



MxCuBE2



WHY A NEW MXCUBE?

- Evaluate and collect of MASSIF samples
- Fully exploit μ beam capabilities
- Describe and perform (automagically) more complex experiments
- A control software shared on different MX beamlines at different SR sources
 - Different hardware same GUI
 - Easy to install and maintain

CONVENTO DO CRISTO, TOMAR, PORTUGAL



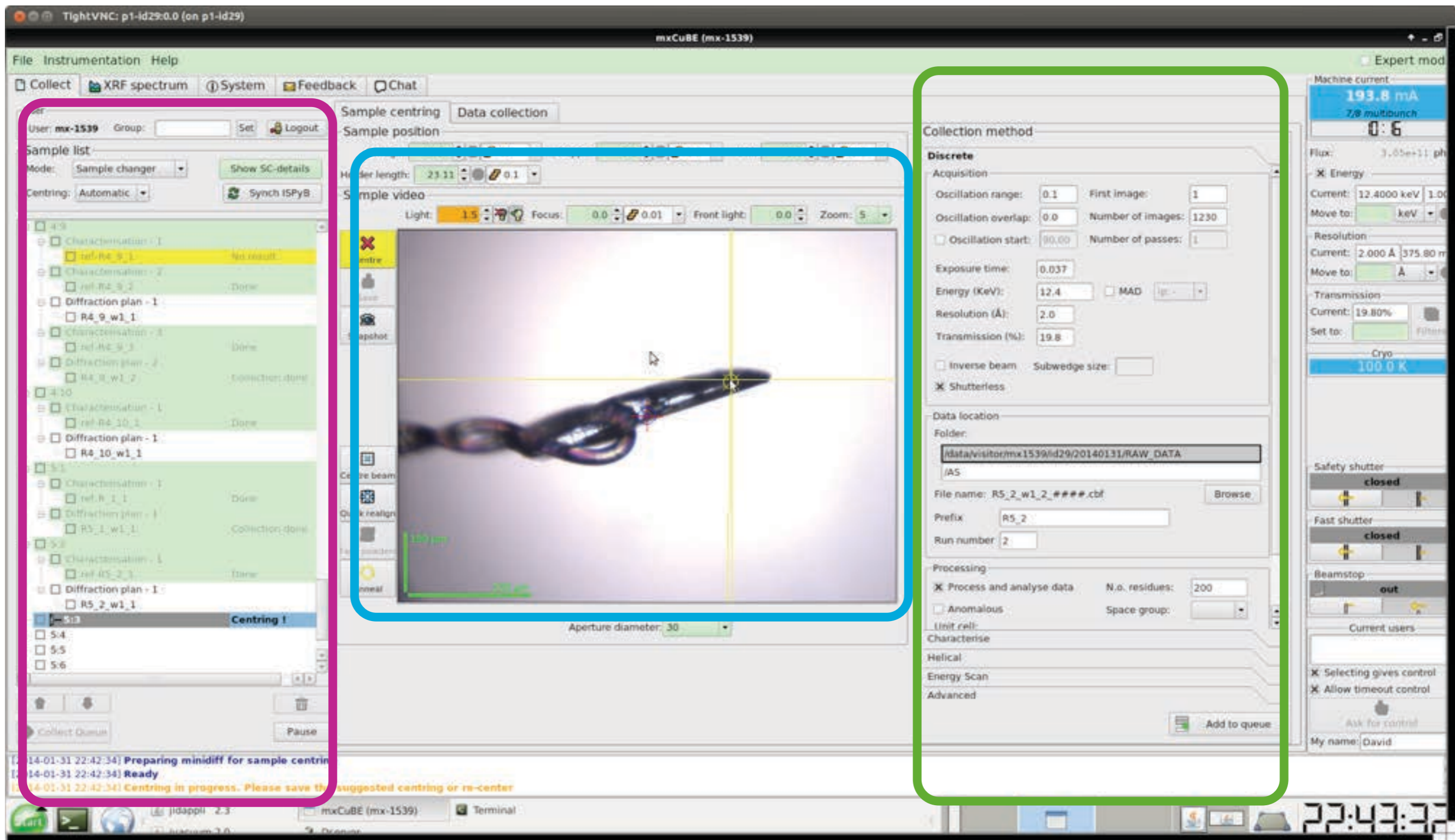
Romanesque, Gothic, Manueline and Renaissance
architectural styles

