

PROXIMA 2A Users Guide

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Please note: Recent modifications are marked in **MAGENTA**

PROXIMA 2A - Remote Access for Users

- Before the remote access session (>1 week):
 - Obtain your SUNSET project number and password (e.g. 20180123, wDvg2ke7Gt)
 - Ask the BL staff to contact the SOLEIL IT group to permit remote access for your project number
 - Test the connection to SOLEIL
 - Use a « decent » network connection (e.g. ADSL, not modem)
 - Download NoMachine
 - Screen resolution 2560 x 1440 (MXCuBE is optimised for this resolution)
 - Mouse with Left-Right buttons and a Scroll-wheel
- Start NoMachine
 - Check the connection parameters (Right-hand click & Edit Connection)
 - Name = PX2A (for example)
 - Protocol = NX
 - Host = nx-vip.synchrotron-soleil.fr
 - Port 4000
 - Open **Custom** session on **proxima2a-10**
 - **Custom** session on **proxima2a-10**
 - Independent display & mouse, which can run a separate instance of MXCuBE or X-terminal for processing
 - Open a terminal window from the side menu/icons
 - **gnome-terminal** & [launches gnome terminals]
 - **mxcube** [launches MXCuBE to control your experiment]
 - **albula** [to display diffraction images]
 - **firefox -P** & [to display webcams]
 - **ssh -X process1** [to process data on the 280-core server]

Starting MXCuBE



1

To start MXCuBE:

- 1) Either click on the MXCuBE icon,
- 2) Or open an X-terminal window (cntl-alt-t)
 - Type "mxcube"
- 3) Enter "proposal id", "password" and/or click "login"

- 4) If the message window "Couldn't contact ISPyB database..." appears,
 - click "OK"

Standard Collection Sample: 3:14

Acquisition

Oscillation start (°):	0	Range per frame (°):	0.1
Number of images:	3600	Total range (°):	360.0
First image:	1	Allowed range:	Full range
Exposure time (s):	0.0044	Detector mode:	9M
Kappa (°):	0	Phi (°):	0
Energy (keV):	11.568	MAD	<input type="checkbox"/>
Resolution (Å):	2.5	Detector distance (mm):	252.92
Transmission (%):	100	Flux (ph/s):	1.38e+12
<input checked="" type="checkbox"/> Shutterless		Estimated dose (MGy):	2.703

Data location

Folder: /nfs/data3/2020_Run5/com-proxima2a/2020-11-21/RAW_DATA

File name: prefix_1_#####.h5

Prefix: prefix

Run number: 1

Processing

N.o. residues: 200 Space group:

Unit cell:

a: b: c:

α: β: γ:

Energy Scan

XRF Spectrum

GPHL Workflows

Advanced

[2020-11-21 11:02:45] Data collection is enabled
[2020-11-21 11:03:43] Diffractometer: Current phase changed to Transfer

ISPyB proposal

Code: mx Password:

Sample tree

Mode:

Sample:

Centring: Double Click n-clicks: 3 step: 120.0

1 2 3

3:1

3:2

3:3

3:4

3:5

3:6

3:7

3:8

3:9

3:10

3:11

3:12

3:13

3:14

3:15

3:16

Puck 4

4:1

4:2

4:3

4:4

4:5

4:6

4:7

4:8

4:9

4:10

Collect Queue

FrontEnd Safety shutter

Machine current

450.8 mA

Machine state

Fri Nov 20 11:27
Shift: Lignes
filling: Hybrid
Dernière perte: Défaut
débitmètre TdL
Beam unstable

Hutch temperature 22.5 C

Flux 2.76e+11 ph/s

Beam size 0.010x0.005 mm

Cryostream In place
temperature: 100.0 K

Sample changer Dewar level in range
refill On

Storage disc space

Total: 1.6TB
Free: 1.4TB (89%)

State: - Diffractometer: Ready Sample changer: Ready Last collect: -

MXCUBE Overview

Description of frames:

- 1) Sample Microscope frame
- 2) Data Collection Methods frame
- 3) Sample Tree frame:
 - the highlighted line shows puck 3: pin 14 is mounted

Description of frames continued:

- 4) Beamline parameters, Machine current, CryoStream temperature, Energy, etc...
- 5) Log messages: please check here for RED error messages
- 6) State frame for diffractometer, sample changer, etc...

The screenshot shows the MXCUBE software interface with several key components highlighted by red boxes and numbered annotations:

- 1:** Sample Microscope frame showing a biological specimen.
- 2:** Data Collection Methods frame containing acquisition parameters such as Range per frame (0.1), Total range (360.0), Number of images (3600), Energy (11.568 keV), and Resolution (2.5 Å).
- 3:** Sample Tree frame showing a list of pucks, with puck 3:14 highlighted.
- 4:** Beamline parameters and Machine current frame, displaying a machine current of 450.8 mA and various operational settings.
- 5:** Log messages frame showing a message: "[2020-11-21 11:03:43] Diffractometer: Current phase changed to Transfer".
- 6:** State frame for diffractometer and sample changer, showing "State: - Diffractometer: Ready Sample changer: Ready Last collect: -".

