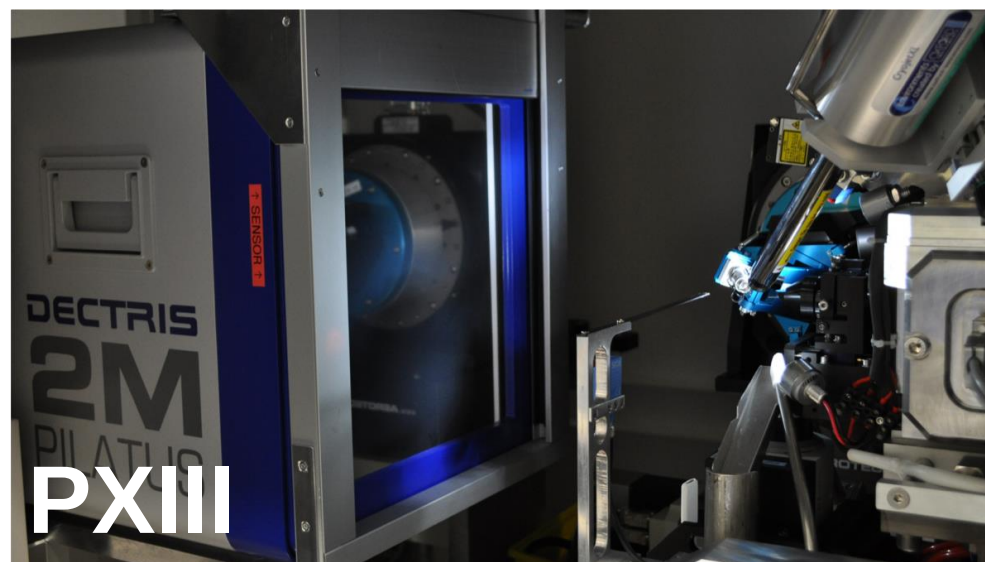




Kate M. Smith :: Postdoctoral Fellow :: MX Data :: Paul Scherrer Institute

User Interfaces and Unattended Data Collection at the Swiss Light Source, PSI

NSLS-II, March 2021



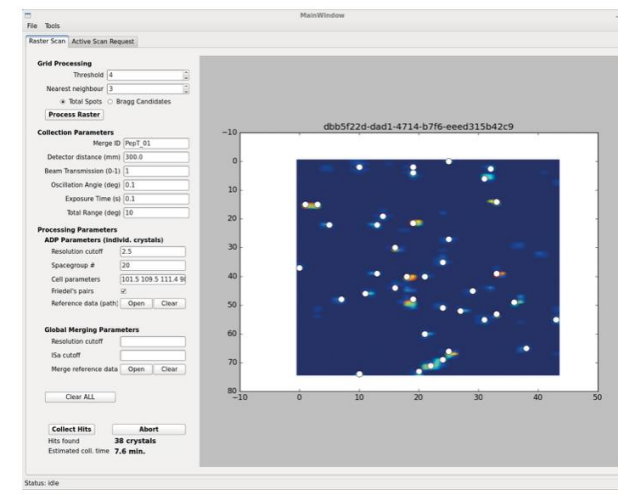
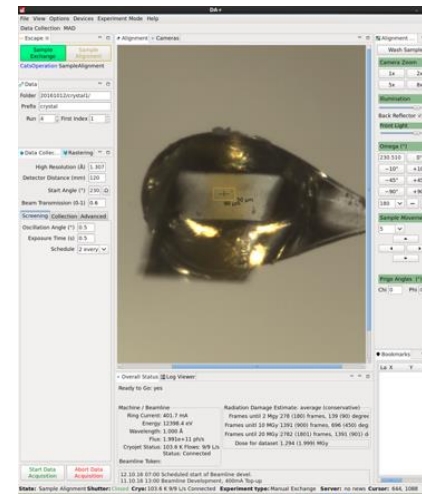
	PXI (X06SA)	PXII (X10SA)	PXIII (X06DA)
Wavelength range [Å]	0.7 - 2.2	0.62 - 2.07	0.71 - 2.07
Source	in-vacuum undulator	in-vacuum undulator	bending magnet
Spectral range	5.7 - 17.5	6.0 - 20.0	6.0 - 17.5
Flux at 12.4 keV [ph/s]	$> 2 \times 10^{12}$	$> 2 \times 10^{12}$	5×10^{11}
Focused spot size h x v [μm^2]	5 x 5 (2 x 1) -> 100 x 100	73 x 16	80 x 45
Detector	EIGER 16M	EIGER2 16M	PILATUS 2M-F -> JUNGFRAU 4M
Frame rates [Hz]	133 750 (4M ROI)	130 500 (4M ROI)	60 -> 2000
Goniometer	single-axis	single-axis	multi-axis PRIGo
Robot & pucks	TELL Unipucks	TELL Unipucks	TELL Unipucks

TELL Sample Changer

- 30 x Unipucks (480 samples) capacity
- Puck barcode scanning station for fast dewar loading
- <20 seconds exchange time
- Dewar is dried during shutdowns (4-6 weeks)
- New gripper can detect pins



- robust, intuitive & user-friendly
- allows exploitation of latest instrumentation
- utilises latest technology
- provides expandable and sustainable solution supported by a small software team



ADP Tracker: Standard & Native-SAD

TestData/omega1adp_dataset_1_20171110_143252

Experimental Parameters				Crystal Parameters: autoPROC			
Detector	0.1	a	88.38	alpha	90		
Exposure Time	0.1	b	88.38	beta	90		
Beam Transmission	1	c	73	gamma	120		
Number of Frames	1800	Space Group	P6322	Space Group Number	182		
Detector Distance	220	Mosaicity	0.2	GA	25.35		
Wavelength	2.0664	Wilson B factor	67.056				
Detector	PLATON 2MP						

Pointless: Space group uniquely determined: P6322, 182

Order	Space Group	Space Group Number	Space Group Confidence
1	P6322	177	0.821
2	P6322	182	0.821

STARANISO Eigenvectors

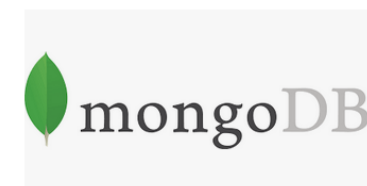
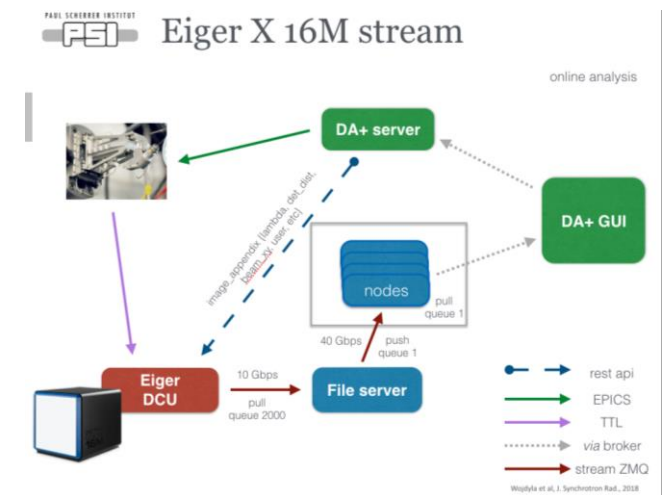
Resolution Limit	Eigenvalue 1	Eigenvalue 2	Eigenvalue 3	Maximal
2.159	1.0000	0.0000	0.0000	0.894, 0.447, 0.000
2.159	0.0000	1.0000	0.0000	0.000, 0.894, 0.447
2.260	0.0000	0.0000	1.0000	0.000, 0.000, 0.894

autoPROC with STARANISO (angular range: 180)

Overall	Inner Shell	Outer Shell
Low Resolution Limit	52.826	2.27
High Resolution Limit	2.18	6.492
Resolution Range	4.8	2.6
Resolution Range (in 1/2)	200	200
Resolution Range (in 1/2)	4.9	2.7
Resolution Range (in 1/2)	1.8	59.4
Resolution Range (in 1/2)	1.2	0.7
Resolution Range (in 1/2)	12.073	6829
Resolution Range (in 1/2)	8405	424
Resolution Range (in 1/2)	52.2	128.5
Resolution Range (in 1/2)	89.4	100
Resolution Range (in 1/2)	91.2	100
Resolution Range (in 1/2)	14.6	16.1

autoPROC (angular range: 180)

Overall	Inner Shell	Outer Shell
Low Resolution Limit	52.826	2.27
High Resolution Limit	2.309	6.264
Resolution Range	4.7	2.6
Resolution Range (in 1/2)	200	200
Resolution Range (in 1/2)	4.9	2.7
Resolution Range (in 1/2)	1.8	59.4
Resolution Range (in 1/2)	1.2	0.7
Resolution Range (in 1/2)	120899	7411
Resolution Range (in 1/2)	7775	465
Resolution Range (in 1/2)	35	107.5
Resolution Range (in 1/2)	99.3	100
Resolution Range (in 1/2)	-	-
Resolution Range (in 1/2)	15.9	15.9

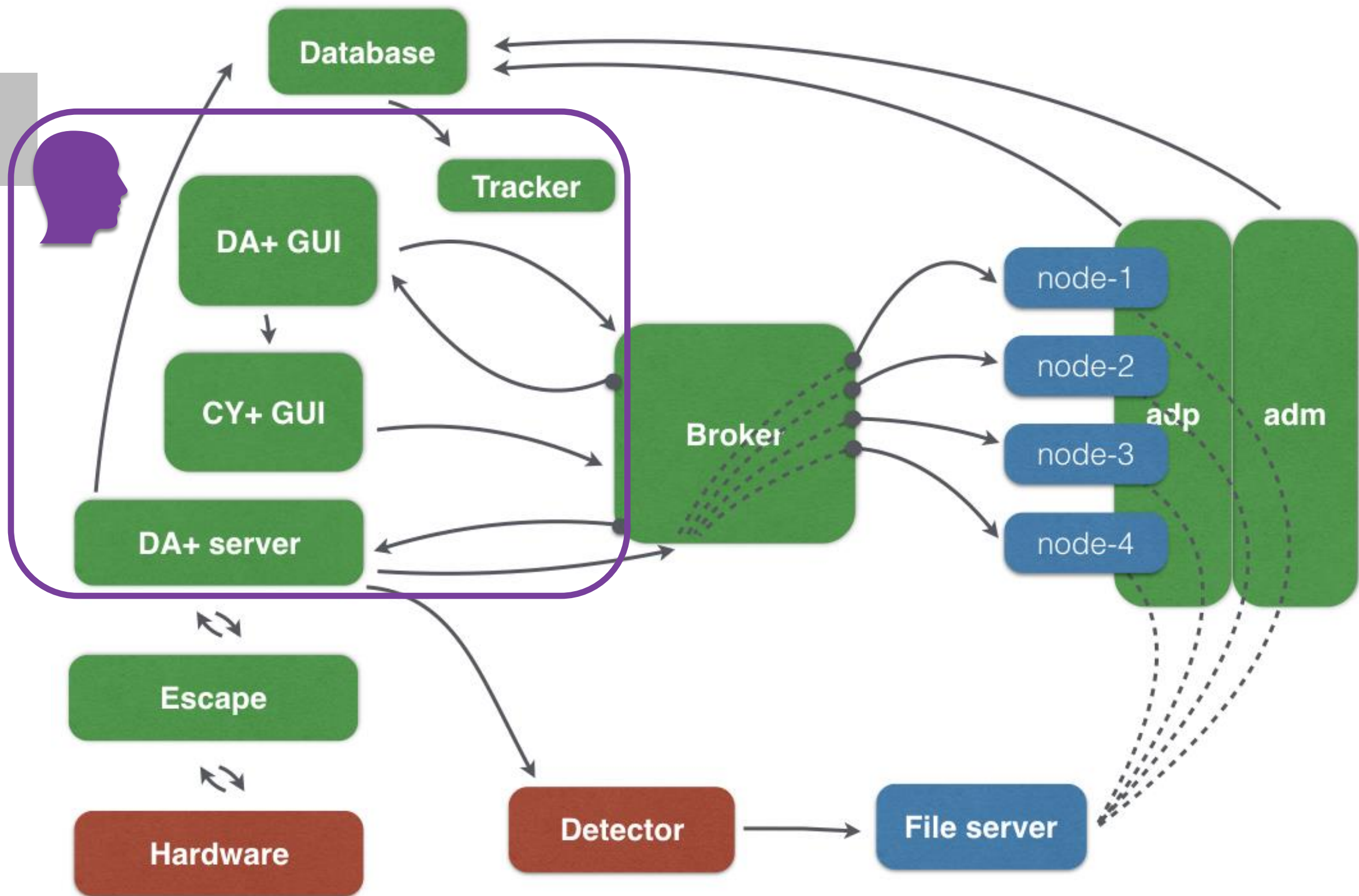


Wojdyla et al, J. Appl. Cryst., 2016. <https://doi.org/10.1107/S1600576716006233>

Wojdyla et al, J. Synchrotron Rad., 2018. <https://doi.org/10.1107/S1600577517014503>

Basu et al, J. Synchrotron Rad., 2019. <https://doi.org/10.1107/S1600577518016570>

Overall infrastructure



DA+
server

DA+
GUI

TELL
GUI

The DA+ GUI interface is shown with a terminal window at the top displaying logs. Below it, the main window is divided into several sections: a left sidebar with 'Data' and 'Collection' tabs, a central camera view showing a sample, and a right sidebar with 'Alignment' and 'Cameras' tabs. The bottom section contains a 'State' bar and a 'Spreadsheet' table.

