MXCuBE user manual
Proxima1

SOLEIL
SYNCHROTRON

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v.2

December 2018

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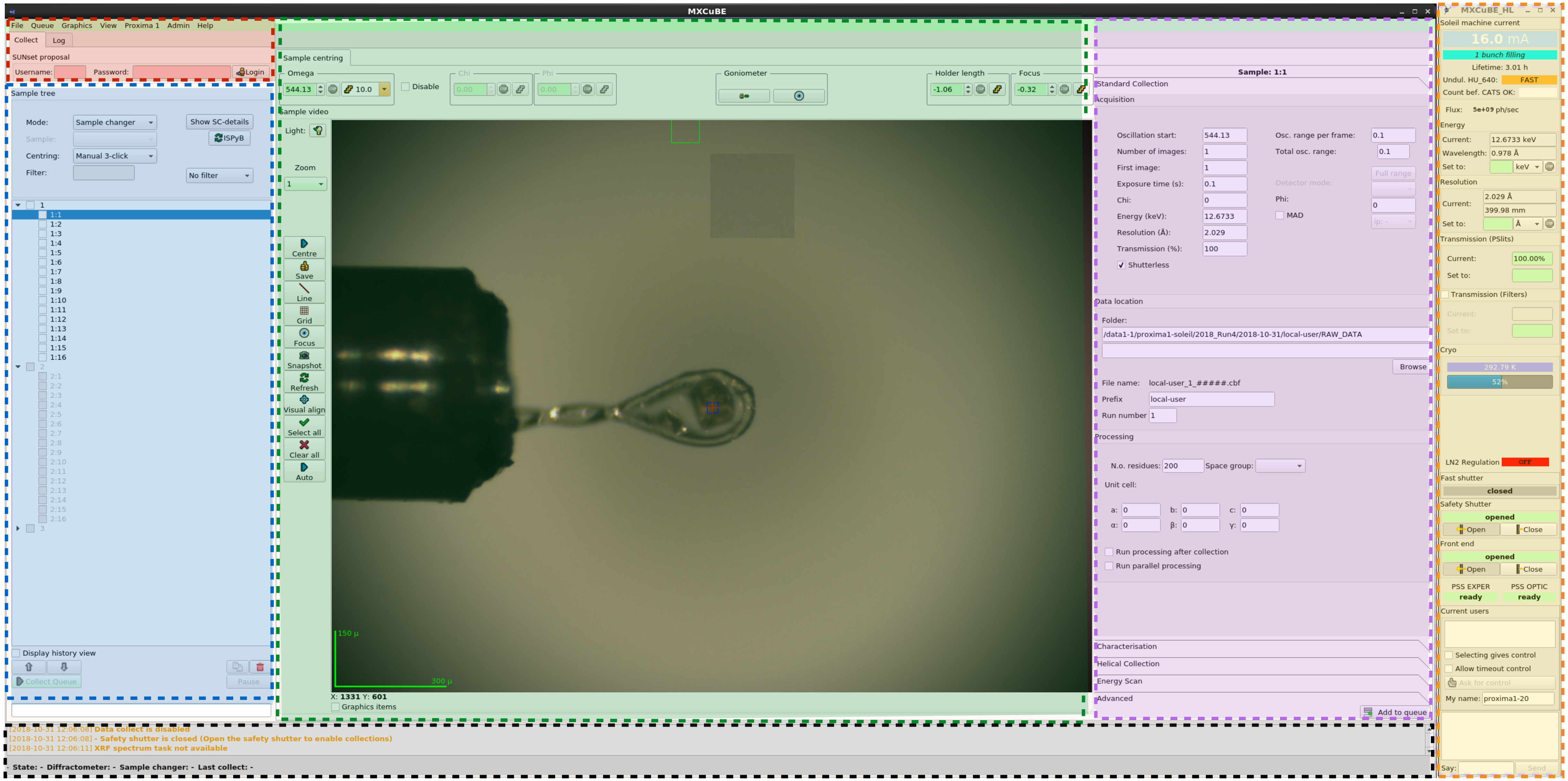
MXCuBE user manual
Proxima1

Part I: The Graphical User Interface (GUI) Description

SOLEIL
SYNCHROTRON

GUI: The “Main” page



Mode: Sample changer

Centring: Manual 3-click

Filter: No filter

Omega: 544.13 — 10.0

Holder length: -1.06

Focus: -0.32

Zoom: 1

X: 1331 Y: 601

Sample: 1:1

Oscillation start: 544.13

Number of images: 1

First image: 1

Exposure time (s): 0.1

Chi: 0

Energy (keV): 12.6733

Resolution (Å): 2.029

Transmission (%): 100

☑ Shutterless

Osc. range per frame: 0.1

Total osc. range: 0.1

Phi: 0

☐ MAD

Folder: /data1-1/proxima1-soleil/2018_Run4/2018-10-31/local-user/RAW_DATA

File name: local-user_1_#####.cbf

Prefix: local-user

Run number: 1

N.o. residues: 200

Space group:

Unit cell:

a: 0 b: 0 c: 0

α: 0 β: 0 γ: 0

☐ Run processing after collection

☐ Run parallel processing

16.0 mA

1 bunch filling

Lifetime: 3.01 h

Undul. HU_640: FAST

Count bef. CATS OK:

Flux: 5e+09 ph/sec

Energy

Current: 12.6733 keV

Wavelength: 0.978 Å

Set to: keV

Resolution

Current: 2.029 Å

399.98 mm

Set to: Å

Transmission (PSlits)

Current: 100.00%

Set to:

☐ Transmission (Filters)

Current:

Set to:

Cryo

292.79 K

52%

LN2 Regulation: OFF

Fast shutter: closed

Safety Shutter: opened

Front end: opened

PSS EXPER: ready

PSS OPTIC: ready

☐ Selecting gives control

☐ Allow timeout control

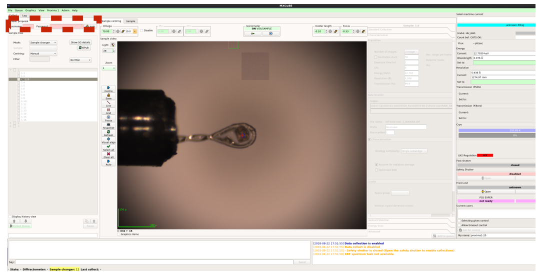
My name: proxima1-20

```
[2018-10-31 12:06:08] Data collect is disabled
[2018-10-31 12:06:08] - Safety shutter is closed (Open the safety shutter to enable collections)
[2018-10-31 12:06:11] XRF spectrum task not available
```

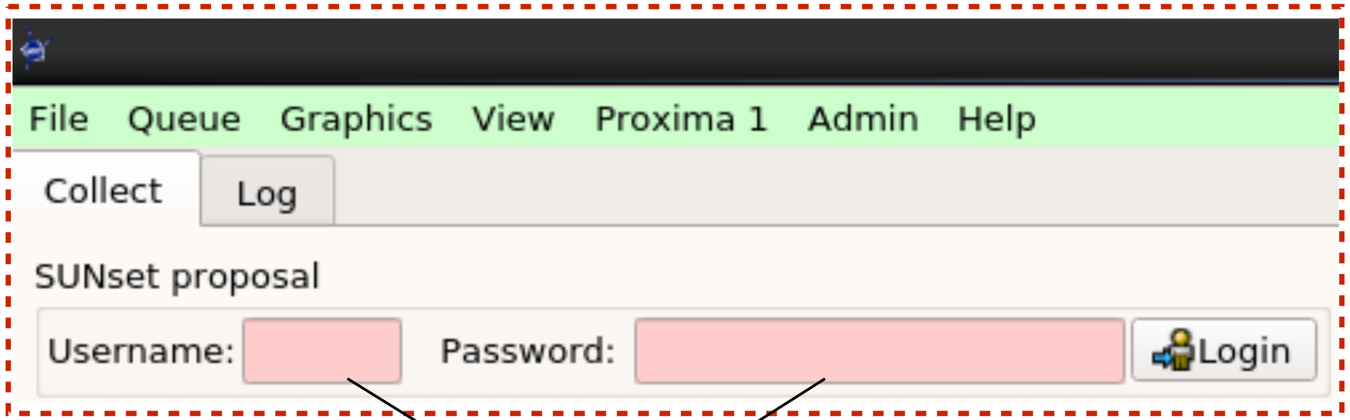
State: - Diffractometer: - Sample changer: - Last collect: -

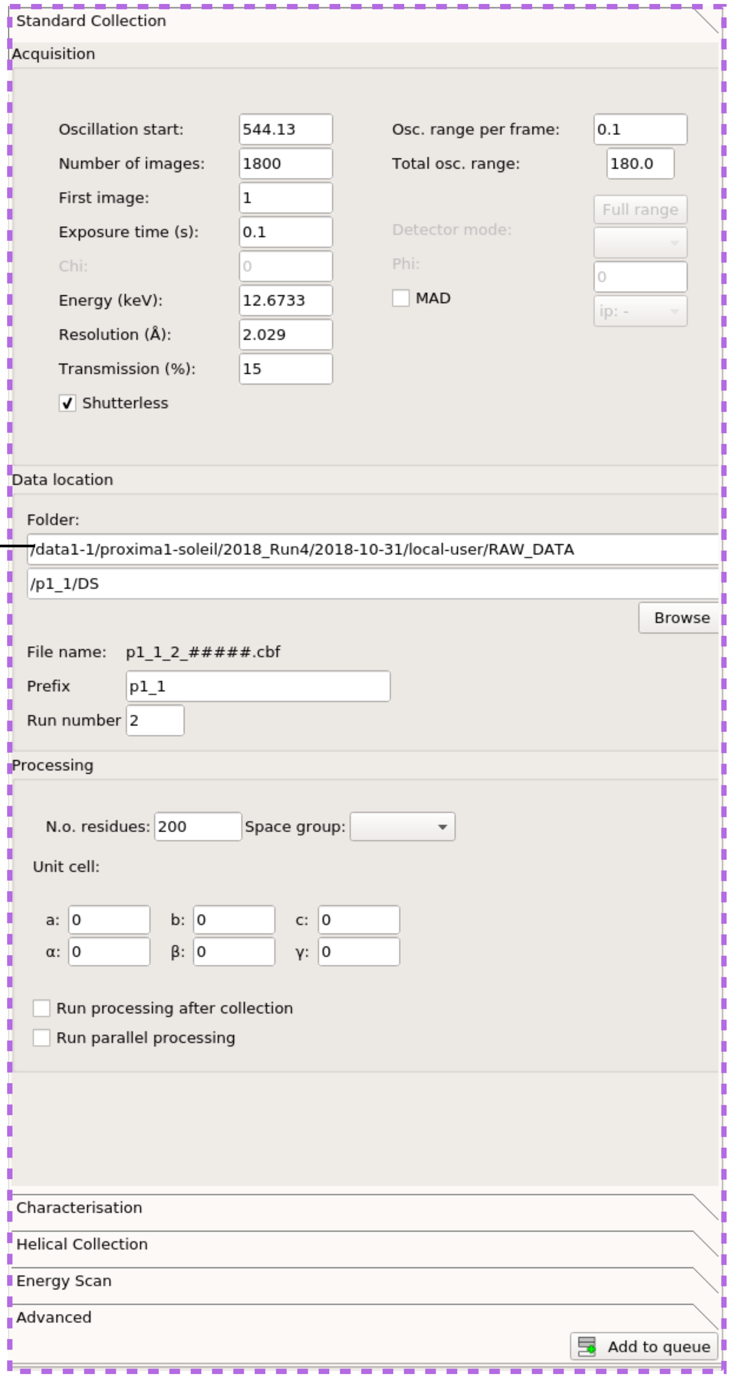
The MxCuBE graphic user interface (GUI) operational areas:

- Login
- Sample tree and data collection queue
- Sample centring
- Collection method
- Machine status
- Dialogue box



GUI: The "Main" page
The login area





Oscillation start: 544.13
Number of images: 1800
First image: 1
Exposure time (s): 0.1
Chi: 0
Energy (keV): 12.6733
Resolution (Å): 2.029
Transmission (%): 15
☑ Shutterless

Osc. range per frame: 0.1
Total osc. range: 180.0
Detector mode:
Phi: 0
☐ MAD
ip: -

Folder: /data1-1/proxima1-soleil/2018_Run4/2018-10-31/local-user/RAW_DATA
/p1_1/DS

File name: p1_1_2_#####.cbf
Prefix p1_1
Run number 2

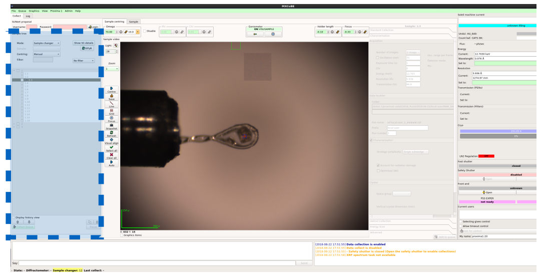
N.o. residues: 200 Space group:
Unit cell:
a: 0 b: 0 c: 0
α: 0 β: 0 γ: 0

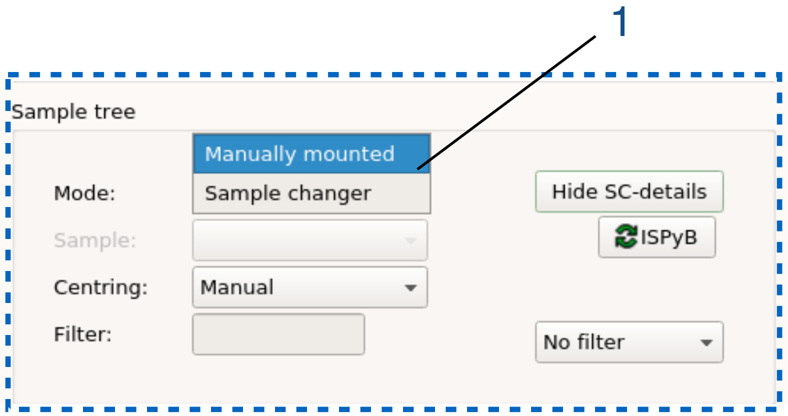
☐ Run processing after collection
☐ Run parallel processing

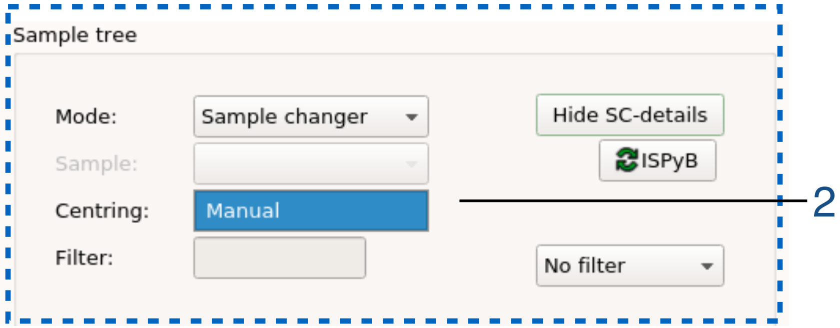
1. Click on the mxCuBE icon on the computer Desktop to open the application
2. Enter your login (proposal number) and password, then click on « Login »

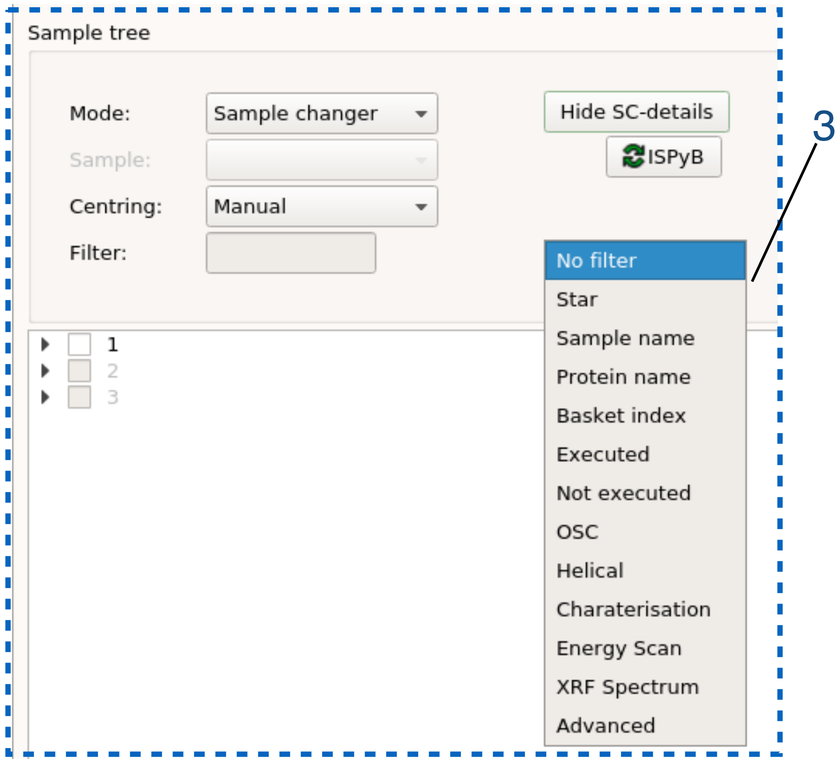
2. The path where your data will be stored will appear in the collection method area

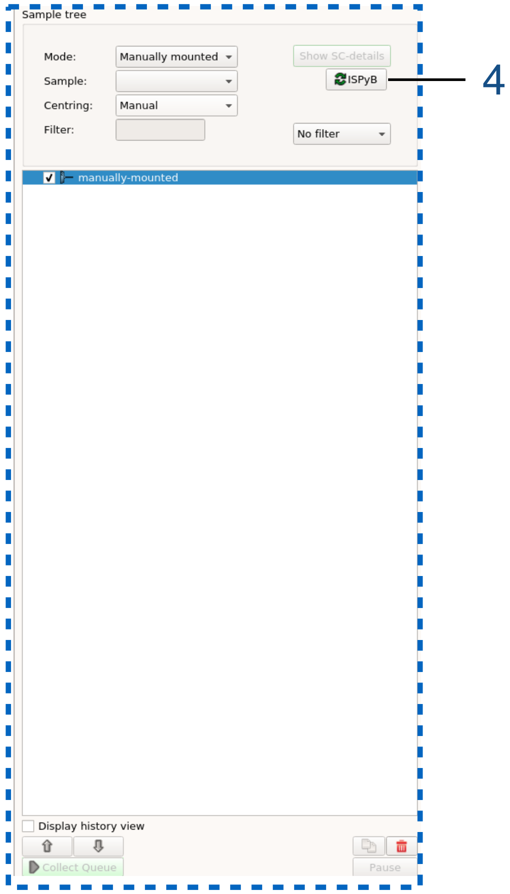
GUI: The “Main” page
The sample tree and queue area (1)