ALBULA

The screenshot shows the ALBULA software interface. The main window displays a diffraction pattern with resolution rings labeled 1.7Å, 2.3Å, and 4.5Å. The interface includes a menu bar (File, Synchronize, Auto Load, Help), a toolbar (New Window, Open, Save As, Export), and a right-hand control panel with various settings and statistics. Red arrows point to the menu bar (4), the resolution rings (2), and the DECTRIS logo (3).

- 1) Open an X-terminal widow and type:
albula or **albula_3.2**
- 2) To set Automatic Loading of images
 - Click on “AutoLoad” then “EIGER Monitor”
 - The latest image will be displayed every second
 - Resolution rings are not possible in this mode
- 3) To change contrast, colour scheme, etc...
 - Click on “Tools” (top right corner)
- 4) To open an HDF5 image file
 - Click “File” then “Open”
 - Select a “master.h5” file
- 5) To zoom in/out
 - Use the mouse scroll wheel

BeamCheck

BeamCheck should be done:

- At the start of each session
- Repeated every few hours
- After large changes in energy
- Potentially for very small or thin crystals

- 1) Open the “Front End” and “Safety Shutter”
- 2) Set the Transmission to **100%**
- 3) Set the Energy (default 12.65 keV)
- 4) Click on “BeamCheck”
 - Wait several seconds for the scintillator to be put in place (10 s)
 - A blue beam spot will flash up in the sample display
- 5) The shift in position is displayed in the log frame

The screenshot displays the ISPyB control interface. The main window shows a sample centring view with a blue beam spot. The interface is divided into several panels:

- Sample centring:** Shows a sample display with a blue beam spot. A red arrow labeled '4' points to the 'Beam check' button in the bottom toolbar.
- Standard Collection:** Contains acquisition parameters such as Oscillation start, Number of images, Exposure time, Energy, Resolution, and Transmission. A red arrow labeled '2' points to the 'Transmission (%)' field, which is set to 100%.
- ISPyB proposal:** Shows the sample tree and filter settings. A red arrow labeled '1' points to the 'FrontEnd open' and 'Safety shutter open' buttons.
- Processing:** Contains options for N.o. residues, Unit cell, and Run processing after collection. A red arrow labeled '3' points to the 'Run processing after collection' checkbox.
- Log:** A log window at the bottom right shows the sequence of events during the BeamCheck process. A red arrow labeled '5' points to the log entries, which include messages like 'Moving scintillator to sample position, please wait...', 'Initial mirror positions (vfm, hfm) [mrad]: 3.9061-4.7577', 'Initial pixel shift from center (vertical, horizontal): 3.0, 4.9', 'Beam position adjustment finished after 4 iterations', 'Final mirror positions (vfm, hfm) [mrad]: 3.9062-4.7578', 'Final pixel shift from center (vertical, horizontal): -0.1, 1.8', and 'Delta in motor positions [mrad]: 0.0001, -0.0001'. A red arrow labeled '1' also points to the 'Collect Now' button.

At the bottom of the interface, the status bar shows: State: Setting energy... Diffractometer: Ready Sample changer: Ready Last collect: -

Sample Changer

- 1) Click on “Show/Hide SC-details”, then on “Sample changer” tab
- 2) Click “Power On/Off” to switch ON/OFF the Robot Arm Power
- 3) Click on OPEN/CLOSE lids
 - If LID 2 does not open, check that Robot Arm Power is ON
- 4) Click “Dry” to dry the Cryotongs
 - This should be done every 8-16 mounts

- 5) Status of the pucks and pins are displayed in the
 - Sample Tree – highlighted in GREY
 - Sample changer Contents – T-shaped icon
- 6) Two ways to load/unload pins
 - Sample Tree: Right-Click to MOUNT/UNMOUNT
 - Sample changer-Contents: Click LOAD/UNLOAD

The screenshot displays the 'Sample changer' control interface. Red arrows and numbers 1 through 6 indicate the following controls:

- 1:** Points to the 'Sample changer' tab at the top left.
- 2:** Points to the 'Power On' and 'Power Off' buttons under 'Arm Power'.
- 3:** Points to the 'Open' buttons for Lid 1, Lid 2, and Lid 3.
- 4:** Points to the 'Dry' button in the 'Commands' section.
- 5:** Points to the 'Sample Tree' on the right side of the interface.
- 6:** Points to the 'Load' and 'Unload' buttons in the 'Contents' section.

The interface includes various sections: 'State' (Ready), 'Contents' (Load/Unload/Abort), 'Arm Power' (Power On/Off), 'LN2 Regulation' (Regulation On), 'Lid 1/2/3' (Open/Close), 'Barcode' (Barcode field, Read Barcode during trajectory checkbox), 'Commands' (Safe, Dry, Home, Recover buttons), 'CATS message' (Reset put/get, Reset Motion, Clear, Abort), 'Standard Collection' (Acquisition parameters like Oscillation start, Number of images, Exposure time, Kappa, Energy, Resolution, Transmission, Shutterless, Data location, Processing), 'Sample tree' (Puck 1-9, Pin 1-28), 'FrontEnd' (Open/Close, Safety shutter), 'Machine current' (500.5 mA), 'Resolution' (2.108 Å, 342.53 mm), 'Transmission' (Current, Set to), 'Energy' (18.0001 keV, 0.689 Å), and 'Machine state' (Thu Nov 15 20:14, Shift Lines, Filling: 4/A, Beam usable, Hutch temperature: 21.4 C, Flux, Remeasure flux!, Cryostream, In place, temperature: 100.0 K, Sample changer, Dewar level in range, refill On, Storage disc space).