Owner	Dewar Loc.	Puck ID	Sample #	Prefix	Folder	Priority	Sample Status	# mounts	Comments
Nai 1	A1	CPS-4861	1	0tacr1Br	20160102/PSL_1	1	not present	0	sfs
Nai 1	A1	CPS-4861	2	0tacr1Br	20160102/PSL_1	1	not present	0	sfs
Nai 1	A1	CPS-4861	3	0tacr1Br	20160102/PSL_1	1	not present	0	sfs
Nai 1	A1	CPS-4861	4	0tacr1Br	20160102/PSL_1	1	not present	0	sfs
Nai 1	A1	CPS-4861	5	0tacr1Br	20160102/PSL_1	1	not present	0	sfs
Nai 1	A1	CPS-4861	6	0tacr1Br	20160102/PSL_1	1	not present	0	sfs
Nai 1	A1	CPS-4861	7	0tacr1Br	20160102/PSL_1	1	not present	0	sfs
Nai 1	A1	CPS-4861	8	0tacr1Br	20160102/PSL_1	1	not present	0	sfs
Nai 1	A1	CPS-4861	9	0tacr1Br	20160102/PSL_1	1	not present	0	sfs
Nai 1	A1	CPS-4861	10	0tacr1Br	20160102/PSL_1	1	not present	0	sfs
Nai 1	A1	CPS-4861	11	0tacr1Br	20160102/PSL_1	1	not present	0	sfs
Nai 1	A1	CPS-4861	12	0tacr1Br	20160102/PSL_1	1	not present	0	sfs
Nai 1	A1	CPS-4861	13	0tacr1Br	20160102/PSL_1	1	not present	0	sfs
Nai 1	A1	CPS-4861	14	0tacr1Br	20160102/PSL_1	1	not present	0	sfs
Nai 1	A1	CPS-4861	15	0tacr1Br	20160102/PSL_1	1	not present	0	sfs

The ALBULA interface shows a diffraction pattern with concentric circles. Below it, the ADP Tracker application window is open, displaying experimental parameters and a table of data.

Experimental Parameters										Crystal Parameters: Fast Processing			
Oscillation Angle	0.1	a	102.83	alpha	90								
Exposure Time	0.1	b	109.81	beta	90								
Beam Transmission	1	c	110.45	gamma	90								
Number of Frames	100	Space Group	C2221	Space Group Number	20								
Detector Distance	300	Mosaicity	0.386	ISA	50								
Wavelength	0.9999	Wilson B Factor	45.511										
Detector	PILATUS 6M												

Albula

Tracker

File View Options Devices Experiment Mode Help

Data Collection MAD

Escape + Alignment o Cameras

Sample Exchange **Sample Alignment**

CatsOperation SampleAlignment

Data

Folder 20161012/crystal1/

Prefix crystal

Run 1 First Index 1

Data Collection Rastering

High Resolution (Å) 2.644

Detector Distance (mm) 300

Start Angle (°) 0 Ω

Beam Transmission (0-1) 1.000

Screening Collection Advanced

Oscillation Angle (°) 0.5

Exposure Time (s) 0.5

Schedule 2 every 90°

Alignment Control

Wash Sample

Camera Zoom

1x 2x

5x 8x

Illumination

Back Reflector ☒ up

Front Light

Omega (°)

-90.000 0°

-10° +10°

-45° +45°

-90° +90°

180 - +

Sample Movement (μm)

5

Prigo Angles (°)

Chi 0 Phi 0

Bookmarks

La X Y Z Ch

Overall Status Log Viewer

Ready to Go: yes

Machine / Beamline

Ring Current: 401.0 mA

Energy: 12398.4 eV

Wavelength: 1.000 Å

Flux: 3.323e+11 ph/s

Cryojet Status: 103.7 K Flows: 9/9 L/s

Status: Connected

Beamline Token:

Radiation Damage Estimate: average (conservative)

Frames until 2 MGy 167 (108) frames, 84 (54) degrees (phasing limit)

Frames until 10 MGy 838 (542) frames, 419 (271) degrees

Frames until 20 MGy 1677 (1085) frames, 839 (543) degrees (Henderson limit)

Dose for dataset 2.146 (3.315) MGy

12.10.16 07:00 Scheduled start of Beamline devel.

11.10.16 13:00 Beamline Development, 400mA Top-up

Start Data Acquisition Abort Data Acquisition

State: Sample Alignment Shutter: Closed Cryo: 103.7 K 9/9 L/s Connected Experiment type: Manual Exchange Server: no news Cursor: 1165, 1147

Choose element

1

Change energy

2

Transmission search

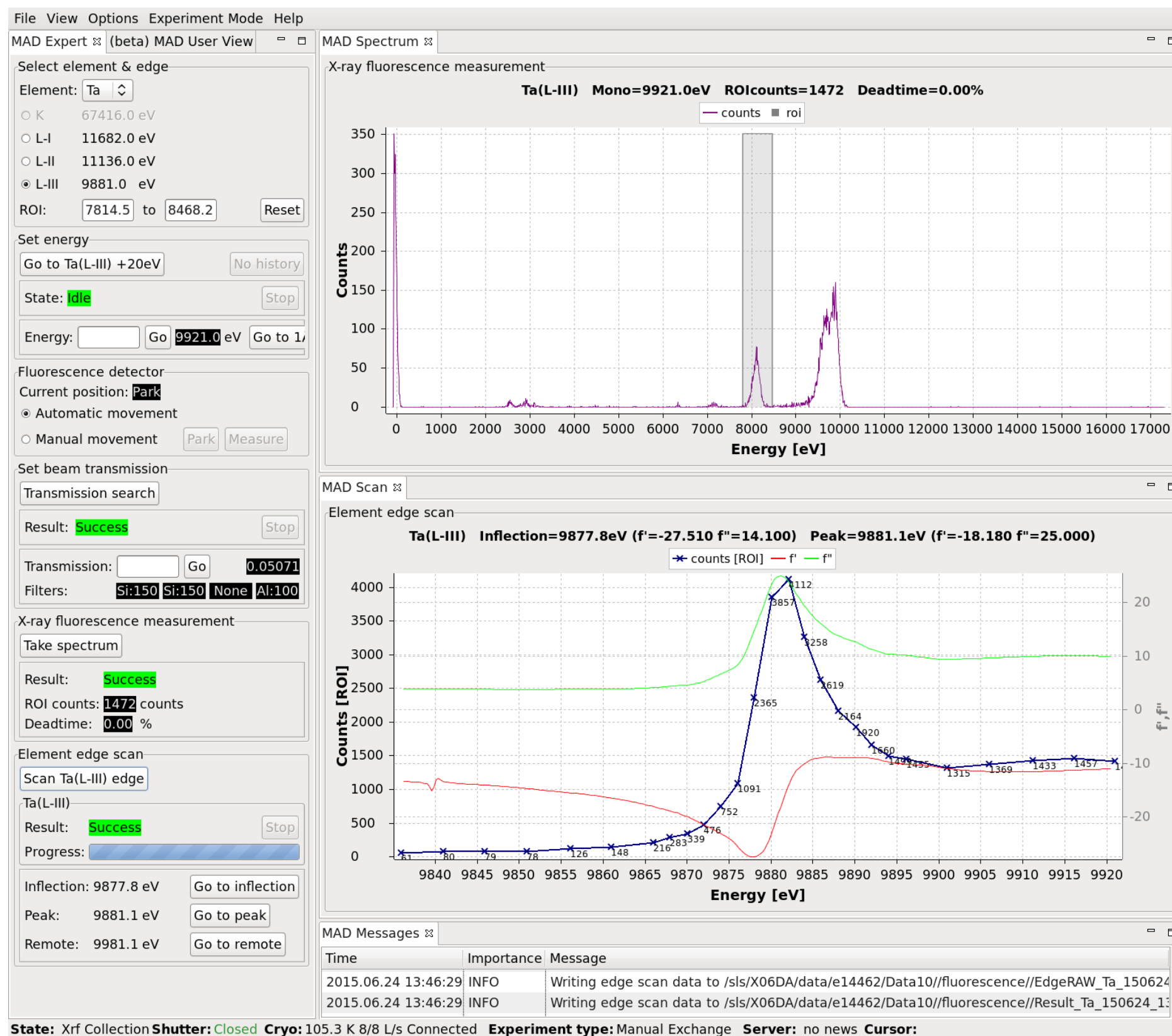
3

Take spectrum

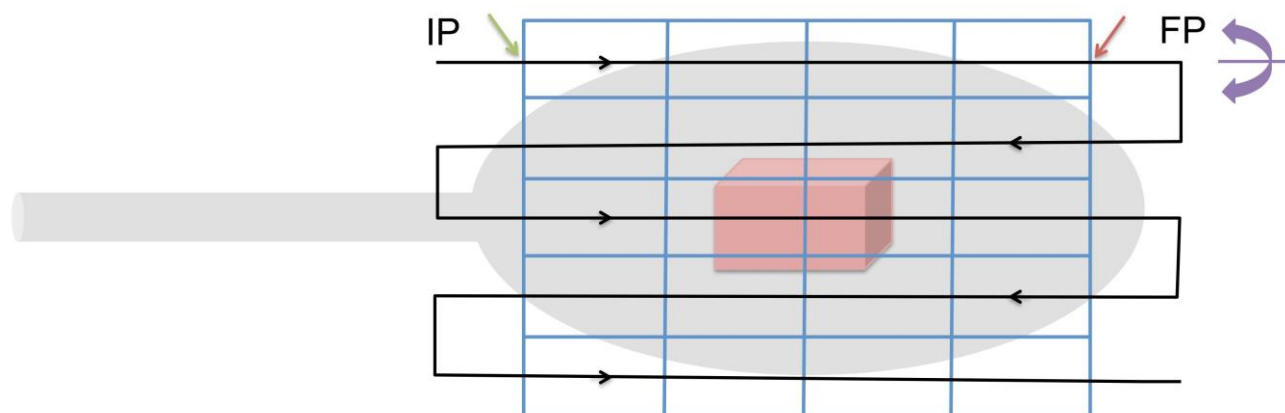
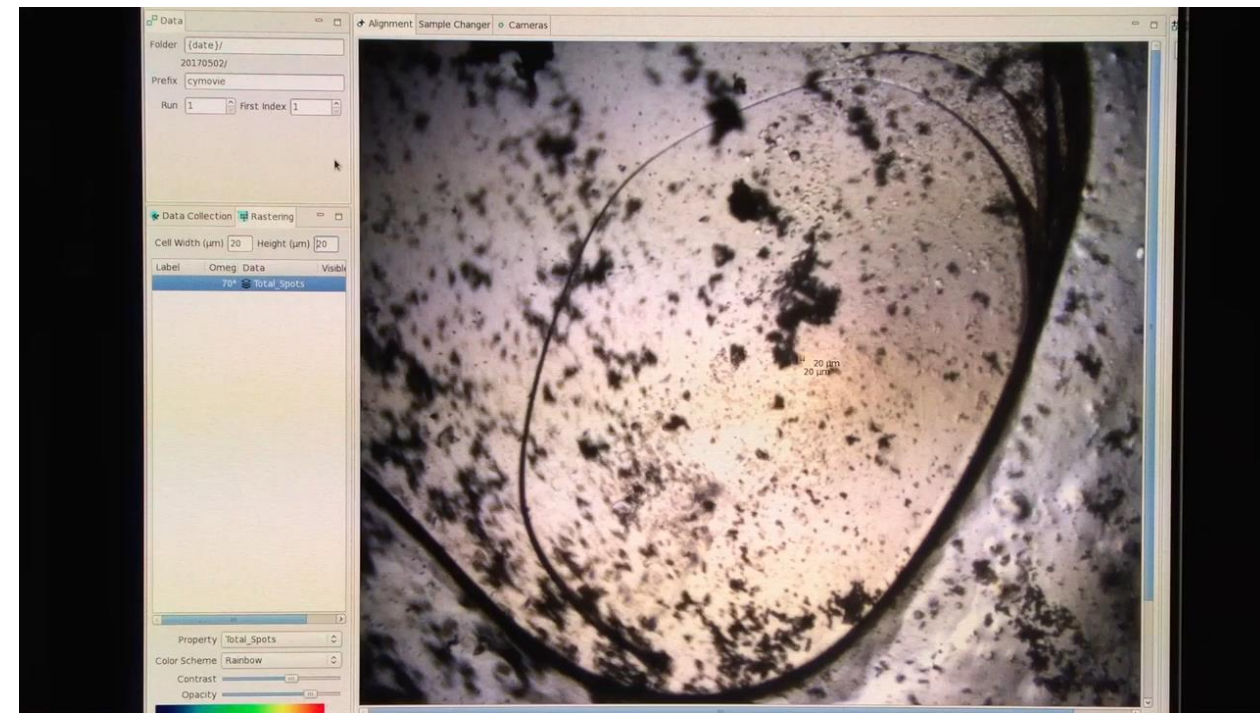
4

