MxDC

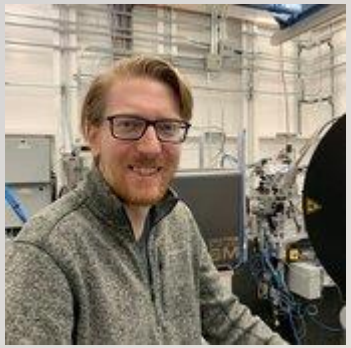
MX Data Collector

User-friendly data collection application for MX Beamlines

Michel Fodje – CMCF

Canadian Light Source | Centre canadien de rayonnement synchrotron

Kathryn

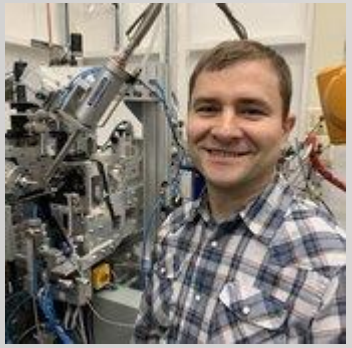

Scott

Shaun

Kiran

Michel

James


Denis

CMCF Team

Joel

Funding

INNOVATION.CA
CANADA FOUNDATION FOR INNOVATION | FONDATION CANADIENNE POUR L'INNOVATION

NSERC CRSNG

NRC · CNRC

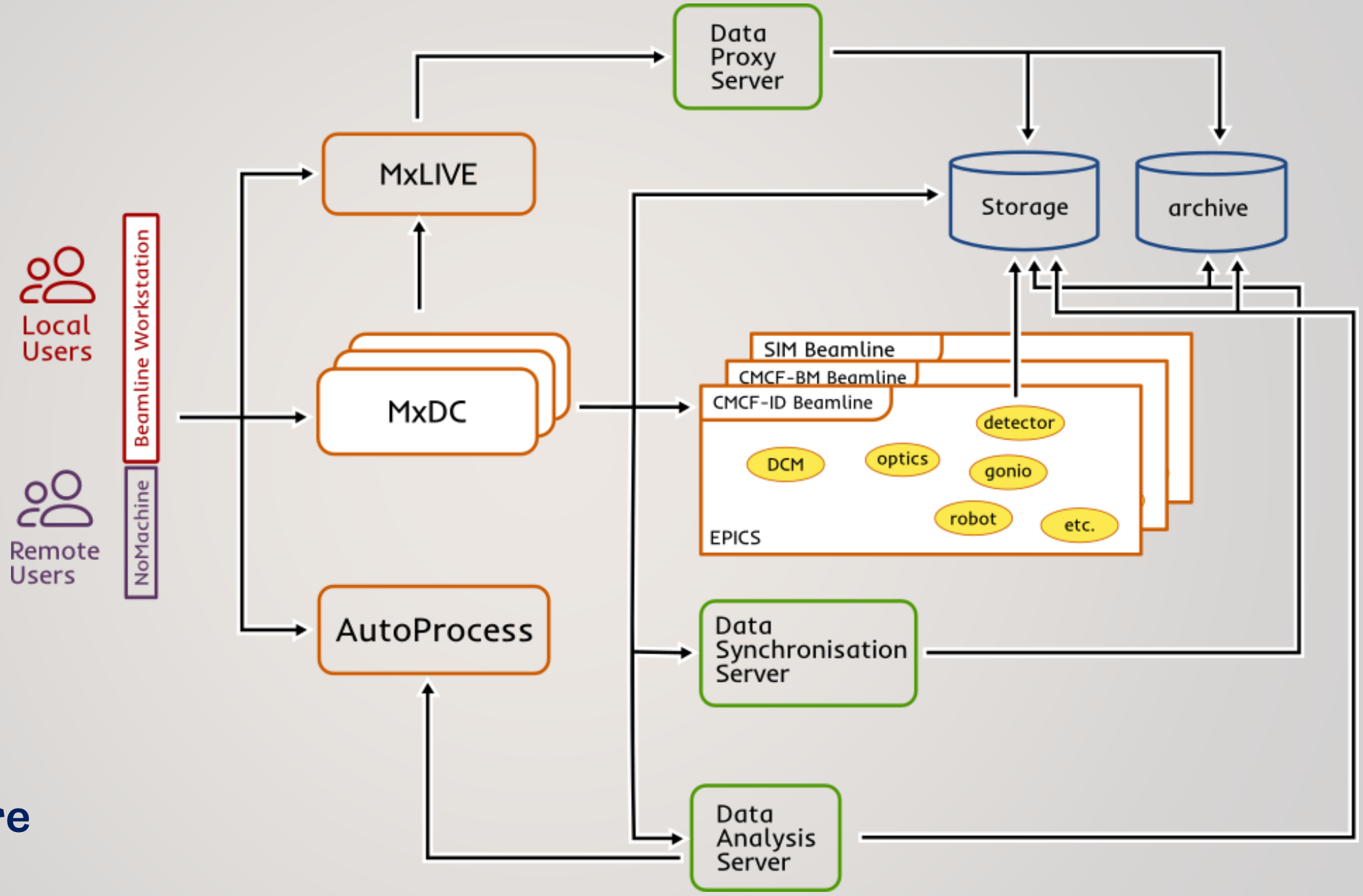
CIHR IRSC
Canadian Institutes of Health Research | Instituts de recherche en santé du Canada

University of Saskatchewan

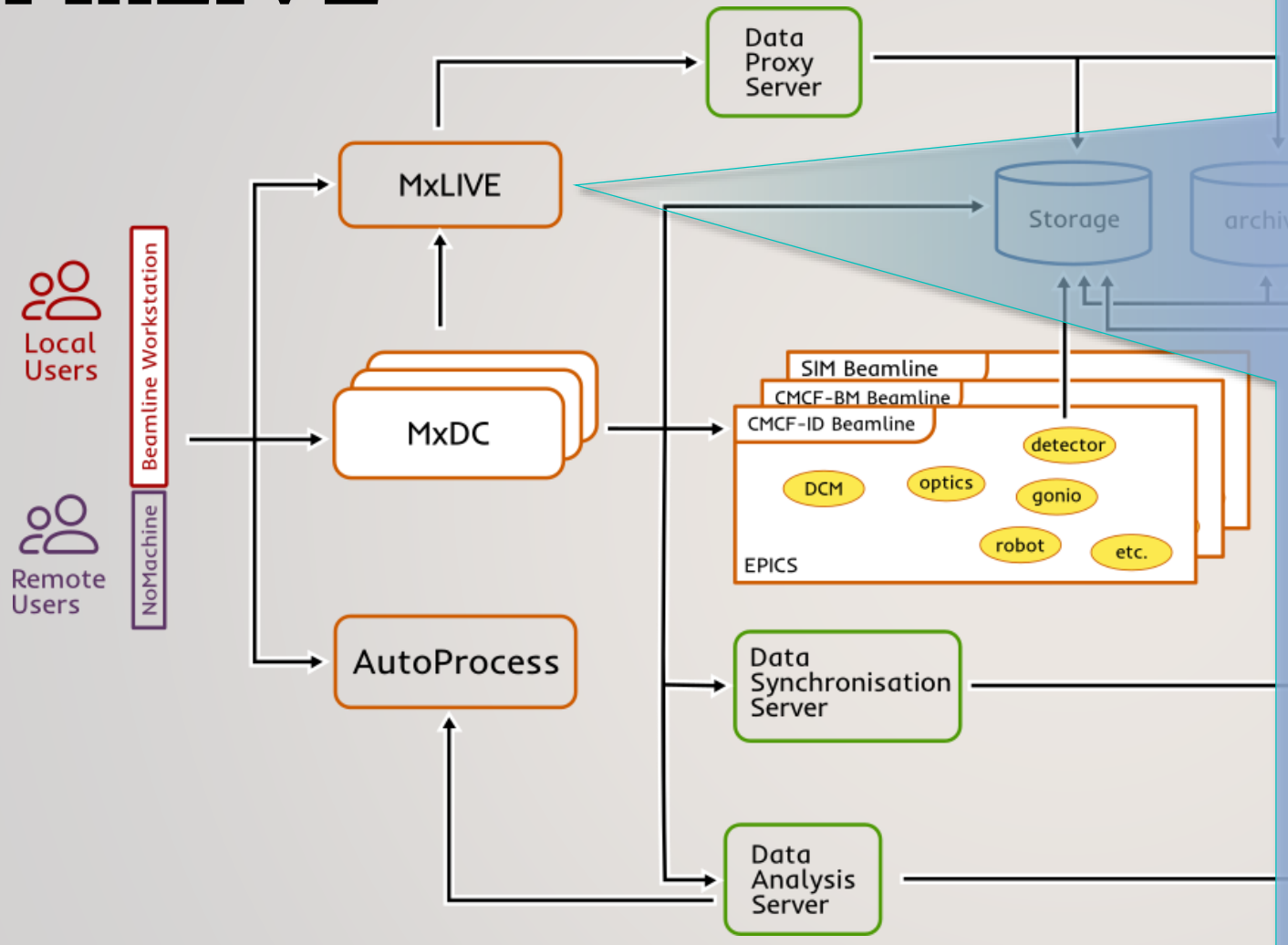
Government of Saskatchewan

Canada

CMCF Software Architecture



MxLIVE

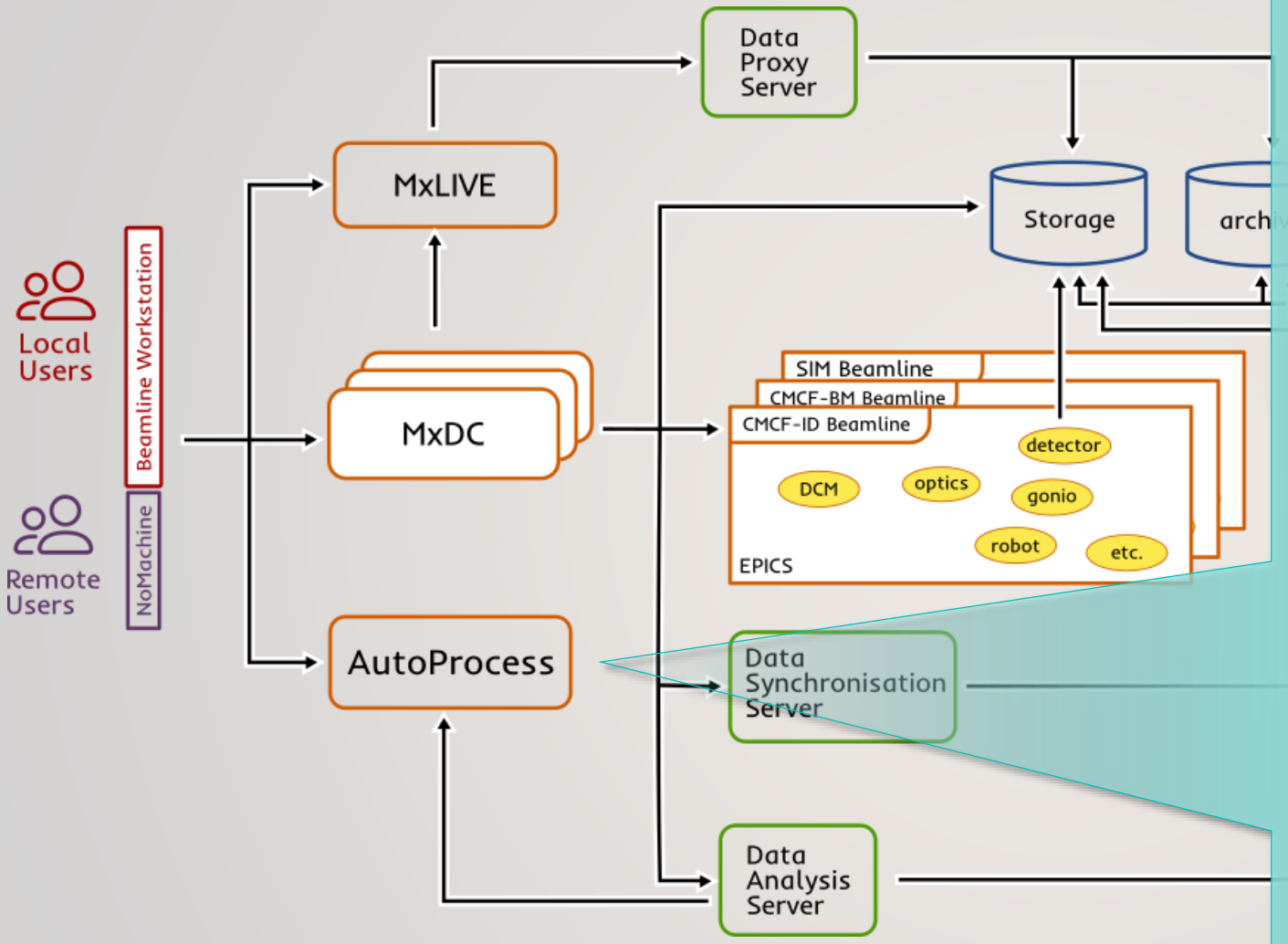


MxLIVE – Mx Lab Information Virtual Environment

- Web-based sample information management
- Meta-data archive
- Secure APIs
- Data access
- Staff Portal
- Since 2011

