

Integrated Sample Management, Data Acquisition and Processing at the Canadian Light Source

Michel Fodje

Canadian Macromolecular Crystallography Facility



Canadian
Light
Source

Centre canadien
de rayonnement
synchrotron

Outline

- Software infrastructure for MX Facility at CLS
 - MxLIVE
 - MxDC
 - Data Analysis
- Re-usable components
 - RPC Framework
 - Data Mining
 - Reporting



CMCF

- Canadian Light Source MX facility
- Two complementary Beamlines
- Techniques
 - **> 95%** MX
 - **< 5%** PXRD, SC-XRD
- Users
 - **60%** Academic
 - **40%** Industrial
 - **90%** Remote access

CMCF-BM

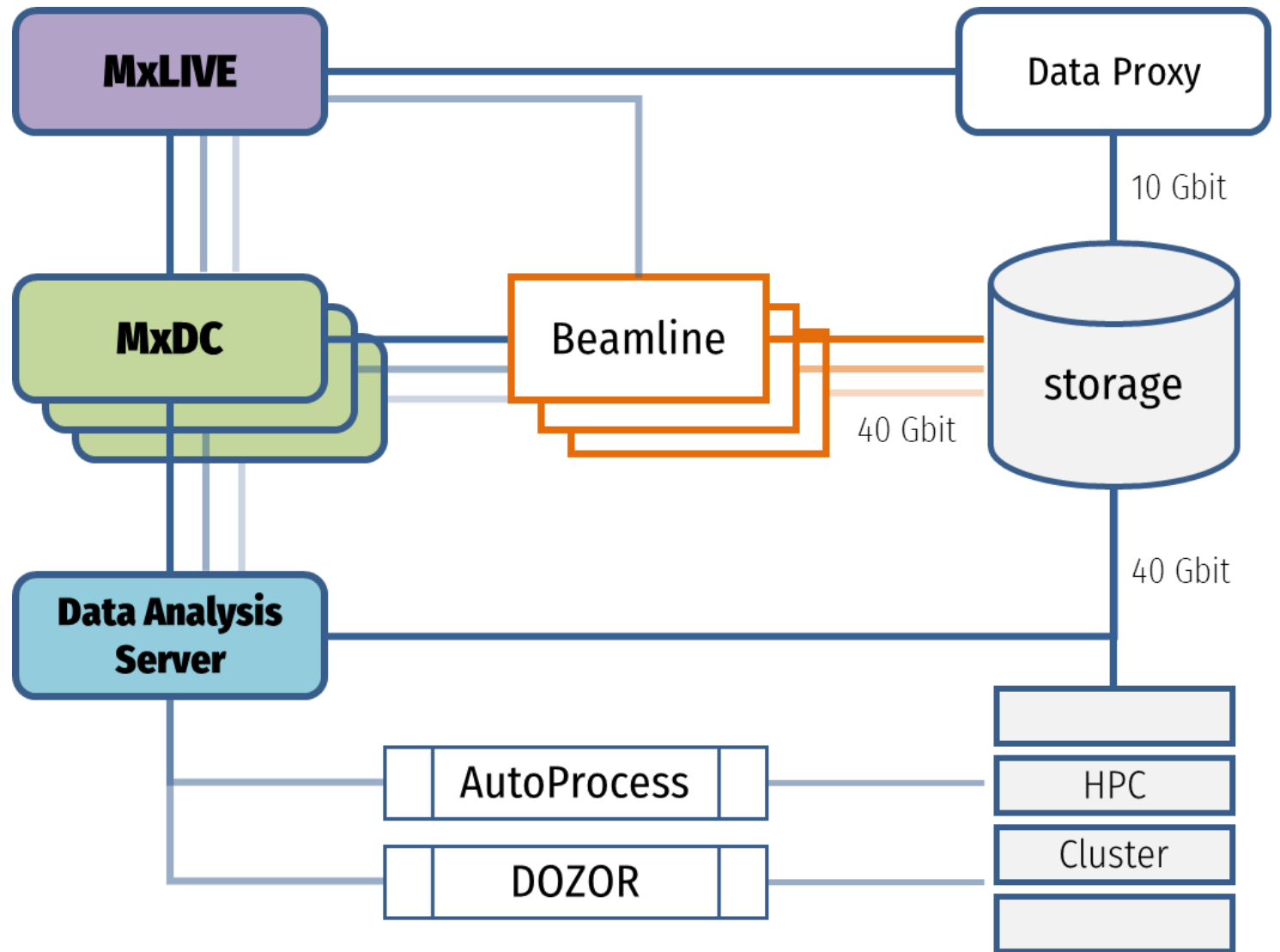
- Bend Magnet Beamline
- Stable Beam
- Macromolecular Crystallography (MX)
- Power Diffraction (PXRD)
- Chemical Crystallography (SC-XRD)
- Operational 2010 / Upgraded 2019

CMCF-ID

- Undulator Beamline
- High Flux
- Macromolecular Crystallography (MX) Only
- Operational 2007 / Upgraded 2020

Software

- MxLIVE - LIMS
 - Samples / Shipping
 - Monitoring / Data retrieval
 - Robot Management
 - Support/Problem Tracking
 - Publications/PDB tracking
- MxDC – Data Collection
 - Integrated
 - User-friendly GUI
- Data Analysis
 - Data Analysis Server
 - AutoProcess
- Computing
 - Centralized GPFS Storage
 - 40 Gbit Network
 - 7 HPC Nodes
 - 680 Cores, 1360 threads



MxLIVE Features

- Shipment Tracking
- Experiment Management
- **Experiment Monitoring**
- Data Transfer
- Statistics
- Publications, Scheduling, User Support, User Feedback

The screenshot displays the MxLIVE web interface with several overlapping panels:

- Main Dashboard:** Shows session information for KATHRYN | SIM1-20200511-RwAfd7Jk, started May 11, 2020. It includes a table of datasets for 'thermolysin' and 'lysozyme' with columns for Sample, Container, Location, and Data Sets.
- Data | LABIUK | 200108-0947:** A plot showing Fluorescence vs. Energy (keV) with a peak at 12.6507 keV. A table on the right lists peak data:

Energy	f'	f''
12.6507 keV	-7.2	5.3
0.9801 Å		
12.6487 keV	-9.3	3.7
0.9802 Å		
12.7287 keV	-3.9	3.6
- Data | LABIUK | 200108-0940:** An XRF dataset plot showing peaks for Co-KL, Co-KM, Zn-KL, and Zn-KM. A table on the right lists elements and their percentages:

Element	%
Zn	28.0
Co	14.5
Yb	9.2
Os	6.8
Gd	2.0
Dy	1.2
Ta	0.7
Lu	0.5
Tb	0.4
Tc	0.4
Cs	0.3
Ne	0.3
K	0.3
Nb	0.3
- Data | LABIUK | thau_dcm_b:** A diffraction pattern image with a resolution of 8.70 Å. A list of image files (thau_dcm_b_0001.img to thau_dcm_b_0011.img) is shown on the right.

Viewing Data

MxLIVE Features

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Analysis Reports

21	tP	3.3	79.0	79.0	36.8	90.0	90.0	90.0	P4, P422
----	----	-----	------	------	------	------	------	------	----------

Table 2 - Lattice Character

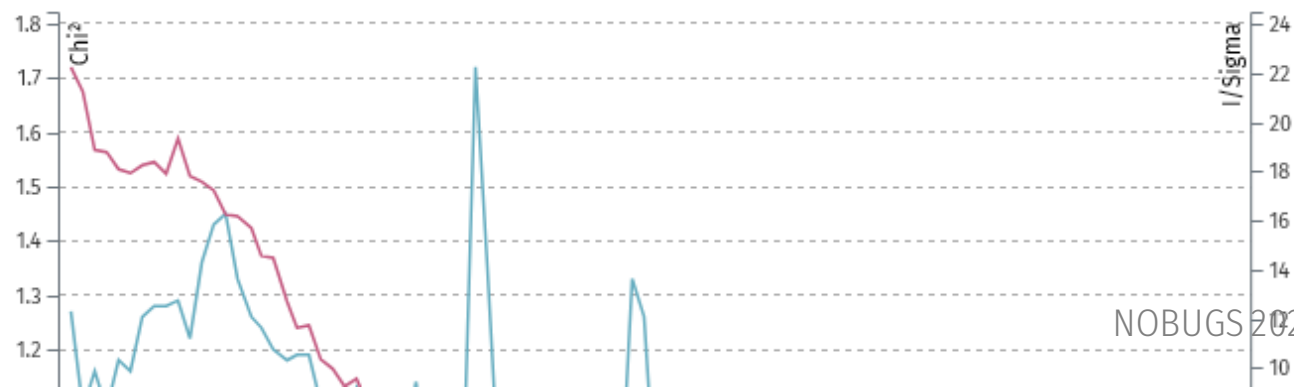
The Lattice Character is defined by the metrical parameters of its reduced cell as described in the International Tables for Crystallography Volume A, p. 746 (Kluwer Academic Publishers, Dordrecht/Boston/London, 1989). Note that more than one lattice character may have the same Bravais Lattice. The error column indicates the quality of fit.