Scan edge

5



- Easily requested by user in the intuitive DA+ GUI
- Hardware (goniometer & detector) and software control allow for fast grid scanning
 - Eiger X 16M 4ROI at 50Hz-100Hz
- PXII computer cluster with 24 nodes (1056 cores) allow for immediate delivery of analysis (*labelit.distl* or Cheetah)
 - 528 workers (24 x 22)
 - Eiger X 16M 4ROI at 100Hz grid with 10.584 images



DA+
server

DA+
GUI

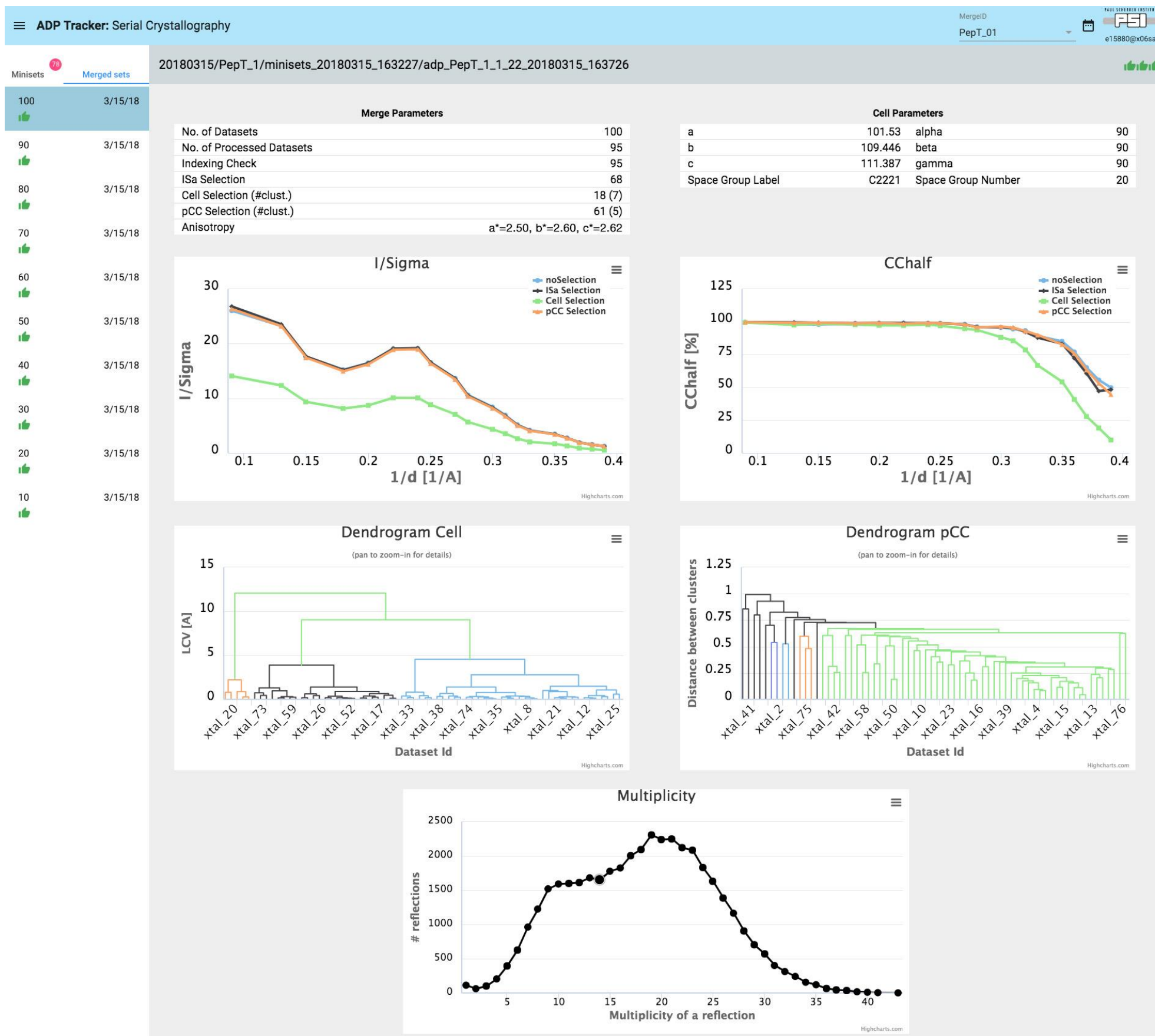
Albula

CY+
GUI

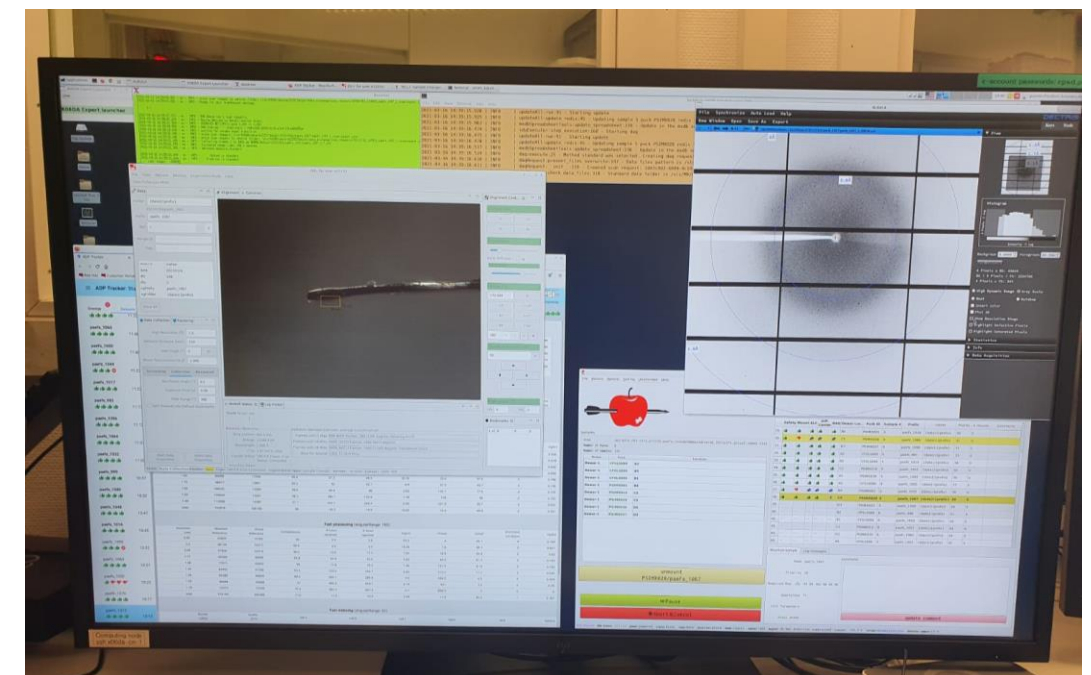
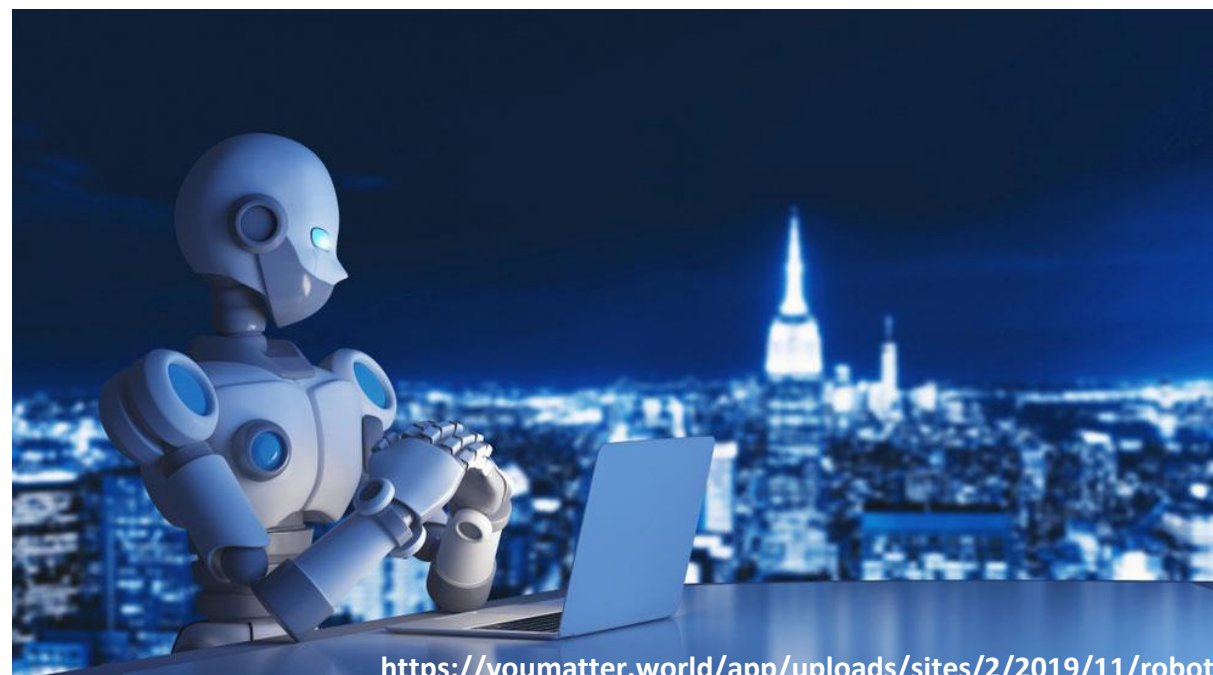
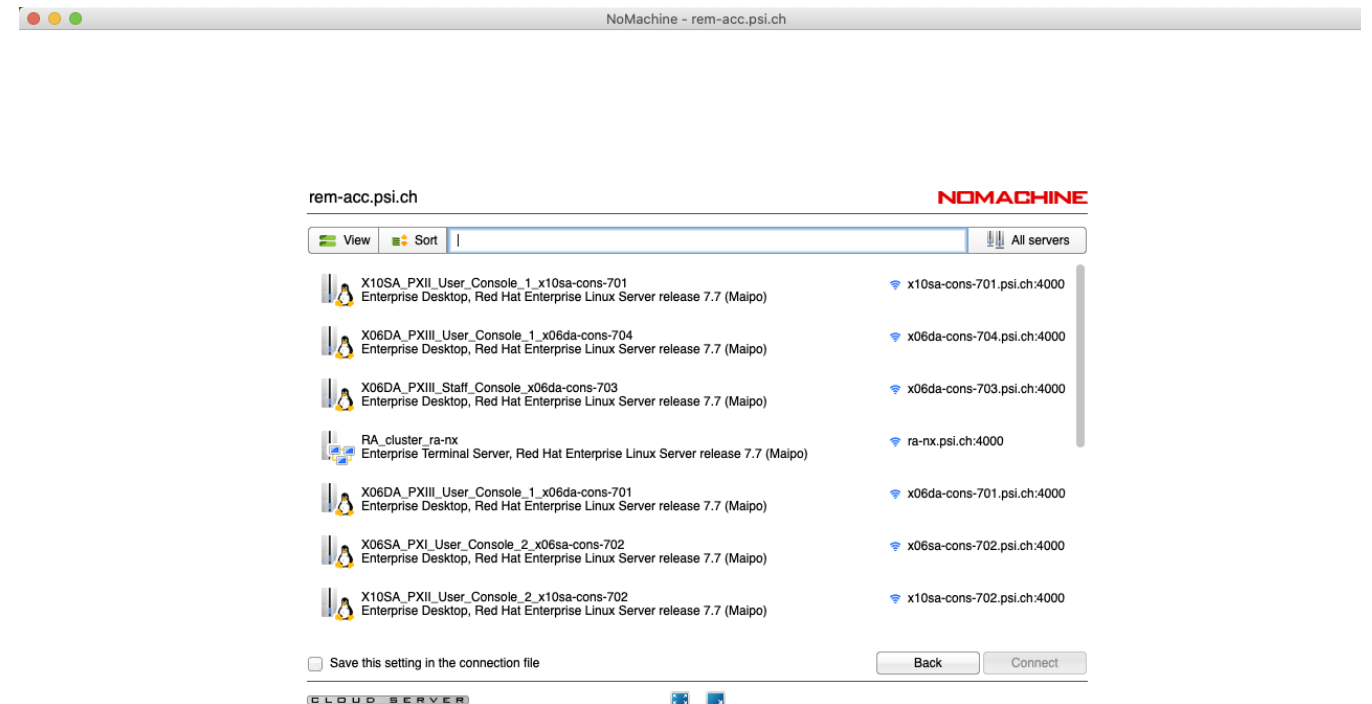
Tracker

