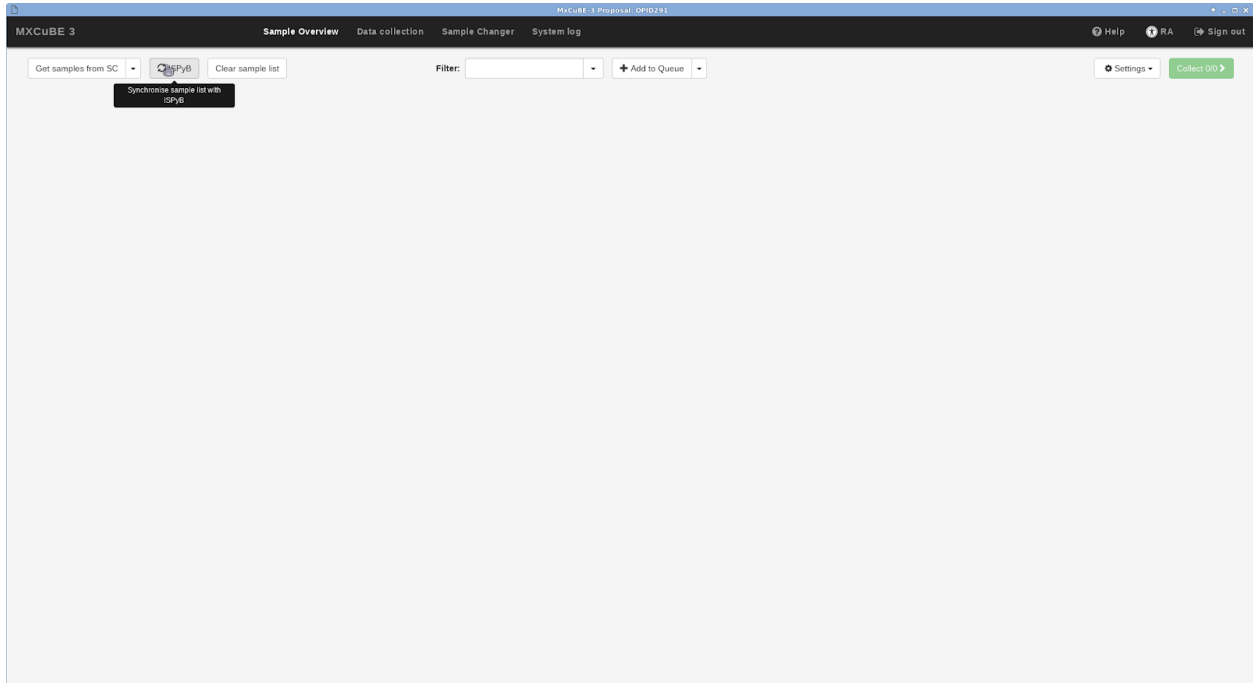


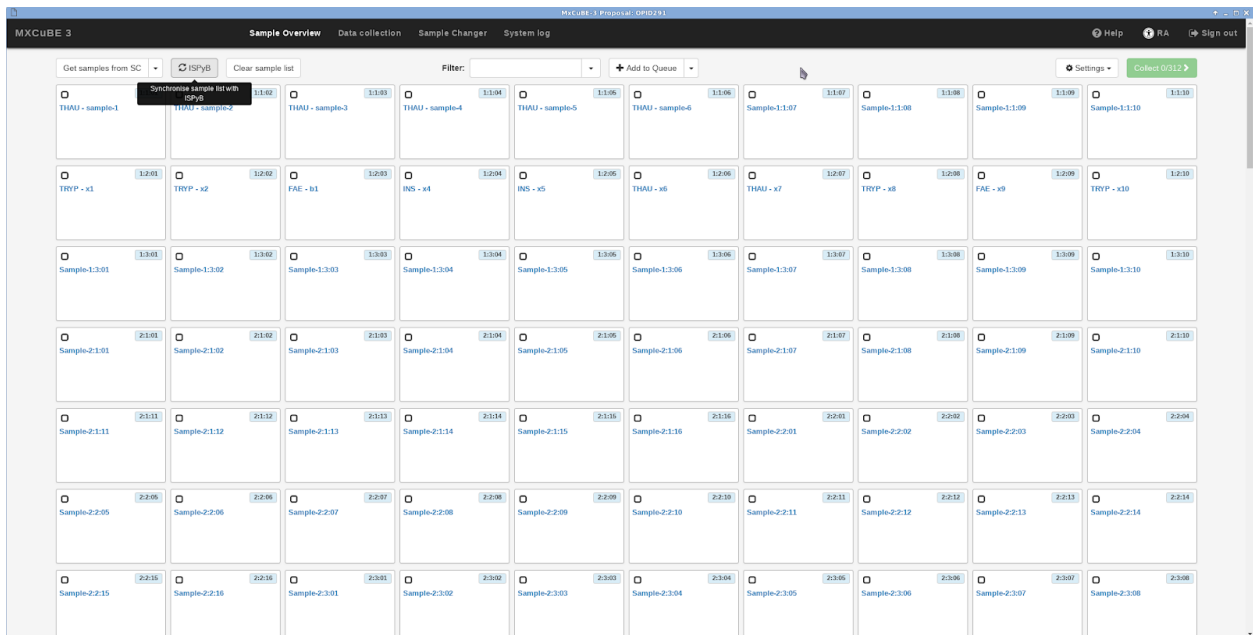
After login:  
Go to Sample overview to Sync ISPyB