Selected	Candidates	Space Group Number	Probability
*	P4 ₁ 2 ₁ 2	92	0.909
	P4 ₃ 2 ₁ 2	96	0.909
	P4 ₁ 22	91	0.038
	P4 ₃ 22	95	0.038
	P4 ₂ 2 ₁ 2	94	0.025
	P4 ₂ 2	90	0.02

Table 3 - Likely Space-Groups and their Probabilities

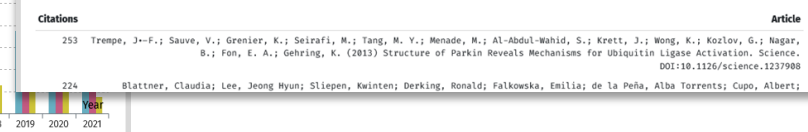
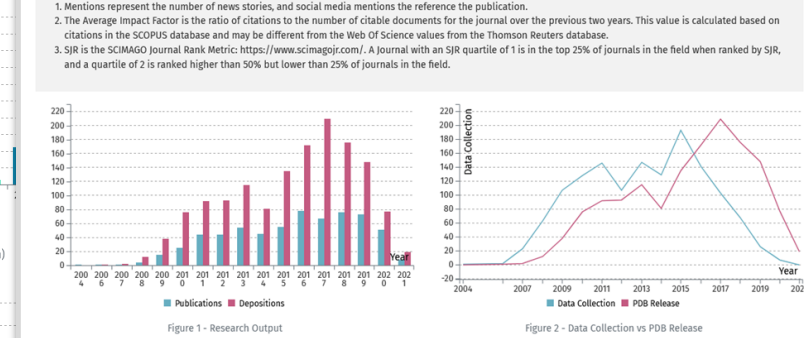
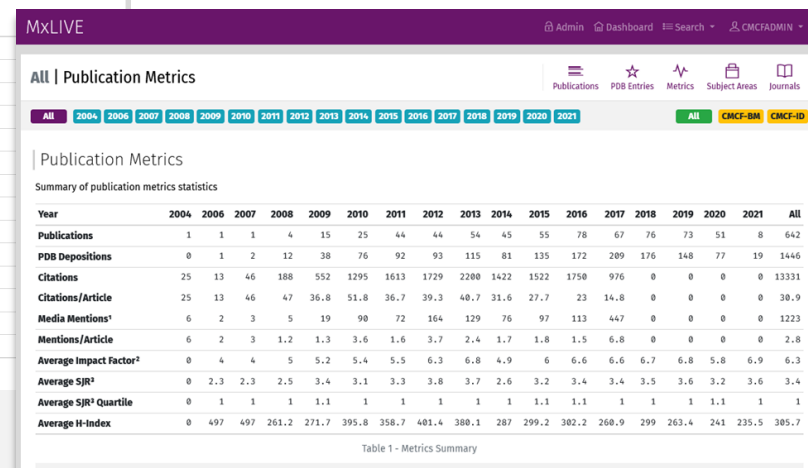
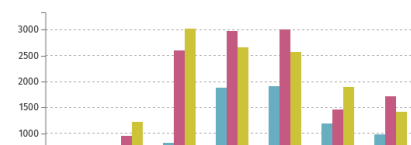
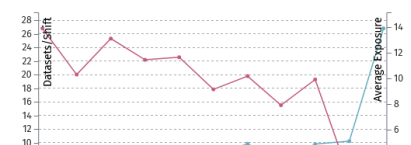
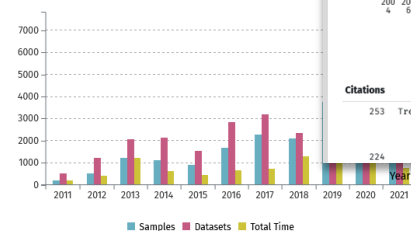
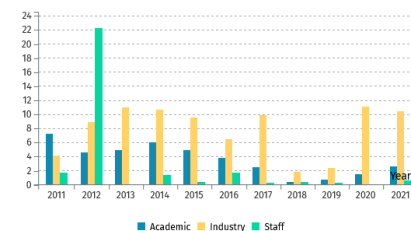
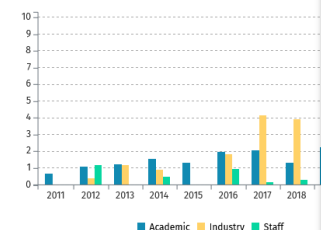
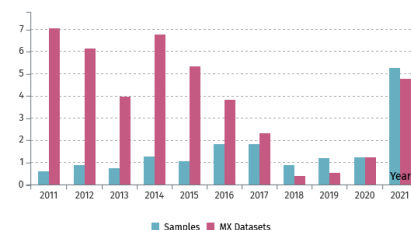
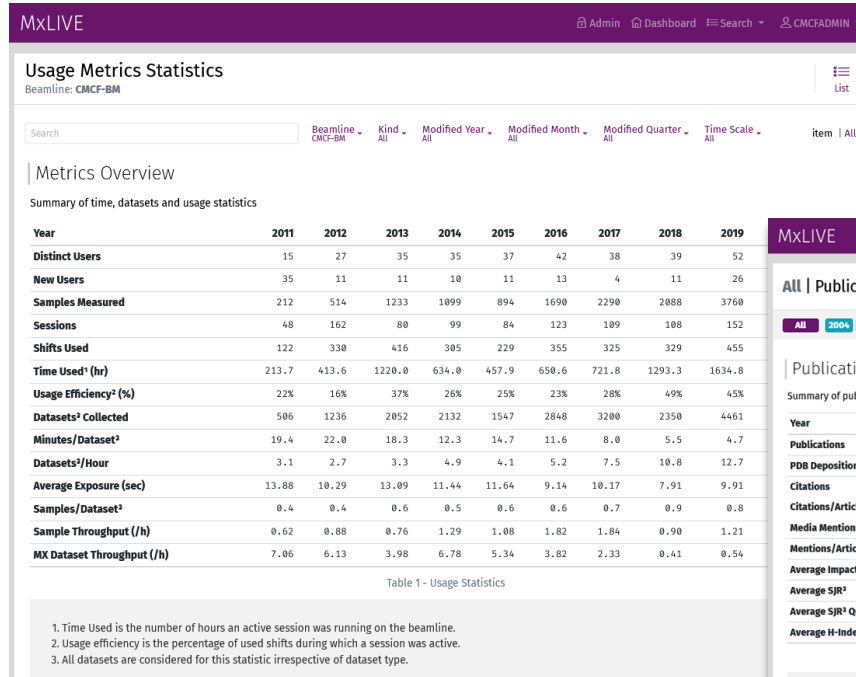
The above table contains results from POINTLESS (see Evans, Acta Cryst. D62, 72-82, 2005). Indistinguishable space groups will have similar probabilities. If two or more of the top candidates have the same probability, the one with the fewest symmetry assumptions is chosen. This usually corresponds to the point group, trying out higher symmetry space groups within the top tier does not require re-indexing the data as they are already in the same setting. For more detailed results, please inspect the output file 'pointless.log'.

Standard Errors of Reflection Intensities by Resolution



MxLIVE Features

- Shipment Tracking
- Experiment Management
- Experiment Monitoring
- Data Transfer
- **Statistics**
- Publications, Scheduling, User Support, User Feedback



MxDC Features

- Single Integrated GUI
- Activity Pages
- Automation
 - AI-assisted Centering
- Data Visualization
- Data Analysis

Hutch Video

The screenshot displays the MxDC GUI interface. At the top, there are tabs for Setup, Samples, Data, Scans, and Analysis. A 'Schematic' label points to a diagram of the X-ray diffraction setup, showing components like attenuation, beam aperture, beam stop, distance, and various angles (Chi, Phi, Kappa, Omega, 2-Theta). A 'Parameters' label points to a control panel with fields for Energy (keV), Attenuation (pct), Beam Aperture (um), Detector Distance, Beam-stop (mm), Detector 2-Theta (deg), and Gonio Omega (deg). Below the schematic is a 'Hutch Video' window showing a live camera feed of the experimental setup, including a yellow robotic arm. To the right is a 'Beamline Status' panel listing various components and their operational status. At the bottom, there is a status bar with fields for Status, Ring Current, I₁ Flux, I₂ Flux, Beam, Beamline Mode, Fast Shutter, and Beamline ID.

Component	Status
ISARA Auto Mounter	Staff Needed
MD2 Diffractometer	OK!
Eiger 9M	OK!
Cryojet	Sample Flow Too Low! Shield Flow Too Low! Temp. to...
Quantax XFlash MCA	OK!
Beamline Enclosures	3 Inactive
Beamline Shutters	SSH1,PSH1,PSH2,SSH2 not open! 1 Inactive
CLS Storage Ring	Beam Unavailable
Data Synchronization Service	OK!
Data Analysis Service	OK!
MxLIVE Server	OK!
Disk Space	34.6 TB (88%) available.

Status: UNKNOWN Ring Current: 10.3 mA I₁ Flux: 4.858·10⁴ I₂ Flux: 3.801·10⁻⁹ Beam: OFF Beamline Mode: Mount Fast Shutter: OFF Beamline ID: CMCF-ID

Beamline Status

MxDC Features

- Single Integrated GUI
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The screenshot displays the MxDC software interface, which is divided into several functional areas:

- Scan Mode:** Located at the top, it includes tabs for Setup, Samples, Data, Scans, and Analysis.
- Parameters:** This section is used for configuring scans. It shows:
 - MAD (Multi-Wavelength Anomalous Dispersion Scan):** Edge: Se-K, Absorption: 12.6567 keV, Emission: 11.2225 keV, Exposure Time: 0.5 sec, Attenuation: 50%.
 - XRF (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%.
- Results:** This area displays the outcomes of the scans.
 - MAD Scan Completed:** A table showing parameters for the Se-K edge:

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
 - XRF Scan Completed:** A table showing the detected elements and their amounts:

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 %
- Feedback:** This section provides status information, including a 'Status' indicator and a 'COL' button.
- Scan Plot:** This area contains two plots:
 - Multi-Wavelength Anomalous Dispersion Scan:** A plot showing fluorescence intensity versus energy, with multiple curves (normfluor, ifluor1-4, i0, fpp, fp) and a legend.
 - X-ray Fluorescence from Excitation at 15.474 keV:** A plot showing fluorescence intensity versus energy (keV). It includes a legend for Fit, Experimental, Smoothed, and Excitation Energy. The plot shows several peaks corresponding to the elements listed in the results table.

MxDC Features

- Single Integrated GUI
- Activity Pages
- Automation
 - AI-assisted Centering
- Data Visualization
- Data Analysis

The screenshot displays the MxDC software interface. The top navigation bar includes tabs for Setup, Samples, Data, Scans, and Analysis. The main window is divided into two primary sections: a Progress Summary on the left and a Data Quality Summary on the right.

Progress Summary: This section lists three data collection strategies for sample lyso_6 (MA6):

- lyso_14 (MA14): SCR / 8 img / lyso_14-30 (SCR: 0.68)
- lyso_5 (MA5): DAT / 60 img / lyso_14-31 (NAT: 0.41, ANO: 0.61, SCR: X)
- lyso_6 (MA6): SCR / 8 img / lyso_6 (SCR: 0.68)

Below the progress summary are buttons for 'Mount Sample' and 'Use Strategy'. The 'Run' button is active, and the 'Anomalous' checkbox is checked. The sample directory is shown as 'Sample: lyso_6|MA6' and 'Directory: ...M1-20230130-8vol9nl8/lyso/lyso_14/proc-screen-20'.

