

# MxLIVE

MX Laboratory Information Virtual Environment

*Kathryn Janzen – CMCF*

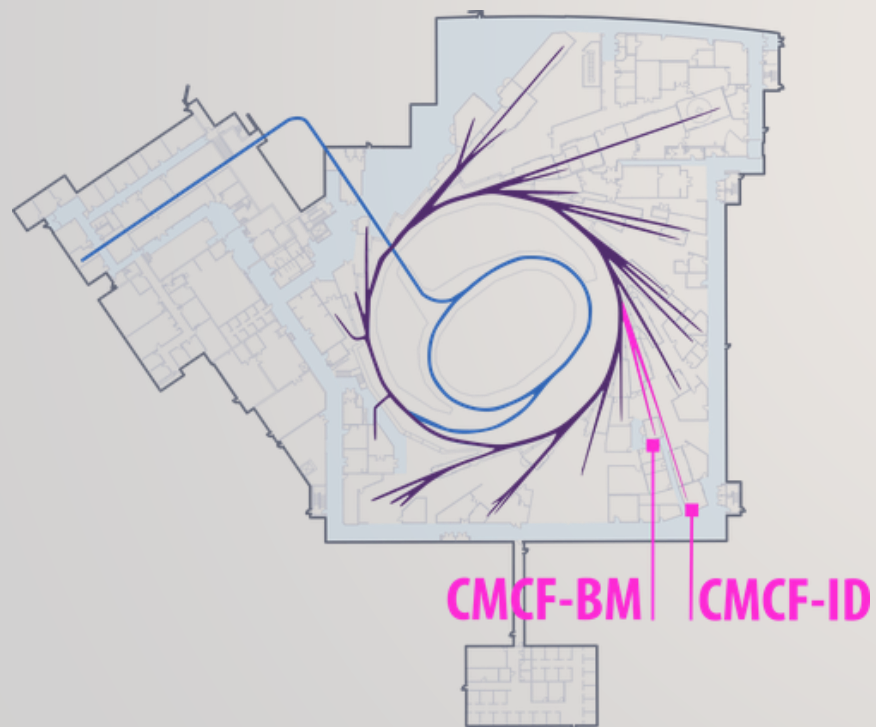


Canadian  
Light  
Source

Centre canadien  
de rayonnement  
synchrotron

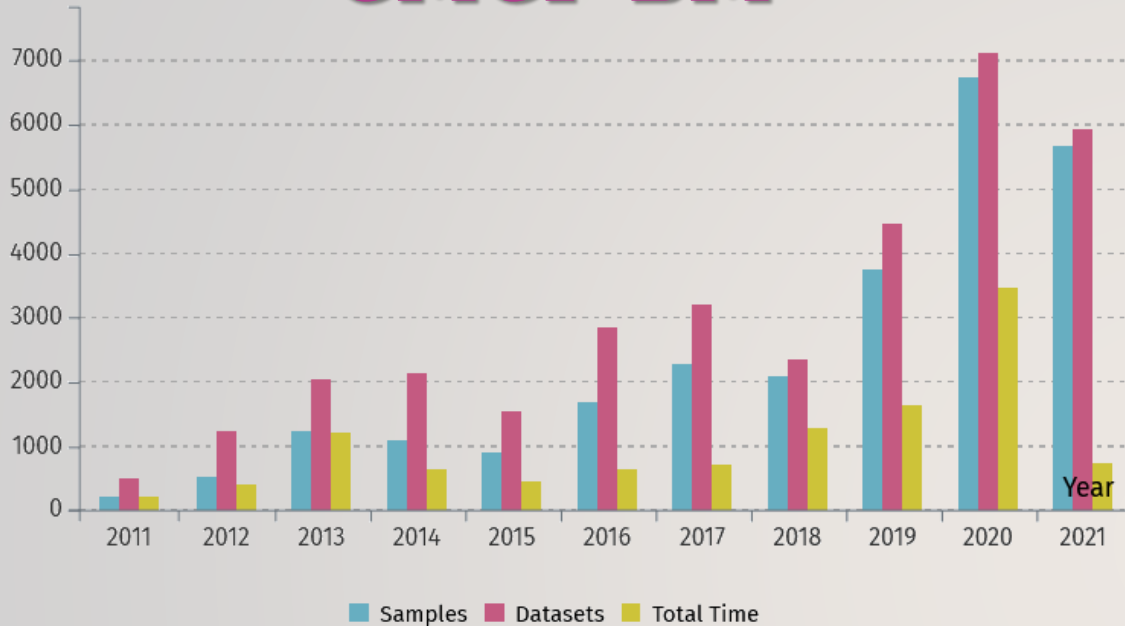
# CMCF

Canadian Macromolecular  
Crystallography Facility





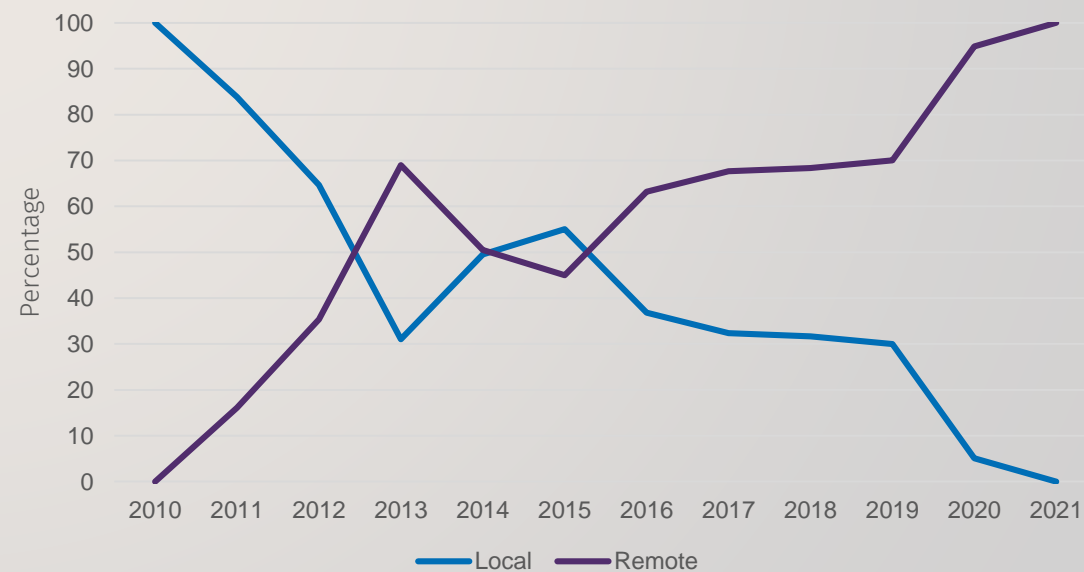
# CMCF-BM



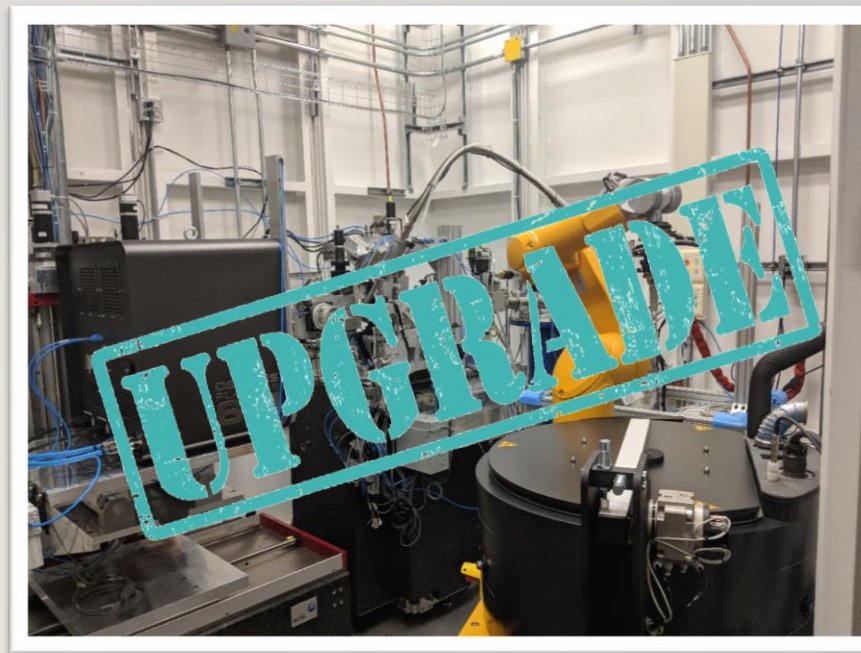
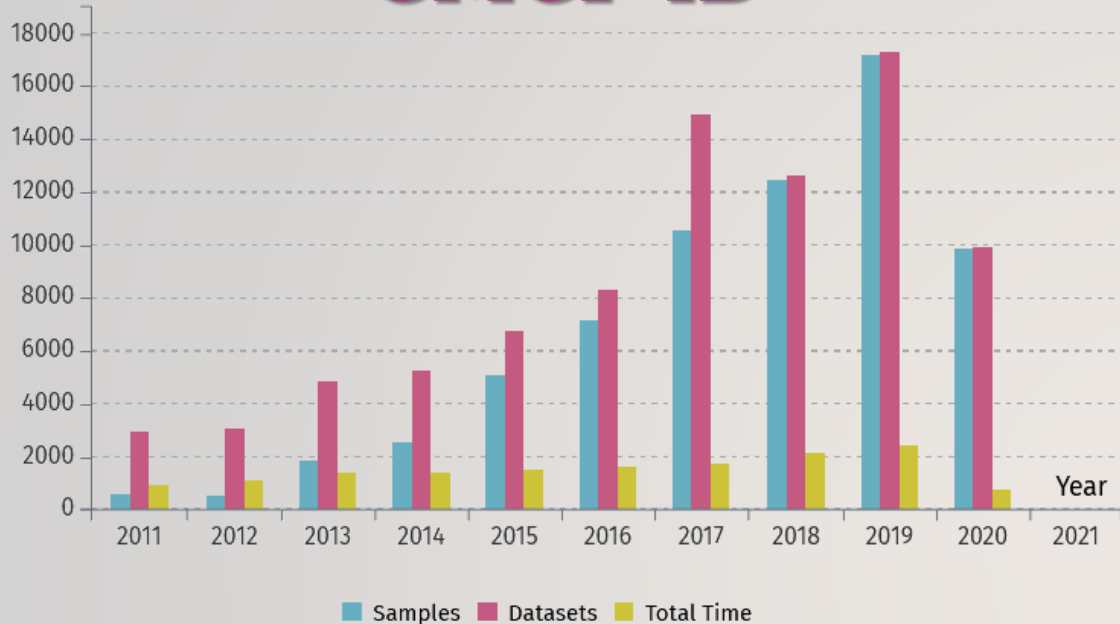
Energy Range	4-18keV
Photon Flux (photons/s)	$>2.5 \times 10^{12}$ DMM @ 8.15keV $>1.5 \times 10^{11}$ DCM @ 12.6keV
Beam Size	20 – 200 $\mu\text{m}$
SAM Automounter	25 second duty cycle with sample pre-fetch
Standards	SSRL Cassettes, Uni-Pucks
Detector	Pilatus3 S 6M
Goniometer	MD2 with miniKappa
Spectroscopy	Vortex ME4 & Bruker XFlash 410



## CMCF-BM Delivered Shifts (Academic and Industrial)

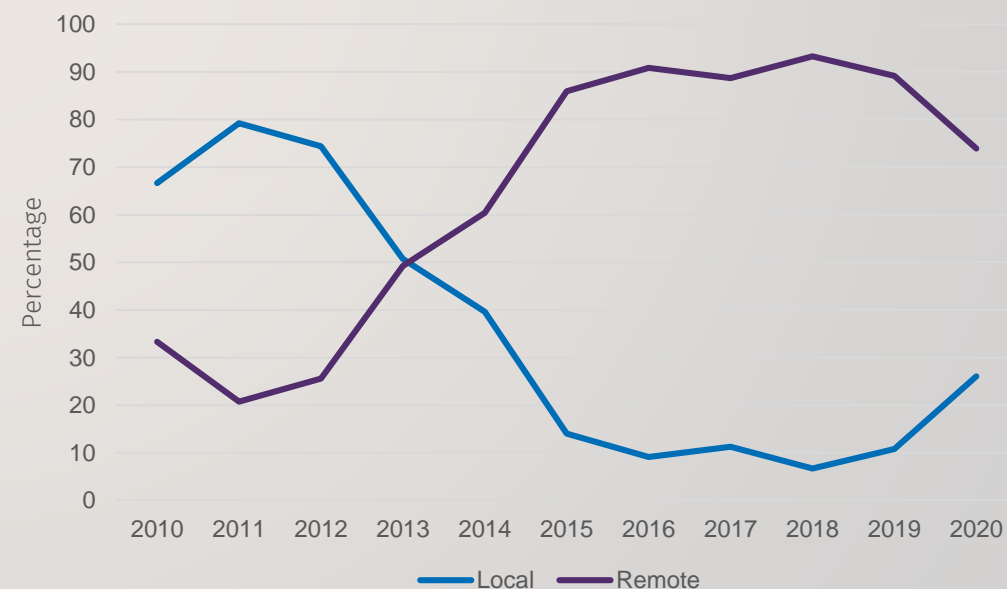


# CMCF-ID



Energy Range	6-18keV
Photon Flux 50 $\mu\text{m}$ @ 12keV (photons/s)	Pre-Upgrade: $1 \times 10^{12}$ After Upgrade: $>1 \times 10^{13}$ $\sim 5 \times 10^{14}$ DMM
Beam Size	5 – 100 $\mu\text{m}$ (after upgrade)
ISARA Automounter	~25 second duty cycle   Installed in 2017
Standards	Uni-Pucks
Detector	Eiger X 9M (install in progress)
Goniometer	MD2-S (install in progress)

## CMCF-ID Delivered Shifts (Academic and Industrial)



# MxLIVE

## Feature Highlights

- Shipment Tracking
