

U[sers] Can't Touch This

Remote Access with SSRL at SLAC

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SSRL-SMB-PX talks at MCE 2021



In case you missed it...

Tuesday March 16th

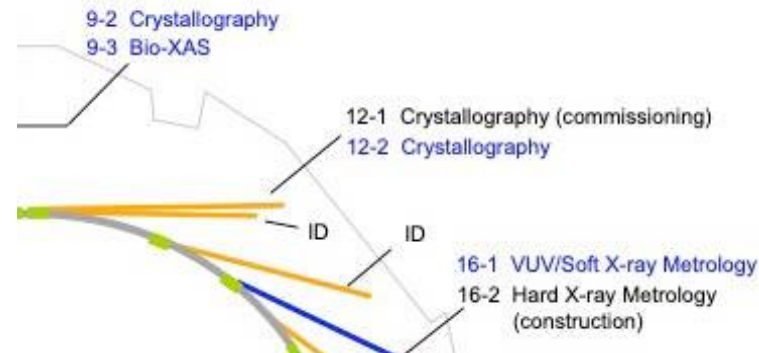
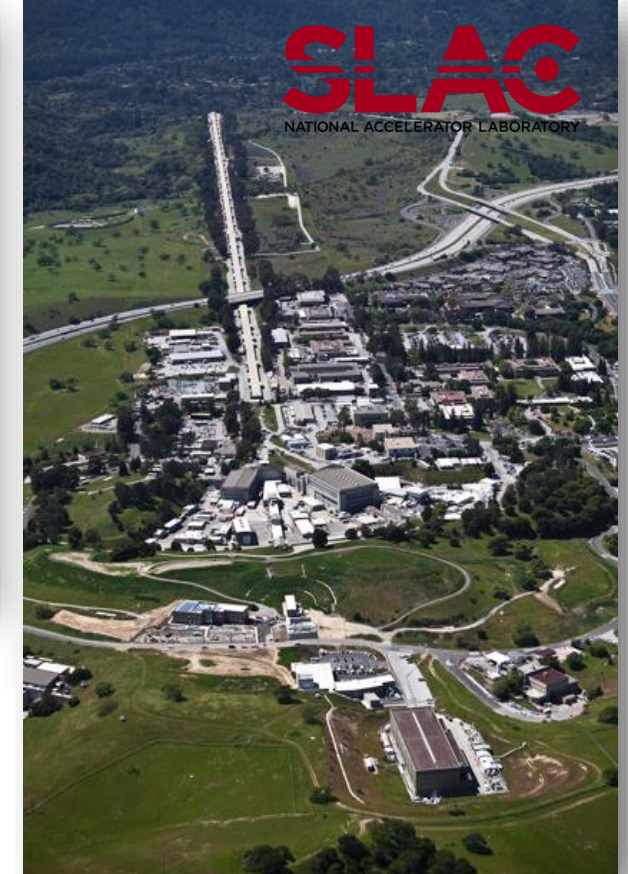
Aina Cohen

Next Generation Remote Experiments

Wednesday March 17th

Art Lyubimov

Crystallography Live: Processing and Analysis
of Xray Diffraction Data in Real Time



Thank you for your attention!



A Rapid Response at SLAC to Combat COVID-19

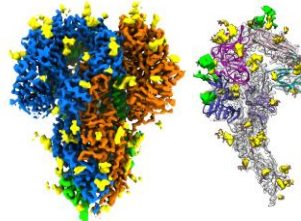
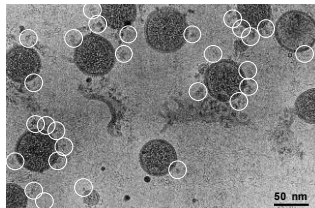
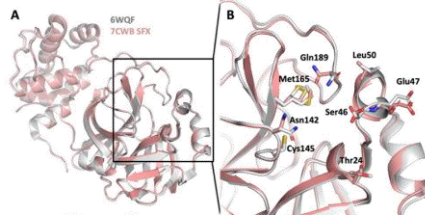
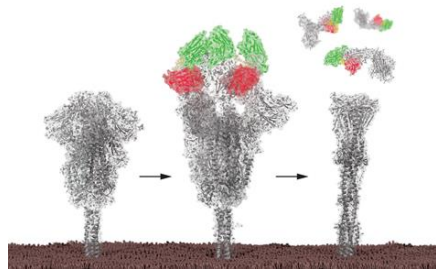


Fast Tracked Research Leads to Drug and Vaccines in Clinical Trials

Synchrotron & CryoEM research started one year ago and LCLS in August 2020

so far

Proposals awarded time: **51**
MC Fragments/inhibitors screened: **> 1088**
MC PDB deposits: **38**
MC Publications: **11**



SSRL BL12-1: Structure-guided inactivation of the SARS-CoV-2 spike protein using nanobodies (Koenig, Science 2021)

LCLS-MFX: SARS-CoV-2 main protease structures at near-physiological temp to guide drug repurposing (Durdagi, bioRxiv/2020)

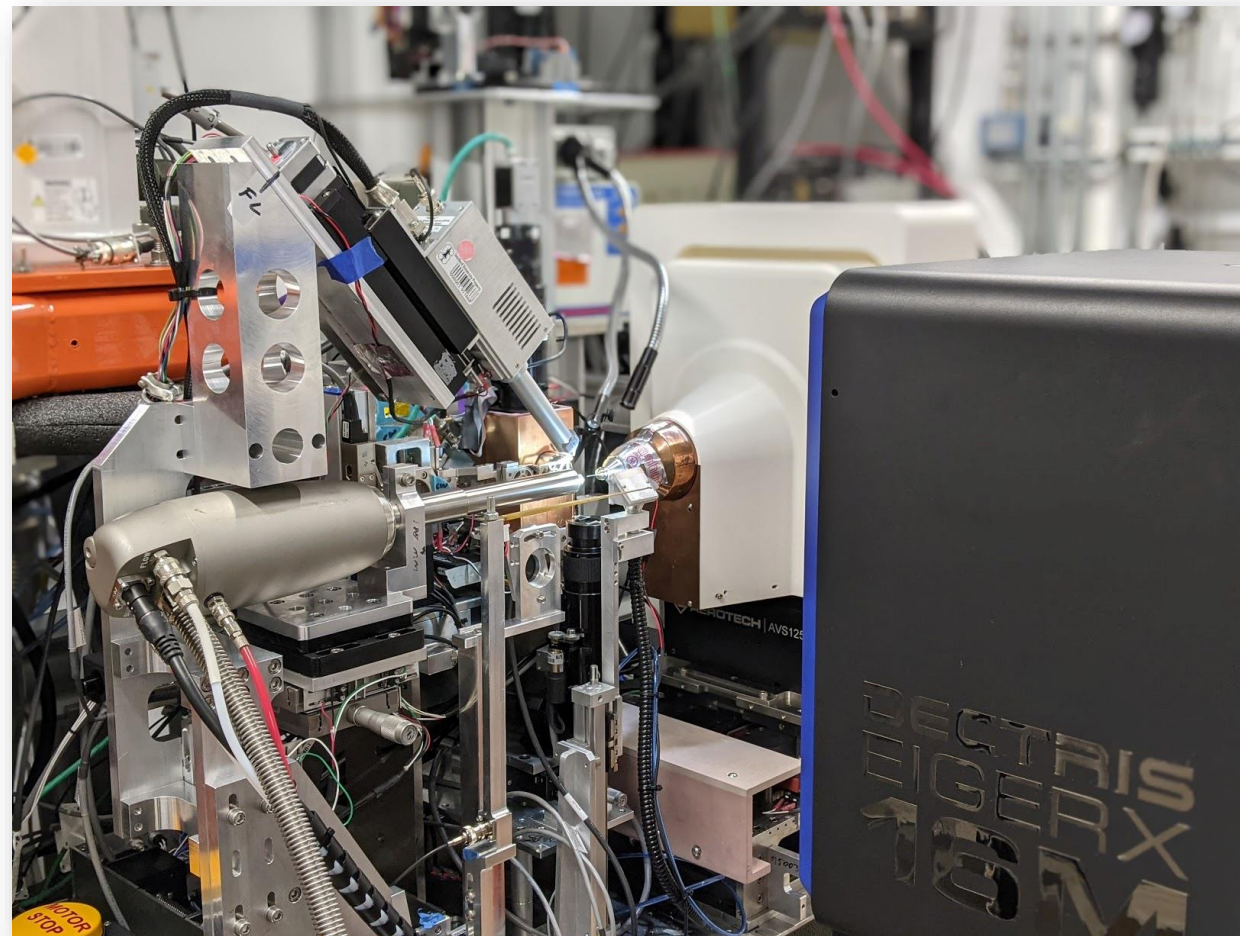
Cryo-EM: Structure of spike proteins and glycans of human coronavirus NL63 directly from virus particles (Zhang, bioRxiv/2020/245696)



Groups from across the US and abroad used SSRL, LCLS and CryoEM facilities at SLAC for COVID-19 related research

Remote Access with SMB at SLAC

- Standard @ SSRL/SMB
 - Stanford Auto-Mounting (SAM) system (Cohen *et al.*, J. Appl. Cryst. 35, 720, 2002)
 - Remote Data Collection from anywhere in the world (Soltis *et al.*, Acta Cryst. D64, 210, 2008)
- Advanced features @ Beamline 12-1
 - Serial and Dynamics
 - Elevated Temperatures
 - Humidity Control
- Look to the future



Standard @ SSRL/SMB – Remote Access



NoMachine NX

- Unix-based
- Access to internal network
 - Beamline control
 - SSRL data storage
 - Data processing

Crystal server

- Sample database
- Spreadsheets

Blu-Ice Control Software

- Experiment control, tcl/tk, C/C++
- Support enables user
- Simple and intuitive graphical interface
- (McPhillips et al., J. Synch. Rad. 9, 401, 2002)

User support

- Zoom, phone, email



Standard @ SSRL/SMB - Shipping



Macromolecular Crystallography
at the Stanford Synchrotron Radiation Lightsource

Home About News Beamlines For Users Become a User R&D Science Training Our Team

Forms

- Users Menu
 - Forms
 - Beam Time
 - Shipping
 - Feedback
 - Access
 - Training
 - Computing
 - Software Development

Shipping Samples to SSRL

General Information

Your Name *

Institution *

Phone *

Access Information

Type of Access ☒ Assigned Beam Time ☐ BeamlineXpress/FCFS ☐ Staff Collaboration

Access Additional Information

Assigned Beamline Leave at SSRL Shipping and Receiving

Proposal Number *

Date of Experimental Start

Are You the Spokesperson on the Proposal? ☒ Yes ☐ No

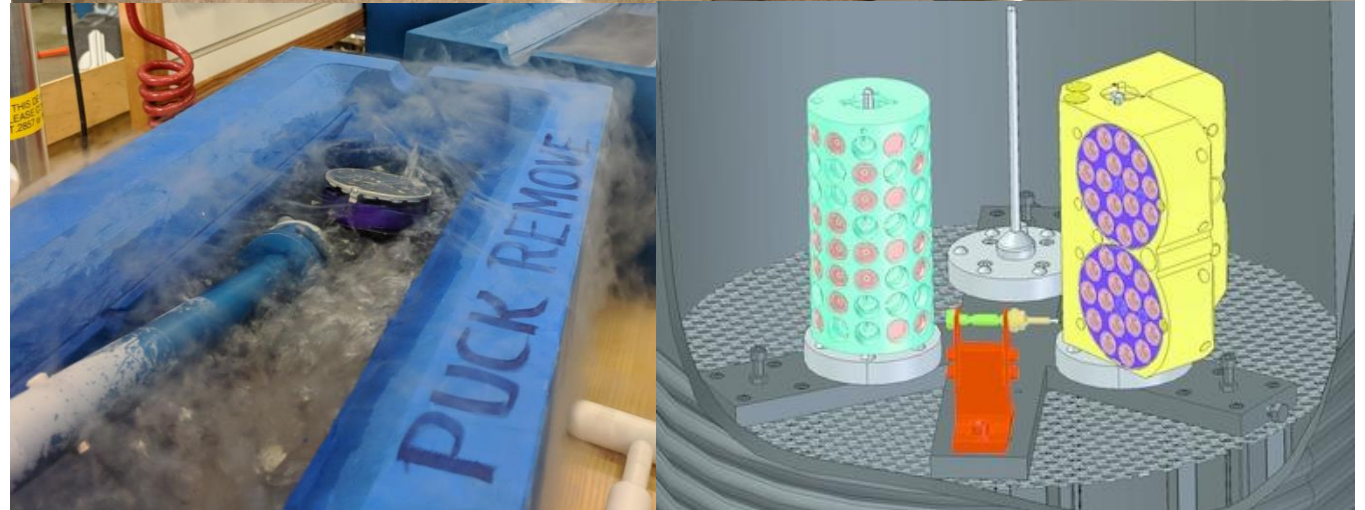
Sample Information

Number of Liquid Nitrogen Dewars 1

Total Number of Cassettes 2

Total Number of Uni-Pucks 0

Number of Blue Shipping Containers for Elevated Temperature 0



Standard @ SSRL/SMB – Sample Database



Spreadsheet based

- Online accessible
 - Editable
 - Upload/download
- Loads into Blu-Ice
 - Through beamline assignment (database or Blu-Ice)