Data Quality Summary: This section displays a table of statistics for the selected data set (lyso_14-31):

Table 1. Data Quality Statistics	
	lyso_14-31
Score ¹	0.41
Wavelength (Å)	1.2398
Space Group ²	P2
Unit Cell (Å)	57.05 57.96 149.85 90.0 90.7 90.0
Resolution ³	1.83
All Reflections	20250
Unique Reflections	18902
Multiplicity	1.1
Completeness	20.1 %
Mosaicity	0.20
I/Sigma(I)	1.2
R-meas	47.1
CC _{1/2} ³	66.4 %
ISA ⁴	50.0

Footnotes for the Data Quality Summary:

1. Data Quality Score for comparing similar data sets. Typically, values > 0.8 are excellent, > 0.6 are good, > 0.5 are acceptable, > 0.4 marginal, and < 0.4 are Barely usable
2. This space group was automatically assigned using POINTLESS (see P.R.Evans, Acta Cryst. D62, 72-82, 2005). This procedure is unreliable for incomplete datasets such as those used for screening. Please Inspect the detailed results below.
3. Percentage correlation between intensities from random half-datasets. (see Karplus & Diederichs (2012), Science. 336 (6084): 1030-1033)
4. The highest I/Sigma(I) that the experimental setup can produce (Diederichs (2010) Acta Cryst D66, 733-740).

The bottom status bar shows the system is 'COLLECTING' with a Ring Current of 0.0 mA, I₁ Flux of 3.502×10⁴, and I₂ Flux of 2.693×10⁴. The Beamline Mode is 'Mount', and the Beamline is 'SIM-1'.

- Request Data Processing
- View Reports
- Scoring

Data Analysis

- Orchestration – Data Analysis Server (Swift RPC)
- Wrapping third-party software – (ParseFire)
- Generating Reports – (MxLIVE Reports)

Data Analysis Server

- **Based on SZRPC Package**
 - Swift RPC – Simple ZMQ RPC
 - Server – Management Node
 - Workers – Compute nodes
- Wraps:
 - AutoProcess – Automated MX Data Processing
 - Fit2D – PXRD integration
 - DOZOR – Signal-strength analysis of MX raster datasets

Swift RPC

- Clean API for servers and clients
- Supports one or more workers
- Load balancing
- Multiple replies per request
- Gtk, Qt integration (signals)



```
from szrpc.server import Service

class MyService(Service):
    def remote__hello_world(self, request, name=None):
        """
        Single reply after a long duration
        """
        request.reply(f'Please wait, {name} ...')
        time.sleep(10)
        return f'Hello, {name}. How is your world today?'

    def remote__date(self, request):
        """
        Single reply after a short duration
        """
        time.sleep(0.1)
        return f"Today's date is {datetime.now()}"

    def remote__progress(self, request):
        """
        Multiple replies to show progress
        """
        for i in range(10):
            time.sleep(0.1)
            request.reply(f'{i*10}% complete')
        return f"Progress done"
```

Swift RPC

- Clean API for servers and clients
- Supports one or more workers
- Load balancing
- Multiple replies per request
- Gtk, Qt integration (signals)



Running a Server

```
from szrpc.server import Server

if __name__ == '__main__':
    service = MyService()
    server = Server(service=service, ports=(9990, 9991))
    server.run()
```

Running a Worker

```
from szrpc import log
from szrpc.server import Server, Service, WorkerManager

from test_server import MyService

if __name__ == '__main__':

    service = MyService()
    log.log_to_console()
    server = WorkerManager(
        service=service, backend="tcp://localhost:9991",
        instances=2
    )
    server.run()
```

Swift RPC

- Clean API for servers and clients
- Supports one or more workers
- Load balancing
- Multiple replies per request
- Gtk, Qt integration (signals)



Writing a Client

```
import time
from szrpc import log
from szrpc.client import Client

# Define response handlers
def on_done(res, data):
    print(f"Done: {res} {data!r}")

def on_err(res, data):
    print(f"Failed: {res} : {data!r}")

def on_update(res, data):
    print(f"Update: {res} {data!r}")

if __name__ == '__main__':
    log.log_to_console()
    client = Client('tcp://localhost:9990')

    # wait for client to be ready before sending commands
    while not client.is_ready():
        time.sleep(.001)

    res = client.hello_world(name='Joe')
    res.connect('done', on_done)
    res.connect('update', on_update)
    res.connect('failed', on_err)
```

Swift RPC

- Clean API for servers and clients
- Supports one or more workers
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Data Analysis Server

- Based on SZRPC Package
 - Swift RPC – Simple ZMQ RPC
 - Server – Management Node
 - Workers – Compute nodes
- Orchestration of Data processing
- Wraps:
 - **AutoProcess – Automated MX Data Processing**
 - DOZOR – Signal-strength analysis of MX raster datasets

AutoProcess

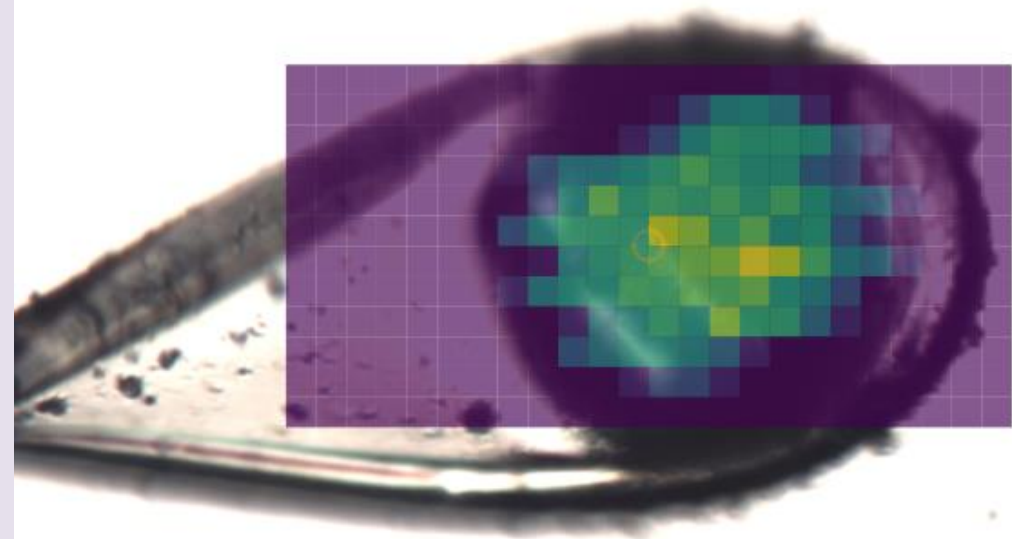
- Expert System for automated MX data reduction after acquisition
- Uses industry standard MX analysis tools behind the scenes
 - XDS (Max-Planck Institute)
 - PHENIX (Berkeley Lab)
 - CCP4 (Rutherford Lab, UK)
- Converts diffraction images to MTZ reflection files
- Graphical analysis reports
- **Users can run AutoProcess manually from CLI**

Data Analysis Server

- Based on SZRPC Package
 - Swift RPC – Simple ZMQ RPC
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- Orchestration of Data processing
- Wraps:
 - AutoProcess – Automated MX Data Processing
 - Fit2D – PXRD integration
 - **DOZOR – Signal-strength analysis of MX raster datasets**

Raster Analysis

- On-the-fly analysis of raster images
- Uses DOZOR
- Directly from Stream (Eiger)
- **Complete within a few seconds of the scan**



ParseFire



Mining log/output files of third-party packages

<https://github.com/michel4j/parsefire>

```
pip install parsefire
```

ParseFire

- Solves a common problem
- Extracting information/data from unstructured text

OUTPUT FILE: XDS_ASCII.HKL

THE CALCULATIONS ASSUME FRIEDEL'S_LAW= TRUE
 TOTAL NUMBER OF CORRECTION FACTORS DEFINED 200
 DEGREES OF FREEDOM OF CHI^2 FIT 54341.0
 CHI^2-VALUE OF FIT OF CORRECTION FACTORS 0.930
 NUMBER OF CYCLES CARRIED OUT 4

CORRECTION FACTORS for visual inspection by XDS-Viewer DECAF.cbfc
 XMIN= 0.3 XMAX= 499.4 NXBIN= 10
 YMIN= 0.00047 YMAX= 0.36404 NYBIN= 20
 NUMBER OF REFLECTIONS USED FOR DETERMINING CORRECTION FACTORS 75145

 CORRECTION FACTORS AS FUNCTION OF X (fast) & Y (slow) IN THE DETECTOR PLANE

RECIPROCAL CORRECTION FACTORS FOR INPUT DATA SETS MERGED TO
 OUTPUT FILE: XDS_ASCII.HKL

THE CALCULATIONS ASSUME FRIEDEL'S_LAW= TRUE
 TOTAL NUMBER OF CORRECTION FACTORS DEFINED 1520
 DEGREES OF FREEDOM OF CHI^2 FIT 54304.5
 CHI^2-VALUE OF FIT OF CORRECTION FACTORS 0.908
 NUMBER OF CYCLES CARRIED OUT 4

CORRECTION FACTORS for visual inspection by XDS-Viewer MODPIX.cbfc
 XMIN= 6.3 XMAX= 4141.5 NXBIN= 38

Anomal_Corr & SigAno. At least two observed reflections for each (+ and -) parity are required.
 LAB COORDINATES OF ROTATION AXIS 0.999975 0.006636 -0.002438
 DIRECT BEAM COORDINATES (REC. ANGSTROM) 0.004803 0.006234 1.024297
 DETECTOR COORDINATES (PIXELS) OF DIRECT BEAM 2081.31 2225.71

SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION

RESOLUTION LIMIT	NUMBER OF REFLECTIONS			COMPLETENESS OF DATA	R-FACTOR observed	R-FACTOR COMPARED expected	I/SIGMA	R-meas	CC(1/2)	Anomal Corr	SigAno	Nano Corr
	OBSERVED	UNIQUE	POSSIBLE									
4.95	824	533	1355	39.3%	3.1%	2.4%	498	23.61	4.1%	99.7*	19	1.489
3.51	1571	947	2243	42.2%	3.1%	2.6%	1042	22.69	4.0%	99.8*	-4	0.844
2.87	1992	1260	2822	44.6%	4.6%	4.0%	1221	13.56	5.9%	99.6*	23	1.191
2.48	2460	1613	3286	49.1%	8.2%	8.1%	1425	6.80	10.6%	98.7*	18	0.970
2.22	2679	1746	3702	47.2%	12.2%	12.2%	1576	4.63	15.7%	97.4*	-17	0.772
2.03	3065	2012	4064	49.5%	21.0%	20.4%	1766	2.88	27.3%	92.6*	-2	0.757
1.88	3054	2016	4385	46.0%	32.7%	36.7%	1692	1.60	41.7%	84.7*	11	0.848
1.76	1970	1317	4686	28.1%	71.4%	79.3%	1055	0.74	90.7%	54.0*	15	0.816
1.66	892	693	4999	13.9%	81.2%	103.7%	346	0.48	107.2%	39.4*	-4	0.724
total	18507	12137	31542	38.5%	5.8%	5.5%	10621	6.64	7.5%	99.8*	8	0.876

NUMBER OF REFLECTIONS IN SELECTED SUBSET OF IMAGES 18675
 NUMBER OF REJECTED MISFITS 142
 NUMBER OF SYSTEMATIC ABSENT REFLECTIONS 26
 NUMBER OF ACCEPTED OBSERVATIONS 18507
 NUMBER OF UNIQUE ACCEPTED REFLECTIONS 12137

 S BETWEEN OBSERVED AND CALCULATED SPOT LOCATIONS

- and Y-coordinates of the spots are depicted in the
 DNS.cbf and DY-CORRECTIONS.cbf for inspection with

 TION PARAMETERS USING ALL IMAGES

RACTION PARAMETERS DERIVED FROM 25907 INDEXED SPOTS
 POSITION BEAM AXIS ORIENTATION CELL
 SPOT POSITION (PIXELS) 1.27
 SPINDLE POSITION (DEGREES) 0.04
 92

58.111 58.111 150.423 90.000 90.000 90.000
 ERS 2.2E-02 2.2E-02 5.0E-02 0.0E+00 0.0E+00 0.0E+00
 0.017208 0.017208 0.006648 90.000 90.000 90.000
 LL A-AXIS -36.751 -24.447 37.797
 LL B-AXIS 29.870 23.258 44.087
 LL C-AXIS -87.169 122.465 -5.548
 REES) 0.096

ParseFire

- Solves a common problem
- Extracting information/data from unstructured text

```
from parsefire.parser import parse_text

specs = {
    'domain': r"Inside:(.*?)(?=Outside|$)",
    'fields': [
        "Age: <int:age>",
        "Name: <str:name>"
    ]
}

text = (
    "Inside:\n"
    "Age: 25\n"
    "Name: John Doe\n"
    "Outside:\n"
    "Age: 30\n"
    "Name: Jane Doe"
)

result = parse_text(specs, text)
print(result) # Output: {'age': 25, 'name': 'John Doe'}
```

- Field Specifications, domains
- Type conversions
- Dictionary output

ParseFire

- Solves a common problem
- Extracting information/data from unstructured text

```
root:
  fields:
    - "!!! ERROR<str:error_code> !!! <str:error>"

  sections:
    quality:
      domain: "REFINEMENT OF DIFFRACTION PARAMETERS USING ALL IMAGES(.+?)THE DATA COLLECTION STATISTICS REPORTED RE
      fields:
        - " STANDARD DEVIATION OF SPOT POSITION (PIXELS) <float:pixel_error>"
        - " STANDARD DEVIATION OF SPINDLE POSITION (DEGREES) <float:angle_error>"
        - " CRYSTAL MOSAICITY (DEGREES) <float:mosaicity>"

    statistics:
      domain: "STATISTICS OF SAVED DATA SET .*? WITH SIGNAL/NOISE >= -3.0(.+?)NUMBER OF REFLECTIONS IN SELECTED"
      table: " <float:shell> <int:observed> <int:unique> <int:possible> <float:completeness>% <float:r_obs>% <float:
<float:cc_half><char:signif> <int:cor_ano><char:asignif> <float:sig_ano> <int:Nano>"

    summary:
      domain: "STATISTICS OF SAVED DATA SET .*? WITH SIGNAL/NOISE >= -3.0(.+?)WILSON STATISTICS OF DATA SET"
      fields:
        - " total <int:observed> <int:unique> <int:possible> <float:completeness>% <float:r_obs>% <float:r_exp>%
<float:cc_half><char:signif> <int:cor_ano><char:asignif> <float:sig_ano> <int:Nano>"
        - " NUMBER OF REFLECTIONS IN SELECTED SUBSET OF IMAGES <int:reflections>"
        - " NUMBER OF SYSTEMATIC ABSENT REFLECTIONS <int:absent>"
        - " NUMBER OF REJECTED MISFITS <int:misfits>"
```

- Complex Specifications Possible
- YAML Files
- Parsing of Tables
- Field Types:
 - Integers
 - Floats
 - Strings, Custom String Patterns, Slugs, Lines

Reporting

Generating Graphical Reports



HTML

Js

CSS

Graphical HTML Analysis Reports

- Takes care of presentation
- Provide data
 - JSON file
 - Python Dictionary

Usage Efficiency² (%)	22%	16%	37%	26%	25%	23%	28%	49%	45%	62%	42%
Datasets² Collected	506	1236	2052	2132	1547	2848	3200	2350	4461	7113	5928
Minutes/Dataset¹	19.4	22.0	18.3	12.3	14.7	11.6	8.0	5.5	4.7	2.5	2.5
Datasets²/Hour	3.1	2.7	3.3	4.9	4.1	5.2	7.5	10.8	12.7	23.6	23.8
Average Exposure (sec)	13.88	10.29	13.09	11.44	11.64	9.14	10.17	7.91	9.91	2.35	1.69
Samples/Dataset²	0.4	0.4	0.6	0.5	0.6	0.6	0.7	0.9	0.8	0.9	1.0
Sample Throughput (/h)	0.62	0.88	0.76	1.29	1.08	1.82	1.84	0.90	1.21	1.25	5.25
MX Dataset Throughput (/h)	7.06	6.13	3.98	6.78	5.34	3.82	2.33	0.41	0.54	1.22	4.76

Table 1 - Usage Statistics

1. Time Used is the number of hours an active session was running on the beamline.
2. Usage efficiency is the percentage of used shifts during which a session was active.
3. All datasets are considered for this statistic irrespective of dataset type.

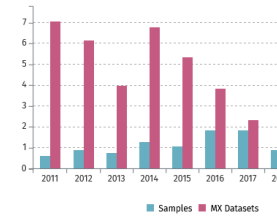


Figure 1 - Throughput by year (h)

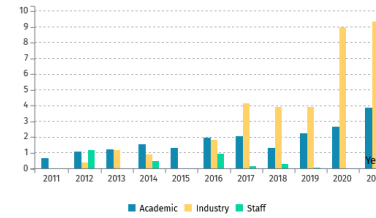


Figure 2 - Sample Throughput by year (h)

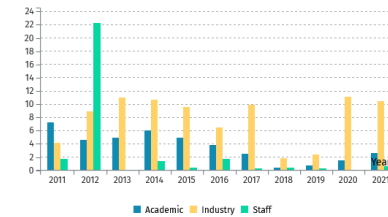


Figure 3 - MX Dataset Throughput by year (h)

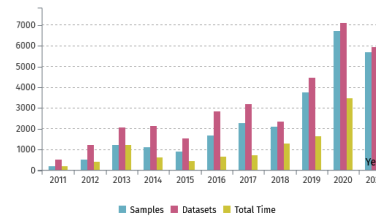


Figure 4 - Usage Statistics

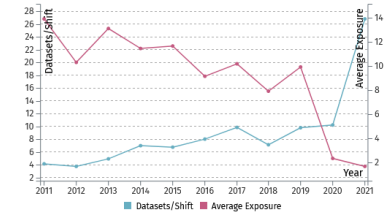


Figure 5 - Productivity

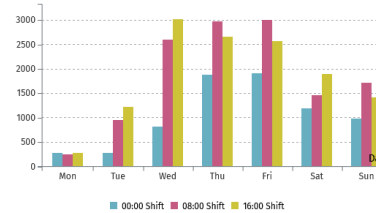


Figure 6 - Datasets by time of week

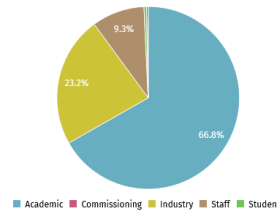


Figure 7 - Datasets by Project Type

Data Summary

	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020	2021	All
MX Screening	278	554	1015	1149	717	2028	2329	1211	2124	4441	4031	19877
MX Dataset	213	546	702	672	544	684	552	331	512	1932	1661	8349
XRD Dataset	0	0	0	0	0	0	28	299	1016	523	100	1966

Summary

	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020	2021	All
MX Screening	278	554	1015	1149	717	2028	2329	1211	2124	4441	4031	19877
MX Dataset	213	546	702	672	544	684	552	331	512	1932	1661	8349
XRD Dataset	0	0	0	0	0	0	28	299	1016	523	100	1966
Rastering	0	0	0	0	0	0	34	52	28	117	126	357
XAS Dataset	0	0	0	0	0	0	0	0	0	0	0	0
XRF Dataset	15	77	228	216	170	74	149	391	663	66	6	2055
MAD Scan	0	59	107	95	116	62	108	66	118	34	4	769
Total	506	1236	2052	2132	1547	2848	3200	2350	4461	7113	5928	33373

Table 2 - Dataset summary by year

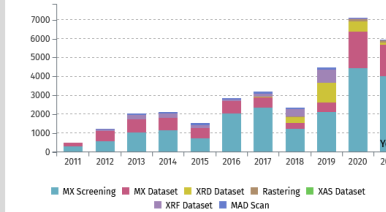


Figure 8 - Dataset summary by year

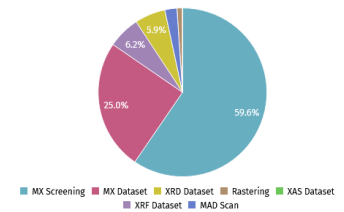


Figure 9 - Dataset Types

User Statistics

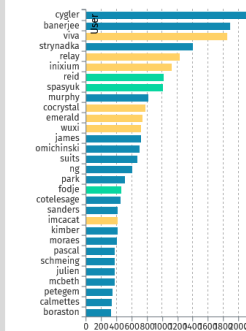


Figure 10 - Datasets

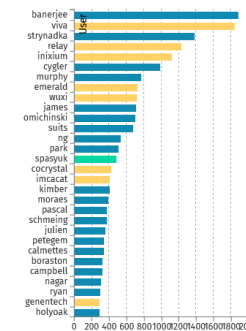


Figure 11 - Samples

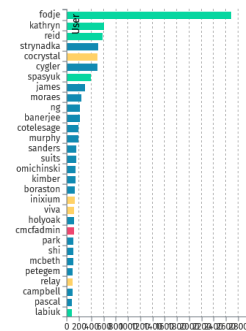


Figure 12 - Time Used

Dataset counts include all types of datasets. Only the top 30 users by number of datasets are shown

Sample counts include only samples measured on the beamline. Only the top 30 users sample count shown

Total time is sum of active session durations for each user. Only the top 30 users are shown.