The image displays four windows from the DA+ serial crystallography software suite:

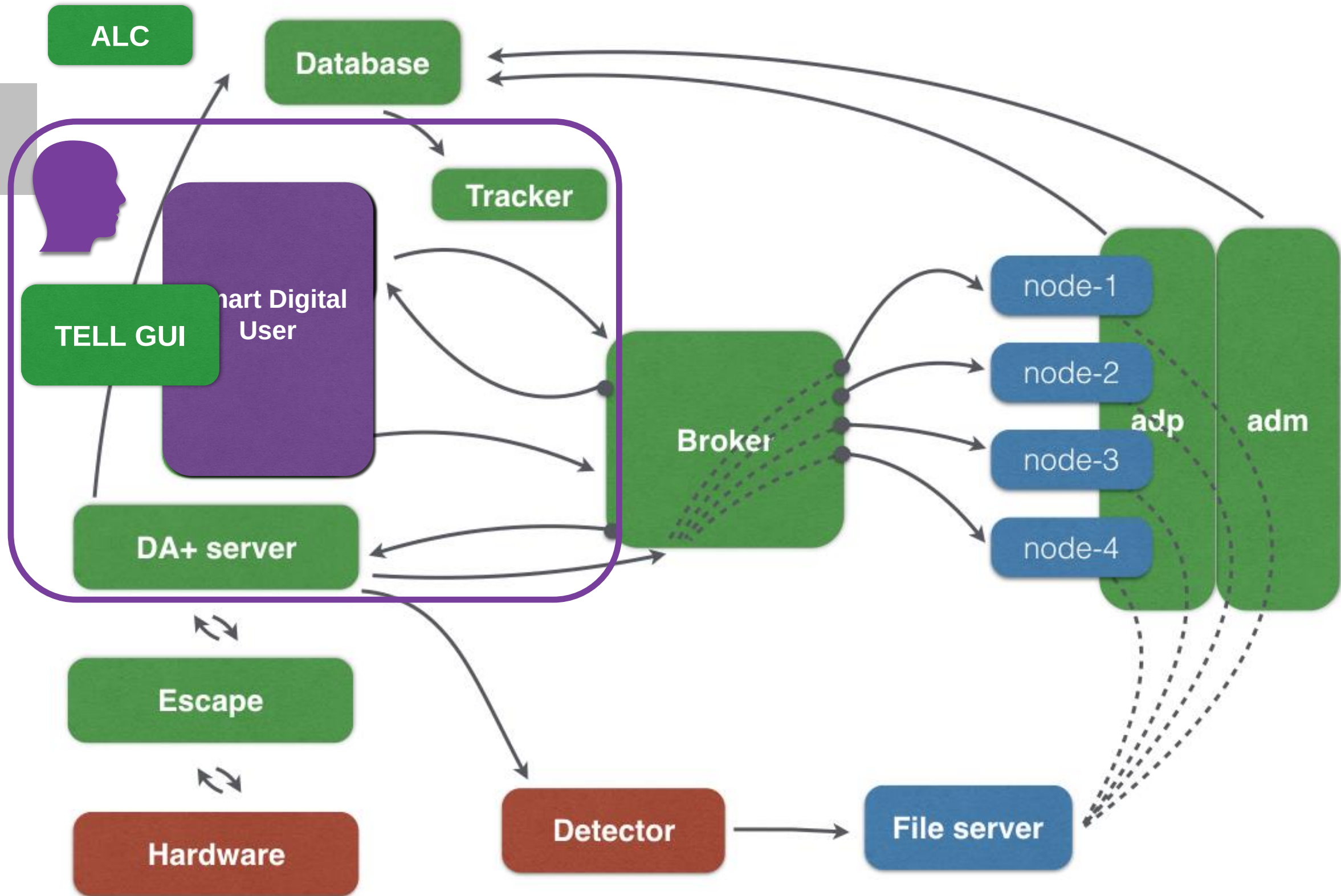
- server.launcher.sh**: A terminal window showing the initialization of various components like the collimator, motor, and detector.
- MainWindow**: The main interface for grid processing, showing a 2D plot of diffraction spots and various control parameters for data collection and processing.
- ALBULA**: A window showing a 2D diffraction pattern with overlaid spot indices (e.g., 3.1A, 4A, 6A, 12A).
- ADP Tracker: Serial Crystallography**: A window providing a detailed summary of experimental parameters, crystal data, and processing statistics.



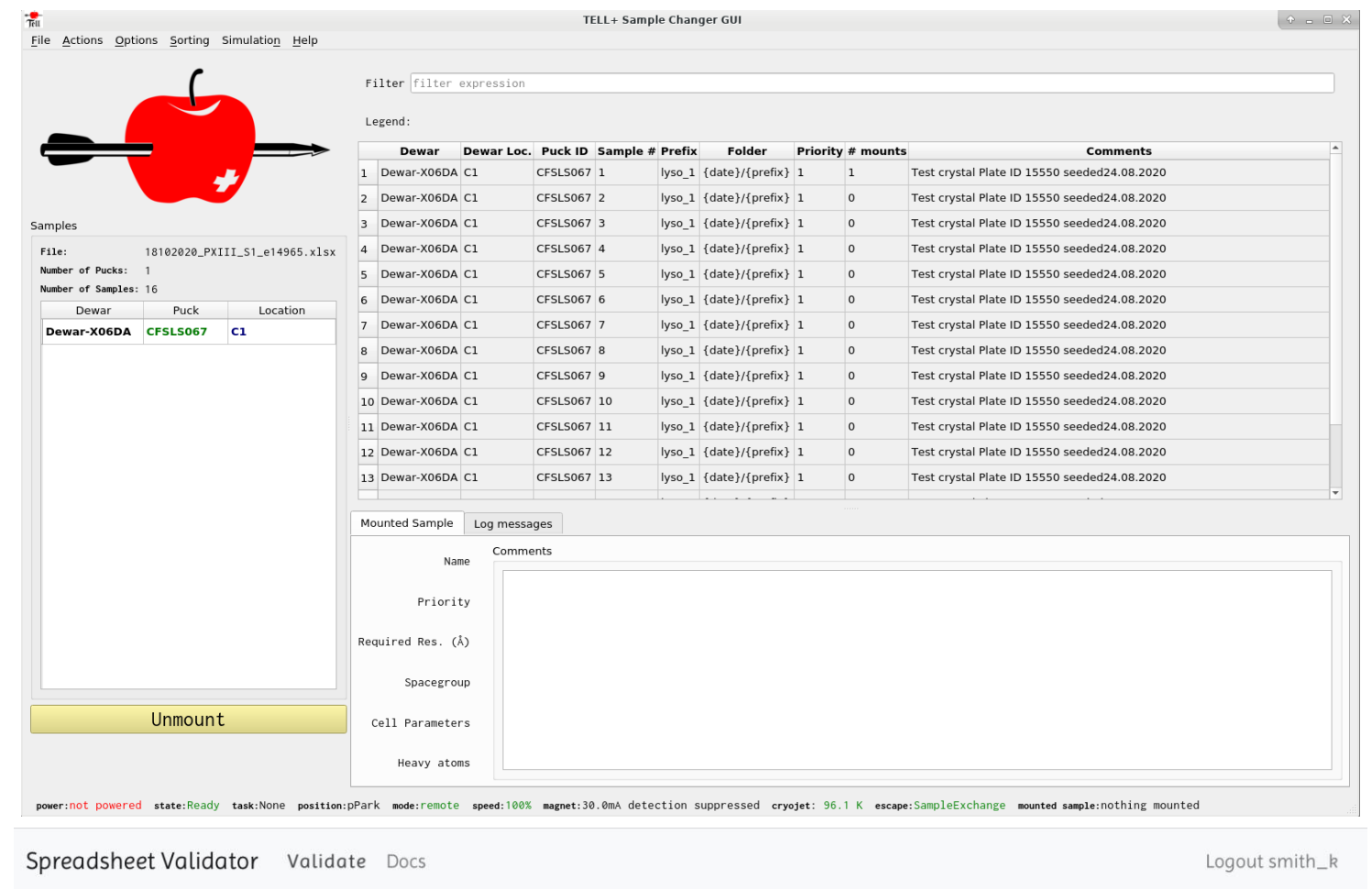
- 100% remote
- automated
- TELL GUI
- Automatic Loop Centring (ALC)
- Smart Digital User (SDU)



Smart Digital User SDU



- PyQt GUI
- Interacts with
 - pshell (TELL robot control)
 - DA+ daq
 - DA+ server
 - escape
 - mxdb
 - automation



Your spreadsheet is valid. You have 15 pucks, 233 samples.