- Experiment Management
- Data Access/Transfer
- Publications, Scheduling, User Support, User Feedback
- Statistics galore

MxLIVE
Admin Dashboard Search CMCADMIN

CMCFADMIN | Staff
Start here to manage shipments, load containers on a beamline, view data, and...
Remote Sessions Accounts Schedule Publications Support Add Guide

BEAMLINES
CMCF-BM | SAM Automounter
L M R
CMCF-ID | ISARA Automounter
1A 2A 3A 4A 5A 1B 2B 3B 4B 5B 6B 1C 2C 3C 4C 5C 1D 2D 3D 4D 5D 6D 1E 2E 3E 4E 5E 1F 2F
SIM-1 | SAM Automounter
L M R

ADAPTORS
CLS-0001 CLS-0002 CLS-0003
A C A C A C

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

SHIPMENTS
MAR 16 7 Containers / 15 Groups / 112 Samples Receive
MAR 17 5 Containers / 5 Groups / 75 Samples Receive
FEB 19 1 Container / 1 Group / ... 20 Data 7 Reports Return
JUL 24 FODJE | 2020-Jul24 #1 1 Container / 1 Group / ... Data Reports Return
SEP 25 SPASYUK | 2020-Sep... 2 Containers / 2 Groups ... 64 Data 20 Reports Return
Click here to start a new shipment! Follow the steps to enter your sample information

LOCAL CONTACT
KATHRYN JANZEN 306-657-3836 Support

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

# Shipment Information Wizard

Create a Shipment: Step 1 of 3

A default name has been chosen for your shipment. This name will be visible to staff at the beamline.