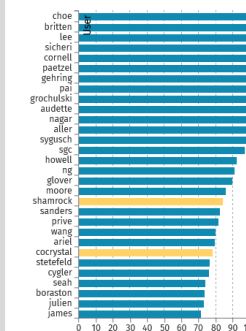


Figure 13 - Efficiency

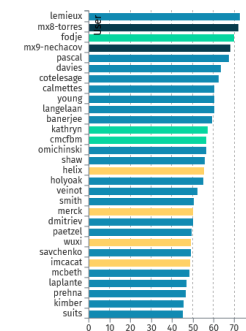


Figure 14 - Schedule Efficiency

Efficiency is the percentage of Time Used during which shutters were open. This measures how

Schedule Efficiency is the percentage of shift time during which a session was active. This measures

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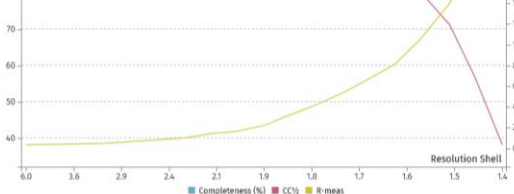


Figure 7 -

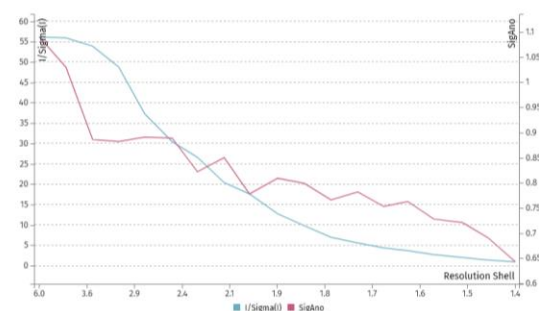
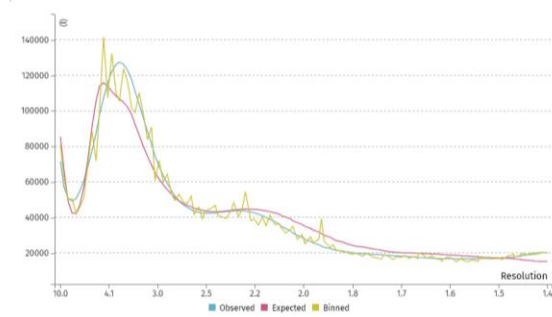


Figure 8 -

Shell	Observed	Unique	Completeness	R_obs	R_meas	CC%	I/Sigma(I) ¹	Sigma(I) ²	CC _{hkl} ³
6.00	3772	357	99.40	3.20	3.40	99.90	56.16	1.09	37.00
4.30	6522	564	100.00	3.70	3.80	99.90	55.91	1.03	23.00
3.52	8140	699	99.70	4.00	4.20	99.90	53.89	0.89	3.00
3.06	9783	798	100.00	4.60	4.80	99.90	48.78	0.88	-2.00
2.74	11489	913	100.00	6.30	6.60	99.90	37.27	0.89	3.00
2.50	12605	994	100.00	8.00	8.30	99.90	30.46	0.89	4.00
2.32	13463	1043	100.00	9.60	10.00	99.80	26.59	0.82	-1.00
2.17	13383	1109	96.90	13.50	14.20	99.70	20.38	0.85	-3.00
2.05	15133	1172	100.00	15.60	16.30	99.50	17.60	0.78	-1.00
1.94	16682	1335	100.00	21.30	22.20	99.30	12.74	0.81	-1.00
1.85	16370	1293	96.90	31.30	32.70	98.40	9.80	0.80	-2.00
1.77	17599	1425	99.90	40.90	42.70	97.30	6.97	0.77	-1.00
1.70	18977	1482	100.00	52.20	54.40	95.20	5.55	0.78	0.00
1.64	17936	1468	100.00	65.20	68.00	91.50	4.36	0.75	0.00
1.59	17432	1389	100.00	77.70	81.00	89.00	3.67	0.76	1.00
1.54	19327	1568	100.00	101.40	105.80	80.10	2.71	0.73	-2.00
1.49	22059	1807	100.00	134.00	139.90	71.20	1.98	0.72	-2.00
1.45	16709	1609	99.90	172.90	181.90	56.80	1.37	0.69	0.00
1.41	13933	1799	100.00	205.70	220.50	38.20	0.93	0.64	-2.00

1. Mean of intensity/Sigma(I) of unique reflections (after merging symmetry-related observations). Where Sigma(I) is the standard deviation of reflection intensity I estimated from sample statistics.
2. Mean anomalous difference in units of its estimated standard deviation (|F(-)-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



1. acceptable, > 0.4 marginal, and < 0.4 are Barely usable
2. POINTLESS was used for automatic spacegroup assignments (see P.R.Evans, Acta Cryst. D62, 72-82, 2005). The procedure is unreliable for incomplete datasets such as those used for screening. Please inspect the detailed results below. Does
3. Percentage correlation between intensities from random half-datasets. (see Karplus & Diederichs (2012), Science. 316 (6084): 1030-1033)
4. The highest I/Sigma(I) that the experimental setup can produce (Diederichs (2010) Acta Cryst D66, 733-740).
5. Anomalous completeness is shown in parentheses.
6. Space group was automatically assigned
7. Resolution limit was set by I/Sigma(I) > 1.0

No.	Character	Error	a	b	c	alpha	beta	gamma	Point Groups
31	aP	0.0	36.8	79.0	79.0	90.0	90.0	90.0	P1
44	aP	0.4	36.8	79.0	79.0	90.0	90.0	90.0	P1
28	mC	1.1	111.8	111.7	36.8	90.0	90.0	90.0	C2
35	mP	1.5	79.0	36.8	79.0	90.0	90.0	90.0	P2
33	mP	1.8	36.8	79.0	79.0	90.0	90.0	90.0	P2
25	mC	2.1	111.8	111.7	36.8	90.0	90.0	90.0	C2
34	mP	2.1	36.8	79.0	79.0	90.0	90.0	90.0	P2
23	oC	2.3	111.7	111.8	36.8	90.0	90.0	90.0	C222
32	oP	2.5	36.8	79.0	79.0	90.0	90.0	90.0	P222
21	tP	3.3	79.0	79.0	36.8	90.0	90.0	90.0	P4, P422

Table 2 - Lattice Character

The Lattice Character is defined by the metrical parameters of its reduced cell as described in the International Tables for Crystallography Volume A, p. 746 (Kluwer Academic Publishers, Dordrecht/Boston/London, 1989). Note that more than one lattice character may have the same Bravais Lattice. The error column indicates the quality of fit.

Selected	Candidates	Space Group Number	Probability
*	P4 ₂ -2	92	0.989
	P4 ₂ -2	96	0.989
	P4 ₂ -2	91	0.038
	P4 ₂ -2	95	0.038
	P4 ₂ -2	94	0.025
	P4 ₂ -2	98	0.02

Table 3 - Likely Space-Groups and their Probabilities

The above table contains results from POINTLESS (see Evans, Acta Cryst. D62, 72-82, 2005). Indistinguishable space groups will have similar probabilities. If two or more of the top candidates have the same probability, the one with the fewest symmetry assumptions is chosen. This usually corresponds to the point group, trying out higher symmetry space groups within the top tier does not require re-indexing the data as they are already in the same setting. For more detailed results, please inspect the output file 'pointless.log'.

Standard Errors of Reflection Intensities by Resolution

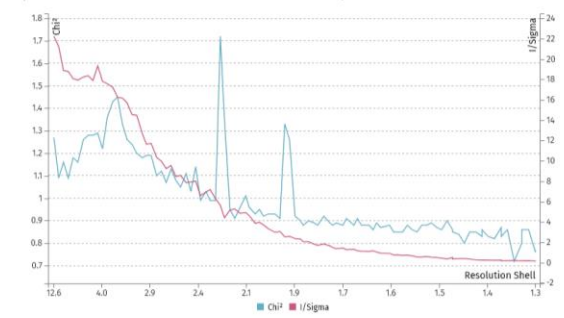
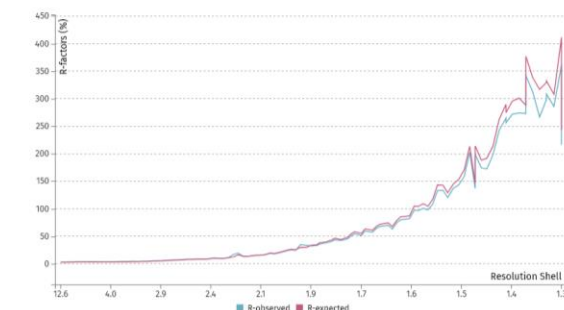


Figure 1 -



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A report is a Python/JSON Dictionary

```
'title': '',
'description': '',
'notes': '',
'style': '',           # CSS class to be applied to the section
'content': []         # list of dictionaries, each one describing a table or plot
to display
```