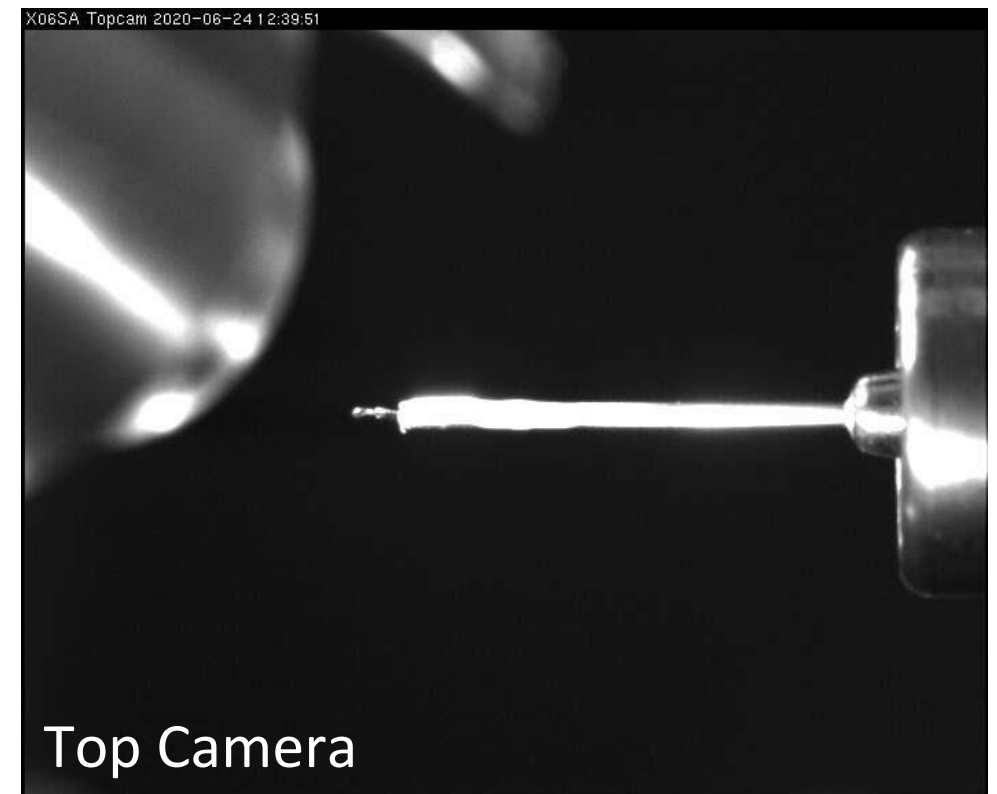
Dewar	Puck ID	Sample #	Prefix	Folder	Priority	Comments
FFCS - Uni-3	CFSLS114	1	20210218_200LDV_100PP_15redo-64	{date}/{beamline}/loop/{sgPuck}/{prefix}	1	
FFCS - Uni-3	CFSLS114	2	20210218_200LDV_100PP_15redo-65	{date}/{beamline}/loop/{sgPuck}/{prefix}	1	
FFCS - Uni-3	CFSLS114	3	20210218_200LDV_100PP_15redo-66	{date}/{beamline}/loop/{sgPuck}/{prefix}	1	
FFCS - Uni-3	CFSLS114	4	20210218_200LDV_100PP_15redo-67	{date}/{beamline}/loop/{sgPuck}/{prefix}	1	
FFCS - Uni-3	CFSLS114	5	20210218_200LDV_100PP_15redo-68	{date}/{beamline}/loop/{sgPuck}/{prefix}	1	

Automatic Loop Centring ALC

Kuba Kaminski, Kate Smith

1st step prelocation (~6 seconds)

- X06SA / X10SA

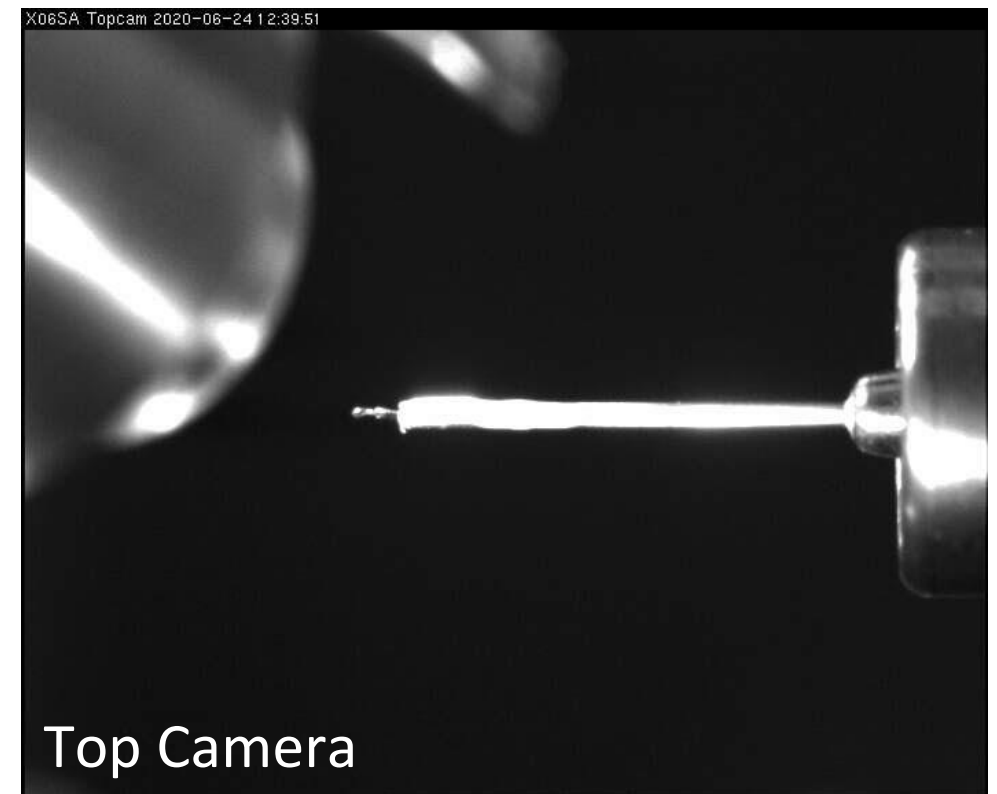


Automatic Loop Centring ALC

Kuba Kaminski, Kate Smith

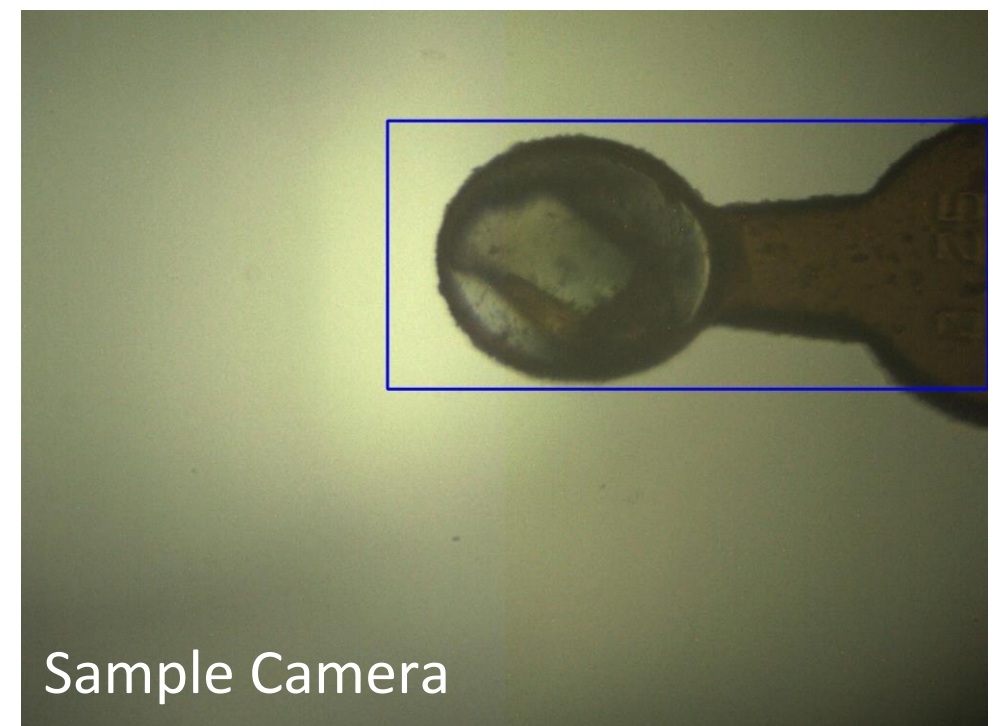
1st step prelocation (~6 seconds)

- X06SA / X10SA



2nd step centerToFlat (~19 seconds)

- 1st centerOnTip
- findFlatFace
- findLoopThickness
- 2nd centerOnTip
- findLoopBoundingBox



Smart Digital User SDU

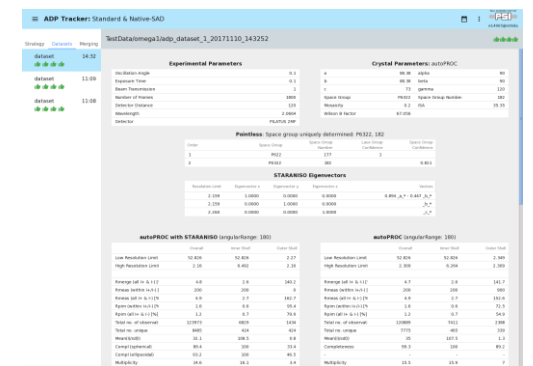
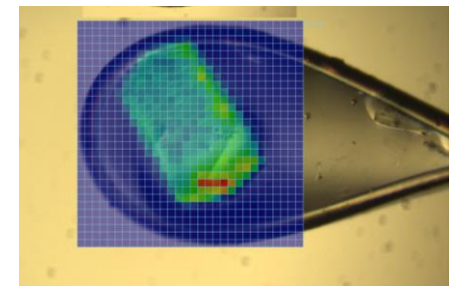
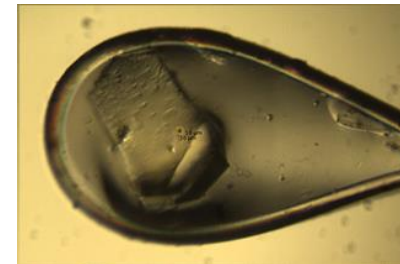
Justyna Wojdyla, Kuba Kaminski, Kate Smith

- Fully automated data collection - python 3.6
 - sample mounting - TELL
 - loop centring - ALC
 - crystal centring - diffraction based with fast grid scan (50-100Hz)
 - data collection - Eiger 16M up to 100Hz
 - data processing - fully automated, live display in tracker, pdf reports