Sample Database

View cassettes of: bluser

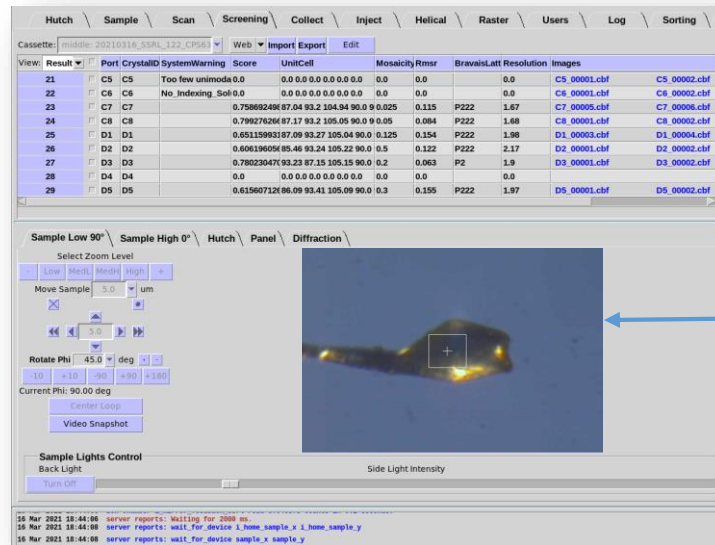
View Cassettes View Beamlines

Search Field: Full List

Cassettes 61 - 75 of 75 (first | prev | next | last)

| SIL ID | Uploaded Spreadsheet | Upload Time | view/edit | Download Results | Commands | Download Original Excel | Delete | Beamline |
|--------|---|-----------------------|---------------------------|----------------------------------|----------|---|------------------------|----------|
| 33229 | BL12_1_Crystal_Testing_cassette_239.xls | 2020-09-09 23:21:59.0 | view/edit | Download Results | | Download Original Excel | Delete | None |
| 33230 | BL12_2_Crystal_Testing_cassette_231.xls | 2020-08-12 15:30:46.0 | view/edit | Download Results | | Download Original Excel | Delete | None |
| 33231 | BL14_1_Crystal_Testing_cassette_082.xls | 2020-09-10 15:13:57.0 | view/edit | Download Results | | Download Original Excel | Delete | None |
| 33475 | cassette_template.xls | 2020-05-04 16:42:40.0 | view/edit | Download Results | | Download Original Excel | Delete | None |
| 33476 | cassette_template.xls | 2020-05-05 20:40:15.0 | view/edit | Download Results | | Download Original Excel | Delete | None |
| 33537 | cassette_template.xls | 2020-06-04 13:30:55.0 | view/edit | Download Results | | Download Original Excel | Delete | None |
| 33563 | BL12_1_Raster_Cas_270_Test.xls | 2020-06-18 15:23:40.0 | view/edit | Download Results | | Download Original Excel | Delete | None |
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| 33697 | cassette_template.xls | 2020-09-21 18:20:43.0 | view/edit | Download Results | | Download Original Excel | Delete | None |
| 33730 | BL7_1_test_cassette_Sept2020.xls | 2020-09-25 14:37:59.0 | view/edit | Download Results | | Download Original Excel | Delete | None |
| 33731 | BL9_2_test_cassette_Sept2020.xls | 2020-12-11 11:44:02.0 | view/edit | Download Results | | Download Original Excel | Delete | None |
| 33732 | BL12_1_test_cassette_Sept2020.xls | 2020-10-16 12:18:43.0 | view/edit | Download Results | | Download Original Excel | Delete | None |
| 33733 | BL12_2_test_cassette_Sept2020.xls | 2021-01-27 20:24:21.0 | view/edit | Download Results | | Download Original Excel | Delete | None |
| 33734 | BL14_1_test_cassette_Sept2020.xls | 2020-11-02 16:28:13.0 | view/edit | Download Results | | Download Original Excel | Delete | None |
| 33780 | BL12_1_test_cassette_October_2020.xls | 2020-12-10 11:04:23.0 | view/edit | Download Results | | Download Original Excel | Delete | None |

Click here to view User's Guide.



Display Type: Display Results Image Display Type: Hide Images Edit Crystal Edit Run Definition

| Row | Port | CrystalID | Protein | GridSampleLocation | Images | Comment | Score | UnitCell | Mosaicity | Rmsr | BravaisLattice | Resolution | SystemWarning | Move |
|-----|------|-----------|----------------|--------------------|--------------------------------|---------------------------------------|-------|---|-----------|-------|----------------|------------|---------------|------|
| 0 | A1 | A1 | Thaumatococcus | | A1_00001.mccd A1_00002.mccd | Please place barcode pin in this port | 0.911 | 57.85 57.85 150.09 90.0 90.0 90.0 | 0.025 | 0.025 | P4,P422 | 1.470 | | |
| 1 | A2 | A2 | Thaumatococcus | | A2_00001.mccd A2_00002.mccd | | 0.878 | 57.74 57.74 150.04 90.0 90.0 90.0 | 0.150 | 0.039 | P4,P422 | 1.320 | | |
| 2 | A3 | A3 | Thaumatococcus | | A3_00001.mccd A3_00002.mccd | | 0.925 | 57.72 57.72 150.11 90.0 90.0 90.0 | 0.025 | 0.022 | P4,P422 | 1.360 | | |
| 3 | A4 | A4 | Thaumatococcus | | A4_00001.mccd A4_00002.mccd | | 0.261 | 57.84 57.64 149.64 90.0 90.0 90.0 | 1.500 | 0.041 | P4,P422 | 1.820 | | |
| 4 | A5 | A5 | Thaumatococcus | | A5_00001.mccd A5_00002.mccd | | 0.880 | 58.66 58.66 149.71 90.0 90.0 90.0 | 0.075 | 0.032 | P4,P422 | 1.600 | | |
| 5 | A6 | A6 | Thaumatococcus | | | | 0.841 | 57.62 | 0.125 | 0.039 | P4,P422 | 1.800 | | |

4/8/2021

MCE 2021Workshop @ NSLSII

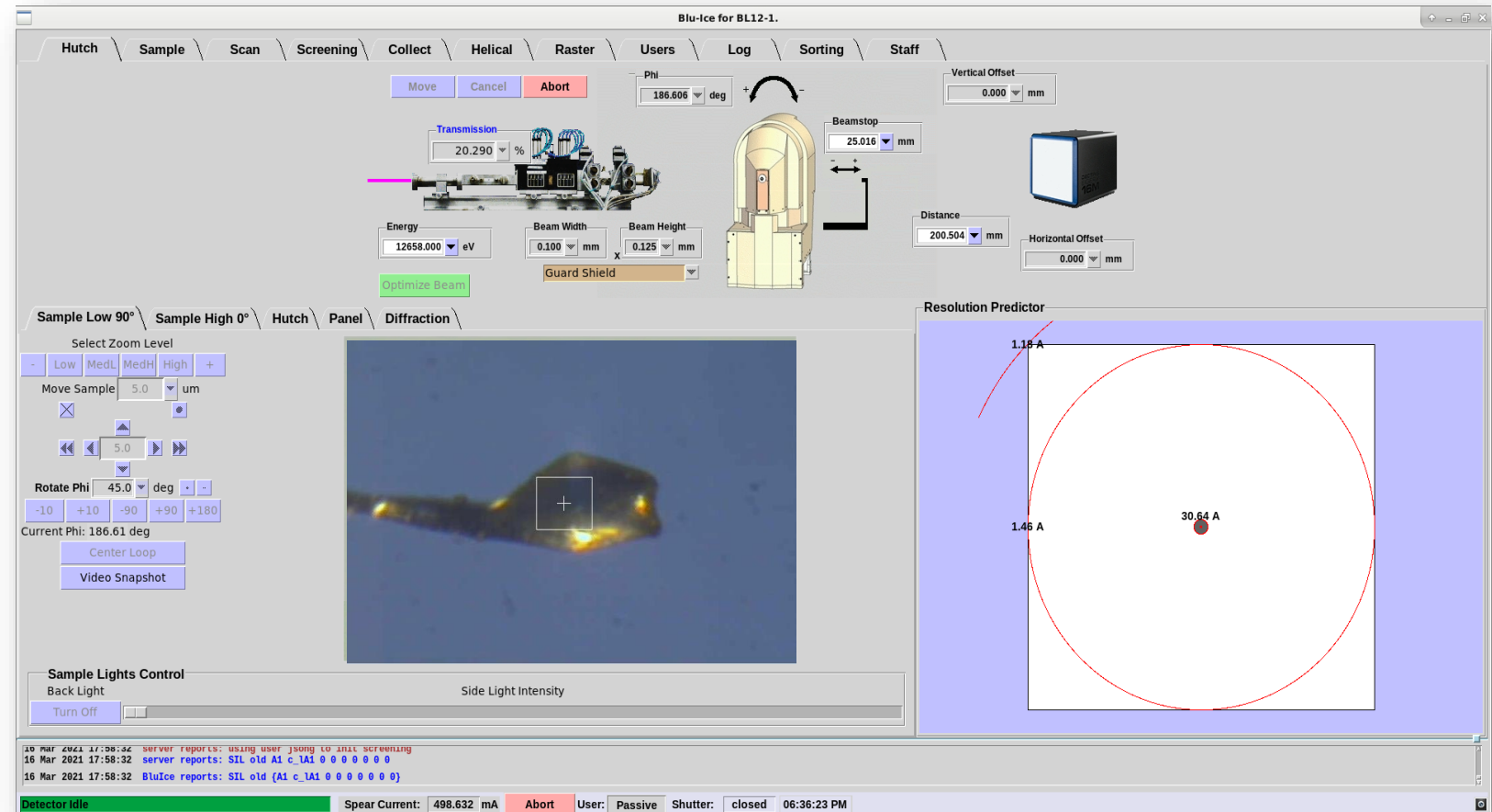
Beamline control

Sample control

- Anneal, wash
- Queue next sample

Scans

- Excitation scans
- MAD scans
 - Runs AutoCHOOCH
 - Displays energies for f' , f'' , plus a calculated remote energy



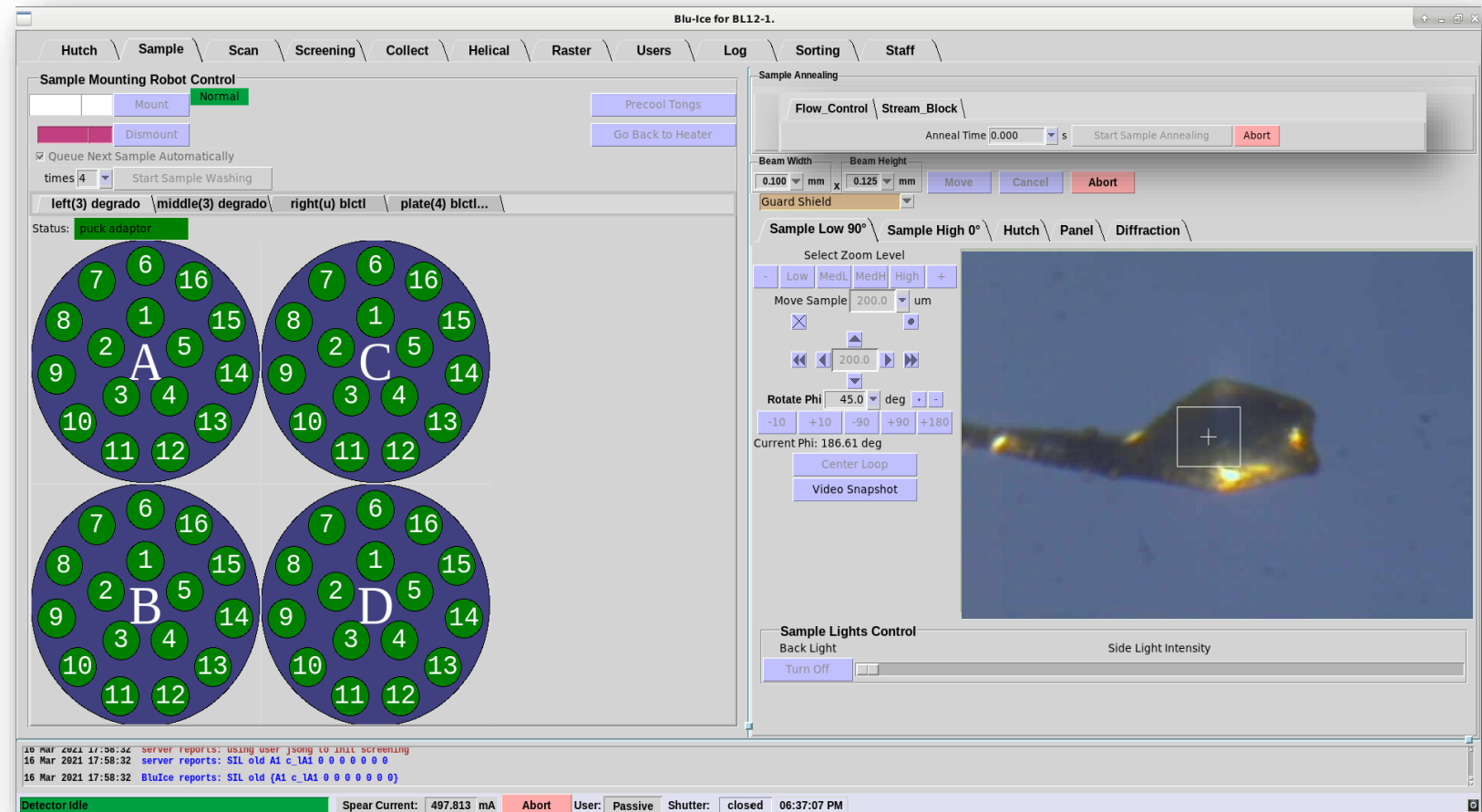
Beamline control

Sample control

- Anneal, wash
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Scans

- Excitation scans
- MAD scans
 - Runs AutoCHOOCH
 - Displays energies for f' , f'' , plus a calculated remote energy