At the bottom left, the status bar reads: - State: - Diffractometer: - Sample changer: - Last collect: -

Sample Centering

- 1) Check "Centring mode" = "3-Click"
- 2) Click "Auto" to centre the loop
- 3) Click "Centre" to launch 3-click centring
 - Click on the crystal at 3 omega angles
- 4) Change the zoom accordingly
- 5) Click "Save" to record a centred position

Other functionalities:

- 6) Adjust the front and back-lighting if necessary
- 7) Double-click anywhere to translate to that position
- 8) Double-click on a YELLOW centred position to move directly to it
- 9) A green saved position is "activated" and recorded for the data collection

The screenshot displays the software interface for sample centering. The main window shows a diffraction image of a sample with a yellow crosshair indicating the current position. Red arrows point to various UI elements corresponding to the numbered instructions:

- 1:** Points to the "Centring" dropdown menu in the "ISPyB proposal" panel, which is set to "Manual 3-click".
- 2:** Points to the "Auto" button in the bottom toolbar.
- 3:** Points to the "Centre" button in the bottom toolbar.
- 4:** Points to the "Zoom" dropdown menu in the bottom toolbar.
- 5:** Points to the "Save" button in the bottom toolbar.
- 6:** Points to the "Front" and "Back" lighting controls in the bottom toolbar.
- 7:** Points to a double-click on the diffraction image to translate to that position.
- 8:** Points to a double-click on a yellow centred position in the diffraction image to move directly to it.
- 9:** Points to a green saved position in the diffraction image, which is "activated" and recorded for data collection.

The interface includes several panels:

- Top Left:** "Collect" and "Log" buttons.
- Top Center:** "Sample centring" header and various control buttons (ur, x, qp, focus).
- Top Right:** "Sample: MA-ma_83117", "Standard Collection", and "ISPyB proposal" information.
- Middle Left:** "Acquisition" and "Data location" settings.
- Middle Right:** "Characterisation" and "Crystal" settings.
- Bottom Left:** "FrontEnd" and "Safety shutter" controls.
- Bottom Center:** "Resolution", "Transmission", and "Energy" settings.
- Bottom Right:** "Machine current" and "Machine state" information.

The status bar at the bottom indicates: "mx20170705@PROXIMA2A State: Setting energy... Diffractometer: Ready Sample changer: Disabled Last collect:-"

Characterisation

- 1) Click CHARACTERISATION
- 2) Click on a saved position
- 3) Enter directory & prefix
 - **NO blanks or special characters!**

- 4) Set parameters: default values [range] :
 - a) Number of wedges = 4 [1-4]
 - b) Oscillation range per frame = 0.1°
 - c) Number of images per wedge = 10 [1 – 14400]
 - d) Exposure time per image = **0.044 s** [>0.0043 s]
 - e) Energy (keV) = 12.650 keV [6 – 18 keV]
 - f) Resolution (Å) = depends upon energy & distance
 - Distance = [120 – 1000 mm]
 - g) Transmission = **100%** [default, 0.1 - 100%]

- 5) Click “Collect Now”, or
 - a) “Add to Queue”, if you wish to add another data collection
 - b) “Collect Queue” to launch all data collections

Standard Data Collections

Standard Collection

Phycocyanin_P1p07_Pt-rm1_1 (Point not defined)