## 1. Login



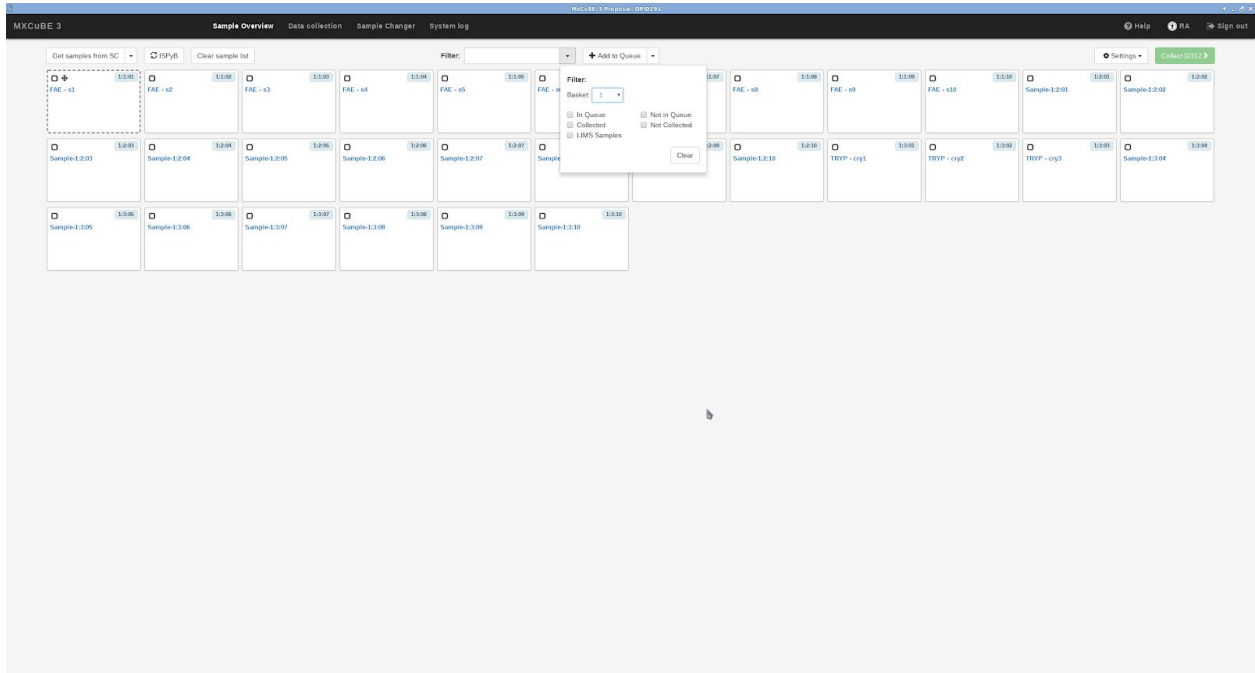
## 2. Sync ISPyB

Sync ISPyB retrieves information on Samples.

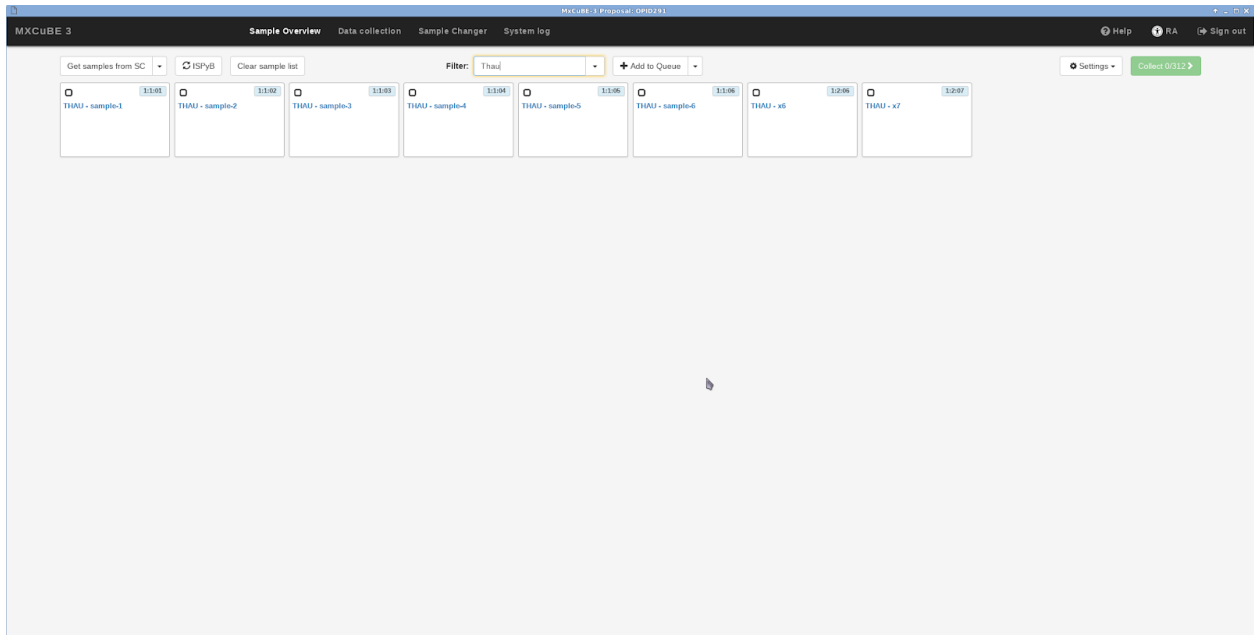


### 3. Filter samples

You can filter the samples by Basket positions (or by collected, non collected, in queue)