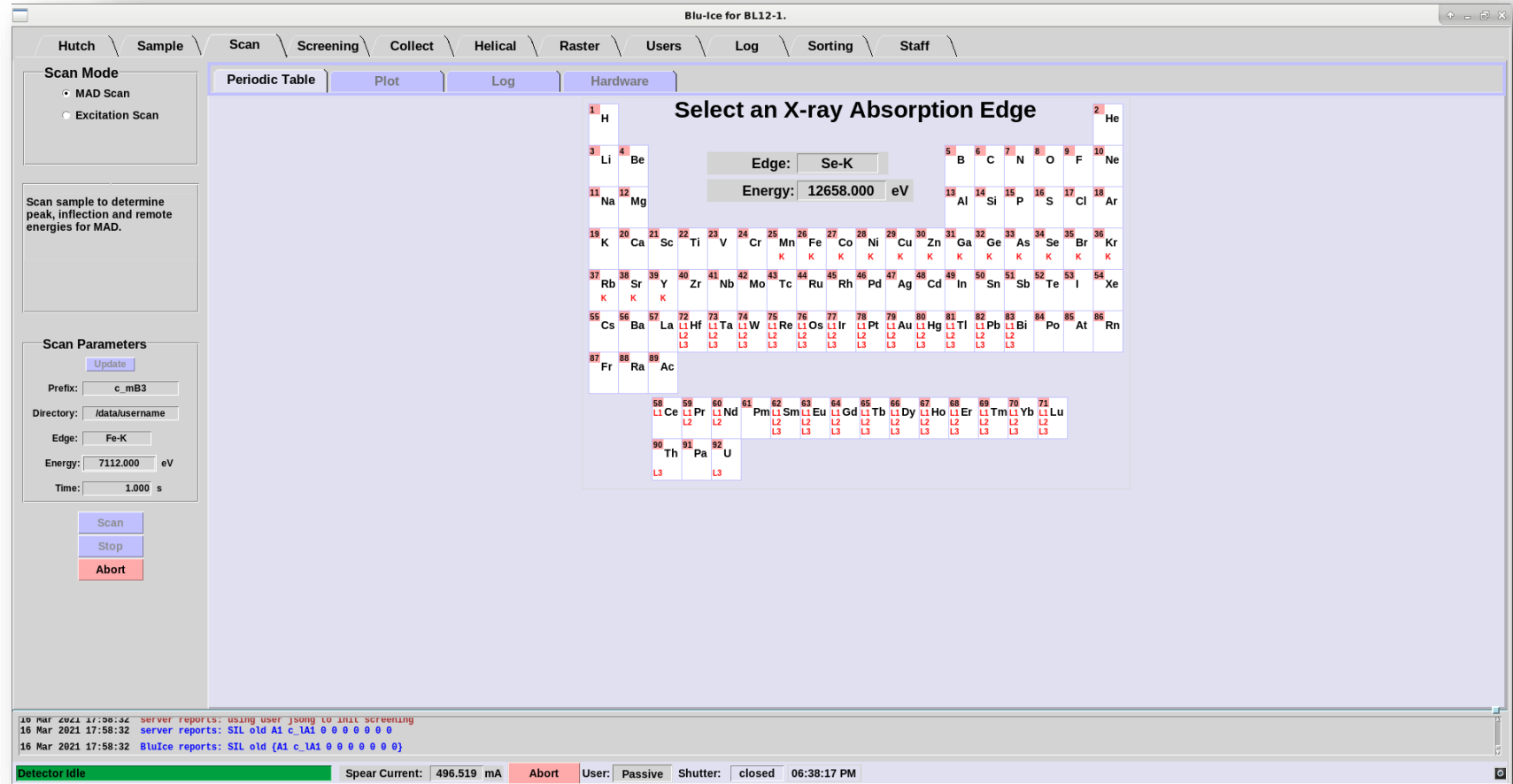
Beamline control

Sample control

- Anneal, wash
- Queue next sample

Scans

- Excitation scans
- MAD scans
 - Runs AutoCHOOCH
 - Displays energies for f' , f'' , plus a calculated remote energy



Blu-Ice for BL12-1.

Hutch | Sample | Scan | Screening | Collect | Helical | Raster | Users | Log | Sorting | Staff

Periodic Table | Plot | Log | Hardware

Select an X-ray Absorption Edge

Edge: Se-K

Energy: 12658.000 eV

Scan Mode

- MAD Scan
- Excitation Scan

Scan sample to determine peak, inflection and remote energies for MAD.

Scan Parameters

Update

Prefix: c_mB3

Directory: /data/username

Edge: Fe-K

Energy: 7112.000 eV

Time: 1.000 s

Scan

Stop

Abort

10 Mar 2021 17:58:54 server reports: USING USER JUSONG TO INIT SCREENING

10 Mar 2021 17:58:32 server reports: SIL old A1 c_lA1 0 0 0 0 0 0

10 Mar 2021 17:58:32 BluIce reports: SIL old (A1 c_lA1 0 0 0 0 0 0)

Detector Idle

Spear Current: 496.519 mA

Abort

User: Passive

Shutter: closed

06:38:17 PM

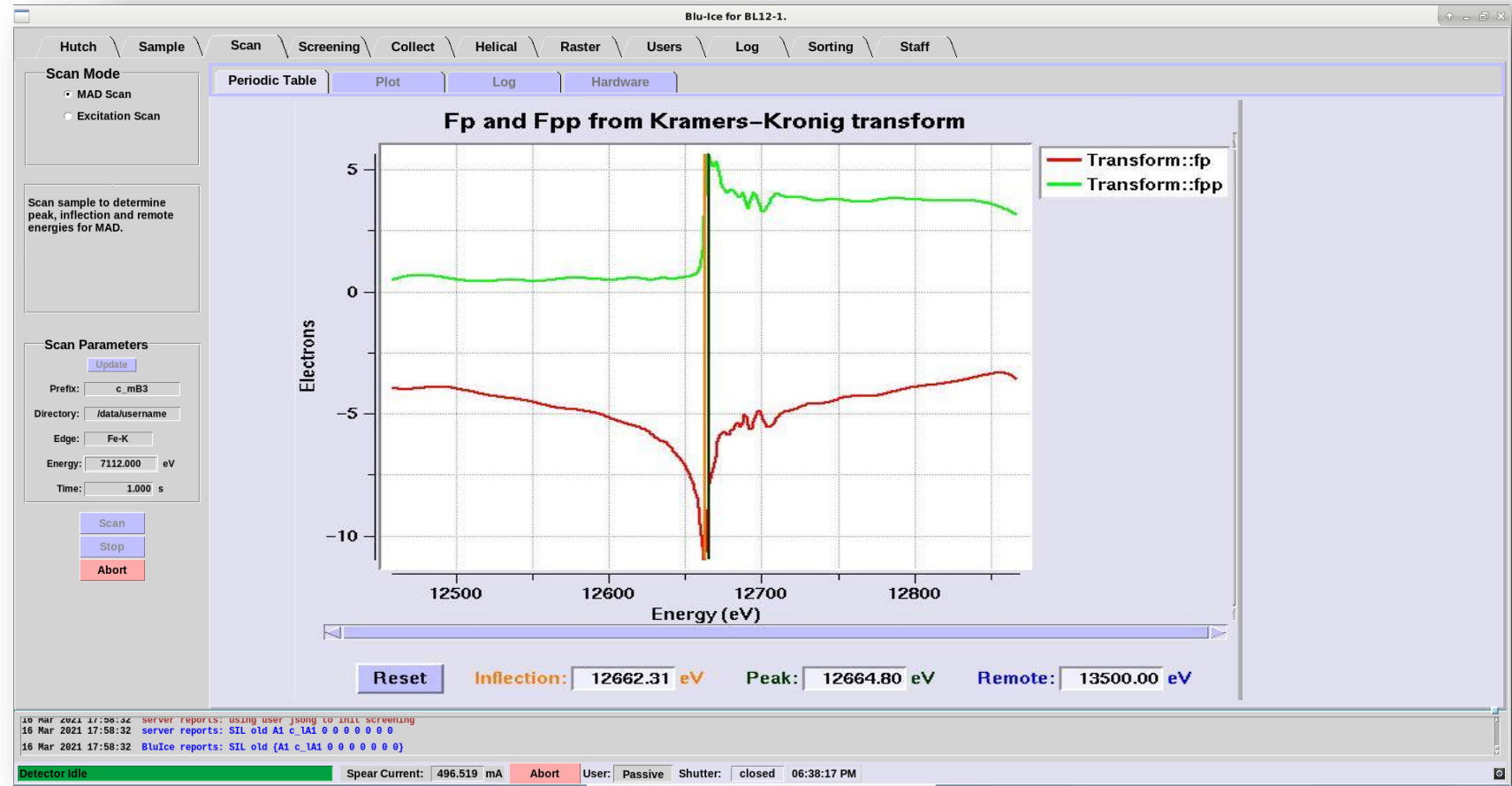
Beamline control

Sample control

- Anneal, wash
- Queue next sample

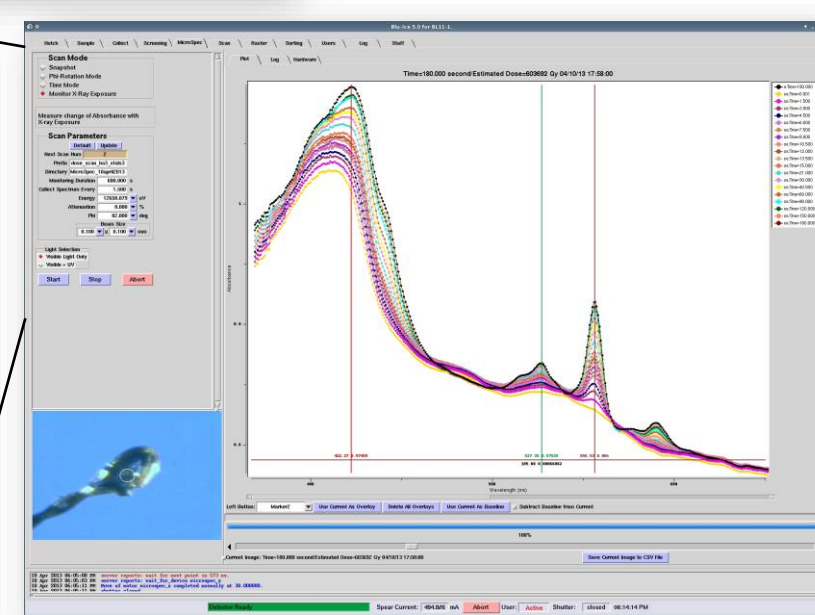
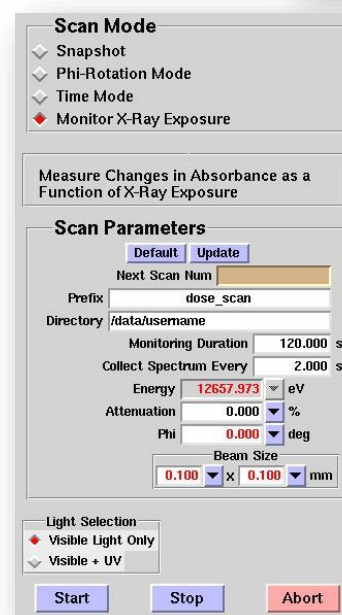
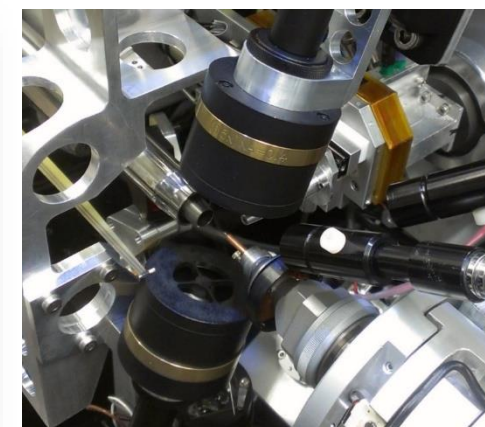
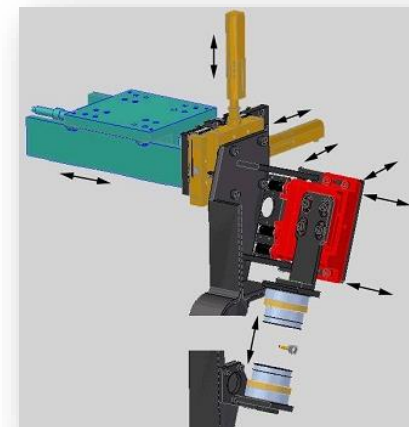
Scans

- Excitation scans
- MAD scans
 - Runs AutoCHOOCH
 - Displays energies for f' , f'' , plus a calculated remote energy



UV-Vis Microspectroscopy @ BL9-2

- Non-invasive
- Confirm identity of reaction intermediates trapped within a crystal
- Monitor reactions occurring in the crystal
 - triggering by lasers or within flow cells
- Monitor X-ray induced structural changes
 - e.g. metalloproteins
 - Radiation damage
- Fully automated for spectroscopy between diffraction data (interweave)
- Both the X-ray exposure time and X-ray dose are recorded for each spectrum measured
- in-situ UV-vis microspectrophotometer
 - (Cohen et al., Protein Pept. Lett. 23, 283 2016)