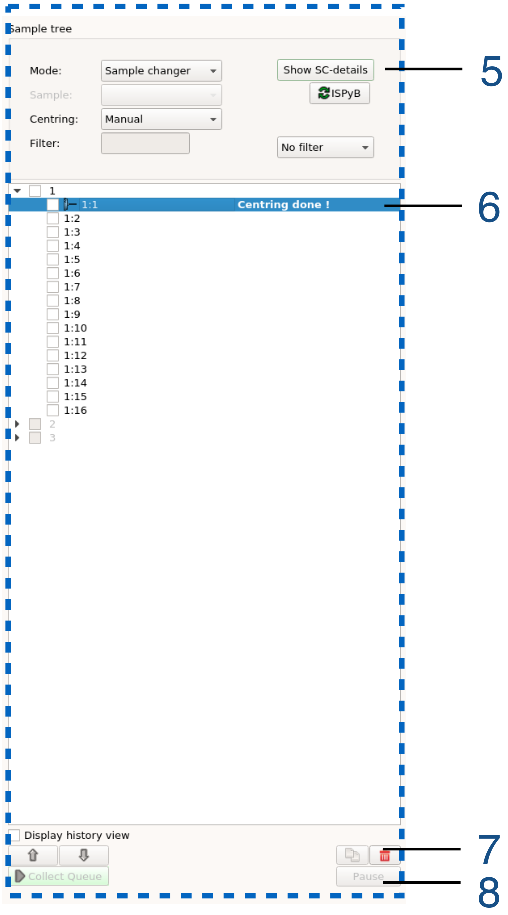




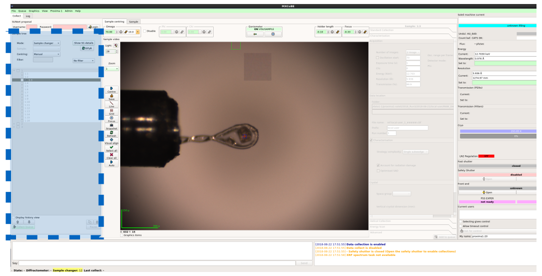




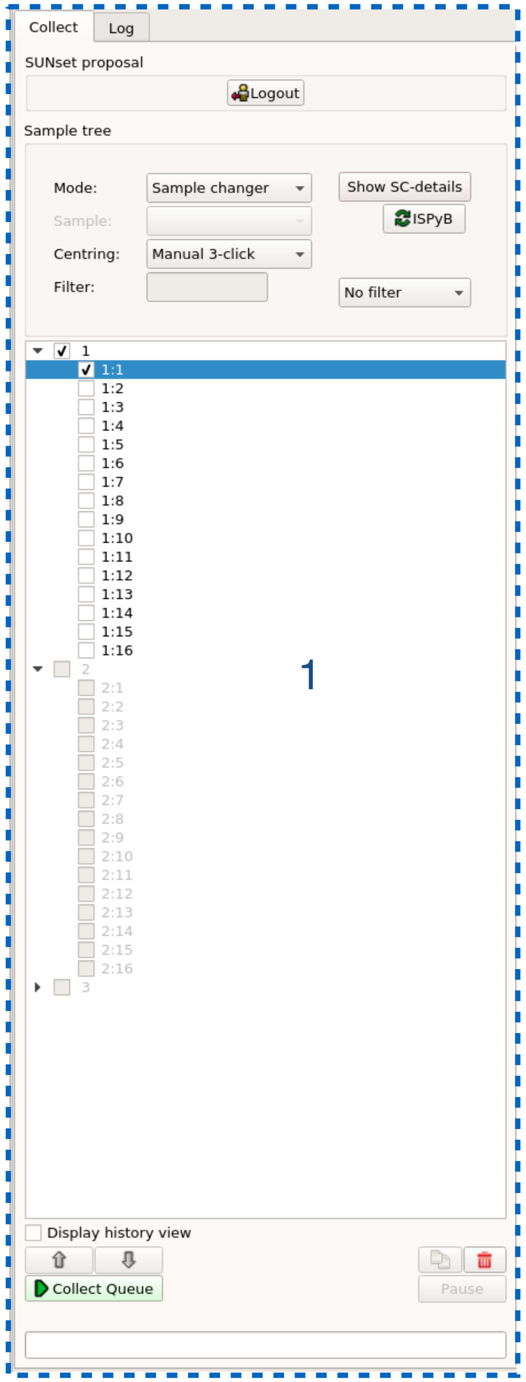




1. Select the sample-mounting mode
2. Choose the sample-centring mode
3. Choose the queue-filtering mode
4. Synchronize with ISPyB database to display a sample list. This mode is not implemented for BAGs yet
5. Show sample changer (SC) details
6. In sample changer mode: sample list is sorted by puck (sample:puck = 1:1)
7. Delete selected collections
8. Pause the running chain of tasks



GUI: The “Main” page
The sample tree and queue area (2)



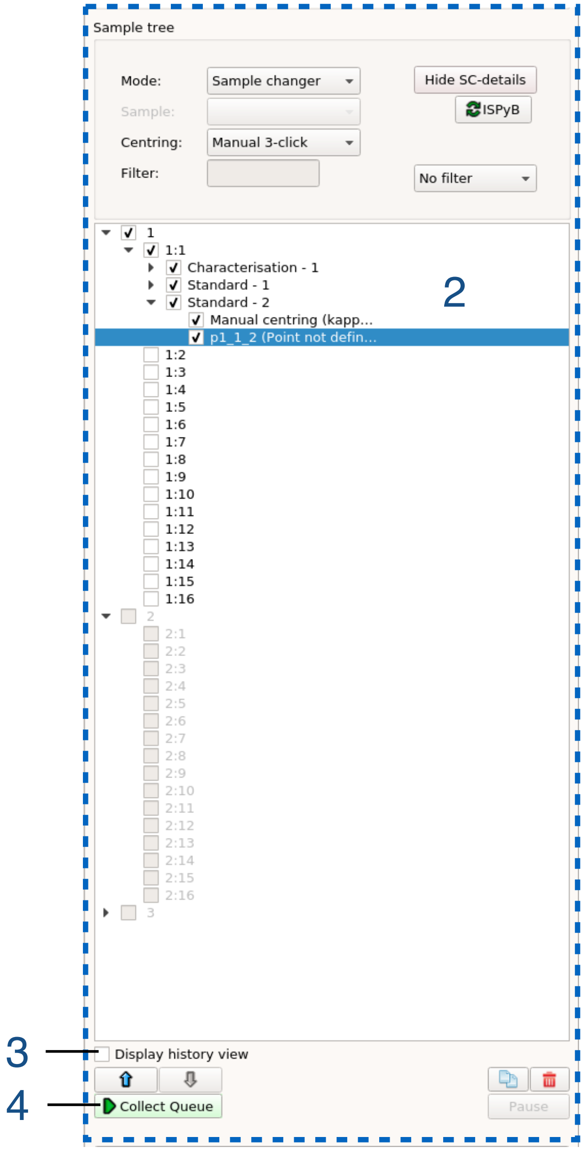
Mode: Sample changer

Sample:

Centring: Manual 3-click

Filter:

No filter



Mode: Sample changer

Sample:

Centring: Manual 3-click

Filter:

No filter

- ☑ 1
  - ☑ 1:1
    - ☑ Characterisation - 1
    - ☑ Standard - 1
    - ☑ Standard - 2
      - ☑ Manual centring (kapp...
      - ☑ p1_1_2 (Point not defin...

1. Sample tree
2. Tick the box corresponding to:

- A puck: to collect all tasks corresponding to this puck when collecting on Collect queue
- First line: to collect all tasks corresponding to this sample when collecting on Collect queue
- A particular task: to collect only this task when collecting on Collect queue

Sample status color code:

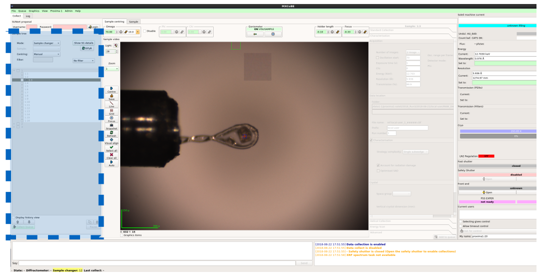
- No color= not selected
- Blue= selected

Task status color code:

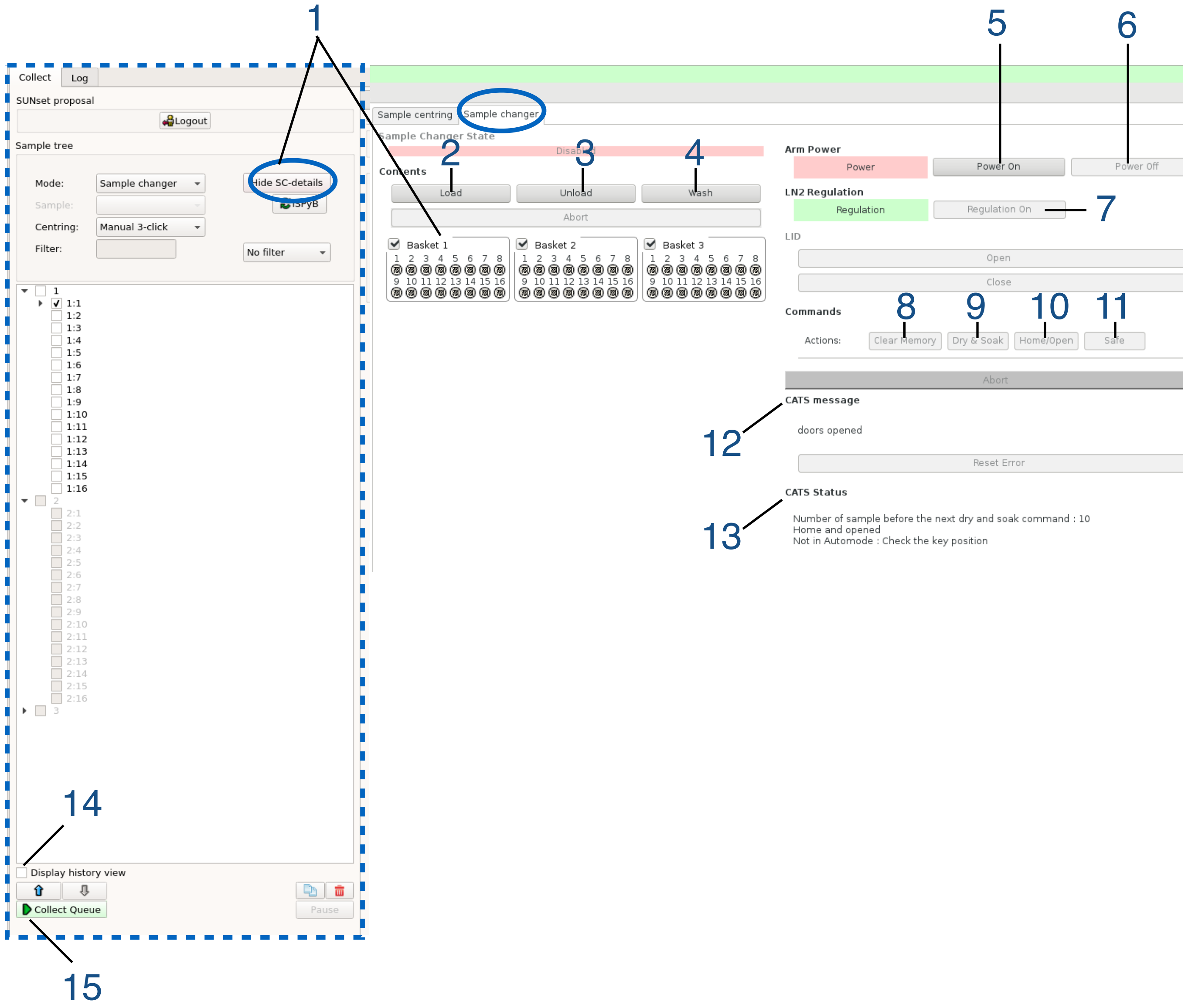
- No color= not selected
- Green= collected
- Red= collection failed

3. Select ‘Display history view’ to see the history of the tasks performed

4. Collect queue starts data collection



GUI: The “Main” page
The sample tree and queue area (3)



Mode: Sample changer
Sample:
Centring: Manual 3-click
Filter: No filter

CATS message

doors opened

CATS Status

Number of sample before the next dry and soak command : 10
Home and opened
Not in Automode : Check the key position

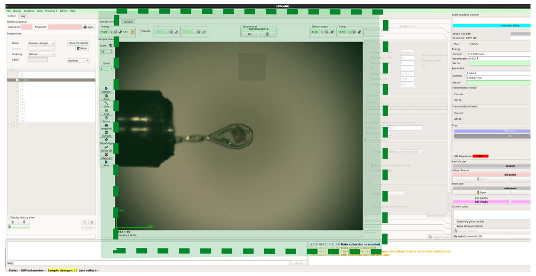
1. The SC-details window allows you to control the sample changer loading:

- Green= Collected samples
- Black= Not collected samples

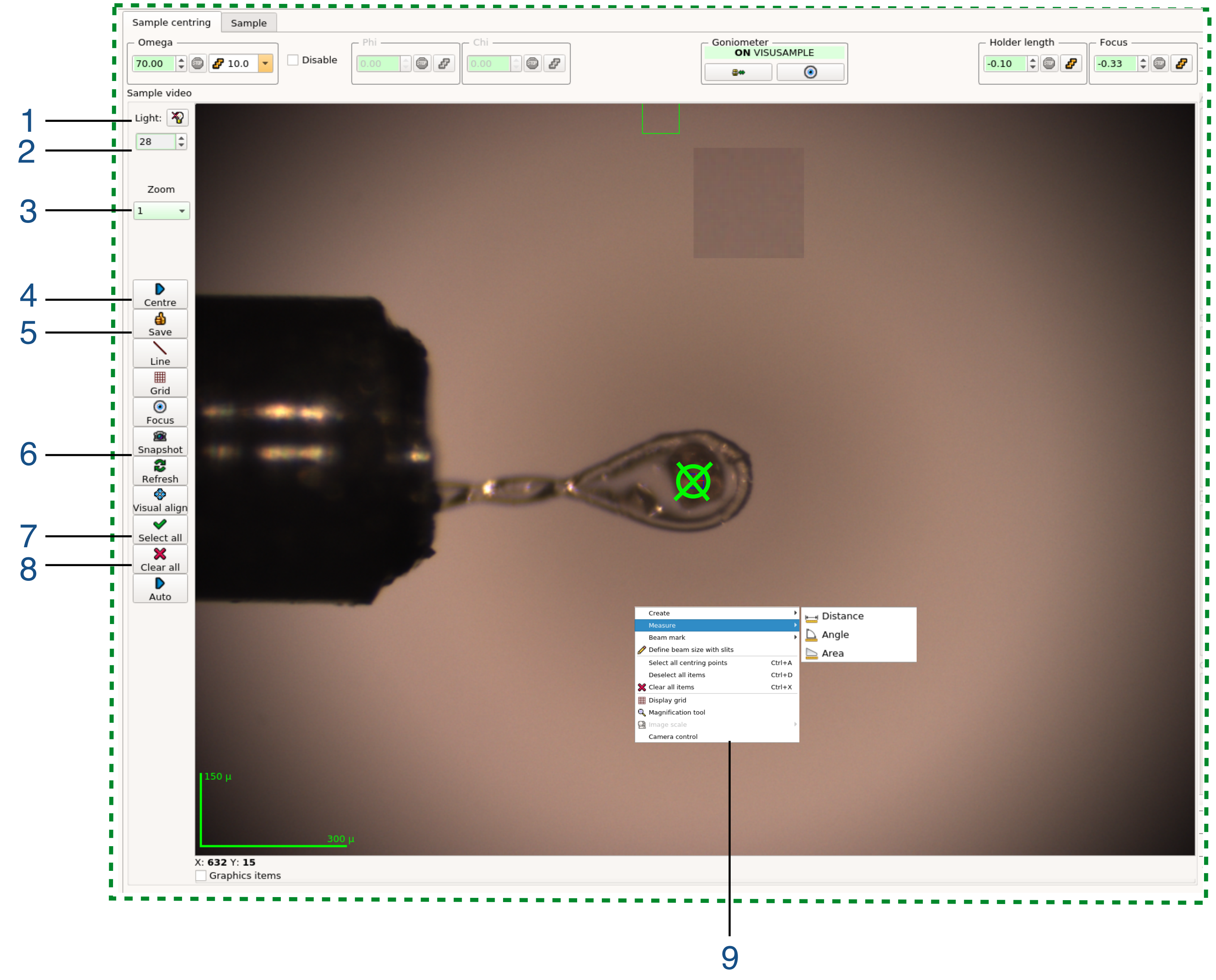
2. Load selected sample
3. Unload selected sample
4. Wash sample. This will unload the sample and quickly reload it. This procedure is often very efficient to get rid of ice
5. Power ON the robot
6. Power OFF the robot
7. Power ON the N2 automatic regulation of the robot dewar
8. ‘Clear Memory’, for the Local Contact
9. ‘Dry and Soak’ dries and cools down the tong of the robot
10. ‘Home/Open’ pulls out of the dewar the arm of the robot and opens the lid of the dewar
11. ‘Safe’ button to recover after soft collision *
12. Error messages form the robot
13. Status messages of the robot. If the key is not in remote mode you will find a message here
14. Display tasks history
15. Collect the queue tasks

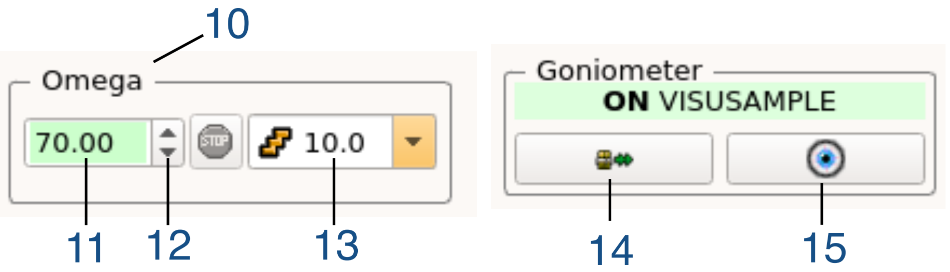
* A soft collision implies that the robot is still power ON after the collision

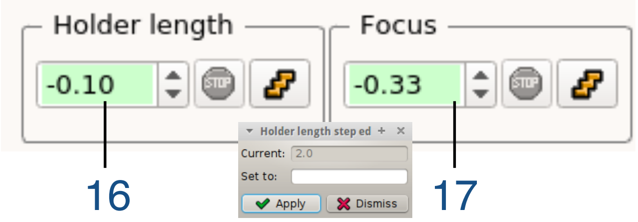
** Attention: This interface is not meant to load the sample. Please see the section ‘Load and unload a sample’. Double click on a sample will load it!



GUI: The “Main” page
Sample centering and video area

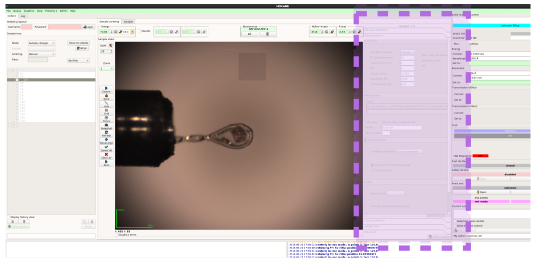




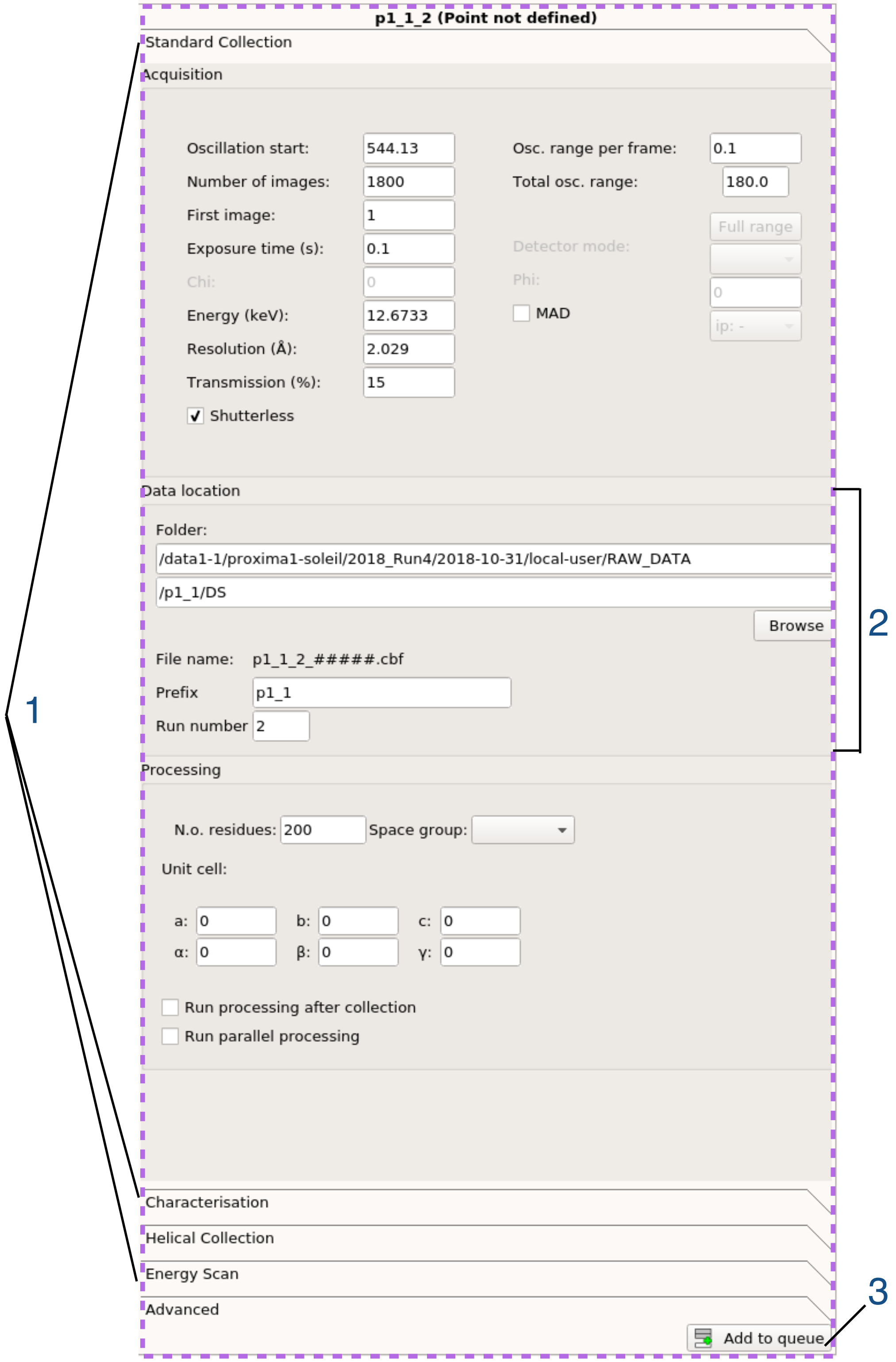


1. Tick to switch the light on
2. Intensity of the light
3. Zoom of the camera
4. Centre the sample
5. Save the centring position
6. Take snapshot of the crystal
7. Select all centring positions
8. Delete all centring positions
9. Measurements tool box (right click)