**Name\***

**Comments**

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*
<input type="text" value="CLS-001"/>	<input type="text" value="Uni-Puck"/>
<input type="text" value="CLS-002"/>	<input type="text" value="Uni-Puck"/>
<input type="text" value="CLS-042"/>	<input type="text" value="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			
<input type="text" value="thermolysin"/>	<input type="text" value="Collect all"/>			
<input type="text" value="lysozyme"/>	<input type="text" value="Collect best"/>			

**Exp. type\***  **Absorption edge**  **Desired Resolution (Å)**

**Comments**

Name	Plan			
<input type="text" value="insulin"/>	<input type="text" value="Collect best"/>			

+ Add Group

Fill Containers

Finish



# Sample Information

MxLIVE

Dashboard Search KATHRYN

Shipment | **My CMCF Shipment**

SHP-002-376 | Created today

Containers Groups Samples Delete Edit Send Labels

Draft

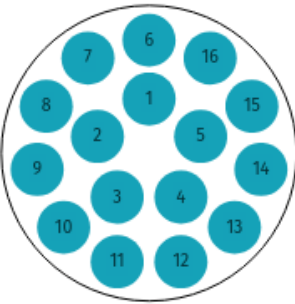
# Containers: 3

# Groups: 3

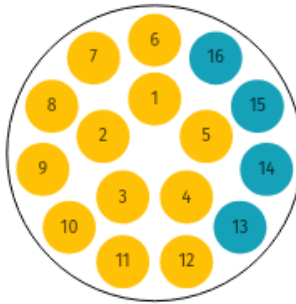
# Samples: 43

Ready to Ship: Yes

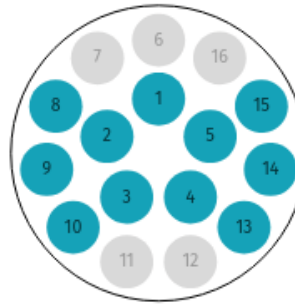
CLS-001



CLS-002



CLS-042



GROUPS

**thermolysin**

Native | Collect all

16 samples assigned.

**lysozyme**

S-SAD | Collect best (1.5Å)

12 samples assigned.

**insulin**

Native | Collect best

15 samples assigned.

KATHRYN

These samples are for our upcoming beamtime.

# Shipping Samples to CLS

- Printable shipping labels
- Tracking numbers visible to staff



Canadian Light Source / Centre canadien de rayonnement synchrotron

SHIPPING LABEL

Print this document and cut out the label to affix to the outside of your transport container (dewar) for shipment.

To: Michel Fodje  
c/o Shipping and Receiving  
Canadian Light Source, Inc.  
44 Innovation Blvd  
Saskatoon  
Canada  
Phone: 306-657-3657

ID: Kathryn Janzen (My CMCF Shipment)  
From: Kathryn Janzen

↑↑  
↑↑  
↑↑

Non-Hazardous  
Frozen Samples In  
Dry-Shipper

Send Shipment

Carrier: Canada Post Tracking code: 12345678

Items included in shipment: External Hard Drive

Comments: These samples are for our upcoming beamtime.

Send



# Receiving Shipments



**MxLIVE** Admin Dashboard Search CMCFADMIN

**CMCFADMIN | Staff**  
Start here to manage shipments, load containers on a beamline, view data, and more.

Remote Accounts Sessions Schedule Publications Add G

**BEAMLINES**  
CMCF-BM | SAM Automounter

**SHIPMENTS**

SHIPMENTS	Receive
<b>KATHRYN   Mail-In May 18</b> 5 Containers / 5 Groups / 80 Samples MAY 12	Receive
ment 6 Samples	Data Reports Return
2 Samples	Data Reports Return
12 Samples	Data Reports Return
ment 3 Samples	Data Reports Return
4 Samples	Data Reports Return

**new shipment!**  
our sample information

**SESSIONS**  
20200511-RwAfD7jk  
st record 51 minutes ago

Data Reports

**USER GUIDE**  
CMCF Remote Connection Guide  
CMCF Remote Connection Guide  
Everything you need to know about remote connections at CMCF is found in our remote control guide. Click to download the document.

- Create a New Shipment
- Add Samples to a Shipment
- Send a Shipment
- Add Sample Information from a
- Download your data

**Receive Shipment?**

Storage location  
CMCF-ID

Staff comments

Receive

# Return Shipping

- Printable return shipping labels/forms
- Tracking numbers visible to user



## MXLIVE | RETURN SHIPPING LABEL

Print this document and cut out the label. Remove the labels currently on the boxes and replace them with this return label.

To: Kathryn Janzen  
CMCF  
Canadian Light Source  
44 Innovation Boulevard  
Saskatoon, Saskatchewan S7N 2V3  
Canada  
Phone: 657-3836  
Fax: 657-3535



Non-Hazardous  
Frozen Samples in  
Dry-Shipper

From: Kathryn Janzen (2020-May12)  
Michael Rudge  
c/o Shipping and Handling  
Canadian Light Source, Inc.  
44 Innovation Blvd  
Saskatoon  
Canada  
Phone: 306-457-3857

Not restricted, as per Special Provision A152

### Shipping Order

Canadian Light Source / Centre canadien de rayonnement synchrotron

Shipper's Name: \_\_\_\_\_ DATE: May 15, 2020

CSI Department: \_\_\_\_\_

Phone: \_\_\_\_\_

SL Account #: \_\_\_\_\_ CSZ Code: \_\_\_\_\_

OPTIONAL: Request for Receipt Complete Date (SL, WP, & L&D Information)

SL Account #: \_\_\_\_\_ CSZ Code: \_\_\_\_\_

FORM: Later provided by Rec'd. Based on: L&D Date, SL, WP, & L&D Information

#### Shipping Information (Consignor)

Company Name: CMCL Canadian Light Source  
Street Address: 44 Innovation Boulevard  
City: Saskatoon Province / State: Saskatchewan  
Country: Canada Postal Code: S7N 2V3  
Attn (Contact Person): Kathryn Janzen Phone Number: 657-3836  
Contact Person Email: kjanzen@lightsource.ca  
CSI Proposal Number: \_\_\_\_\_ Federal Tax # (GST): \_\_\_\_\_  
Consignee's Country: FedEx Courier Account #: \_\_\_\_\_  
On Load: Chargeable Weight: Return to Sender: Other:  
Return of Load: Warranty Weight: US Goods Returned: Other:  
Return to Vendor: Other: Other (Specify):

Qty	Item or Lot # (Chemical)	Model # / Serial # / Description	Country of Manufacture	Value
1		Non-Hazardous Frozen Protein Samples in Dry Shipping Box	Canada	\$200

City Total: \_\_\_\_\_ U.S. Code: \_\_\_\_\_

#### Any Hazards?

Yes	No	Yes	No	Yes	No	Total	U.S.
Explosives		Flammable Liquid		Poisonous Material		CAFS	1000
Dangerous When Wet		Flammable Solid		Poisonous Gas		USAG	5000
Corrosive Material		Combustible Liquid		Radioactive Material		USAG	5000
Organic Peroxides		Infectious Substances		Quarantine		USAG	5000
Lead Acid Battery		Spontaneously Combustible Liquid		Other Category			
Lithium Metal Battery		Nonflammable Compressed Gas					
Lithium Ion Battery		Flammable Compressed Gas					

Please Supply True Copies Of Safety Data Sheet For Each Element Shipped

Package Label with Mark	Weight	Measurement: Box (L)	Box (W)	Box (H)
Package 1				
Package 2				
Package 3				
Package 4				

Canadian Light Source - 44 Innovation Boulevard - University of Saskatchewan, Saskatoon, SK Canada - S7N 2V3