Standard @ SSRL/SMB – Experimental Setup



Screening

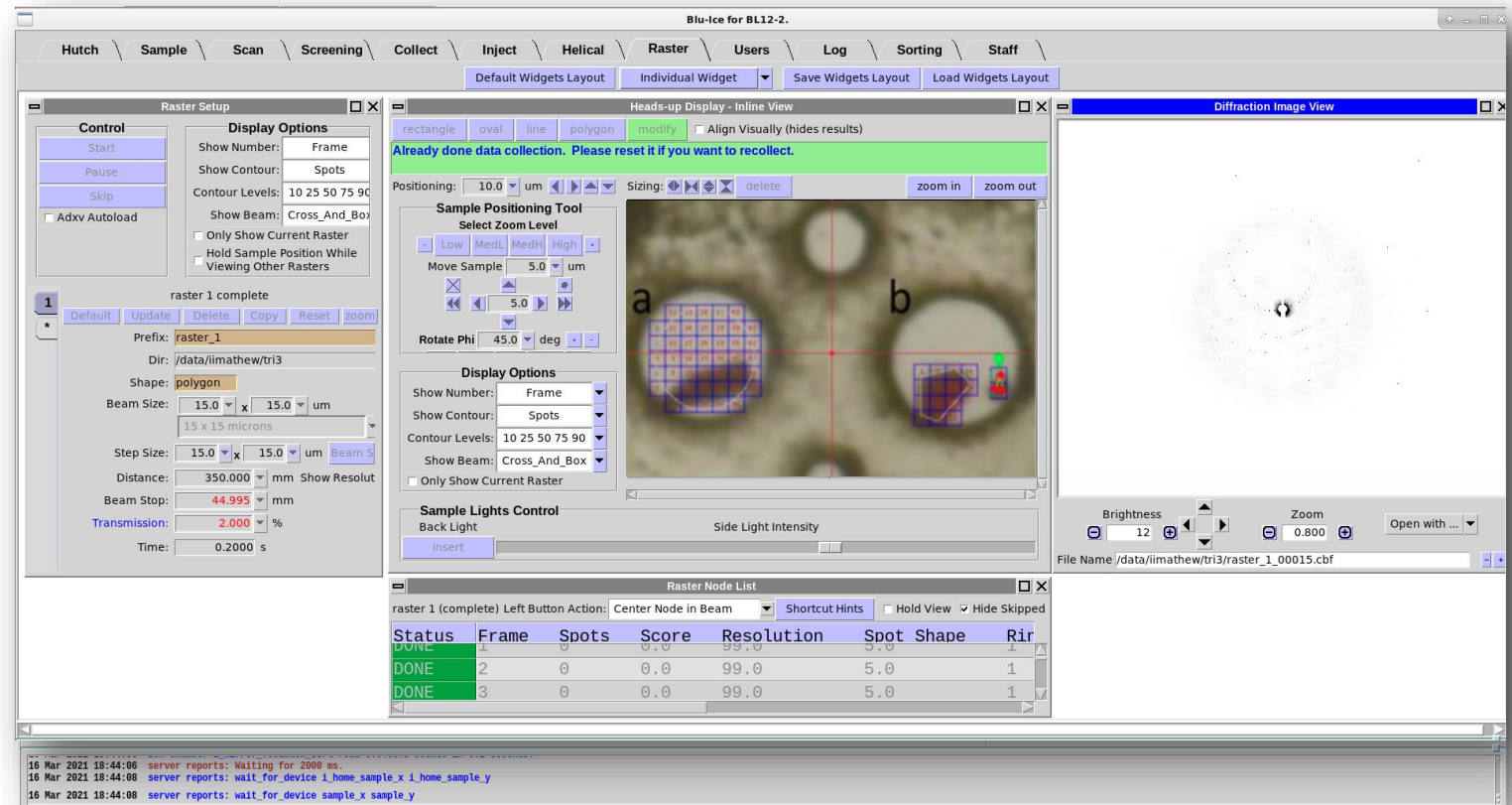
- Automatic
 - Exchange samples in 25 seconds
- Loop centering (15 seconds)
- Raster alignment
- Weblce strategy
 - Requires 2 images

Rastering

- Microbeam, matching crystal size
- Polygon, oval, line
- 90° line raster for centering
- Scoring
- Diffraction-based crystal alignment (Song et al., J. Synch. Rad. 14, 191, 2007)



Art Lyubimov
(talked yesterday)



Diffraction images scored automatically

Results are displayed in Blu-Ice and Weblce and saved in spreadsheet

Standard @ SSRL/SMB – Weblce and Strategy



Weblce

- Mosaicity
- Oscillation
- Resolution
- Exposure time
- Number of images
- Detector, beamstop distances
- Energy(s)
- Attenuation
- Inverse beam
- Absorbed dose

> Import collection strategy into Blu-Ice

Coming Soon

- Integrate into Blu-Ice

Cassette: right: Cassette_00263_BL11-1_121

Web Import Export Edit

Directory Spreadsheet CrystalCond Metal

D3 Weblce

| bluser Runs New Run Selected Run | | | | | | | | | |
|---|-------------------|--|-------|--------|--------------|------------|----------------------|----------------|----------|
| Sort By: Run Name Ascending Descending Update Run 1 - 7 of 7 first prev next last | | | | | | | | | |
| Run Name | Creation Time | Images | Score | #Spots | #Bragg Spots | #Ice Rings | Predicted Resolution | Bravais Choice | Commands |
| A2-BL7-1-Feb2007 | 07/02/07 14:36:54 | autoindex_myo-A2_001.img, autoindex_myo-A2_002.img | 0.76 | 628 | 585 | 0 | 1.66 | P3 | [Delete] |
| A2-BL1-5-Nov06 | 06/12/01 10:51:29 | A2_005.img, A2_006.img | 0.92 | 1673 | 1392 | 1 | 0.61 | P3 | [Delete] |
| B2-BL7-1-Feb2007 | 07/02/07 23:00:20 | autoindex_myo-B2_003.img, autoindex_myo-B2_004.img | 0.87 | 1883 | 1701 | 0 | 1.25 | P3 | [Delete] |
| B2-Feb2007 | 07/02/07 20:41:45 | autoindex_myo-B3_001.img, autoindex_myo-B3_002.img | 0.83 | 1683 | 1489 | 1 | 0.81 | P3 | [Delete] |
| B3-BL7-1-Feb2007 | 07/02/08 18:26:55 | autoindex_myo-B3_001.img, autoindex_myo-B3_002.img | 0.86 | 1799 | 1655 | 0 | 1.31 | P3 | [Delete] |
| test | 07/02/08 12:37:02 | autoindex_test_001.img, autoindex_test_002.img | 0.81 | 1625 | 1490 | 0 | 0.93 | P3 | [Delete] |

Choose Dir and Images >> Choose Strategy Options >> Choose Experiment >> Choose Other Options >> Finish

Choose Directory and Images

Prev Next

Please choose image directory and images.

Directory: /data/bluser/BL9-2/Nov-2006/A2

Image1 A2_8_001.mccd

Image2 A2_8_012.mccd

Hutch | Sample | Scan | Screening | Collect | Helical | Raster

Diffraction | Strategy | Dev

▼ Setup

Directory: /data/blstaff/BL12-1/Commissioning/2020-5-14

Image 1: C1_300_2_00001.cbf

Image 2: C1_300_2_00100.cbf

Laue Group: Unknown

Crystal size: x: mm y: mm z: mm

Native SAD MAD

Run Strategy Cancel

▼ Strategy Results

Solutions: Solution 9 Spacegroup P4 Create Run

Unique Phi 171.00° - 528.00°, 100.0% completeness, 1.76e+05 Gy

Anomalous Phi 72.00° - 438.00°, 100.0% completeness, 1.76e+05 Gy

Experiment Type: Native

Score: 0.64 (score = 1.0 - 0.7e-4/d - 1.5rmsd - 0.2mosaicity)

Mosaicity: 0.00 (predicts 80% of spots in images)

Completeness: 100.0%

Redundancy: 13.0%

Delta: 0.10°

Wedge: 180.00°

Resolution: 2.07Å The predicted resolution from the diffraction images is 1.56 Å

Time: 1.00 seconds

Attenuation: 98.32 %

Distance: 282.59 mm To measure higher resolution data, move the detector to 190.8 mm and recollect test images.

Beamstop: 32.7 mm

Energy: 12658.00 eV

FGSP | Setup | Logs | Autoindex Summary | Solution | Predictions | Strategy | Details | Update

Run Status

Waiting for collect status from DCSS

System Status: collectWeb - Detector Ready

Abort

Collect Options | Scan Options | Autoindex & Strategy Options | Edit Setup

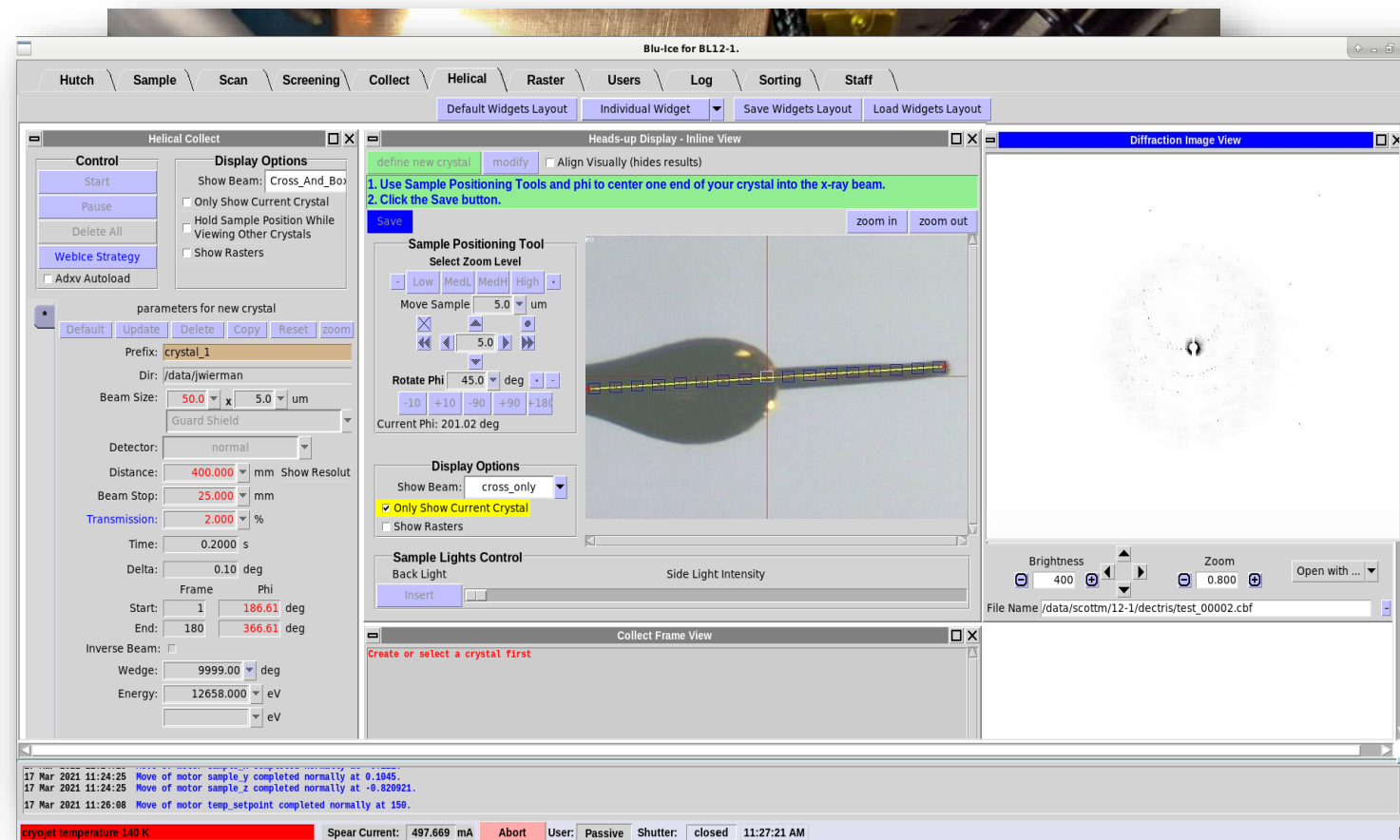
| | |
|-------------------|--------------------------------|
| Image Directory | /data/bluser/BL9-2/Nov-2006/A2 |
| Image1 | To be collected |
| Image2 | To be collected |
| Generate Strategy | Yes |
| For Beamline | SIM1-5 |
| Experiment Type | MAD |
| LaueGroup | Unknown |
| Unit Cell | Unknown |

