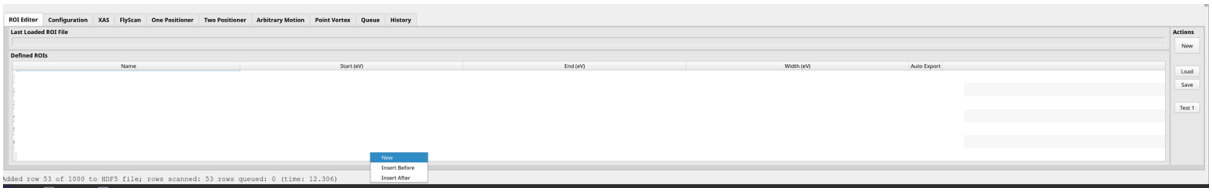


12.3 Exporting XAS Data Recorded in Fluorescence Mode

XAS data recorded in fluorescence mode requires an appropriate ROI (Region of Interest) to be selected on the fluorescence spectrum before the data can be exported.

It is important to use a consistent ROI across different datasets to maintain the integrity of comparative data analysis.

To configure an ROI, open the **ROI Editor** tab and right-click within the tab to create a new ROI.



Configure an ROI with an appropriate width based on the fluorescence peaks of interest and give it a name. The selected width should be chosen carefully to ensure accurate and consistent analysis. Multiple ROIs can be configured to target different elements of interest.

Select the appropriate XAS dataset from the **History** tab. In the corresponding fluorescence spectrum, right-click and place the ROI on the region of interest.

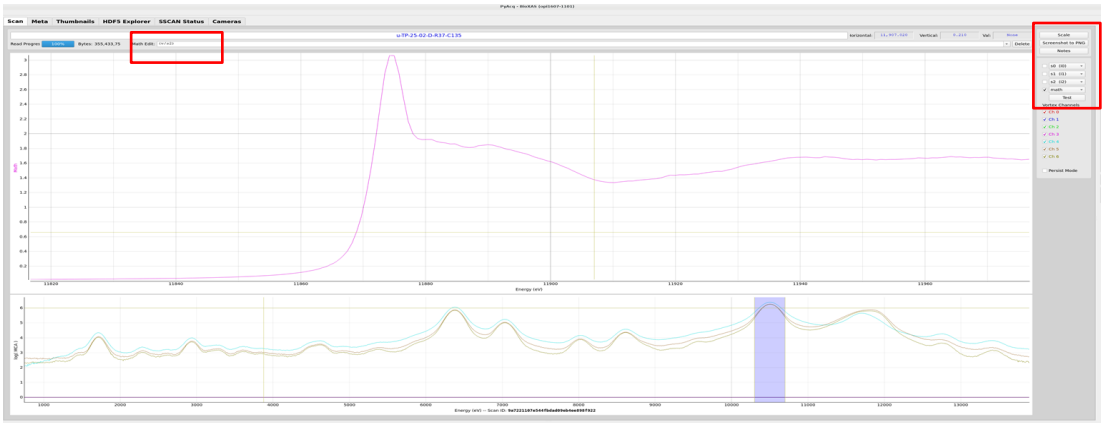


Once an ROI is placed, a shaded region will appear over the corresponding area of the spectrum, indicating the selected region of interest. Make sure the correct math operation is selected to obtain the appropriate view of the data. In addition, ensure that all **Vortex channels** are selected.

Note: The selection of a math operation and Vortex channels has no effect on the exported data. However, the correct choice of an ROI is important, so make your expert judgment on how wide your ROI has to be.