## Return Shipment

### Carrier

FedEx

### Return code

87632512

### Staff comments

Save

# Loading Samples

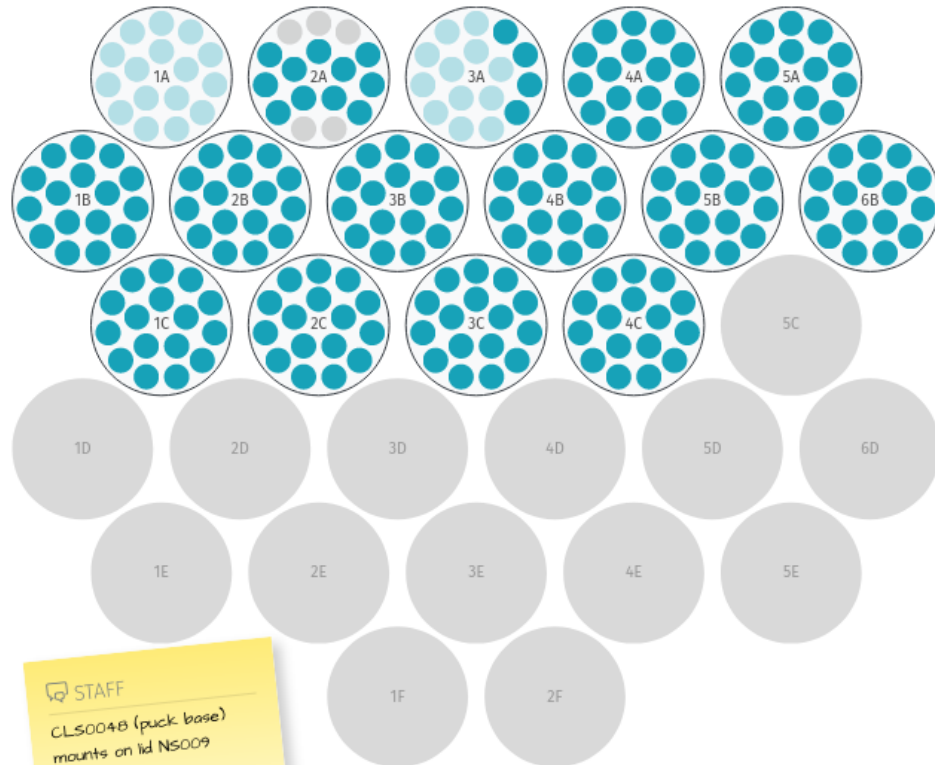
MxLIVE

Admin

## CMCF-ID | ISARA Automounter

Canadian Macromolecular Crystallography Facility - Insertion Device

306-657-3610

Energy Range:  
6.0 - 18.5

STAFF

CLS004B (puck base)  
mounts on lid NS009

### Loaded Locations

5B	CLS-57
6B	CLS-58
3B	CLS-55
4B	CLS-56
4A	CLS-1
1A	CLS-001
2A	CLS-002
2B	CLS-5
3A	CLS-042
1B	CLS-4
5A	CLS-2
4C	SIM-005
2C	SIM-002





# Managing Remote Connections

MxLIVE Admin Dashboard Search CMCFADMIN


## 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)				CMCF-BM	True
NX-2221	CMCF-ID Ctrl Rm				CMCF-ID	True
NX-2222	CMCF-BM Ctrl Rm				CMCF-BM	True
NX-2224	CMCF-BM (VM) NX1 Port 2224				CMCF-BM	True
Old DATA-2223	Data Transfer Server Port 2223				CMCF-BM	False
Old NX-2223	CMCF-ID (VM) NX2 Port 2223				CMCF-ID	False
Old NX-2224	CMCF-BM (VM)				CMCF-ID	False




## ACTIVE CONNECTIONS


 Support


CMCF-BM | No scheduled beamtime / 0 Shipments

 MAR 14


 Support


CMCF-BM | FODJE | Michel Fodje  
No scheduled beamtime / 1 Shipment

 2  
NX-2222


 Support


CMCF-BM | KATHRYN | Kathr...  
No scheduled beamtime / 0 Shipm...

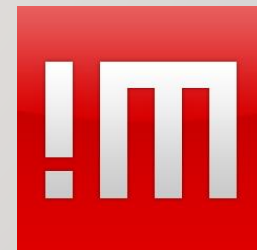
 NX-2224

 2  
NX-2222

## SSH KEYS

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

 Delete



# Reviewing Data & Processing Reports

MxLIVE

Admin Dashboard Search CMCADMIN

Session | KATHRYN | SIM1-20200511-RwAfD7jk

SES-002-839 | Started May 11, 2020

7 Reports

30 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 0.45
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	
thermolysin_10	CLS-001	CMCF-ID 1A10	SCR 8 imgs	
thermolysin_11	CLS-001	CMCF-ID 1A11	SCR 8 imgs	SCR 0.66
thermolysin_12	CLS-001	CMCF-ID 1A12	SCR 8 imgs	
thermolysin_13	CLS-001	CMCF-ID 1A13	SCR 8 imgs	
thermolysin_14	CLS-001	CMCF-ID 1A14	SCR 8 imgs	
thermolysin_15	CLS-001	CMCF-ID 1A15	SCR 8 imgs	
thermolysin_16	CLS-001	CMCF-ID 1A16	SCR 8 imgs	

lysozyme | S-SAD(1.5Å) | Collect best

Sample	Container	Location	Data Sets	Analysis Reports
lysozyme_1	CLS-042	1	SCR 12 imgs	
lysozyme_2	CLS-042	2	SCR 12 imgs	
lysozyme_3	CLS-042	3	SCR 12 imgs	
lysozyme_4	CLS-042	4	SCR 9 imgs	

Data | LABIUK | 200108-0947

DAT-097-959 — MAD Scan from Jan. 8, 2020

Session: CMCFID-20200107-ORxCF8Uz

Beamline / Energy: CMCF-ID at 12.6567 keV

Beam: 0.5s / 50.0% / 50 µm

Group / Sample: None / None

Download

Data | LABIUK | 200108-0940

DAT-097-958 — XRF Dataset from Jan. 8, 2020

Session: CMCFID-20200107-ORxCF8Uz

Beamline / Energy: CMCF-ID at 12.6580 keV

Beam: 0.5s / 50.0% / 50 µm

Group / Sample: None / None

Download

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

DAT-099-435 — MX Dataset from Jan. 14, 2020

Session: CMCFBM-20200114-e5...

Beamline / Energy: CMCF-BM at 8.1570 keV

Beam: 1.0s / 50.0% / 200 µm

Group / Sample: None / None

Reports: 0.77

Download

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

thau\_dcm\_b\_0012.img

Res: 8.70 Å

Dark Normal Light

thau\_dcm\_b\_0001.img

0 deg to 0.5 deg

Energy

f

f'

PEAK	12.6507 keV	-7.2	5.3
	0.9801 Å		
INFL	12.6487 keV	-9.3	3.7
	0.9802 Å		
REMO	12.7287 keV	-3.9	3.6
	0.9741 Å		

Meta

Data

Roi	[11.1475, 11.2975]
Edge	Se-K

# Data Transfer

**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 0.45
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	
thermolysin_10	CLS-001	CMCF-ID 1A10	SCR 8 imgs	
thermolysin_11	CLS-001	CMCF-ID 1A11	SCR 8 imgs	SCR 0.66
thermolysin_12	CLS-001	CMCF-ID 1A12	SCR 8 imgs	
thermolysin_13	CLS-001	CMCF-ID 1A13	SCR 8 imgs	
thermolysin_14	CLS-001	CMCF-ID 1A14	SCR 8 imgs	
thermolysin_15	CLS-001	CMCF-ID 1A15	SCR 8 imgs	
thermolysin_16	CLS-001	CMCF-ID 1A16	SCR 8 imgs	