python
django
docker

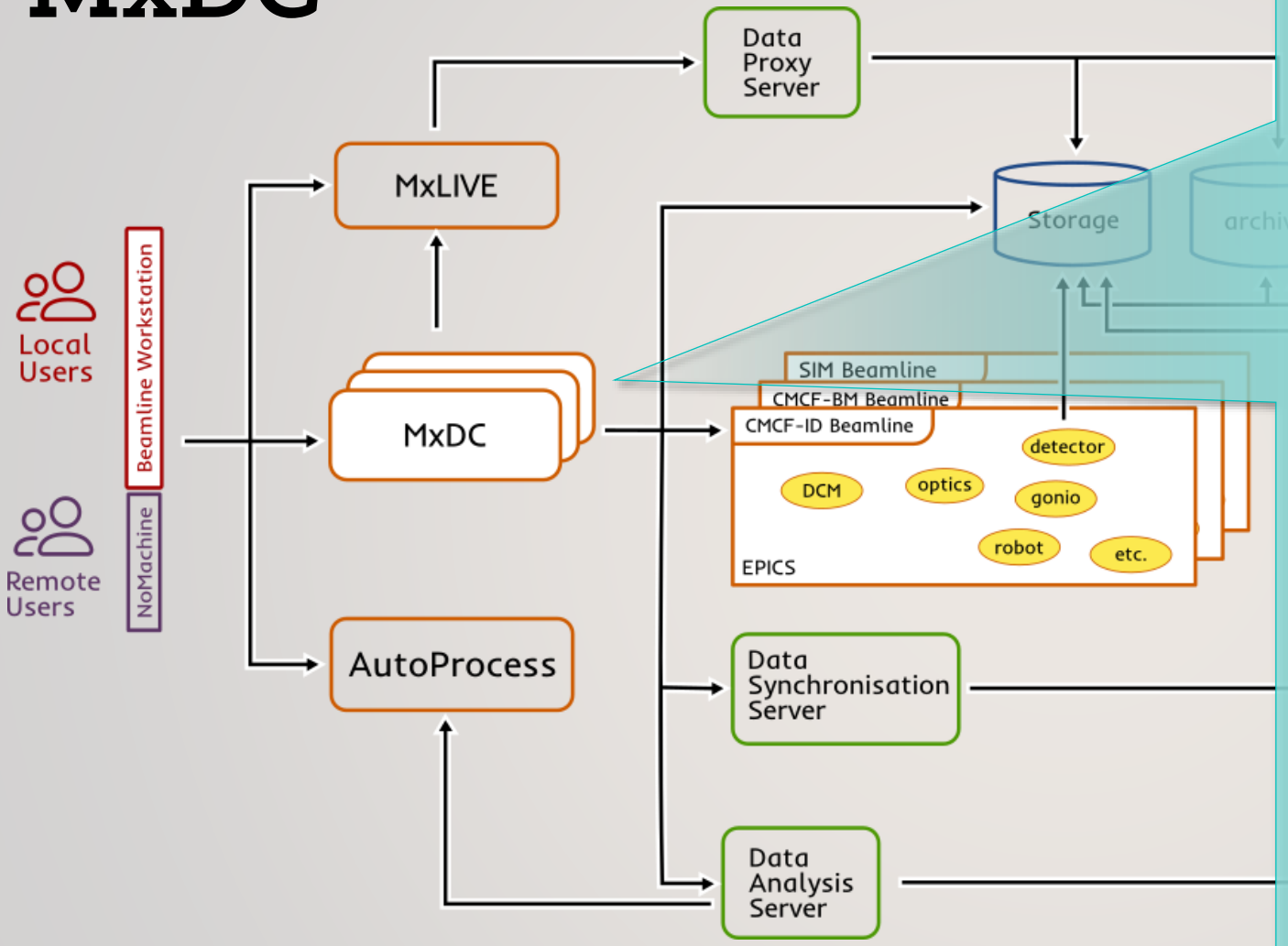
AutoProcess



- A set of command line utilities for automated reduction of diffraction data to “mtz”
- *Data Analysis Server* - an RPC server for automated data analysis from MxDC.
- Automated analysis of datasets from
  - MX
  - Powder Diffraction
- Integrated with MxDC
- Since 2007

python™

MxDC



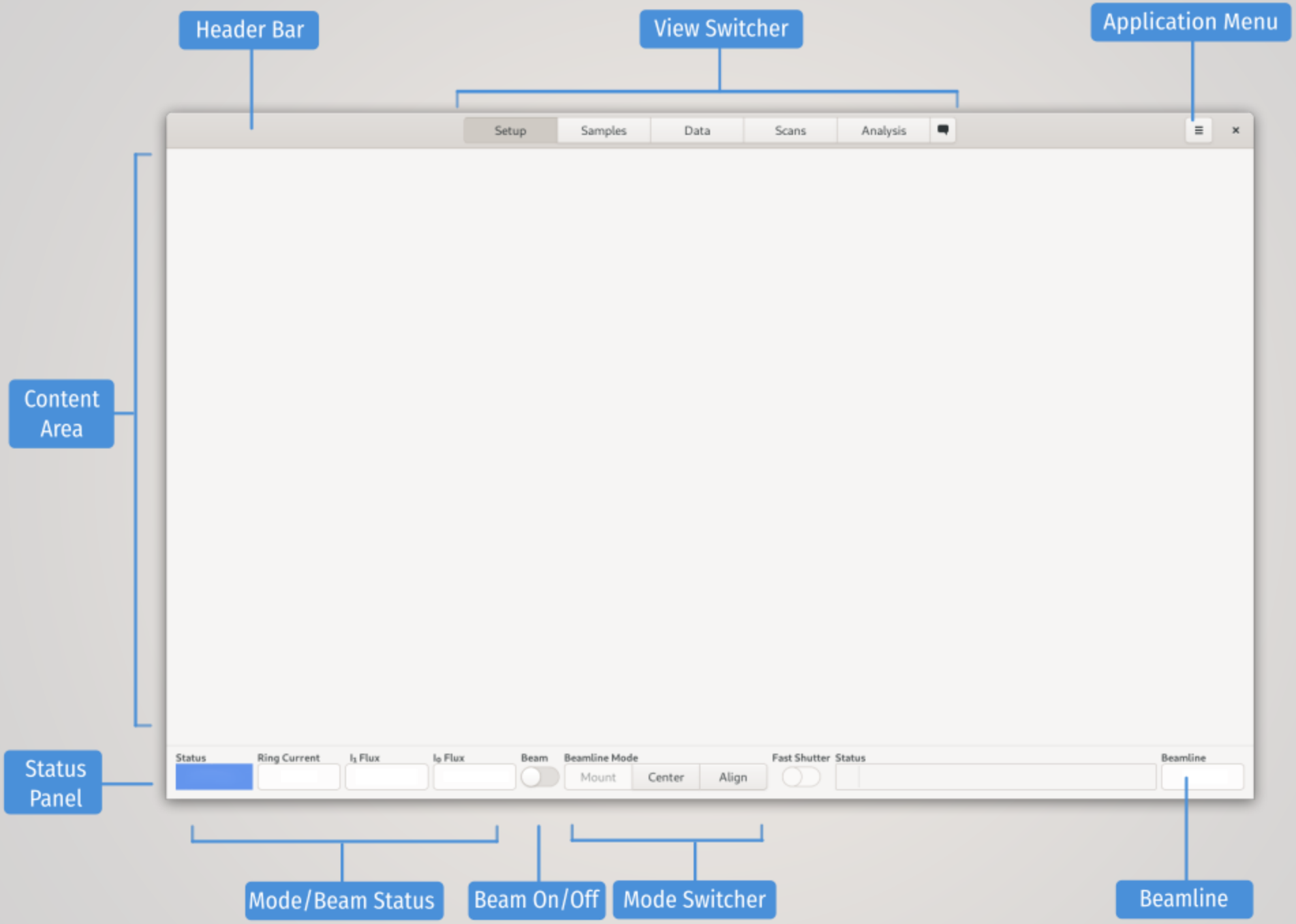
MxDC – Mx Data Collector

- Experiment management,
- Interactive and automated data acquisition
- One instance per beamline
  - Configuration file
- Single-window, multi-paged GUI
  - Setup, Samples, Data, Scans, Analysis Pages
- Separate Python-based SPEC-like Beamline console for staff and commissioning
- Since 2007

python™

Design Principles

- Users First!
  - Experiment focused, NOT beamline focused
  - User friendly, intuitive & familiar GUI
  - Make common techniques easy, and complex schemes possible, without sacrificing usability.
  - Integration (Single GUI for all techniques)
- Separation of Concerns
  - Pluggable components
  - Versatile interfaces between components
- Ease of deployment
  - Focus on common functional aspect of devices relevant for experimental technique
  - Support different beamlines with different hardware devices
  - One Python Config file per beamline

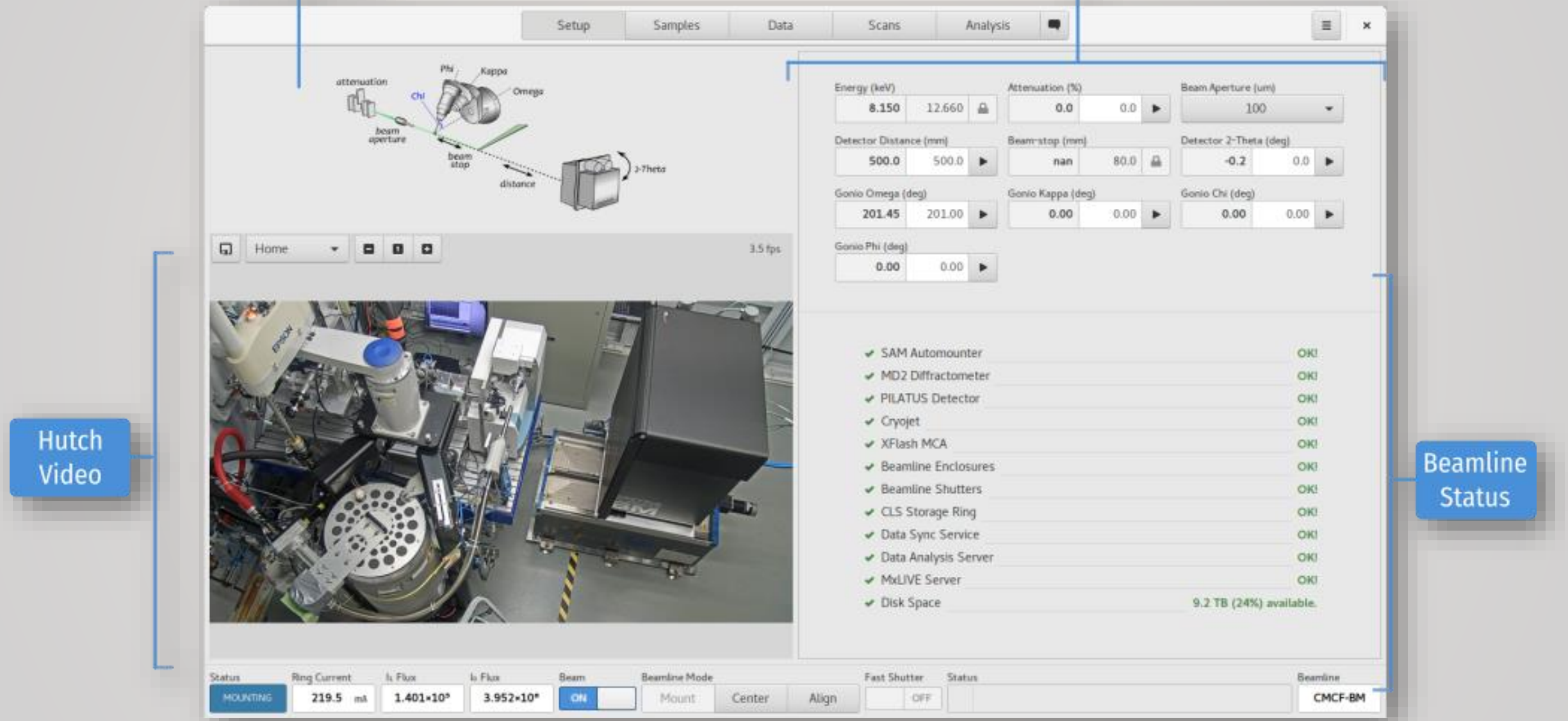

Header Bar
View Switcher
Application Menu
Content Area
Status Panel
Setup
Samples
Data
Scans
Analysis
Status
Ring Current
I_1 Flux
I_0 Flux
Beam
Beamline Mode
Mount
Center
Align
Fast Shutter
Status
Beamline
Mode/Beam Status
Beam On/Off
Mode Switcher
Beamline