Standard Collection

Acquisition

Oscillation start: 270 Osc. range per frame: 0.1

Number of images: 1800 Total osc. range: 180.0

First image: 1 Full range

Exposure time (s): 0.025 Detector mode: 0

Kappa: 0 Phi: 0

Energy (keV): 11.604 MAD rm1: 11.6

Resolution (Å): 2.717

Transmission (%): 10

Shutterless

Data location

Folder: /nfs/data2/2018_Run5/2018-11-07/local-user/RAW_DATA

/phycocyanin-Pt

File name: Phycocyanin_P1p07_Pt-rm1_1_#####.h5 Browse

Prefix Phycocyanin_P1p07_Pt

Characterisation

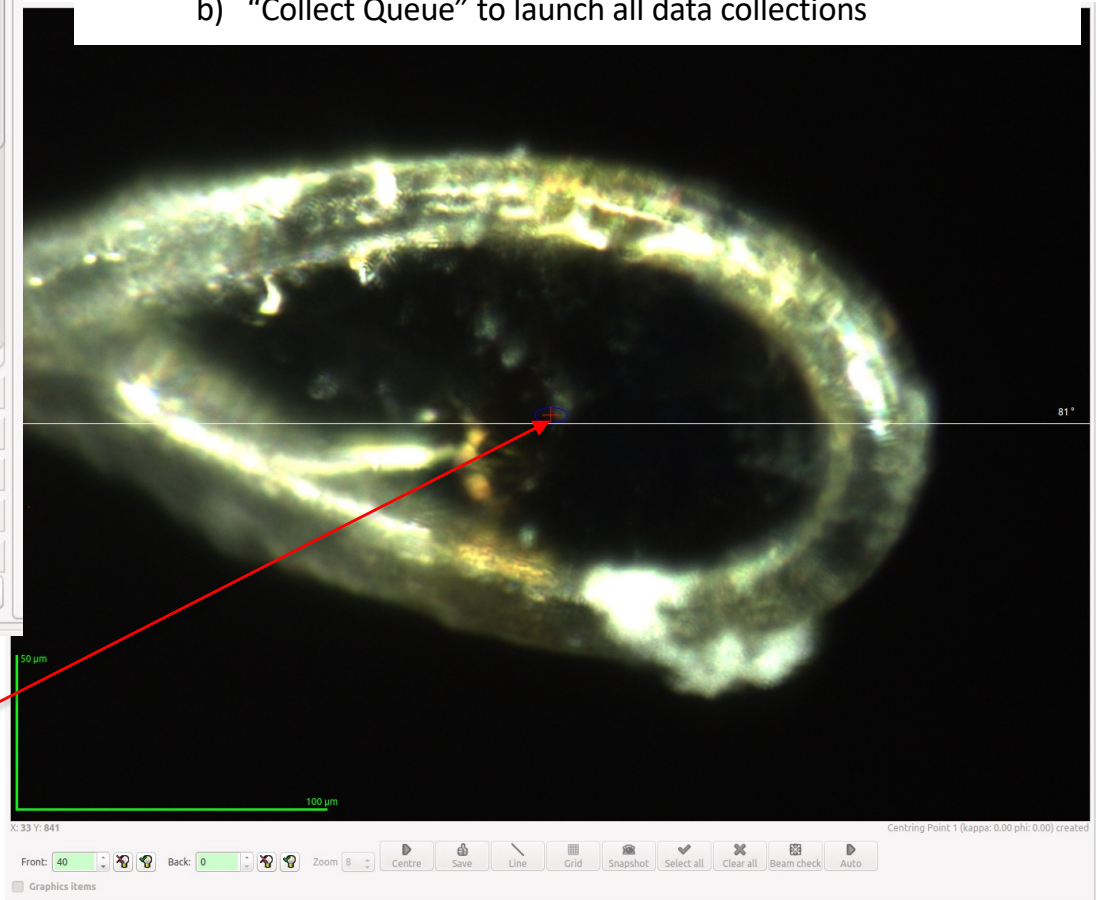
Helical Collection

Energy Scan

XRF Spectrum

Advanced

- 1) Click STANDARD COLLECTION
- 2) Click on a SAVED centred position
- 3) Check & set all parameters, typical values [range in brackets] are:
 - a) Oscillation range per frame = 0.1° [0.01 - 720°]
 - b) Number of images = 3600 [1 - 14400]
 - c) Exposure time = **0.044 s** [default, range: >0.0043 s]
 - d) Energy (keV) = 12.650 keV [6 - 18 keV]
 - e) Resolution (Å) = depends upon energy & distance
 - Distance = [110 - 1000 mm]
 - f) Transmission = **100%** [default, range: 0.1 - 100%]
- 4) Enter directory & prefix
 - NO blanks or special characters!
- 5) Click “Collect Now”, or
 - a) “Add to Queue”, if you wish to add another data collection
 - b) “Collect Queue” to launch all data collections



Helical Data Collections

- 1) Click HELICAL COLLECTION
- 2) Centre and SAVE TWO positions
- 3) Click on one SAVED position
- 4) CNTL-click on a second SAVED position
 - a) This will create a GREEN line
- 5) Check & set all parameters as for Standard Collections
 - a) Transmission = **100%** [default]
- 6) Enter directory & prefix
- 7) Click "Collect Now"

The screenshot displays the software interface for helical data collection. The left panel shows a microscope image of a specimen with a green line connecting two points, labeled 2, 3, 4, and 4a. The right panel shows the 'Standard Collection' configuration window with various parameters and buttons, labeled 1, 5, 5a, 6, and 7. The bottom panel shows a status bar and a log window.

Standard Collection Configuration:

- Sample: 1:2
- Characterisation: Helical Collection (1)
- Line:

Name	Start point	End point
Line 2	2	4
Line 3	4	5
- Acquisition:
 - Oscillation start: 0.02, Osc. range per frame: 0.1
 - Number of images: 1800, Total osc. range: 180.0
 - First image: 1, Full range: [checkbox]
 - Exposure time (s): 0.025, Detector mode: 0
 - Kappa: 0.0023, Phi: 0.0042
 - Energy (keV): 12.6681, MAD: [checkbox]
 - Resolution (Å): 2.5, Ip: [dropdown]
- Transmission (%): None (5a)
- Shutterless: [checked]
- Data location:
 - Folder: /ifs/data2/2018_Run5/2018-11-12/local-user/RAW_DATA
 - File name: local-user_1_#####.h5 (6)
 - Prefix: local-user (6)
 - Run number: 1
 - Compress data: [checked]
- Processing:
 - N.o. residues: 200, Space group: [dropdown]
 - Unit cell: [input]
- Energy Scan: [checkbox]
- XRF Spectrum: [checkbox]
- Advanced: Collect Now (7)