10. Parameter
11. Current value of parameter
12. Tune up and down the parameter by the step defined in 13
13. Tuning step
14. Enter the hutch and manual mounting of the sample
15. Activate the centring mode
16. Holder length (click on ladder, insert value and Apply)
17. Focus (click on ladder, insert value and Apply)



GUI: The “Main” page
Collection method area



Oscillation start: 544.13
Osc. range per frame: 0.1
Number of images: 1800
Total osc. range: 180.0
First image: 1
Exposure time (s): 0.1
Detector mode:
Chi: 0
Phi: 0
Energy (keV): 12.6733
☐ MAD
ip: -
Resolution (Å): 2.029
Transmission (%): 15
☑ Shutterless

Folder: /data1-1/proxima1-soleil/2018_Run4/2018-10-31/local-user/RAW_DATA
/p1_1/DS
File name: p1_1_2_#####.cbf
Prefix p1_1
Run number 2

N.o. residues: 200
Space group:
Unit cell:
a: 0 b: 0 c: 0
α: 0 β: 0 γ: 0
☐ Run processing after collection
☐ Run parallel processing

1. Collection methods (Characterisation, Energy Scan, Standard Collection, Helical Collection)

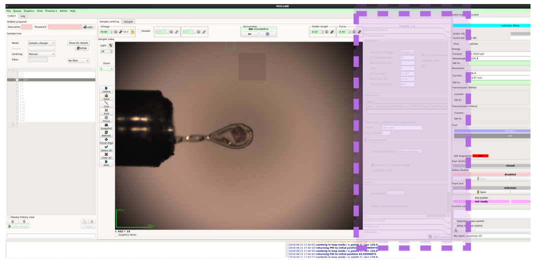
2. Pathway for your data. Diffraction images will typically be stored in a subdirectory of your choice under RAW_DATA:

   The pathway is automatically filled once you are logged in with your Proposal number and password. Fill in the subdirectory name

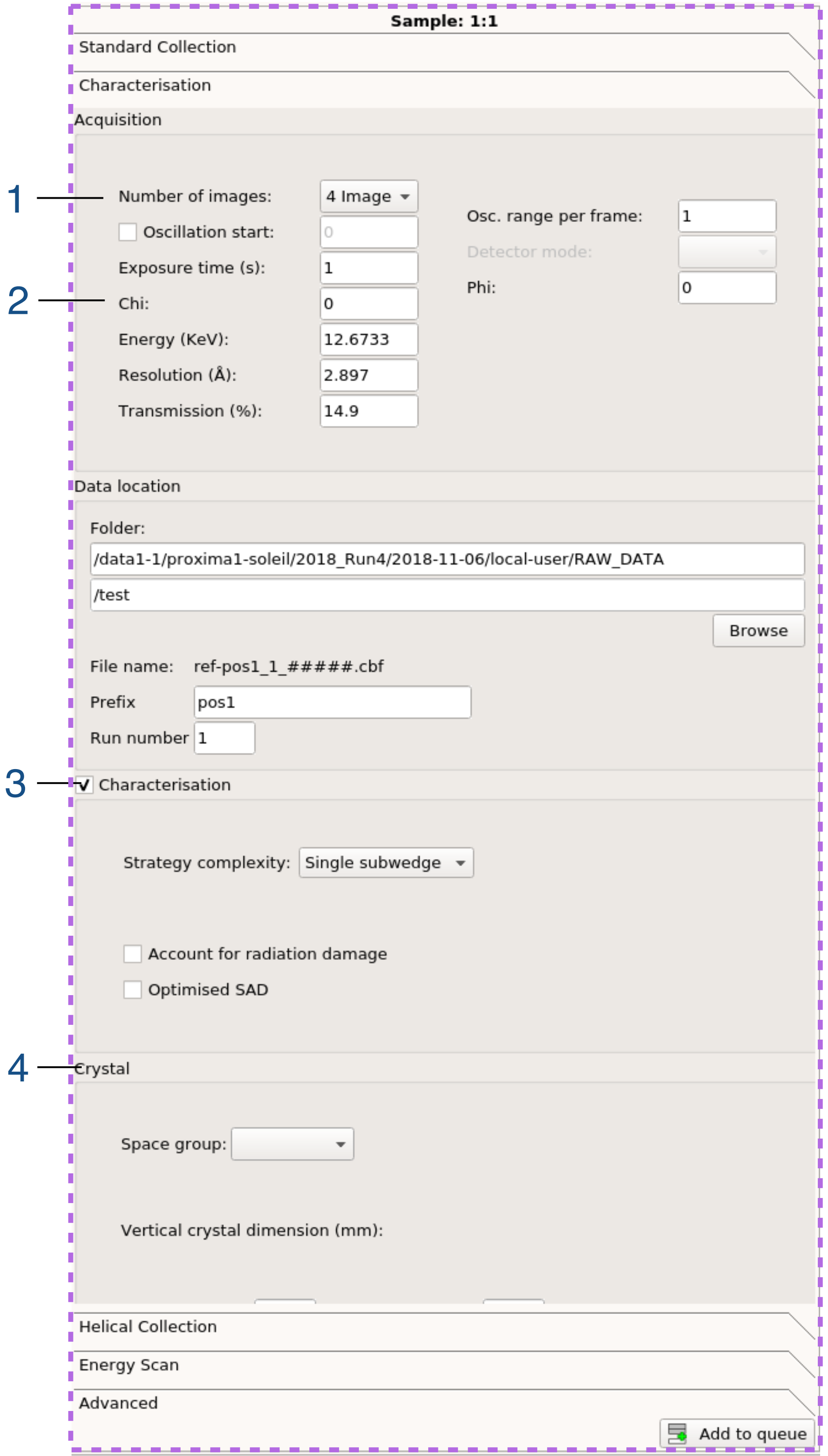
   Fill in the prefix of the sample

   The Run number is automatically incremented at the end of each experiment of the same type

3. For each collection method, « Add to queue » will add the collection to the selected samples and display it in the sample tree and queue area



GUI: The “Main” page
Collection method area
« Characterisation »



Sample: 1:1

Standard Collection

Characterisation

Acquisition

Number of images: 4 Image
☐ Oscillation start: 0
Exposure time (s): 1
Chi: 0
Energy (KeV): 12.6733
Resolution (Å): 2.897
Transmission (%): 14.9
Osc. range per frame: 1
Detector mode:
Phi: 0

Data location

Folder: /data1-1/proxima1-soleil/2018_Run4/2018-11-06/local-user/RAW_DATA
/test
Browse
File name: ref-pos1_1_#####.cbf
Prefix pos1
Run number 1

☑ Characterisation

Strategy complexity: Single subwedge
☐ Account for radiation damage
☐ Optimised SAD

Crystal

Space group:
Vertical crystal dimension (mm):

Helical Collection

Energy Scan

Advanced

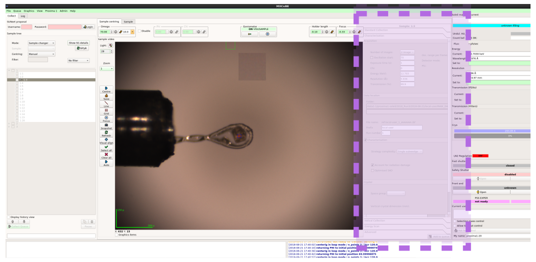
Add to queue

Use the Characterisation method when you want to test the diffraction of your crystal or run a data collection strategy with xdsme

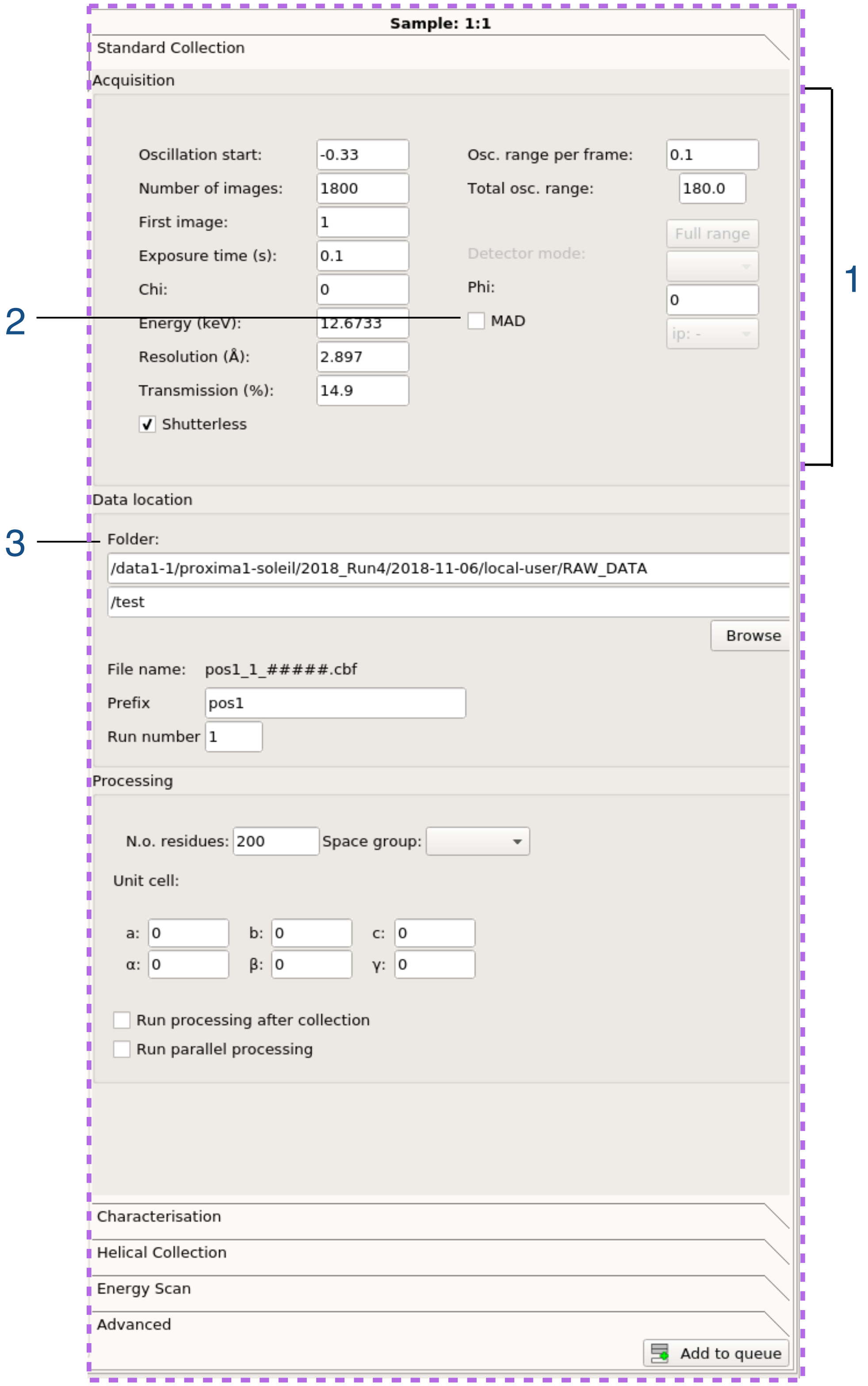
1. Number of images taken to characterize the crystal (1, 2 or 4) corresponding to the angles: (0°, 0°- 90°, 0°- 90°- 180° - 270°).

2. The value of Chi used in the Characterisation is the same as that used for sample centring

3, 4. Not implemented yet



GUI: The “Main” page
« Standard Collection »



Sample: 1:1

Standard Collection

Acquisition

Oscillation start: -0.33
Number of images: 1800
First image: 1
Exposure time (s): 0.1
Chi: 0
Energy (keV): 12.6733
Resolution (Å): 2.897
Transmission (%): 14.9
☑ Shutterless

Osc. range per frame: 0.1
Total osc. range: 180.0
Full range
Detector mode:
Phi: 0
☐ MAD
ip: -

Data location

Folder:
/data1-1/proxima1-soleil/2018_Run4/2018-11-06/local-user/RAW_DATA
/test
Browse

File name: pos1_1_#####.cbf
Prefix pos1
Run number 1

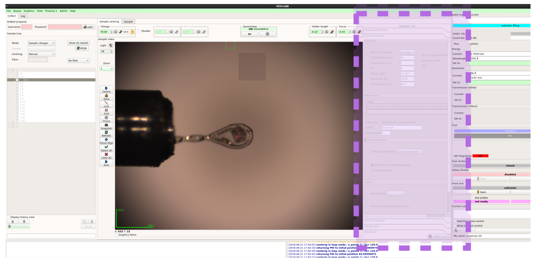
Processing

N.o. residues: 200 Space group:
Unit cell:
a: 0 b: 0 c: 0
α: 0 β: 0 γ: 0
☐ Run processing after collection
☐ Run parallel processing

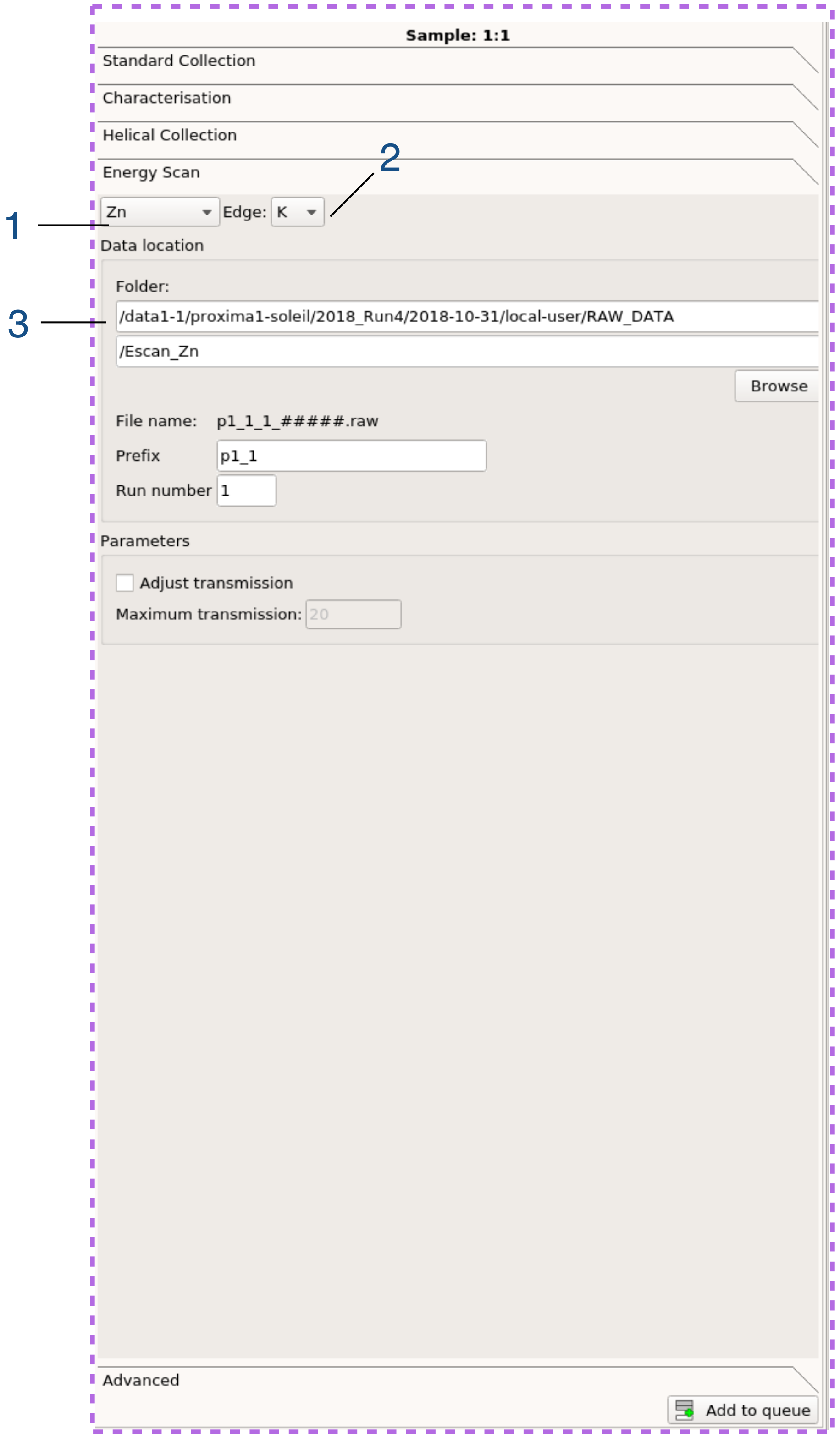
Characterisation
Helical Collection
Energy Scan
Advanced
Add to queue

Use the Standard Collection to collect a complete data set of your crystal based onto the xds data collection strategy plan

1. Data collection parameters obtained from the strategy plan
2. Tick if you want to collect MAD dataset at the energies of peak, inflection point and remote from an Energy Scan
3. Directory where the images will be stored.
   Processing information will be automatically filled if a isample list is synchronized from ISPyB (not implement for BAGs yet)



GUI: The “Main” page « Energy Scan »



Sample: 1:1

Zn Edge: K

Data location

Folder:
/data1-1/proxima1-soleil/2018_Run4/2018-10-31/local-user/RAW_DATA
/Escan_Zn

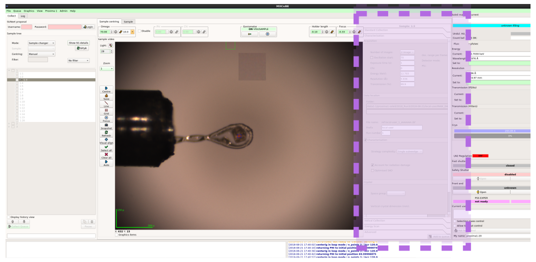
File name: p1_1_1_#####.raw
Prefix: p1_1
Run number: 1

