

# MXCuBE user manual



# Table of content

Part I: Graphical User Interface Description	3	Part II: How to's	21
"Collect" homepage	4	Use the basics of MXCuBE	22
Login area	5	Link your sample list in MXCuBE with IPSyB	23
Sample list and collection queue	6	Select a sample from the sample changer and mount it	24
Sample centring and video area	9	Centre your sample and save a position	25
Collection method area (general)	10	Associate a task to a selected position of one sample	26
Collection method area (Standard Collection)	11	Perform same collection method on several positions of one sample	27
Collection method area (Characterisation)	12	Perform same collection method on multiple samples	28
Collection method area (Helical Collection)	13	Measure distances or angles	29
Collection method area (Energy Scan)	14	Measure your crystal size (ex: for a characterisation)	30
Collection method area (Advanced)	15	Perform a helical data collection	31
Machine status and Dialogue areas	16	Define a grid for a mesh scan or a X-ray centring	32
XRF spectrum tab	17	Perform a mesh scan	33
System tab	18	Perform a X-ray centring	34
Feedback tab	19	Do a kappa re-orientation	35
Chat tab	20	Do a visual re-orientation	36
		Measure an energy scan (MAD/SAD)	37
		Measure a X-ray fluorescence (XRF) spectrum	38
		Trouble shooting	39

**Part I:** 

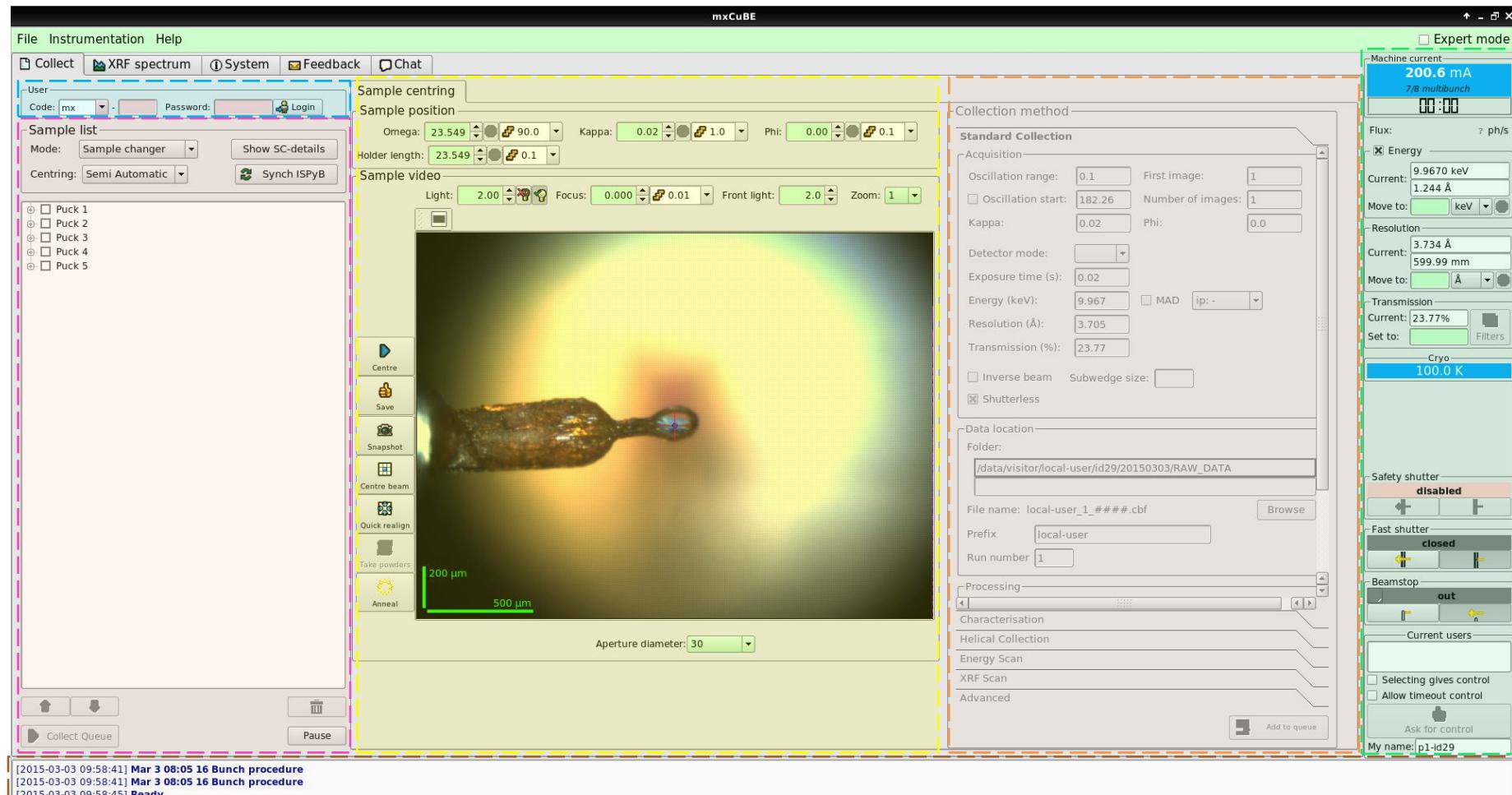
Click on a title to directly go  
to the corresponding page

# MXCuBE user manual

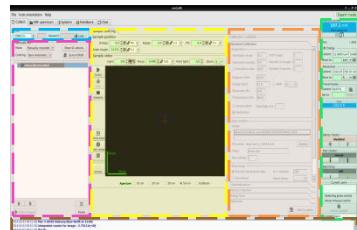
## Part I: Graphical User Interface Description



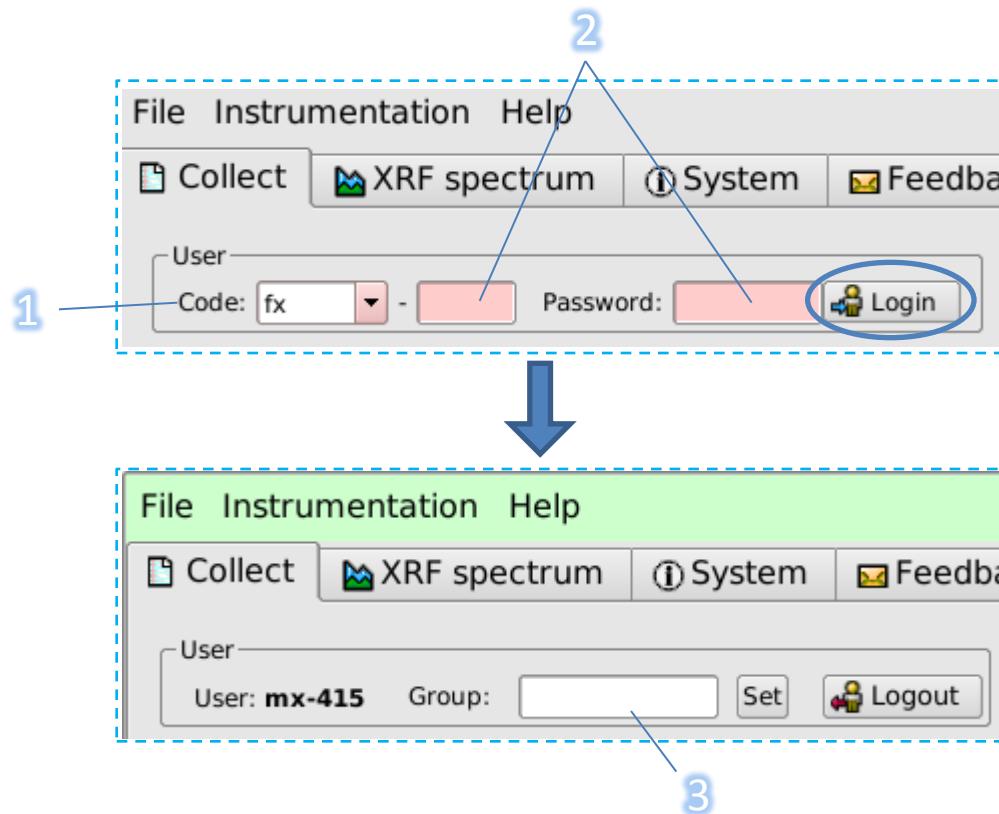
# GUI description: “Collect” homepage



- MXCuBE is divided into definite areas :
- Login
  - Sample list and data collection queue
  - Sample centring and video
  - Collection method
  - Machine status
  - Dialogue box



## GUI description: Login area



**Collection method**

**Standard Collection**

**Acquisition**

- Oscillation range: 0.1
- First image: 1
- Oscillation start: 183.39
- Number of images: 1
- Kappa: 0.02
- Phi: 0.0
- Detector mode:
- Exposure time (s): 0.02
- Energy (keV): 9.967
- MAD: ip: -
- Resolution (Å): 3.705
- Transmission (%): 23.77
- Inverse beam
- Subwedge size:
- Shutterless

**Data location**

Folder: /data/visitor/mx415/id29/20150303/RAW\_DATA

File name: mx415\_1\_####.cbf

Browse

Prefix: mx415

Run number: 1

**Processing**

**Characterisation**

**Helical Collection**

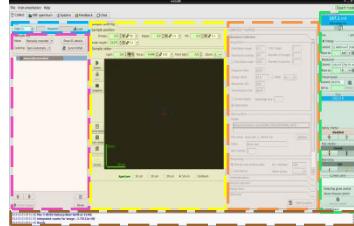
**Energy Scan**

**XRF Scan**

**Advanced**

Add to queue

## GUI description: Sample list and collection queue



**1** Sample list

Mode: Sample changer

Centring: Semi Automatic

1:1

Sample changer  
Mounted sample  
Manually mounted  
Plate

Show SC-details

Synch ISPyB

**2** Sample list

Mode: Sample changer

Centring: Manual

1:1

Manual  
Semi Automatic  
Fully Automatic

Show SC-details

Synch ISPyB

**3** Sample list

Mode: Manually mounted

Centring: Semi Automatic

**4** Sync ISPyB

**5**

**6**

**7**

manually-mounted

Collect Queue

Pause

**3** Sample list

Mode: Sample changer

Centring: Semi Automatic

**4** Sync ISPyB

**5**

**6**

**7**

Puck 1

1:1

1:2

1:3

1:4

1:5

1:6

1:7

1:8

1:9

1:10

Puck 2

2:1

2:2

2:3

2:4

2:5

2:6

2:7

2:8

2:9

2:10

Puck 3

Puck 4

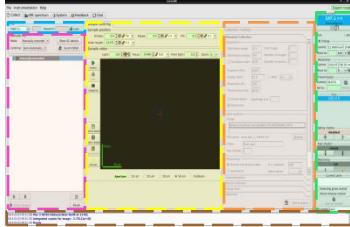
Puck 5

Collect Queue

Pause

- 1 Select the sample mounting mode
- 2 Select the default sample centring mode:
  - Manual: no automatic centring performed
  - Semi automatic: auto-loop centring requesting user validation (most common option)
  - Fully automatic: auto-loop centring without user validation (for automatic pipeline)
- 3 Show sample changer details (see next page)
- 4 Synchronize with ISPyB database to display a sample list (see "how to" section)
- 5 In sample changer mode: sample list sorted by puck appears, 1:1 = puck1: sample1
- 6 Delete the selected collection(s)
- 7 Pause the running chain of tasks

## GUI description: Sample list and collection queue (2)



**Sample list**

Mode: Sample changer ▾ Show SC-details  
Centring: Semi Automatic ▾ Synch ISPyB

- Puck 1
  - 1:1
  - 1:2
  - 1:3
  - 1:4
  - 1:5
  - 1:6
  - 1:7
  - 1:8
  - 1:9
  - 1:10
- Puck 2
  - 2:1
  - 2:2
  - 2:3
  - 2:4
  - 2:5
  - 2:6
  - 2:7
  - 2:8
  - 2:9
  - 2:10
- + Puck 3
- + Puck 4
- + Puck 5

↑ ↓ Delete Collect Queue Pause

**Sample list**

Mode: Sample changer ▾ Centring: Semi Automatic ▾

- Puck 1
  - 1:1 - Mnth-sample-E01
  - 1:2 - Mnth-sample-E02
  - 1:3 - Mnth-sample-E03
  - 1:4 - Mnth-sample-E04
  - 1:5 - Mnth-sample-E05
  - 1:6 - Mnth-sample-E06
  - 1:7 - Mnth-sample-E07
  - 1:8 - Mnth-sample-E08
  - 1:9 - Mnth-sample-E09
  - 1:10 - Mnth-sample-E10
- + Puck 2
- + Puck 3
- + Puck 4
- + Puck 5

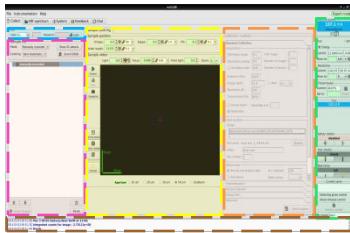
- 1 Sample list not updated with ISPyB content  
2 Sample list updated with ISPyB content

- 3 Tick the box corresponding to:
- a puck, to collect every tasks for this puck when clicking on “collect queue”
  - the first sample line, to collect every tasks for this sample when clicking on “collect queue”
  - a particular task, to collect only this task when clicking on “collect queue”
- 4 Sample status: - blue = mounted  
- black = selected  
- no color = not selected
- 5 List of tasks done or to be performed. Task status: - green = done  
- red = failed  
- yellow = collection done but no result  
- no color = to be done
- 6 Double click on task to see task plan/details (if not performed yet) or results (if performed)