Schematic

Parameters

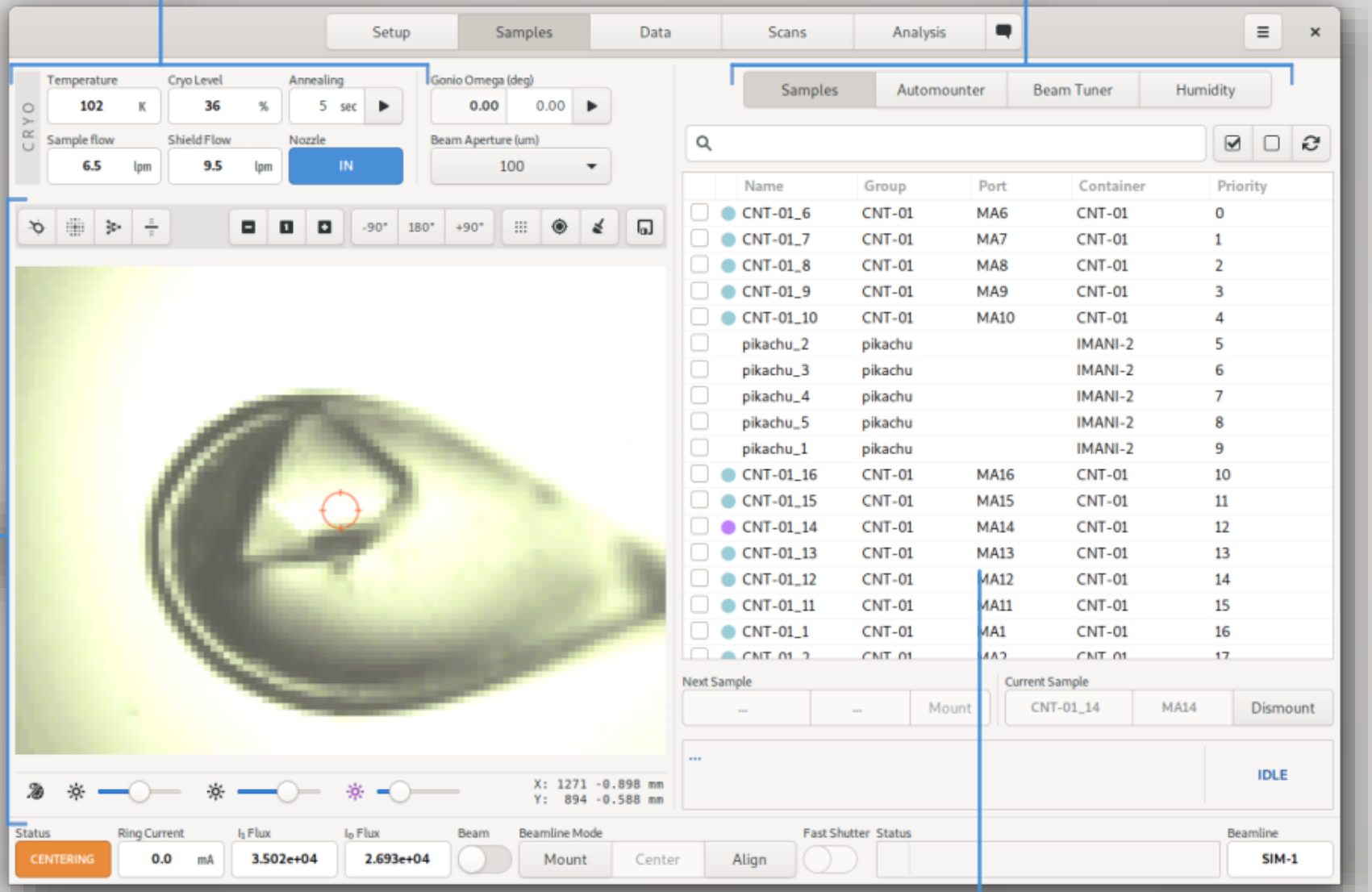
Hutch Video

Beamline Status



Cryo Tool

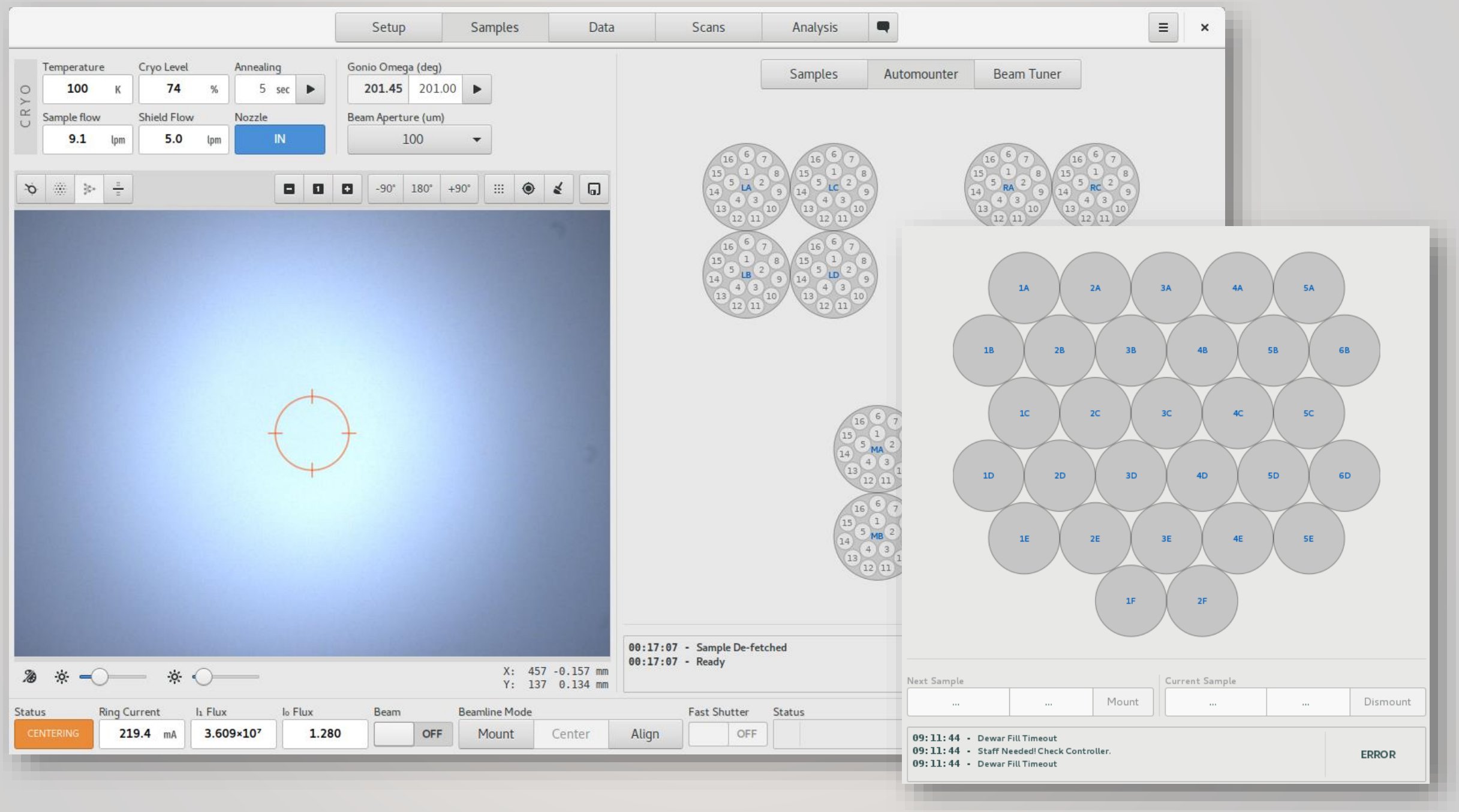
Tools



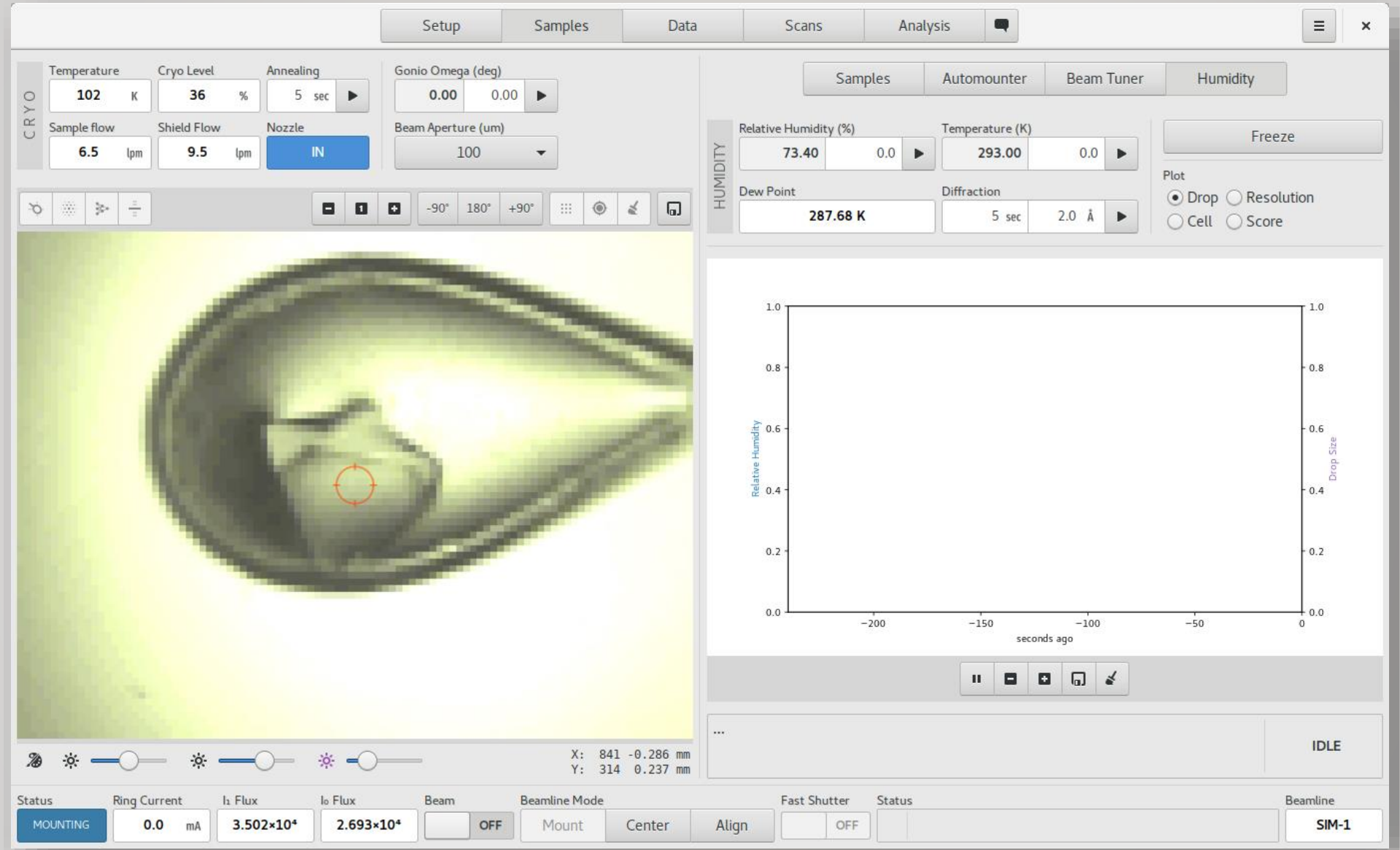
Sample Microscope

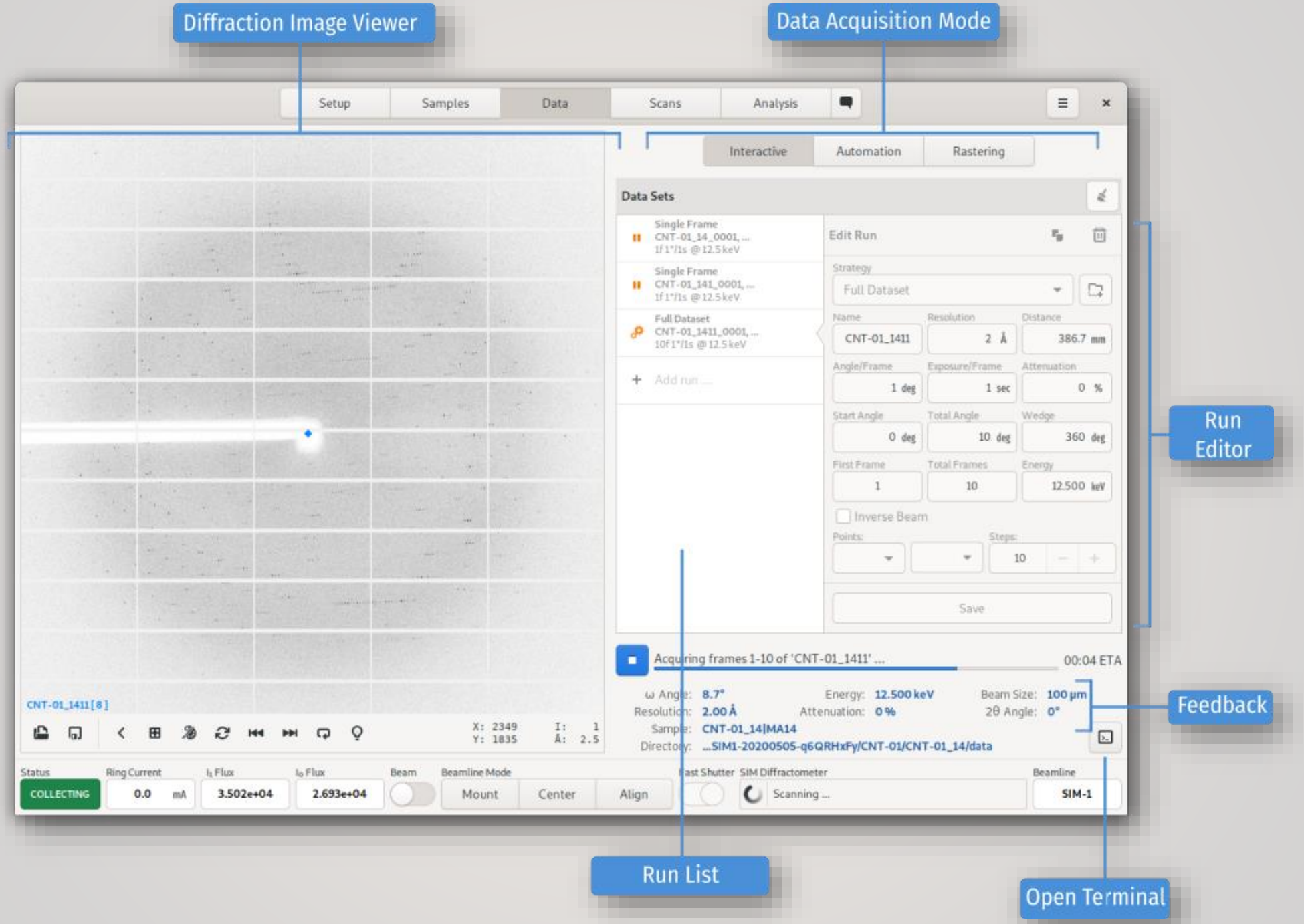
Sample List

SAMPLES – AUTOMOUNTER



SAMPLES – HUMIDITY CONTROL




Diffraction Image Viewer
Data Acquisition Mode
Setup
Samples
Data
Scans
Analysis
Interactive
Automation
Rastering
Data Sets
Single Frame
CNT-01_14_0001, ...
1f 1°/1s @12.5keV
Single Frame
CNT-01_141_0001, ...
1f 1°/1s @12.5keV
Full Dataset
CNT-01_1411_0001, ...
10f 1°/1s @12.5keV
Add run ...
Edit Run
Strategy
Full Dataset
Name
CNT-01_1411
Resolution
2 Å
Distance
386.7 mm
Angle/Frame
1 deg
Exposure/Frame
1 sec
Attenuation
0 %
Start Angle
0 deg
Total Angle
10 deg
Wedge
360 deg
First Frame
1
Total Frames
10
Energy
12.500 keV
Inverse Beam
Points:
Steps:
10
Save
Run Editor
Acquiring frames 1-10 of 'CNT-01_1411' ...
00:04 ETA
ω Angle: 8.7°
Energy: 12.500 keV
Beam Size: 100 µm
Resolution: 2.00 Å
Attenuation: 0 %
2θ Angle: 0°
Sample: CNT-01_14|MA14
Directory: ...SIM1-20200505-q6QRHxFy/CNT-01/CNT-01_14/data
Feedback
CNT-01_1411[8]
X: 2349
Y: 1835
I: 1
Å: 2.5
Status
COLLECTING
Ring Current
0.0 mA
I1 Flux
3.502e+04
I0 Flux
2.693e+04
Beam
Beamline Mode
Mount
Center
Align
Fast Shutter
SIM Diffractometer
Scanning ...
Beamline
SIM-1
Run List
Open Terminal