Content blocks

```
'title': '',
'description': '',
'notes': '',
'style': '',           # CSS class to be applied to the content
'kind': ,              # Supported types are 'barchart', 'columnchart',
'histogram', 'pie', 'scatterplot', 'lineplot', 'timeline'
'header': 'row',      # For tables only. Options are 'row', 'column', or 'column
row'
'data':                # {} for plots / [] for tables
```

Graphical HTML Analysis Reports

```
{
  "title": "Metrics Overview",
  "style": "row",
  "content": [
    {
      "title": "Usage Statistics",
      "kind": "table",
      "data": [
        ["Year", 2011, 2012, 2013, 2014, 2015, 2016, 2017, 2018, 2019, 2020],
        ["Users", 36, 28, 41, 44, 42, 54, 51, 67, 58, 31],
        ["New Users", 38, 12, 12, 6, 10, 14, 6, 26, 18, 1],
        ["Samples Measured", 555, 509, 1826, 2529, 5094, 7180, 10552, 12448, 17190, 9856],
        ["Sessions", 112, 73, 131, 149, 169, 184, 222, 205, 234, 102],
        ["Shifts Used", 434, 428, 598, 588, 674, 771, 727, 593, 726, 319],
        ["Usage Efficiency\u00b2 (%)", "27%", "32%", "29%", "29%", "28%", "26%", "29%", "45%", "42%", "30%"],
        ["Datasets\u00b3 Collected", 2939, 3046, 4866, 5265, 6737, 8313, 14942, 12637, 17289, 9930],
        ["Minutes/Dataset\u00b3", "9.0", "9.9", "9.0", "7.7", "6.7", "5.6", "1.8", "1.4", "1.6", "1.4"],
        ["Datasets\u00b3/Hour", "6.7", "6.0", "6.7", "7.8", "9.0", "10.6", "33.3", "42.8", "37.6", "44.3"],
        ["Average Exposure (sec)", "1.09", "1.11", "1.28", "1.62", "1.56", "1.72", "0.93", "0.92", "1.03", "0.79"],
        ["Samples/Dataset\u00b3", "0.2", "0.2", "0.4", "0.5", "0.8", "0.9", "0.7", "1.0", "1.0", "1.0"]],
      "style": "col-12",
      "header": "column row",
      "description": "Summary of time, datasets and usage statistics",
      "notes": "
        1. Time Used is the number of hours an active session was running on the beamline. \n
        2. Usage efficiency is the percentage of used shifts during which a session was active. \n
        3. All datasets are considered for this statistic irrespective of dataset type."
    },
  ],
}
```

Summary of time, datasets and usage statistics

Year	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020
Users	36	28	41	44	42	54	51	67	58	31
New Users	38	12	12	6	10	14	6	26	18	1
Samples Measured	555	509	1826	2529	5094	7180	10552	12448	17190	9856
Sessions	112	73	131	149	169	184	222	205	234	102
Shifts Used	434	428	598	588	674	771	727	593	726	319
Time Used¹ (hr)	930.8	1107.3	1388.7	1373.1	1487.1	1595.2	1705.5	2142.3	2414.7	759.5
Usage Efficiency² (%)	27%	32%	29%	29%	28%	26%	29%	45%	42%	30%
Datasets³ Collected	2939	3046	4866	5265	6737	8313	14942	12637	17289	9930
Minutes/Dataset³	9.0	9.9	9.0	7.7	6.7	5.6	1.8	1.4	1.6	1.4
Datasets³/Hour	6.7	6.0	6.7	7.8	9.0	10.6	33.3	42.8	37.6	44.3
Average Exposure (sec)	1.09	1.11	1.28	1.62	1.56	1.72	0.93	0.92	1.03	0.79
Samples/Dataset³	0.2	0.2	0.4	0.5	0.8	0.9	0.7	1.0	1.0	1.0

Table 1 - Usage Statistics

- 1. Time Used is the number of hours an active session was running on the beamline.
- 2. Usage efficiency is the percentage of used shifts during which a session was active.
- 3. All datasets are considered for this statistic irrespective of dataset type.