**lysozyme** | S-SAD(1.5Å) | Collect best

Sample	Container	Location	Data Sets	Analysis Reports
lysozyme_1	CLS-042	1	SCR 12 imgs	
lysozyme_2	CLS-042	2	SCR 12 imgs	
lysozyme_3	CLS-042	3	SCR 12 imgs	
lysozyme_4	CLS-042	4	SCR 9 imgs	

**Data | LABIUK | 200108-0947**  
DAT-097-959 — MAD Scan from Jan. 8, 2020

Session: CMCFID-20200107-ORxCF8Uz Beamline / Energy: CMCF-ID at 12.6567 keV Beam: 0.5s / 50.0% / 50 µm Group / Sample: None / None

Download

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

Session: CMCFID-20200107-ORxCF8Uz Beamline / Energy: CMCF-ID at 12.6580 keV Beam: 0.5s / 50.0% / 50 µm Group / Sample: None / None

Download

**Data | LABIUK | thau\_dcm\_b**  
DAT-099-435 — MX Dataset from Jan. 14, 2020

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

Download

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

**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

**Meta Data**

Meta	Data
Roi	[11.1475, 11.2975]
Edge	Se-K

**Energy f f'**

PEAK	12.6507 keV	-7.2	5.3
	0.9801 Å		
INFL	12.6487 keV	-9.3	3.7
	0.9802 Å		
REMO	12.7287 keV	-3.9	3.6
	0.9741 Å		



# Publications

- Automatic fetching of PDB depositions, articles, metrics

MxLIVE

[Admin](#) [Dashboard](#) [Search](#) [CMCFADMIN](#)

## PDB Depositions

[Publications](#) [PDB Entries](#) [Metrics](#) [Subject Areas](#) [Journals](#)

<input type="text" value="Search"/>						Created Any date	Modified Any date	Released Year All	Released Month All	Tags All	1446 items
Id	Code	Released	Title	Resolution	Deposited						
1446	6XOG	2021-03-09	Structure of SUMO1-ML786519 adduct bound to SAE	1.98	2020-07-06						
1445	7JKR	2021-03-09	GTP-specific succinyl-CoA synthetase complexed with Mg-GMPPNP, phosphohistidine loop pointing towards nucleotide binding site	2.64	2020-07-27						
1444	7JJ0	2021-03-09	GTP-specific succinyl-CoA synthetase complexed with Mg-GMPPCP	2.25	2020-07-23						
1443	7DHz	2021-03-02	Arsenic-bound p53 DNA-binding domain mutant R249S	1.74	2020-11-17						
1442	7LJ7	2021-02-23	Crystal structure of MtCNNM with C-terminal deletion in complex with Mg <sup>2+</sup> -ATP	3.26	2021-01-27						
1441	7KHL	2021-02-23	BRD4-BD1 Compound6 (methyl 4-(3,5-difluoropyridin-2-yl)-10-methyl-7-((methylsulfonyl)methyl)-11-oxo-3,4,10,11-tetrahydro-1H-1,4,10-triazadibenzo[cd,f]azulene-6-carboxylate)	1.29	2020-10-20						
1440	6XCS	2021-02-16	Erythromycin esterase mutant EreC H289N in its open conformation	2.4	2020-06-08						
1439	7KLG	2021-02-09	SARS-CoV-2 RBD in complex with Fab 15033	3.2	2020-10-29						
1438	7KLH	2021-02-09	SARS-CoV-2 RBD in complex with Fab 15033-7	3.0	2020-10-29						
1437	7JJV	2021-01-26	Crystal waters on the nine polyproline type II helical bundle springtail antifreeze protein from <i>Granosotoma rainieri</i> match the ice lattice	1.21	2020-07-26						
1436	7DNB	2021-01-26	Crystal structure of PhoCl barrel	2.81	2020-12-08						
1435	7DNA	2021-01-26	Photocleavable Fluorescent Protein in green and red form	2.3	2020-12-08						
1434	7DMX	2021-01-26	Photocleavable Fluorescent Protein in green form	2.1	2020-12-07						
1433	7JU2	2021-01-19	Crystal structure of the monomeric ETV6 PNT domain	1.85	2020-08-18						
1432	6VUV	2021-01-19	Scabin (S117A) toxin from <i>Streptomyces scabies</i>	1.55	2020-02-15						
1431	6VVF	2021-01-19	Scabin (Y129H) toxin from <i>Streptomyces scabies</i>	1.75	2020-02-16						
1430	6VV4	2021-01-19	Scabin (V109G) toxin from <i>Streptomyces scabies</i>	1.7	2020-02-15						

MxLIVE

[Admin](#) [Dashboard](#) [Search](#) [CMCFADMIN](#)

## All | Publication Metrics

[Publications](#) [PDB Entries](#) [Metrics](#) [Subject Areas](#) [Journals](#)

[All](#) [2004](#) [2006](#) [2007](#) [2008](#) [2009](#) [2010](#) [2011](#) [2012](#) [2013](#) [2014](#) [2015](#) [2016](#) [2017](#) [2018](#) [2019](#) [2020](#) [2021](#) [All](#) [CMCF-BM](#) [CMCF-ID](#)

## Publication Metrics

Summary of publication metrics statistics

Year	2004	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020	2021	All
Publications	1	1	1	4	15	25	44	44	54	45	55	78	67	76	73	51	8	642
PDB Depositions	0	1	2	12	38	76	92	93	115	81	135	172	209	176	148	77	19	1446
Citations	25	13	46	188	552	1295	1613	1729	2200	1422	1522	1750	976	0	0	0	0	13331
Citations/Article	25	13	46	47	36.8	51.8	36.7	39.3	40.7	31.6	27.7	23	14.8	0	0	0	0	30.9
Media Mentions <sup>1</sup>	6	2	3	5	19	90	72	164	129	76	97	113	447	0	0	0	0	1223
Mentions/Article	6	2	3	1.2	1.3	3.6	1.6	3.7	2.4	1.7	1.8	1.5	6.8	0	0	0	0	2.8
Average Impact Factor <sup>2</sup>	0	4	4	5	5.2	5.4	5.5	6.3	6.8	4.9	6	6.6	6.6	6.7	6.8	5.8	6.9	6.3
Average SJR <sup>3</sup>	0	2.3	2.3	2.5	3.4	3.1	3.3	3.8	3.7	2.6	3.2	3.4	3.4	3.5	3.6	3.2	3.6	3.4
Average SJR <sup>3</sup> Quartile	0	1	1	1	1.1	1	1	1	1	1	1.1	1.1	1	1	1	1.1	1	1
Average H-Index	0	497	497	261.2	271.7	395.8	358.7	401.4	380.1	287	299.2	302.2	260.9	299	263.4	241	235.5	305.7

Table 1 - Metrics Summary

- Mentions represent the number of news stories, and social media mentions the reference the publication.
- The Average Impact Factor is the ratio of citations to the number of citable documents for the journal over the previous two years. This value is calculated based on citations in the SCOPUS database and may be different from the Web Of Science values from the Thomson Reuters database.
- SJR is the SCIMAGO Journal Rank Metric: <https://www.scimagojr.com/>. A Journal with an SJR quartile of 1 is in the top 25% of journals in the field when ranked by SJR, and a quartile of 2 is ranked higher than 50% but lower than 25% of journals in the field.