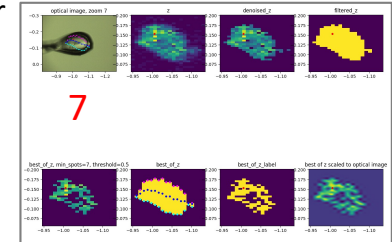
Log Window:

```
sample_info None [2018-11-12 10:08:51] start_centring_method 2018-11-12 10:08:51, method Manual 3-click, sample_info None [2018-11-12 10:09:17] start_centring_method 2018-11-12 10:09:17, method Computer automatic, sample_info None [2018-11-12 10:10:21] start_centring_method 2018-11-12 10:10:21, method Manual 3-click, sample_info None [2018-11-12 10:10:59] MicrodifMotor stop [2018-11-12 10:11:02] MicrodifMotor stop [2018-11-12 10:11:06] MicrodifMotor stop [2018-11-12 10:11:12] MicrodifMotor stop [2018-11-12 10:14:54] start_centring_method 2018-11-12 10:14:54, method Manual 3-click, sample_info None
```

Grid & Mesh Scans

- 1) Click ADVANCED
- 2) Click "Grid"
- 3) Click-drag the mouse from the Top-Left down to Bottom-Right to select an area to scan

- 4) Check & set all parameters as for Standard Collections
 - Verify the starting angle
 - Exposure time > 0.010 s [recommended]
- 5) Enter directory & prefix
- 6) Click "Collect Now" & wait for the scan to finish
- 7) The calculation may take a few minutes:
 - A results window will appear
- 8) Results can be recalculated:
 - raster_scan_analysis.py -h



State: - Diffractometer: Ready Sample changer: - Last collect: -

Processing Data

- Open an X-terminal window on proxima2a-10 or SRV4 terminal
 - Note: the cluster process1 is not available on the machines proxima2a-6 and proxima2a-7
- Log on to the calculation cluster by typing:
 - `ssh -X process1`
- Go to current directory where data were collected by typing:
 - `goimg`
- Launch XDS on the current or most recent collected data with:
 - `goxdsme`
- Launch XDS on older data from the process directory with:
 - `xdsme [options] ../my_crystal_1_master.h5`
 - `-h` [help shows all options]
 - `-a` [anomalous]
 - `-s P21` [spacegroup name or number]
 - `-c "43 55 289 90 90 90"` [unit cell in quotes]
 - `--brute` [for difficult indexing cases]
 - `--weak` [for cases with weak diffraction]
 - `-r 1.2` [sets the high resolution limit]
 - `-3` [relaunch from IDXREF step]
 - `-5` [relaunch from CORRECT step]

X-ray Fluorescence Spectra

- 1) Set Energy to 15 keV
- 2) Set Transmission to 1%
- 3) Click on "XRF" tab to specify folder & prefix
- 4) Set count time to 10 s
- 5) Click "Collect Now"
- 6) The display of X-ray Fluorescence spectra
- 7) Click "Fit Again" to automatically fit of common elements
- 8) Click "Configure" and "Peaks" tab to change the selected elements
- 9) Click "Fit Again" to refit the spectrum
- 10) Click "Peaks Spectrum"???

The screenshot displays the MXCuBE software interface for X-ray Fluorescence (XRF) data collection and analysis. The interface is divided into several sections:

- Data location:** Shows the folder path `/nfs/data2/2018_Run5/2018-11-16/local-user/RAW_DATA` and the file name `x2_1_#####.raw`.
- Parameters:** Includes fields for **Count time (s):** 10.0 and **Excitation energy (keV):** 15.0. A **Collect Now** button is visible at the bottom of this section.
- GRAPH:** Displays the XRF spectrum with **Counts** on the y-axis (0 to 500) and **Energy** on the x-axis (0 to 14). A prominent peak is labeled **K_LBM2**. A **Fit Again!** button is located below the graph.
- Sample tree:** A hierarchical view on the right showing the current sample configuration, including **Characterisation - 1** and **XRF spectrum - 1**.
- Machine status:** A panel on the bottom right showing **Machine current: 500.2 mA** and other operational parameters.

Red arrows and numbers (1-10) indicate the steps for setting up and analyzing the XRF spectrum:

- 1) Set Energy to 15 keV
- 2) Set Transmission to 1%
- 3) Click on "XRF" tab to specify folder & prefix
- 4) Set count time to 10 s
- 5) Click "Collect Now"
- 6) The display of X-ray Fluorescence spectra
- 7) Click "Fit Again" to automatically fit of common elements
- 8) Click "Configure" and "Peaks" tab to change the selected elements
- 9) Click "Fit Again" to refit the spectrum
- 10) Click "Peaks Spectrum"???