Standard data collection

- Rotation, wedge
- Helical

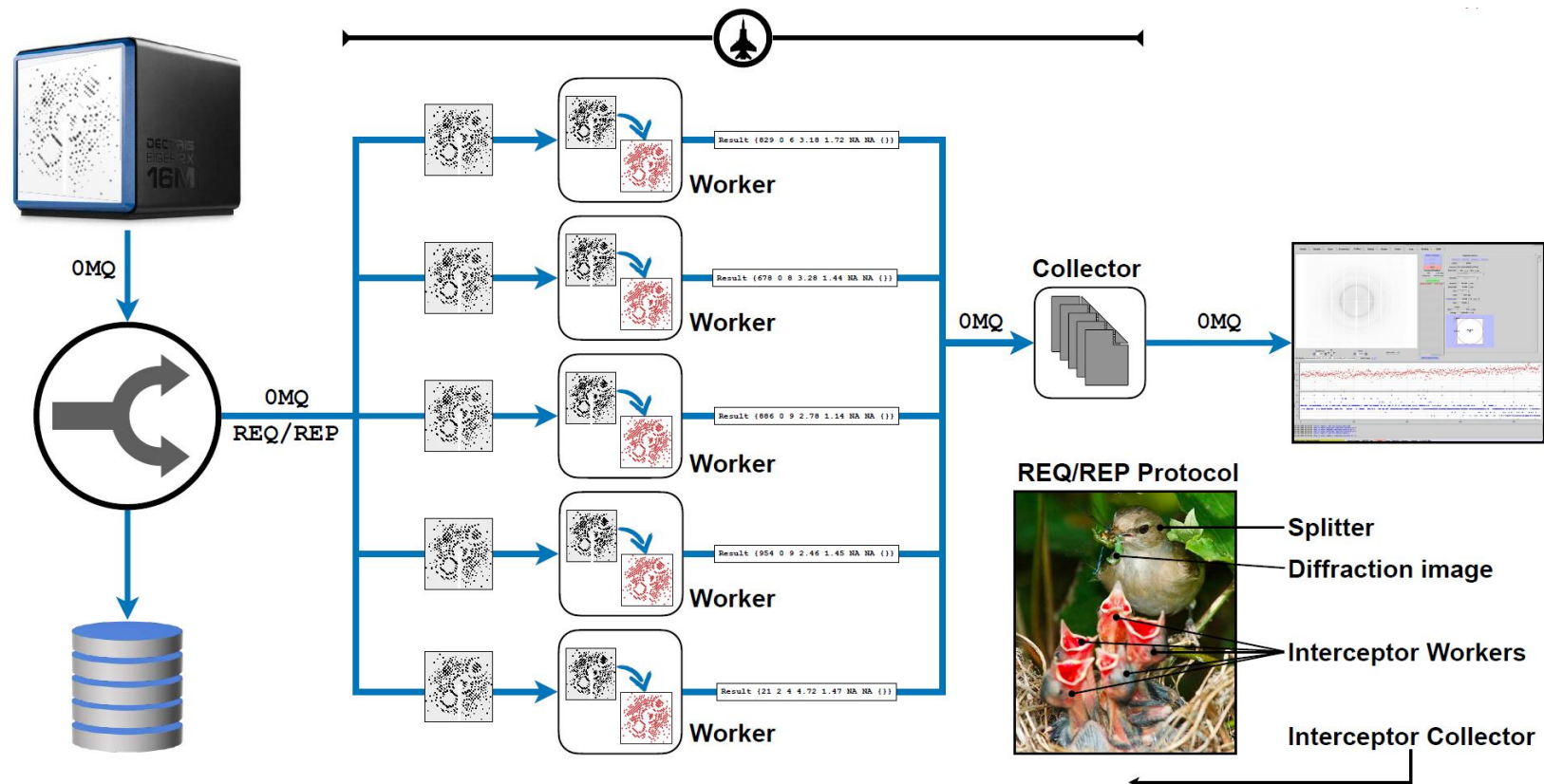
Beamline 12-1

- Microbeam: 5 μm^2 to 100 μm^2
- High Intensity: 5 x10¹² photons/sec
- 5-15 keV range, S-SAD phasing optimized
- EIGER 16M (133 Hz or 750 ROI)
- Crystal rotation speeds <90°/s
- Instant feedback
- Automated hit finding + data processing
 - Any dataset more than 5 frames is fully autoprocessed in users' directory
 - XDS, POINTLESS, XTRIAGE, AIMLESS, TRUNCATE
 - MOLREP, REFMAC5

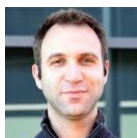


The Interceptor

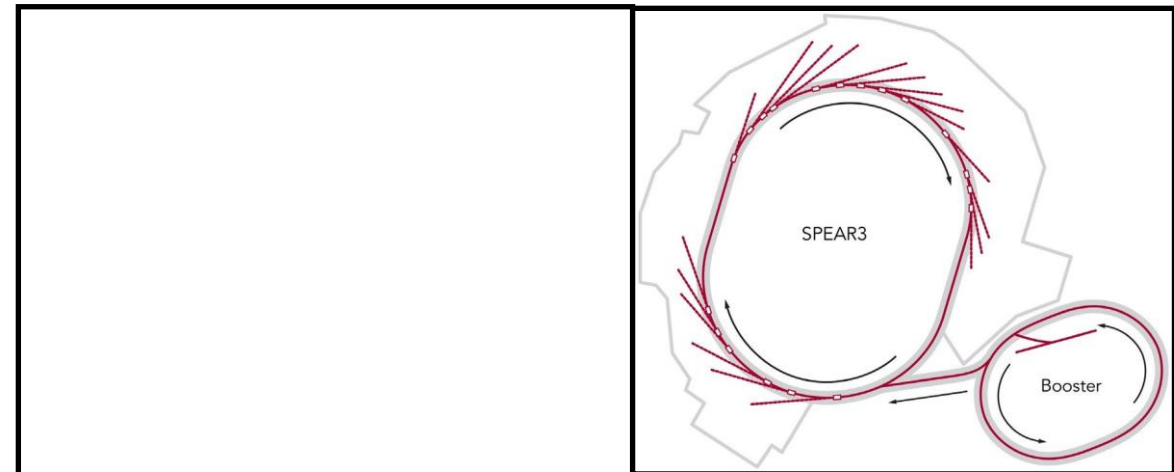
- Live processing and scoring to track basic diffraction properties of a single crystals in real time
 - Resolution score
 - +max diffraction intensity score
 - Ice ring penalty
 - Elongated spot penalty
- Fully automated, persists in background
- Can handle high-speed bursts (~300 images) up to 100Hz



Art Lyubimov
(talked yesterday)



Serial Crystallography at SLAC



Serial Crystallography

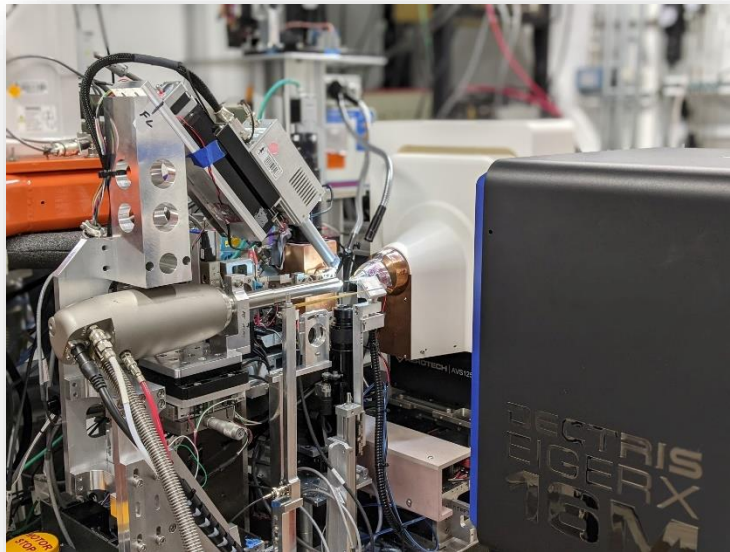


Five Beamlines at SSRL dedicated to Macromolecular Crystallography Research

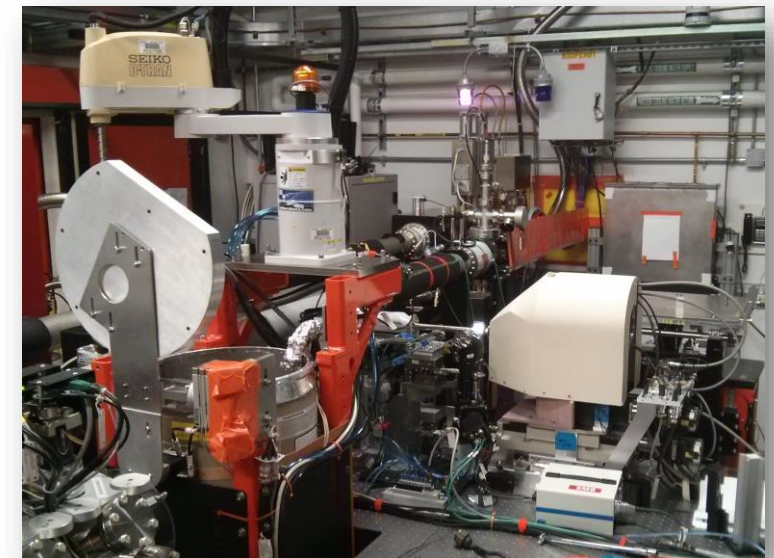
X-ray Free Electron Laser – LCLS-MFX Instrument



Aina Cohen
(talked Tuesday)



New Rapid Access Proposal Mechanism
BL12-1 / Gateway to LCLS



Standard setups for goniometer and injector

Collaboration between SSRL-SMB & LCLS-HXR staff

Blu-Ice Control Software (developed at SSRL)

- User friendly - familiar to the user community
- Highly automated

High Speed Microcrystal Goniometer

- Rapid sample motions with $\pm 0.5 \mu\text{m}$ SOC

Automated Sample Exchange with Stanford Robot

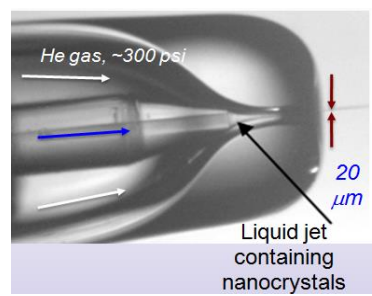
- Highly reliable (>1M samples mounted at SSRL)
- Cryogenic studies enable safe transport & storage
- Support room temperature samples at controlled humidity

UV-fluorescence microscopy and visual mapping of crystal samples (Barnes et al., PNAS. 116(19), 9333-9339, 2019)



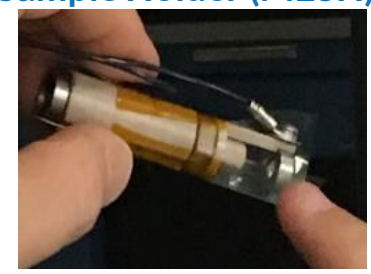
Advanced Features – Serial Crystallography

Gas Dynamic Virtual Nozzle



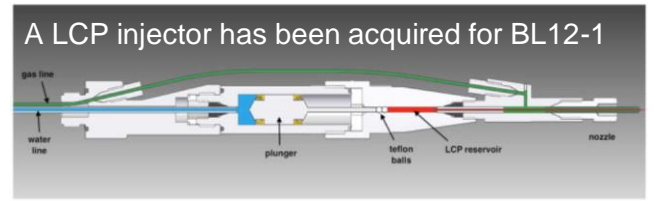
Rev. Sci. Instr. **83**, 35108, 2012

Mobile Electro-spinning Sample Holder (MESH)



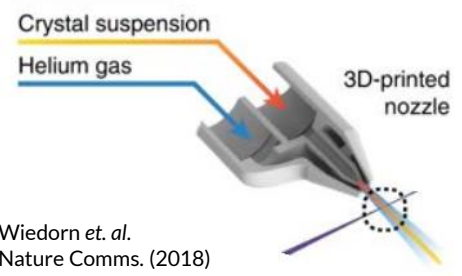
Sierra, *Acta Cryst D* (2012)

LCP/Viscous Media Injector



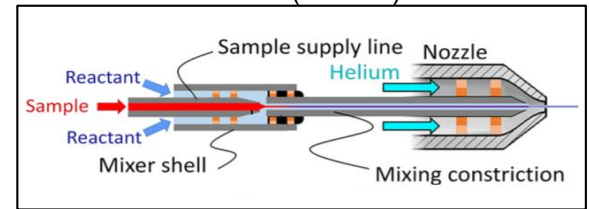
Weierstall, Uwe et al. *Nature communications* 5 (2014)

Mixing Injectors

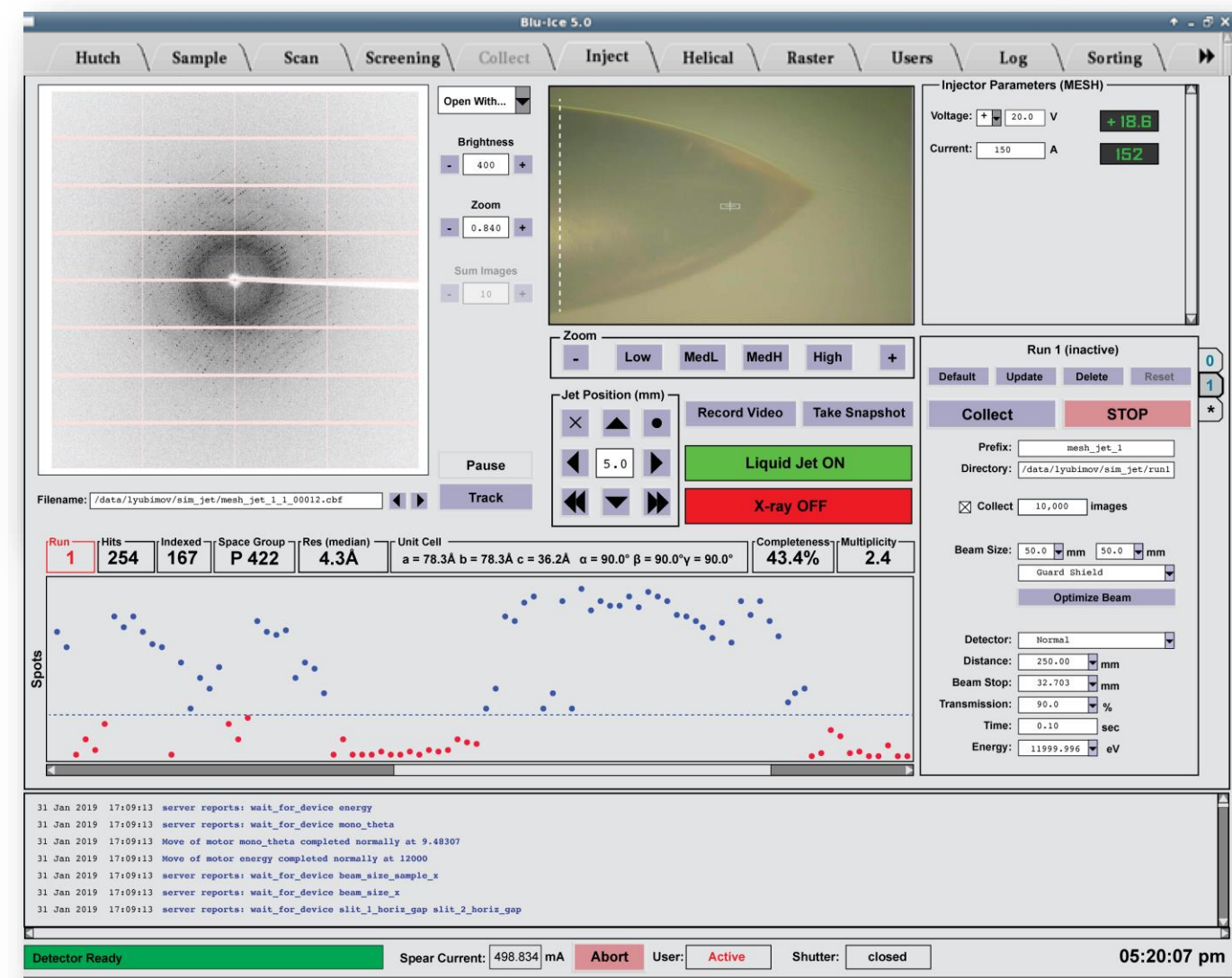


Wiedorn et. al.
Nature Comms. (2018)