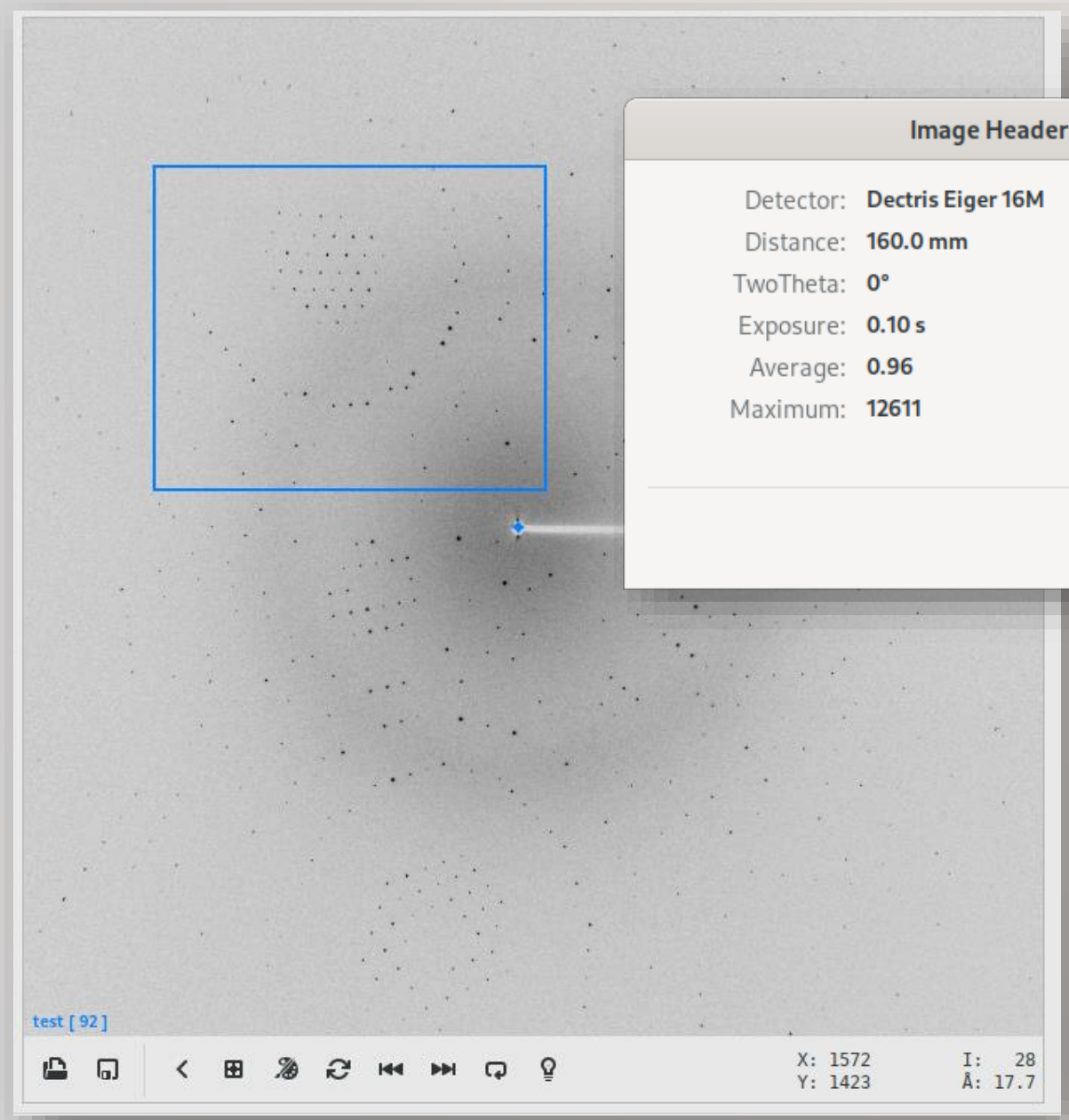
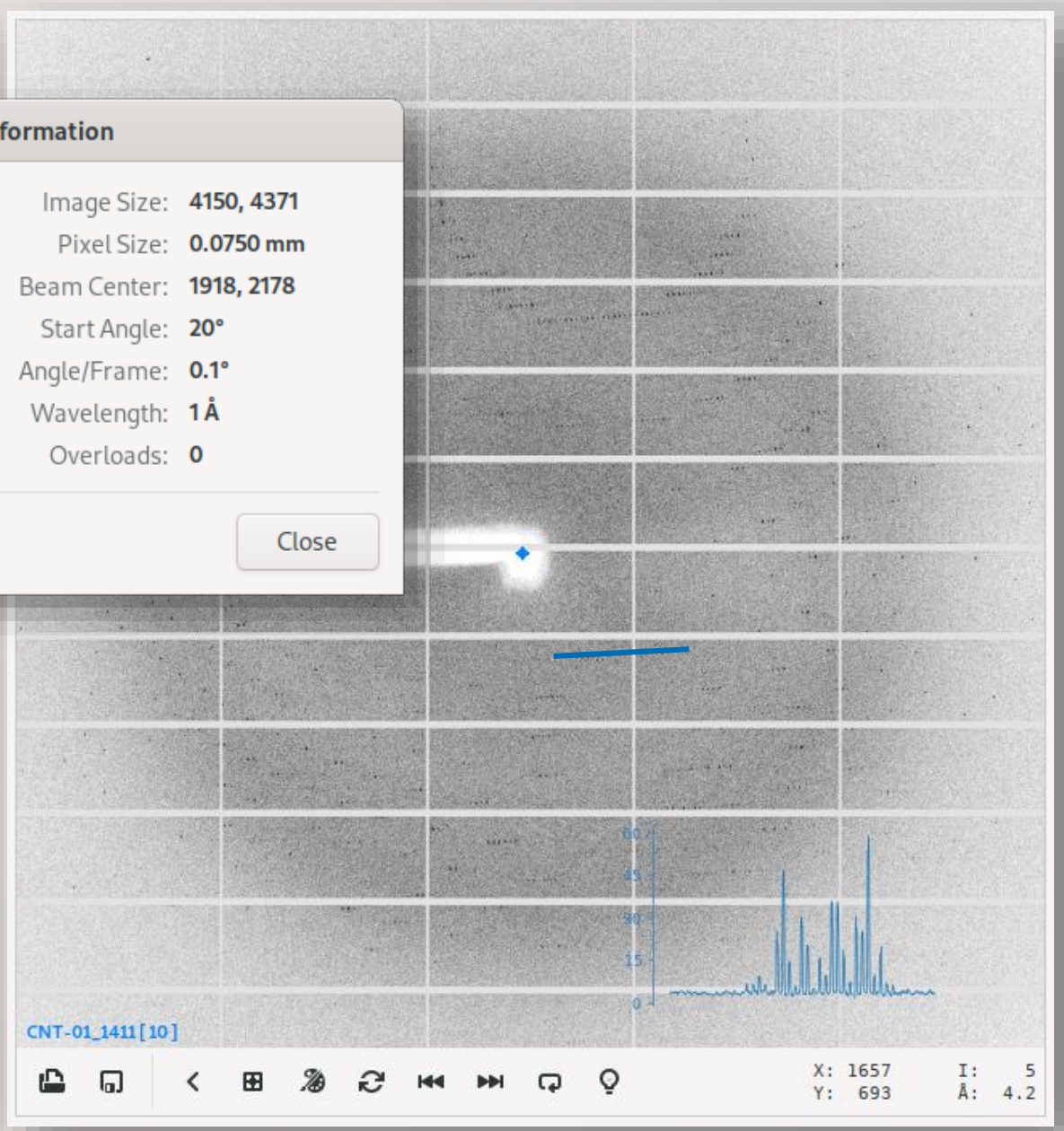
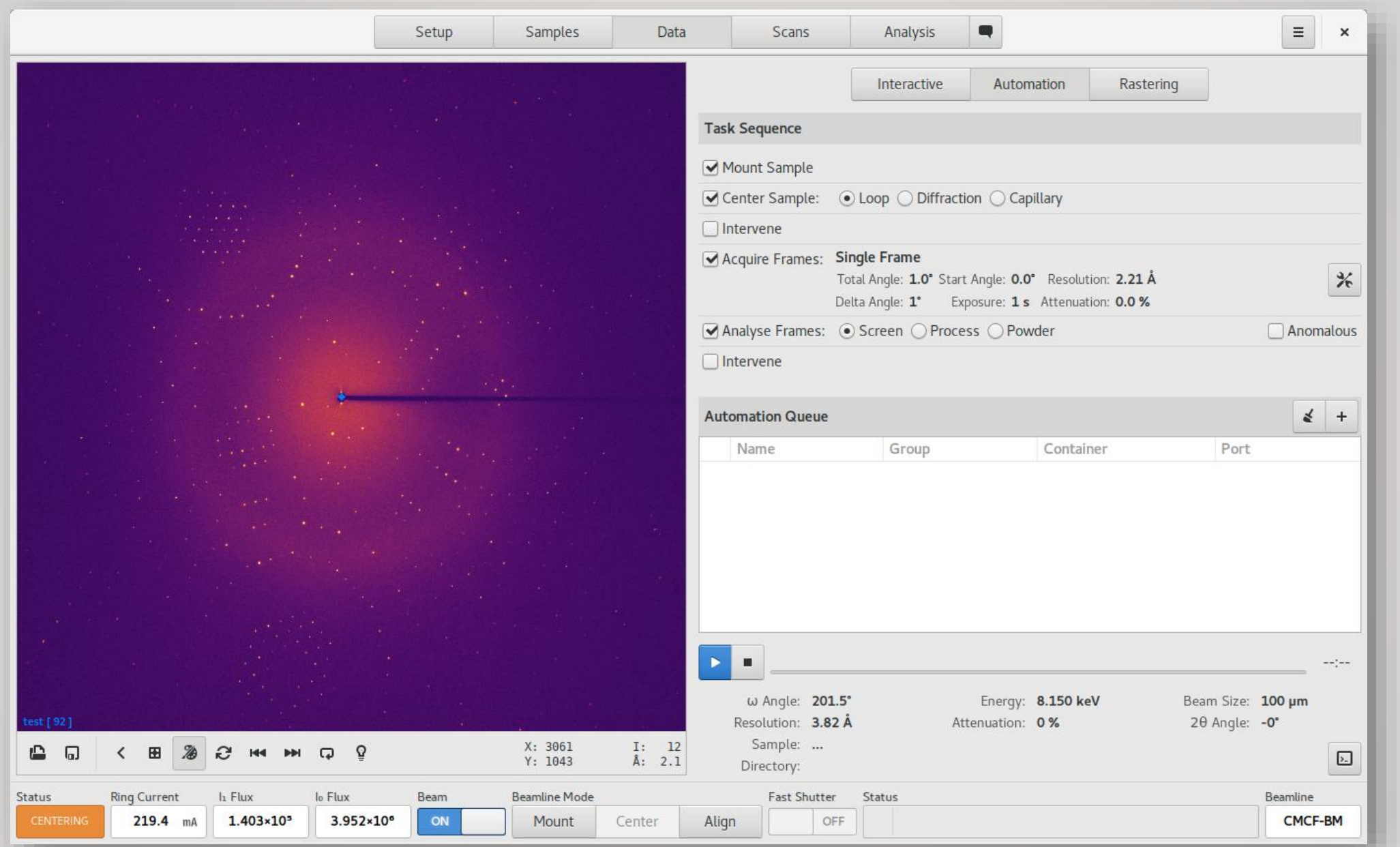
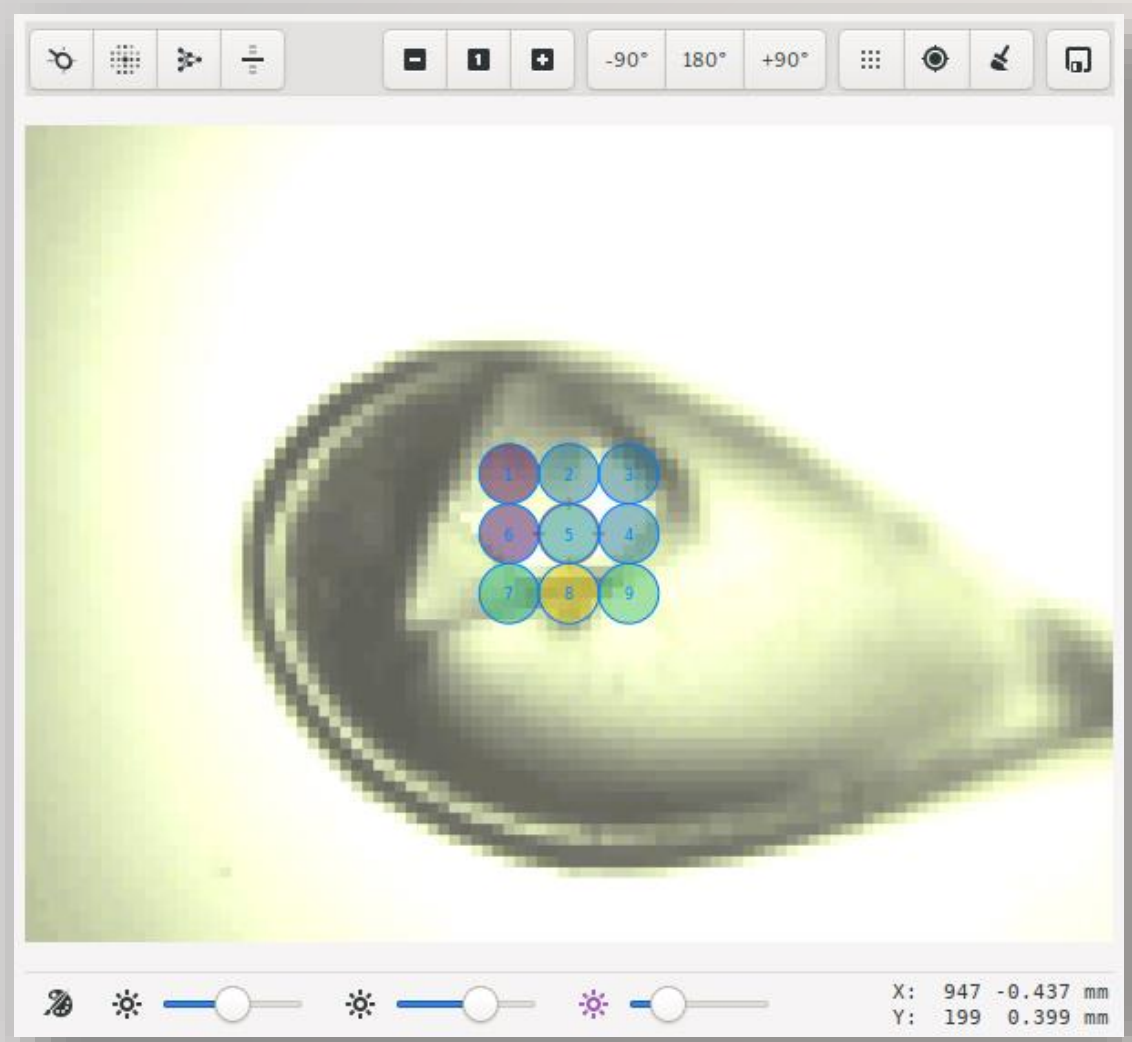


Image Header Information
Detector: Dectris Eiger 16M
Distance: 160.0 mm
TwoTheta: 0°
Exposure: 0.10 s
Average: 0.96
Maximum: 12611
Image Size: 4150, 4371
Pixel Size: 0.0750 mm
Beam Center: 1918, 2178
Start Angle: 20°
Angle/Frame: 0.1°
Wavelength: 1 Å
Overloads: 0
Close
test [92]
X: 1572
Y: 1423
I: 28
Å: 17.7


CNT-01_1411 [10]
X: 1657
Y: 693
I: 5
Å: 4.2


Setup
Samples
Data
Scans
Analysis
Interactive
Automation
Rastering
Task Sequence
Mount Sample
Center Sample: Loop Diffraction Capillary
Intervene
Acquire Frames: Single Frame
Total Angle: 1.0° Start Angle: 0.0° Resolution: 2.21 Å
Delta Angle: 1° Exposure: 1 s Attenuation: 0.0 %
Analyse Frames: Screen Process Powder Anomalous
Intervene
Automation Queue
Name
Group
Container
Port
test [92]
X: 3061 I: 12
Y: 1043 Å: 2.1
ω Angle: 201.5°
Resolution: 3.82 Å
Sample: ...
Directory:
Energy: 8.150 keV
Attenuation: 0 %
Beam Size: 100 µm
2θ Angle: -0°
Status
CENTERING
Ring Current
219.4 mA
I₁ Flux
1.403×10⁵
I₀ Flux
3.952×10⁶
Beam
ON
Beamline Mode
Mount
Center
Align
Fast Shutter
OFF
Status
Beamline
CMCF-BM