Energy Scans

- 1) Set Transmission to 1%
- 2) Click on Energy Scan
- 3) Select an element
- 4) Specify the folder & prefix
- 5) Click "Collect Now"

- 6) The Energy scan will plot the XANES spectra in real-time
- 7) CHOOCH will be displayed automatically
 - The pk, ip and rm energies will be updated in the Standard Collection tab in the MAD menu
- 8) If the Energy scan or CHOOCH fail, click STOP
- 9) If the Energy scan was completed, then in a terminal window type (the option `-e` specifies the element):
`chooch -e Se MyEScan.raw`

The screenshot displays the ISPyB control interface with several key components:

- Top Left:** "Sample centring" and "Energy scan" tabs. A periodic table highlights Selenium (Se) as the selected element.
- Top Right:** "Snapshot" window showing a real-time image of the sample.
- Middle Left:** "Element: Se Edge: K" plot showing the XANES spectrum with counts on the y-axis and energy on the x-axis.
- Bottom Left:** A large empty plot area labeled "7".
- Center:** Configuration panel for "x2 - 2 (Se K, Point - not defined)". It includes fields for "Folder" and "File name", and a "Collect Now" button.
- Right Panel:** "ISPyB proposal" section with a "Sample tree" showing the scan configuration and a "Stop" button.
- Bottom Right:** Machine status panel showing "FrontEnd open", "Safety shutter open", and "Machine current 500.8 mA".
- Terminal:** A log window at the bottom showing the execution of the energy scan and CHOOCH commands.

Red arrows indicate the following steps:

- 2: Arrow pointing to the "Energy Scan" button in the top center.
- 3: Arrow pointing to the Selenium (Se) element in the periodic table.
- 4: Arrows pointing to the "Folder" and "File name" input fields.
- 5: Arrow pointing to the "Collect Now" button.
- 6: Arrow pointing to the "Element: Se Edge: K" plot.
- 7: Arrow pointing to the large empty plot area.
- 8: Arrow pointing to the "Stop" button in the right panel.

Terminal Log:

```
[2018-11-16 16:58:20] Energy scan started. (['title': 'Element: Se Edge: K', 'scaletype': 'normal', 'xlabel': 'energy', 'ylabel': 'counts'],)
[2018-11-16 16:58:24] get_edge_energy in energy_scan.py K
[2018-11-16 16:58:24] optimizing transmission at 12.698 keV
[2018-11-16 16:58:33] current_transmission 0.500
[2018-11-16 16:58:37] Transmission optimized after 2 steps to 0.125
[2018-11-16 16:58:37] get_edge_energy in energy_scan.py K
[2018-11-16 17:00:45] parse_chooch_output
```

Status Bar: State: Queue started Diffractionmeter: Ready Sample changer: Ready Last collect: Sample centering : Successful (2018-11-16 16:58:20)

MAD Data Collections

Phycocyanin_P1p07_Pt-rm1_1 (Point not defined)

Standard Collection

1 Acquisition

Oscillation start: 270 Osc. range per frame: 0.1

Number of images: 1800 Total osc. range: 180.0

First image: 1 Full range

Exposure time (s): 0.025 Detector mode: 0

Kappa: 0 Phi: 0

Energy (keV): 11.604 MAD 3 rm1: 11.61 4,6,8

Resolution (Å): 2.717

Transmission (%): 10

Shutterless

Data location

Folder: /nfs/data2/2018_Run5/2018-11-07/local-user/RAW_DATA

/phycocyanin-Pt

File name: Phycocyanin_P1p07_Pt-rm1_1_#####.h5 Browse

Prefix: Phycocyanin_P1p07_Pt

Characterisation

Helical Collection

Energy Scan

XRF Spectrum

Advanced

5,7,9

- 1) Click on Standard Collection
- 2) Enter directory and prefix
- 3) Click the "MAD" radio button
- 4) Select an Energy (e.g. rm1, 11.609 keV)
- 5) Click "Add to Queue"
- 6) Select second Energy (e.g. pk)
- 7) Click "Add to Queue"
- 8) Select a third Energy (e.g. ip)
- 9) Click "Add to Queue"
- 10) Each data collection will appear in the Queue
- 11) Click the "Collect Now/Stop" button

Collect Log

Sample tree

Mode: Sample changer Show SC-details

Sample: ISPyB

Centring: Manual 3-click

Filter: No filter

1:4

1:5

1:6

1:7

Energy scan - 1

escan - 1 (Pt L... Done

Standard - 1

Manual centri...

Phycocyanin... Collection done 10

Phycocyanin... Collecting

Phycocyanin...

1:8

1:9

1:10

Queue history

11

Collection 94%

Manual Raster/Grid Scans

For those unafraid of keyboards, raster/grid scans can be done via command line on p10:

```
raster_scan.py
-d /data2/2018_Run5/2018-11-25/local-user/RAW_DATA/crystal1/raster1 [directory]
-n prefix_1 [prefix NAME]
-x 0.1 [Horizontal scan width in mm]
-y 0.1 [Vertical scan height in mm]
-c 50 [number of COLUMNS, 500 * x = 2 µm steps]
-r 50 [number of ROWS, 500 * y = 2 µm steps]
-a 123.25 [start ANGLE in degrees]
-A [ANALYSE]
```