Parameters

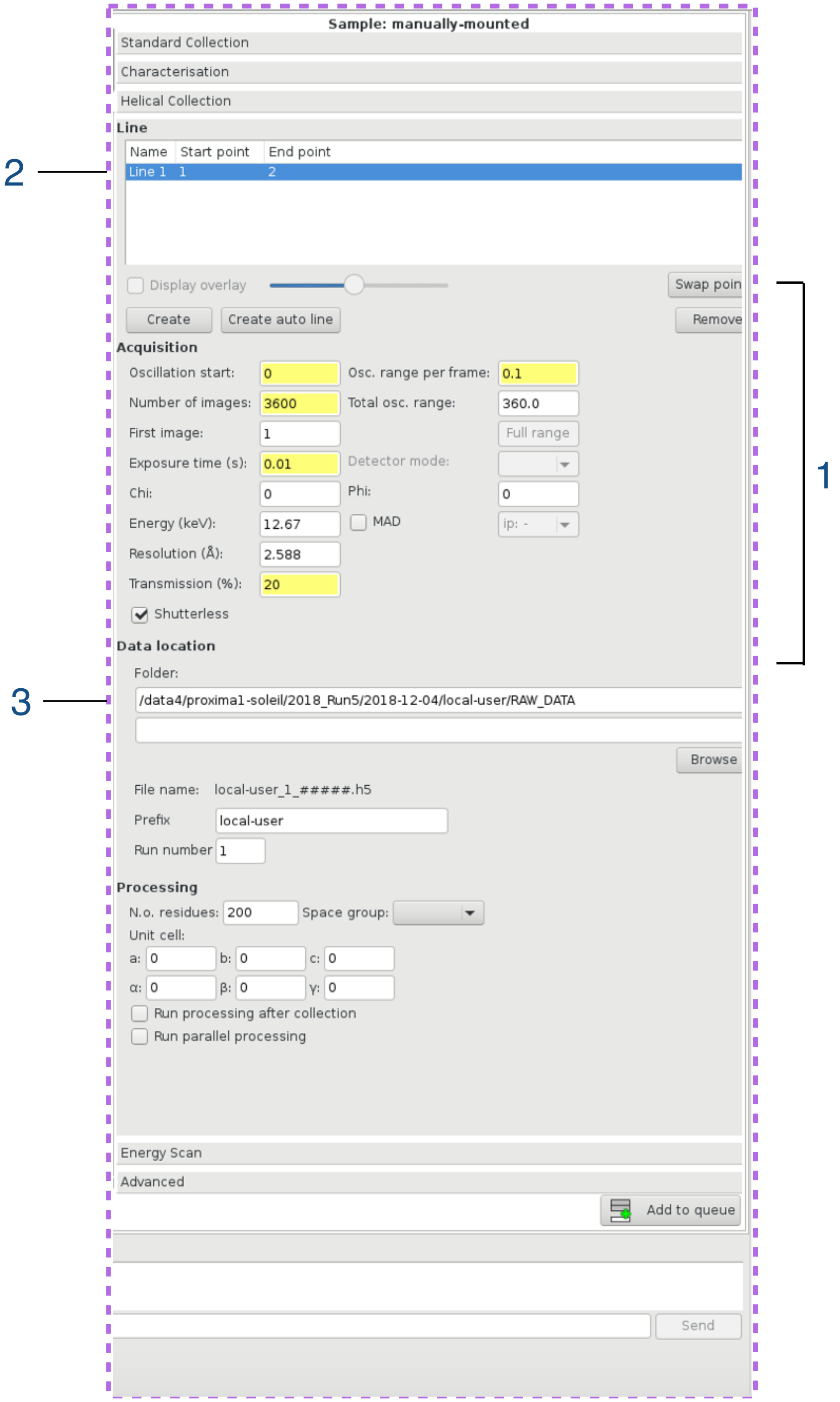
☐ Adjust transmission
Maximum transmission: 20

Use the Energy Scan if your crystal contains anomalous scatterers (Fe, Cu, Zn…)

1. List of the anomalous scatterers
2. List of the absorption Edges
3. Directory where the images will be stored



GUI: The “Main” page « Helical Collection »



Sample: manually-mounted

Standard Collection

Characterisation

Helical Collection

Line

Name	Start point	End point
Line 1	1	2

Acquisition

Oscillation start: 0
Osc. range per frame: 0.1
Number of images: 3600
Total osc. range: 360.0
First image: 1
Exposure time (s): 0.01
Detector mode:
Chi: 0
Phi: 0
Energy (keV): 12.67
☐ MAD
ip: -
Resolution (Å): 2.588
Transmission (%): 20
☑ Shutterless

Data location

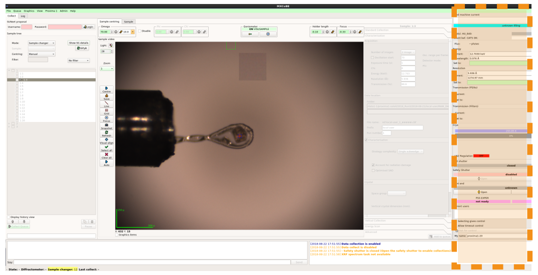
Folder: /data4/proximal1-soleil/2018_Run5/2018-12-04/local-user/RAW_DATA
File name: local-user_1_#####.h5
Prefix local-user
Run number 1

Processing

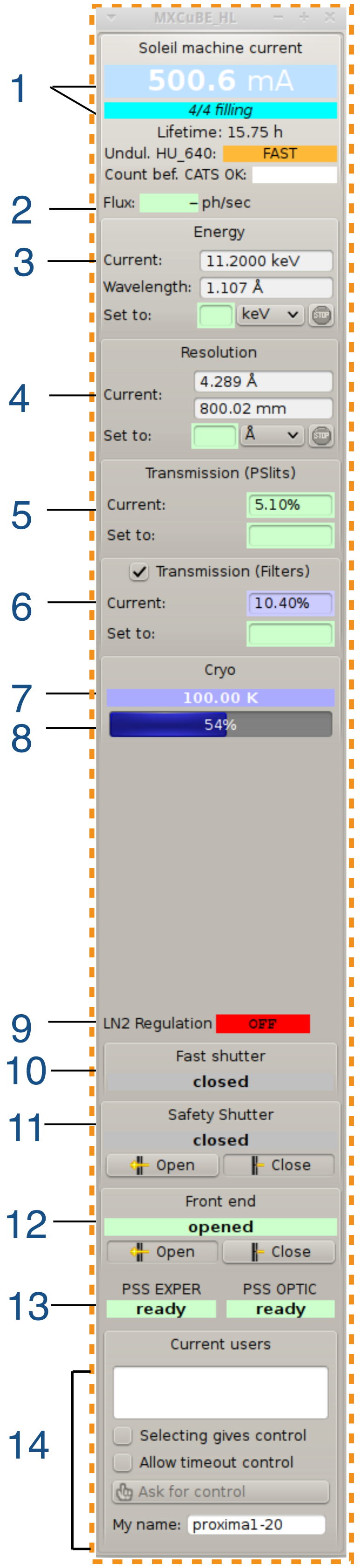
N.o. residues: 200
Space group:
Unit cell:
a: 0 b: 0 c: 0
α: 0 β: 0 γ: 0
☐ Run processing after collection
☐ Run parallel processing

Use the Helical Collection if you want to collect your sample along a straight line (recomended for samples in the shape of rods)

1. Data collection parameters
2. Helical collection task
3. Directory where the images will be stored.



GUI: The “Main” page
Machine status



MXCuBE_HL

Soleil machine current
500.6 mA
4/4 filling
Lifetime: 15.75 h
Undul. HU_640: FAST
Count bef. CATS OK:
Flux: - ph/sec

Energy
Current: 11.2000 keV
Wavelength: 1.107 Å
Set to: keV

Resolution
Current: 4.289 Å
800.02 mm
Set to: Å

Transmission (PSlits)
Current: 5.10%
Set to:

☑ Transmission (Filters)
Current: 10.40%
Set to:

Cryo
100.00 K
54%

LN2 Regulation OFF

Fast shutter
closed

Safety Shutter
closed

Front end
opened

PSS EXPER ready
PSS OPTIC ready

Current users
☐ Selecting gives control
☐ Allow timeout control

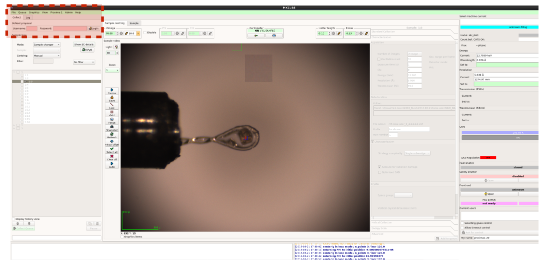
My name: proxima1-20

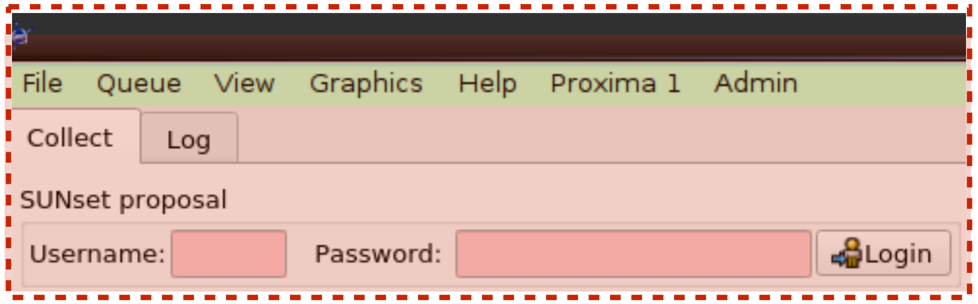
1. Machine current and filling mode
2. Flux of photons at sample position
3. Beamline energy. Nominal energy of the beamline is 12.67 keV.
   To tune the energy beamline enter a value in the « Set to » box and press enter then select the corresponding units (Å or keV)
4. Maximum resolution (recorded at the edge of the detector).
   To change resolution enter the new value in the « Set to » box and press enter then select the corresponding units (Å or keV)
5. Beam Transmission by the primary slits (PSlits).
   To adjust the transmission of the beam, enter a new value in the « Set to » box and press enter
6. Beam Transmission by the Filters.
   Change only when doing XRF scans or energy scans (please ask the Local Contact)
7. Cryogenic stream temperature at the sample position
8. N2 level in the CryoCane dewar
9. N2 regulation of the robot dewar
10. Open/Close the Fast shutter
11. Open/Close the Safety shutter
12. Open/Close the Front end
13. State of the PSS of Experimental and Optical hutch (green= PSS is running, red= PSS is not running)
14. Remote access menu (for the Local Contact)

<u>Open/Close color code:</u>
grey= closed
green=opened

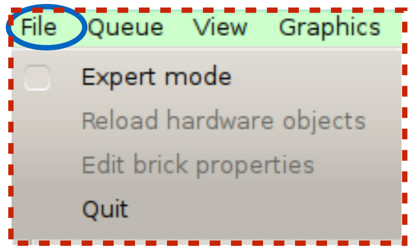
<u>PSS color code:</u>
green= PSS is running
red= PSS is not running

GUI: The “Main” page
Sub-menus

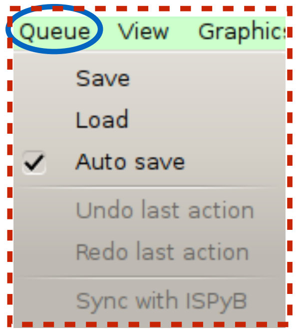




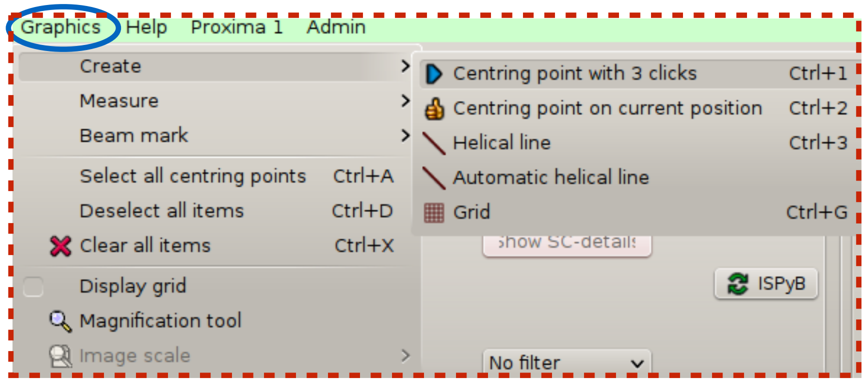
1



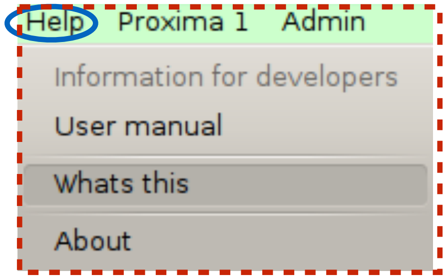
2



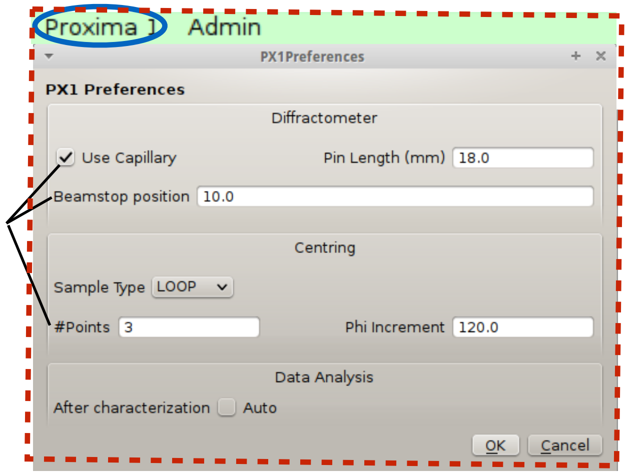
3



4



5



☑ Use Capillary

Pin Length (mm) 18.0

Beamstop position 10.0

Sample Type LOOP

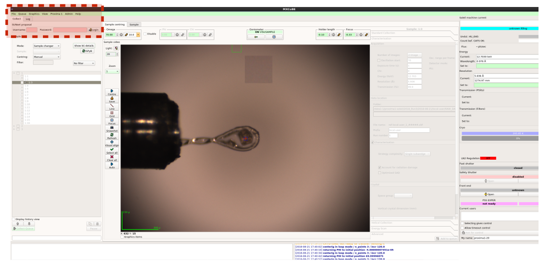
#Points 3

Phi Increment 120.0

After characterization ☐ Auto

1. Expert mode (for the local contact)
2. Sample tree mode
3. Centring, measurement and item selection tools
4. Access to MXCuBE manual and Information for Developers
5. Go in Proxima1 -> Edit Preferences to access the following options:
   - Use capillary: Ticked by default. Untick if you don’t want to use the capillary
   - Beamstop position: Default value is 10mm but you can move it up to 30 mm to collect the low resolution
   - #Points: Select the number of points used for centring and the corresponding Phi angle increment

GUI: The “Main” page
System tabs



```
Level      Date         Time        Message
WARNING    2018-10-31   13:28:15    i10-c-cx1/dt/pilatus/State (state): could not complete init. (hint: device server is not running, or has to be restarted)
WARNING    2018-10-31   13:28:15    i10-c-cx1/dt/pilatus/threshold (threshold): could not complete init. (hint: device server is not running, or has to be restarted)
ERROR      2018-10-31   13:28:15    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:16    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:17    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
WARNING    2018-10-31   13:28:18    i10-c-cx1/dt/pilatus/State (state): could not complete init. (hint: device server is not running, or has to be restarted)
WARNING    2018-10-31   13:28:18    i10-c-cx1/dt/pilatus/threshold (threshold): could not complete init. (hint: device server is not running, or has to be restarted)
ERROR      2018-10-31   13:28:18    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:19    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:20    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
WARNING    2018-10-31   13:28:21    i10-c-cx1/dt/pilatus/State (state): could not complete init. (hint: device server is not running, or has to be restarted)
WARNING    2018-10-31   13:28:21    i10-c-cx1/dt/pilatus/threshold (threshold): could not complete init. (hint: device server is not running, or has to be restarted)
ERROR      2018-10-31   13:28:21    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:22    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:23    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
WARNING    2018-10-31   13:28:24    i10-c-cx1/dt/pilatus/State (state): could not complete init. (hint: device server is not running, or has to be restarted)
WARNING    2018-10-31   13:28:24    i10-c-cx1/dt/pilatus/threshold (threshold): could not complete init. (hint: device server is not running, or has to be restarted)
ERROR      2018-10-31   13:28:24    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:25    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:26    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
WARNING    2018-10-31   13:28:27    i10-c-cx1/dt/pilatus/State (state): could not complete init. (hint: device server is not running, or has to be restarted)
WARNING    2018-10-31   13:28:27    i10-c-cx1/dt/pilatus/threshold (threshold): could not complete init. (hint: device server is not running, or has to be restarted)
ERROR      2018-10-31   13:28:28    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:29    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:30    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
WARNING    2018-10-31   13:28:30    i10-c-cx1/dt/pilatus/State (state): could not complete init. (hint: device server is not running, or has to be restarted)
WARNING    2018-10-31   13:28:30    i10-c-cx1/dt/pilatus/threshold (threshold): could not complete init. (hint: device server is not running, or has to be restarted)
ERROR      2018-10-31   13:28:31    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:32    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:33    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
WARNING    2018-10-31   13:28:33    i10-c-cx1/dt/pilatus/State (state): could not complete init. (hint: device server is not running, or has to be restarted)
WARNING    2018-10-31   13:28:33    i10-c-cx1/dt/pilatus/threshold (threshold): could not complete init. (hint: device server is not running, or has to be restarted)
ERROR      2018-10-31   13:28:34    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:35    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:36    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
WARNING    2018-10-31   13:28:36    i10-c-cx1/dt/pilatus/State (state): could not complete init. (hint: device server is not running, or has to be restarted)
WARNING    2018-10-31   13:28:36    i10-c-cx1/dt/pilatus/threshold (threshold): could not complete init. (hint: device server is not running, or has to be restarted)
ERROR      2018-10-31   13:28:37    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:38    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:39    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
WARNING    2018-10-31   13:28:40    i10-c-cx1/dt/pilatus/State (state): could not complete init. (hint: device server is not running, or has to be restarted)
WARNING    2018-10-31   13:28:40    i10-c-cx1/dt/pilatus/threshold (threshold): could not complete init. (hint: device server is not running, or has to be restarted)
ERROR      2018-10-31   13:28:40    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:41    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:42    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
WARNING    2018-10-31   13:28:43    i10-c-cx1/dt/pilatus/State (state): could not complete init. (hint: device server is not running, or has to be restarted)
WARNING    2018-10-31   13:28:43    i10-c-cx1/dt/pilatus/threshold (threshold): could not complete init. (hint: device server is not running, or has to be restarted)
ERROR      2018-10-31   13:28:43    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:44    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:45    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
WARNING    2018-10-31   13:28:46    i10-c-cx1/dt/pilatus/State (state): could not complete init. (hint: device server is not running, or has to be restarted)
WARNING    2018-10-31   13:28:46    i10-c-cx1/dt/pilatus/threshold (threshold): could not complete init. (hint: device server is not running, or has to be restarted)
ERROR      2018-10-31   13:28:47    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:48    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:49    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
WARNING    2018-10-31   13:28:49    i10-c-cx1/dt/pilatus/State (state): could not complete init. (hint: device server is not running, or has to be restarted)
WARNING    2018-10-31   13:28:49    i10-c-cx1/dt/pilatus/threshold (threshold): could not complete init. (hint: device server is not running, or has to be restarted)
ERROR      2018-10-31   13:28:50    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:51    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:52    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
WARNING    2018-10-31   13:28:52    i10-c-cx1/dt/pilatus/State (state): could not complete init. (hint: device server is not running, or has to be restarted)
WARNING    2018-10-31   13:28:52    i10-c-cx1/dt/pilatus/threshold (threshold): could not complete init. (hint: device server is not running, or has to be restarted)
ERROR      2018-10-31   13:28:53    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:54    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
ERROR      2018-10-31   13:28:55    no attribute Att_transmission in Tango device i10-c-c00/ex/att_parser
WARNING    2018-10-31   13:28:55    i10-c-cx1/dt/pilatus/State (state): could not complete init. (hint: device server is not running, or has to be restarted)
WARNING    2018-10-31   13:28:55    i10-c-cx1/dt/pilatus/threshold (threshold): could not complete init. (hint: device server is not running, or has to be restarted)
```

```
[2018-10-31 13:07:13] Path valid
[2018-10-31 13:19:57] The current path settings will overwrite data from another task. Correct the problem before adding to queue
[2018-10-31 13:20:00] Path valid
```

State: - **Diffractometer:** Phase is COLLECT (state=ON) **Sample changer:** - **Last collect:** -

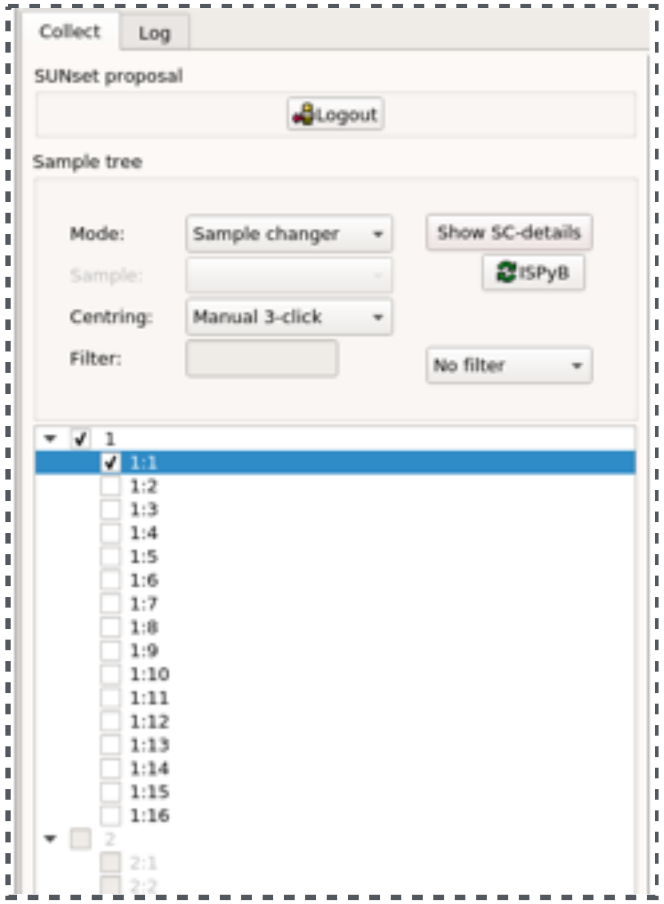
1. MXCuBE errors and warning are reported here in greater details compared to the Dialogue area below (4)
2. General information about the beamline status are reported
3. MXCuBE debug information is reported
4. MXCuBE Dialogue area: general status and warning messages are reported here
5. Diffractometer and sample changer state and last collection status are notified here