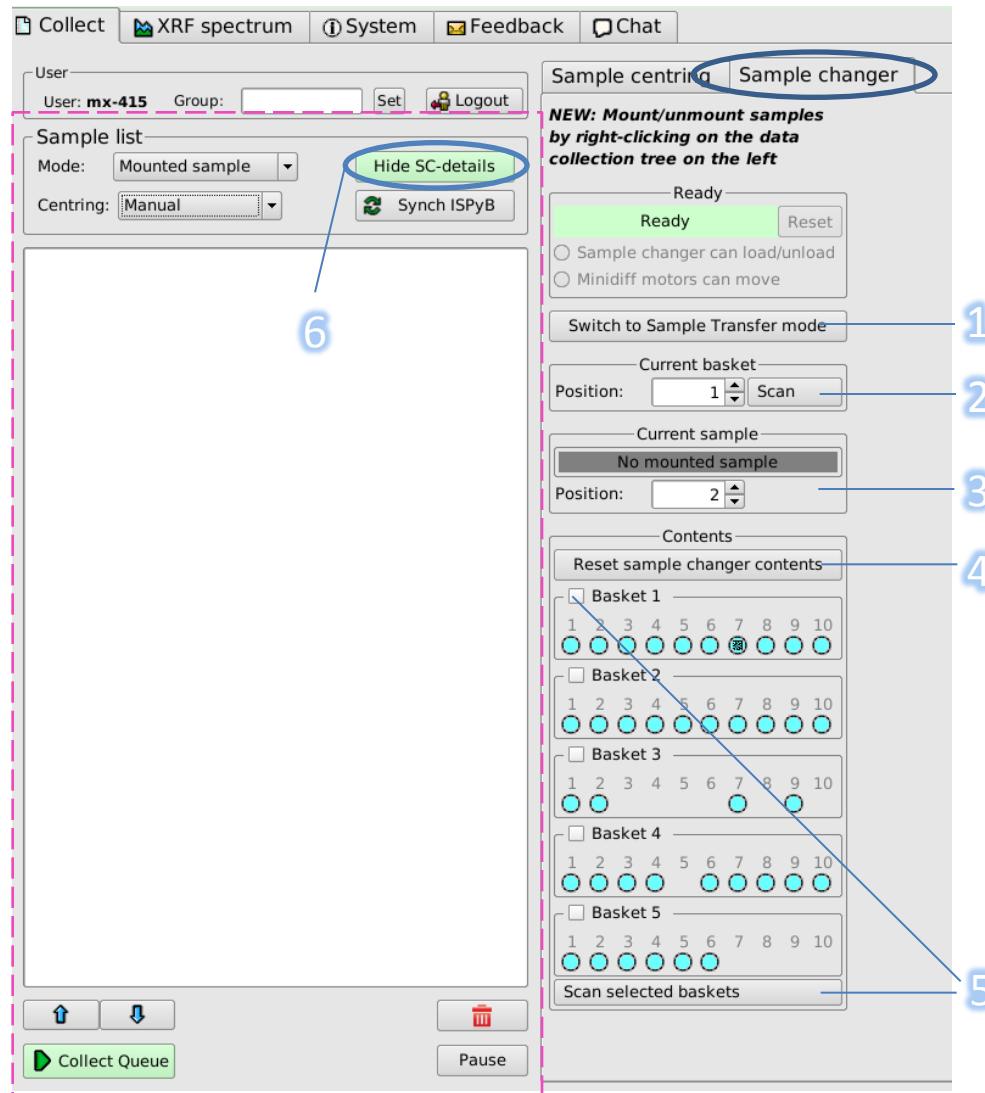
**Sample list**

Mode: Sample changer ▾ Show SC-details  
Centring: Semi Automatic ▾ Synch ISPyB

- Puck 1
  - 1:1 - Mnth-sample-E01
  - 1:2 - Mnth-sample-E02
  - Characterisation - 3
    - ref-Mnth-sample-E02\_1 (P... No result)
  - Standard - 2
    - Mnth-sample-E02\_1 (Point... Collection done)
  - 1:3 - Mnth-sample-E03
  - 1:4 - Mnth-sample-E04
  - 1:5 - Mnth-sample-E05



## GUI description: Sample list and collection queue (3)



The screenshot shows the MX-1 software interface with a pink dashed border around the central control area. At the top, there are tabs for Collect, XRF spectrum, System, Feedback, and Chat. Below the tabs, the user information shows 'User: mx-415' and 'Group: [ ]'. There are buttons for 'Set' and 'Logout'. The main area is titled 'Sample list' and includes fields for 'Mode: Mounted sample' and 'Centring: Manual'. A button 'Syncr ISPvB' is also present. On the right, there are two tabs: 'Sample centring' (circled in blue) and 'Sample changer' (circled in blue). A note below says: 'NEW: Mount/unmount samples by right-clicking on the data collection tree on the left'. The 'Sample changer' tab is active, showing a 'Ready' status with a 'Reset' button. It has sections for 'Current basket' (Position: 1, Scan button), 'Current sample' (No mounted sample), and 'Contents' (Basket 1 to Basket 5, each with a 10x10 grid of numbered circles). Buttons include 'Switch to Sample Transfer mode', 'Reset sample changer contents', and 'Scan selected baskets'. Navigation icons at the bottom include arrows for up/down, a trash can, and a 'Collect Queue' button.

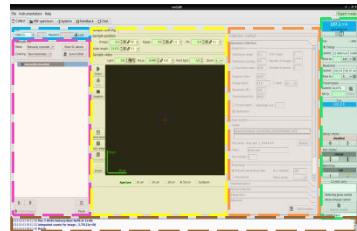
- 1 Switch sample changer state from basket transfer to sample transfer mode
- 2 View/Change basket position or scan current basket
- 3 View/Change sample position
- 4 Erase all barcodes previously read
- 5 Tick basket box and scan selected baskets
- 6 Hide the sample changer details

Here you can control the sample changer loading :

- 1 Switch sample changer state from basket transfer to sample transfer mode
- 2 View/Change basket position or scan current basket
- 3 View/Change sample position
- 4 Erase all barcodes previously read
- 5 Tick basket box and scan selected baskets
- 6 Hide the sample changer details

NB: This interface is not used to load sample (see "How to: Select a sample from the sample changer and mount it "section)

## GUI description: Sample centring and video area



**Sample centring**

**Sample position**

Omega: 23.56 ▾ ⚙ 90.0 ▾    Kappa: 0.02 ▾ ⚙ 1.0 ▾    Phi: 0.00 ▾ ⚙ 0.1 ▾

Holder length: 23.439 ▾ ⚙ 0.1 ▾

**Sample video**

Light: 1.00 ▾ ⚙ Focus: 0.000 ▾ ⚙ 0.01 ▾ Front light: 2.0 ▾ Zoom: 5 ▾

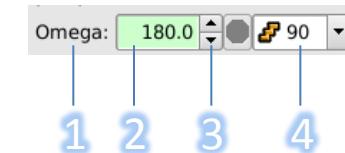
5 Centre  
 6 Save  
 7 Snapshot  
 8 Centre beam  
 9 Quick realign  
 10 Take powders  
 11 Anneal

12   
 13   
 14   
 15

17

Point no. 1 (kappa: 0.02 phi: 0.00) selected

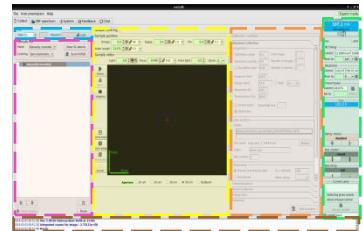
Aperture diameter: 30 ▾



- 1 Parameter
- 2 Current value. To change it write a value and press enter
- 3 Move the current value up or down by a step defined in (4)
- 4 Change tuning step

- 5 Three clicks centering of the sample
- 6 Save current centered position
- 7 Take a snapshot (automatically done at data collection start)
- 8 Align beam at sample position
- 9 Realign the beamline
- 10 Block the cryostream for a time length defined by the user
- 11 Select the beam aperture
- 12 Turn light on/off, adjust brightness
- 13 Adjust focus
- 14 Adjust front light intensity
- 15 Zoom in or out (1=far to 10=close)
- 16 Size and shape of the beam
- 17 Do a right click on the screen to show tools options

## GUI description: Collection method area (general)



**Collection method**

**Standard Collection**

**Acquisition**

- Oscillation range: 0.1
- First image: 1
- Oscillation start: 23.56
- Number of images: 1
- Kappa: 0.02
- Phi: 0.00
- Detector mode:
- Exposure time (s): 0.02
- Energy (keV): 9.967
- MAD ip: -
- Resolution (Å): 3.705
- Transmission (%): 0.0
- Inverse beam Subwedge size: [ ]
- Shutterless

**Data location**

Folder: /data/visitor/mx415/d29/20150303/RAW\_DATA

/test

File name: test\_2\_####.cbf

Browse

Prefix test

Run number 2

**Processing**

Characterisation

Helical Collection

Energy Scan

XRF Scan

Advanced

Add to queue

### 1 Collection method options

NB : For more information on the different options please refer to the “How to” section

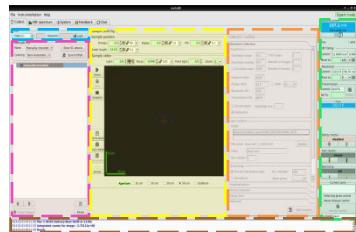
### 2 Data location is a common brick for all collection methods:

Folder-> subdirectories below the RAW\_DATA directory of your session. Automatically filled with “ACRONYM-samplename” if a sample list from ISPyB is synchronised

Prefix of your image: Automatically filled with “ACRONYM-samplename” if a sample list from ISPyB is synchronised

Run number-> incremented for each experiment from the same method

3 For each collection method, once you have adjusted the parameters, “Add to queue” will add the collection to the selected sample(s) and display it in the queue of the sample list area



## GUI description: Collection method area (Standard Collection)

**Collection method**

**Standard Collection**

**Acquisition**

- 2 Oscillation range:  First image:
- 3  Oscillation start:  Number of images:
- 4 Kappa:  Phi:
- 5 Detector mode:
- 6 Exposure time (s):
- 7 Energy (keV):   MAD
- Resolution (Å):
- Transmission (%):
- 8 Inverse beam  Subwedge size:
- 6 Shutterless

**Data location**

Folder:   
  
  
File name: test\_2\_####.cbf   
Prefix   
Run number

**Processing**

Characterisation  
Helical Collection  
Energy Scan  
XRF Scan  
Advanced

Use the standard collection when you know your diffraction plan.

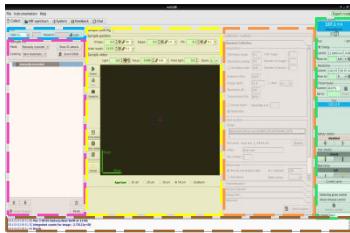
- 1 Fill in the different parameters from your diffraction plan
- 2 Tick if you want to start the oscillation at a particular angle (default is current angle)
- 3 To do a data collection with the same parameters but at different kappa angles please see the “how to” section
- 4 Tick if you want to use peak, inflection point and an energy from an energy scan
- 5 Tick if you want to perform a MAD data collection with Friedel paired reflections collected close in time
- 6 Tick to collect in a shutterless mode (ticked by default)
- 7 Number of frames in a subwedge
- 8 Fill in **both** if you want to force a particular space group in the EDNA auto-processing.

**Processing**

N.o. residues:  Space group:

Unit cell:

a: <input type="text" value="0"/>	b: <input type="text" value="0"/>	c: <input type="text" value="0"/>
$\alpha$ : <input type="text" value="0"/>	$\beta$ : <input type="text" value="0"/>	$\gamma$ : <input type="text" value="0"/>



## GUI description: Collection method area (Characterisation)

Collection method

**Characterisation**

Acquisition

- Number of images: 2 Images
- Exposure time: 0.05
- Oscillation range: 1.0
- Oscillation start: 23.56
- Kappa: 0.02
- Phi: 0.00
- Detector mode:
- Resolution (Å): 3.705
- Energy (KeV): 9.967
- Transmission (%): 0.0

Data location

Folder: /data/visitor/mx415/id29/20150303/RAW\_DATA

/test

File name: ref-test\_2\_####.cbf

Browse

Prefix: test

Run number: 2

Characterisation

Strategy complexity: Single subwedge

Account for radiation damage

Optimised SAD

Crystal

Helical Collection

Energy Scan

XRF Scan

Advanced

Add to queue

Use the characterisation option when you want to automatically obtain a diffraction plan from EDNA.

- Choose the number of images taken to characterise the crystal (1, 2 or 4)
- Tick if you want to start the oscillation at a particular angle
- To do a data collection with the same parameters but at different kappa angles please see the "how to" section
- Select the complexity of the diffraction plan you accept (1 or multiple subwedges)
- Tick if you want that EDNA takes the radiation damage into account (ticked by default)
- Tick if you want a diffraction plan for anomalous phasing
- Force EDNA to use the space group you provide
- Provide vertical dimensions of your crystal (2 measures 90° apart, see "How to: measure a crystal" section). It will be used by RADDose for dose absorption prediction

Crystal

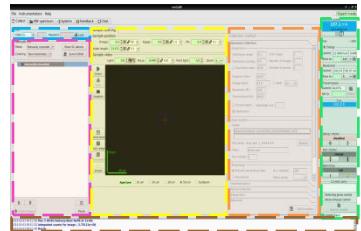
Space group:

Vertical crystal dimension (mm):

Min: 0.05 Max: 0.05

w at min: 0.0 w at max: 90.0

## GUI description: Collection method area (Helical Collection)



**Collection method**

- Standard Collection**
- Characterisation**
- Helical Collection**

**Lines**

1. Add line(s) to define path of the helical collection (see how to section)

**Acquisition**

Oscillation range: 0.1 First image: 1

Oscillation start: 183.39 Number of images: 1

Kappa: 0.02 Phi: 0.0

Detector mode:

Exposure time (s): 0.02

Energy (keV): 9.967 MAD ip: -

Resolution (Å): 3.705

Transmission (%): 0.0

5. Shutterless

**Data location**

Folder: /data/visitor/mx415/id29/20150303/RAW\_DATA

/test

File name: test\_2 #####.chf

Add to queue

Use the helical collection to collect along a specified line to minimize radiation damage

1. Add line(s) to define path of the helical collection (see how to section)
2. Fill in the different parameters from your diffraction plan
3. Tick if you want to start the oscillation at a particular angle
4. Tick if you want to perform MAD experiment
5. Tick to collect in shutterless mode (ticked by default)
6. Fill in if you want to force a particular space group in the EDNA auto-processing

**Processing**

N.o. residues: 200 Space group:

Unit cell:

a: 0	b: 0	c: 0
$\alpha$ : 0	$\beta$ : 0	$\gamma$ : 0

6

## GUI description: Collection method area (Energy Scan)

**Collection method**

- Standard Collection
- Characterisation
- Helical Collection
- Energy Scan**

**Available elements**

H										He								
Li	Be																	
Na	Mg																	
K	Ca	Sc	Ti	V	G	Mn	Fe	Co	Ni	Cu	Zn	B	C	N	O	F	Ne	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Ge	As	Se	Br	Kr
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	J	Xe
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt										
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu					
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr					

**Data location**

Folder:

File name: Mnth-sample-E02\_2\_####.raw

Prefix

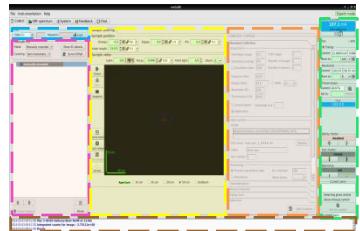
Run number

**XRF Scan**

Advanced

Perform an energy scan if you expect your crystal to contain a particular element that might be excited (Selenium, Iron, Magnesium...)