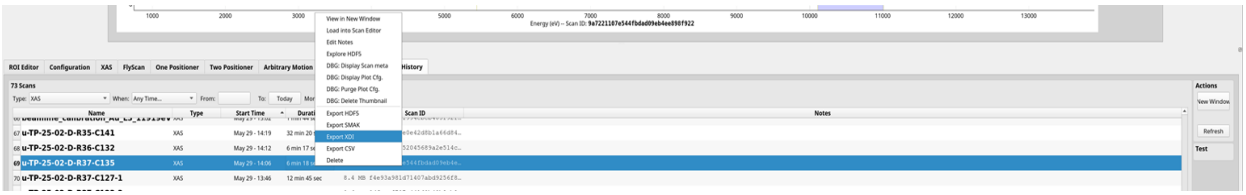
For **micro-mode**, common math options include: **(v/s2), (np.log(v/s2)), or (grad(v/s2))**

For **macro-mode**, common math options include: **(v/s1), (np.log(v/s1)), or (grad(v/s1))**

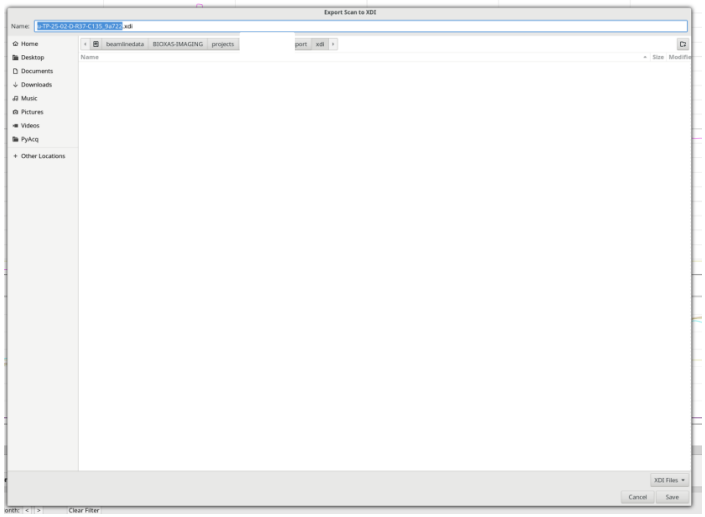


Once the appropriate ROI has been selected, right-click on the scan and choose **Export XDI** to export the XAS data. To export multiple scans, first ensure that an appropriate ROI has been applied to the fluorescence spectra. Then, hold **Ctrl** and click each scan individually to select multiple scans. Alternatively, click the first scan, hold **Shift**, and then click the last scan to select all scans in between.

Once the desired scans are selected, right-click and choose **Export XDI** to export the XAS data.



A new window will pop up. Select the appropriate directory where you would like to export the data and then proceed with the export.



The **Exporter** window will display the message **"Exporting..."**, indicating that the data export process has started. Once the export is complete, the status will return to **"Idle"**.

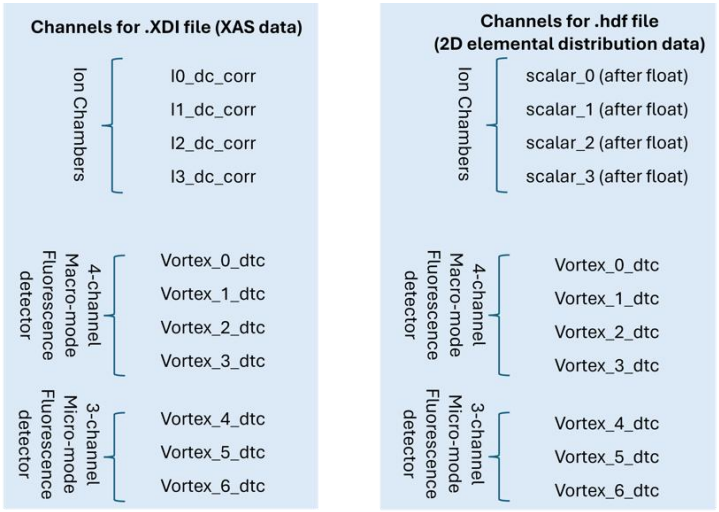


The exported data can then be downloaded to your local computer using the **Globus** platform. Separate instructions for using Globus and transferring data will be provided by the beamline staff.
The exported data then can be downloaded to your local computer using Globus platform. Separate instructions on this shall be provided by the beamline staff.