DATA - RASTERING

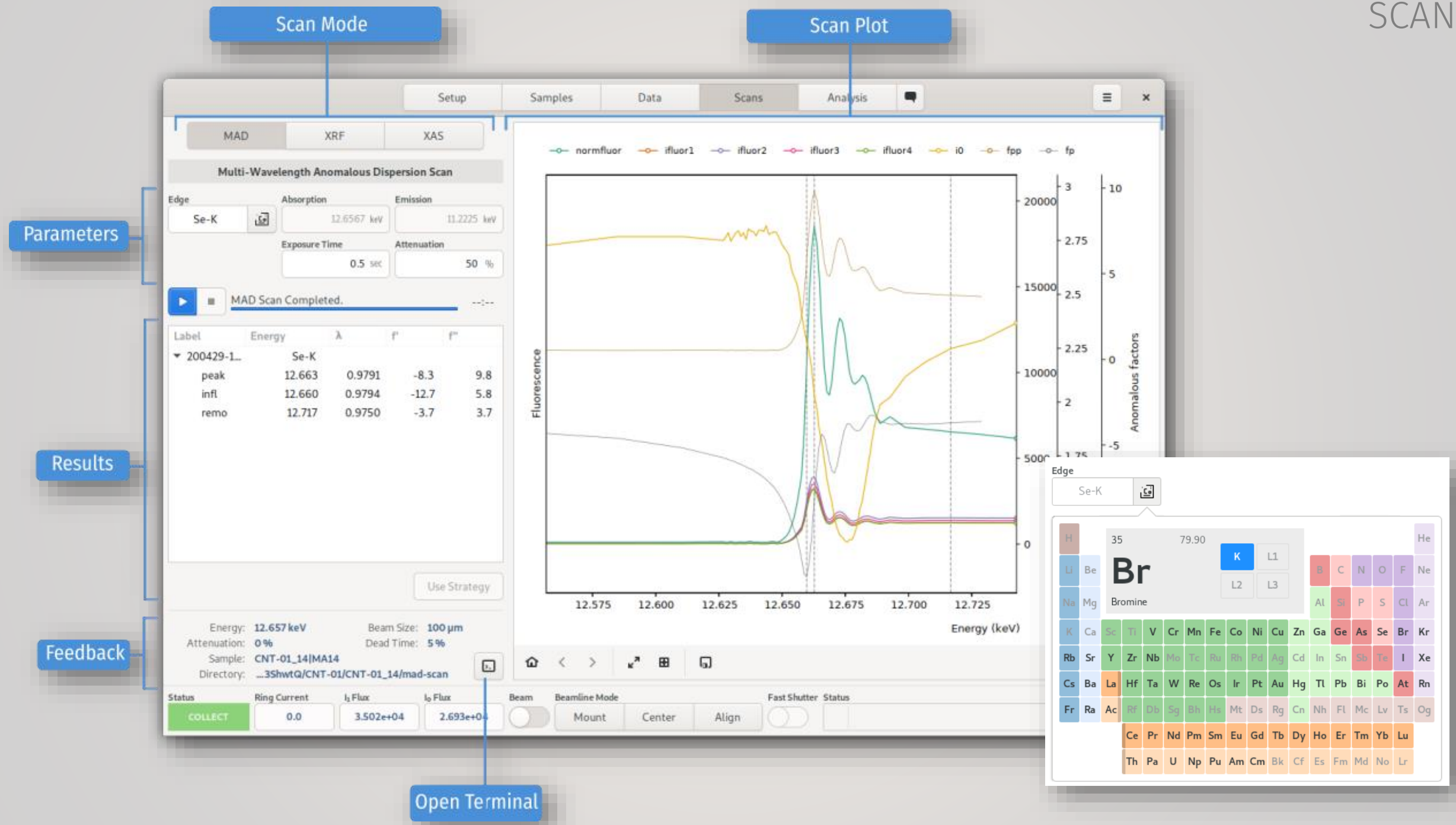


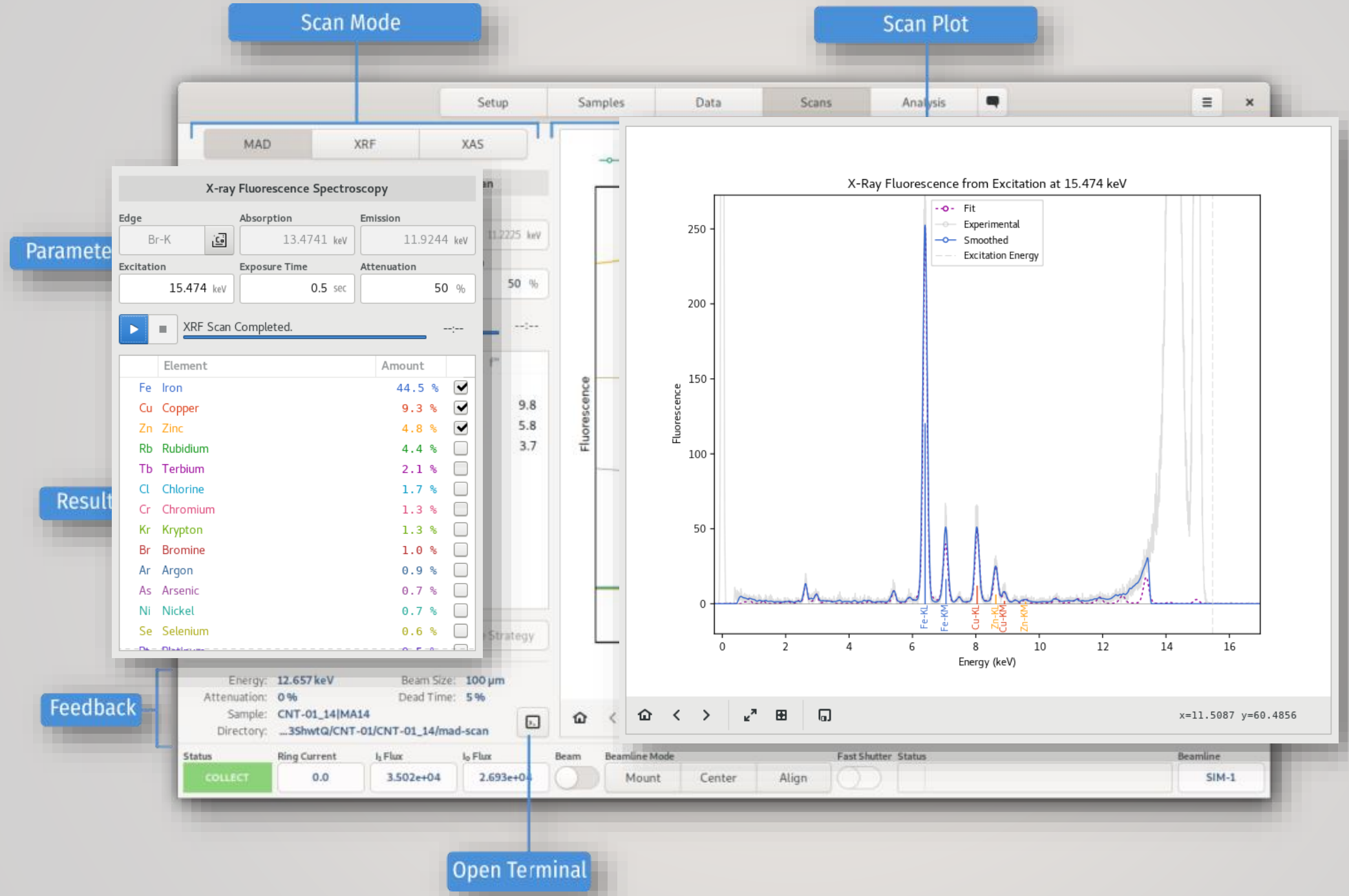
Interactive | Automation | Rastering

Grid Width	Grid Height	Exposure/Frame	Max Resolution
200 µm	200 µm	0.5 sec	2 Å

Frames/Line	Total Lines	Start Angle	Aperture
3	3	0 deg	100 µm

Label	Angle	X (mm)	Y (mm)	Z (mm)	Score
▼ 20050...					
1	0.0°	-0.1000	-0.1000	0.0000	370.0
2	0.0°	0.0000	-0.1000	0.0000	408.3
3	0.0°	0.1000	-0.1000	0.0000	407.5
4	0.0°	0.1000	0.0000	0.0000	411.2
5	0.0°	0.0000	0.0000	0.0000	418.2
6	0.0°	-0.1000	0.0000	0.0000	374.3
7	0.0°	-0.1000	0.1000	0.0000	432.7
8	0.0°	0.0000	0.1000	0.0000	467.7
9	0.0°	0.1000	0.1000	0.0000	440.1


Scan Mode
Scan Plot
Parameters
Results
Feedback
Open Terminal
Setup
Samples
Data
Scans
Analysis
MAD
XRF
XAS
Multi-Wavelength Anomalous Dispersion Scan
Edge
Se-K
Absorption
12.6567 keV
Emission
11.2225 keV
Exposure Time
0.5 sec
Attenuation
50 %
MAD Scan Completed.
Label
Energy
λ
f'
f"
200429-1...
Se-K
peak 12.663 0.9791 -8.3 9.8
infl 12.660 0.9794 -12.7 5.8
remo 12.717 0.9750 -3.7 3.7
Use Strategy
Energy: 12.657 keV
Attenuation: 0 %
Sample: CNT-01_14|MA14
Directory: ...3ShwtQ/CNT-01/CNT-01_14/mad-scan
Beam Size: 100 µm
Dead Time: 5 %
Status
COLLECT
Ring Current
0.0
Beam
Beamline Mode
Mount
Center
Align
Fast Shutter
Status
normfluor
ifluor1
ifluor2
ifluor3
ifluor4
i0
fpp
fp
Fluorescence
Anomalous factors
Energy (keV)
12.575
12.600
12.625
12.650
12.675
12.700
12.725
Edge
Se-K
35
79.90
Br
Bromine
K
L1
L2
L3


Scan Mode
Scan Plot
Paramete
Result
Feedback
Open Terminal
Setup
Samples
Data
Scans
Analysis
MAD
XRF
XAS
X-ray Fluorescence Spectroscopy
Edge
Br-K
Absorption
13.4741 keV
Emission
11.9244 keV
Excitation
15.474 keV
Exposure Time
0.5 sec
Attenuation
50 %
XRF Scan Completed.
Element
Amount
Fe Iron 44.5 %
Cu Copper 9.3 %
Zn Zinc 4.8 %
Rb Rubidium 4.4 %
Tb Terbium 2.1 %
Cl Chlorine 1.7 %
Cr Chromium 1.3 %
Kr Krypton 1.3 %
Br Bromine 1.0 %
Ar Argon 0.9 %
As Arsenic 0.7 %
Ni Nickel 0.7 %
Se Selenium 0.6 %
Energy: 12.657 keV
Beam Size: 100 µm
Attenuation: 0 %
Dead Time: 5 %
Sample: CNT-01_14|MA14
Directory: ...3ShwtQ/CNT-01/CNT-01_14/mad-scan
Fluorescence
X-Ray Fluorescence from Excitation at 15.474 keV
Fit
Experimental
Smoothed
Excitation Energy
Fluorescence
Energy (keV)
Fe-KL
Fe-KM
Cu-KL
Zn-KL
Cu-KM
Zn-KM
x=11.5087 y=60.4856
Status
COLLECT
Ring Current
0.0
I1 Flux
3.502e+04
I0 Flux
2.693e+04
Beam
Beamline Mode
Mount
Center
Align
Fast Shutter Status
Beamline
SIM-1

Setup | Samples | Data | Scans | Analysis

Analysis Reports

Name	Title	Type	Score
rc-bchi-01	Data Analysis Report	proc-n...	0.69
rc-bchi-02	Data Analysis Report	proc-n...	0.69
rc-bchi-03	MX analysis in progress ...	proc-n...	0.00

Single | Merge | MAD | Calibrate (LaB6) | Run
Screen | Anom | Integrate

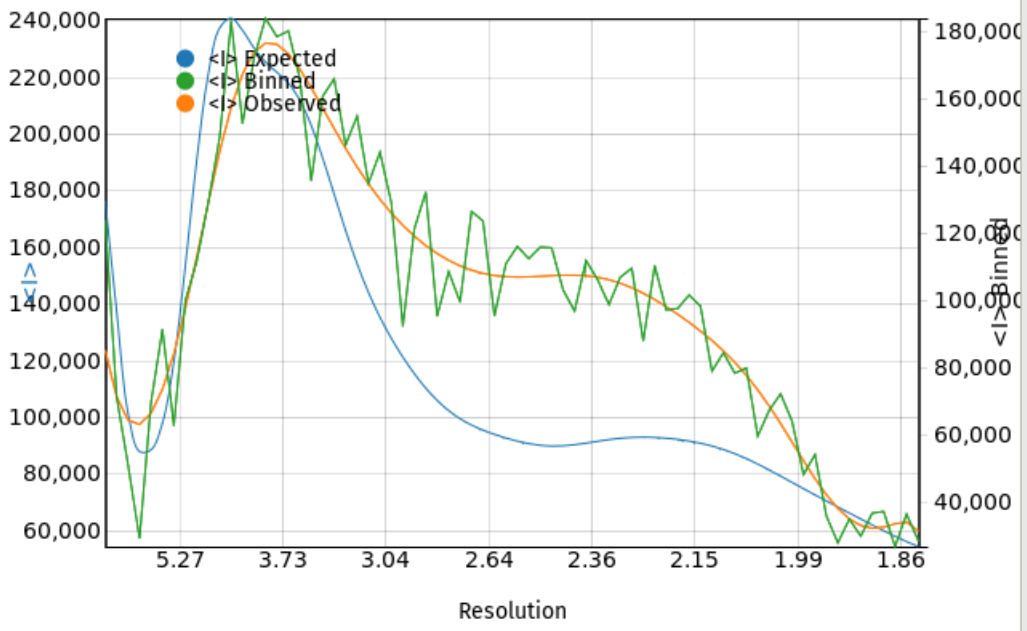
Sample: rc-bchi-01|MC1
Directory: ~/SIM1-20171019/rc-bchi/rc-bchi-01/proc-native

Mount Sample | Use Strategy

F(-)|/Sigma). F(+), F(-) are structure factor estimates obtained from the merged intensity observations in each parity class.