MXCuBE user manual

Part II: Practical guidelines

SOLEIL
SYNCHROTRON

Practical guidelines:
Prepare the robot for sample charging



SUNset proposal

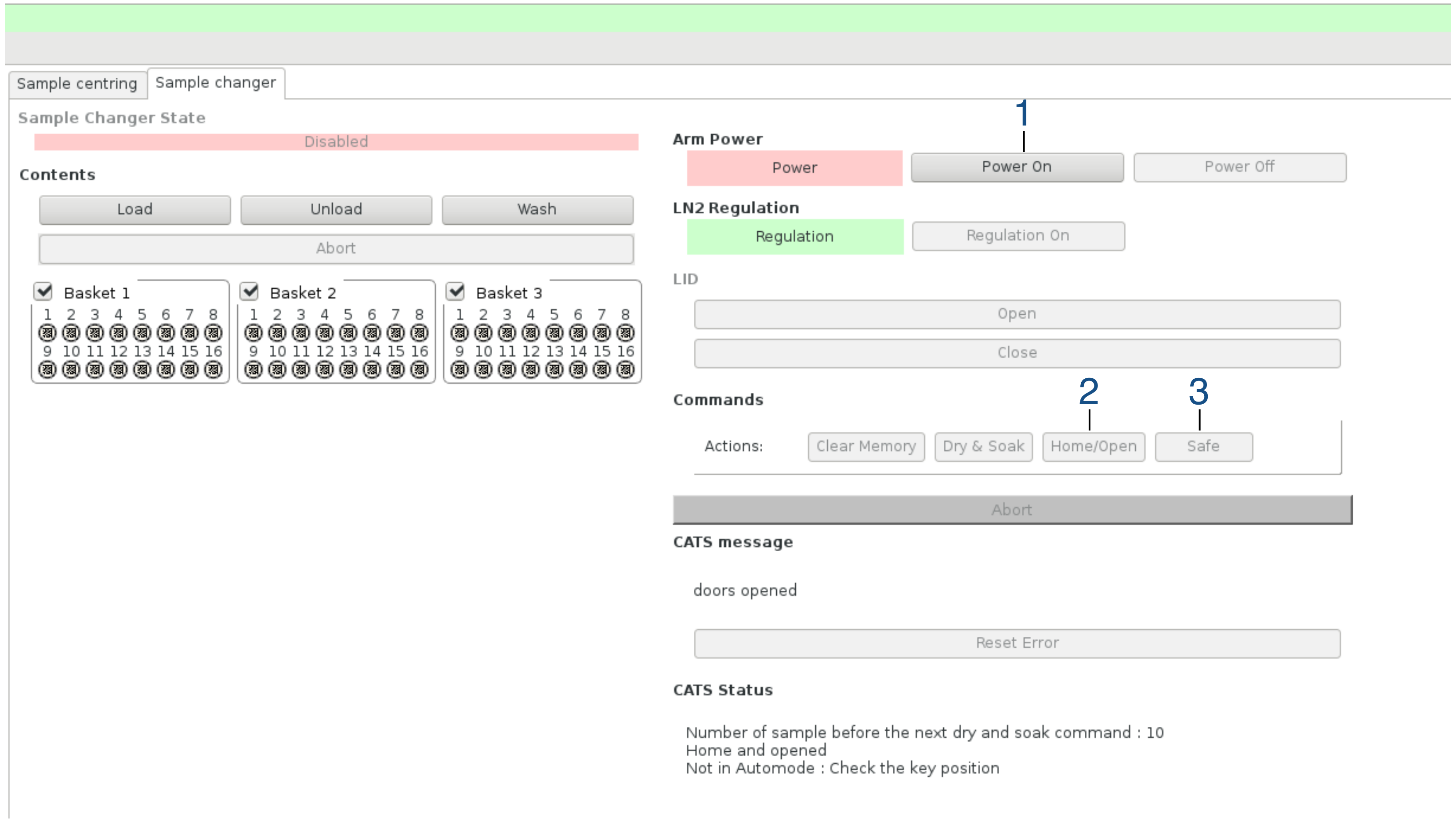
Sample tree

Mode: Sample changer

Sample:

Centring: Manual 3-click

Filter: No filter



Sample Changer State

Disabled

CATS message

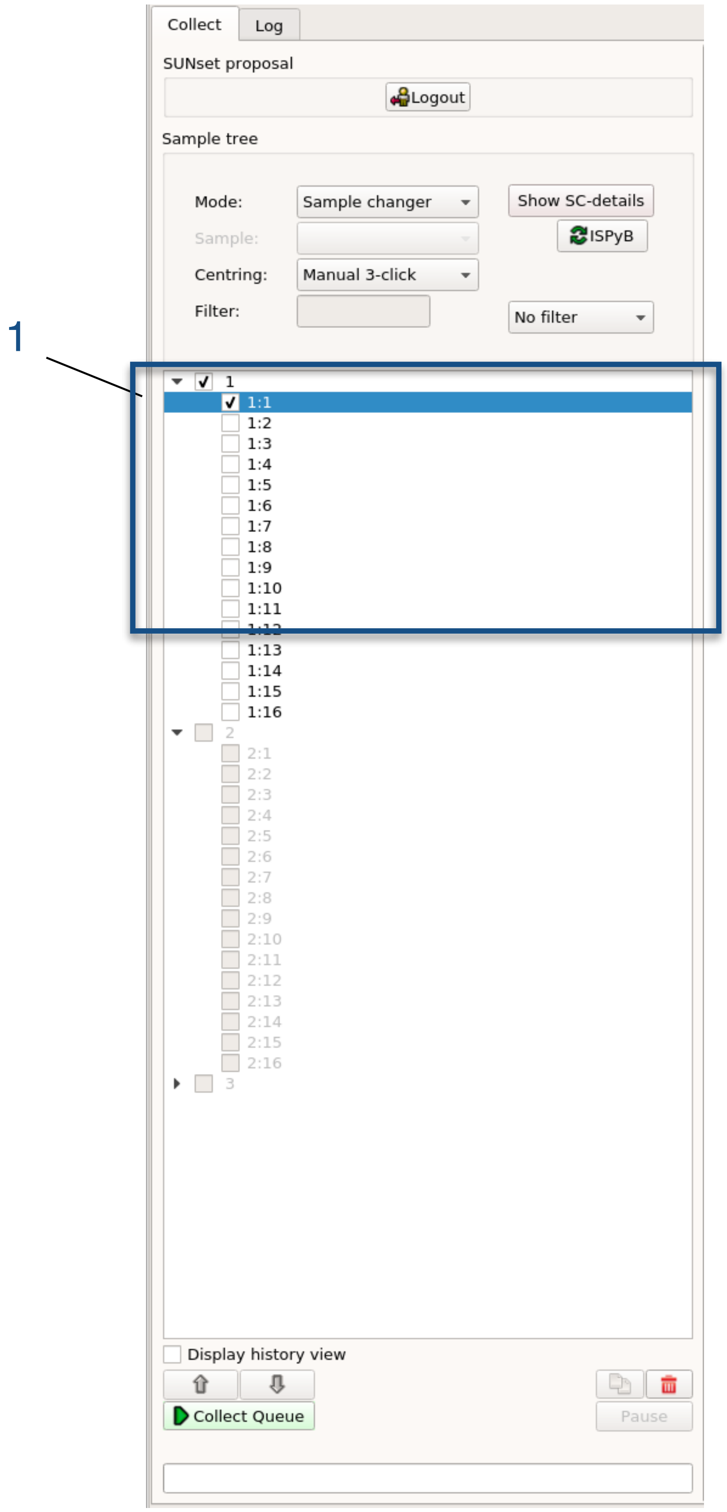
doors opened

CATS Status

Number of sample before the next dry and soak command : 10
Home and opened
Not in Automode : Check the key position

1. Cick on the « Show SC-details » to access to the
2. Click on Power ON to switch the robot ON
3. Click on Dry & Soak to dry and cool down the arm of the robot before charging the first sample.
   - The dry and soak procedure is mandatory the first time after loading the pucks. Afterwards it is automatically performed every 10 samples and after a Safe procedure
   - At the end of the dry and soak the lid of the dewar is closed and the arm of the robot plunges inside the dewar
4. Load the sample
5. Centre the sample and save
6. Select « Characterisation » and run the task (please see section Run a task associated to a position on a sample)

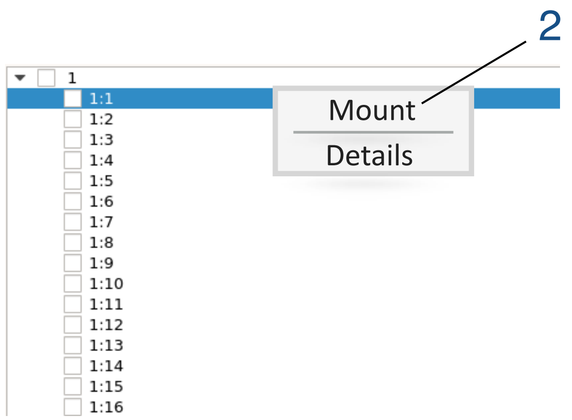
Practical guidelines:
Load and unload a sample

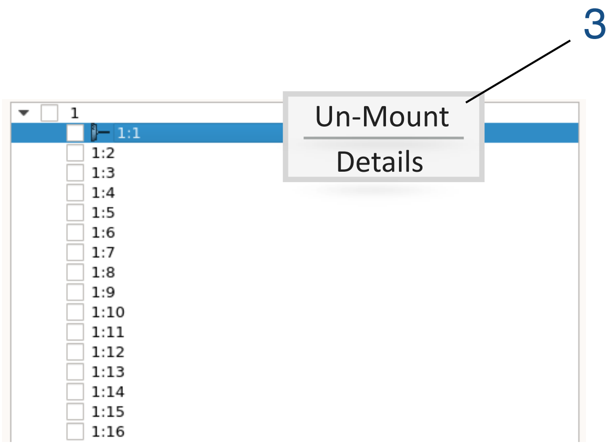


Mode: Sample changer

Centring: Manual 3-click

Filter: No filter

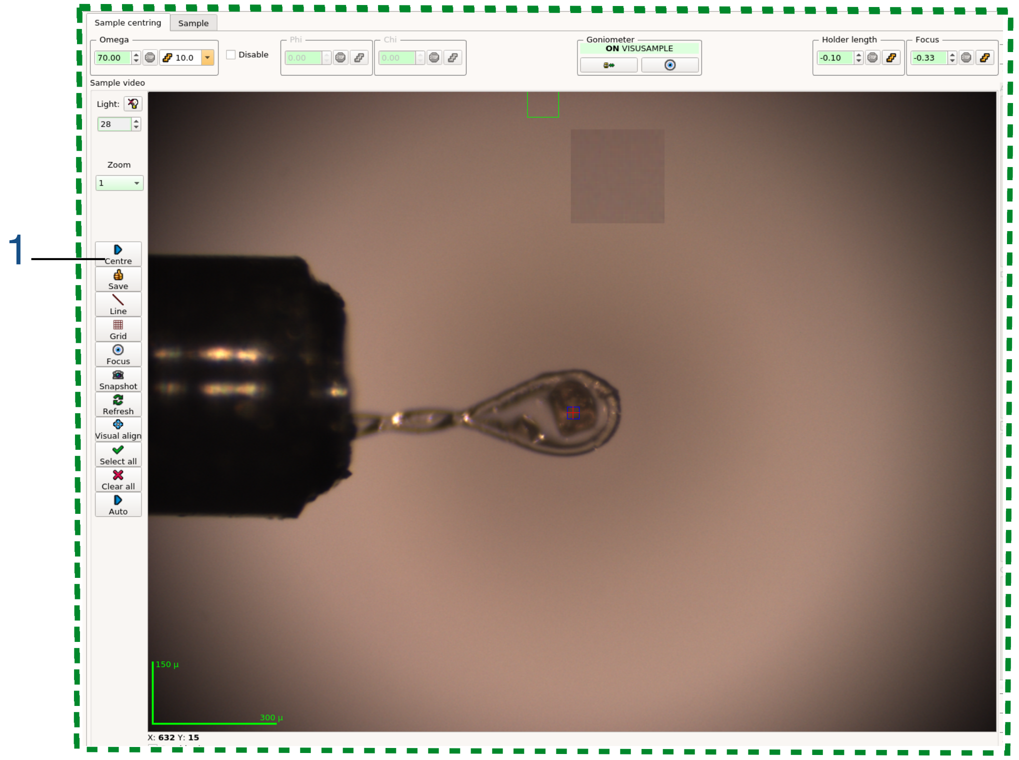




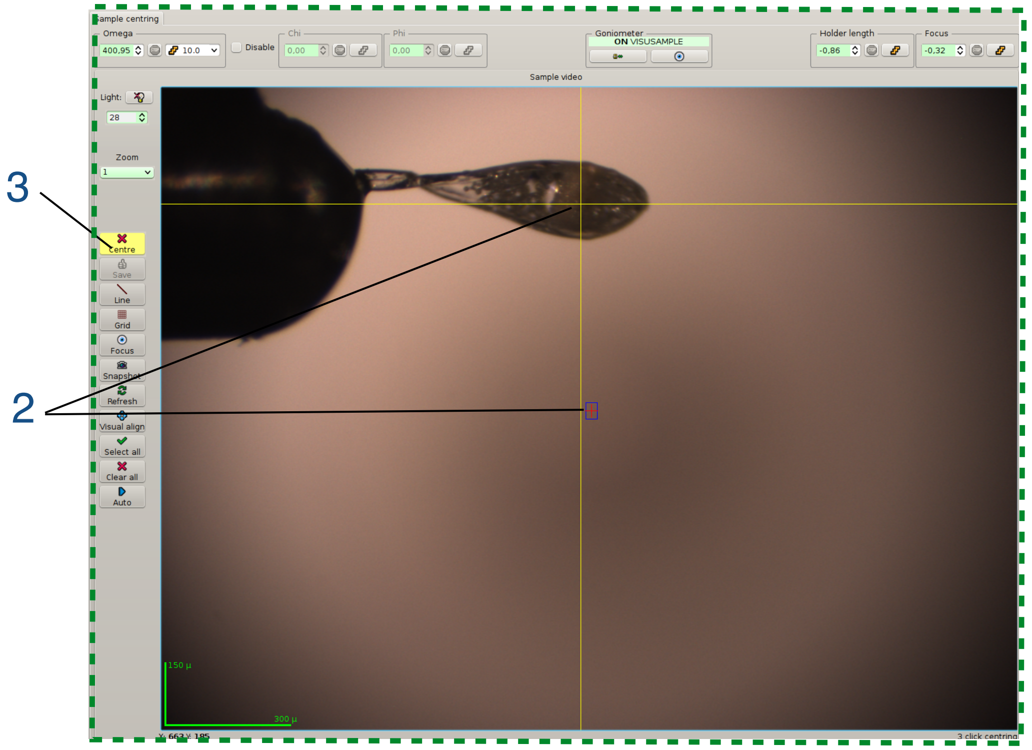
To load/un-load a sample the Sample changer mode must be selected

1. Click on a sample. The sample will be highlighted in blue
2. To mount a sample: right click on sample name to open to the sample changer menu and click on Mount
3. To unmount a sample: right click to open to the sample changer menu and click on Un-Mount

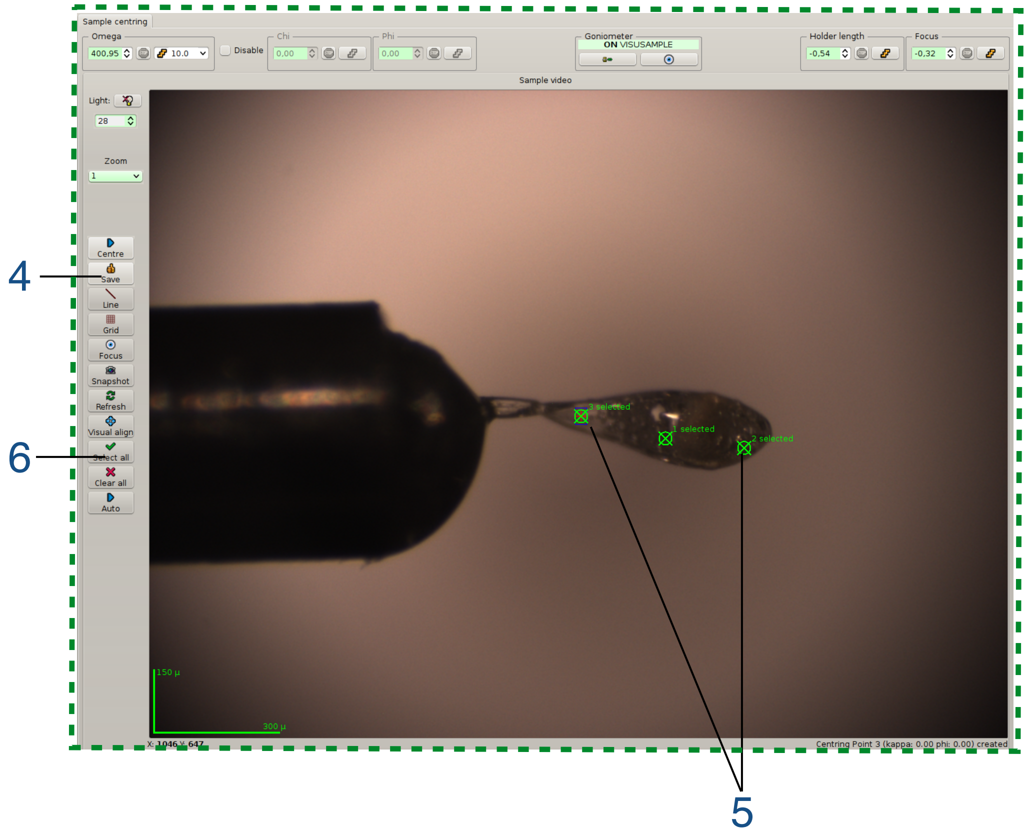
Practical guidelines:
Centre the sample and save one (or more) position(s)