all together

as MxCuBE v1

- After ESRF long shutdown (May 2012)
 - Abstraction level introduced
 - Roots for new version
- Design of new GUI
 - New functionalities
 - New concept
- April 2013 - third mxCuBE workshop
 - Agreements on common and specific needs
- September 2013 - deployment
- February 2014 - release of v2.0.9

- Which sample(s)?
- Where? (Which position(s)?)
- What? (Which task(s)?)



SC - Queue

Sample - Position

Tasks - Data Collection

Which? Where? What?

Combinations are infinite. For example:

- Collect a MAD with energy scan at N different positions
- Collect the same Data collection (or characterisation, or ...) over N samples
- Collect the same Data collection over N positions on one sample
- Any parameter (including centered position) can still be edited before collection
-

Sample list

Mode: Sample changer Show SC-details

Centring: Automatic Synch ISPyB

- 4.9
 - Characterisation - 1
 - ref-R4_9_1 No result
 - Characterisation - 2
 - ref-R4_9_2 Done
 - Diffraction plan - 1
 - R4_9_w1_1
 - Characterisation - 3
 - ref-R4_9_3 Done
 - Diffraction plan - 2
 - R4_9_w1_2 Collection done
- 4.10
 - Characterisation - 1
 - ref-R4_10_1 Done
 - Diffraction plan - 1
 - R4_10_w1_1
- 5.1
 - Characterisation - 1
 - ref-R_1_1 Done
 - Diffraction plan - 1
 - R5_1_w1_1 Collection done
- 5:2 Centring done !
- 5:3
- 5:4
- 5:5
- 5:6
- 5:7
- 5:8
- 5:9
- 5:10

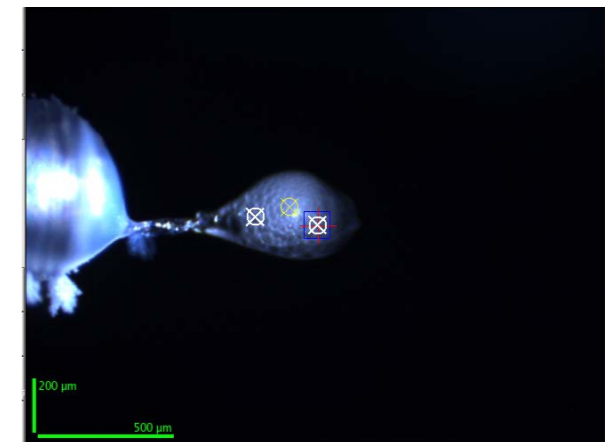
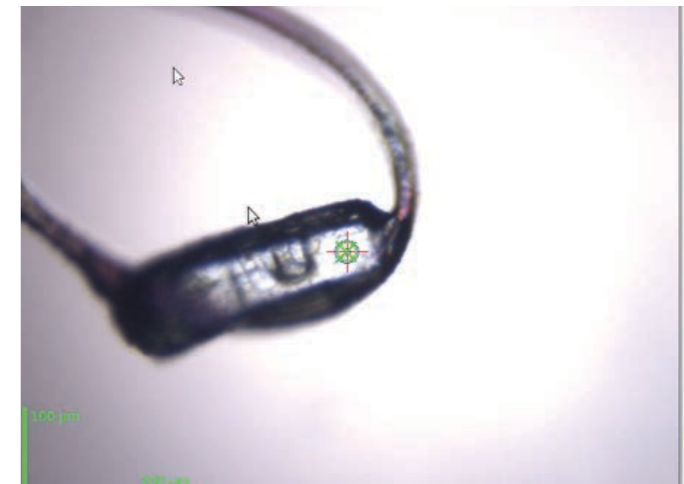
Characterization no strategy