3. Percentage of correlation between random half-sets of anomalous intensity differences.

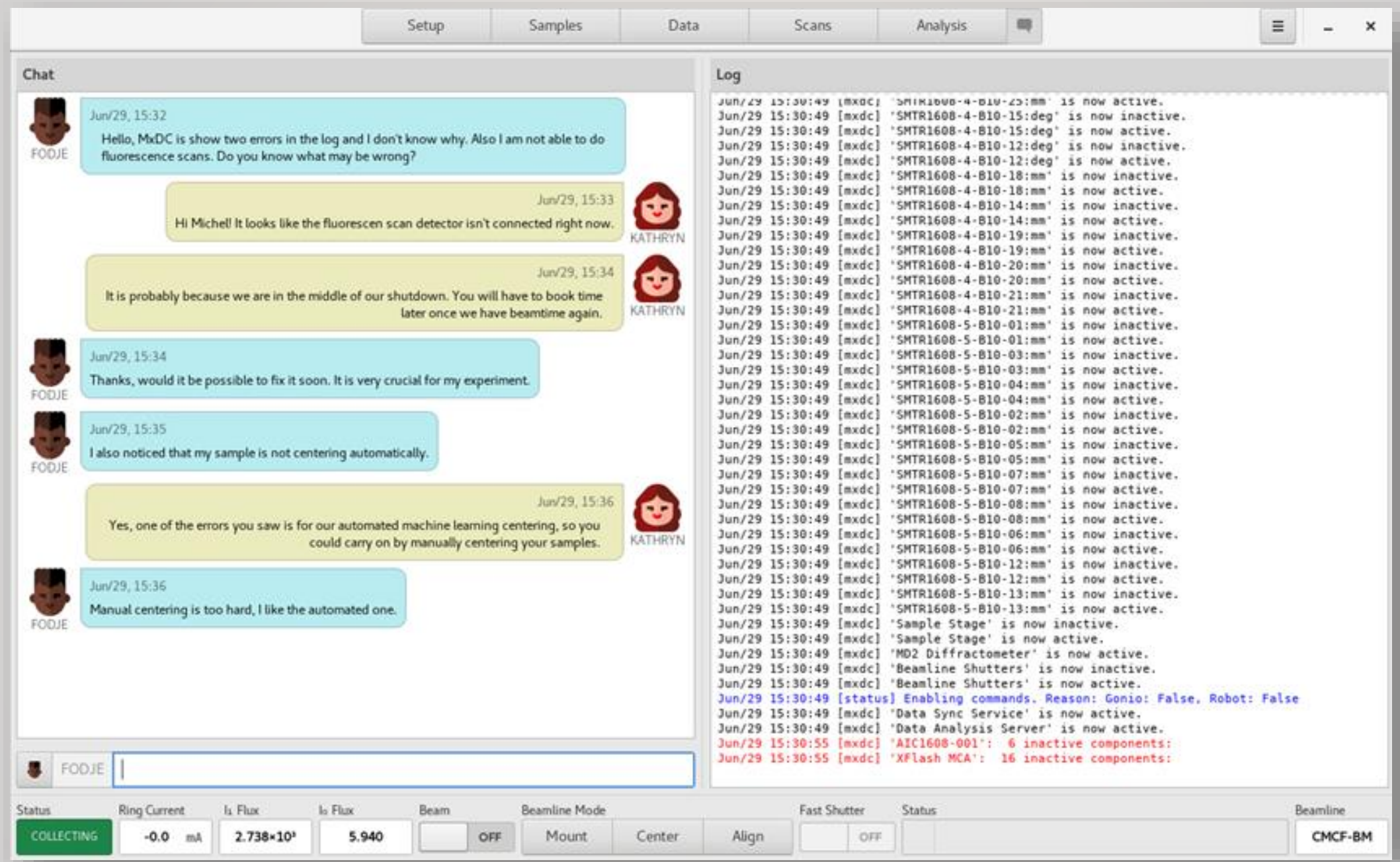
Wilson Statistics



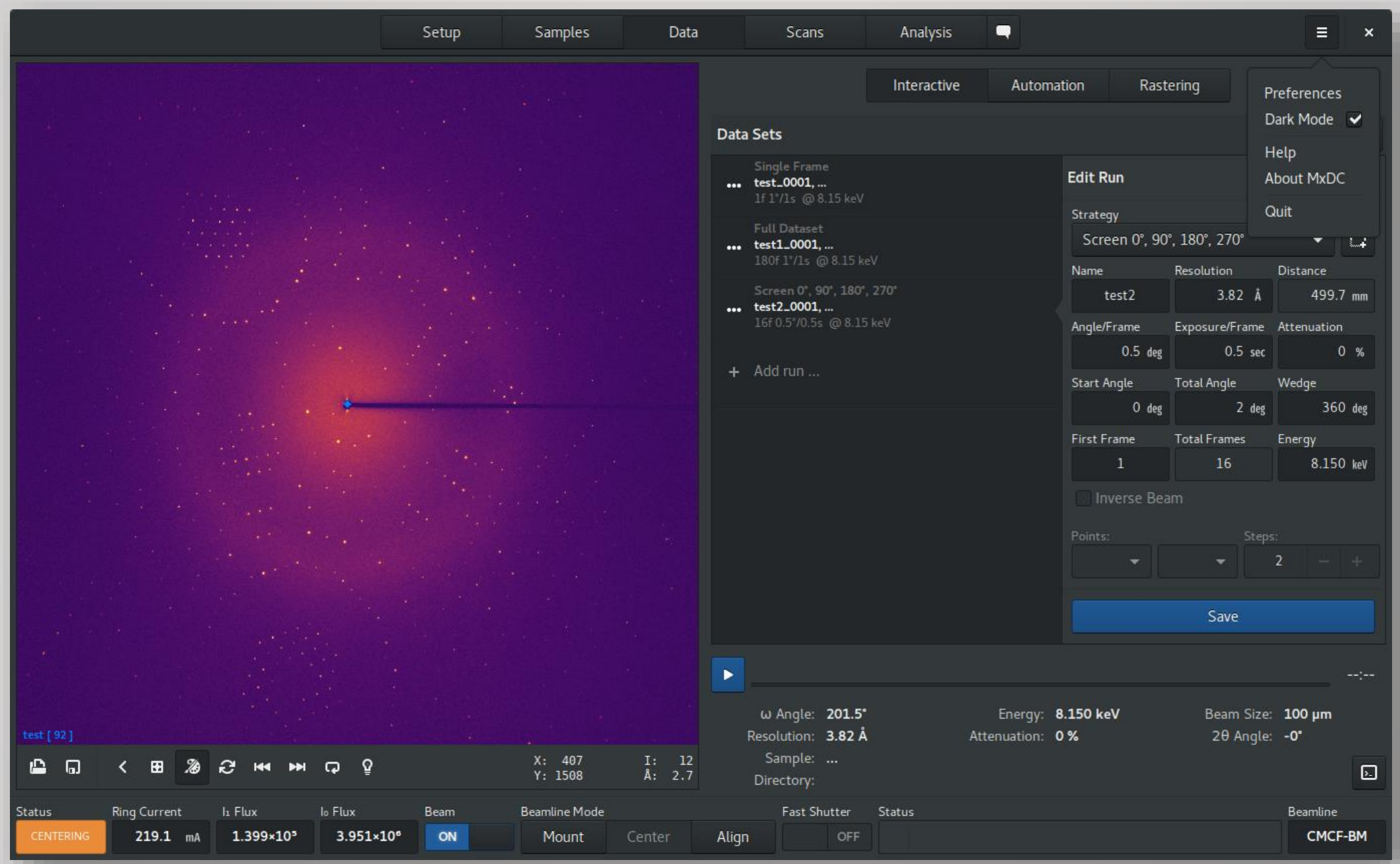
Twinning Analysis

Status: MOUNTING | Ring Current: 157.8 mA | I_1 Flux: 3.501e+04 | I_0 Flux: 2.693e+04 | Beam: OFF | Beamline Mode: Mount | Center | Beam | Fast Shutter: ON | Beamline: SIM-1