- 1 Select an element in the periodic table and click on “Add to queue”



## GUI description: Collection method area **(Advanced)**

**Collection method**

- Standard Collection
- Characterisation
- Helical Collection
- Energy Scan
- XRF Scan
- Advanced**

Workflow type

X-ray Centring

Data location

Folder:

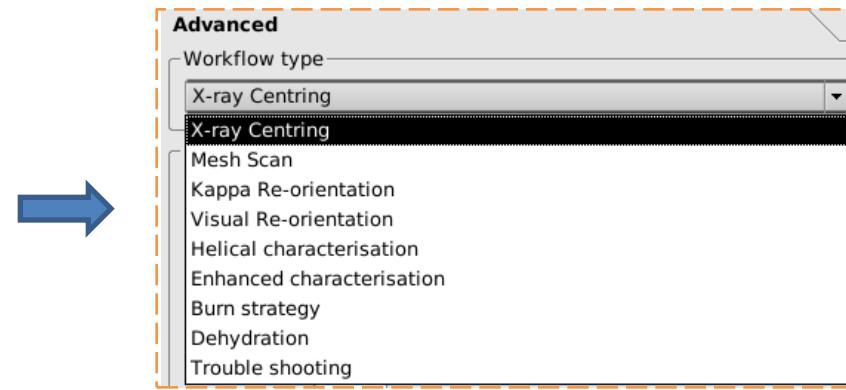
/data/visitor/mx415/id29/20150303/RAW\_DATA

/test

Browse

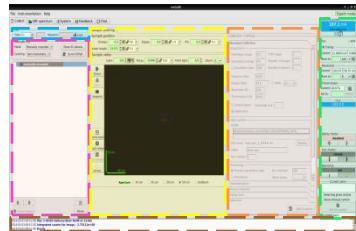
Prefix test

Run number 2

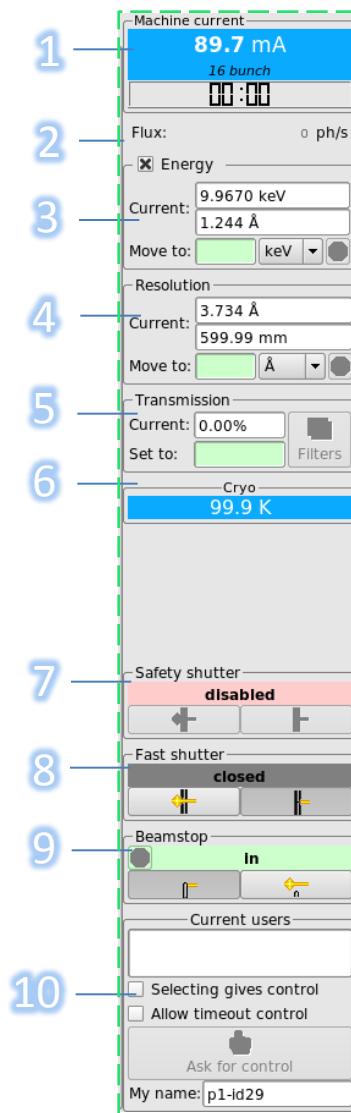


“Advanced” displays collection types made of task and decision series. Example: “X-ray centering” will center the best part of your crystal in the beam by doing a MESH scan followed by a line scan at 90° and will analyse the diffraction images

For more information on the different advanced options please refer to “How to” section



## GUI description: Machine status and Dialogue areas



- 1 Machine current and Synchrotron filling mode
- 2 Photon flux at sample position
- 3 Beamline energy. To adjust on tunable beamline: enter a value in the green box and press enter
- 4 Maximum resolution recorded at the edge of the detector. To adjust: enter a value in the green box and press enter
- 5 Beam transmission. To adjust: enter a value in the green box and press enter
- 6 Cryogenic stream temperature at sample position
- 7 Open/ Close the safety shutter. Not accessible when the experimental hutch door is open
- 8 Open/ Close the Fast shutter
- 9 Move the beamstop in or out of the beam
- 10 Remote access menu (local contact only)

[2014-03-03 09:51:29] Mar 3 09:03 Delivery:Next Refill at 21:00;  
[2014-03-03 09:51:33] Integrated counts for image : 2.75111e+08  
[2014-03-03 09:51:34] Ready

Dialogue area : here MXCuBE indicates what it is doing or its status. It will flash orange when a new information is displayed or when user input is required

# GUI description: XFR Scan and XRF spectrum tab

**Collection method**

- Standard Collection
- Characterisation
- Helical Collection
- Energy Scan
- XRF Scan**

**Data location**

Folder:

File name: Mnth-sample-E02

Prefix: Mnth-sample-E02

Run number: 2

**Parameters**

Count time: 1

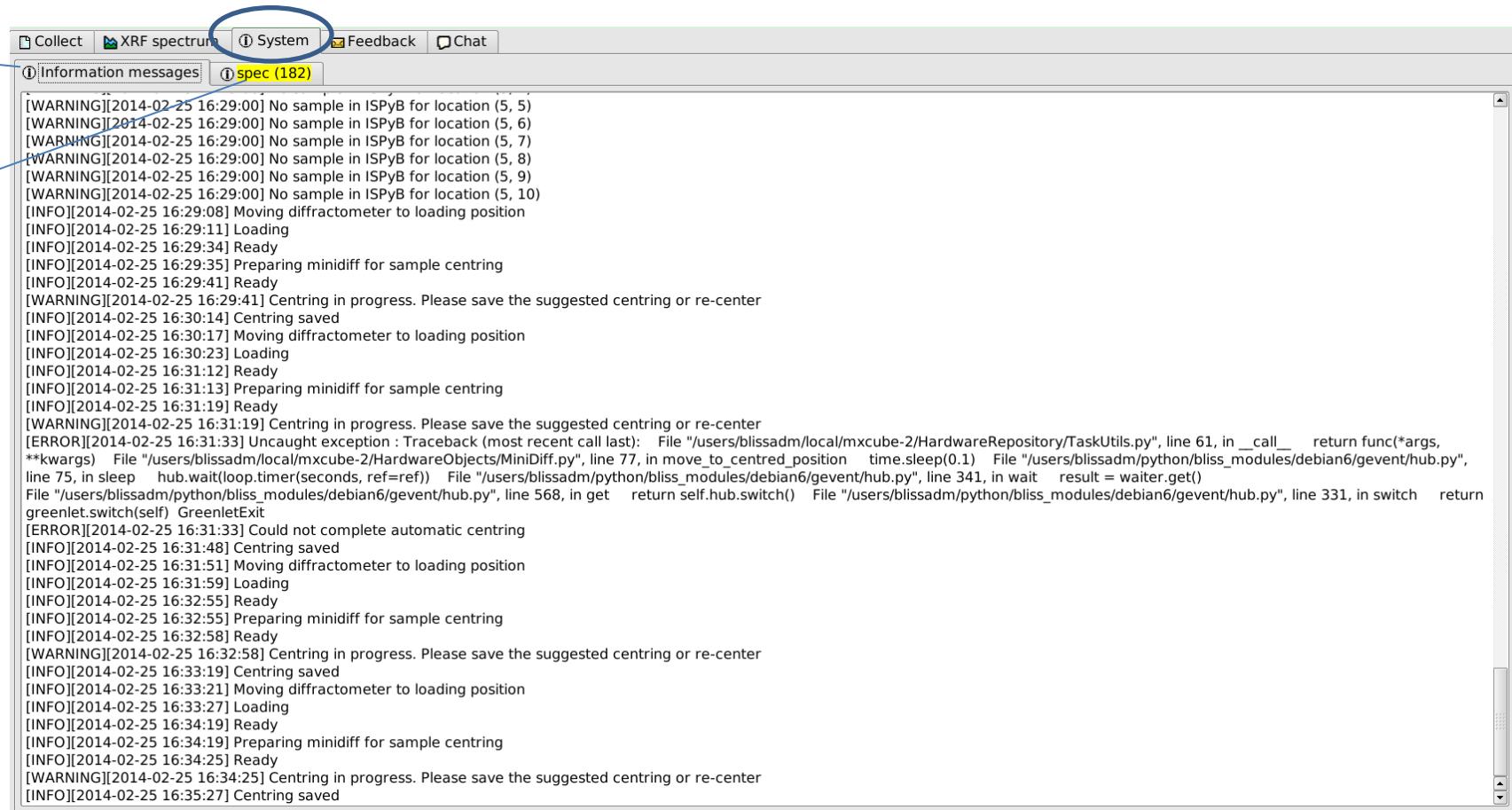
**Advanced**



A XRF scan can be started either from the queue or from the XRF spectrum tab (see "how to" section)

- 1 Enter the count time and add to queue
- 2 and 2' Tick the XRF spectrum parameters box and choose where to save your data  
NB : to know more about XRF spectrum go to "how to" section

# GUI description: System tab



- 1 MXCuBE log file with more details than the dialogue box area
- 2 Spec terminal

# GUI description: Feedback tab

Collect XRF spectrum System Feedback Chat

Feel free to report any comment about this software, an email will be sent to the people concerned. Do not forget to put your name or email address if you require an answer.

Your email:

Message:

1

2

Submit

Use this form to give us feedback.

- 1 Fill in your e-mail address if you wish to get an answer
- 2 After typing your message, click on submit

We value your opinion and advices on MXCuBE and we will use your feedback to improve its operation. We will be happy to help you use MXCuBE if necessary.  
You can also contact the MXCuBE team through : [mxcube-feedback@esrf.fr](mailto:mxcube-feedback@esrf.fr)

## GUI description: Chat tab



The screenshot shows a software window with a toolbar at the top containing icons for Collect, XRF spectrum, System, Feedback, and Chat. The 'Chat' icon is highlighted with a blue oval. The main area displays a chat log with the following messages:

(09:37:09) *[?]jopid29 has joined the conversation.*  
(09:40:45) Emilie: Hello, it's Emilie  
(09:41:01) Emilie: everything is ready here  
(09:41:17) Emilie: position 1 = Puck aaa226a  
(09:41:33) Emilie: position 2= puck cc397a  
(09:41:42) Emilie: position3 = cb252a  
(09:41:53) Emilie: pos4= cc394a  
(09:42:04) Emilie: pos5= cc393a  
(09:44:18) Emilie: my phone number is +33 (0) 4 76 88 24 77  
(09:45:02) *[?]jopid29 has changed to [ix Jopid29.*  
(09:45:12) *[ix Jopid29 wants to have control!*  
(09:45:12) *[ix Jopid29 has control.*  
(09:45:12) *I've lost control...*

At the bottom, there is a text input field labeled "Say:" and a "Send" button, both circled in blue.

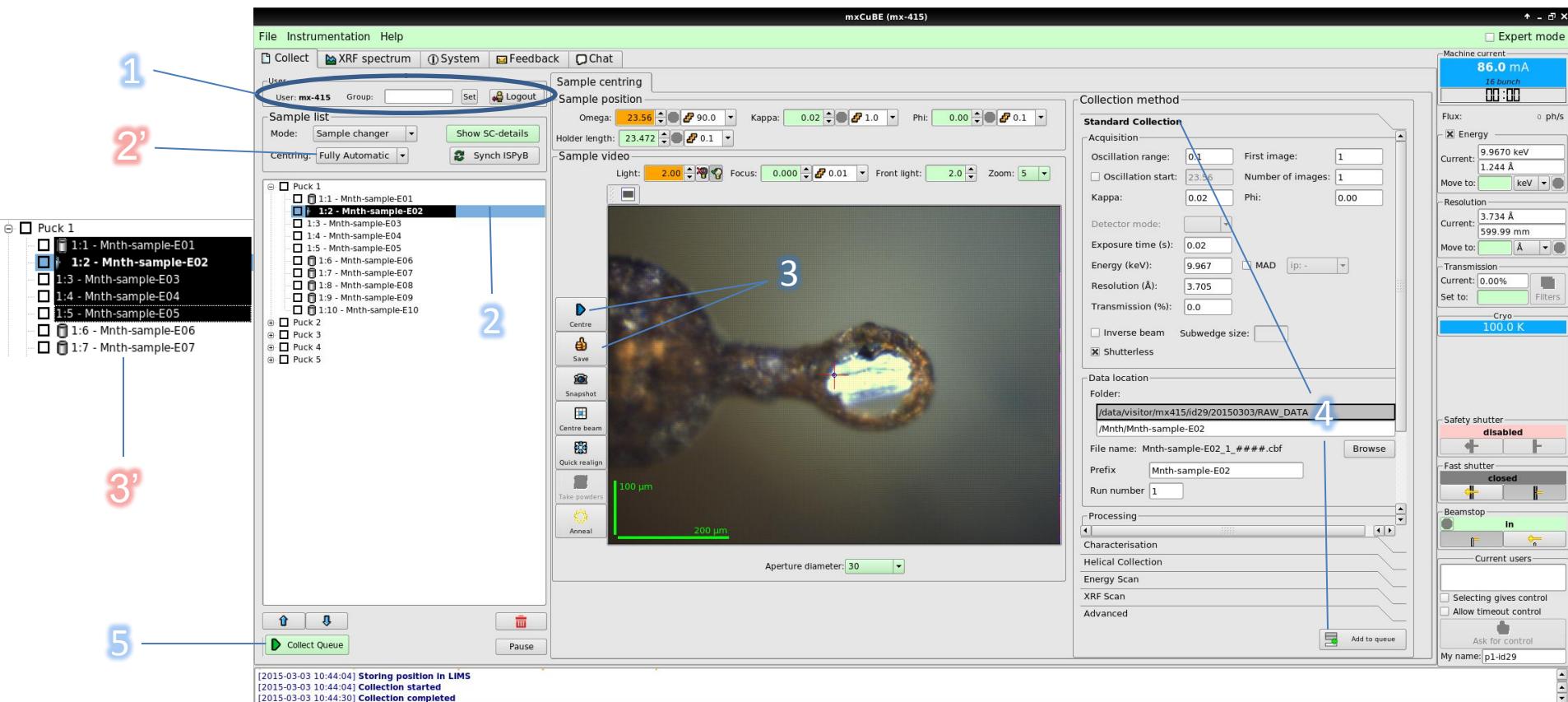
Use this page to discuss with your local contact when connected as a remote access user

# MXCuBE user manual

## Part II: How to's



# How to: Use the basics of MXCuBE



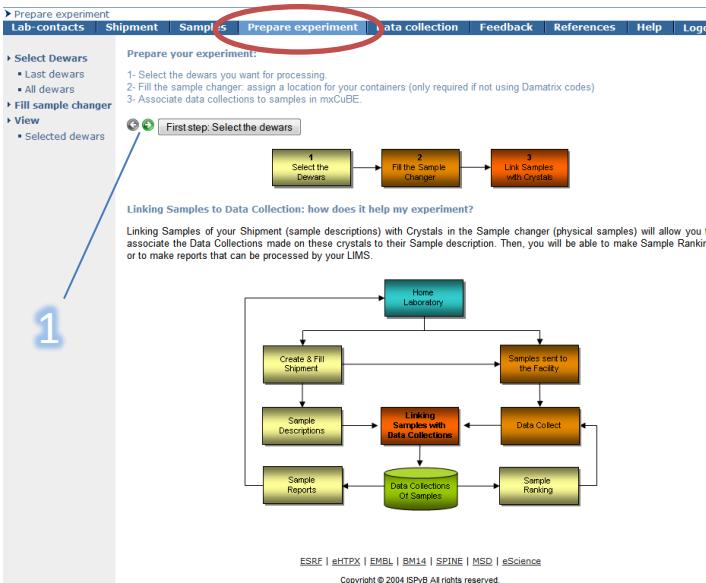
## In basic mode:

- 1 Log-in in MXCuBE
- 2 Select a sample
- 3 Center it and save
- 4 Select a collection method and add to queue
- 5 Collect queue

## In pipeline mode (semi or fully automatic):

- 1 Log-in MXCuBE
- 2' Select the semi or fully automatic centring mode
- 3' Select a list of sample: Press Ctrl key while clicking on sample name or Press shift key and select 1<sup>st</sup> and last sample name or Select the first sample name and drag to the last sample name
- 4 Select a collection method, adjust parameters as required and add to queue
- 5 Collect queue

1



Prepare your experiment:

- Select the dewars you want for processing
- Fill the sample changer; assign a location for your containers (only required if not using Damatrix codes)
- Associate data collections to samples in mxCuBE.

First step: Select the dewars

Linking Samples to Data Collection: how does it help my experiment?