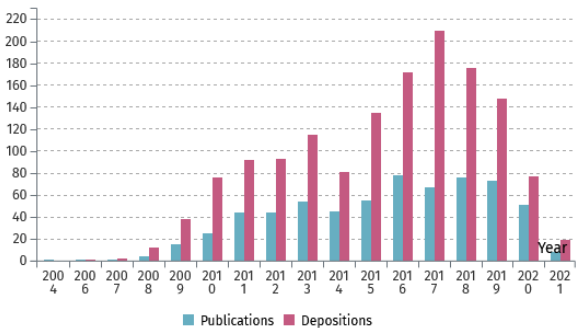


Figure 1 - Research Output

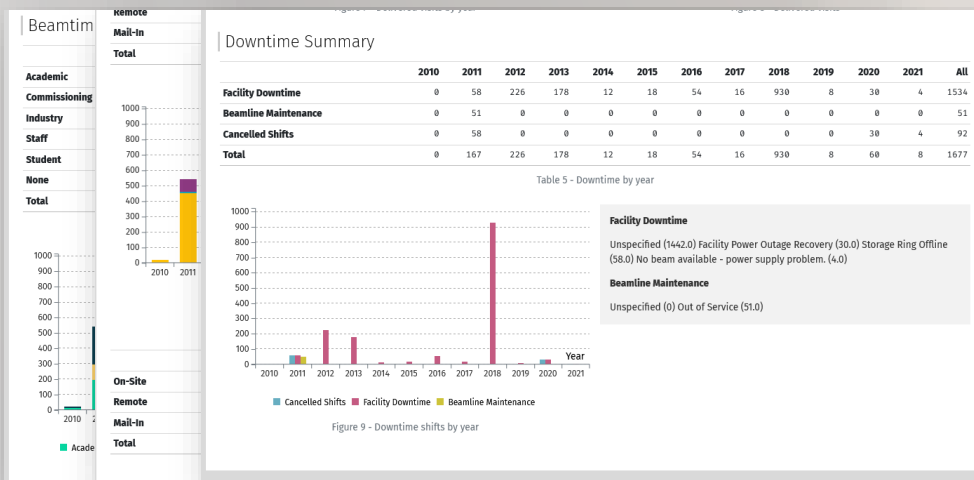


Figure 2 - Data Collection vs PDB Release

Citations	Article
253	Trempe, J.-F.; Sauve, V.; Grenier, K.; Seirafi, M.; Tang, M. Y.; Menade, M.; Al-Abdul-Wahid, S.; Krett, J.; Wong, K.; Kozlov, G.; Nagar, B.; Fon, E. A.; Gehring, K. (2013) Structure of Parkin Reveals Mechanisms for Ubiquitin Ligase Activation. Science. DOI:10.1126/science.1237908
224	Blattner, Claudia; Lee, Jeong Hyun; Sliepen, Kwinten; Derking, Ronald; Falkowska, Emilia; de la Peña, Alba Torrents; Cupo, Albert; Julian, Jean-Philippe; van Gils, Marit; Lee, Peter S.; Peng, Wenjie; Paulson, James C.; Poignard, Pascal; Burton, Dennis P.; Moore, ...

# Scheduling

- Local contacts
- Imported facility modes
  - Configurable for any facility
- Sanitized public display
- Downtime tracking
- Email notifications



Week of 2020-03-09

	TIME	CMCF-BM	CMCF-ID	STAFF 08:00 - 22:00
MARCH 09 MON	00:00			
	08:00			
	16:00			
MARCH 10 TUE	00:00			
	08:00			
	16:00			
MARCH 11 WED	00:00			Michel Fodje
	08:00	Maintenance (CMCFADMIN)	DAVIES   davies	306-657-3758
	16:00	DMITRIEV   Michal	DAVIES   davies	
MARCH 12 THU	00:00	DMITRIEV   Michal	DAVIES   davies	Kathryn Janzen
	08:00	TREMPE   SAD	BURKE	306-657-3836
	16:00	Maintenance (CMCFADMIN)		
MARCH 13 FRI	00:00	Maintenance (CMCFADMIN)		
	08:00	Maintenance (CMCFADMIN)		
	16:00	BANERJEE   powder, WARM ROBOT		
MARCH 14 SAT	00:00	BANERJEE   powder, WARM ROBOT		
	08:00	REID   powder		
	16:00	HOURY		
MARCH 15 SUN	00:00	MOORE   manual mounting by Stan		
	08:00	powder, WARM ROBOT		
	16:00	powder, WARM ROBOT		

## New Beamtime

### Project

KATHRYN

### Start\*

2021-03-16 00:00:00

### End\*

2021-03-17 16:00:00

### Access\*

Remote

☒ Schedule email notification

### Comments

Revert Save

# User Support

- Record of events to rely on
- Knowledge transfer
- Expose recurring issues quickly



MxLIVE Admin Dashboard Search CMCADMIN

### Support Record

New Record of User Support

Staff\* FODJE Beamline\* CMCF-BM Project\* GROCHULSKI

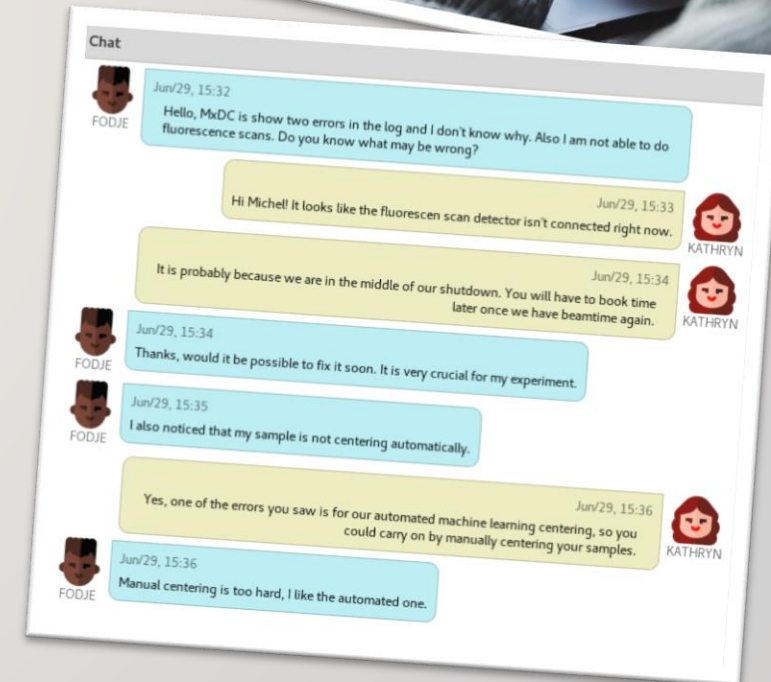
Kind\* Problem Time Lost (hours)\* 1.0

Areas  
x Beamline Performance

Comments  
Question/Concern from User:  
My Response/Action Taken:

Revert Save

Project / Name	Beamline	Status	Time Lost (Hours)
shi	CMCF-BM	LA	148 items
pascal	CMCF-BM	FO	3.0
pascal	CMCF-BM	FO	0.2
pascal	CMCF-BM	FO	0.0
pascal	CMCF-BM	FO	0.0





# User Support Statistics

## User Support Interactions and Problem Recovery

Summary of user support records

	Info	Problem	MTBF <sup>[1]</sup> (h)	MRT <sup>[2]</sup> (h)	Time Lost (h)
<b>SAM Automounter</b>	8	27	54.81	0.77	20.91
<b>[*] Storage Ring Reliability</b>	0	14	95.55	1.3	18.2
<b>MD2 Goniometer</b>	7	13	119.17	0.27	3.45
<b>MxDC</b>	8	5	194.54	0.53	2.66
<b>Beamline Performance</b>	12	10	132.91	0.24	2.4
<b>Data Acquisition Software</b>	1	5	167.04	0.23	1.16
<b>Data Analysis Support</b>	1	1	-	1	1
<b>Computers and IT</b>	4	4	111.82	0.2	0.8
<b>Detector</b>	0	6	196.71	0.13	0.76
<b>[*] Facility Access</b>	0	1	-	0.5	0.5
<b>Sample Handling / Shipping</b>	0	1	-	0.25	0.25
<b>Training / Documentation</b>	6	0	-	-	0.2
<b>MxLIVE</b>	3	1	-	0.15	0.15
<b>AutoProcess</b>	2	2	369.1	-	0
<b>Beamline Readiness</b>	2	1	-	-	0
<b>Data Access / Data Transfer</b>	1	1	-	-	0
<b>User Support / Staff Interactions</b>	1	0	-	-	0
<b>Overall</b>	56	92	17.33	0.57	52.44
<b>Beamline Overall</b>	56	77	21.36	0.44	33.74