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```
{
  "title": "MAD Scan",
  "kind": "lineplot",
  "data": {
    "x": ["Energy (keV)", 12.5567, 12.5847, ..., 12.7167, 12.7287],
    "y1": [["Experiment", 154, 145, ..., 6386, 6290]],
    "y2": [["f", -4.13, -4.34, ..., 3.51, 3.46]],
    "x-label": "Energy (keV)",
    "y1-label": "Fluorescence",
    "y2-label": "Anomalous Scattering Factors",
    "aspect-ratio": 1.5,
    "annotations": [
      {"value": 12.662700000000001, "text": "PEAK"},
      {"value": 12.6597, "text": "INFL"},
      {"value": 12.7287002, "text": "REMO"}
    ]
  }
},
"id": "mad",
"style": "col-12"
}
```



Figure 1 - MAD Scan

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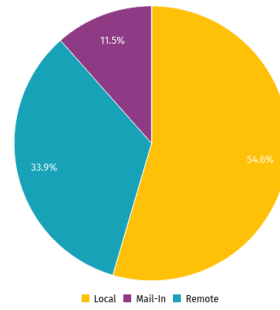


Figure 8 - Beamtime by access type

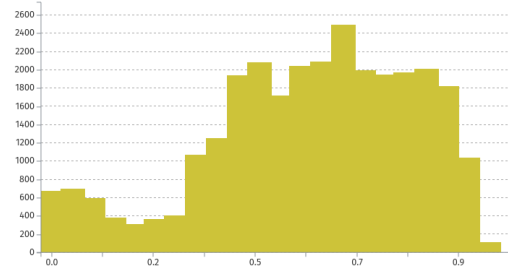


Figure 2 - Analysis Report Score

- Multiple Chart Types
- Annotations
- Notes

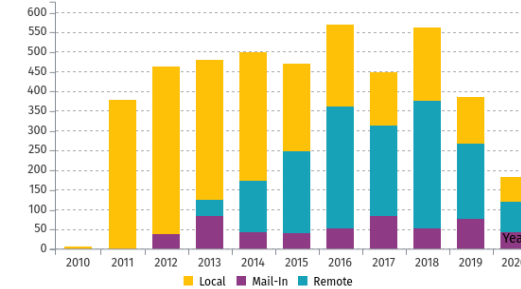


Figure 7 - Beamtime access type shifts by year

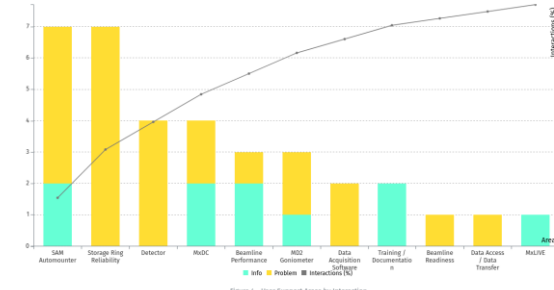
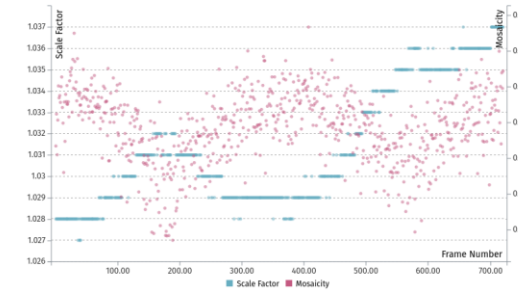


Figure 4 - User Support Areas by Interaction

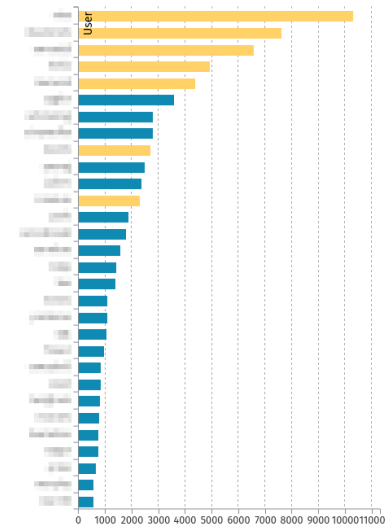


Figure 14 - Datasets

Dataset counts include all types of datasets. Only the top 30 users by number of datasets are shown

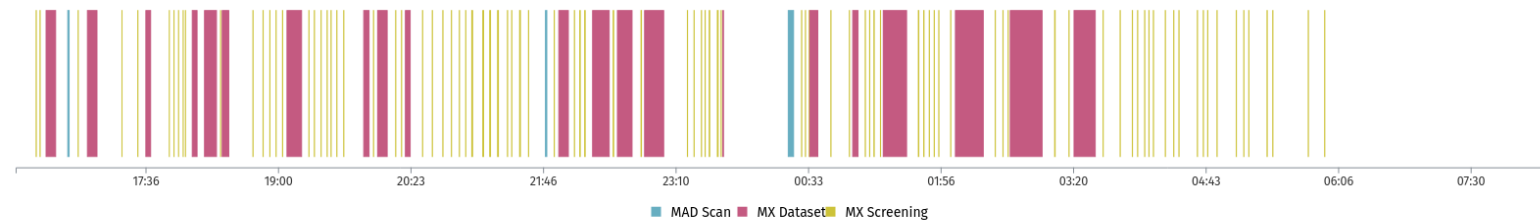


Figure 7 - Session Timeline

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Usage

Grab three files to include with each report to use as is (no edits needed):

- `report.html`
- `report.min.js`
- `report.min.css`

Generate data file according to report API

- `report.json`



Developed by

- Michel Fodje
- Kathryn Janzen

Contact me at:
Michel.Fodje@lightsource.ca

Special thanks To

- Zachary Arthur, Stuart Read, Pawel Grochulski, James Gorin
- Scott Colville, Denis Spasyuk, Kurt Nienaber, Joel Reid,
- Cuylar Conly, Shaun Labiuk, Dean Lang, CMCF Users



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SASKATCHEWAN**



Government
of
Saskatchewan


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

Canada

MxLIVE Features

- Shipment Tracking
- Experiment Management
- Experiment Monitoring
- Data Transfer
- Statistics
- Publications, Scheduling, User Support, User Feedback

The screenshot displays the MxLIVE user interface. At the top, the 'MxLIVE' logo is on the left, and navigation links for 'Dashboard', 'Search', and 'FODJE' are on the right. Below the header, the user is identified as 'FODJE | User' with a subtitle: 'Start here to manage and monitor shipments, review recent sessions, view and download data, an...'. A navigation bar contains icons for 'New Shipment', 'Sessions', 'Schedule', 'My Stats', and 'My Profile'. The main content area is divided into two sections: 'RECENT SHIPMENTS' and 'RECENT SESSIONS'. The 'RECENT SHIPMENTS' section includes a 'Start Now' button and a link to 'Click here to start a new shipment!'. It lists six shipments with details such as ID, date, containers, groups, and samples, along with data and report counts. The 'RECENT SESSIONS' section lists two sessions with details like ID, duration, and last record time, also with data and report counts. A 'USER GUIDE' sidebar on the right lists various help topics like 'Remote Connection Guide', 'NX Connection Settings', and 'Download your data'.

RECENT SHIPMENTS			
+ Start Now	Click here to start a new shipment! Follow the steps to enter your sample information		
 MAR 20	SHP-003-890 2024-Mar20 #1 4 Containers / 1 Group / 64 Samples	15 Data	12 Reports
 MAR 20	SHP-003-774 2024-Feb07 #1 2 Containers / 2 Groups / 32 Samples	18 Data	2 Reports
 FEB 7	SHP-003-645 2023-Dec08 #1 1 Container / 1 Group / 16 Samples	1 Data	1 Reports
 FEB 7	SHP-003-489 2023-Oct11 #1 2 Containers / 3 Groups / 16 Samples	Data	Reports
 FEB 7	SHP-003-105 2023-Feb01 #1 1 Container / 1 Group / 16 Samples	1 Data	Reports
 FEB 7	SHP-003-068 2023-Jan15 #1 1 Container / 1 Group / 16 Samples	135 Data	48 Reports

RECENT SESSIONS			
 AUG 15	CMCF-ID CMCFID-20240815-XcRw0t59 Duration 1 hour 5 mins / Last record 2 weeks, 5 days ago	Data	Reports
 AUG 15	CMCF-BM CMCFBM-20240815-8SFr4G8l Duration 10 mins 58 secs / Last record 2 weeks, 5 days ago	2 Data	Reports

USER GUIDE	
Remote Connection Guide	>
NX Connection Settings	>
Create a New Shipment	>
Send a Shipment	>
Add Samples to a Shipment	>
Add Sample Information from a Spread...	>
Download your data	>

MxLIVE Features

Creating Shipments

- **Shipment Tracking**
- Experiment Management
- Experiment Monitoring
- Data Transfer
- Statistics
- Publications, Scheduling, User Support, User Feedback

Create a Shipment: Step 1 of 3

A default name has been chosen for your shipment. You can modify it as needed. This name will be visible to staff at the beamline.

Name*

Comments

Continue

My CMCF Shipment | Sample Seat Selection

GROUPS

- thermolysin
- lysozyme
- insulin

Click on a group to select it, then click the locations of the corresponding samples in each container. Click previously selected samples to remove them.

Save Samples

Create a Shipment: Step 2 of 3

Add the containers you are sending!

To avoid confusion, use labels that are externally visible on your containers. It is possible to add more containers later.

Name*	Kind*	
CLS-001	Uni-Puck	-
CLS-002	Uni-Puck	-
CLS-042	Uni-Puck	-

+ Add Container

Create a Shipment: Step 3 of 3

Add Groups

Specify groups for similar samples. Use the tool to add samples after your shipment is created. "Fill Containers" to auto-create one group per container filled with samples ignoring the groups defined below.

Name	Plan			
thermolysin	Collect all	+/-	>>	-
lysozyme	Collect best	+/-	>>	-

Exp. type* S-SAD **Absorption edge** **Desired Resolution (Å)** 1.5

Comments

Name	Plan			
insulin	Collect best	+/-	>>	-

+ Add Group

Fill Containers Finish

MxLIVE Features

- **Shipment Tracking**
- Experiment Management
- Experiment Monitoring
- Data Transfer
- Statistics
- Publications, Scheduling, User Support, User Feedback

Printing
Shipping
Labels

Send Shipment

Carrier **Tracking code**

Items included in shipment

Comments

Send



MxLIVE Features

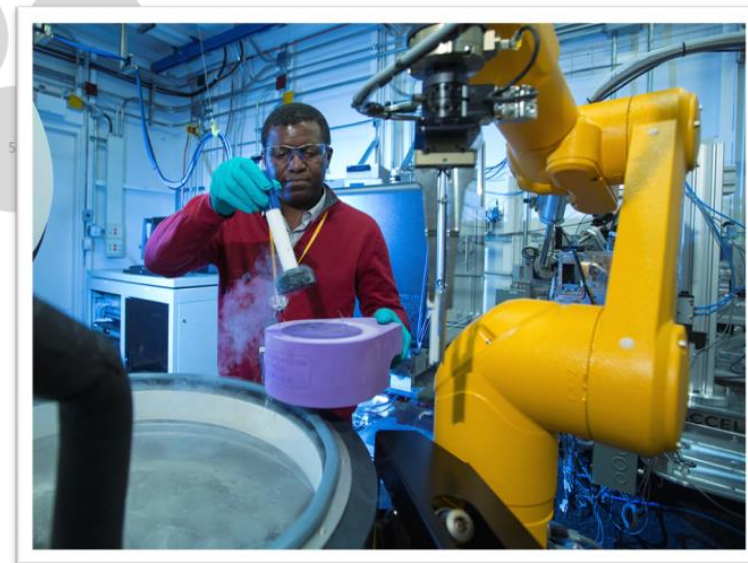
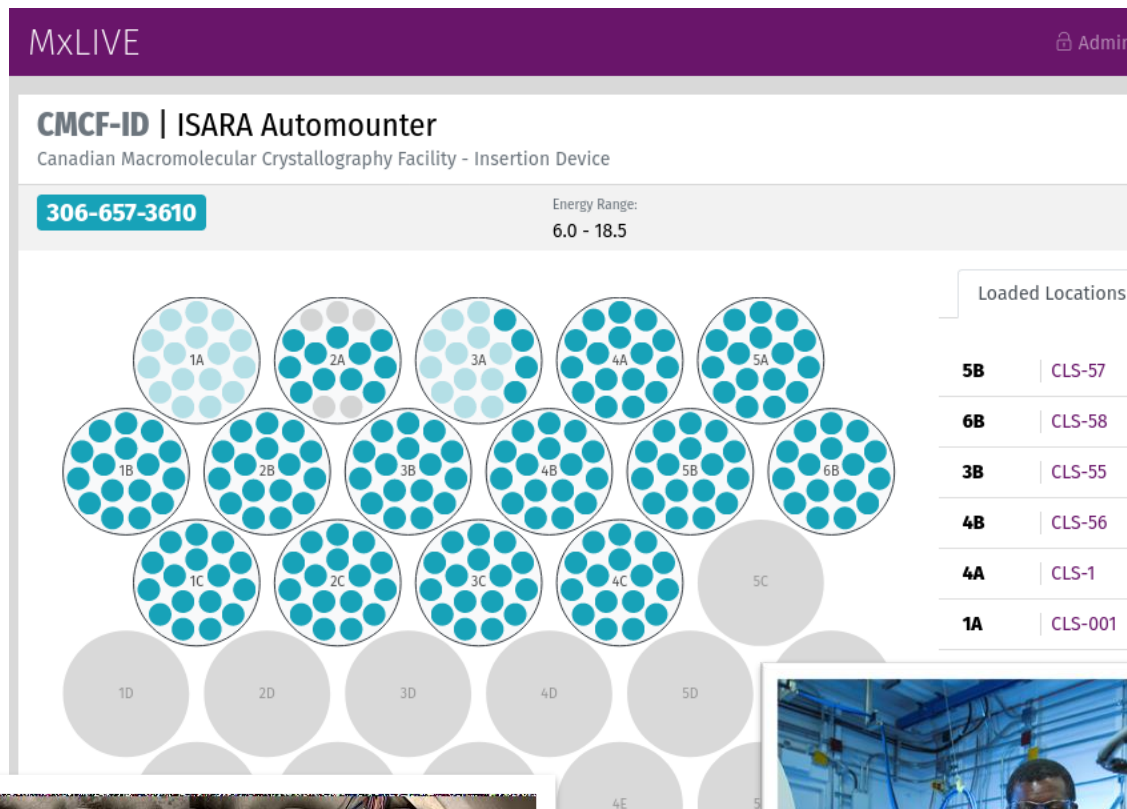
- **Shipment Tracking**
- Experiment Management
- Experiment Monitoring
- Data Transfer
- Statistics