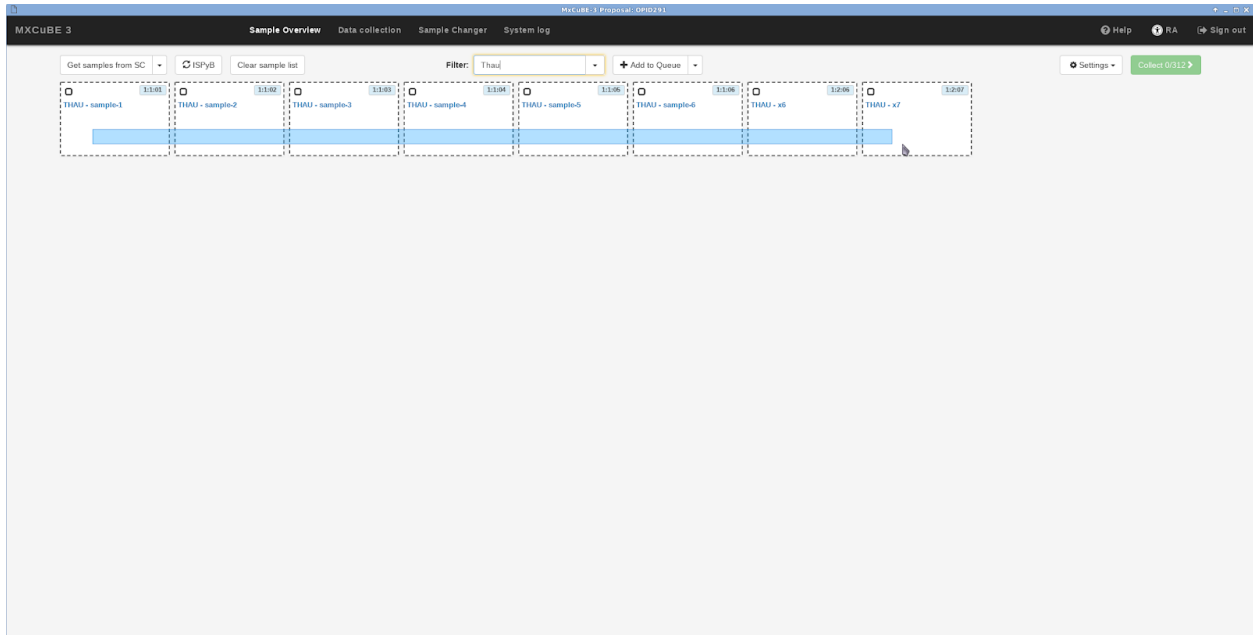


Or by sample name (typing name in filter)