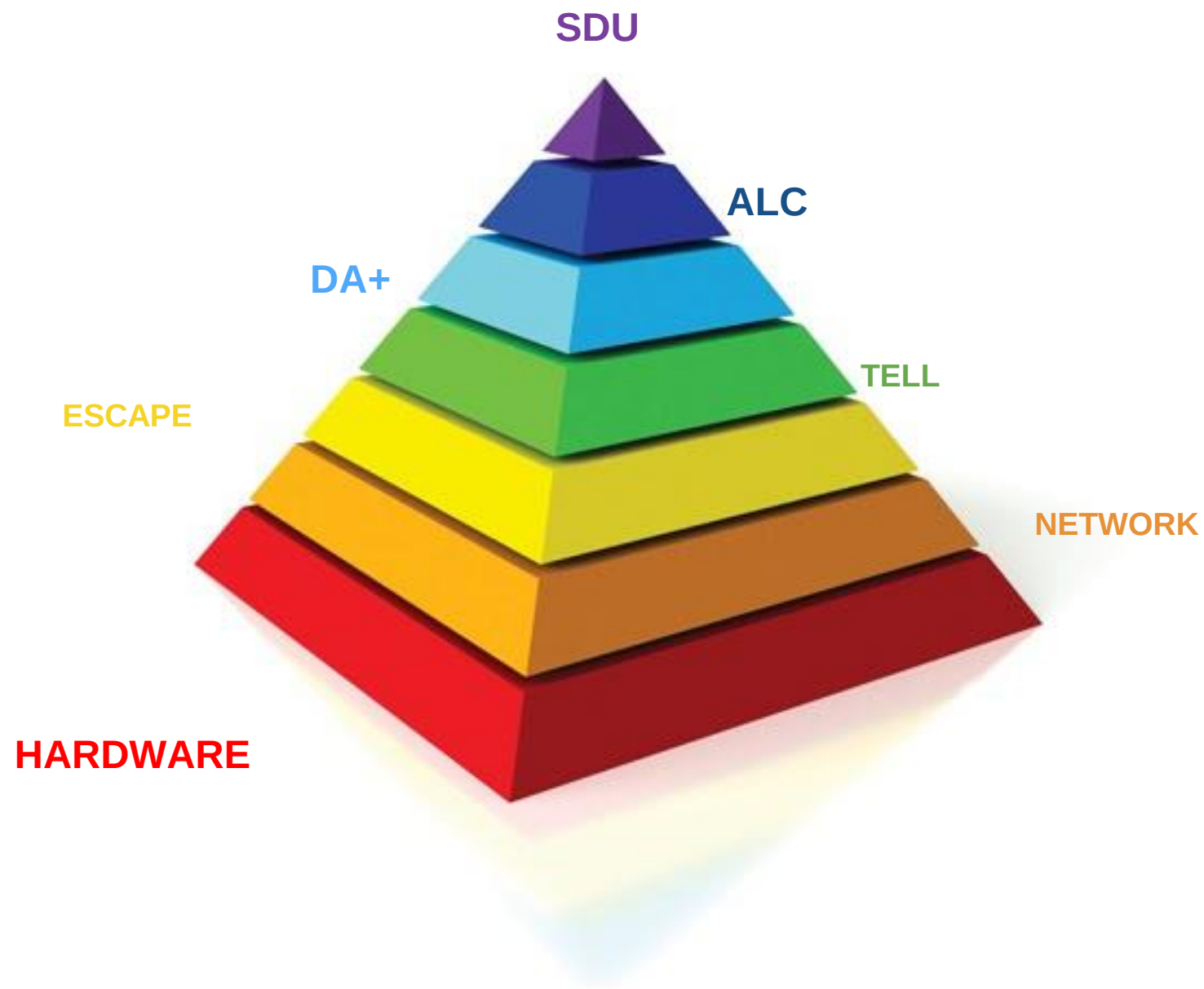


redis

Digital user



Smart Digital User SDU



- SDU automation control & progress via TELL GUI

TELL+ Sample Changer GUI

File Actions Options Sorting **Unattended** Simulation Help

Filter

Legend: running success skipped failed unknown

Samples

File: 20200928_V4_TELL_ALC_COPY01.xlsx
Number of Pucks: 5
Number of Samples: 79

Dewar	Puck	Location
Dewar-1	PSIMX119	C1
Dewar-1	PSIMX120	C2
Dewar-1	PSIMX121	C3
Dewar-1	PSIMX122	C4
Dewar-1	PSIMX091	C5

Safety	Mount	ALC	Diff. Center	DAQ	Dewar Loc.	Puck ID	Sample #	Prefix	Folder	Priority	# mounts	Comments
1	—	—	—	—	C1	PSIMX119	1	Nylon01	{date}/{prefix}	1	0	Empty
2	—	—	—	—	C1	PSIMX119	2	Nylon02	{date}/{prefix}	1	0	Empty
3	—	—	—	—	C1	PSIMX119	3	Nylon03	{date}/{prefix}	1	0	Empty
4	—	—	—	—	C1	PSIMX119	4	Nylon04	{date}/{prefix}	2	0	Empty
5	—	—	—	—	C1	PSIMX119	5	Nylon05	{date}/{prefix}	2	0	Empty
6	—	—	—	—	C1	PSIMX119	6	Nylon06	{date}/{prefix}	2	0	Empty
7	—	—	—	—	C1	PSIMX119	7	Nylon07	{date}/{prefix}	2	0	Empty
8	—	—	—	—	C1	PSIMX119	8	Nylon08	{date}/{prefix}	3	0	Empty
9	—	—	—	—	C1	PSIMX119	9	Nylon09	{date}/{prefix}	3	0	Empty
10	—	—	—	—	C1	PSIMX119	10	Nylon10	{date}/{prefix}	3	0	Empty
11	—	—	—	—	C1	PSIMX119	11	Nylon11	{date}/{prefix}	88	0	Empty
12	—	—	—	—	C1	PSIMX119	12	Nylon12	{date}/{prefix}	88	0	Empty
13	—	—	—	—	C1	PSIMX119	13	Nylon13	{date}/{prefix}	999	0	Empty
14	—	—	—	—	C1	PSIMX119	14	Nylon14	{date}/{prefix}	999	0	Empty

Mounted Sample Log messages

Name Comments

Priority

Required Res. (Å)

Spacegroup

Cell Parameters

Heavy atoms

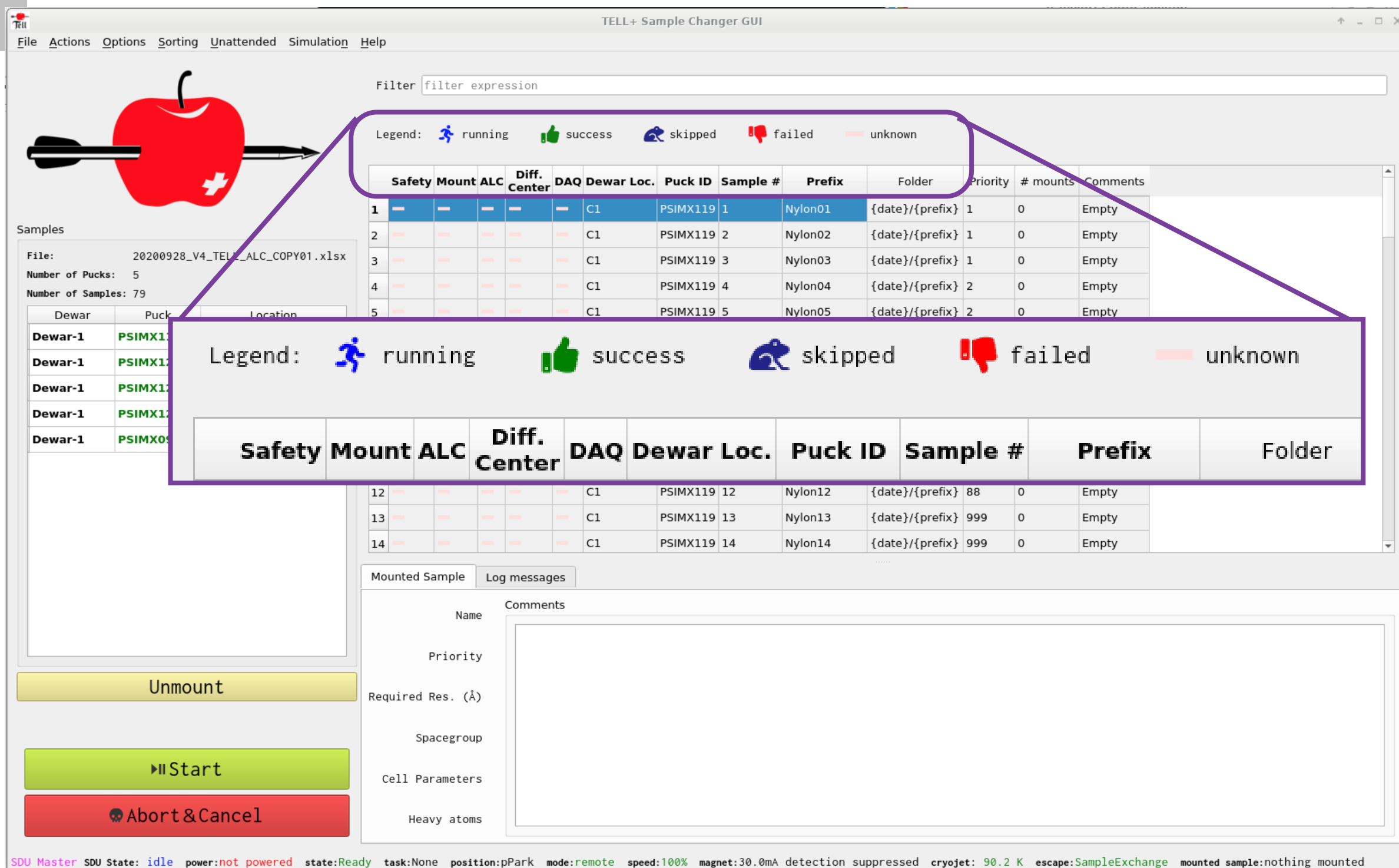
Unmount

▶ Start

⚠ Abort & Cancel

SDU Master SDU State: idle power: not powered state: Ready task: None position: pPark mode: remote speed: 100% magnet: 30.0mA detection suppressed cryojel: 90.2 K escape: SampleExchange mounted sample: nothing mounted

- SDU automation start & progress via TELL GUI



TELL+ Sample Changer GUI

File Actions Options Sorting Unattended Simulation Help

Filter

Legend: running success skipped failed unknown

	Safety	Mount	ALC	Diff. Center	DAQ	Dewar Loc.	Puck ID	Sample #	Prefix	Folder	Priority	# mounts	Comments
1	—	—	—	—	—	C1	PSIMX119	1	Nylon01	{date}/{prefix}	1	0	Empty
2	—	—	—	—	—	C1	PSIMX119	2	Nylon02	{date}/{prefix}	1	0	Empty
3	—	—	—	—	—	C1	PSIMX119	3	Nylon03	{date}/{prefix}	1	0	Empty
4	—	—	—	—	—	C1	PSIMX119	4	Nylon04	{date}/{prefix}	2	0	Empty
5	—	—	—	—	—	C1	PSIMX119	5	Nylon05	{date}/{prefix}	2	0	Empty
12	—	—	—	—	—	C1	PSIMX119	12	Nylon12	{date}/{prefix}	88	0	Empty
13	—	—	—	—	—	C1	PSIMX119	13	Nylon13	{date}/{prefix}	999	0	Empty
14	—	—	—	—	—	C1	PSIMX119	14	Nylon14	{date}/{prefix}	999	0	Empty

Mounted Sample Log messages

Name Comments

Priority

Required Res. (Å)