Lois Pollack (Cornell) collaboration



Calvey, Katz, Pollack. *Analytical Chemistry* 91-11, (2019)



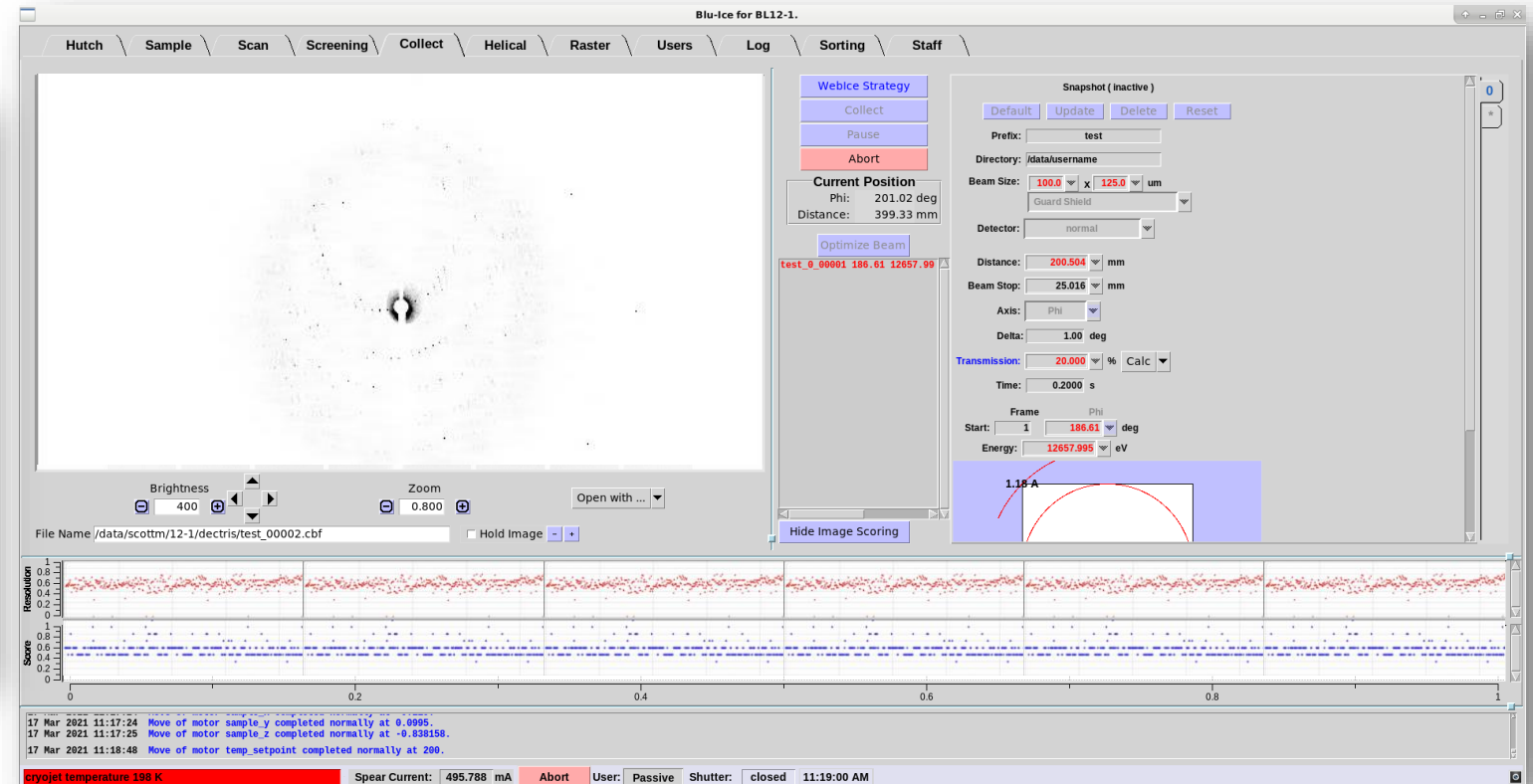
Advanced Features – Serial Crystallography



Thin polymer crystallization chip



Megan Shelby, Deepshika Shamraj Gilbile,
Matthew Coleman, Matthias Frank, Tonya Kuhl
LLNL, UC Davis



Advanced Features – Serial Crystallography



Fixed target

Full automation is possible if it fits within the robot gripper



If it has known dimensions and fiducials, we can automate it!

<http://www.mitegen.com/>

Cohen, et al., *PNAS* (2014)

Gati et al. *IUCrJ* (2014)

Feld, et al., *J Appl Cryst* (2015)

Roedig, et al., *Sci Rep* (2015)

Lyubimov, et al., *Acta Cryst D* (2015)

Murray, et al., *Acta Cryst D* (2015)

Gati et al., *IUCrJ* (2014)

Heymann et al. *IUCrJ* (2014)

Murray et al. *Acta Cryst D* (2015)

Baxter et al. *Acta Cryst D* (2015)

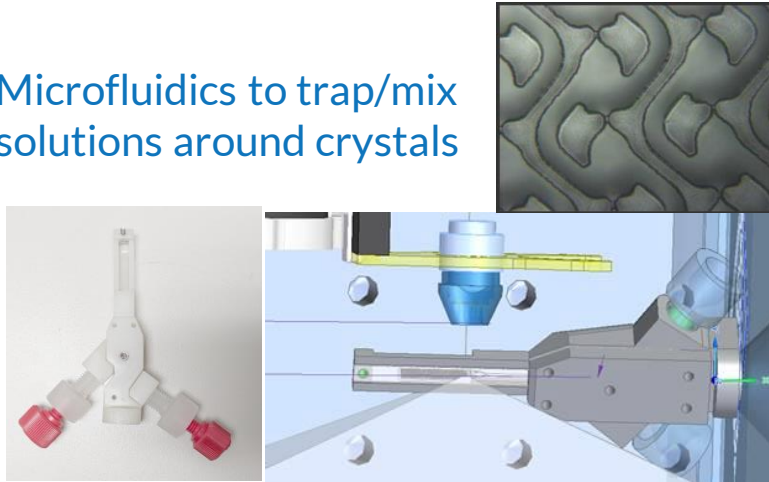
Sui et al. *Lab Chip*, 16 (2016)

Advanced Features - Studies of Protein Dynamics



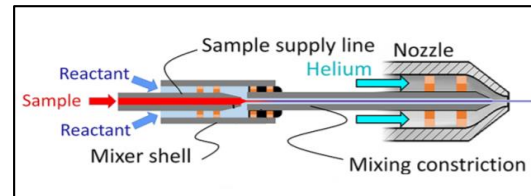
Reactions triggered within crystals during (or *prior to*) data collection (μs to ms time scale)

Microfluidics to trap/mix solutions around crystals



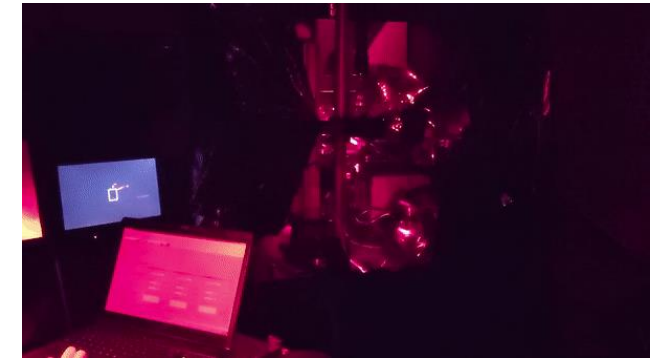
Liquid/Crystal Mixing Injectors

Lois Pollack (Cornell) collaboration



Calvey, Katz, Pollack. Analytical Chemistry 91-11, (2019)

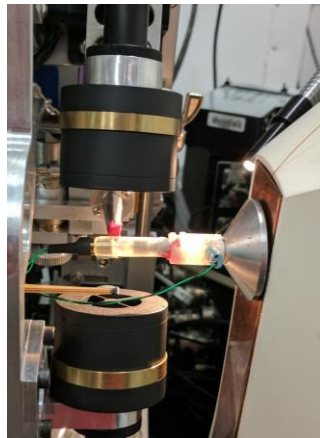
Light activation/Caged Compounds



Jonathan Clinger (Cornell U)
SMB-MX Group (SLAC/SSRL)

High voltage jump

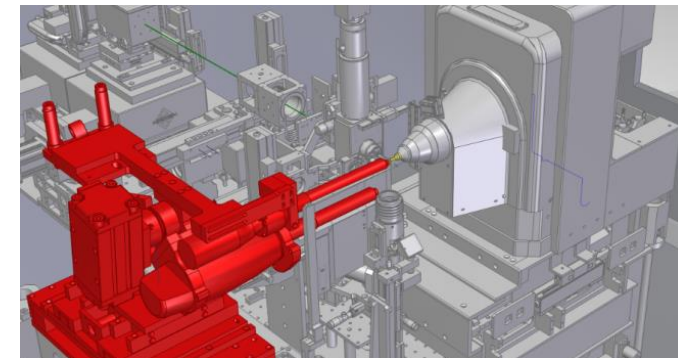
Sarah Perry and Shuo Sui
(UMass Amherst)
SMB-MX Group
(SLAC/SSRL)



“Kinetic crystallography”

Cryo-trap intermediates

In assembly for BL12-1



Validating intermediate states

Freeze-trap reactions in cryostream at fixed time-delays after adding substrate to crystal

Monitor/Follow Radiation Damage

Radiation damage is accrued site-specifically around metal centers

Support for photo-triggered reactions

UV light for uncaging compounds, activating reactions
All automated!

Fully remote pump probe (timing control)

**On-axis system to be installed at BL12-1
and in planning for MFX**



Option for UV-light (or other light sources)
for time-resolved measurements

crystals exposed to UV light (breaking cage)
temperature increase from 100K to 170K
rapid helical data collection (2sec/dataset)

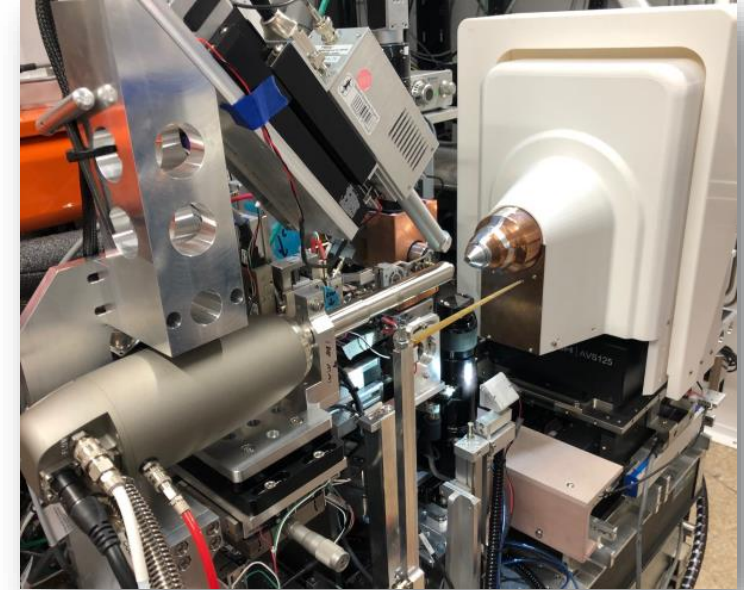
The Calero Lab (University of Pittsburgh)



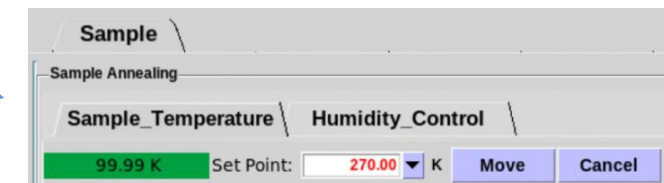
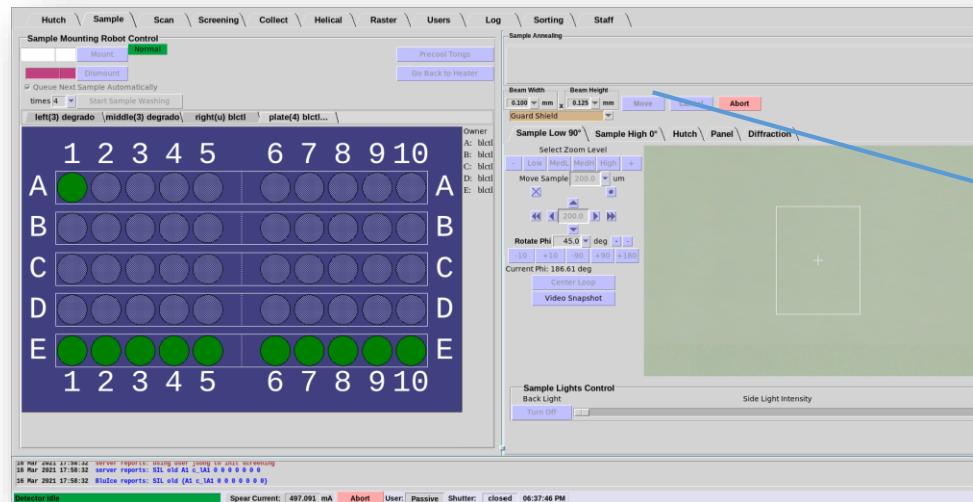
Advanced Features – Elevated Temperatures