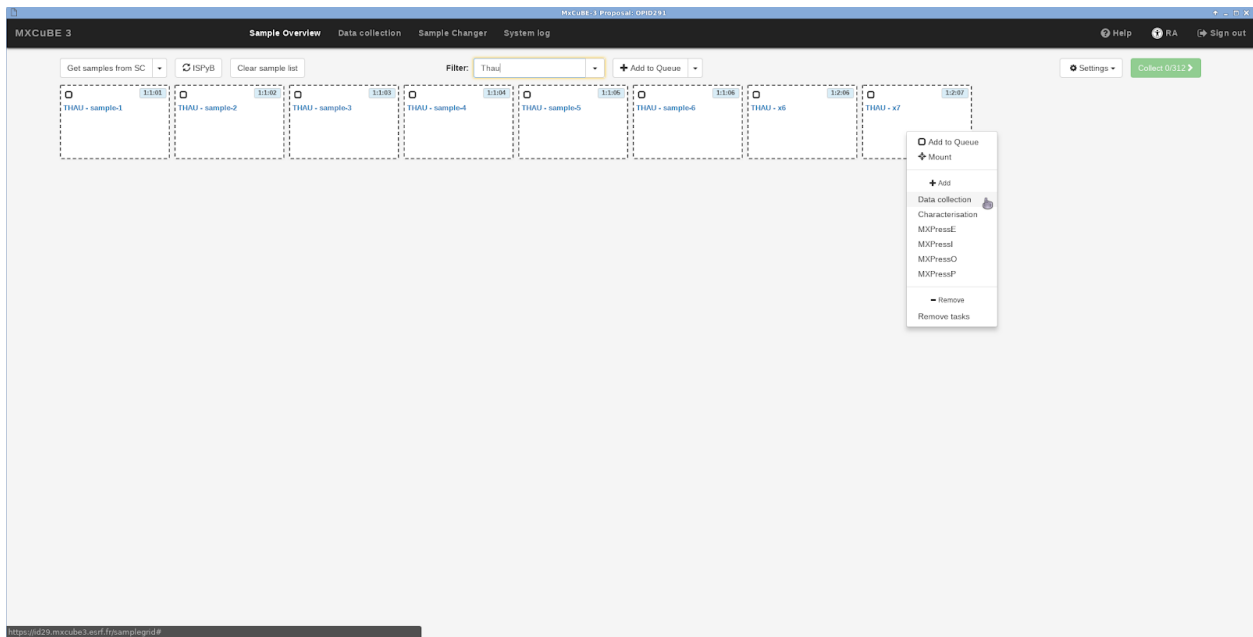


## 4. Add Data collection to samples - Pipeline mode

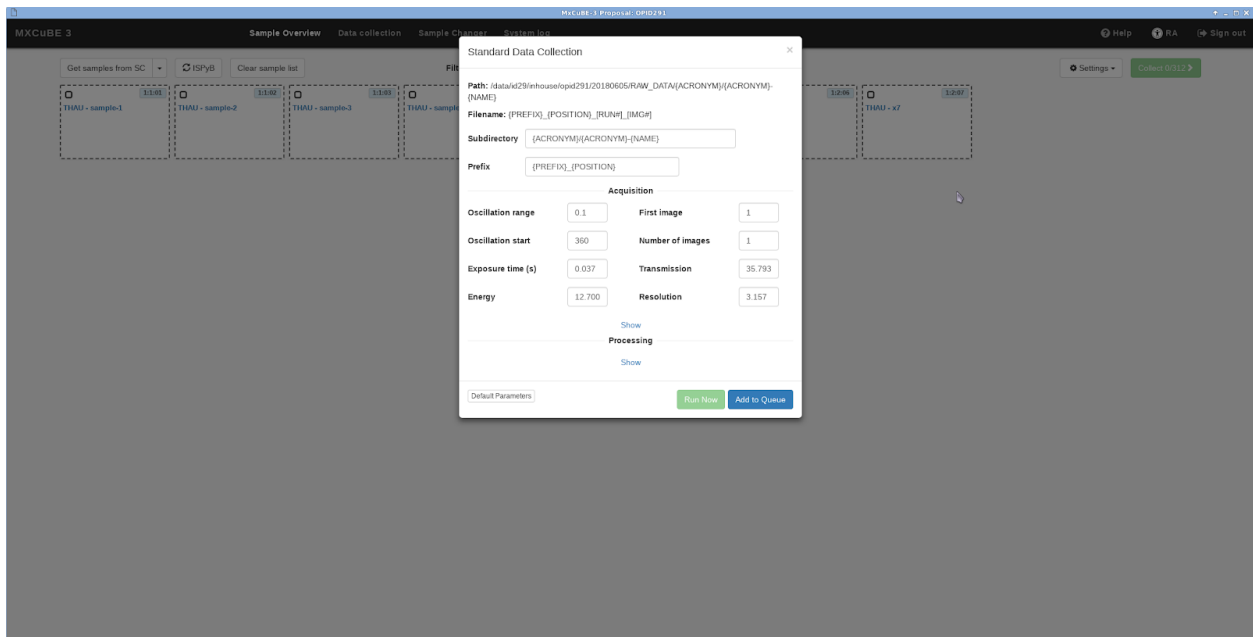
Select the samples you want to work on



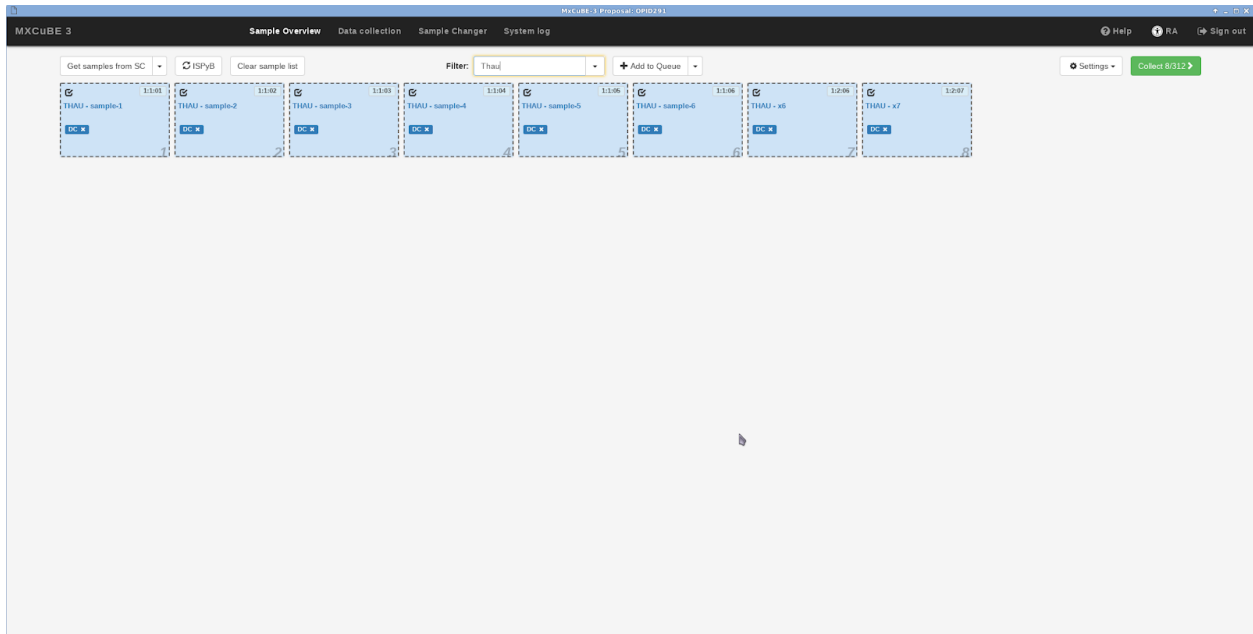
And add a Data collection to them (this is the best strategy if you are going to perform data collections with the same strategy)



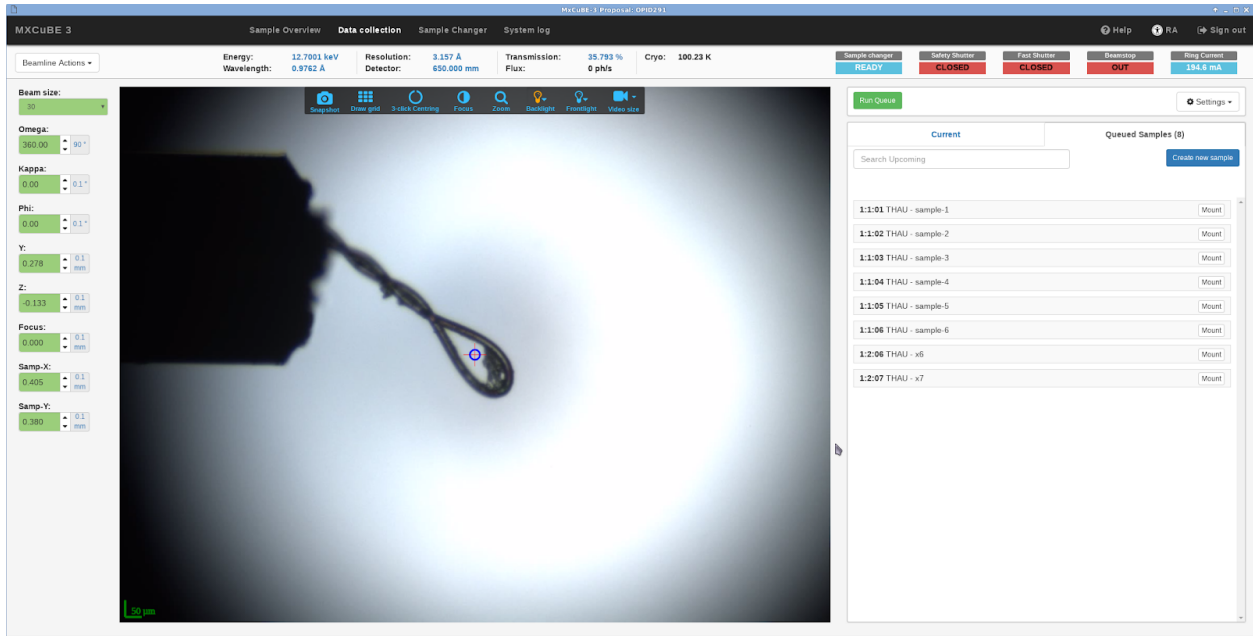
Specify the data collection parameters (same for all selected samples) and Add to Queue