Linking Samples of your Shipment (sample descriptions) with Crystals in the Sample changer (physical samples) will allow you to associate the Data Collections made on these crystals to their Sample description. Then, you will be able to make Sample Ranking or to make reports that can be processed by your LIMS.

```

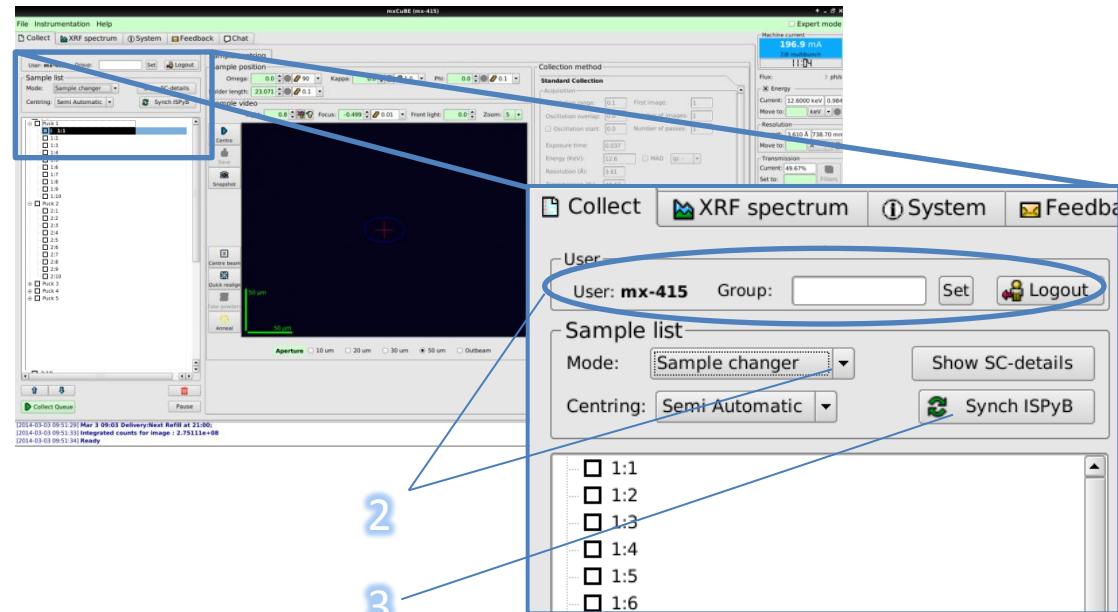
graph TD
    Home[Home] --> Create[Create & Fill Shipment]
    Create --> Samples[Samples Descriptions]
    Create --> SamplesFacility[Samples sent to the facility]
    Samples --> Linking[Linking Samples with Data Collections]
    SamplesFacility --> Linking
    SamplesFacility --> DataCollect[Data Collect]
    Linking --> DataCollect
    Linking --> SampleReports[Sample Reports]
    DataCollect --> SampleReports
    DataCollect --> SampleRanking[Sample Ranking]
    SampleReports --> DataCollection[Data Collections Of Samples]
    SampleRanking --> DataCollection
    
```

ESRF | eHTPX | EMBL | BM14 | SPINE | MSD | eScience  
Copyright © 2004 ISPyB All rights reserved.

2

3

4



mxCuBE (mx-415)

User: mx-415 Group: Set Logout

Sample list

Mode: Sample changer Show SC-details

Centring: Semi Automatic Synch ISPyB

<input type="checkbox"/> 1:1
<input type="checkbox"/> 1:2
<input type="checkbox"/> 1:3
<input type="checkbox"/> 1:4
<input type="checkbox"/> 1:5
<input type="checkbox"/> 1:6

Centring done!

### Why linking my samples from ISPyB to MXCuBE ?

This action will allow you to view your samples (described in ISPyB) in the MXCuBE sample list and link your samples to the data collections

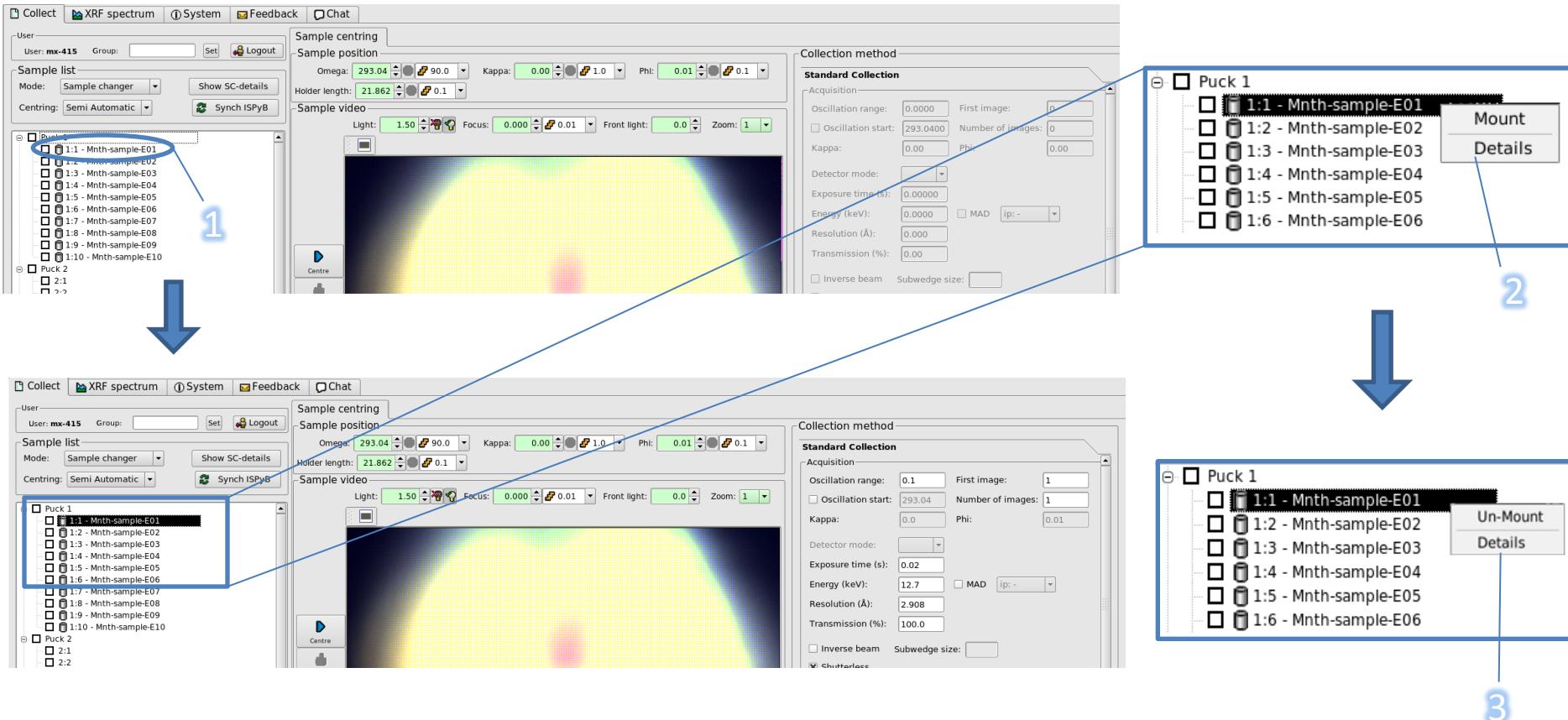
=> Facilitate your experiment (image prefix and directories are automatically filled in MXCuBE)

In ISPyB:

=> Easy grouping of your data collections per sample  
=> Easy searches by sample and/or by protein acronym to list all experiments performed over the various sessions

- 1 Prepare experiment in ISPyB (as described in ISPyB manual)
- 2 Log-in in MXCuBE – Choose sample changer mode
- 3 Synchronize with ISPyB
- 4 View your sample list -> "1:1" becomes "1:1-Acronym-sample1"

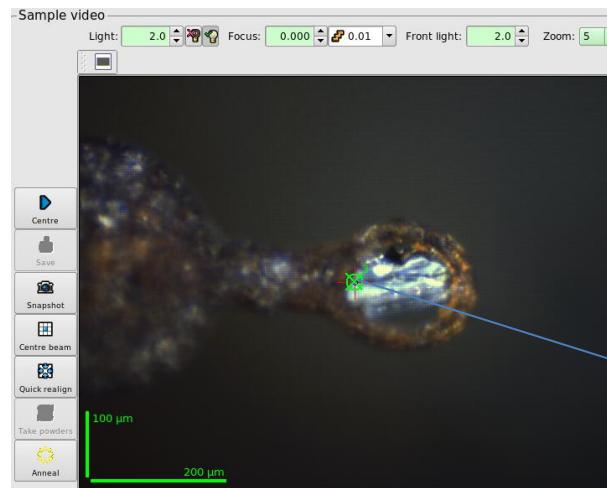
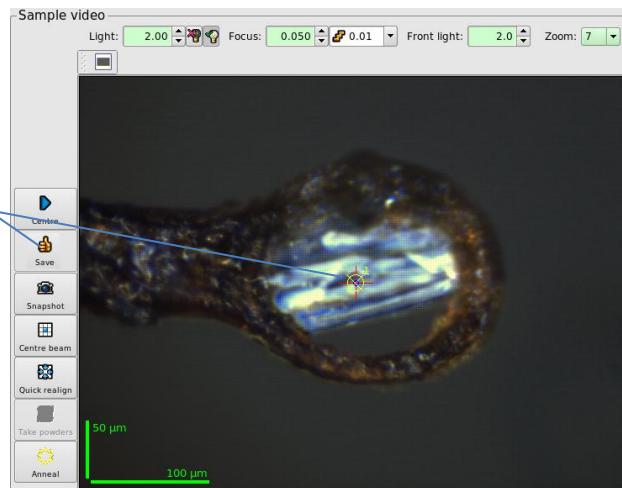
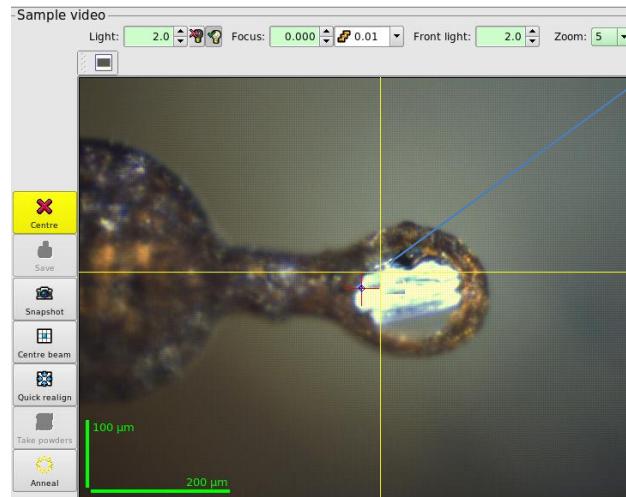
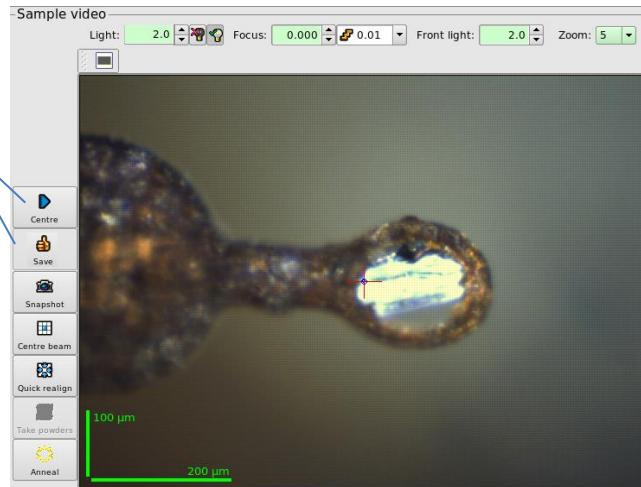
# How to: Select a sample from the sample changer and mount it



- 1 Click on a sample to select it. The sample name will be highlighted in black
- 2 Right click to access the sample changer mounting menu and click on mount
- 3 To un-mount manually a mounted sample, right click on the sample name to access the sample changer mounting menu then select un-mount

# How to: Centre your sample and save a position

[2014-03-03 10:09:04] Centring in progress. Please save the suggested centring or re-center



2

1 Dialogue box : After auto loop-centring is finished you can save the current position or re-center

2 To re-center, click 3 times on the point you want to center in the beam (red cross)

3 Save this position (mandatory to start a collection), a yellow circle with a number appears

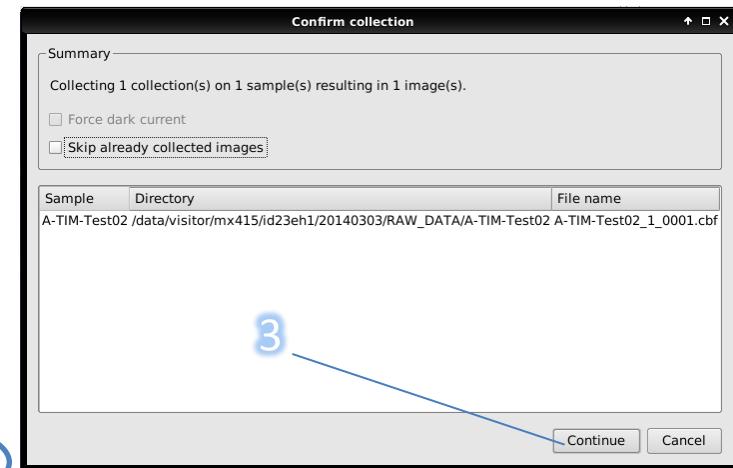
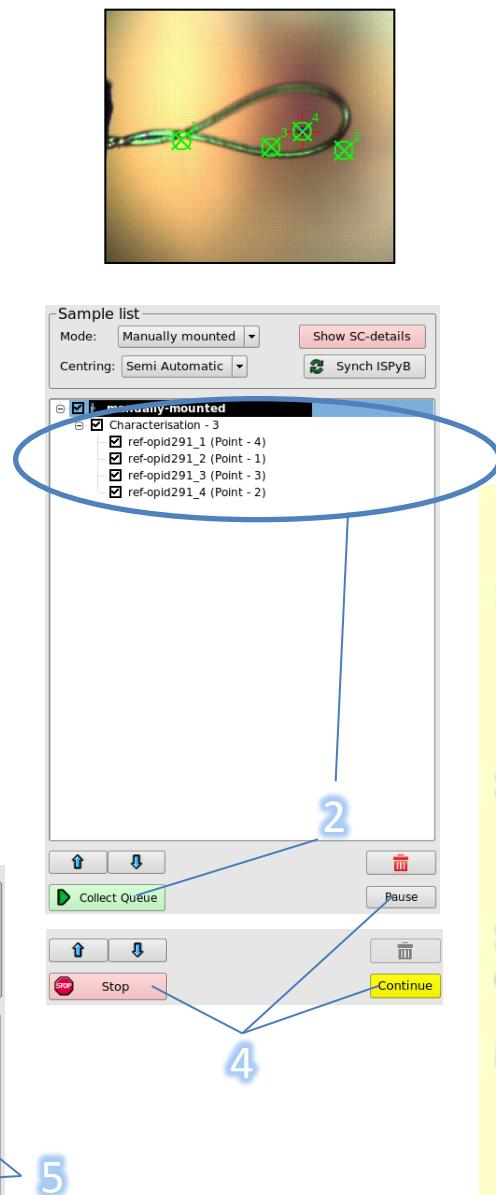
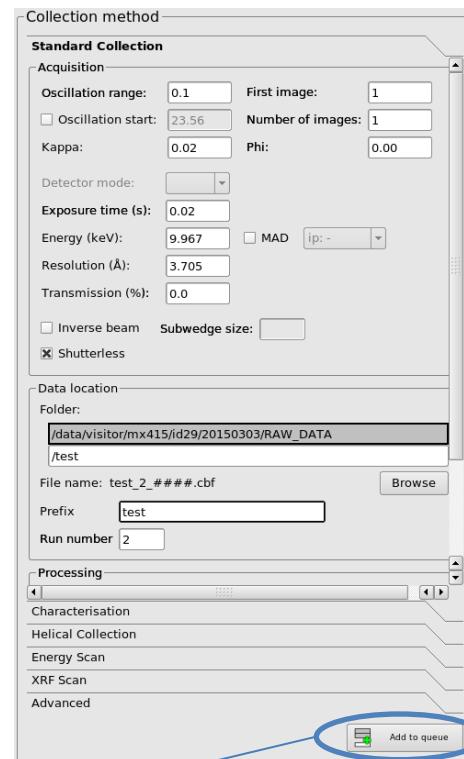
4 Once selected, the yellow crossed circle becomes bold green