Table 1 - Support Records by Area

**[\*] External Area:** External factor out of the beamline's control; excluded from **Beamline Overall** calculations

**[1] MTBF:** Mean Time Between Failures

**[2] MRT:** Mean Recovery Time

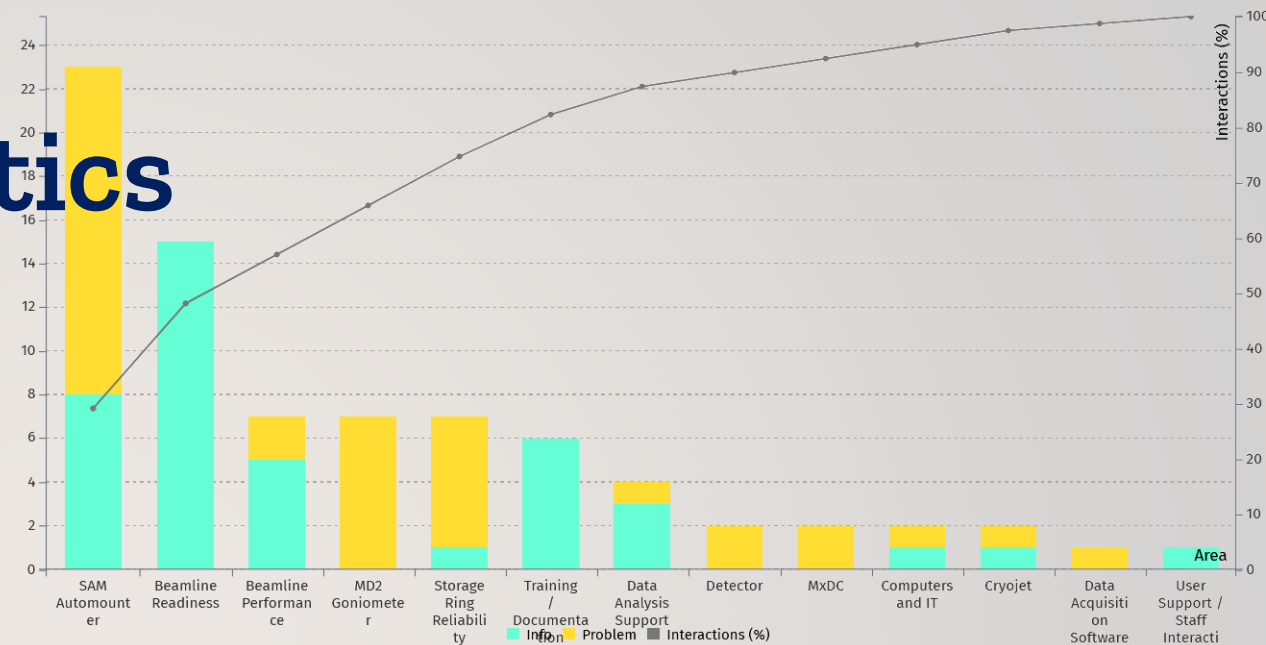


Figure 2 - User Support Areas by Interaction

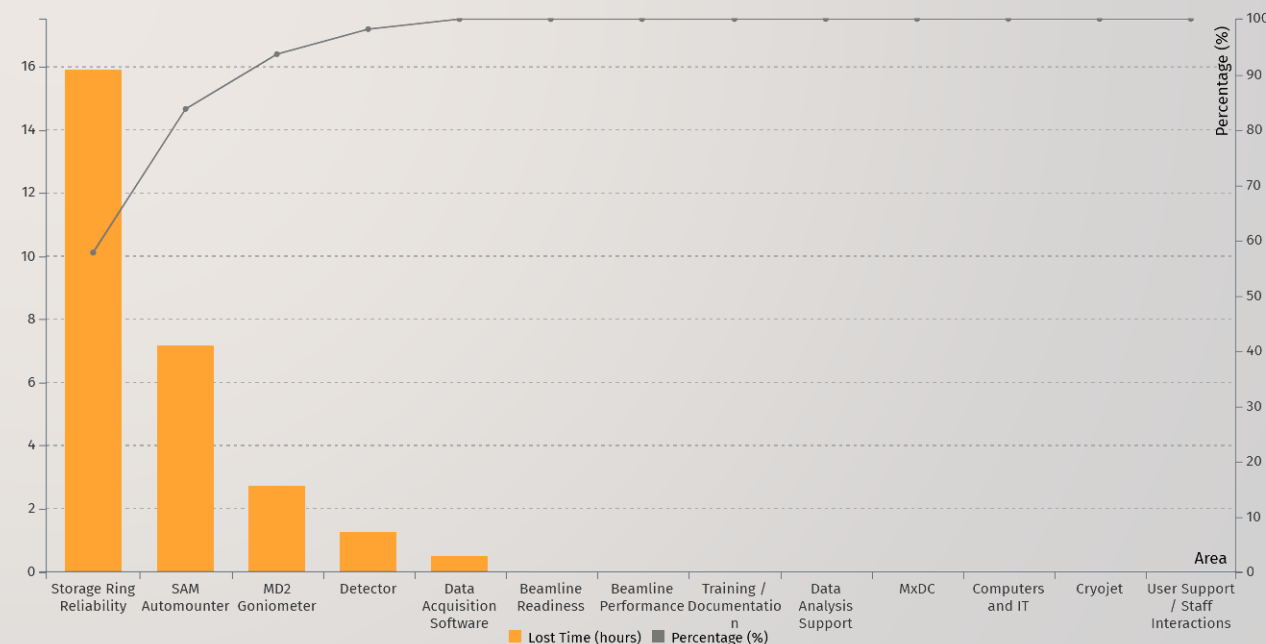
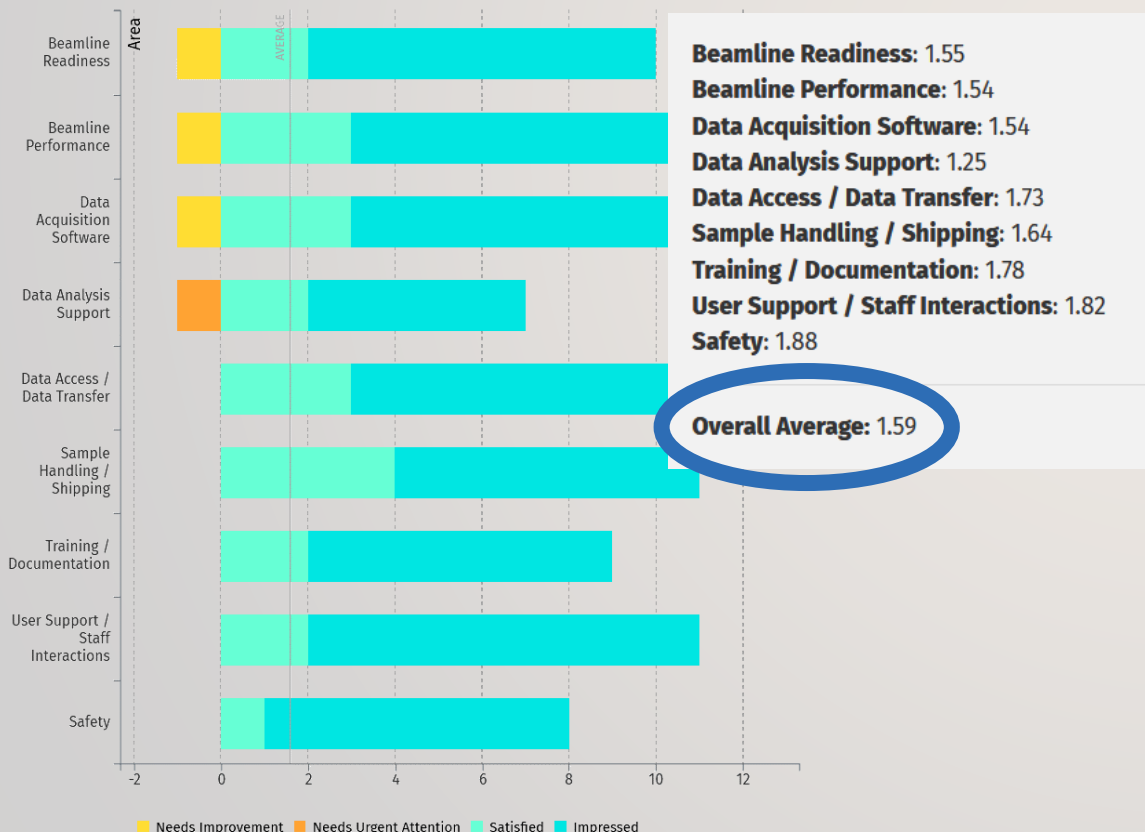