12.4 Important Information Regarding Exported Data format

The exported data contains multiple channels corresponding to different detectors. The data from all the channels shall be exported. Refer to the setup schematic in **Section - 1** to identify the detector positions and select the appropriate data channels for your analysis in Athena, Larch, PyMCA or any other software of your choice.

For macro-mode experiments, use I1_dc_corr/scalar_1 (after_float) for data normalization. For micro-mode experiments, use I2_dc_corr/scalar_2 (after_float). In both cases, the selected signal is from the ion chamber located immediately upstream of the sample.



dc_corr and **dtc** imply dark-current corrected and dead-time corrected, respectively

13. Remote Access to the BioXAS Beamline Computer

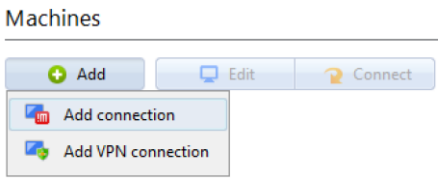
Remote access to the beamline computers is provided through the NoMachine server.

13.1 Install NoMachine Enterprise Client:

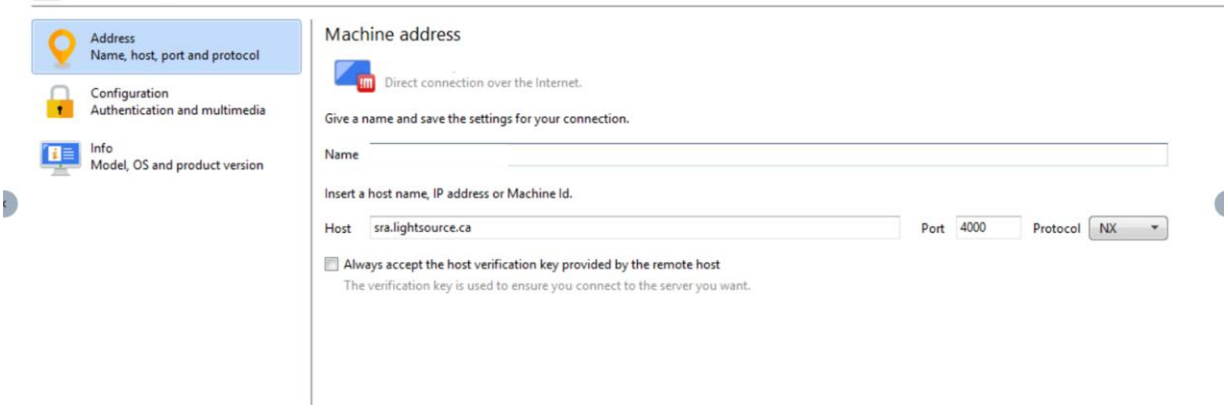
Download and install NoMachine client:

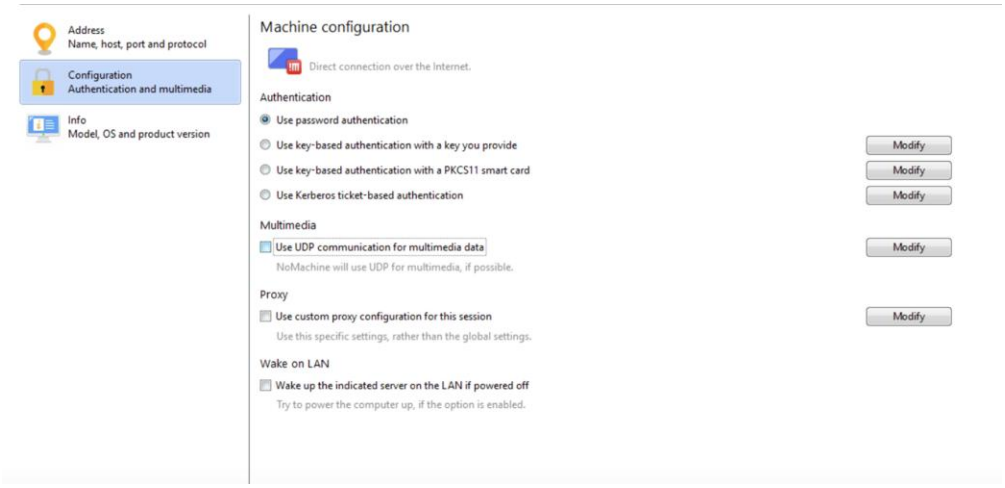
- On your PC, navigate to: https://download.nomachine.com/
- Follow the download instructions for the NoMachine Enterprise Client appropriate to your computer and operating system
- Install the Client onto your computer

13.2 Setup your connection:



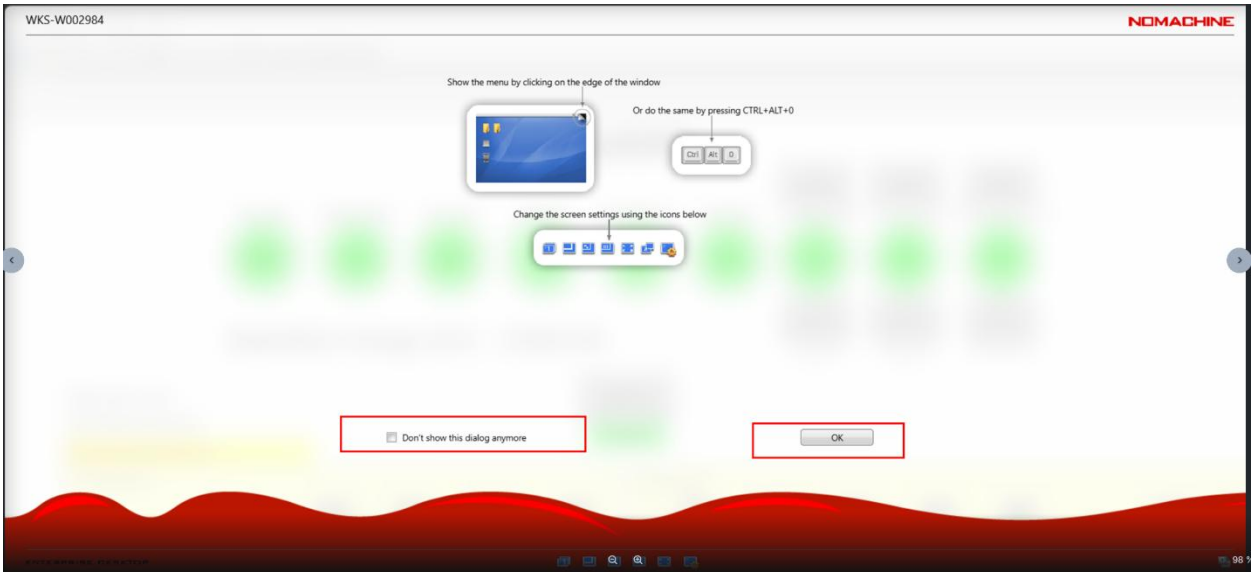
- Start NoMachine Enterprise Client
- Select Add under machines → Add connection
- Set connection settings:
  - **Name:** your choice
  - **Host Address:** sra.lightsource.ca
  - Port Number: 4000
  - Protocol: NX
- Accept the host verification key
- Un-check UDP.
- If prompted about proxy settings, choose **Don't use a proxy** (unless you are on a proxied network), Continue
- Click 'Add'.