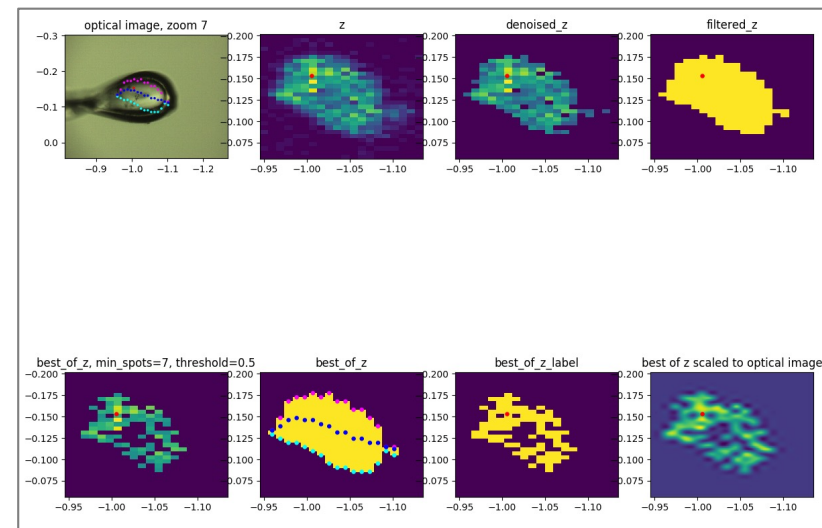
A Figure_1 window will open and display :

For more information, type:

```
raster_scan.py -h
```

or

```
raster_scan_analyse.py -h
```



Manual Area Scans

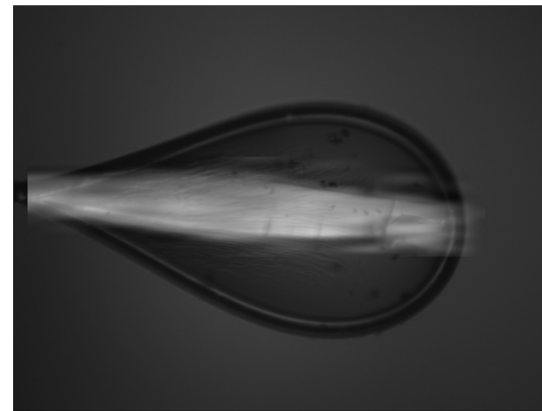
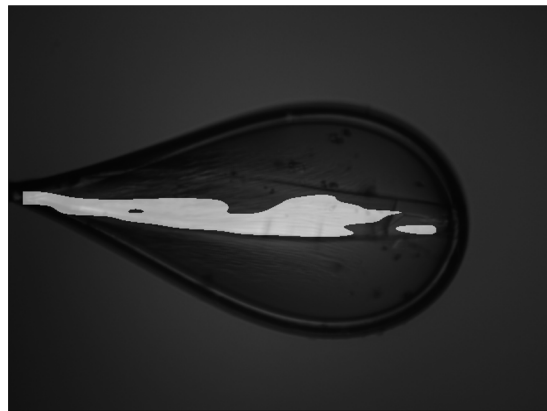
The older version of raster/grid scans can be done via command line on p10:

```
area_scan.py
-d /data2/2018_Run5/2018-11-25/local-user/RAW_DATA/crystal1/raster1 [directory]
-n prefix_1 [prefix NAME, default = « grid_ »]
-x 0.1 [Horizontal scan width in mm]
-y 0.1 [Vertical scan height in mm]
-c 50 [number of COLUMNS, 500 * x = 2 µm steps]
-r 50 [number of ROWS, 500 * y = 2 µm steps]
-p 331.25 [start ANGLE in degrees]
```

A window will open and display :

For more information, type:

```
area_scan.py -h
```



X-ray Centering (excenter)

X-ray centering can be accomplished via command line on p10:

```
excenter.py  
-d /data2/2018_Run5/2018-11-25/local-user/RAW_DATA/crystal1/raster1 [directory]  
-n prefix_1 [prefix NAME, default = « excenter_ »]  
-l 0.1 [scan LENGTH in mm]  
-a '(60,150,240,330)' [scan ANGLES in degrees in 'tuple' format]
```

The goniometer should automatically move the calculated center position. Then click **SAVE** in MXCuBE.

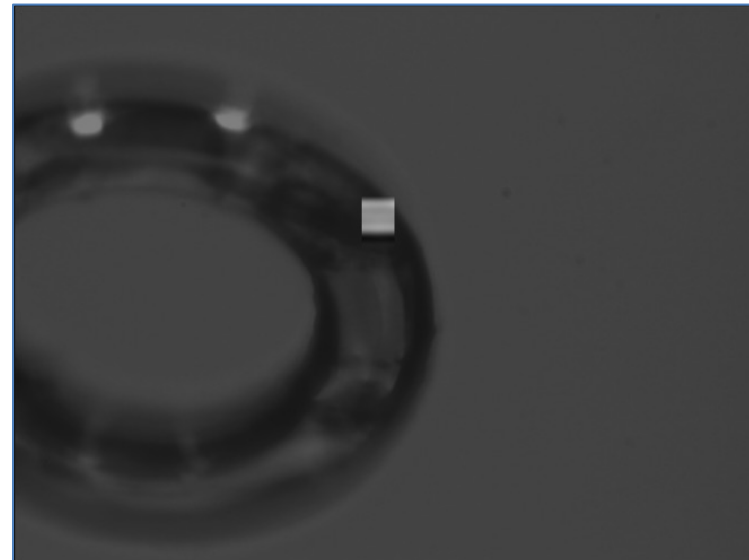
A window for each angle will open and display (note that the windows may display behind other windows) :