- Publications, Scheduling, User Support, User Feedback

The screenshot displays the MxLIVE web interface. At the top, the header includes 'MxLIVE' on the left and navigation links for 'Admin', 'Dashboard', 'Search', and 'CMCFADM' on the right. Below the header, the user is identified as 'CMCFADMIN | Staff'. A navigation bar contains icons for 'Remote', 'Accounts', 'Sessions', 'Schedule', 'Publications', and 'Add G'. The main content area is divided into sections: 'BEAMLINES' (showing 'CMCF-BM | SAM Automounter'), 'SHIPMENTS' (showing a shipment for 'KATHRYN | Mail-In May 18' with 5 Containers, 5 Groups, and 80 Samples), and 'USER GUIDE' (showing 'CMCF Remote Connection Guide'). A modal dialog titled 'Receive Shipment?' is overlaid on the shipment list. The dialog has a close button (X) in the top right corner. It contains a 'Storage location' field with 'CMCF-ID' entered, and a 'Staff comments' text area. A purple 'Receive' button is located at the bottom right of the dialog. A purple circle highlights the 'Receive' button in the shipment list, with a line pointing to the modal's 'Receive' button.

Receiving Shipments

MxLIVE Features

- Shipment Tracking
- **Experiment Management**
- Experiment Monitoring
- Data Transfer
- Statistics
- Publications, Scheduling, User Support, User Feedback



Loading
automounters

MxLIVE Features

- Shipment Tracking
- **Experiment Management**
- Experiment Monitoring
- Data Transfer
- Statistics
- Publications, Scheduling, User Support, User Feedback

MxLIVE Admin Dashboard - Remote Access

Search [] Beamline: All Active: All item

Name	Description	Scheduled Users	Allowed Users	Address	Beamlines	Active
DATA-2223	Data Transfer Server Port 2223 (srv-cmcf3)					
NX-2221	CMCF-ID Ctrl Rm					
NX-2222	CMCF-BM Ctrl Rm					
NX-2224	CMCF-BM (VM) NX1 Port 2224					
Old DATA-2223	Data Transfer Server Port 2223					
Old NX-2223	CMCF-ID (VM) NX2 Port 2223					
Old NX-2224	CMCF-BM (VM) NX2 port 2224					

ACTIVE CONNECTIONS

- Support CMCF-BM | No scheduled beamtime / 0 Shipments MAR 14
- Support CMCF-BM | FODJE | Michel Fodje No scheduled beamtime / 1 Shipment NX-2222
- Support CMCF-BM | KATHRYN | Kathr... No scheduled beamtime / 0 Shipm... NX-2224 NX-2222

SSH KEYS

- localhost-live | Nov. 30, 2020, 12:43... Delete



MxLIVE Features

- Shipment Tracking
- Experiment Management
- Experiment Monitoring
- **Data Transfer**
- Statistics
- Publications, Scheduling, User Support, User Feedback

MxLIVE

Admin Dashboard Search CMCADMIN

Session | KATHRYN | SIM1-20200511-RwAfd7jk
SES-002-839 | Started May 11, 2020

Reports Data History Statistics Download

Datasets: 30 Reports: 7 Total Time: 4 hours 15 mins Start: May 11, 2020

thermolysin | Native | Collect all

Sample	Container	Location	Data Sets	Analysis Reports
thermolysin_1	CLS-001	CMCF-ID 1A1	SCR 8 imgs	
thermolysin_2	CLS-001	CMCF-ID 1A2	DAT 673 imgs SCR 8 imgs	NAT 0.38
thermolysin_3	CLS-001	CMCF-ID 1A3	SCR 8 imgs	
thermolysin_4	CLS-001	CMCF-ID 1A4	SCR 8 imgs	
thermolysin_5	CLS-001	CMCF-ID 1A5	SCR 8 imgs	SCR 0.75
thermolysin_6	CLS-001	CMCF-ID 1A6	SCR 8 imgs	SCR 0.48
thermolysin_7	CLS-001	CMCF-ID 1A7	SCR 8 imgs	SCR 0.56
thermolysin_8	CLS-001	CMCF-ID 1A8	SCR 8 imgs	SCR 0.75
thermolysin_9	CLS-001	CMCF-ID 1A9	SCR 8 imgs	

Downloading Data

Data | LABIUK | thau_dcm_b
DAT-099-435 — MX Dataset from Jan. 14, 2020

Session: CMCFBM-20200114-e5... Beamline / Energy: CMCFBM at 8.1570 keV Beam: 1.0s / 50.0% / 200 μm Group / Sample: None / None Reports: 0.77

719 Frames (1-719) Meta-Data

- thau_dcm_b_0001.img
- thau_dcm_b_0002.img
- thau_dcm_b_0003.img
- thau_dcm_b_0004.img
- thau_dcm_b_0005.img
- thau_dcm_b_0006.img
- thau_dcm_b_0007.img
- thau_dcm_b_0008.img
- thau_dcm_b_0009.img
- thau_dcm_b_0010.img
- thau_dcm_b_0011.img

Res: 8.70 Å

Dark Normal Light

thau_dcm_b_0001.img
0 deg to 0.5 deg

Data | LABIUK | 200108-0940
DAT-097-958 — XRF Dataset from Jan. 8, 2020

Session: CMCFID-20200107-0RxCF8Uz Beamline / Energy: CMCFID at 12.6580 keV Beam: 0.5s / 50.0% / 50 μm Group / Sample: None / None

Fluorescence

Energy (keV)

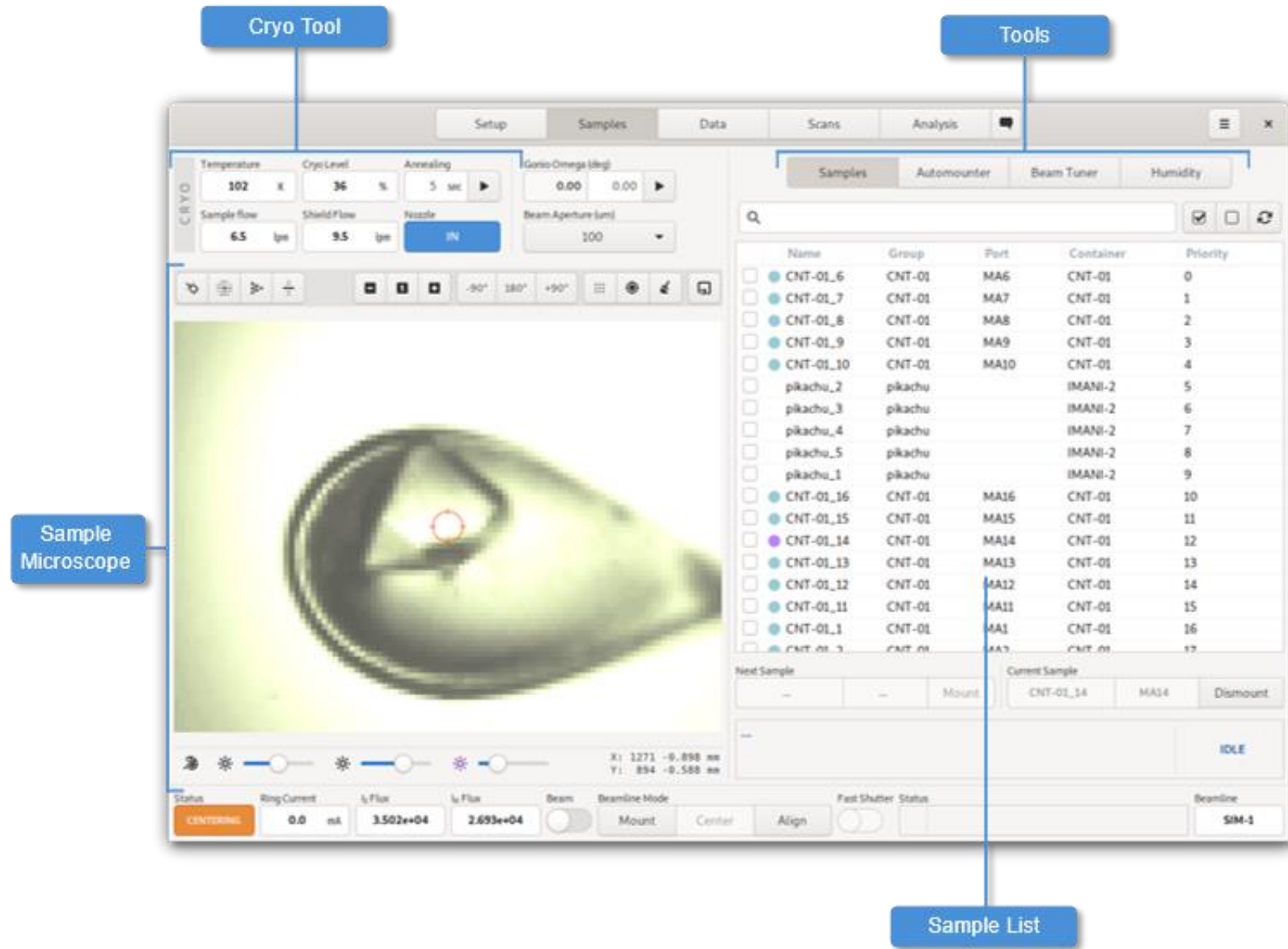
Experiment Fit

Figure 1 - XRF Spectrum, select elements on the right to show/hide emission lines

Element	%
Zn	28.0
Co	14.5
Yb	9.2
Os	6.8
Gd	2.0
Dy	1.2
Ta	0.7
Lu	0.5
Tb	0.4
Tc	0.4
Cs	0.3
Ne	0.3
K	0.3
Nb	0.3

MxDC Features

- Single Integrated GUI
- Activity Pages
- Automation
 - AI-assisted Centering
- Data Visualization
- Data Analysis



MxDC Features

- Single Integrated GUI
- Activity Pages
- Automation
 - AI-assisted Centering
- Data Visualization
- Data Analysis

The screenshot displays the MxDC software interface, which is divided into several functional areas:

- Diffraction Image Viewer:** Located at the top left, it shows a diffraction pattern with overlaid concentric circles and a grid. The circles are labeled with values: 1.55, 1.71, 1.93, 2.24, 2.72, 3.54, 5.21, and 10.31.
- Data Acquisition Mode:** Located at the top right, it contains tabs for 'Interactive', 'Automation', and 'Rastering'.
- Data Sets:** A list on the right side showing three datasets: 'Screen 0°, 90° @ 12.5 keV lyso-0', 'Full Dataset @ 12.5 keV lyso-1', and 'Full Dataset @ 12.5 keV lyso-2'. Each entry includes a play button, a gear icon, and a duration.
- Edit Run:** A panel on the right for configuring a run. It includes fields for Name (lyso-2), Resolution (1.08 Å), Distance (150.1 mm), Angle/Frame (0.25 deg), Exposure/Frame (0.25 sec), Attenuation (0 %), Start Angle (0 deg), Total Angle (360 deg), Wedge (720 deg), First Frame (1), Total Frames (1440), and Energy (12.500 keV). It also has an 'Inverse Beam' checkbox, 'Points' and 'Steps' dropdowns, and a 'Notes' field.
- Run Editor:** A blue callout box on the right side of the interface.
- Run List:** A blue callout box pointing to the 'Data Sets' list.
- Feedback:** A blue callout box pointing to the 'Notes' field in the 'Edit Run' panel.
- Open Terminal:** A blue callout box pointing to the 'Beamline' dropdown menu at the bottom right, which is currently set to 'SIM-1'.
- Status Bar:** At the bottom, it shows 'Status: COLLECTING', 'Ring Current: 248.6 mA', 'I₁ Flux: 3.502*10⁴', 'I₂ Flux: 2.693*10⁴', 'Beam: ON', 'Beamline Mode: Mount', 'Center', 'Align', 'Fast Shutter Status: SIM Diffractometer - Scanning ...', and 'Beamline: SIM-1'.