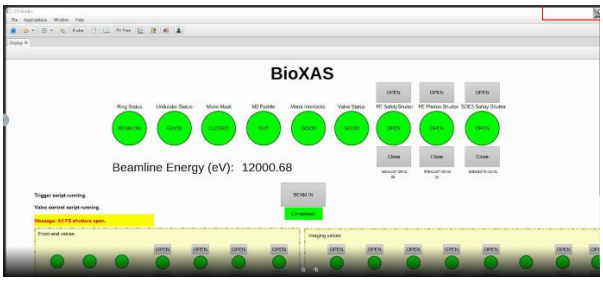


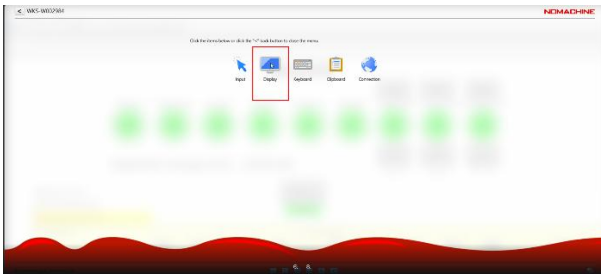
13.3 Log Into the Beamline Computer

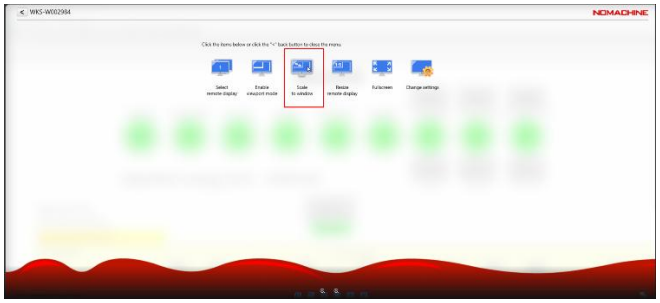
- Double-click the new connection to launch it.
- Ent**er Username and Password**
  - Enter the nm- username and password provided by your beamline staff.
- Accept the presented certificate fingerprint.
- Double-Click the new connection to launch it.
- Username/Password: The nm- user and password.
- Continue through the remaining prompts by selecting **OK** and **Do Not Show Again** where applicable. Leave all default settings unchanged.



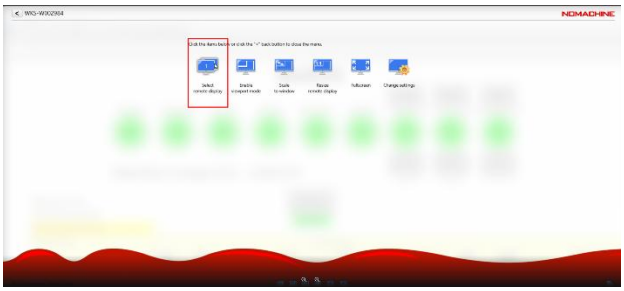
Follow the steps below to adjust the display scale to fit your computer screen:

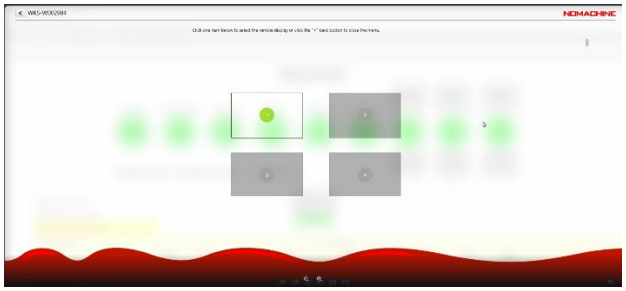






- Alternatively, use the shortcut **Ctrl + Alt + F** to go full screen. Or use a shortcut specific to your browser to activate full screen mode. For Microsoft edge, the full screen mode shortcut is the press of the single button F11.
- If the computer has multiple displays connected, follow the steps below to switch between the displays (or use the shortcut **Ctrl + Alt + 2** to go to the second display).