To only interpret images already collected:

```
excenter.py -i
```

For more information, type:

```
excenter.py -h
```



Sample Changer – « Error messages »

MXCuBE will display error messages returned by the CATS robot in the Sample Changer tab:

- CATS message window : **incoherent diffracto detection**. This means that the goniometer and the robot disagree whether a sample is mounted or not...
 - Check the CATS robot arm position
 - SOAK? – Then **ABORT, CLEAR**
 - OTHER? – Then contact the BL staff ASAP!
 - Check if the sample is in the CryoTongs
 - **ABORT, CLEAR, HOME, DRY**
 - Is a sample mounted on the MD2?
 - YES? – Then the previous sample was manually mounted, remove it manually and try again.
 - NO? – Then the CATS failed to pick up the SPINE pin (similar to the **Missing Sample** condition)
 - Try to **MOUNT** or **LOAD** again
 - If it fails again,
 - Check that the sample is really present via webcam “CAM8”
 - Click **DRY** to dry the cryotongs (3 min), and then **MOUNT** again
 - If it fails a third time,
 - Move the puck to another position in the CATS Dewar
- CATS message window: **WAIT for TrfGtd condition**:
 - The robot is waiting for the “transfer granted condition” to be given by the MD2
 - Check if the MD2 really is in Transfer Phase
 - Select **TRANSFER** in the Phase menu
 - **ABORT**
 - Try to **MOUNT** again

Sample Changer – Missing Samples, Collisions, Arm Power, etc...

If the robot fails to mount a sample pin:

- This is known as a **MISSING SAMPLE** or **INCOHERENT DIFFRACTO** condition
- Try to **MOUNT** or **LOAD** again
- If it fails again,
 - Check that the sample is really present via webcam “CAM8”
 - Click **DRY** to dry the cryotongs (3 min), and then **MOUNT** again
- If it fails a third time,
 - Move the puck to another position

There are two types **ROBOT COLLISIONS** (usually in the Dewar):

- **SOFT** collisions
 - Symptom: the robot arm simply stops
 - These collisions can be recovered easily
 - Click the **SAFE** button (untested in MXCuBE Qt4)
 - Wait several minutes as the robot arm dries and recalibrates
 - Check that the sample is still present in the Dewar
 - Try to **MOUNT** again
- **HARD** collisions require manual intervention:
 - Symptom: the robot arm stops, but the cryotong is dislocated
 - The SAFE command will not run
 - When entering the hutch cryotongs will make a hissing noise
 - Ask for help from the BL staff or call 9797 (Hall Coordinator)
 - They will move the robot arm away from the collision point and to the HOME position

If the robot fails to move after you have been in the hutch (loading pucks):

- This might be because the **Arm Power** is **OFF** condition
 - Check that the ROBOT KEY is turned to the DOWN position
 - Click the POWER ON button
 - Try to **MOUNT** again
- If it fails again
 - Contact the BL staff or Hall Coordinator (9797)

The screenshot displays the 'Sample changer' control interface. At the top, the 'State' is 'Ready'. Below this, the 'Contents' section shows a grid of 9 pucks (Puck 1 to Puck 9), each with a 3x4 grid of sample positions (1-16). Each puck has a checked box and a 'Load' button. An 'Abort' button is located above the puck grid. Below the puck grid, the 'Arm Power' section shows 'Power' (green), 'Power On', and 'Power Off' buttons. The 'LN2 Regulation' section shows 'Regulation' (red) and 'Regulation On' buttons. The 'Lid' section shows three columns (Lid 1, Lid 2, Lid 3) with 'Open' and 'Close' buttons. The 'Barcode' section has a 'Barcode:' input field and a 'Read Barcode during trajectory' checkbox. The 'Commands' section has 'Actions:' (Safe, Dry, Home) and 'Recovery:' (Reset put/get, Reset Motion, Clear) buttons. An 'Abort' button is also present below the commands. At the bottom, the 'CATS message' section shows 'Remote Mode requested'.

Before You Leave PX2-A

- 1) UNMOUNT the sample with the robot via MXCuBE
 - It is impossible to open a lid with a sample on the goniometer!
- 2) OPEN the LIDS via MXCuBE
- 3) CLOSE the Safety Shutter via MXCuBE
- 4) ENTER the hutch
 - Press the blue PSS button & turn the CATS key to the top position (manual)
- 5) Remove your pucks
 - a) Screw on a puck cover on to a puck-loading-tool
 - b) Push the puck cover down onto the puck base
 - c) Tilt the puck loading tool slightly towards the center of the lid
 - d) Lift the tool up, the base should be attached
 - If the base does not come up, try « girating » the tool to dislodge the base
 - e) Unscrew the puck from the tool
- 6) CLOSE the hutch door
- 7) TURN the CATS key to the bottom position (remote)
- 8) **CLOSE the LIDS and DRY-SOAK via MXCuBE**
 - **This keeps ice from forming in the Dewar!**