Spacegroup

Cell Parameters

Heavy atoms

Unmount

▶ Start

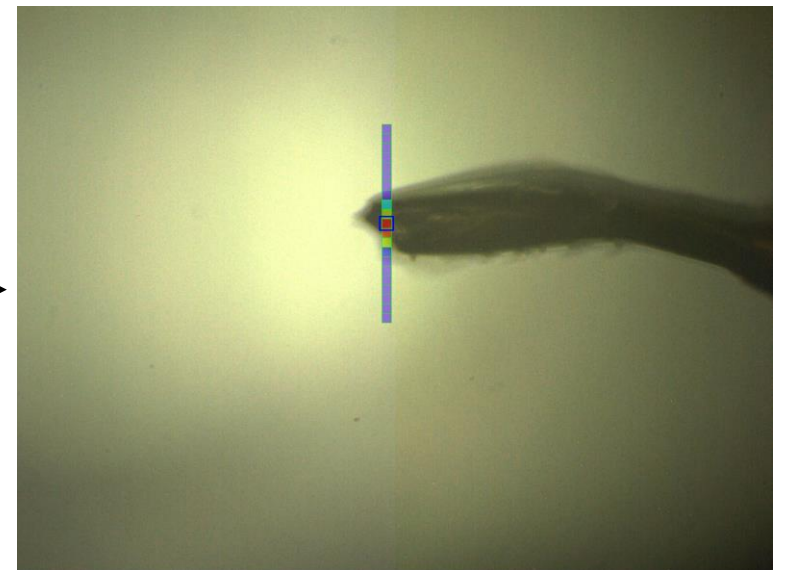
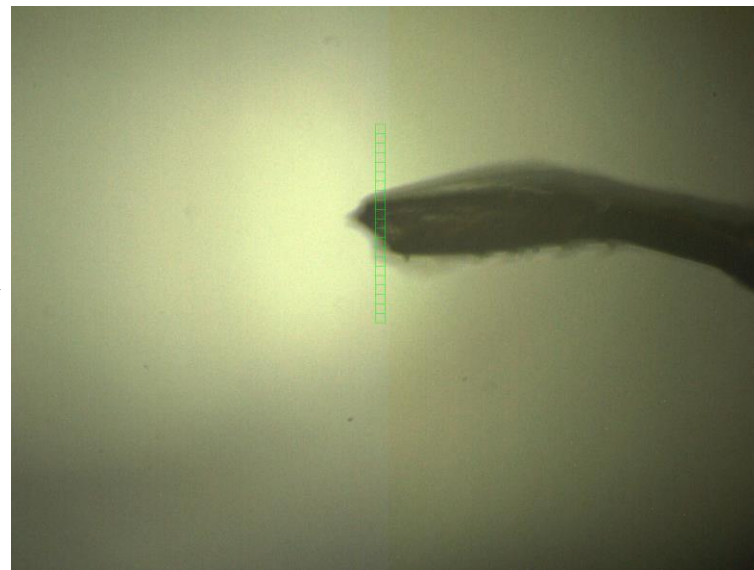
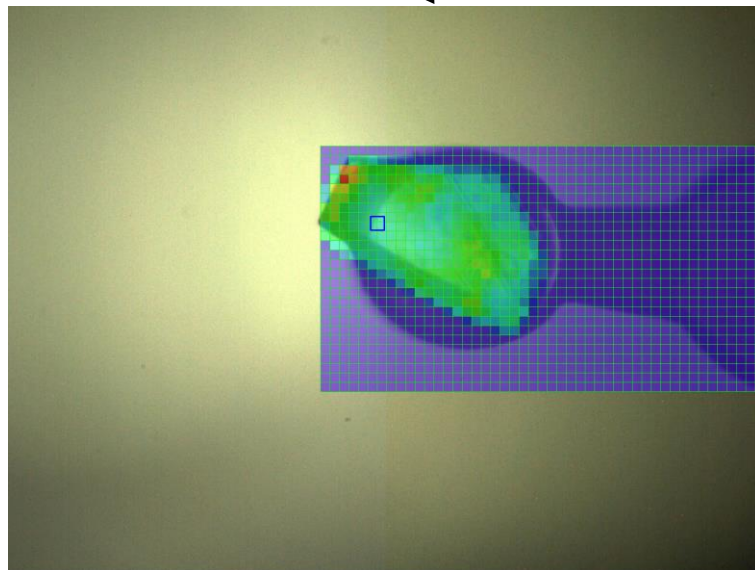
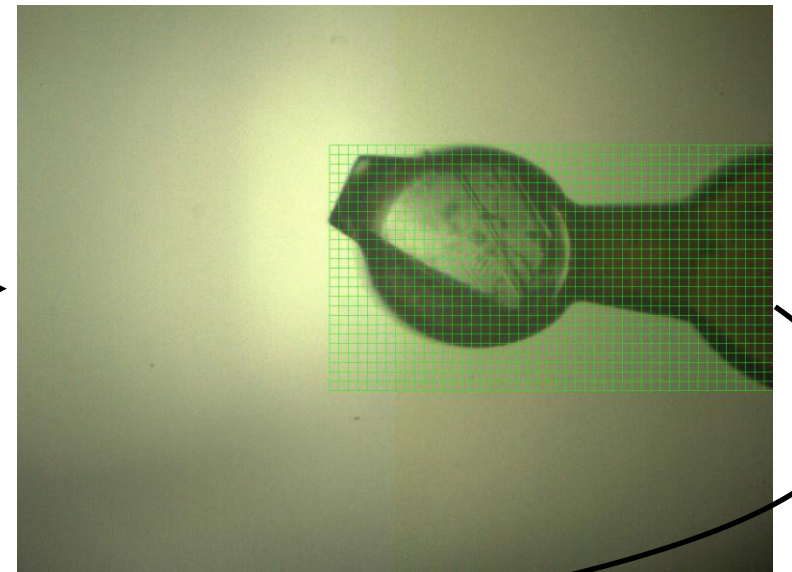
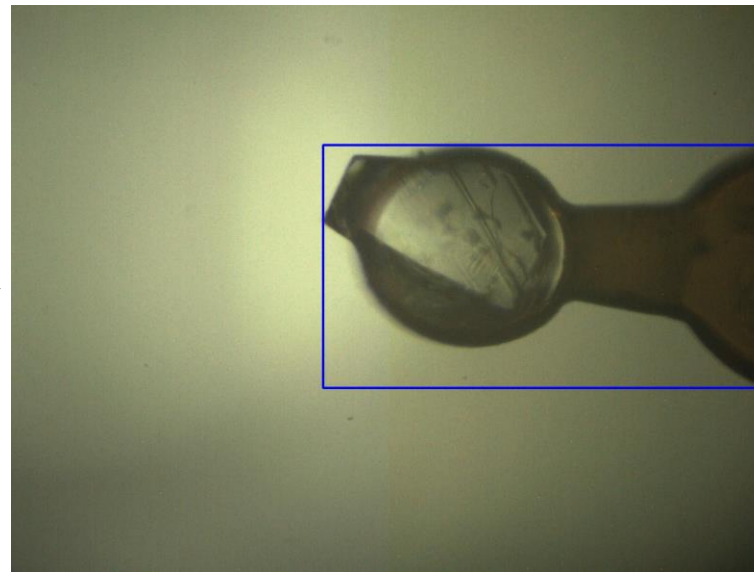
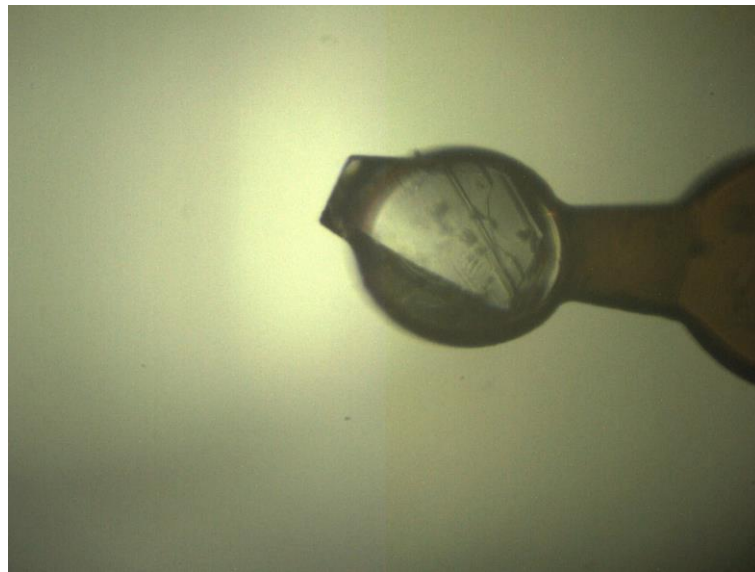
⚠ Abort & Cancel

SDU Master SDU State: idle power: not powered state: Ready task: None position: pPark mode: remote speed: 100% magnet: 30.0mA detection suppressed cryojet: 90.2 K escape: SampleExchange mounted sample: nothing mounted

Smart Digital User SDU

Legend:  running  success  skipped  failed  unknown

Safety Mount ALC	Diff. Center	DAQ Dewar Loc.	Puck ID	Sample #	Prefix	Folder
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Smart Digital User SDU

- SDU parameters are provided in the sample spreadsheet

Data Processing										
Processing Pipeline [str]	Space Group Number [1x int]	Cell Parameters [6x real number]	Res Cut Key [str]	Res Cut Value [float]	PDB Model [str]	Autoproc Full [bool]	Proc Full [bool]	No Ano [bool]	Trusted High [float]	FFCS campaign [bool]
autoproc	89	78 78 60 90 90 90	cchalf	60	my_lysozyme_model	True	False	True	0.9	True
autoproc	89	78 78 60 90 90 90	cchalf	30	my_lysozyme_model	True		False	0.9	True
autoproc	89	78 78 60 90 90 90	cchalf	20	my_lysozyme_model	True		False	0.9	True
autoproc	89	78 78 60 90 90 90	cchalf	20	my_lysozyme_model	True		False	0.9	True
autoproc	89	78 78 60 90 90 90	cchalf	20	my_lysozyme_model	True		False	0.9	True
autoproc	89	78 78 60 90 90 90	cchalf	20	my_lysozyme_model	True		False	0.9	True
autoproc	89	78 78 60 90 90 90	cchalf	20	my_lysozyme_model	True		False	1.1	True
autoproc	89	78 78 60 90 90 90	cchalf	20		True		False	1.1	True
autoproc	89	78 78 60 90 90 90	cchalf	20		True		False	1.1	True
autoproc	89	78 78 60 90 90 90	cchalf	20		True		True	1.1	True
autoproc	89	78 78 60 90 90 90	cchalf	20		True		True	1.1	True
autoproc	89	78 78 60 90 90 90	cchalf	20		True		True	1.1	True
autoproc	89	78 78 60 90 90 90	is	1.5		True		True	1.1	True
autoproc	89	78 78 60 90 90 90	is	1.5		True		True	1.1	True
autoproc	89	78 78 60 90 90 90	is	2.0		True		True	1.1	True
autoproc	89	78 78 60 90 90 90	is	2.0		True		True	1.1	True
autoproc	89	78 78 60 90 90 90	is	1.5	4y39_MOD.pdb				1.1	
autoproc	89	78 78 60 90 90 90	is	1.5	4y39_MOD.pdb		False		1.1	
autoproc	89	78 78 60 90 90 90	is	2.0	4y39_MOD.pdb		False		1.1	
autoproc	89	78 78 60 90 90 90	is	2.0	4y39_MOD.pdb		False		1.1	
gopy			is	2.0	4y39_MOD.pdb		False		1.1	
gopy			is	2.0	4y39_MOD.pdb				1.1	
gopy			is	2.0					1.1	
gopy			is	2.0					1.1	
gopy			is	2.0					1.1	
gopy			is	2.0					1.1	
gopy			is	2.0					1.1	
gopy			is	2.0					1.1	
gopy			cchalf	20	4y39_MOD.pdb				1.1	
gopy			cchalf	20	4y39_MOD.pdb				1.1	
Dewar-2	project078	0.1	0.02	180	20	1.5		standard	{prefix}	
Dewar-2	project078	0.1	0.02	180	20	1.5		standard	{prefix}	
Dewar-2	project078	0.1	0.02	180	20	2.5		standard	{prefix}	
Dewar-2	project078	0.1	0.02	180	20	2.5		standard	{prefix}	
Dewar-2	project078	0.1	0.02	180	20	2.5		standard	{prefix}	
Dewar-2	project078	0.1	0.02	180	20	2.5		standard	{prefix}	
Dewar-2	project078	0.1	0.02	180	20	2.5		standard	{prefix}	
Dewar-2	project078	0.1	0.02	180	20	2.5		standard	{prefix}	
Dewar-2	project078	0.1	0.02	180	20	2.5		standard	{prefix}	
Dewar-2	project078	0.1	0.02	180	20	2.5		standard	{prefix}	
Dewar-2	project078	0.1	0.02	180	20	2.5		standard	{prefix}	
Dewar-2	PSIMX-042	Unipuck	2	4504889	1	3	ZZZ- we can sort on comments too		{date}	{prefix}



Samples

File: 20200615_PX1_S1_evotec_sdu03.xlsx
Number of Pucks: 12
Number of Samples: 173

Dewar	Puck	Location
DLS-IN-0238	CPS-1528	B2
DLS-IN-0238	CPS-5496	B3
DLS-IN-0238	CPS-5502	B4
DLS-IN-0238	CPS-1103	B5
DLS-IN-0238	CPS-5499	C1
DLS-IN-0238	CPS-5501	C2
DLS-IN-0804	CPS-1106	A1
DLS-IN-0804	CPS-2238	A2
DLS-IN-0804	CPS-1527	A3
DLS-IN-0804	CPS-2239	A4
DLS-IN-0804	CPS-5497	A5
DLS-IN-0804	CPS-1525	B1