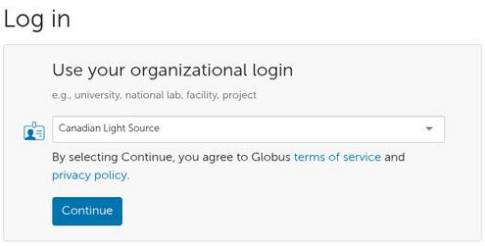


Precaution: Please avoid having multiple people remotely connected to the same computer at the same time. When two or more users attempt to control the mouse simultaneously, it can result in unintended clicks and selections. To prevent these issues, ensure that only one person has control of the computer at a time unless coordination between users is required and clearly established.

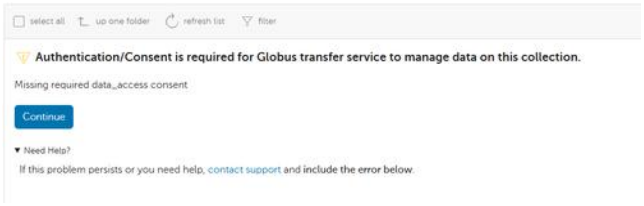
14. Access CLS Data on Globus

Globus delivers advanced file transfer and sharing capabilities to researchers no matter where their data live. Globus Connect Server makes it easy to add your lab cluster, campus research computing system, or other multiuser HPC facility to the Globus ecosystem. The CLS provides a Globus Connect Server endpoint that connects to our beamline data share, allowing users associated with scientific proposals access to their data.

14.1 Logging into Globus

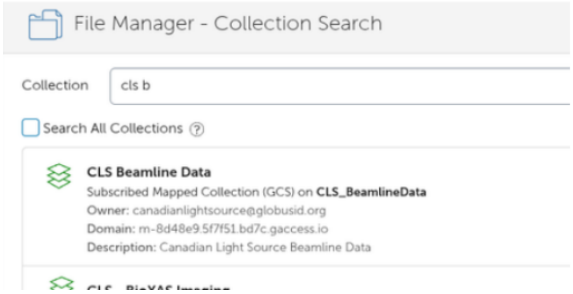


- Access **Globus at http://app.globus.org/.**
- Select the **Canadian Light Source** as your institution. Click **Continue**. You will receive the familiar CLS sign-in page.
- Enter your **CLS username and password**. Your first log-in will register you with Globus' systems, which is important if other users want to share with you.



- Authentication/Consent authorization may be required upon the first login. Click **Continue** to proceed.

14.2 File Manager | CLS Beamline Data



- Go to the **File Manager** view and select "SEARCH"
- Search for the "**CLS Beamline Data**" Collection - this is our CLS endpoint on Globus

14.3 Path to Project Data

- The **CLS Beamline Data** Collection will open with your CLS username as the Path and display any project folders you are involved in.
- You will see the project you are interested in transferring data from.

14.4 Set-up Personal Endpoint

- To transfer the data to your personal computer, institution workstation or computing system you must first setup a personal endpoint. Your institution/you may already have this configured. If not:
- Navigate to Globus Connect Personal at https://www.globus.org/globus-connect-personal
- Install the Globus Connect Personal for your operating system
- Launch Globus Connect Personal and 'Log In' to authenticate with Globus and begin the Collection Setup process.
- Enter Collection Details for your Personal Setup and 'Save'

14.5 Transfer Data from CLS to Your Endpoint

- Select the files you wish to transfer to your computer

An important note: Once you are on Globus, for a project number such as **prj123456**, and a username **user_abc,** download files from the following directories:

- **2D scan data:**
  /user_abc/prj123456/BIOXAS_IMAGING/export/hdf5/
- **XAS data:**
  /user_abc/prj123456/BIOXAS_IMAGING/export/xdi/

(**Note:** the "e" in **export** is lowercase.)

- Select the desired destination
- Click Start on CLS Beamline Data side.
- The two-pane view works well for this.