Samples now are blue (which means they are in the queue) and a data collection item (DC) has been added to them

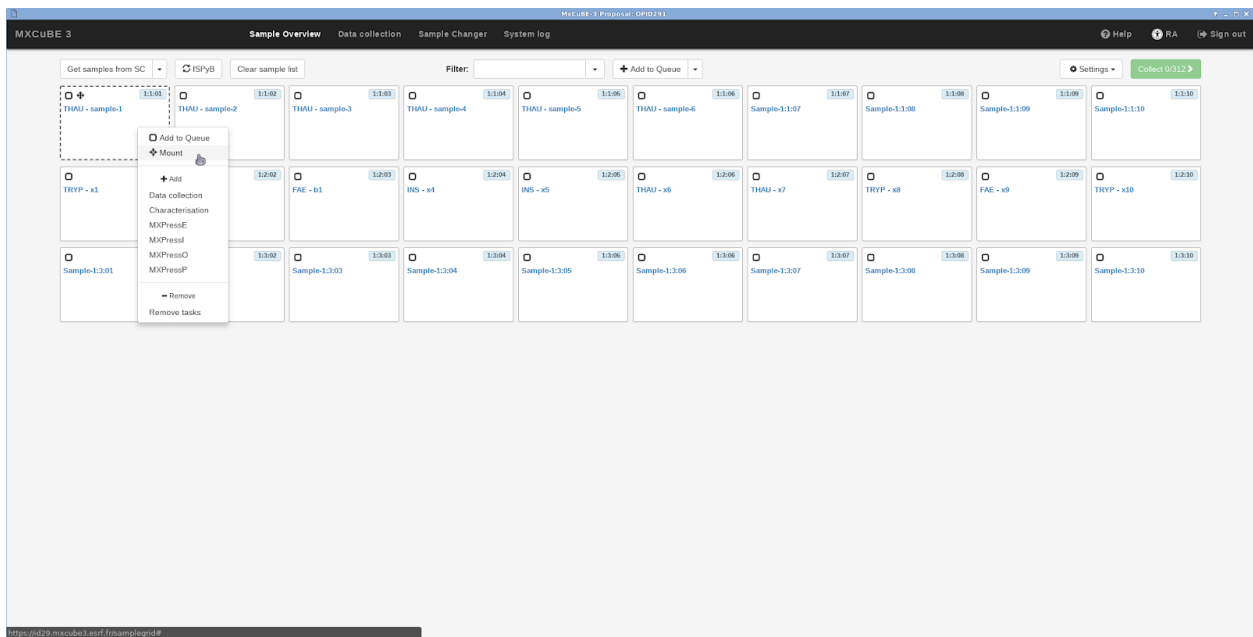


When you click on Collect (green button) the first sample is mounted

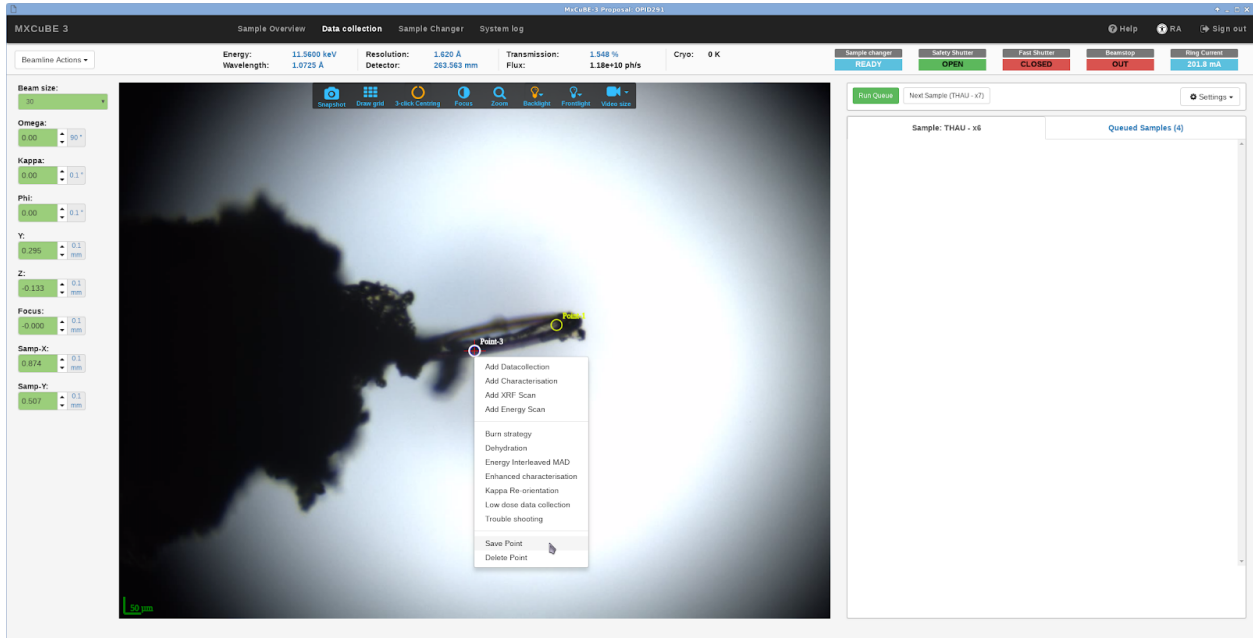


## 5. Mount Sample by Sample

Alternatively you can decide what to do sample by sample and mount them directly from Sample Overview