Filter

	Safety	Mount	ALC	Diff. Center	DAQ	Dewar Loc.	Puck ID	Sample #	Prefix	Folder	Priority	# mounts	Comments
121	👍	👍	👍	👍	👍	A5	CPS-5497	12	0026194_1_4257b	SLS_15-06-2020/bk/Ursa/0026194_1_4257b	2	1	
122	👍	👍	👍	👍	👍	A5	CPS-5497	14	0026196_1_4469b	SLS_15-06-2020/bk/Ursa/0026196_1_4469b	2	1	
123	👍	👍	👍	👍	👍	A5	CPS-5497	16	0026198_1_5093b	SLS_15-06-2020/bk/Ursa/0026198_1_5093b	2	1	
124	👍	👍	👍	👍	👍	C1	CPS-5499	3	0026218_1_LC4_3	SLS_15-06-2020/nbk/lapis/0026218_1_LC4_3	2	1	
125	👍	👍	👍	👍	👍	C1	CPS-5499	5	0026220_1_D866b	SLS_15-06-2020/bk/dolly/0026220_1_D866b	2	1	
126	👍	👍	👍	👍	👍	C1	CPS-5499	8	0026223_1_D866c	SLS_15-06-2020/bk/dolly/0026223_1_D866c	2	1	
127	👍	👍	👍	👍	👍	C1	CPS-5499	10	0026225_1_K797b	SLS_15-06-2020/nbk/keanu/0026225_1_K797b	2	1	
128	👍	👍	👍	👍	👍	C1	CPS-5499	12	0026227_1_K797d	SLS_15-06-2020/nbk/keanu/0026227_1_K797d	2	1	
129	👍	👍	👍	👍	👍	C1	CPS-5499	14	0026229_1_K797f	SLS_15-06-2020/nbk/keanu/0026229_1_K797f	2	1	
130	👍	👍	👍	👍	👍	C2	CPS-5501	6	0026098_1_3413f	SLS_15-06-2020/bk/celin/0026098_1_3413f	2	1	
131	👍	👍	👍	👍	👍	C2	CPS-5501	7	0026099_1_3413g	SLS_15-06-2020/bk/celin/0026099_1_3413g	2	1	
132	👍	👍	👍	👍	👍	C2	CPS-5501	9	0026101_1_5144a	SLS_15-06-2020/bk/celin/0026101_1_5144a	2	1	
133	👍	👍	👍	👍	👍	C2	CPS-5501	10	0026102_1_5144b	SLS_15-06-2020/bk/celin/0026102_1_5144b	2	1	
134	👍	👍	👍	👍	👍	C2	CPS-5501	11	0026103_1_5144c	SLS_15-06-2020/bk/celin/0026103_1_5144c	2	1	
135	👍	👍	👍	👍	👍	C2	CPS-5501	12	0026104_1_5144d	SLS_15-06-2020/bk/celin/0026104_1_5144d	2	1	
136	👍	👍	👍	👎	👎	B4	CPS-5502	15	0026120_1_C0051	SLS_15-06-2020/bk/tyran2/0026120_1_C0051	2	1	
137	👍	👎	👎	👎	👎	B4	CPS-5502	16	0026121_1_C0052	SLS_15-06-2020/bk/tyran2/0026121_1_C0052	2	2	
138	👍	👍	👍	👍	👍	B5	CPS-1103	3	0026145_1_4093c	SLS_15-06-2020/bk/molly/0026145_1_4093c	3	1	
139	👍	👍	👍	👎	👎	A1	CPS-1106	1	0026262_1_x1080	SLS_15-06-2020/bk/Odin/0026262_1_x1080	3	1	
140	👍	👍	👍	👍	👍	A1	CPS-1106	2	0026263_1_x1081	SLS_15-06-2020/bk/Odin/0026263_1_x1081	3	1	
141	👍	👍	👍	👍	👍	A1	CPS-1106	3	0026264_1_x1082	SLS_15-06-2020/bk/Odin/0026264_1_x1082	3	1	
142	👍	👍	👍	👍	👍	A1	CPS-1106	4	0026265_1_x1083	SLS_15-06-2020/bk/Odin/0026265_1_x1083	3	1	
143	👍	👍	👍	👍	👍	A1	CPS-1106	5	0026266_1_x1084	SLS_15-06-2020/bk/Odin/0026266_1_x1084	3	1	
144	👍	👍	👍	👍	👍	B1	CPS-1525	2	0026231_1_x1065	SLS_15-06-2020/bk/Odin/0026231_1_x1065	3	1	
145	👍	👍	👍	👍	👍	B1	CPS-1525	3	0026236_1_x1066	SLS_15-06-2020/bk/Odin/0026236_1_x1066	3	1	
146	👍	👍	👍	👍	👍	B1	CPS-1525	5	0026240_1_x1068	SLS_15-06-2020/bk/Odin/0026240_1_x1068	3	1	
147	👍	👍	👍	👍	👍	B1	CPS-1525	6	0026241_1_x1069	SLS_15-06-2020/bk/Odin/0026241_1_x1069	3	1	
148	👍	👍	👍	👍	👍	B1	CPS-1525	8	0026244_1_x1071	SLS_15-06-2020/bk/Odin/0026244_1_x1071	3	1	
149	👍	👍	👍	👎	👎	B1	CPS-1525	10	0026248_1_x1073	SLS_15-06-2020/bk/Odin/0026248_1_x1073	3	1	
150	👍	👍	👍	👍	👍	B1	CPS-1525	11	0026250_1_x1074	SLS_15-06-2020/bk/Odin/0026250_1_x1074	3	1	

Mounted Sample

Name 0026255_1_x1076

Priority 3

Required Res. (Å)

Spacegroup P1

Cell Parameters

Heavy atoms

Comments

CPS-1525/0026255_1_x1076

SDU Master SDU State: active power:powered state:Ready task:None position:pCold mode:remote speed:100% magnet:50.0mA detection suppressed cryojel: 100.0 K escape:DataCollection mounted sample:B1-13

TELL+ Sample Changer GUI

File Actions Options Sorting Unattended Help

Filter



Samples

File: 20200615_PX1_S1_evotec_sdu03.xlsx
Number of Pucks: 12
Number of Samples: 173

Dewar	Puck	Location
DLS-IN-0238	CPS-1528	B2
DLS-IN-0238	CPS-5496	B3
DLS-IN-0238	CPS-5502	B4
DLS-IN-0238	CPS-1103	B5
DLS-IN-0238	CPS-5499	C1
DLS-IN-0238	CPS-5501	C2
DLS-IN-0804	CPS-1106	A1
DLS-IN-0804	CPS-2238	A2
DLS-IN-0804	CPS-1527	A3
DLS-IN-0804	CPS-2239	A4
DLS-IN-0804	CPS-5497	A5
DLS-IN-0804	CPS-1525	B1

Safety	Mount	ALC	Diff. Center	DAQ	Dewar Loc.	Puck ID	Sample #	Prefix	Folder	Priority	# mounts	Comments
121	👍	👍	👍	👍	A5	CPS-5497	12	0026194_1_4257b	SLS_15-06-2020/bk/Ursa/0026194_1_4257b	2	1	
122	👍	👍	👍	👍	A5	CPS-5497	14	0026196_1_4469b	SLS_15-06-2020/bk/Ursa/0026196_1_4469b	2	1	
123	👍	👍	👍	👍	A5	CPS-5497	16	0026198_1_5093b	SLS_15-06-2020/bk/Ursa/0026198_1_5093b	2	1	
124	👍	👍	👍	👍	C1	CPS-5499	3	0026218_1_LC4_3	SLS_15-06-2020/nbk/lapis/0026218_1_LC4_3	2	1	
125	👍	👍	👍	👍	C1	CPS-5499	5	0026220_1_D866b	SLS_15-06-2020/bk/dolly/0026220_1_D866b	2	1	
126	👍	👍	👍	👍	C1	CPS-5499	8	0026223_1_D866c	SLS_15-06-2020/bk/dolly/0026223_1_D866c	2	1	
127	👍	👍	👍	👍	C1	CPS-5499	10	0026225_1_K797b	SLS_15-06-2020/nbk/keanu/0026225_1_K797b	2	1	
128	👍	👍	👍	👍	C1	CPS-5499	12	0026227_1_K797d	SLS_15-06-2020/nbk/keanu/0026227_1_K797d	2	1	
129	👍	👍	👍	👍	C1	CPS-5499	14	0026229_1_K797f	SLS_15-06-2020/nbk/keanu/0026229_1_K797f	2	1	
130	👍	👍	👍	👍	C2	CPS-5501	6	0026098_1_3413f	SLS_15-06-2020/bk/celin/0026098_1_3413f	2	1	
131	👍	👍	👍	👍	C2	CPS-5501	7	0026099_1_3413g	SLS_15-06-2020/bk/celin/0026099_1_3413g	2	1	
132	👍	👍	👍	👍	C2	CPS-5501	9	0026101_1_5144a	SLS_15-06-2020/bk/celin/0026101_1_5144a	2	1	
133	👍	👍	👍	👍	C2	CPS-5501	10	0026102_1_5144b	SLS_15-06-2020/bk/celin/0026102_1_5144b	2	1	
134	👍	👍	👍	👍	C2	CPS-5501	11	0026103_1_5144c	SLS_15-06-2020/bk/celin/0026103_1_5144c	2	1	
135	👍	👍	👍	👍	C2	CPS-5501	12	0026104_1_5144d	SLS_15-06-2020/bk/celin/0026104_1_5144d	2	1	
136	👍	👍	👍	🐼	B4	CPS-5502	15	0026120_1_C0051	SLS_15-06-2020/bk/tyran2/0026120_1_C0051	2	1	
137	👍	👎	🐼	🐼	B4	CPS-5502	16	0026121_1_C0052	SLS_15-06-2020/bk/tyran2/0026121_1_C0052	2	2	
138	👍	👍	👍	👍	B5	CPS-1103	3	0026145_1_4093c	SLS_15-06-2020/bk/molly/0026145_1_4093c	3	1	
139	👍	👍	👍	👍	A1	CPS-1106	1	0026262_1_x1080	SLS_15-06-2020/bk/Odin/0026262_1_x1080	3	1	
140	👍	👍	👍	👍	A1	CPS-1106	2	0026263_1_x1081	SLS_15-06-2020/bk/Odin/0026263_1_x1081	3	1	
141	👍	👍	👍	👍	A1	CPS-1106	3	0026264_1_x1082	SLS_15-06-2020/bk/Odin/0026264_1_x1082	3	1	

135	👍	👍	👍	👍	👍	C2	CPS-5501	12
136	👍	👍	👍	🐼	🐼	B4	CPS-5502	15
137	👍	👎	🐼	🐼	🐼	B4	CPS-5502	16
138	👍	👍	👍	👍	👍	B5	CPS-1103	3

CPS-

Required Res. (Å)

Spacegroup P1

Cell Parameters

Heavy atoms

▶Pause

⏏Abort & Cancel

SDU Master SDU State: active power:powered state:Ready task:None position:pCold mode:remote speed:100% magnet:50.0mA detection suppressed cryojet: 100.0 K escape:DataCollection mounted sample:B1-13

Summary for all Samples

Sample Name	Initial Checks	Optical Alignment	Diffraction align.		Thumbnails		
			Grid Scan	Line Data Collection	Sample	Grid Scan	Line Scan
lyso_1							
lyso_2							
lyso_3							
lyso_4							
lyso_5							
lyso_6							
lyso_7							

- v1.0 released at PXI and PXIII
 - 18-20 samples/hr PXI
 - 10-12 samples/hr PXIII
- Future
 - PXII
 - beam size & energy changes (PXI)
 - serial-xtal

Summary

- Continuous MX software development
- Towards full automation
 - TELL GUI
 - Automatic Loop Centring ALC
 - Smart Digital User SDU

Acknowledgements

- MX Data
 - Justyna Wojdyla
 - Zac Panepucci
 - Filip Leonarski
 - Kate Smith
- Jakub Kaminski
- Shibom Basu
- Simon Ebner
- Isabelle Martiel
- MX team
- Controls
- IT support



<https://www.psi.ch/macromolecular-crystallography/>

Thank you



- setup modes (when do we skip samples)
 - default
 - weak
 - always-collect

```
if self.type == 'weak':
    my_hub.put(sdu_grid_lowResSpotThreshold=5.0)
    my_hub.put(sdu_grid_threshold=10.0)
    my_hub.put(sdu_grid_override=False)
elif self.type == 'always-collect':
    my_hub.put(sdu_grid_lowResSpotThreshold=20.0)
    my_hub.put(sdu_grid_threshold=30.0)
    my_hub.put(sdu_grid_override=True)
else:
    my_hub.put(sdu_grid_lowResSpotThreshold=20.0)
    my_hub.put(sdu_grid_threshold=30.0)
    my_hub.put(sdu_grid_override=False)
```

```
{
  "x06sa": {
    "sdu_grid_lowResSpotThreshold": "20.0",
    "sdu_grid_verticalExposure": "0.05",
    "sdu_grid_boxExposure": "0.02",
    "sdu_grid_threshold": "30.0",
    "sdu_grid_verticalTransmission": "1",
    "sdu_grid_override": "False",
    "sdu_grid_boxTransmission": "1"
  }
}
```