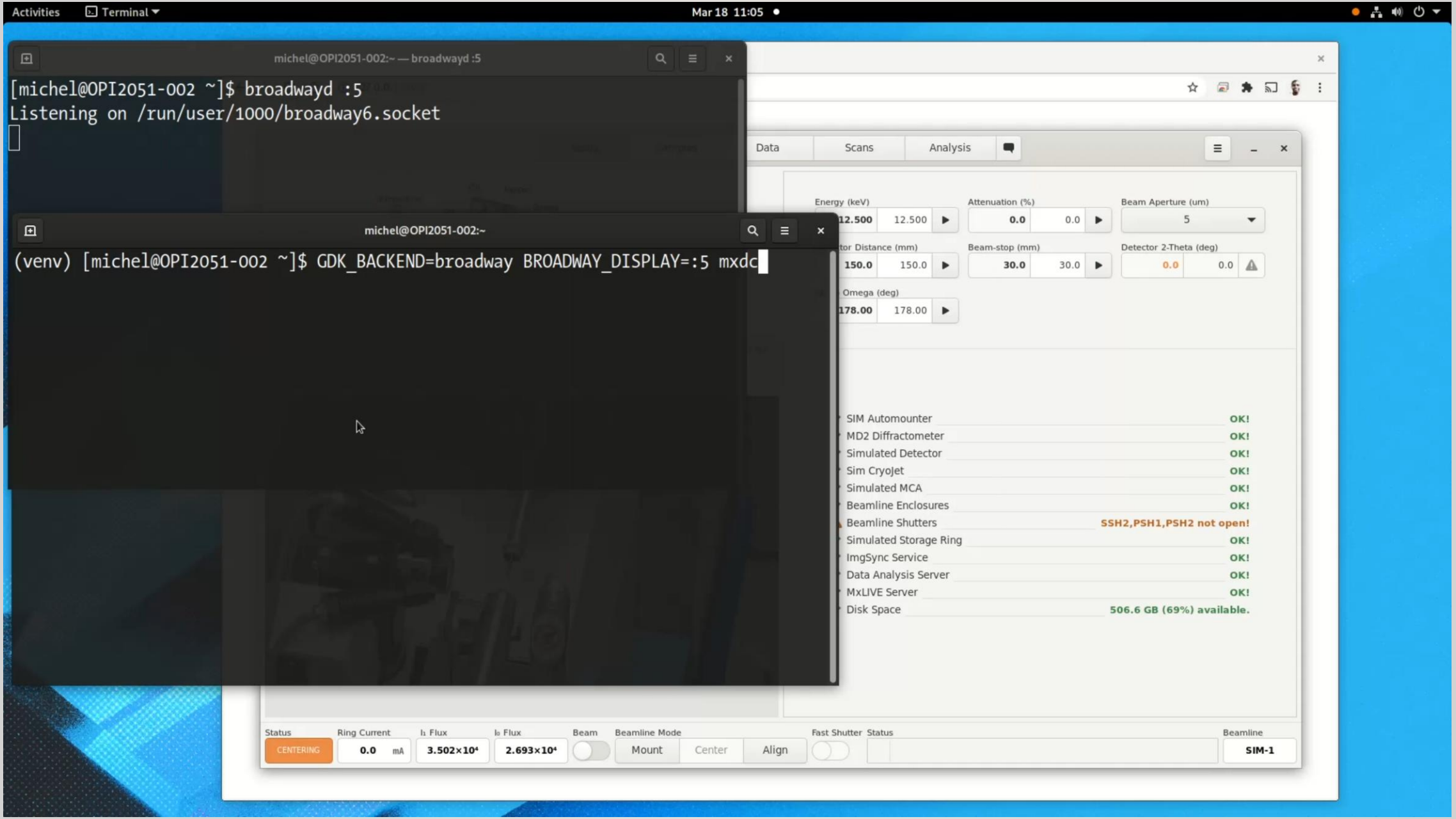
CHAT & LOG

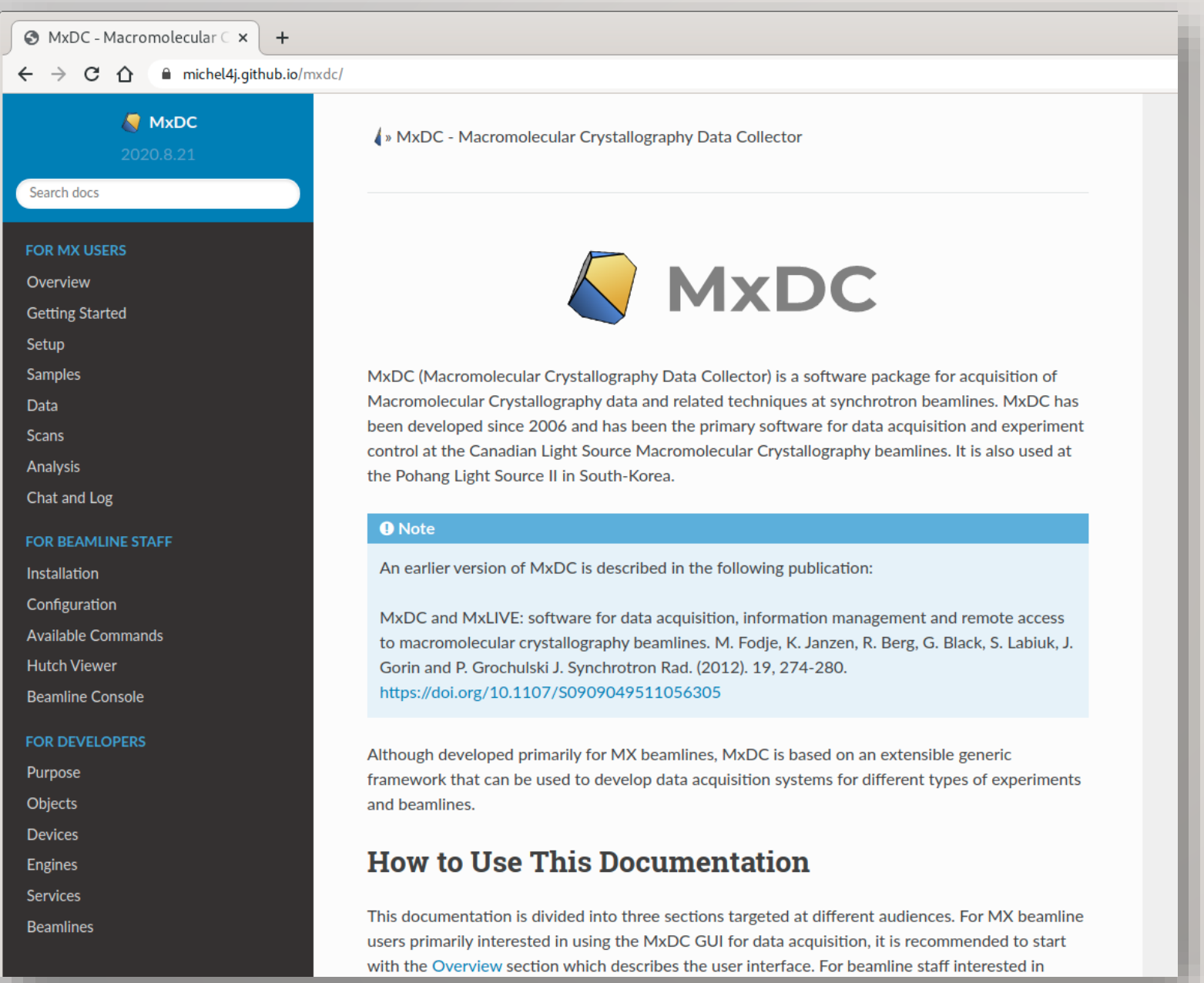

Setup
Samples
Data
Scans
Analysis
Chat
FODJE
Jun/29, 15:32
Hello, MxDC is show two errors in the log and I don't know why. Also I am not able to do fluorescence scans. Do you know what may be wrong?
KATHRYN
Jun/29, 15:33
Hi Michel! It looks like the fluorescen scan detector isn't connected right now.
KATHRYN
Jun/29, 15:34
It is probably because we are in the middle of our shutdown. You will have to book time later once we have beamtime again.
FODJE
Jun/29, 15:34
Thanks, would it be possible to fix it soon. It is very crucial for my experiment.
FODJE
Jun/29, 15:35
I also noticed that my sample is not centering automatically.
KATHRYN
Jun/29, 15:36
Yes, one of the errors you saw is for our automated machine learning centering, so you could carry on by manually centering your samples.
FODJE
Jun/29, 15:36
Manual centering is too hard, I like the automated one.
FODJE
Log
Jun/29 15:30:49 [mxdc] 'SMTR1608-4-B10-15:deg' is now inactive.
Jun/29 15:30:49 [mxdc] 'SMTR1608-4-B10-15:deg' is now active.
Jun/29 15:30:49 [mxdc] 'SMTR1608-4-B10-12:deg' is now inactive.
Jun/29 15:30:49 [mxdc] 'SMTR1608-4-B10-12:deg' is now active.
Jun/29 15:30:49 [mxdc] 'SMTR1608-4-B10-18:mm' is now inactive.
Jun/29 15:30:49 [mxdc] 'SMTR1608-4-B10-18:mm' is now active.
Jun/29 15:30:49 [mxdc] 'SMTR1608-4-B10-14:mm' is now inactive.
Jun/29 15:30:49 [mxdc] 'SMTR1608-4-B10-14:mm' is now active.
Jun/29 15:30:49 [mxdc] 'SMTR1608-4-B10-19:mm' is now inactive.
Jun/29 15:30:49 [mxdc] 'SMTR1608-4-B10-19:mm' is now active.
Jun/29 15:30:49 [mxdc] 'SMTR1608-4-B10-20:mm' is now inactive.
Jun/29 15:30:49 [mxdc] 'SMTR1608-4-B10-20:mm' is now active.
Jun/29 15:30:49 [mxdc] 'SMTR1608-4-B10-21:mm' is now inactive.
Jun/29 15:30:49 [mxdc] 'SMTR1608-4-B10-21:mm' is now active.
Jun/29 15:30:49 [mxdc] 'SMTR1608-5-B10-01:mm' is now inactive.
Jun/29 15:30:49 [mxdc] 'SMTR1608-5-B10-01:mm' is now active.
Jun/29 15:30:49 [mxdc] 'SMTR1608-5-B10-03:mm' is now inactive.
Jun/29 15:30:49 [mxdc] 'SMTR1608-5-B10-03:mm' is now active.
Jun/29 15:30:49 [mxdc] 'SMTR1608-5-B10-04:mm' is now inactive.
Jun/29 15:30:49 [mxdc] 'SMTR1608-5-B10-04:mm' is now active.
Jun/29 15:30:49 [mxdc] 'SMTR1608-5-B10-02:mm' is now inactive.
Jun/29 15:30:49 [mxdc] 'SMTR1608-5-B10-02:mm' is now active.
Jun/29 15:30:49 [mxdc] 'SMTR1608-5-B10-05:mm' is now inactive.
Jun/29 15:30:49 [mxdc] 'SMTR1608-5-B10-05:mm' is now active.
Jun/29 15:30:49 [mxdc] 'SMTR1608-5-B10-07:mm' is now inactive.
Jun/29 15:30:49 [mxdc] 'SMTR1608-5-B10-07:mm' is now active.
Jun/29 15:30:49 [mxdc] 'SMTR1608-5-B10-08:mm' is now inactive.
Jun/29 15:30:49 [mxdc] 'SMTR1608-5-B10-08:mm' is now active.
Jun/29 15:30:49 [mxdc] 'SMTR1608-5-B10-06:mm' is now inactive.
Jun/29 15:30:49 [mxdc] 'SMTR1608-5-B10-06:mm' is now active.
Jun/29 15:30:49 [mxdc] 'SMTR1608-5-B10-12:mm' is now inactive.
Jun/29 15:30:49 [mxdc] 'SMTR1608-5-B10-12:mm' is now active.
Jun/29 15:30:49 [mxdc] 'SMTR1608-5-B10-13:mm' is now inactive.
Jun/29 15:30:49 [mxdc] 'SMTR1608-5-B10-13:mm' is now active.
Jun/29 15:30:49 [mxdc] 'Sample Stage' is now inactive.
Jun/29 15:30:49 [mxdc] 'Sample Stage' is now active.
Jun/29 15:30:49 [mxdc] 'MD2 Diffractometer' is now active.
Jun/29 15:30:49 [mxdc] 'Beamline Shutters' is now inactive.
Jun/29 15:30:49 [mxdc] 'Beamline Shutters' is now active.
Jun/29 15:30:49 [status] Enabling commands. Reason: Gonio: False, Robot: False
Jun/29 15:30:49 [mxdc] 'Data Sync Service' is now active.
Jun/29 15:30:49 [mxdc] 'Data Analysis Server' is now active.
Jun/29 15:30:55 [mxdc] 'AIC1608-001': 6 inactive components:
Jun/29 15:30:55 [mxdc] 'XFlash MCA': 16 inactive components:
FODJE
Status
COLLECTING
Ring Current
-0.0 mA
I1 Flux
2.738×10³
I0 Flux
5.940
Beam
OFF
Beamline Mode
Mount
Center
Align
Fast Shutter
OFF
Status
Beamline
CMCF-BM

DARK MODE


Setup
Samples
Data
Scans
Analysis
Interactive
Automation
Rastering
Preferences
Dark Mode
Help
About MxDC
Quit
Data Sets
Single Frame
test_0001, ...
1f 1°/1s @ 8.15 keV
Full Dataset
test1_0001, ...
180f 1°/1s @ 8.15 keV
Screen 0°, 90°, 180°, 270°
test2_0001, ...
16f 0.5°/0.5s @ 8.15 keV
Add run ...
Edit Run
Strategy
Screen 0°, 90°, 180°, 270°
Name
test2
Resolution
3.82 Å
Distance
499.7 mm
Angle/Frame
0.5 deg
Exposure/Frame
0.5 sec
Attenuation
0 %
Start Angle
0 deg
Total Angle
2 deg
Wedge
360 deg
First Frame
1
Total Frames
16
Energy
8.150 keV
Inverse Beam
Points:
Steps:
2
Save
test [92]
X: 407
Y: 1508
I: 12
Å: 2.7
--:--
ω Angle: 201.5°
Resolution: 3.82 Å
Sample: ...
Directory:
Energy: 8.150 keV
Attenuation: 0 %
Beam Size: 100 µm
2θ Angle: -0°
Status
CENTERING
Ring Current
219.1 mA
I1 Flux
1.399×10³
I0 Flux
3.951×10⁶
Beam
ON
Beamline Mode
Mount
Center
Align
Fast Shutter
OFF
Status
Beamline
CMCF-BM

BROWSER ACCESS





Resources

GitHub

https://github.com/michel4j/mxdc/

Documentation:

https://michel4j.github.io/mxdc/

Canadian Light Source
Centre canadien de rayonnement synchrotron