Successful Characterization

Proposed Diffraction plan

Collected Diffraction plan

Mounted sample and status



DETAILS - DATA COLLECTION


Sample centring | **Data collection**

Data location
Folder: /data/visitor/mx1539/id29/20140131/RAW_DATA /AS
File name: R5_2_w1_1_####.cbf
Prefix: R5_2 Run number: 1

Acquisition
 Oscillation start: 63.0 Oscillation range: 0.1 Oscillation overlap: 0.0
First image: 1 Number of images: 1230 Number of passes: 1
Transmission (%): 42.62 Resolution (Å): 2.23 Energy (KeV): 12.4
Exposure time: 0.037 MAD ip: -
 Shutterless

Processing
 Process and analyse data N.o. residues: 200
 Anomalous Space group:
Unit cell:
a: 0 b: 0 c: 0
 α : 0 β : 0 γ : 0

Centred position



Diffraction plan details

DETAILS - CHARACTERIZATION

Sample centring Characterisation

Reference images

Acquisition parameters

Data location

Folder: /data/id14eh4/inhouse/opid144/20131030/RAW_DATA/

File name: ref-opid144_1_###.img

Prefix: Run number:

Acquisition


Oscillation start: Oscillation range: Oscillation overlap:

First image: Number of images: Number of passes:

Transmission (%): Resolution (Å): Energy (KeV):

Exposure time: MAD

Centred position



Characterisation type

Routine-DC

Use min dose Dose limit MGy:

Use min time Total time limit (s):

Account for radiation damage

SAD

Radiation damage

Radiation damage model

β Å²/MGy:

γ 1/MGy:

Sensetivity:

Crystal

Space group:

Vertical crystal dimension (mm):

Min: Max:

ω at min: ω at max:

Optimization parameters

Aimed l/σ at highest resolution: Strategy complexity:

Aimed completeness: Use permitted rotation range:

Maximum resolution: ω -start:

Aimed multiplicity: ω -end:

Calculate low resolution pass strategy

Characterization details

DETAILS - CHARACTERIZATION RESULTS

Sample centring Characterisation

Forced space group	Anomalous data	Aimed multiplicity	Aimed completeness	Aimed I/sigma at highest res.	Aimed resolution (Å)
	False	4.00	0.99	3.00	1.00

Characterization details (results)

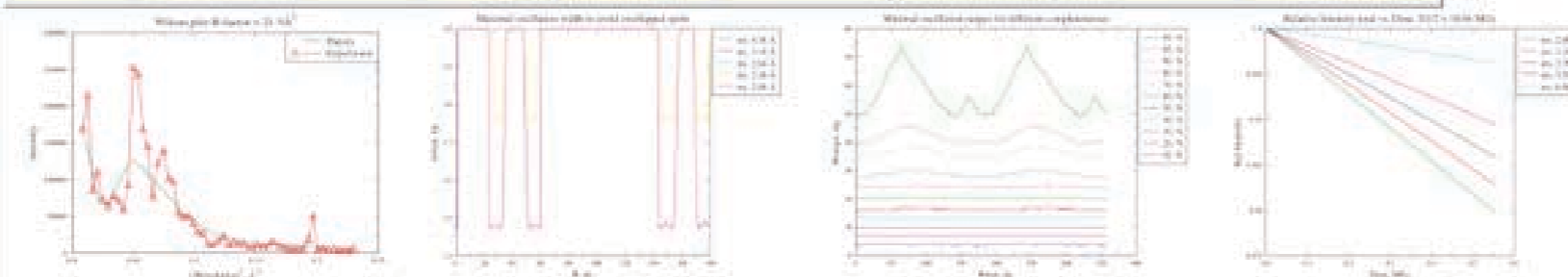
Collection plan strategy ([RADDPOSE log file](#) , [BEST log file](#))

Best has detected that the sample can diffract to 1.73 Å!

The current strategy is calculated to 2.06 Å. In order to calculate a strategy to 1.73 Å move the detector to collect 1.73 Å data and re-launch the EDNA characterisation.