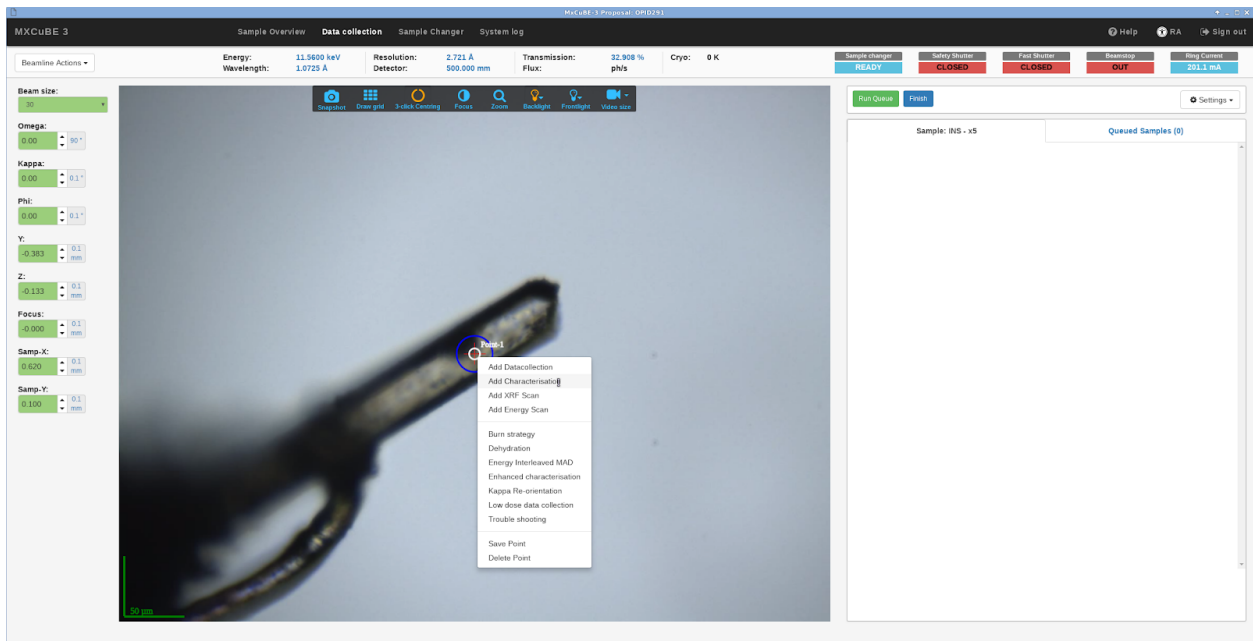


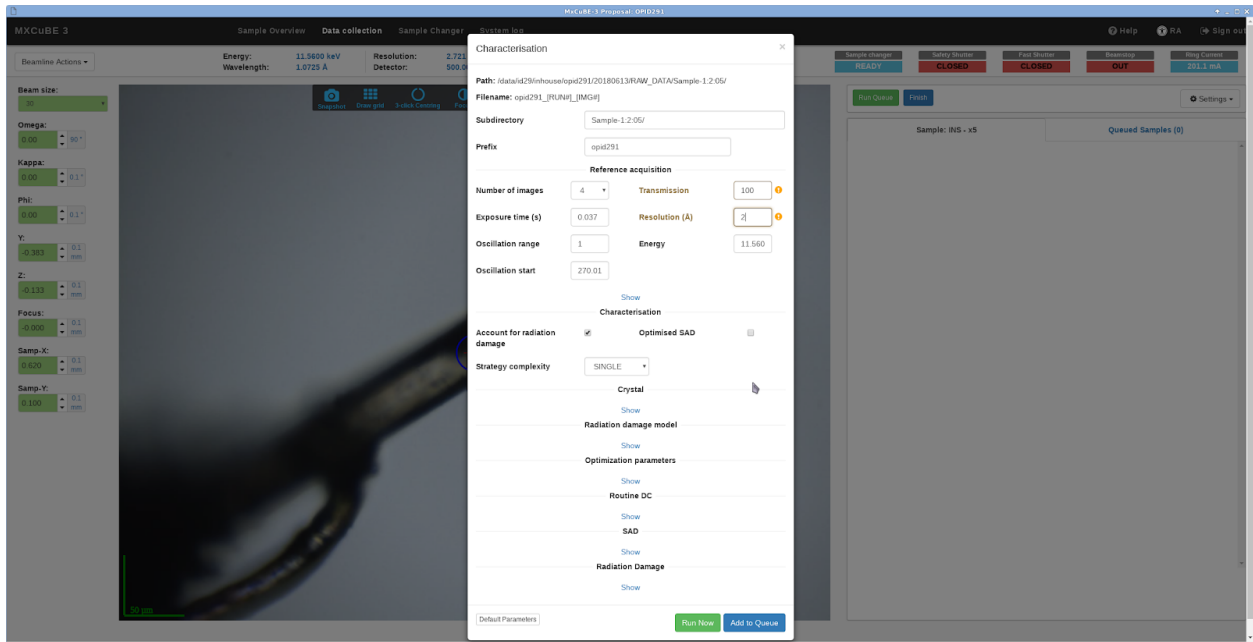
When the sample is mounted and centered any possible data collection can be added to a point, or the point can be saved for later use. Right click on the point to open the menu. If you add any data collection the point will be saved automatically