3

4

# How to:

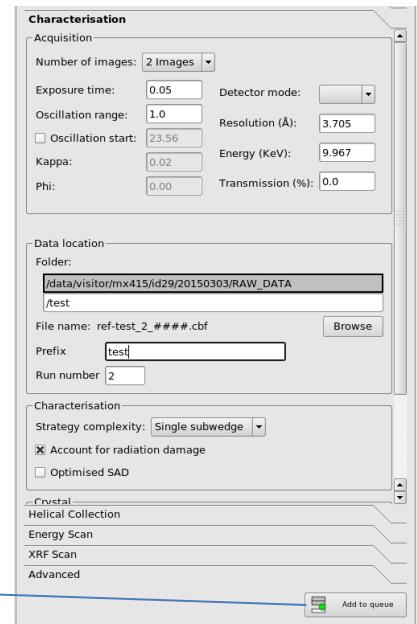
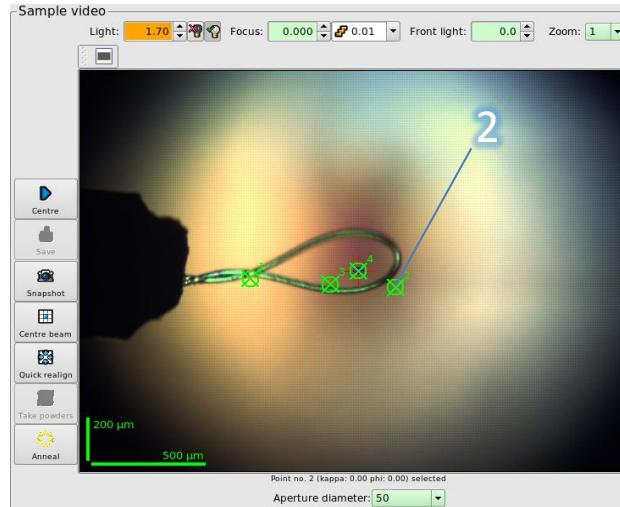
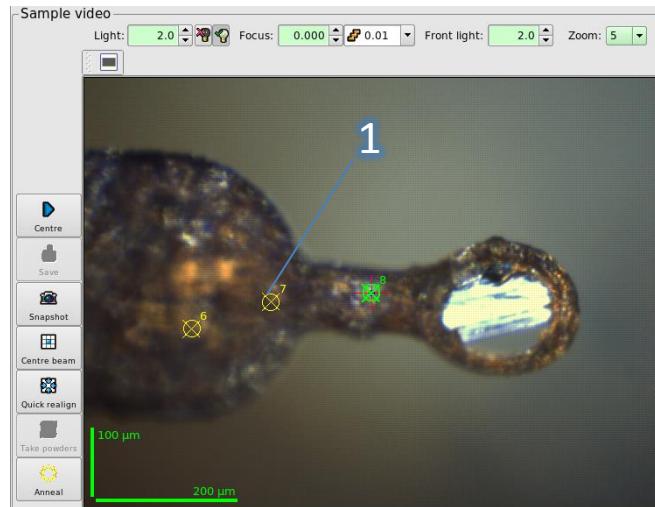
## Associate a task to a selected position of one sample



Having a sample selected and a position saved and selected for this sample (see previous page):

- 1 Fill in the parameters and Add to queue  
NB : If you did not center your sample or select the centered position before starting your collection, MXCuBE will automatically add a centring task to the queue
- 2 The corresponding collection will be added to the queue on the sample list -> Click on "Collect queue"  
NB: In the queue, each task will be associated to the corresponding number of the selected position
- 3 A confirmation message will appear -> Click continue
- 4 You can stop, pause or continue the process at any time (effective at the end of the current task)
- 5 When finished, sample list will become green (if successful), yellow or red. If results are expected (EDNA characterisation...) double click on the result line to view them

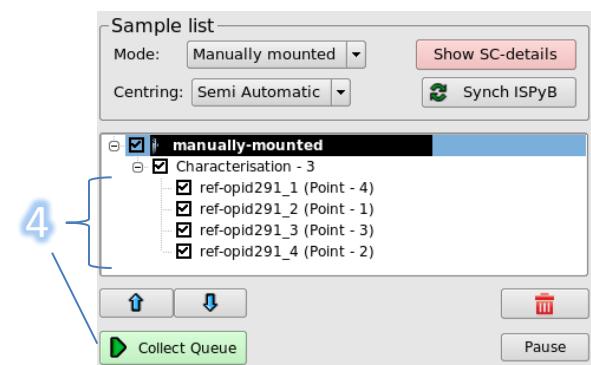
# How to: Perform same collection method on several positions of one sample



Follow this process to perform the same action on various parts of the same sample.  
Example: EDNA characterisation

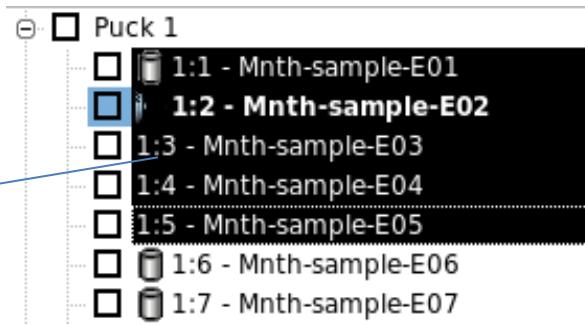
- 1 On the mounted sample centre and save several positions (all numbered and yellow except the last one, bold and green)
- 2 Select all : press ctrl key + select each yellow ring on sample view
- 3 Select a task to add (here EDNA characterisation) and press “Add to queue”
- 4 Collect queue: in that particular case, an EDNA characterisation is performed on each saved position and a diffraction plan is proposed for each position.

NB: It is possible at this level to rank the positions automatically within ISPyB (see ISPyB manual) and to select the crystal part which is of best quality.

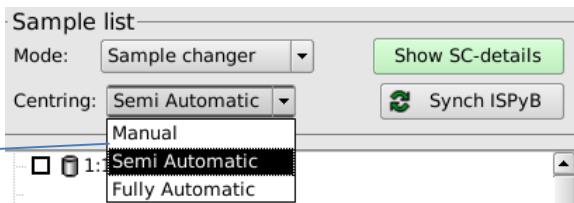


# How to:

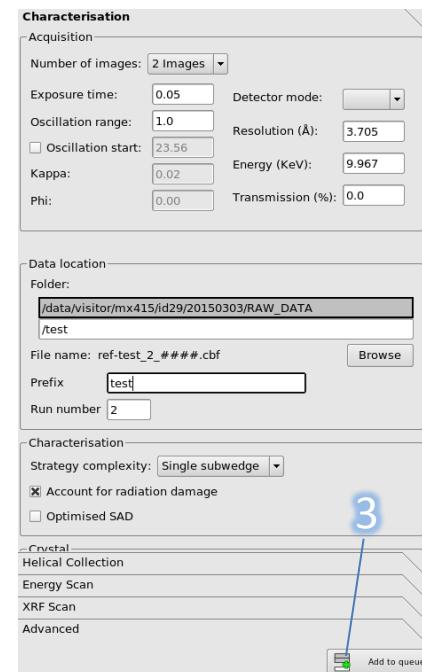
## Perform same collection method on multiple samples



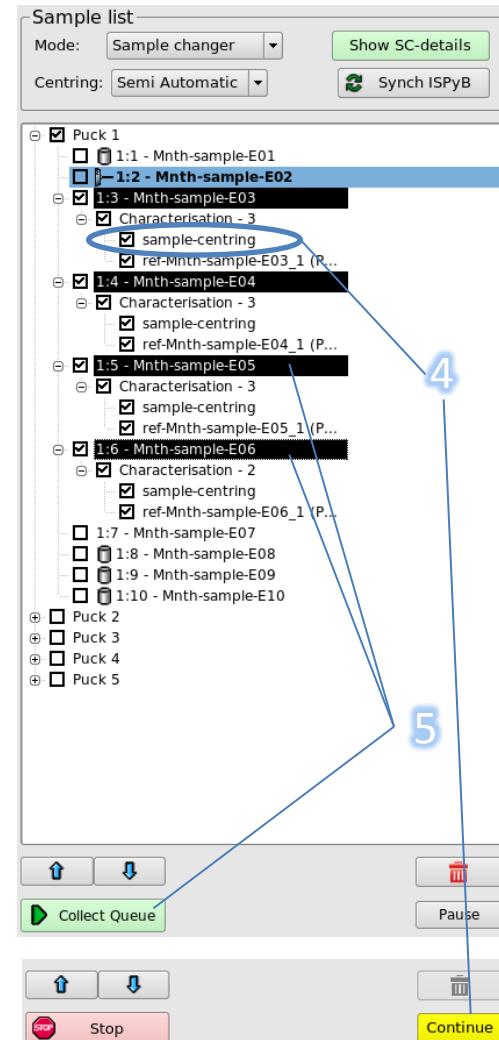
1



2



3



4

5

Follow this process to perform the same action(s) on each sample of a selected pool.  
 Example: EDNA characterisation on each sample to select the best suitable crystal of the pool.

1 Select the samples of interest in the sample list:

- by selecting the 1<sup>st</sup> one of the series and pressing shift key while selecting the last one
- or by selecting all samples of interest one by one while pressing the Ctrl key

2 Above sample list, select fully automatic or semi-automatic (Centring type)

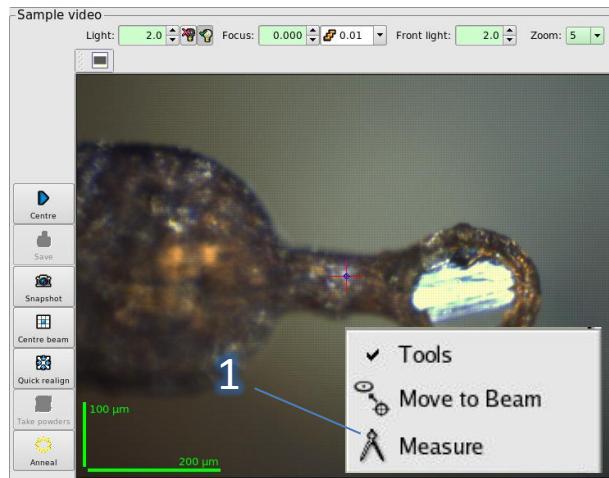
3 Select a task to add (here EDNA characterisation...) and press "Add to queue"

4 If semi-automatic centring was selected, a centring step is added to the queue. For each sample, press continue to accept the automatic centring or re-center.

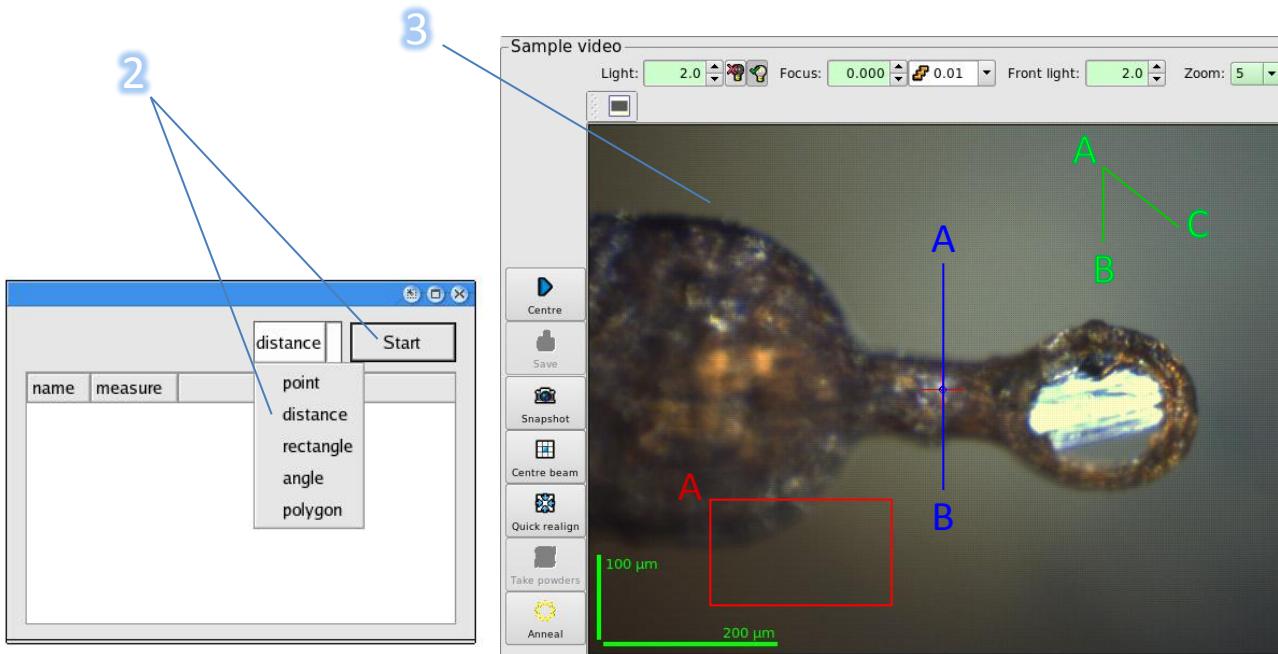
This is not the case in fully automatic mode

5 "Collect queue" will collect all ticked tasks from the queue (untick a task if you do not want it to be performed straightaway)

# How to: Measure distances or angles



- 1 Right click on the video screen and click on measure to open the measure tool
- 2 Choose the type of measure that you want to perform (ex: distance) and click on start
- 3 To measure :
  - **Distances** : Click on the starting point **A** then on the ending point **B**
  - **Angles**: Click on the peak of the angle **A**, then on the end of the first branch **B** and on the end of the second branch **C**
  - **Rectangle** or **Polygon**: Click on the starting point of your rectangle **A** and drag until you obtain the desired shape
- 4 The value will appear in the measure box
- 5 Right click on the name of a measure to remove it or to change its color



name	measure
Mes 1	distance -> 30.29 µm
Mes 2	distance -> 102.40 µm
Mes 3	angle -> 50.973978 deg
Mes 4	distance (x,y) -> (68.10 µm, 41.35 µm), surface 0.00m2

name	measure
Mes 1	distance -> 30.29 µm
Mes 2	remove -> 102.40 µm

colors :

- black
- white
- red
- green
- blue
- yellow
- More color ...