X: 632 Y: 15



3 click centring

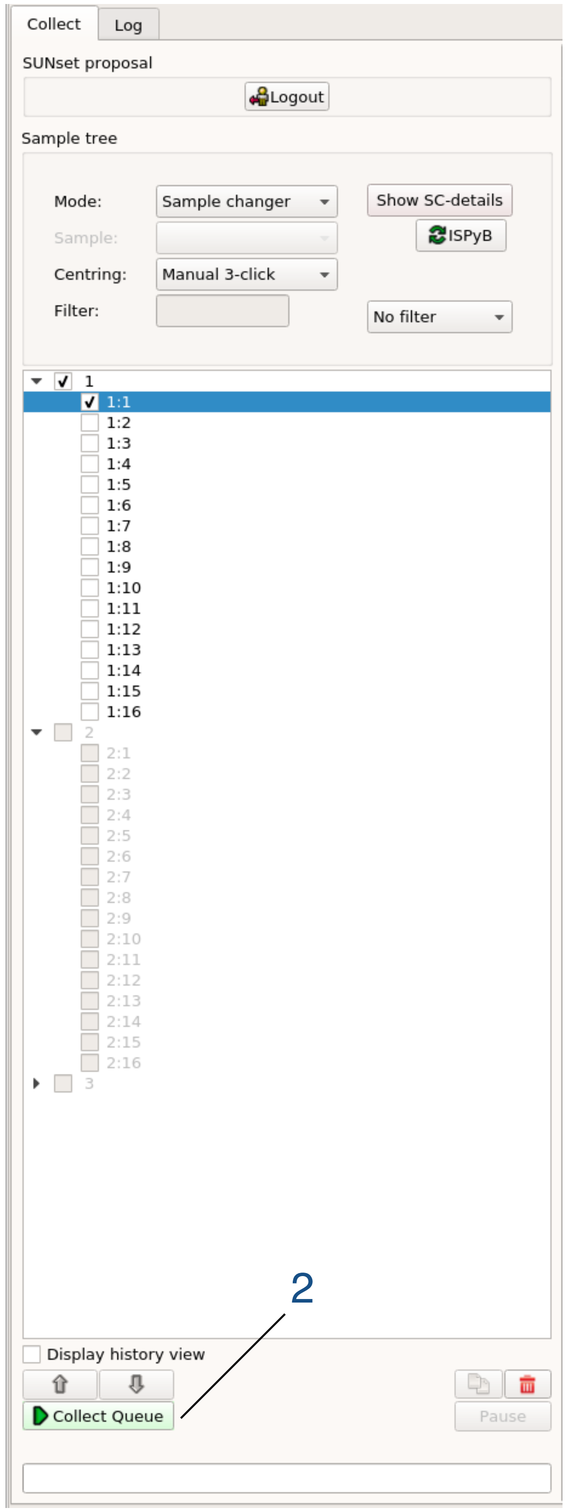


X: 1046 Y: 647

Centring Point 3 (kappa: 0.00 phi: 0.00) created

1. Load the sample and click on Centre
2. To centre click 3 times on the point of the sample you want to centre in the beam (the beam is represented by the red cross)
3. To reject the position click on Centre
4. To save the postion click on Save (mandatory to start the data collection). The yellow circle becomes bold green and a number apprears beside (selected position)
5. Repeat point 2, 3 and 5 to save additional positions.
6. To select all the centring points click left and drag or click on Select all

Practical guidelines:
Run a task associated to a position on a sample



SUNset proposal

Sample tree

Mode: Sample changer

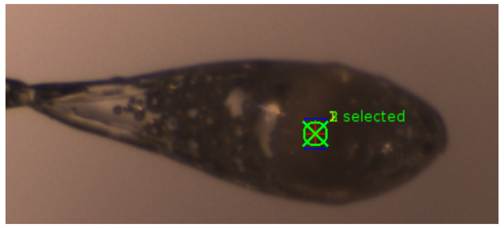
Sample:

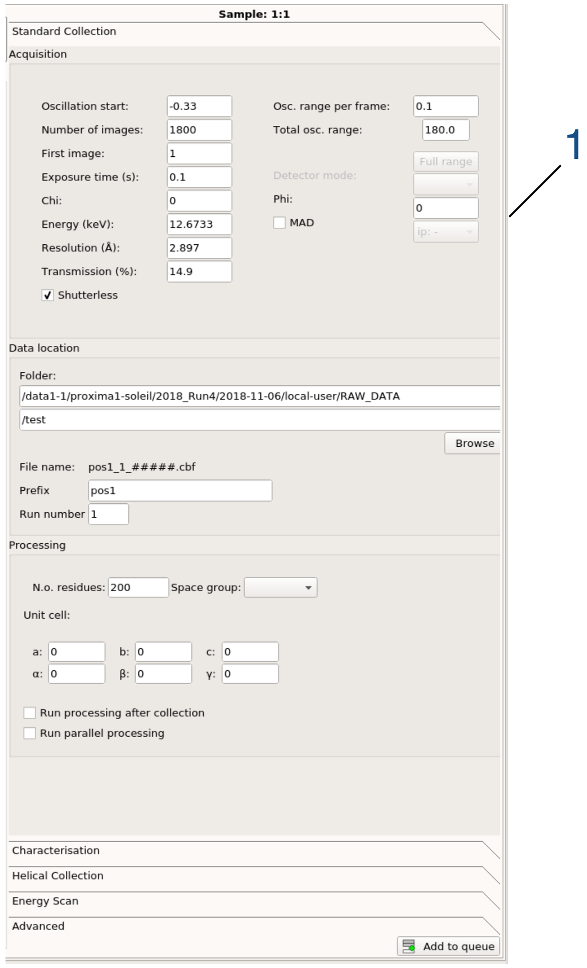
Centring: Manual 3-click

Filter:

- ☑ 1
  - ☑ 1:1
  - ☐ 1:2
  - ☐ 1:3
  - ☐ 1:4
  - ☐ 1:5
  - ☐ 1:6
  - ☐ 1:7
  - ☐ 1:8
  - ☐ 1:9
  - ☐ 1:10
  - ☐ 1:11
  - ☐ 1:12
  - ☐ 1:13
  - ☐ 1:14
  - ☐ 1:15
  - ☐ 1:16
- ☐ 2
  - ☐ 2:1
  - ☐ 2:2
  - ☐ 2:3
  - ☐ 2:4
  - ☐ 2:5
  - ☐ 2:6
  - ☐ 2:7
  - ☐ 2:8
  - ☐ 2:9
  - ☐ 2:10
  - ☐ 2:11
  - ☐ 2:12
  - ☐ 2:13
  - ☐ 2:14
  - ☐ 2:15
  - ☐ 2:16
- ☐ 3

☐ Display history view





Sample: 1:1

Oscillation start: -0.33

Number of images: 1800

First image: 1

Exposure time (s): 0.1

Chi: 0

Energy (keV): 12.6733

Resolution (Å): 2.897

Transmission (%): 14.9

☑ Shutterless

Osc. range per frame: 0.1

Total osc. range: 180.0

Detector mode:

Phi: 0

☐ MAD

ip: -

Data location

Folder: /data1-1/proxima1-soleil/2018_Run4/2018-11-06/local-user/RAW_DATA

/test

File name: pos1_1_#####.cbf

Prefix pos1

Run number 1

Processing

N.o. residues: 200 Space group:

Unit cell:

a: 0 b: 0 c: 0

α: 0 β: 0 γ: 0

☐ Run processing after collection

☐ Run parallel processing

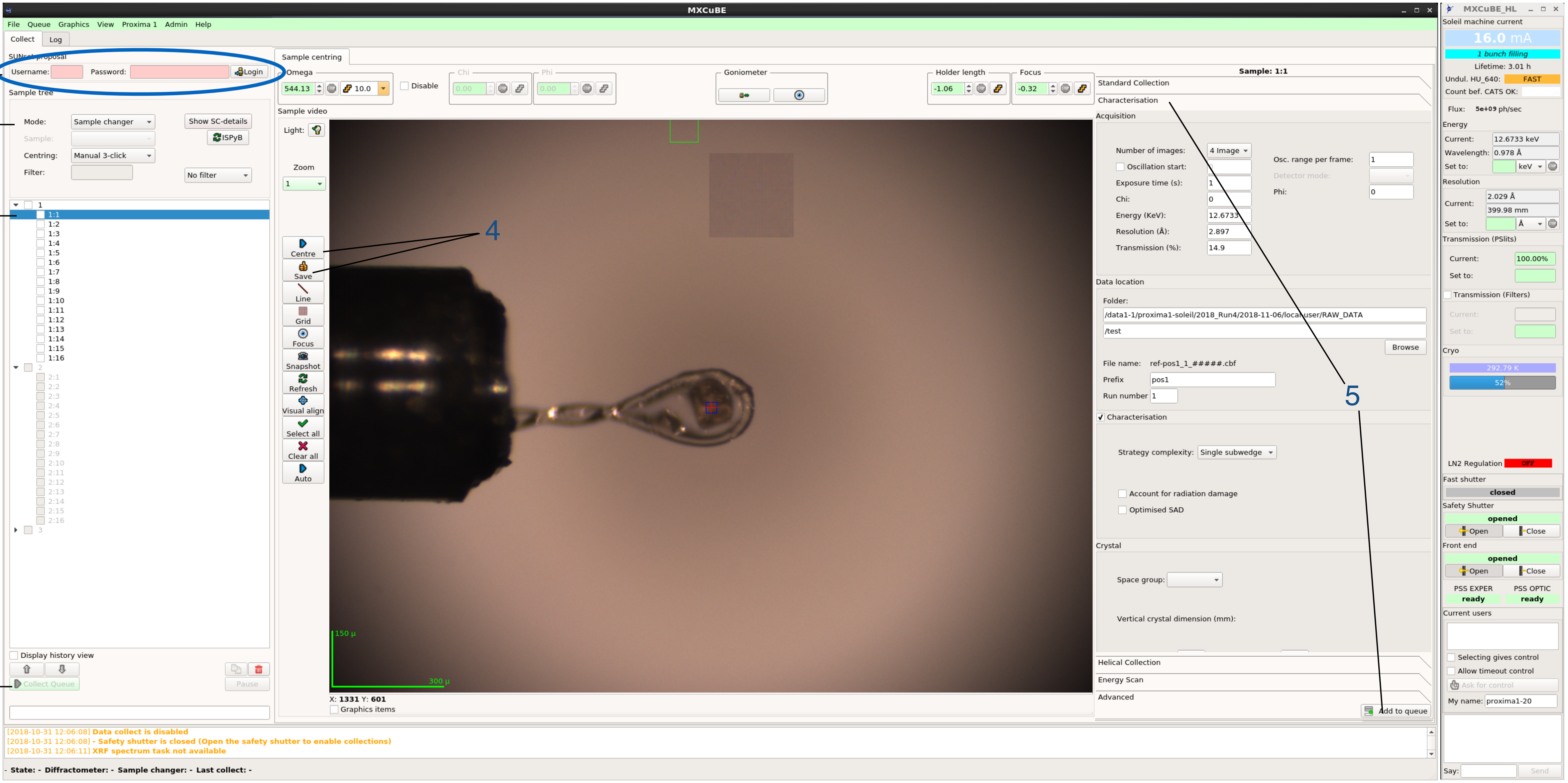
The sample and a saved position must be selected (please see section Centre the sample and save the position)

1. Fill in the parameters in the collection method associated to that position and click on « Add to queue »
2. The data collection is added to the sample list. Click on « Collect queue »

A confirmation message will appear, click on « Continue «

Please remember that each task is associated to the corresponding selected position

Practical guidelines
Collection mode: Characterisation



Mode: Sample changer

Centring: Manual 3-click

Filter: No filter

Sample: 1:1

Acquisition

Number of images: 4 Image

☐ Oscillation start:

Exposure time (s): 1

Chi: 0

Energy (KeV): 12.6733

Resolution (Å): 2.897

Transmission (%): 14.9

Osc. range per frame: 1

Phi: 0

Data location

Folder: /data1-1/proxima1-soleil/2018_Run4/2018-11-06/local-user/RAW_DATA /test

File name: ref-pos1_1_#####.cbf

Prefix: pos1

Run number: 1

☑ Characterisation

Strategy complexity: Single subwedge

☐ Account for radiation damage

☐ Optimised SAD

```
[2018-10-31 12:06:08] Data collect is disabled
[2018-10-31 12:06:08] - Safety shutter is closed (Open the safety shutter to enable collections)
[2018-10-31 12:06:11] XRF spectrum task not available
```

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

1. Log-in using your Proposal number and Password
2. Choose the charging mode
3. Load the sample
4. Centre the sample and save
5. Select « Characterisation » and run the task (please see section Run a task associated to a position on a sample)

Default parameters for sample Characterisation:

Numb. of images = 1, 2 or 4

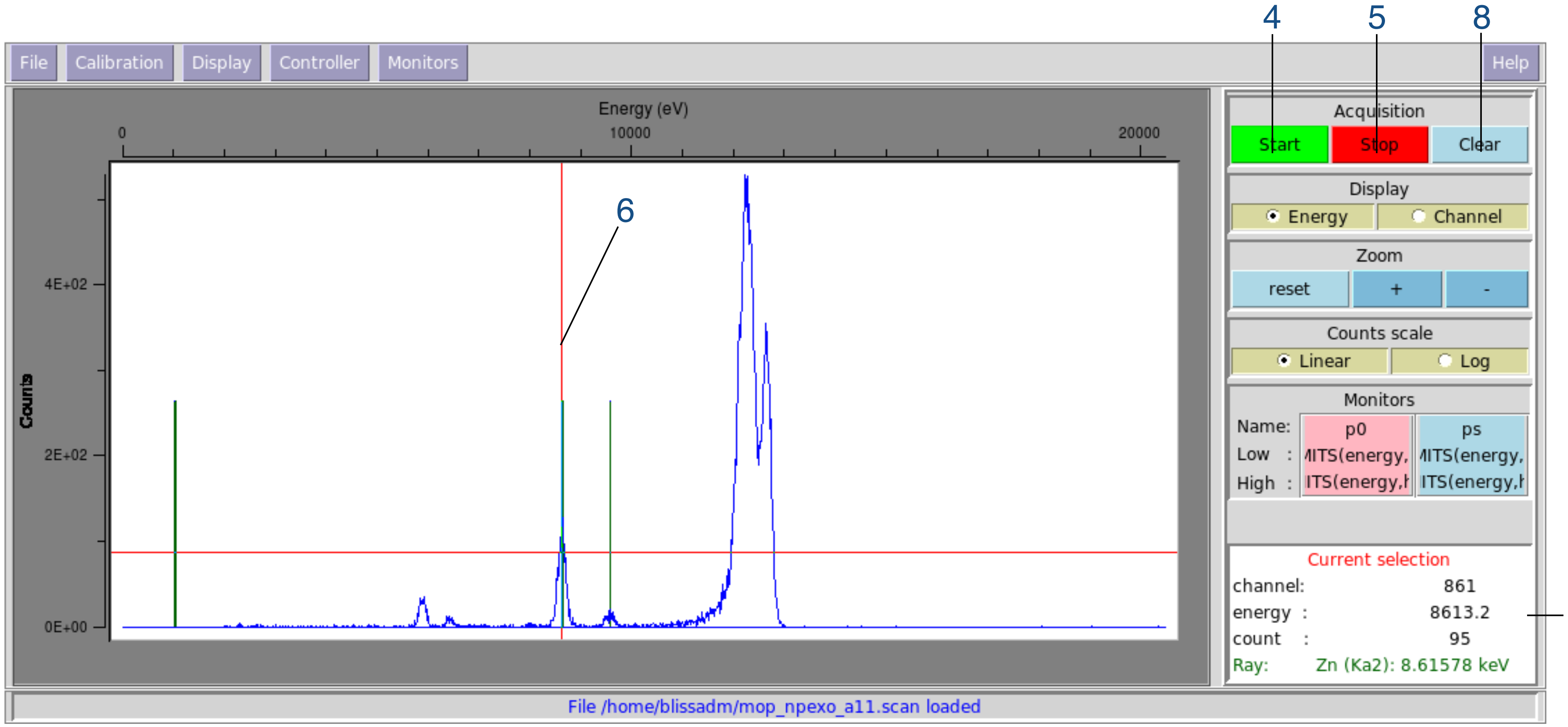
Oscillation start = 0°

Oscillation range per frame = 1°

Exposure time = 1 sec

Transmission = 10 - 15%

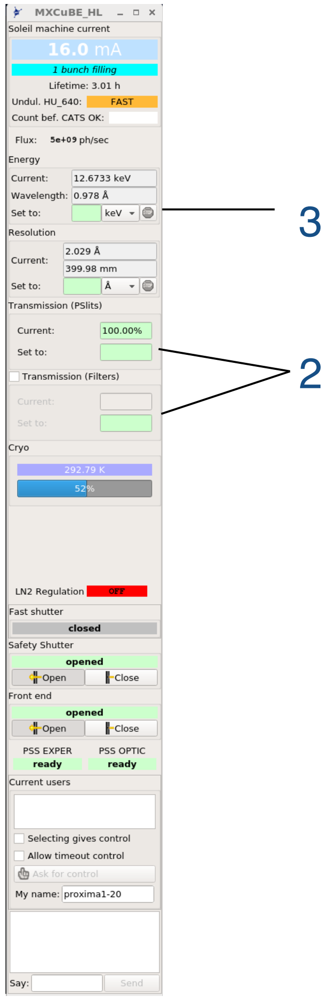
Practical guidelines:
Measure a XRF spectrum



Name: p0 ps
Low : IITS(energy, IITS(energy,
High : ITS(energy,I ITS(energy,I

Current selection
channel: 861
energy : 8613.2
count : 95
Ray: Zn (Ka2): 8.61578 keV

File /home/blissadm/mop_npexo_a11.scan loaded

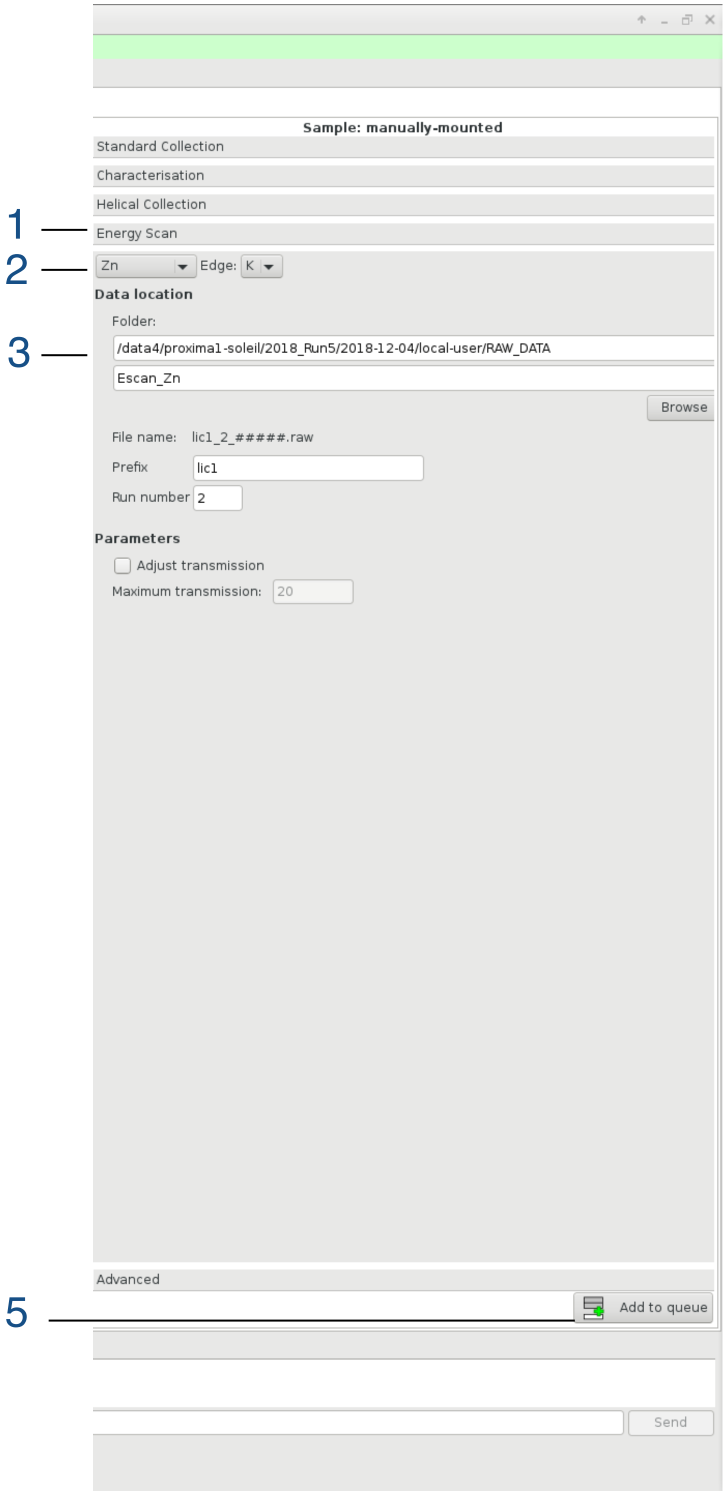


Soleil machine current
16.0 mA
1 bunch filling
Lifetime: 3.01 h
Undul. HU_640: FAST
Count bef. CATS OK:
Flux: 5e+09 ph/sec
Energy
Current: 12.6733 keV
Wavelength: 0.978 Å
Set to: keV
Resolution
Current: 2.029 Å 399.98 mm
Set to: Å
Transmission (PSlits)
Current: 100.00%
Set to:
☐ Transmission (Filters)
Current:
Set to:
Cryo
292.79 K
52%
LN2 Regulation OFF
Fast shutter
closed
Safety Shutter
opened
Front end
opened
PSS EXPER ready
PSS OPTIC ready
Current users
☐ Selecting gives control
☐ Allow timeout control
Ask for control
My name: proxima1-20
Say:

Use the XRF external application when you want to detect the presence of metals in your sample

1. Click onto the « FluoX Ketek » icon on the computer Desktop to open the XRF Program
2. Set up the suitable beam line energy (the value of the energy should be above the absorption edge of the metal you want to detect)
3. Set up the suitable attenuation for the Primary Slits (PSlits) and the Filters in the Machine Status panel (roughly 5% and 10% respectively)
4. Click Start
5. You can Stop your XRF measurement at any time
6. Left click on a peak to display the corresponding characteristic X-ray, energy and fluorescent element
7. The result of the XRF spectrum is displayed in the bottom right window
8. Click on « Clear » before starting a new measurement

Practical guidelines:
Energy Scan (SAD or MAD)



Sample: manually-mounted

Zn Edge: K

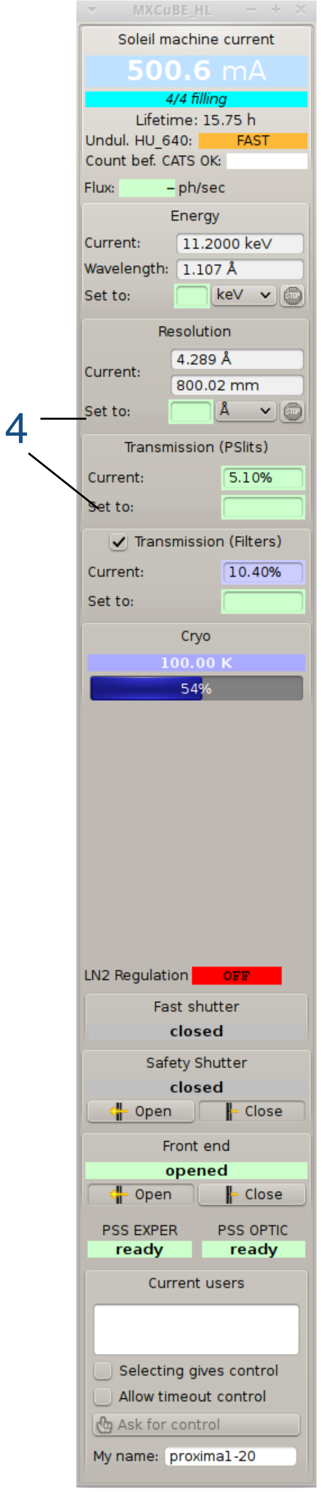
Data location

Folder:
/data4/proxima1-soleil/2018_Run5/2018-12-04/local-user/RAW_DATA
Escan_Zn

File name: lic1_2_#####.raw
Prefix: lic1
Run number: 2

Parameters

☐ Adjust transmission
Maximum transmission: 20



Soleil machine current
500.6 mA
4/4 filling
Lifetime: 15.75 h
Undul. HU_640: FAST
Count bef. CATS OK:
Flux: – ph/sec

Energy
Current: 11.2000 keV
Wavelength: 1.107 Å
Set to: keV

Resolution
Current: 4.289 Å
800.02 mm
Set to: Å

Transmission (PSlits)
Current: 5.10%
Set to:

☑ Transmission (Filters)
Current: 10.40%
Set to:

Cryo
100.00 K
54%

LN2 Regulation OFF

Fast shutter
closed

Safety Shutter
closed

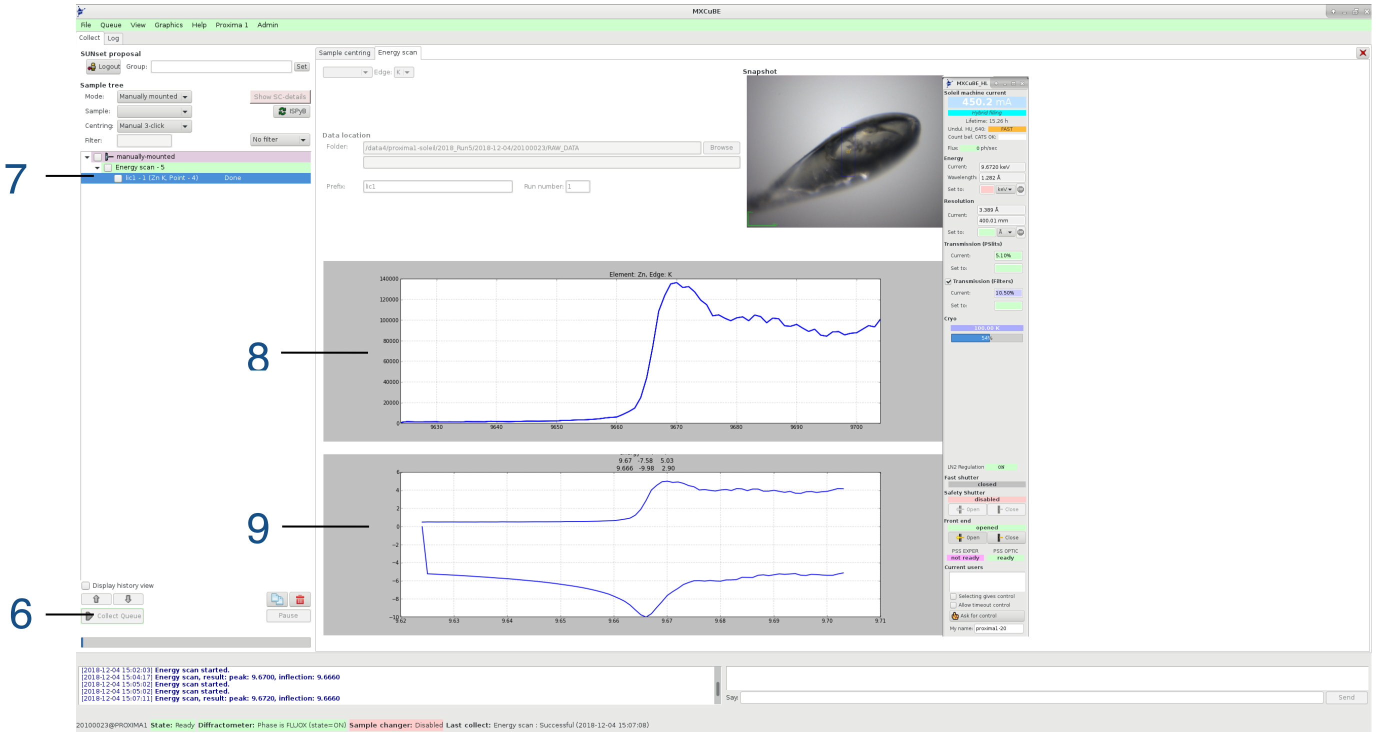
Front end
opened

PSS EXPER ready
PSS OPTIC ready

Current users

☐ Selecting gives control
☐ Allow timeout control

My name: proxima1-20



SUNset proposal
Group:

Sample tree
Mode: Manually mounted
Sample:
Centring: Manual 3-click
Filter: No filter

manually-mounted
Energy scan - 5
lic1 - 1 (Zn K, Point - 4) Done

☐ Display history view

Edge: K

Data location
Folder: /data4/proxima1-soleil/2018_Run5/2018-12-04/20100023/RAW_DATA
Prefix: lic1 Run number: 1

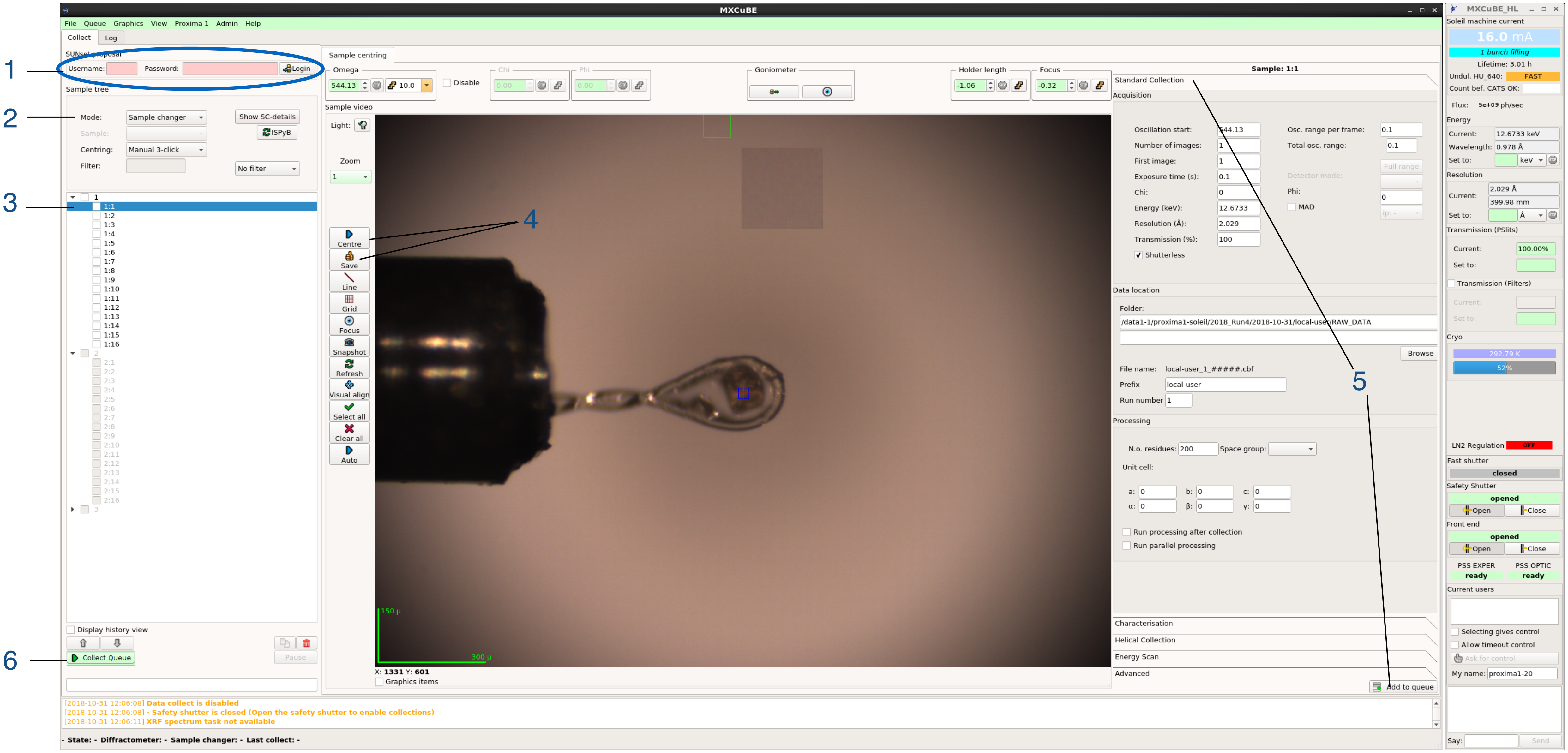
9.67 -7.58 5.03
9.666 -9.98 2.90

```
[2018-12-04 15:02:03] Energy scan started.
[2018-12-04 15:04:17] Energy scan, result: peak: 9.6700, inflection: 9.6660
[2018-12-04 15:05:02] Energy scan started.
[2018-12-04 15:05:02] Energy scan started.
[2018-12-04 15:07:11] Energy scan, result: peak: 9.6720, inflection: 9.6660
```

20100023@PROXIMA1 **State:** Ready **Diffractometer:** Phase is FLUOX (state=ON) **Sample changer:** Disabled **Last collect:** Energy scan : Successful (2018-12-04 15:07:08)

1. Select « Energy Scan»
2. Select the anomalous scatterer present in your sample and the desired absorption edge
3. Enter the sample name
4. Select the suitable primary slits and filters attenuation (please ask your Local Contact)
5. Click on Add to queue
6. Click on Queue in the sample list menu
7. Double click on the prefix name in the sample list to display the Energy scan
8. Energy scan for the selected element
9. Result of the CHOOCH program with computed Energy, f', f'' values for the peak and inflection point
   At the end of CHOOCH the Beam line Energy will automatically be set up at the peak value

Practical guidelines
Collection mode: Standard Collection



Sample: 1:1

Standard Collection

Acquisition

Oscillation start: 544.13
Number of images: 1
First image: 1
Exposure time (s): 0.1
Chi: 0
Energy (keV): 12.6733
Resolution (Å): 2.029
Transmission (%): 100
☑ Shutterless
Osc. range per frame: 0.1
Total osc. range: 0.1
Phi: 0
☐ MAD

Data location

Folder: /data1-1/proxima1-soleil/2018_Run4/2018-10-31/local-user/RAW_DATA
File name: local-user_1_#####.cbf
Prefix local-user
Run number 1

Processing

N.o. residues: 200
Unit cell: a: 0 b: 0 c: 0 α: 0 β: 0 γ: 0
☐ Run processing after collection
☐ Run parallel processing

X: 1331 Y: 601
☐ Graphics items

```
[2018-10-31 12:06:08] Data collect is disabled
[2018-10-31 12:06:08] - Safety shutter is closed (Open the safety shutter to enable collections)
[2018-10-31 12:06:11] XRF spectrum task not available
```

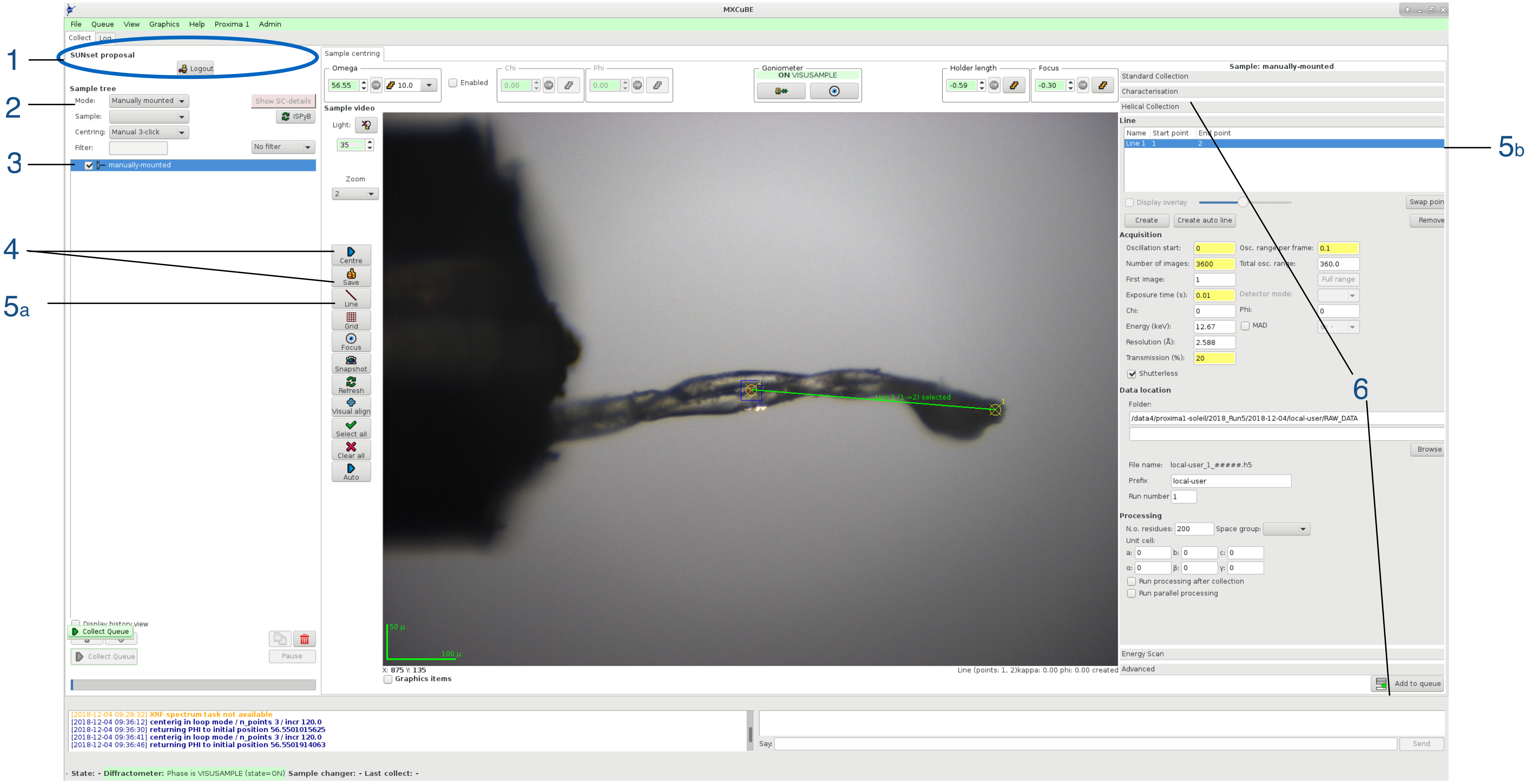
- State: - Diffractometer: - Sample changer: - Last collect: -

1. Log-in using your Proposal number and Password
2. Choose the charging mode
3. Load the sample
4. Centre the sample and save
5. Select « Standard Collection » and run the task (please see section <u>Run a task associated to a position on a sample</u>)

<u>Standard parameters for Collection:</u>

Oscillation start = Suggested by the strategy plan
N. of Images = Suggested by the strategy plan
Oscillation range per frame = 0.1°
Total oscillation range = 0.1°
Exposure time = 0.0125 sec
Transmission = 60%

Practical guidelines
Collection mode: Helical Collection



SUNset proposal

Sample tree

Mode: Manually mounted

Sample:

Centring: Manual 3-click

Filter: No filter

☑ manually-mounted

Omega: 56.55 — 10.0

Goniometer: ON VISUSAMPLE

Holder length: -0.59

Focus: -0.30

Sample video — Light: 35 — Zoom: 2

X: 875 Y: 135

☐ Graphics items

Line (points: 1, 2)kappa: 0.00 phi: 0.00 created

Sample: manually-mounted

Line

Name	Start point	End point
Line 1	1	2

☐ Display overlay

Acquisition

Oscillation start: 0 — Osc. range per frame: 0.1

Number of images: 3600 — Total osc. range: 360.0

First image: 1

Exposure time (s): 0.01 — Detector mode:

Chi: 0 — Phi: 0

Energy (keV): 12.67 — ☐ MAD

Resolution (Å): 2.588

Transmission (%): 20

☑ Shutterless

Data location

Folder: /data4/proxima1-soleil/2018_Run5/2018-12-04/local-user/RAW_DATA

File name: local-user_1_#####.h5

Prefix: local-user

Run number: 1

Processing

N.o. residues: 200 — Space group:

Unit cell:

a: 0 b: 0 c: 0

α: 0 β: 0 γ: 0

☐ Run processing after collection

☐ Run parallel processing

```
[2018-12-04 09:28:32] XRF spectrum task not available
[2018-12-04 09:36:12] centerig in loop mode / n_points 3 / incr 120.0
[2018-12-04 09:36:30] returning PHI to initial position 56.5501015625
[2018-12-04 09:36:41] centerig in loop mode / n_points 3 / incr 120.0
[2018-12-04 09:36:46] returning PHI to initial position 56.5501914063
```

- State: - **Diffractometer:** Phase is VISUSAMPLE (state=ON) **Sample changer:** - **Last collect:** -

1. Log-in using your Proposal number and Password
2. Choose the charging mode
3. Load the sample
4. Centre the sample in one end of the line (point1) and save the position

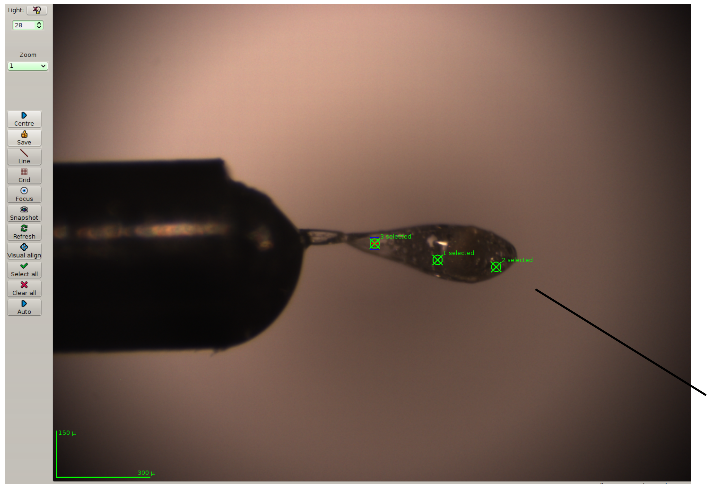
   Centre the sample in the second end of the line (point2) and save the position
5. Select both the centring points and click on the button Line (5a). A green line will appear connecting the two centring points as well as a description of the task (5b)
6. Select « Helical Collection » and run the task (please see section Run a task associated to a position on a sample)