- Measurements at physiological temperatures
- Understanding temperature effects in protein structure and interactions
- Potentially no additional disorder from cryoprotectants
- Side chain conformation insights
- Time scale resolution, transient steps



Aina Cohen
(talked Tuesday)

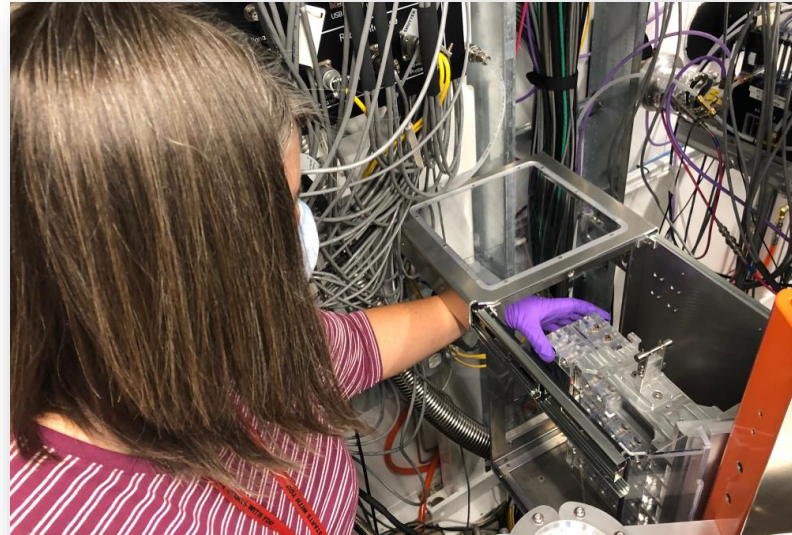


Advanced Features – Elevated Temperatures

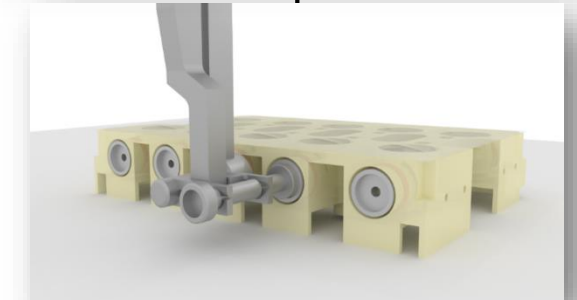
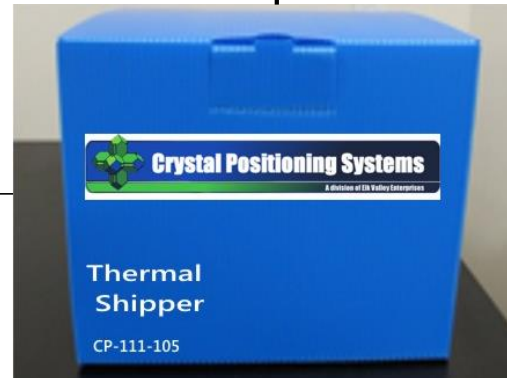


First used at LCLS-MFX,
but now standard at 12-1

Aina Cohen
(talked Tuesday)



Samples inside at
controlled humidity



Advanced Features – Elevated Temperatures



Fraser Group (UCSF - QBI Corona Virus Research Group)

- Studies of conserved “macro domain,” enzyme shown to promote virulence in coronavirus
- Screening of fragments done at BL9-2 and BL12-2
- Measurements at physiological temperatures associated with infection in humans were done at BL12-1
- Understanding how temperature affects the enzyme structure and interactions may provide insight to develop of antiviral therapeutics

UCSF

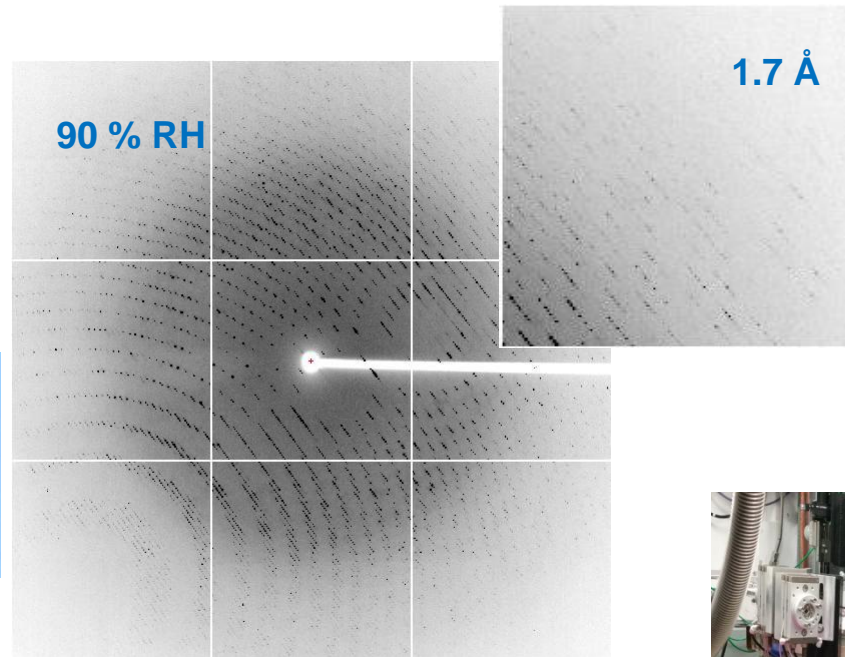
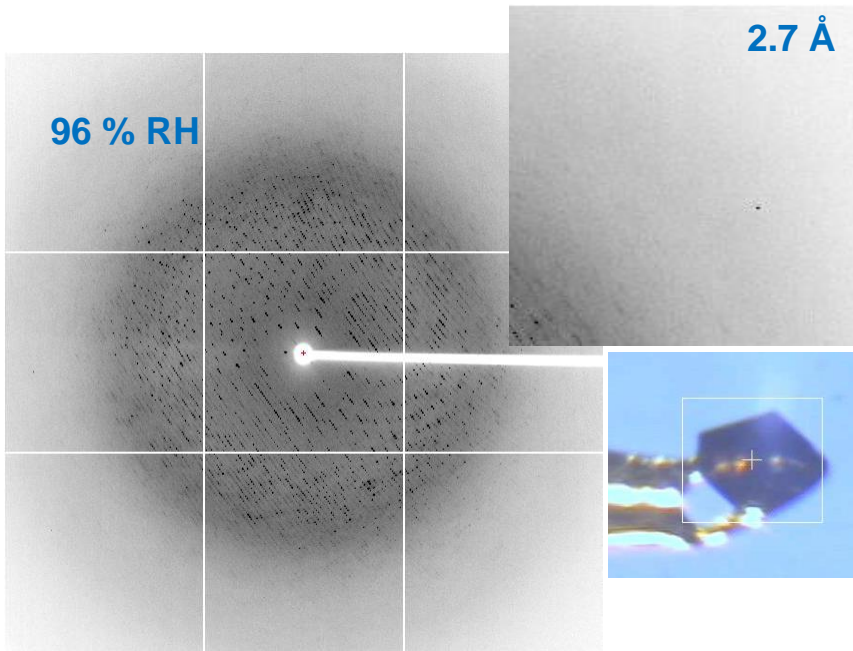
QBI



James Fraser (PI), Michael Thompson Support: Jeney Wierman and Silvia Russi



Advanced Features – Hydration/Dehydration

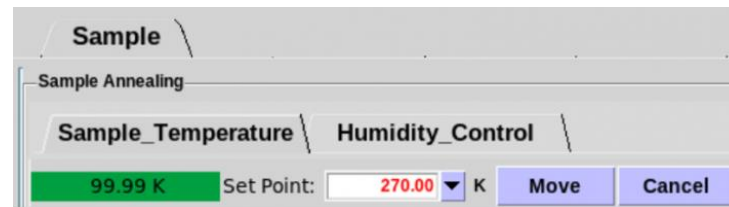


$a=87.8 \text{ Å}$, $b=140.8 \text{ Å}$, $c=233.1 \text{ Å}$, P212121

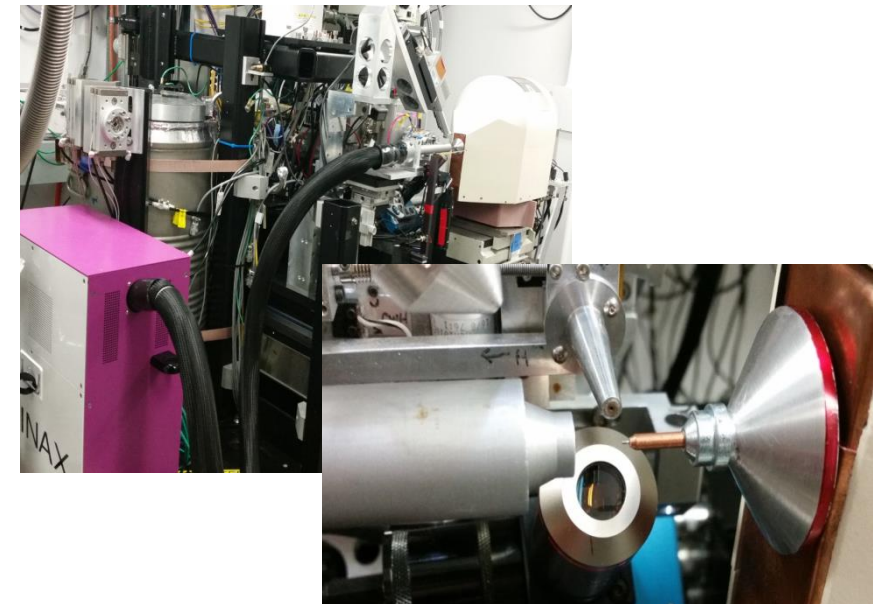
$a=84.6 \text{ Å}$, $b=142.0 \text{ Å}$, $c=233.8 \text{ Å}$, P212121

Bovine Liver Catalase

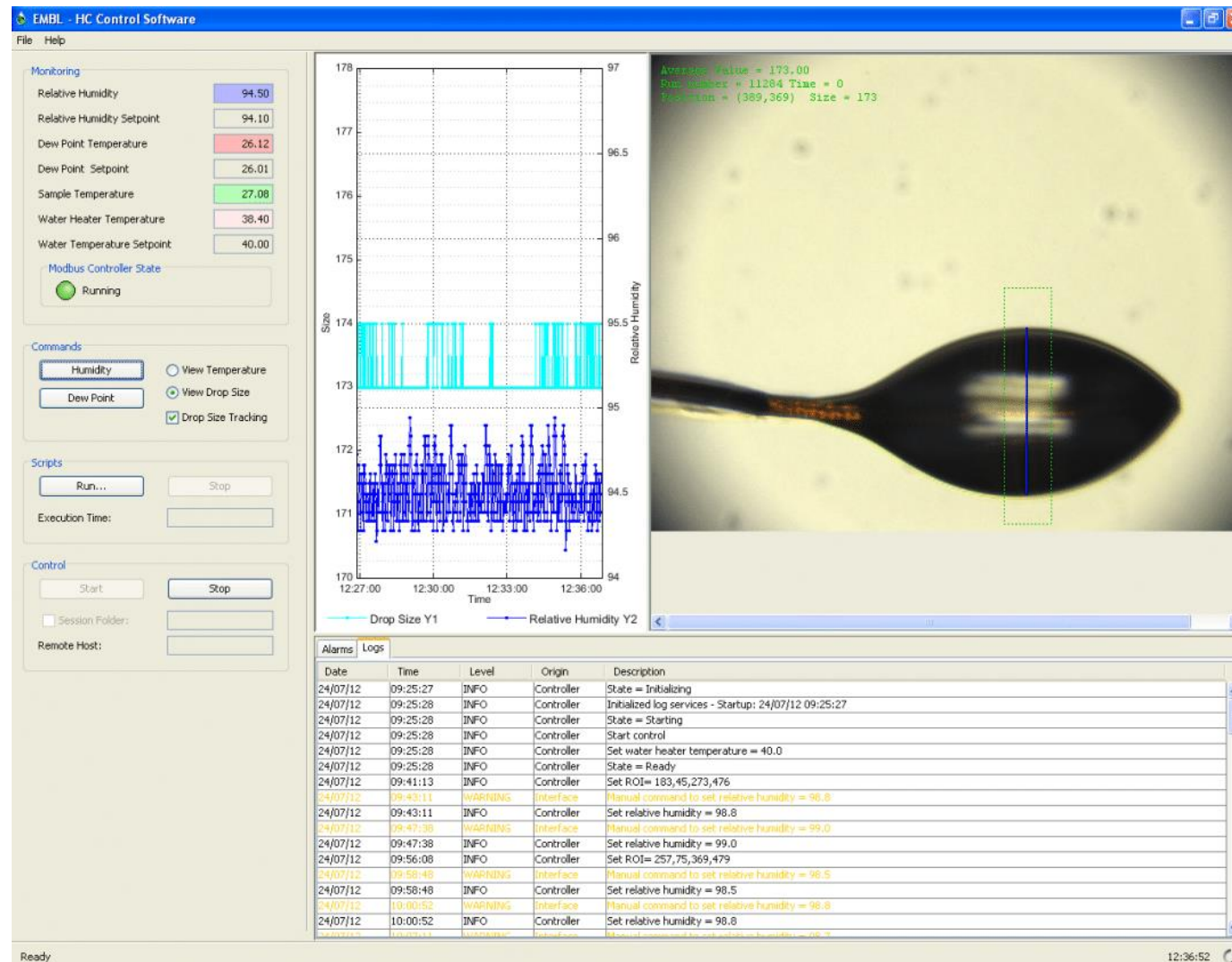
- starting RH=96%, final RH=90%, 1 % RH steps,
- 300 seconds equilibration time between steps