# How to: Measure your crystal size (ex: for a characterisation)

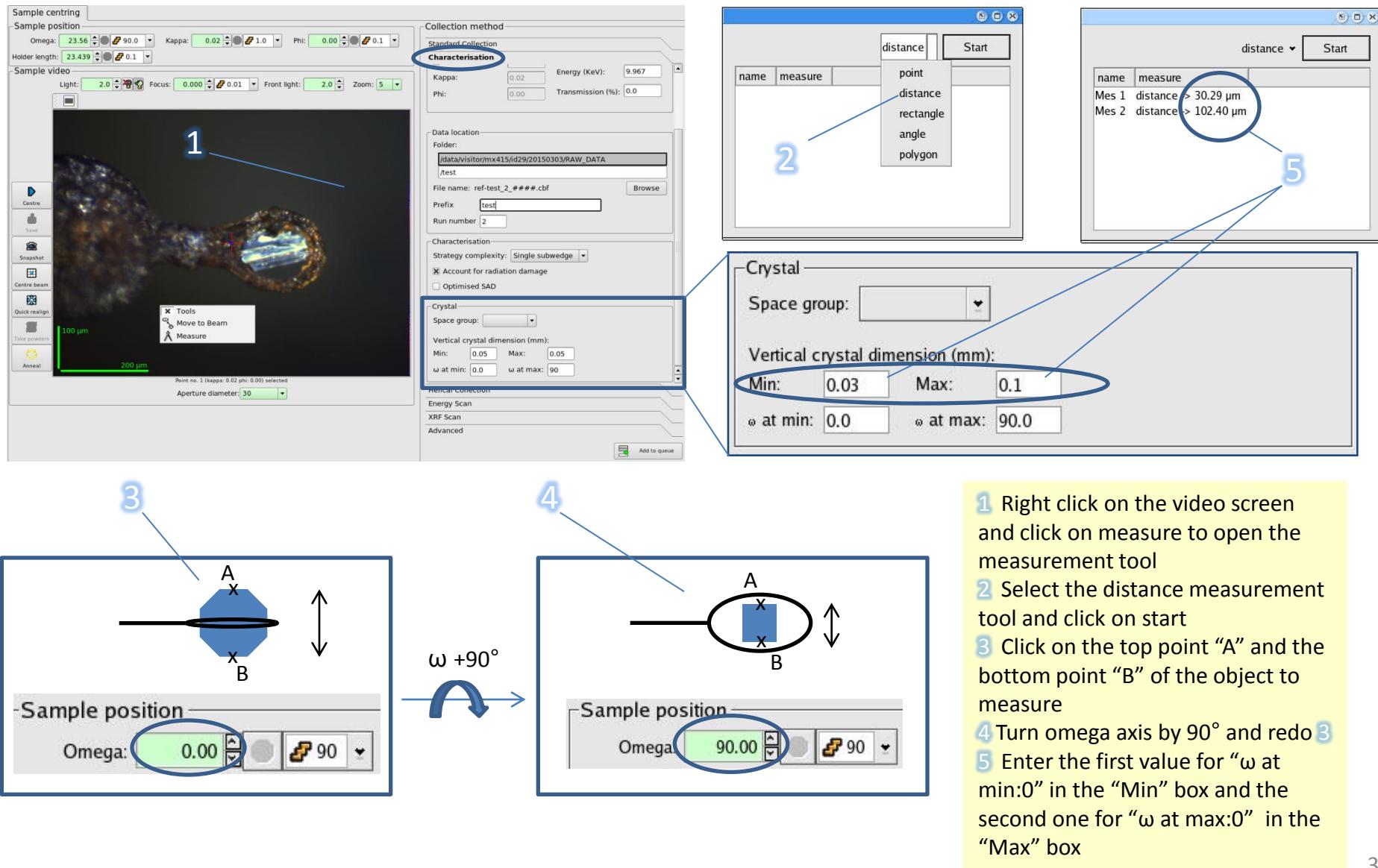
**1** Right click on the video screen and click on measure to open the measurement tool

**2** Select the distance measurement tool and click on start

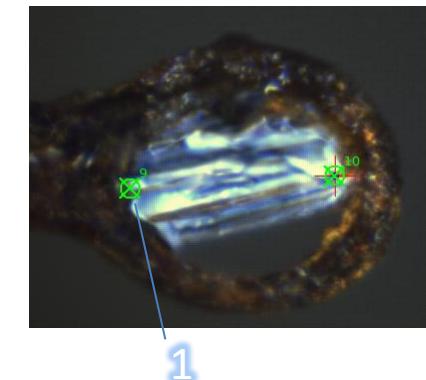
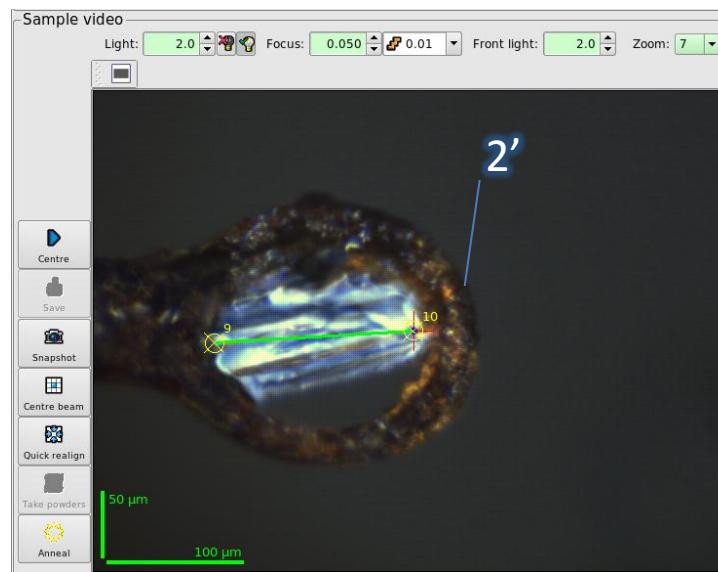
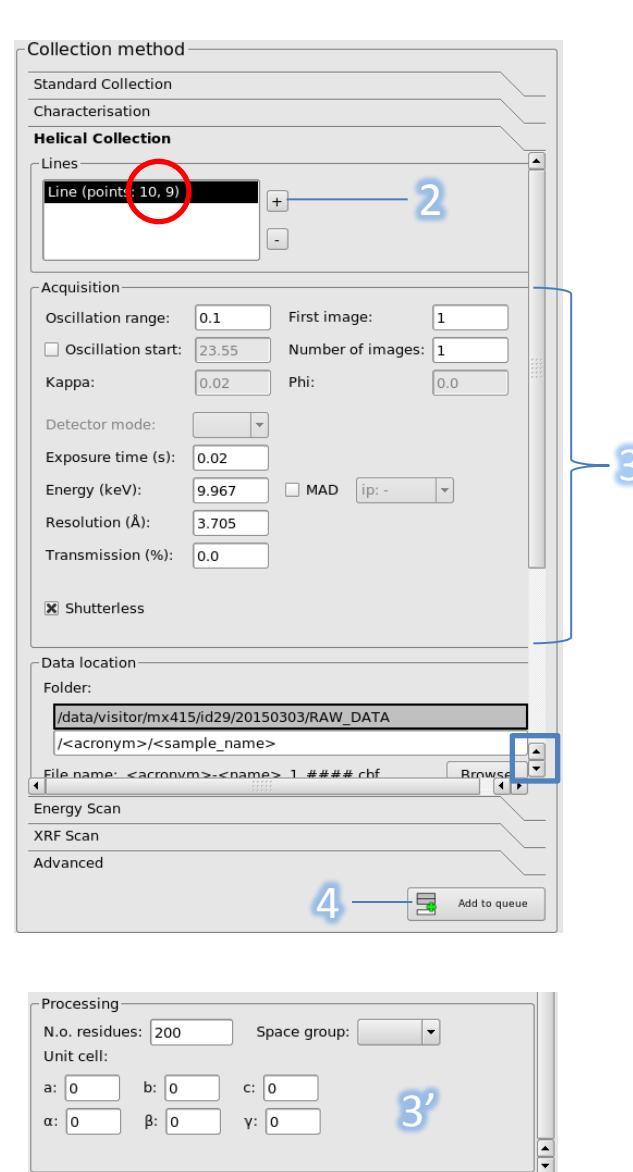
**3** Click on the top point "A" and the bottom point "B" of the object to measure

**4** Turn omega axis by 90° and redo **3**

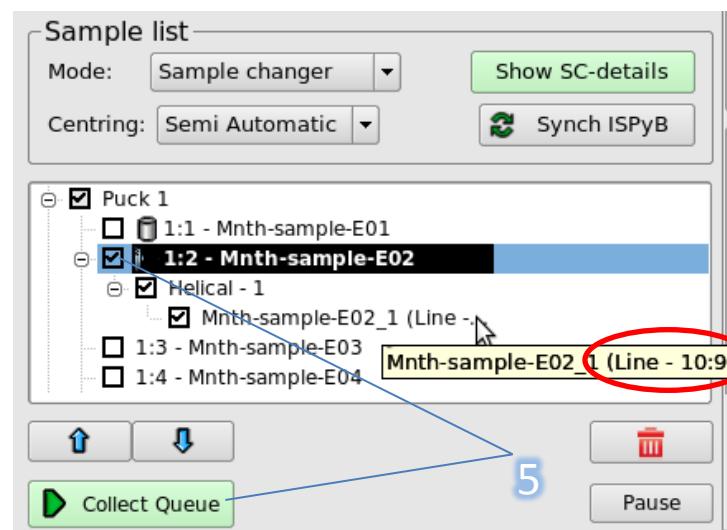
**5** Enter the first value for "ω at min:0" in the "Min" box and the second one for "ω at max:0" in the "Max" box



# How to: Perform a helical data collection



Use the helical data collection to collect along a specified axis along the spindle axis (--->)



1 Save two positions at the two extremities of the axis on which you want to perform helical data collection and select them (ctrl + click)

2 And 2' Add a guiding line for the helical collection

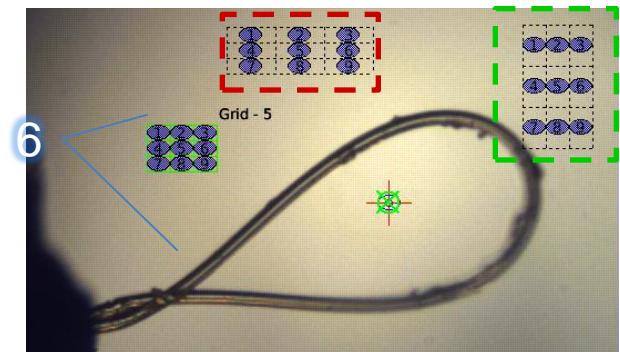
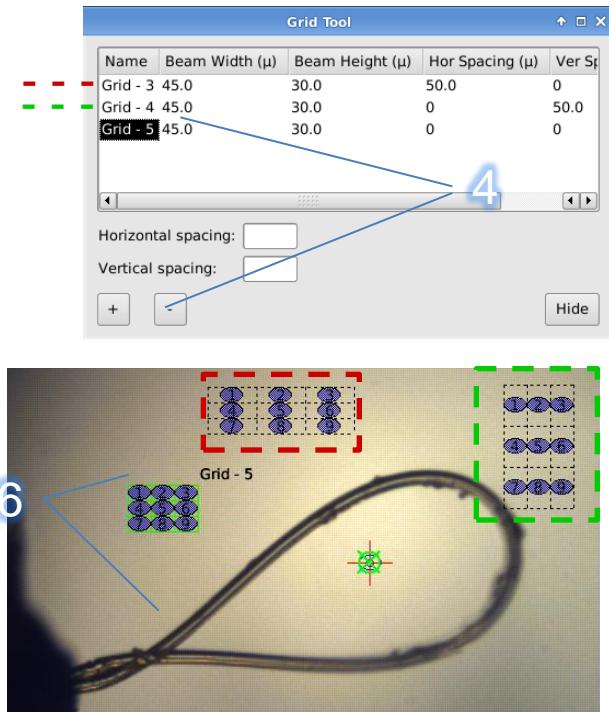
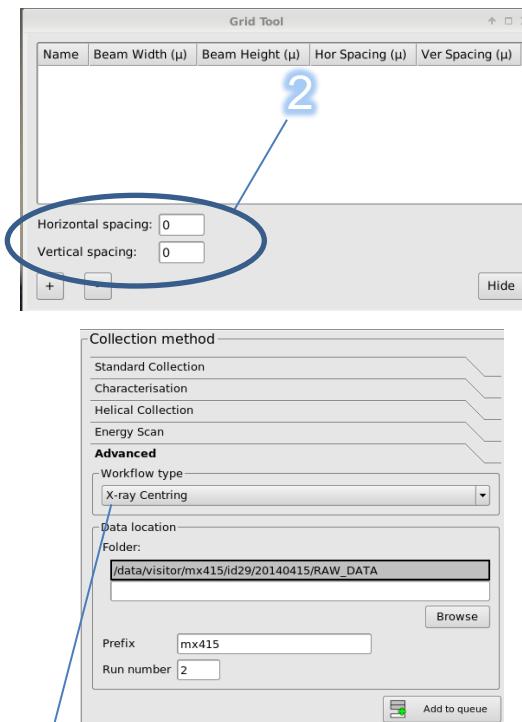
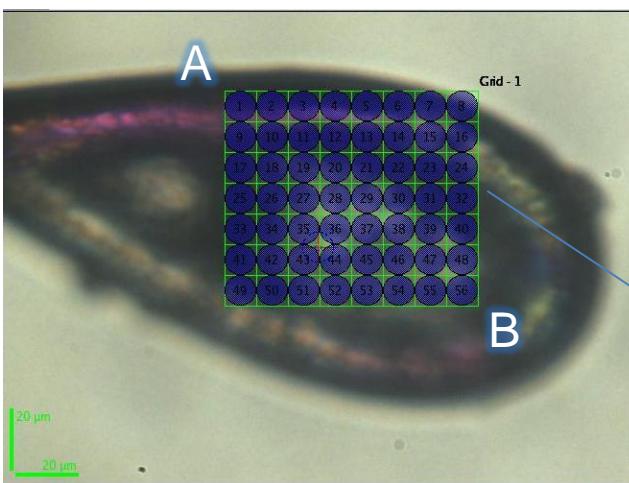
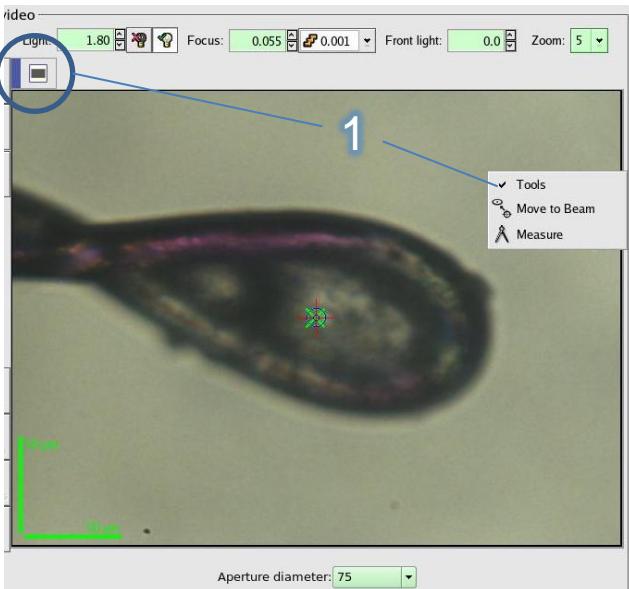
3 and 3' Fill in the parameters