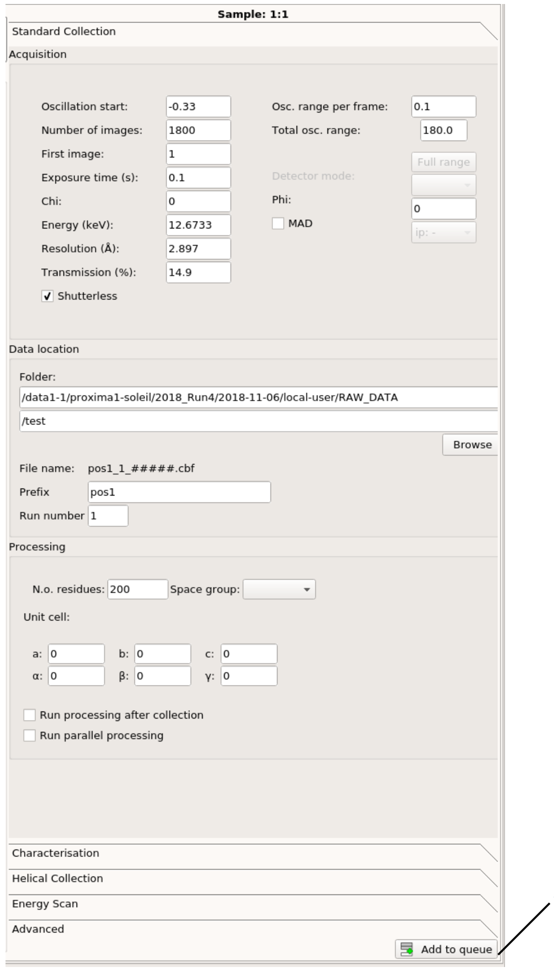
Practical guidelines:
Run the same collection method on multiple positions on the same sample

Follow these guidelines to perform for example a Characterisation on multiple centred positions on the same sample

Centre the sample and save several positions (please see <u>Centre the sample and save one (or more) position(s)</u>)

1. Select all saved position: left click and drag or click on Select all
2. Select a collection method (ex. Characterisation), fill the parameters, click on Add to queue
3. All the tasks will appear in the Sample tree, click on Collect Queue





Sample: 1:1

Standard Collection

Acquisition

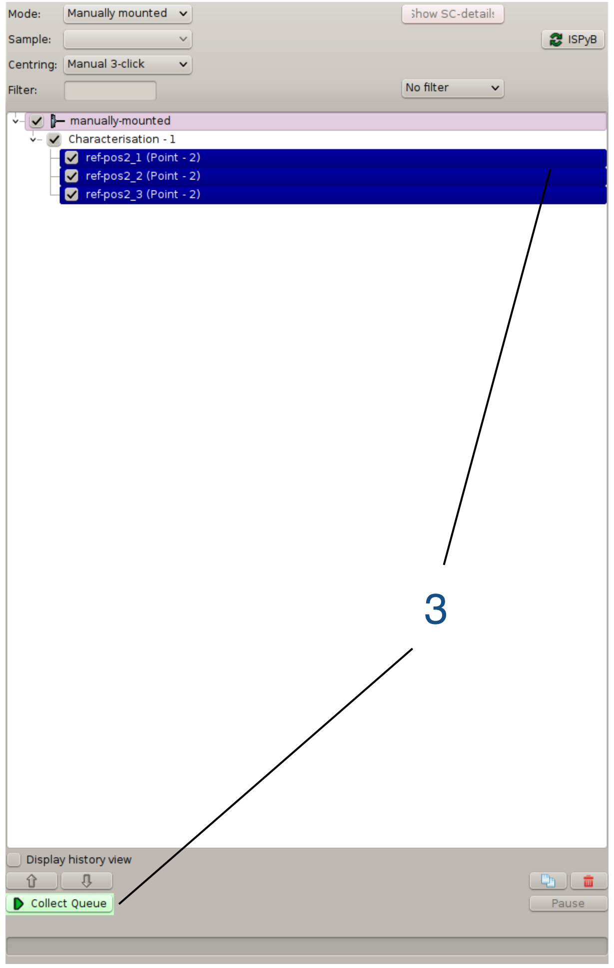
Oscillation start: -0.33
Number of images: 1800
First image: 1
Exposure time (s): 0.1
Chi: 0
Energy (keV): 12.6733
Resolution (Å): 2.897
Transmission (%): 14.9
☑ Shutterless
Osc. range per frame: 0.1
Total osc. range: 180.0
Detector mode:
Phi: 0
☐ MAD

Data location

Folder:
/data1-1/proxima1-soleil/2018_Run4/2018-11-06/local-user/RAW_DATA
/test
File name: pos1_1_#####.cbf
Prefix pos1
Run number 1

Processing

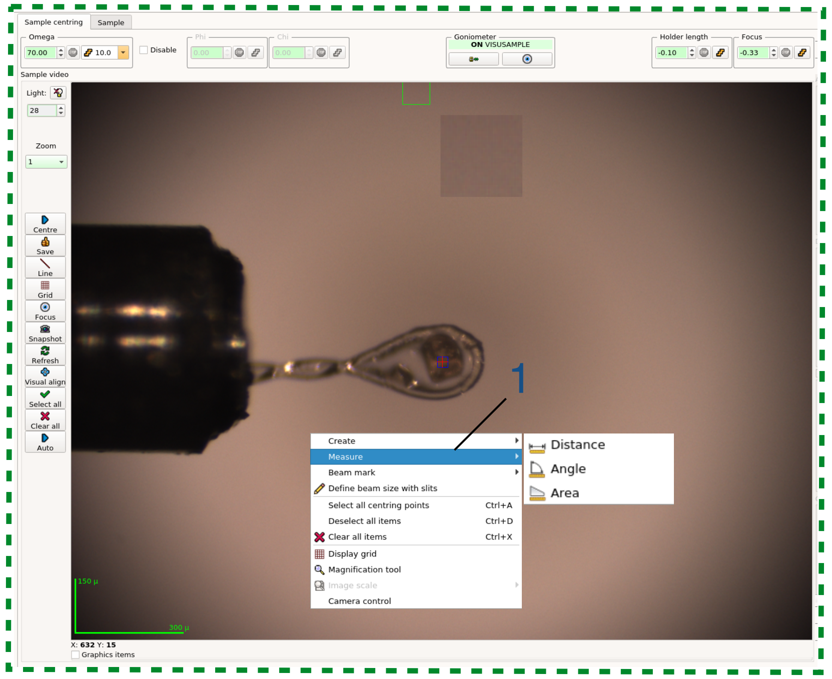
N.o. residues: 200 Space group:
Unit cell:
a: 0 b: 0 c: 0
α: 0 β: 0 γ: 0
☐ Run processing after collection
☐ Run parallel processing

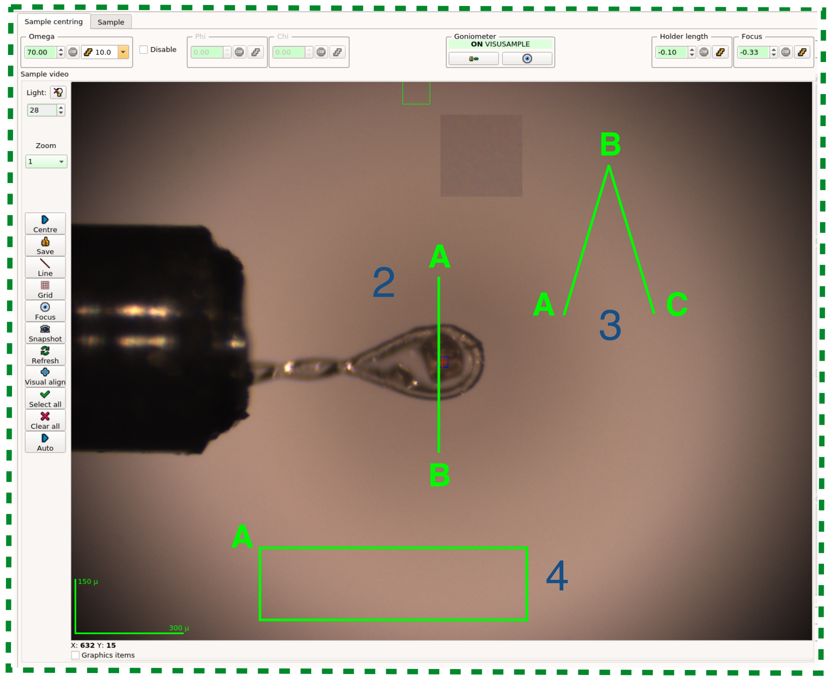


Mode: Manually mounted
Sample:
Centring: Manual 3-click
Filter:
No filter

- ☑ manually-mounted
  - ☑ Characterisation - 1
    - ☑ ref-pos2_1 (Point - 2)
    - ☑ ref-pos2_2 (Point - 2)
    - ☑ ref-pos2_3 (Point - 2)

Practical guidelines:
Measure distances, angles and areas





1. Right click on the sample view to open the measure menu
   Click on the measure you want to perform (distance, angle, area)

2. Measure distances: Click on the starting point (A) and the ending point (B)

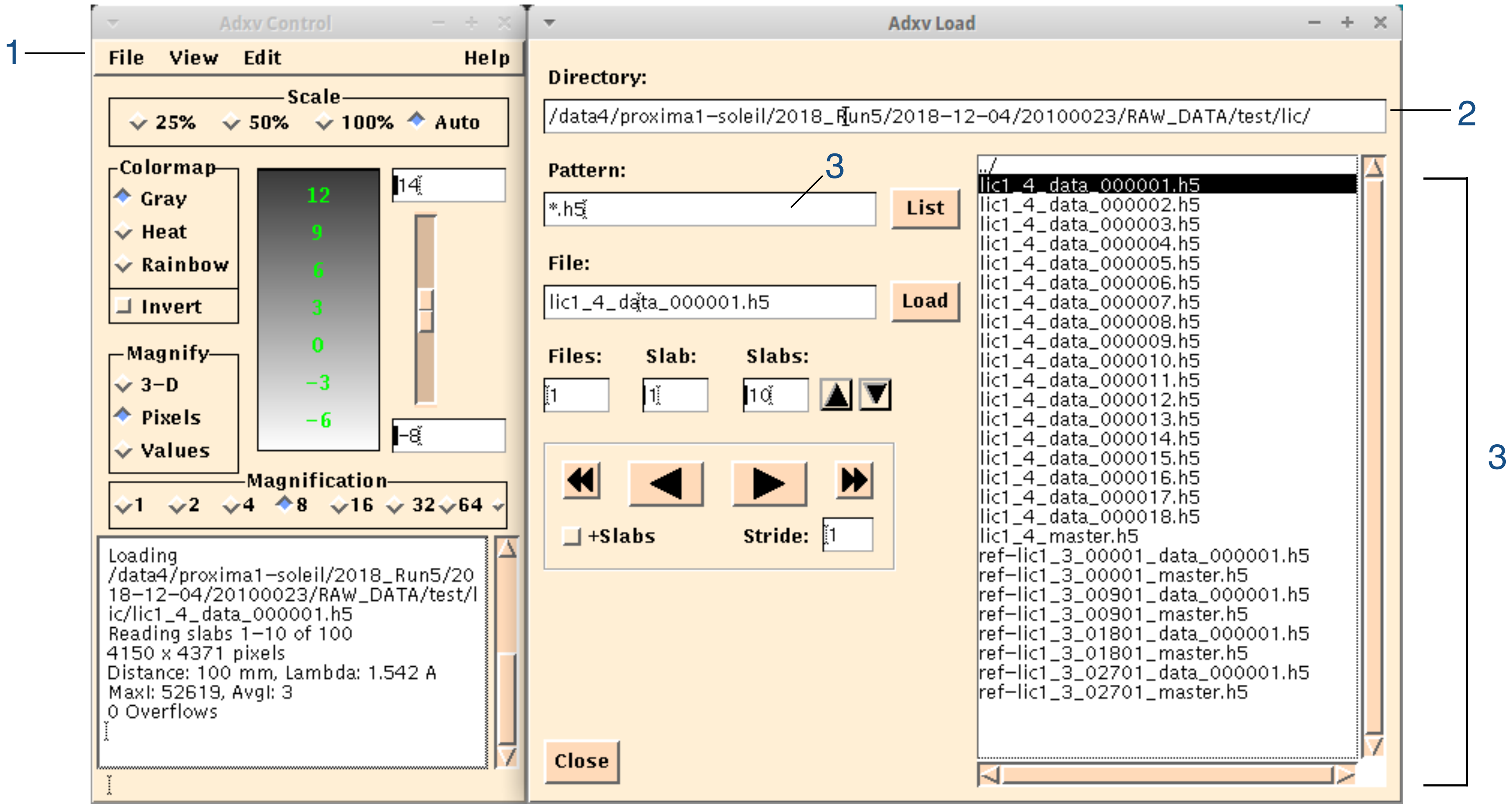
3. Measure angles: click on the end of the first branch (A), then on the peak of the angle (B) and finally on the end of the second branch (C)

4. Measure areas: click on the first point (A) and draw the desired polygon

- The value of the measurement will appear beside the measure on the sample view (not for area measurements)

- To delete a measurement double click on the sample view

Practical guidelines:
Visualise the diffraction images with ADXV



Scale: ● Auto

Colormap: ● Gray

Magnify: ● Pixels

Magnification: ● 8

14

-8

```
Loading
/data4/proxima1-soleil/2018_Run5/20
18-12-04/20100023/RAW_DATA/test/l
ic/lic1_4_data_000001.h5
Reading slabs 1-10 of 100
4150 x 4371 pixels
Distance: 100 mm, Lambda: 1.542 A
MaxI: 52619, AvgI: 3
0 Overflows
```

Directory: /data4/proxima1-soleil/2018_Run5/2018-12-04/20100023/RAW_DATA/test/lic/

Pattern: *.h5

File: lic1_4_data_000001.h5

Files: 1 Slab: 1 Slabs: 10

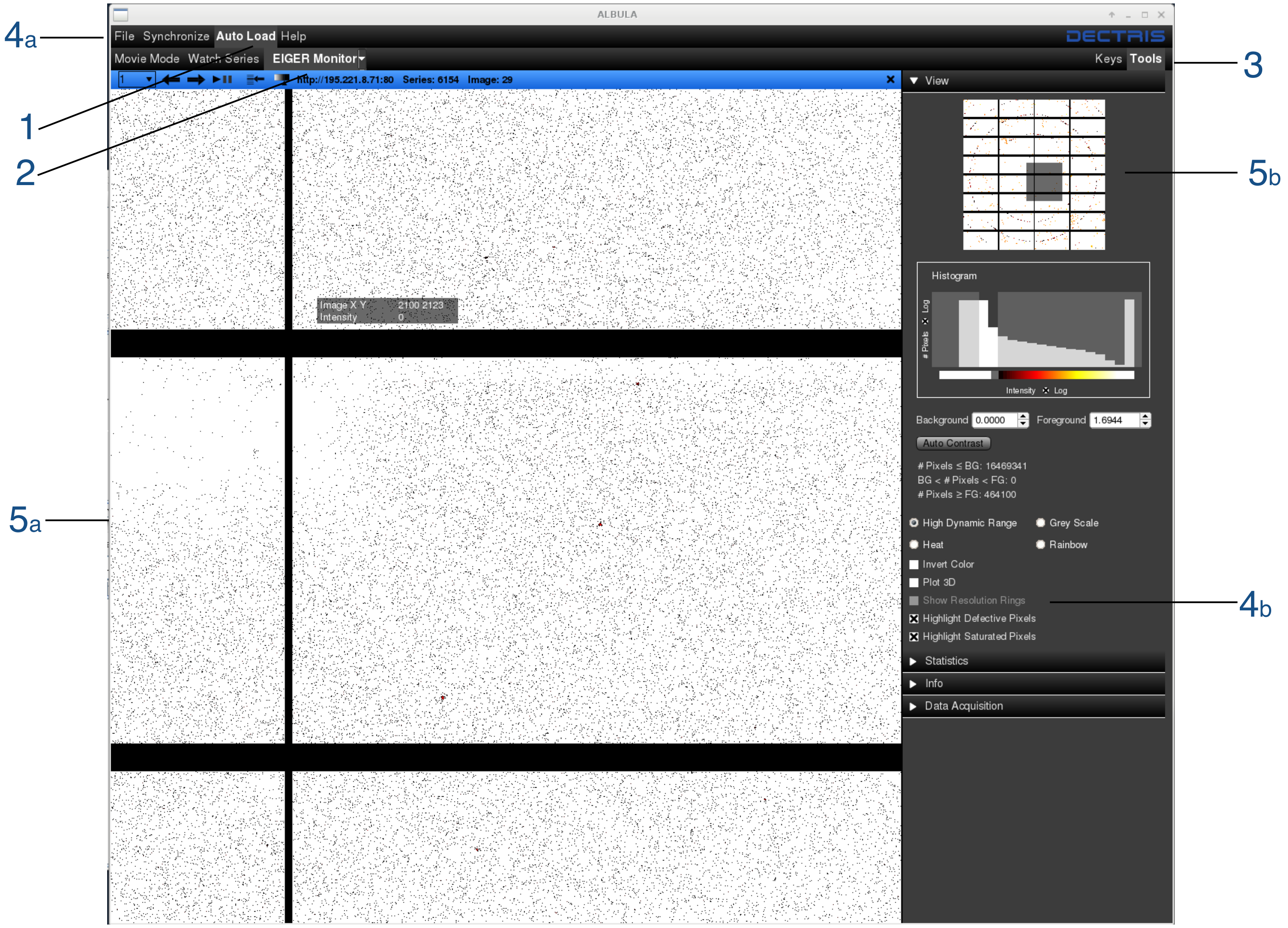
☐ +Slabs Stride: 1

```
../
lic1_4_data_000001.h5
lic1_4_data_000002.h5
lic1_4_data_000003.h5
lic1_4_data_000004.h5
lic1_4_data_000005.h5
lic1_4_data_000006.h5
lic1_4_data_000007.h5
lic1_4_data_000008.h5
lic1_4_data_000009.h5
lic1_4_data_000010.h5
lic1_4_data_000011.h5
lic1_4_data_000012.h5
lic1_4_data_000013.h5
lic1_4_data_000014.h5
lic1_4_data_000015.h5
lic1_4_data_000016.h5
lic1_4_data_000017.h5
lic1_4_data_000018.h5
lic1_4_master.h5
ref-lic1_3_00001_data_000001.h5
ref-lic1_3_00001_master.h5
ref-lic1_3_00901_data_000001.h5
ref-lic1_3_00901_master.h5
ref-lic1_3_01801_data_000001.h5
ref-lic1_3_01801_master.h5
ref-lic1_3_02701_data_000001.h5
ref-lic1_3_02701_master.h5
```

Use ADXV to inspect the diffraction images: (You won't be able to follow the progression of the diffraction images during the data collection)

1. Click on File, then click on Load
2. Retrieve your diffraction images directory
3. List diffraction images by sorting the h5 files
4. To load an image from the sample Characterisation:
   Click on the corresponding ref-XXX_master.h5 file, then click on the corresponding data_??????.h5 file and insert Slabs value = 10
5. To load an image from the sample Standard Collection:
   Click on the corresponding XXX_master.h5 file, then click on the corresponding data_??????.h5 file

Practical guidelines:
Visualise the diffraction images with ALBULA



http://195.221.8.71:80 Series: 6154 Image: 29

Image X Y 2100 2123
Intensity 0

Background 0.0000 Foreground 1.6944

Pixels ≤ BG: 16469341
BG < # Pixels < FG: 0
Pixels ≥ FG: 464100

● High Dynamic Range ○ Grey Scale
○ Heat ○ Rainbow
☐ Invert Color
☐ Plot 3D
☐ Show Resolution Rings
☒ Highlight Defective Pixels
☒ Highlight Saturated Pixels

Use ALBULA to inspect diffraction images: (You will be able to follow the progression of the diffraction images during the data collection)

1. Click on Auto Load
2. Click on EIGER Monitor
3. Click on Tools to open up the right panel
4. To show the resolution rings click on « File » (4a) then on « Show Resolution Rings » (4b)
   Please remember to scroll on the image to refresh the resolution rings values
5. To move on the diffraction image click left and drag on the diffraction image (5a) or click left and drag on the small window (5b)

Most frequent BUGs