Figure 3 - User Support Areas by Lost Time

# User Experience Feedback

- Link to facilitate integration in data collection software



Setup Samples Data Scans Analysis

CRYO Temperature 102 K Cryo Level 36 % Annealing 5 sec

Sample flow 6.5 lpm Shield Flow 9.5 lpm Nozzle IN

Gonio Omega (deg)

Feedback

### User Experience Survey

Help us improve your next visit or session by letting us know how we did this time.

Please evaluate the following aspects of your recent beamline experience.

	Needs Urgent Attention	Needs Improvement	Satisfied	Impressed	N/A
Beamline Performance*	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>
Data Acquisition Software*	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>
Data Analysis Support*	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>
Data Access / Data Transfer*	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>
Sample Handling / Shipping*	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>
Training / Documentation*	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>
User Support / Staff Interactions*	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>
Safety*	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>
Beamline Readiness*	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	<input checked="" type="radio"/>

Choose the level of impact that best describes the following:

Negligible Small Significant Extreme N/A

What level of impact would your research program face with a loss of access to our facility?\*

What impact could these facilities have on the research of others in your field who might not know about us yet?\*

Status MOUNTING Ring Current 0.0 mA Is Flux 3.502×10<sup>4</sup> Is Flux 2.693×10<sup>4</sup> Beam OFF Beamline Mode Mount Center Align Fast Shutter OFF Status

# Statistics

- Beamline Parameters
- Beamline Usage
- Publication Metrics
- Individual User Statistics
- Session Statistics
- User Support Records
- User Feedback
- ...

## KATHRYN | Project Statistics

Your history in numbers

My Profile

### Data Collection Summary

<b>Visits Scheduled</b>	0	<b>Sessions</b>	88
<b>Shifts Scheduled</b>	0 (0 minutes)	<b>First Session</b>	9 years, 8 months ago
<b>Shifts Used</b>	286 (2 months 4 weeks)	<b>Last Session</b>	6 days, 15 hours ago
<b>Actual Time</b>	34% (4 weeks 4 days)	<b>Shipments / Containers</b>	51 / 108
<b>Shutters Open</b>	4 days 3 hours	<b>Groups / Samples</b>	112 / 1817

Table 1 - Time Usage

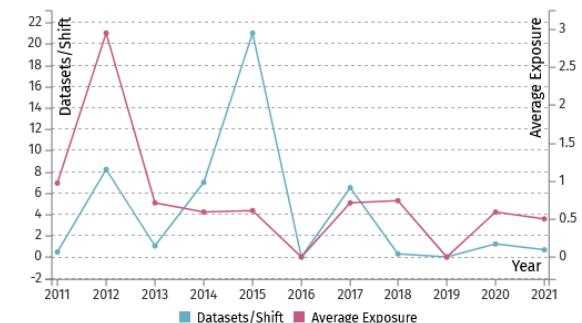
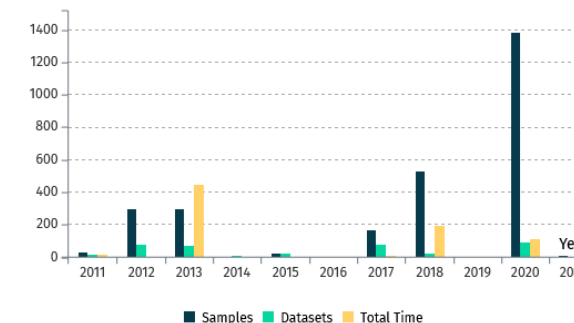
Table 2 - Overall Statistics

Summary of time, datasets and usage statistics

Year	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020	2021
<b>Samples Measured</b>	28	297	293	3	25	1	165	530	0	1379	9
<b>Sessions</b>	1	8	5	0	0	0	8	30	0	30	6
<b>Visits Scheduled</b>	0	0	0	0	0	0	0	0	0	0	0
<b>Shifts Scheduled</b>	0	0	0	0	0	0	0	0	0	0	0
<b>Shifts Used</b>	39	9	68	0	0	0	12	79	0	73	6
<b>Time Used<sup>1</sup> (hr)</b>	12.0	1.2	442.1	0.0	0.0	0.0	8.2	192.6	0.0	113.2	1.8
<b>Usage Efficiency<sup>2</sup> (%)</b>	4%	2%	81%	0%	0%	0%	9%	30%	0%	19%	4%
<b>Datasets<sup>3</sup> Collected</b>	18	74	71	7	21	0	78	23	0	89	4
<b>Minutes/Dataset<sup>3</sup></b>	0.5	1.0	0.7	0.7	0.6	0.0	0.6	0.8	0.0	64.9	0.4
<b>Datasets<sup>3</sup>/Hour</b>	118.1	61.8	89.3	82.9	92.6	0.0	99.7	74.9	0.0	0.9	150.5
<b>Average Exposure (sec)</b>	0.97	2.94	0.71	0.59	0.61	0.00	0.71	0.74	0.00	0.59	0.50
<b>Samples/Dataset<sup>3</sup></b>	1.6	4.0	4.1	0.4	1.2	1.0	2.1	23.0	0.0	15.5	2.2

Table 3 - 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.





# Development

- Open Source
- Simple deployment
- Secure APIs for integration
- Facility/technique agnostic
- Easily extendible



GitHub

[katyjg/mxlive](https://github.com/katyjg/mxlive)

MX Laboratory Information Virtual Environment. Contribute to katyjg/mxlive development by creating an account on GitHub.

**Detailed Documentation:**

<https://katyjg.github.io/mxlive/>



python™

django



PostgreSQL



docker

# Acknowledgments

- Michel Fodje
  - CMCF Beamline Responsible
- The CMCF Team
  - Shaun Labiuk, Scott Colville, Kiran Mundboth, Denis Spasyuk, Joel Reid, James Gorin
- CMCF User Community



[katyjc/mlive](#)

MX Laboratory Information Virtual Environment. Contribute to katyjc/mlive development by creating an account on GitHub.

**Detailed Documentation:**

<https://katyjc.github.io/mlive/>



Canadian  
Light  
Source

Centre canadien  
de rayonnement  
synchrotron

INNOVATION.CA  
CANADA FOUNDATION  
FOR INNOVATION

UNIVERSITY OF  
SASKATCHEWAN



**IRCC - CMRC**

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

Canada