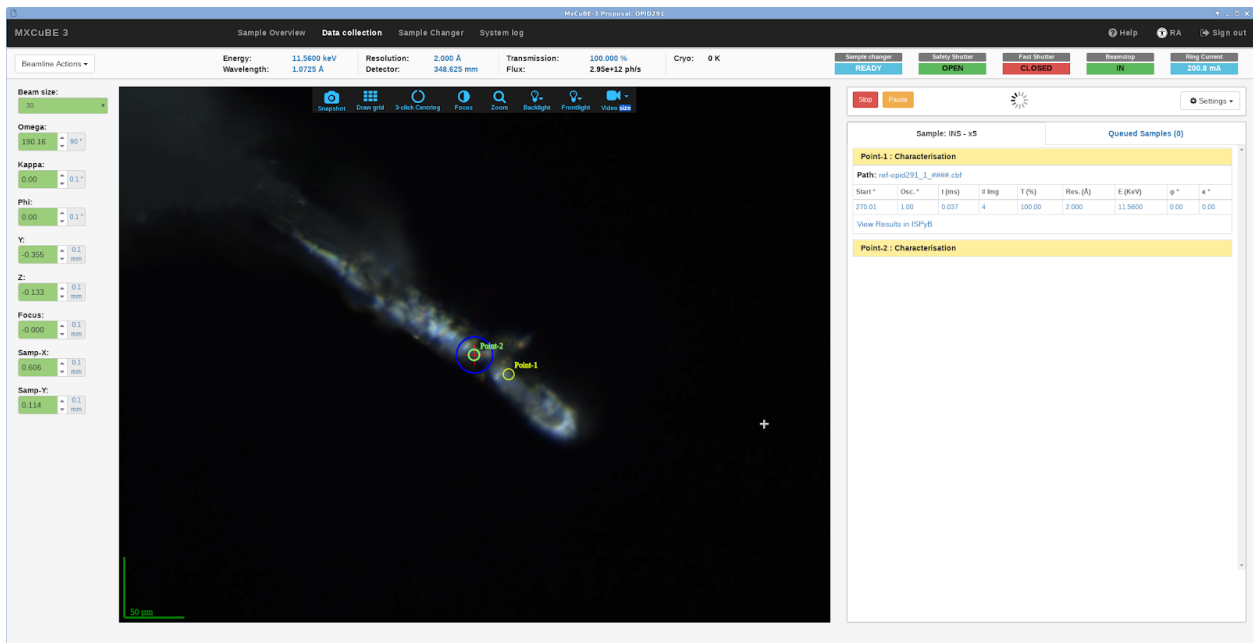
## 6. Characterisation

When adding a characterisation all BEST parameters can be specified





While Characterisation is running the Queue is busy



If the Characterisation ends up with a strategy the queue task is green and a Add diffraction plan and access the data collection parameters

MXCUBE 3

Sample Overview Data collection Sample Changer System log

Energy: 11.3600 keV Resolution: 2.000 Å  
Wavelength: 1.0725 Å Detector: 948.823

Beamline Actions

Beam size: 30  
Omega: 190.16  
Kappa: 0.00  
Phi: 0.00  
Y: -0.305  
Z: -0.113  
Focus: -0.000  
Samp-X: 0.005  
Samp-Y: 0.114

Standard Data Collection

Path: /state428/inhouse/ops291/0180613/RAW\_DATA/Sample-1.2.05/  
Filename: ops291\_w1\_[RUN#]\_[IMG#]  
Subdirectory: Sample-1.2.05/  
Prefix: ops291\_w1

Acquisition

Oscillation range: 0.05 First image: 1  
Oscillation start: 01 Number of images: 2580  
Exposure time (s): 0.037 Transmission: 1.5651  
Energy: 11.56 Resolution: 1.62

Processing

Run Now Add Diffraction Plan to Queue

Sample: /WS - x5

Queued Samples (0)

Point-1 : Characterisation

Path: /self-ops291\_1\_####.csl

Start <sup>o</sup>	Dec. <sup>o</sup>	T (ms)	# img	T (%)	Res. (Å)	E (KeV)	$\phi$ °	$\kappa$ °
270.01	1.00	0.037	4	100.00	2.000	11.5600	0.00	0.00

View Results in ISPyB

Point-2 : Characterisation

Path: /self-ops291\_2\_####.csl

Start <sup>o</sup>	Dec. <sup>o</sup>	T (ms)	# img	T (%)	Res. (Å)	E (KeV)	$\phi$ °	$\kappa$ °
270.01	1.00	0.037	4	100.00	2.000	11.5600	0.00	0.00