Resolution limit is set by the initial image resolution

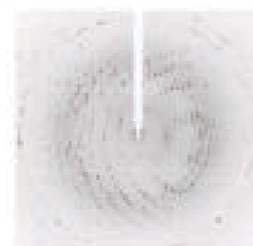
Wedge	Subwedge	Start (°)	Width (°)	No images	Exp time (s)	Max res (Å)	Rel trans (%)	Distance (mm)
1	1	48.00	1.45	86	0.10	2.06	49.63	302.23



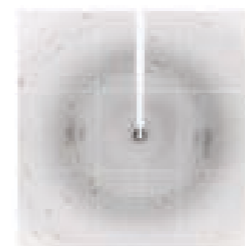
Indexing summary: Selected spacegroup: P3, forced space group:

Refined unit cell parameters (Å/degrees)					
a (Å)	b (Å)	c (Å)	alpha (°)	beta (°)	gamma (°)
54.745	54.745	107.776	90.000	90.000	120.000

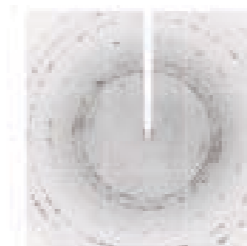
[Indexing log file](#)



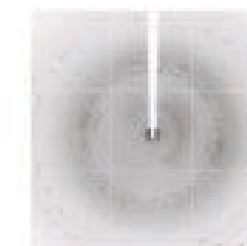
ref-opid144_1_0003.img



ref-opid144_1_0004.img



ref-opid144_1_0002.img



ref-opid144_1_0001.img

- [Integration log file 1](#)
- [Integration log file 2](#)
- [Integration log file 3](#)
- [Integration log file 4](#)