4 Add to queue

5 Check that the corresponding box is ticked and collect Queue

NB: The saved positions are numbered and the helical collection will start at the first selected point (here "10")

# How to: Define a grid for a mesh scan or a X-ray centring



5

1 Click on this icon to open the grid tool in a pop up window. If you do not see it, do a right click on the video and click on "Tools"

2 Grid tool pop up window. Enter the horizontal and vertical values of the step between two points of the grid

3 To set the grid: click on the first corner (A) then drag until you obtain the desired shape (B)

4 Click on "+" to add this grid and click on the grid name to select it

5 Select the appropriate workflow in "Collection method/ Advanced" and "Add to queue"

6 Each node of the grid will be the location of a data collection.

----- Positive horizontal step. - - - - Positive vertical step

NB: You can draw several grid to work on different part of your crystal

# How to: Perform a mesh scan

**Advanced**

Workflow type **Mesh Scan** (1)

Data location  
Folder: /data/visitor/mx415/id23eh1/20141203/RAW\_DATA  
/A/A-TIM-toto01

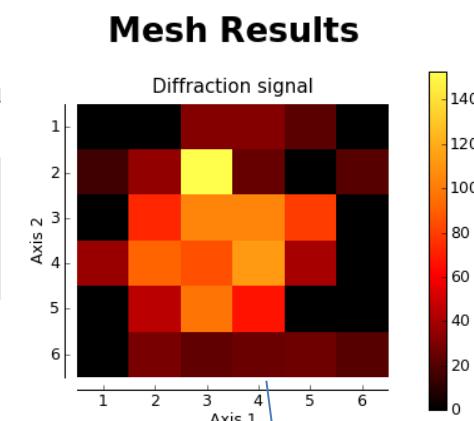
Prefix A-TIM-toto01  
Run number 1

Add to queue (2)

[2014-03-06 14:34:29] Workflow: phiz: -0.119  
[2014-03-06 14:34:29] Workflow waiting for input, verify parameters and press continue.

Exposure time	0.037
Total oscillation range	1.0
Transmission	100.0

Continue (4)



### Best position

The sample has automatically been moved to the best position.  
In order to move the sample to an other position please copy/paste the commands from the right column into SPEC EXP.

Axis 1	Axis 2	Image file	Signal 1	Signal 2	Bravais lattice	SPEC command for moving sample to position
3	2	mesh-xth10-blu60-01_1_0009.cbf	153	92784	P1	mv sampx 0.449; mv sampy 0.117; mv phiy -0.785

Signal 1: Criteria that uses intensities over background vs resolution. Popov 2014, to be published.

Signal 2: Labelit distl distl spotfinder total integrated intensity.

### All positions

Axis 1	Axis 2	Image file	Signal 1	Signal 2	Bravais lattice	SPEC command for moving sample to position
9	1	line-tryp-sampA09_2_0009.cbf	1.05e+03	1211617	P222	mv sampx 0.872; mv sampy 0.108; mv phiy -0.391
8	1	line-tryp-sampA09_2_0008.cbf	622	862583	P222	mv sampx 0.904; mv sampy 0.109; mv phiy -0.391
10	1	line-tryp-sampA09_2_0010.cbf	484	541628	P222	mv sampx 0.840; mv sampy 0.108; mv phiy -0.391
7	1	line-tryp-sampA09_2_0007.cbf	194	121427	P222	mv sampx 0.936; mv sampy 0.110; mv phiy -0.391

Define the grid as shown previously (p.32)

- 1 Select the Mesh scan in the Advanced pull down menu for the workflow type
- 2 Add to queue
- 3 Collect queue
- 4 Verify the input parameters and press continue
- 5 In the data collection tab, view the result of the MESH, the best position and all other positions

NB : MXCuBE will directly center the crystal on the best position determined but if you want to move to another position, check its SPEC command in All positions table (last column) and copy it to the SPEC EXP window

**Sample list**

Mode: Sample changer  
Centring: Semi Automatic

Show SC-details  
Synch ISPyB

<input type="checkbox"/> 1:1 - A-TIM-Test01
<input checked="" type="checkbox"/> 1:2 - A-TIM-Test02
<input checked="" type="checkbox"/> Mesh Scan - 1
<input checked="" type="checkbox"/> Workflow task - 0
<input type="checkbox"/> 3:1

Collect Queue (3)  
Pause

# How to: Perform a X-ray centring

**Advanced**

Workflow type: **X-ray Centring** (1)

Data location:

Folder: **/data/visitor/mx415/id23eh1/20141203/RAW\_DATA**

Prefix: **A-TIM-toto01**

Run number: **1**

**Add to queue**

**Sample list**

Mode: **Sample changer** Show SC-details

Centring: **Semi Automatic** Synch ISPyB

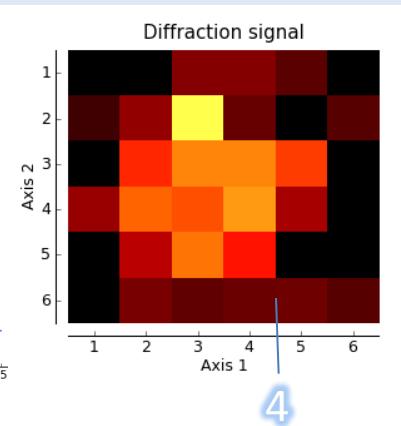
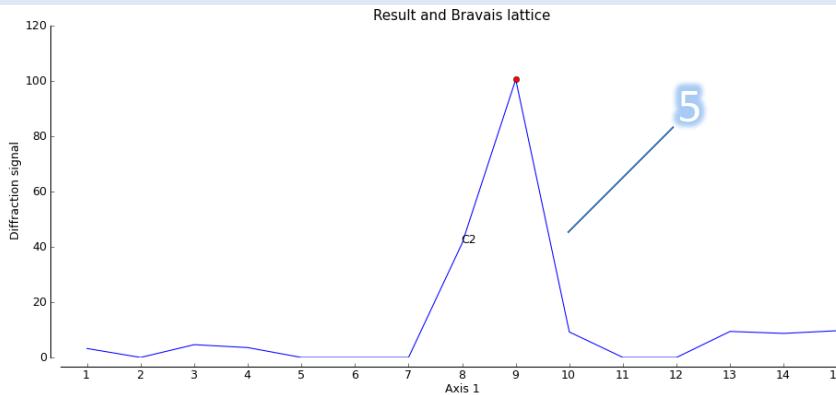
- 1:1 - A-TIM-Test01
- 1:2 - A-TIM-Test02 (2)
- X-ray Centring - 1
  - Workflow task - 0
- 3:1

Collect Queue

[2014-03-06 14:34:29] Workflow: phiz: -0.119  
[2014-03-06 14:34:29] Workflow waiting for input, verify parameters and press continue.

Exposure time	0.037
Total oscillation range	1.0
Transmission	100.0

**Continue** (3)



Signal 1: Criteria that uses intensities over background vs resolution. Popov 2014, to be published.  
Signal 2: Labelit distl spotfinder total integrated intensity.

#### All positions

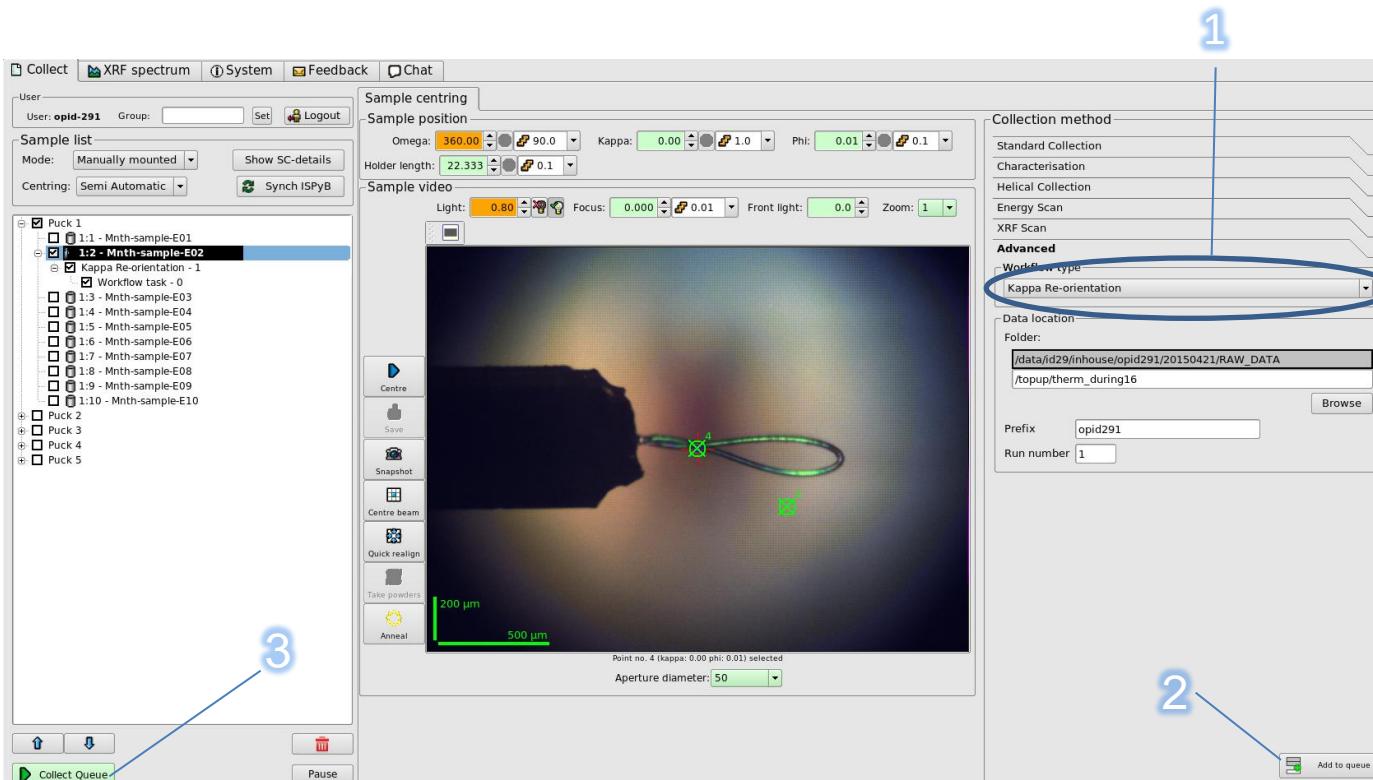
Axis 1	Axis 2	Image file	Signal 1	Signal 2	Bravais lattice	SPEC command for moving sample to position
3	2	mesh-xth10-blu60-01_1_0009.cbf	153	92784	P1	mv sampx 0.449; mv sampy 0.117; mv phiy -0.785
9	1	line-tryp-sampA09_2_0009.cbf	1.05e+03	1211617	P222	mv sampx 0.872; mv sampy 0.108; mv phiy -0.391
8	1	line-tryp-sampA09_2_0008.cbf	622	862583	P222	mv sampx 0.904; mv sampy 0.109; mv phiy -0.391
10	1	line-tryp-sampA09_2_0010.cbf	484	541628	P222	mv sampx 0.840; mv sampy 0.108; mv phiy -0.391
7	1	line-tryp-sampA09_2_0007.cbf	194	121427	P222	mv sampx 0.936; mv sampy 0.110; mv phiy -0.391

Define the grid as shown previously (p.32)

- Select the X-Ray centring in the Advanced pull down menu for the workflow type and Add to queue (1)
- Collect queue (2)
- Verify the input parameters and press continue (3)
- In the data collection tab, view the result of the MESH, the best position and all other positions (4)
- At the end of the MESH a line scan is performed at 90° from the best position (5)

NB : MXCuBE will directly center the crystal on the best position determined but if you want to move to another position, check its SPEC command in All positions table and copy it to the SPEC EXP window