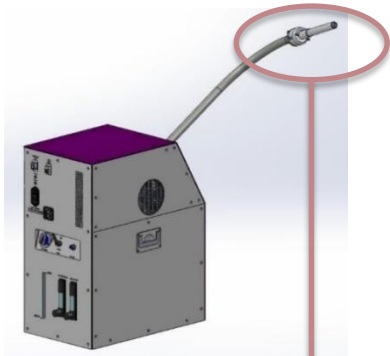


Humidity range of 30.0% to 99.8% $\pm 0.05\%$ RMS



Advanced Features– Hydration/Dehydration

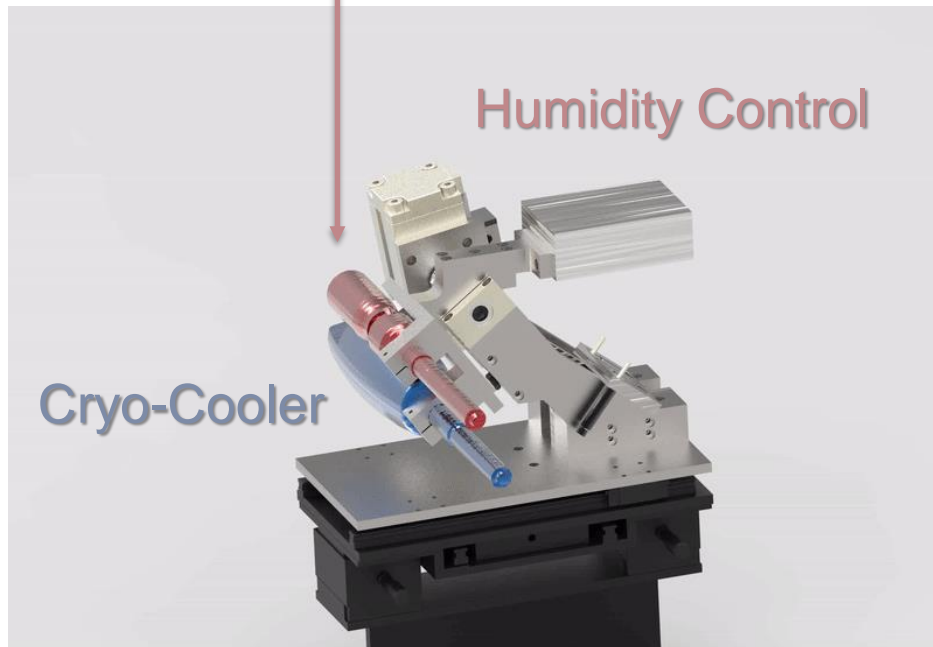




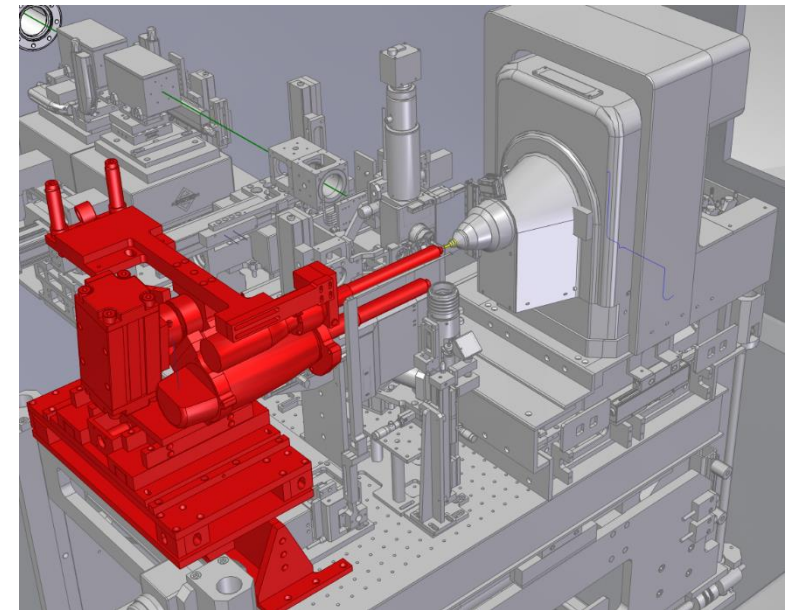
Arinax Humidity Control Device

Automated switch between humid RT or cryo-conditions

- Flash cooling after controlled dehydration experiments
- Samples both cryo and RT supported for same beamtime
- Flash-cooling experiments to trap reaction intermediates



**Flash-cooling
60 ms to switch**



In assembly for BL12-1

Advanced Features – Nozzle Switcher



Cryo-trapping Dynamics

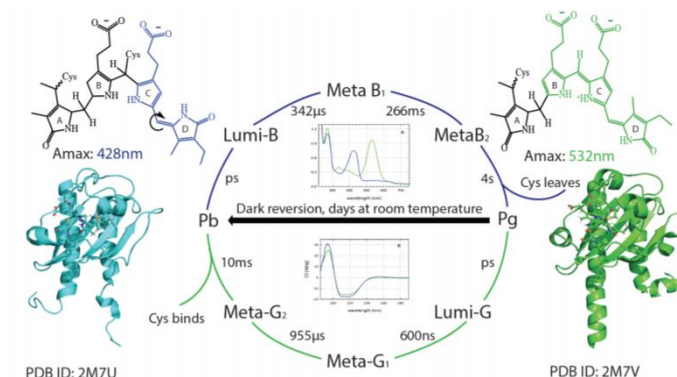
Use in conjunction with light, spray, drop



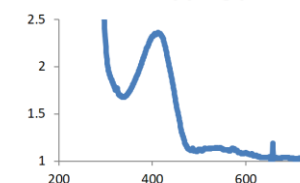
Cryo-trapping Experiment to Observe Phytochrome Photoconversion Intermediates



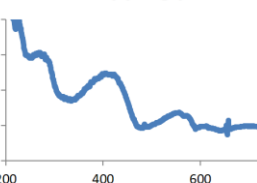
Jonathan Clinger, Sethe Burgie,
Rick Vierstra, and George N.
Phillips Jr.



300ms trapping point

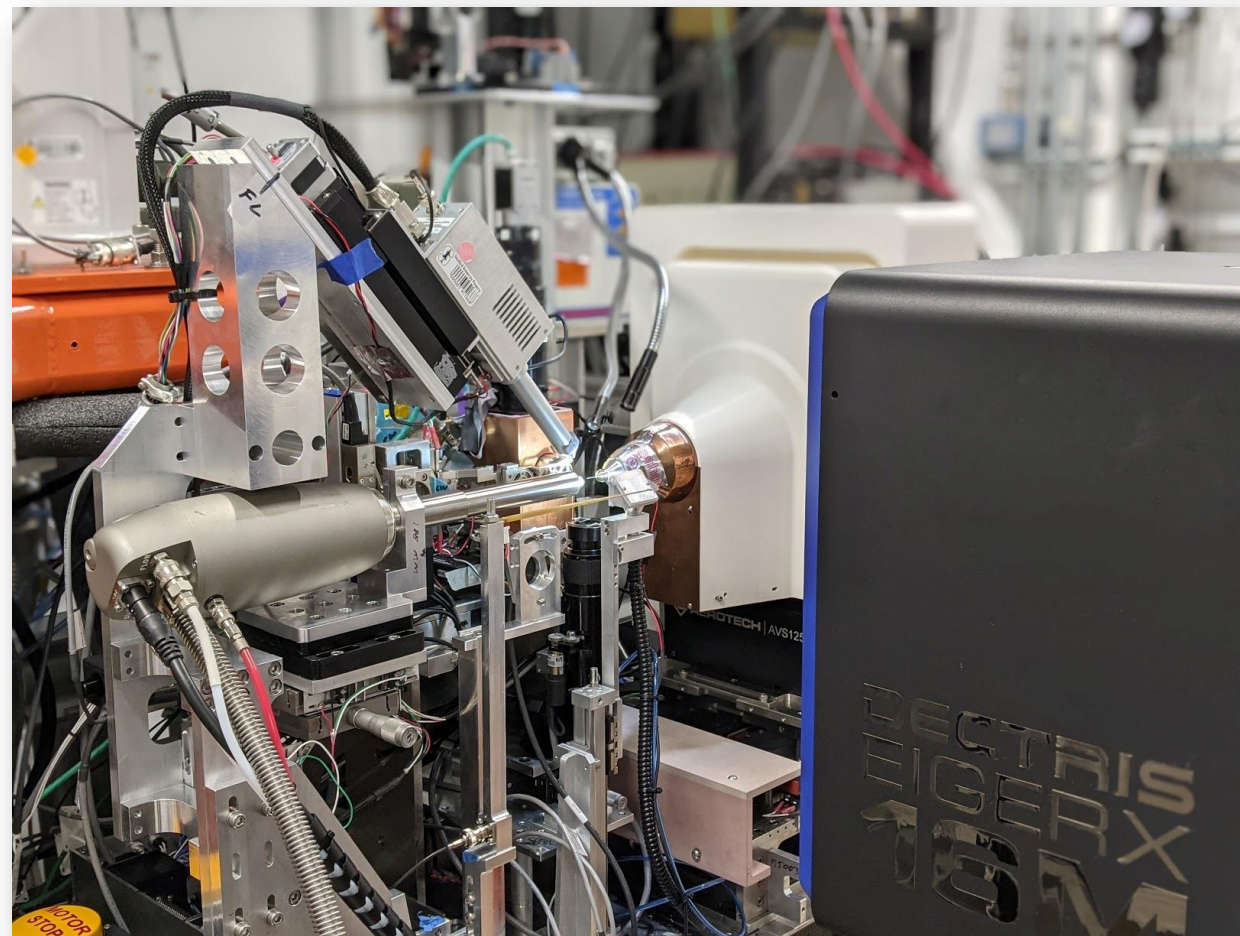


1.2s trapping point



Remote Access with SMB at SLAC

- Standard @ SSRL/SMB
 - Stanford Auto-Mounting (SAM) system (Cohen *et al.*, J. Appl. Cryst. 35, 720, 2002)
 - Remote Data Collection from anywhere in the world (Soltis *et al.*, Acta Cryst. D64, 210, 2008)
- Advanced features @ Beamline 12-1
 - Serial and Dynamics
 - Elevated Temperatures
 - Humidity Control
- Look to the future



- Multi-crystal database
- Blu-Ice Strategy
- Dynamics automation
 - Timing
 - Automate EIGER with gonio
 - 90°/second, fast framing, all remote
- Optical sources, Raman installment
 - More sources! More fibers!
- Nozzle switcher installment
- New optics: CRLs, multilayer monochromator
- EIGER2 XE 16M
 - move EIGER 16 to BL12-2

| Display Type: Display Results Image Display Type: Hide Images Edit Crystal Edit Run Definition | | | | | | | | | | | | | | | | | |
|--|------|-----------|----------------|--------------------|--------------------------------|---------------------------------------|-------|---|-----------|-------|----------------|------------|---------------|------|--|--|--|
| Row | Port | CrystalID | Protein | GridSampleLocation | Images | Comment | Score | UnitCell | Mosaicity | Rmsr | BravaisLattice | Resolution | SystemWarning | Move | | | |
| 0 | A1 | A1 | Thaumatococcus | | A1_00001.mccd A1_00002.mccd | Please place barcode pin in this port | 0.911 | 57.85 57.85 150.09 90.0 90.0 90.0 | 0.025 | 0.025 | P4,P422 | 1.470 | | | | | |
| 1 | A2 | A2 | Thaumatococcus | | A2_00001.mccd A2_00002.mccd | | 0.878 | 57.74 57.74 150.04 90.0 90.0 90.0 | 0.150 | 0.039 | P4,P422 | 1.320 | | | | | |
| 2 | A3 | A3 | Thaumatococcus | | A3_00001.mccd A3_00002.mccd | | 0.925 | 57.72 57.72 150.11 90.0 90.0 90.0 | 0.025 | 0.022 | P4,P422 | 1.360 | | | | | |
| 3 | A4 | A4 | Thaumatococcus | | A4_00001.mccd A4_00002.mccd | | 0.261 | 57.64 57.64 149.64 90.0 90.0 90.0 | 1.500 | 0.041 | P4,P422 | 1.820 | | | | | |
| 4 | A5 | A5 | Thaumatococcus | | A5_00001.mccd A5_00002.mccd | | 0.880 | 58.66 58.66 149.71 90.0 90.0 90.0 | 0.075 | 0.032 | P4,P422 | 1.600 | | | | | |
| 5 | A6 | A6 | Thaumatococcus | | | | 0.841 | 57.62 | 0.125 | 0.039 | P4,P422 | 1.800 | | | | | |

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Acknowledgements



SSRL SMB

| | |
|-----------------|-------------------|
| Aina Cohen | Edgar Estebanez |
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| Clyde Smith | Renato Avelar |
| Tzanko Doukov | Robin Frank |
| Jinhu Song | Scott Mitchell |
| Irimpan Mathews | Henry Meier |

LBNL/ALS

James Holton

If you have additional questions, please email me at jwierman@slac.stanford.edu



- How much processing do we automate?
- How much data collection automation/autonomous?
 - The thought: the further the user gets from the nuts and bolts of data collection, the less they appreciate intricacies in the data.
 - “Automation is more work for staff, less for users” - N.P.
- When do we intervene with data collection?
 - e.g. “Yikes, they are totally missing the crystal!”
- Where does data come from for strategy?
 - Can users override acquired data?
 - Does every collection generate a strategy?
- How do we handle storing data?
 - Cloud?
 - Massive physical storage?
 - Junk it!
- How to teach new users?
- How much is too much? More widgets? More tabs? More options?

Front End Glamour Shot