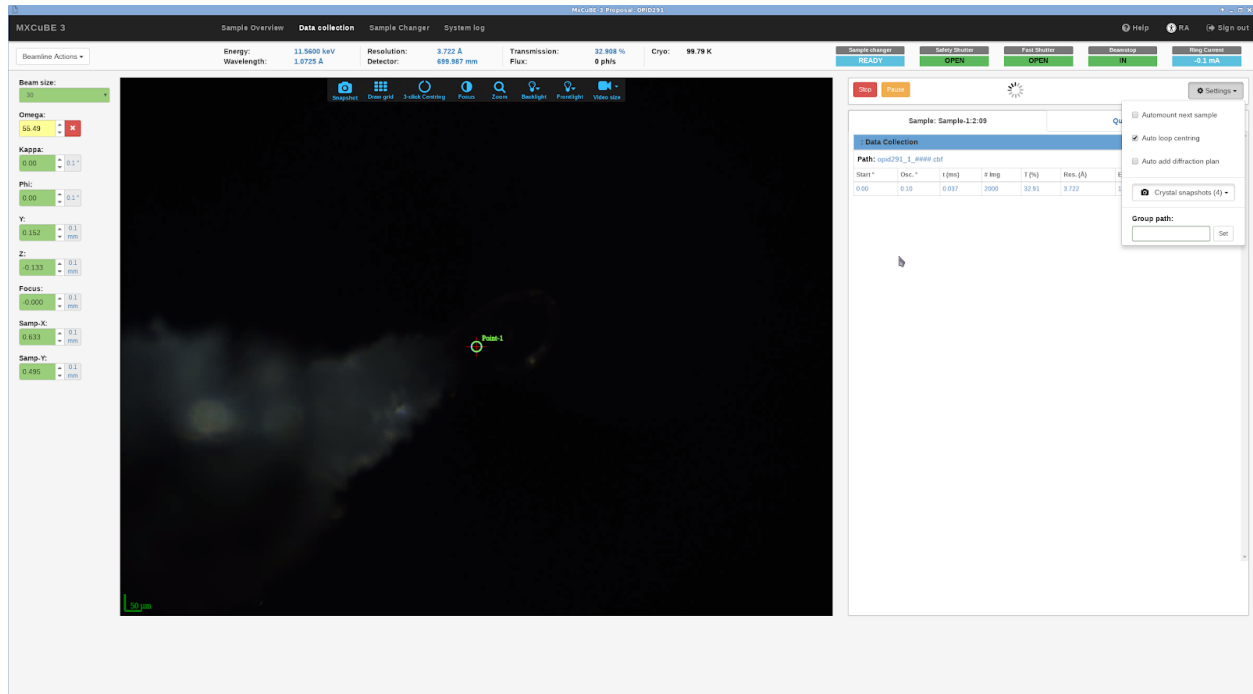
View Results in ISPyB

↓ Add Diffraction Plan



## 7. Settings

The Settings menu in the Data collection (and in the Sample overview) contains additional options. Autoloop centring performs automatic centring (default on). Automount next sample automatically mount the following sample as soon as the data collection is over. AutoAdd diffraction plan adds the result of the Characterisation and performs data collection without user intervention. It is also possible to specify a Group ID, which adds a subfolder below RAW\_DATA. It is possible to specify different subfolders (ex. TestData/Test1/Test2)



The screenshot displays the MXCuBE 3 software interface. The main window is titled "MXCuBE 3" and shows the "Data collection" tab. The interface is divided into several sections:

- Top Bar:** Displays "Sample Overview", "Data collection", "Sample Changer", and "System log". It also shows "Energy: 12.5800 keV", "Wavelength: 1.0725 Å", "Resolution: 3.722 Å", "Detector: 689.887 mm", "Transmission: 52.868 %", "Flux: 8 ph/s", and "Cryo: 99.79 K".
- Left Panel:** Contains "Beam size" (32) and various alignment parameters: Omega (55.49), Kappa (0.00), Phi (0.00), Y (-0.152 mm), Z (-0.133 mm), Focus (-0.000 mm), Samp. X (0.633 mm), and Samp. Y (0.246 mm).
- Center:** A large dark area representing the diffraction pattern, with a small green circle labeled "Point 1" and a scale bar of 100 μm.
- Right Panel:** Shows the "Data Collection" settings for "Sample: Sample-1:2:05". It includes a table for the diffraction plan:

Start	Disc.	t (ms)	t (mg)	t (%)	Res. (Å)
0.00	0.18	0.037	2000	32.91	3.722

Additional settings on the right include "Automount next sample" (checked), "Auto loop centring" (checked), "Auto add diffraction plan" (checked), and "Crystal snapshots (4)". A "Group path:" field is also visible.

## 8. Beamline alignment etc

Beamline related functions are under the Beamline Actions menu and are beamline specific. Here user can find Centre beam, Quick realign, Annealing, etc.

The screenshot displays the MXCuBE 3 software interface. At the top, there are tabs for 'Sample Overview', 'Data collection', 'Sample Changer', and 'System log'. The 'Data collection' tab is active, showing parameters: Energy: 11.5600 keV, Wavelength: 1.0725 Å, Resolution: 2.721 Å, Detector: 500.000 mm, Transmission: 1.548 %, Flux: ph/s, and Cryo: 0 K. Below these are status indicators for 'Sample changer' (READY), 'Safety shutter' (CLOSED), 'Fast shutter' (CLOSED), 'Beamstop' (OUT), and 'Ring Current' (200.7 mA).

The main interface is divided into three sections:

- Beamline Actions:** A vertical menu on the left containing 'Centre beam' (Run), 'Quick realign' (Run), 'Anneal' (Run), 'Detector cover' (OUT), 'Scintillator' (OUT), 'Aperture' (OUT), 'Hutchtrigger' (ENABLED), and 'Cryo' (IN). Below this are sliders for 'Samp-X' (1.541 mm) and 'Samp-Y' (0.109 mm).
- Image View:** A large central window showing a dark, blurry image of a sample. A red circle labeled 'Point-1' is positioned on the sample. A scale bar in the bottom left corner indicates 1.00 mm.
- Sample Queue:** A panel on the right titled 'Sample: TRYP - x8' and 'Queued Samples (2)'. It contains a search field and a list of samples: '1:2:09 FAE - x9' and '1:2:10 TRYP - x10', each with a 'Mount' button.

## 9. Helical Data collection

Helical Data collection requires two points to be saved, when selected at the same time, right click on any of them and select Helical data collection