# How to: Do a kappa re-orientation



**Kappa strategy option**

**Number of reference images**

**Angle between reference images**

**Exposure time**

**Total oscillation range**

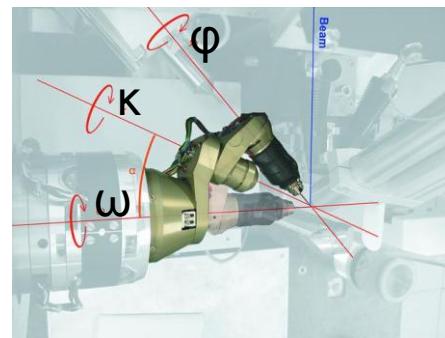
**Transmission**

**Resolution**

**Do data collection?**

true  
 false

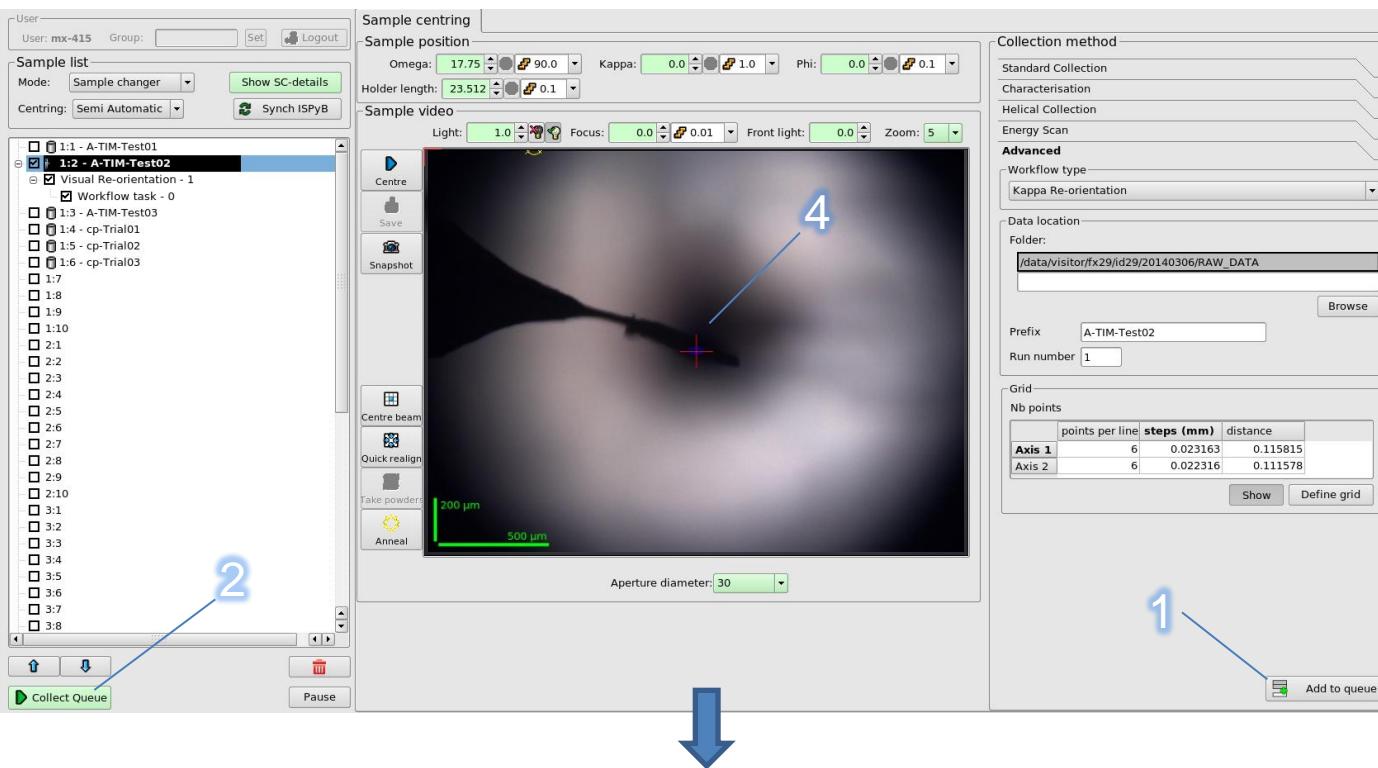
**Continue**



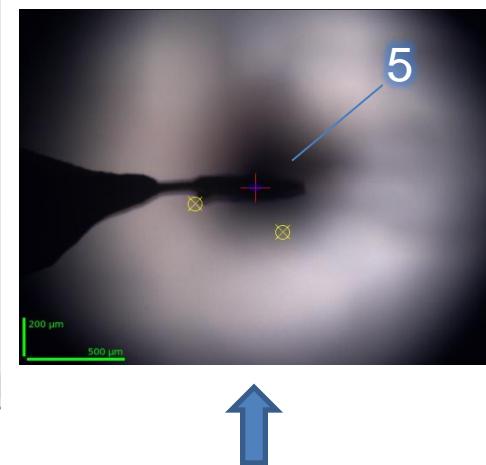
- 1 Select the kappa re-orientation in the Advanced pull down menu for the workflow type
  - 2 Add to queue
  - 3 Collect queue
  - 4 Verify the input parameters and press continue
  - 5 Before kappa re-orientation
  - 6 After kappa re-orientation
- NB : you can also view the kappa re-orientation results in the data collection tab



# How to: Do a visual re-orientation



- 1 Add a visual re-orientation workflow to queue
- 2 Collect queue
- 3 Center two positions along the axis you want to re-align
- 4 Before visual re-orientation
- 5 After visual re-orientation



[2014-03-06 14:23:47] Workflow: phiy: -0.813  
[2014-03-06 14:23:47] Workflow: phiz: -0.109  
[2014-03-06 14:23:48] Workflow waiting for input, verify parameters and press continue.

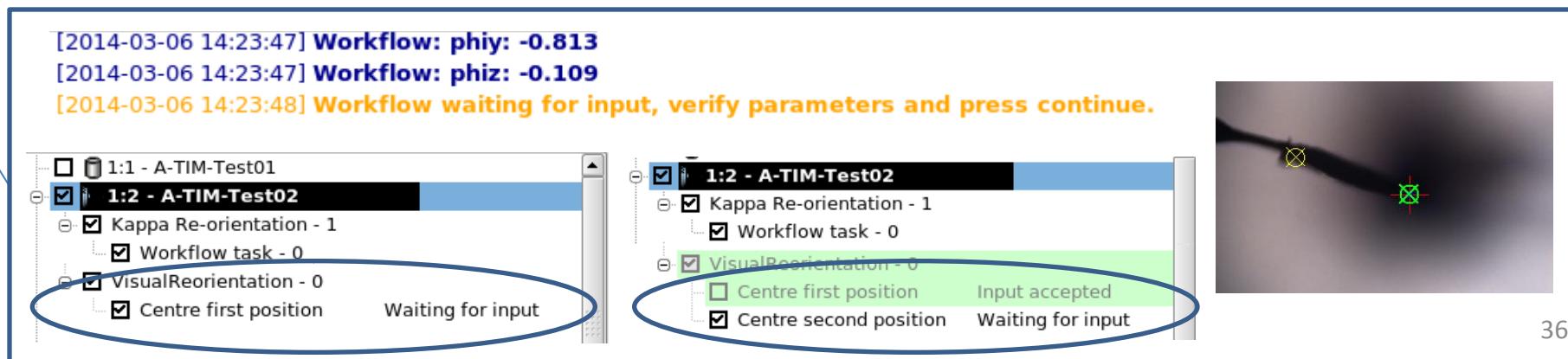
3

Waiting for input

Waiting for input

Input accepted

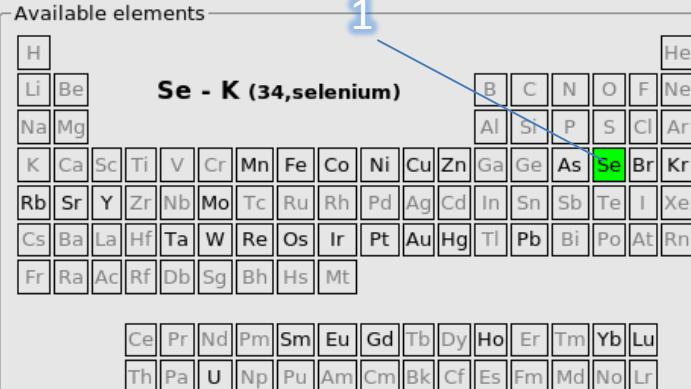
Waiting for input



# How to: Measure an energy scan (MAD or SAD)

**Energy Scan**

Available elements



**Se - K (34,selenium)**

Data location

Folder: /data/visitor/mx1545/id29/20140305/RAW\_DATA

File name: A-TIM-Test01\_1\_####.raw

Browse

Prefix: A-TIM-Test01

Run number: 1

Advanced

Add to queue

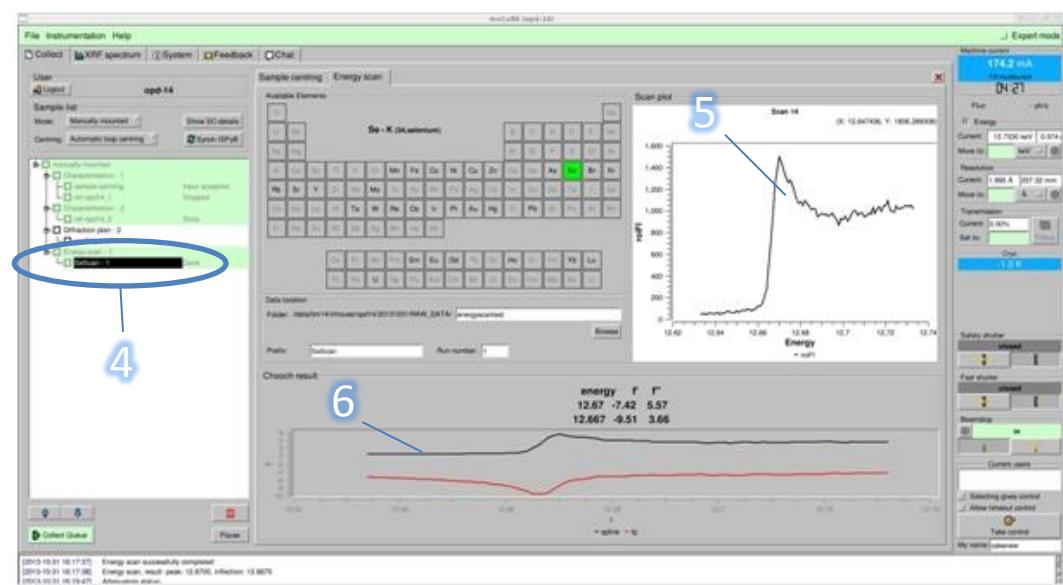
Sample list

Mode: Sample changer  
Centring: Fully Automatic  
Show SC-details  
Synch ISPyB

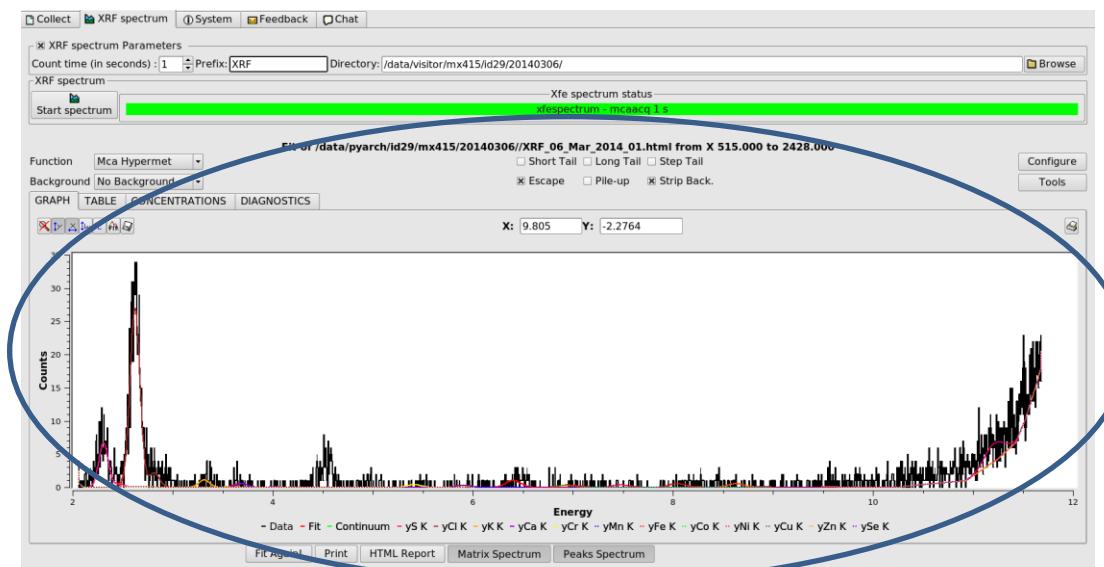
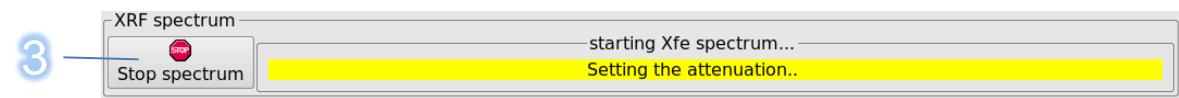
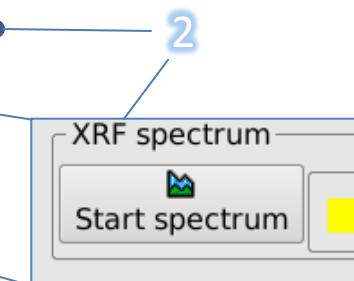
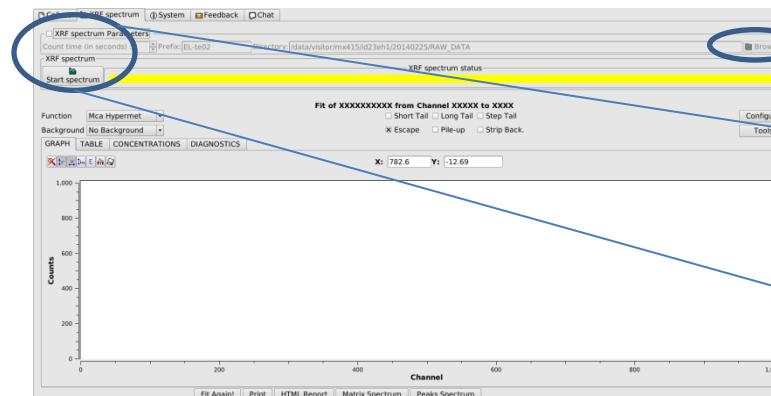
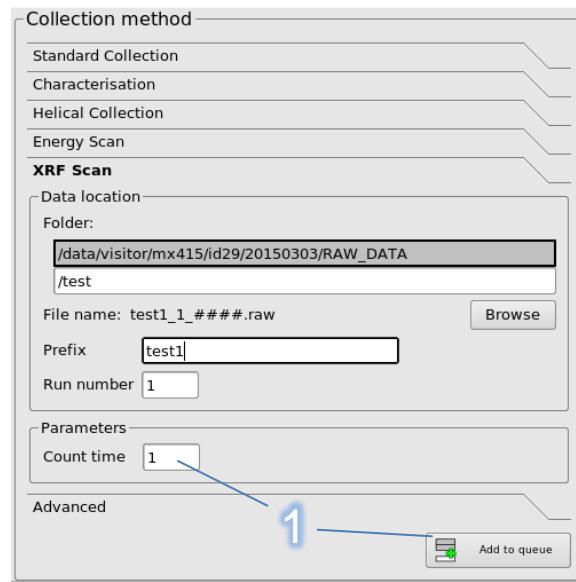
- 1:1 - A-TIM-Test01
- 1:2 - A-TIM-Test02** (selected)
- 1:3 - A-TIM-Test03
- 1:4 - cp-Trial01
- 1:5 - cp-Trial02
- 1:6 - cp-Trial03
- 3:7
- 3:8

Collect Queue

- In Energy Scan (listed in collection methods area):
- 1 Select the element you expect to be present in your sample
  - 2 Add to queue
  - 3 Collect queue
  - 4 Double click on the prefix name to view results
  - 5 Energy scan measured for that sample
  - 6 CHOOCH results : Energy, f', f'' for the peak and inflection



# How to: Measure a X-ray fluorescence (XRF) spectrum



- From the collection panel:

1 Fill in the parameters, add to queue and Collect queue

- From the XRF tab:

2 Choose your directory and click on start XRF spectrum

3 You can stop the XRF spectrum measurement at any time

- For both cases:

4 Display of the results in the XRF spectrum tab or in the PyMca window automatically opened on the right screen

## Trouble shooting

=> Collection method is not available (all options are light grey): No sample is selected

Hint: [Select one or several samples from the sample list](#)

=> MXCuBE does not respond anymore

Hint: [Kill MXCuBE and restart it](#)

=> My sample is not mounted/unmounted when I click on mount/unmount

Hint: [Check sample changer status through a VNC to the sample changer interface](#)

[Check that nothing is blocked on the path of the sample or underneath the arm of the sample changer](#)

[Manually turn the pin of your sample on the magnet by 20 °](#)

[Try to mount/unmount your sample again](#)

[After 2-3 times call your local contact](#)

=> The queue is interrupted because the sample changer failed to upload or download a sample

Hint: [Select the tasks by ticking them in the queue after having fixed the problem and Collect queue again](#)

=> I added to the queue a wrong collection method

Hint: [Tick the box corresponding to this collection and remove it by clicking on the red bin](#)

=> I started a wrong collection method

Hint: [Click on the stop button \(replacing the “Collect queue” button\) and trash the method by clicking on the red bin](#)

=> I would like to change few parameters of a collection method already added to the queue

Hint: [Click on the line corresponding to this method in the queue. This will open tab where you can edit parameters](#)