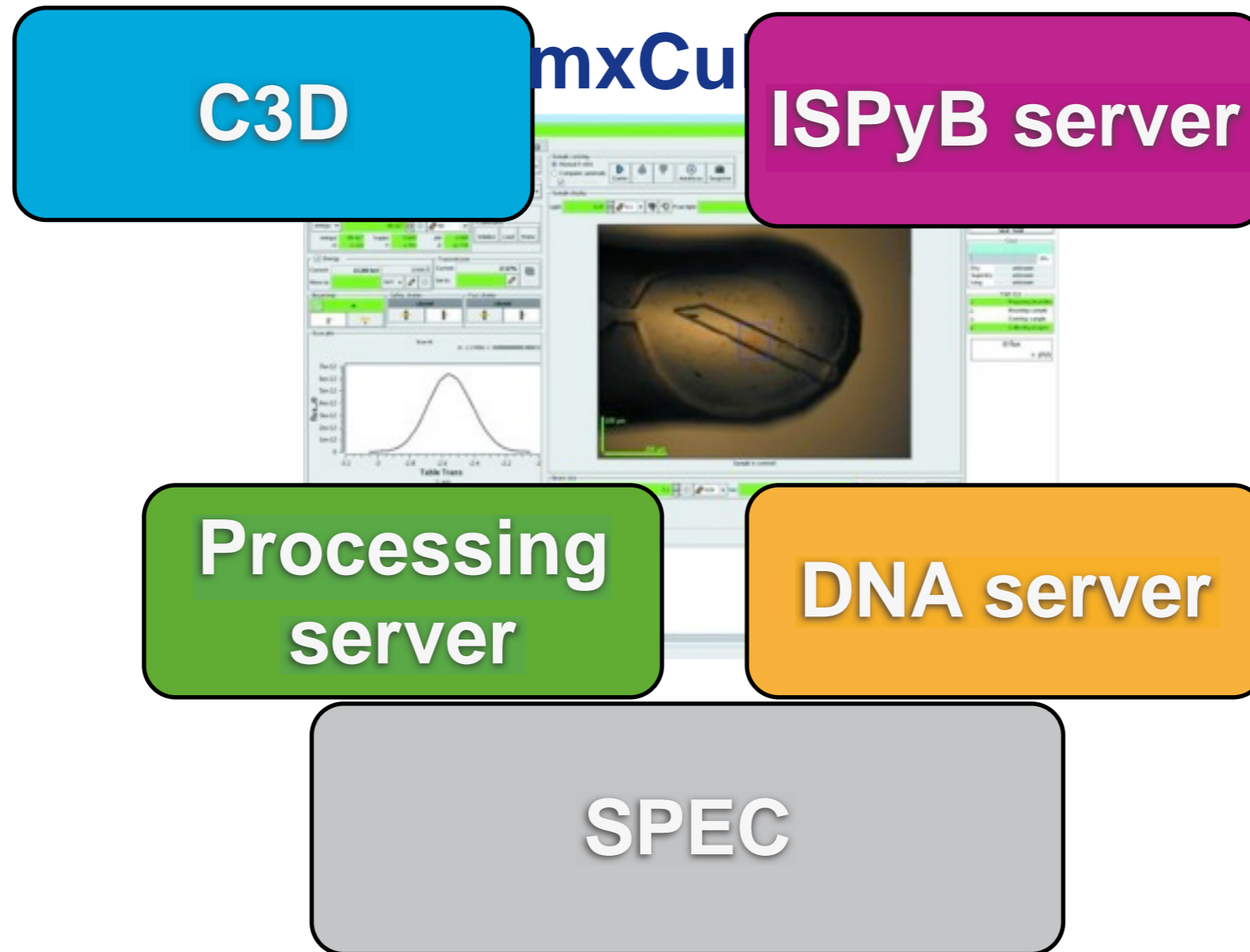
Image quality indicators

File	Tot integr signal	Spot total	In-Res Total	Good Bragg	Ice Rings	Meth 1 Res	Meth 2 Res	Max unit cell
ref-opid144_1_0001.img	593418	398	297	207	9	2.70	3.44	444.0
ref-opid144_1_0002.img	13704880	964	885	528	10	2.10	2.09	205.2

View parameter



SIMPLER AND ROBUST

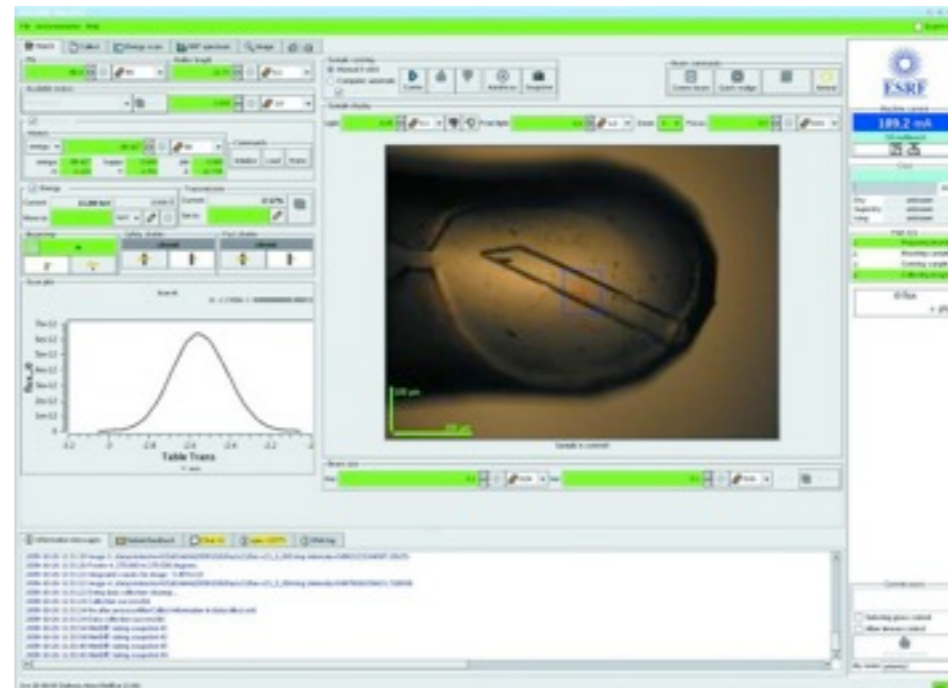


SIMPLER AND ROBUST

C3D

ISPyB server

mxCuBE



Processing
server

SPEC

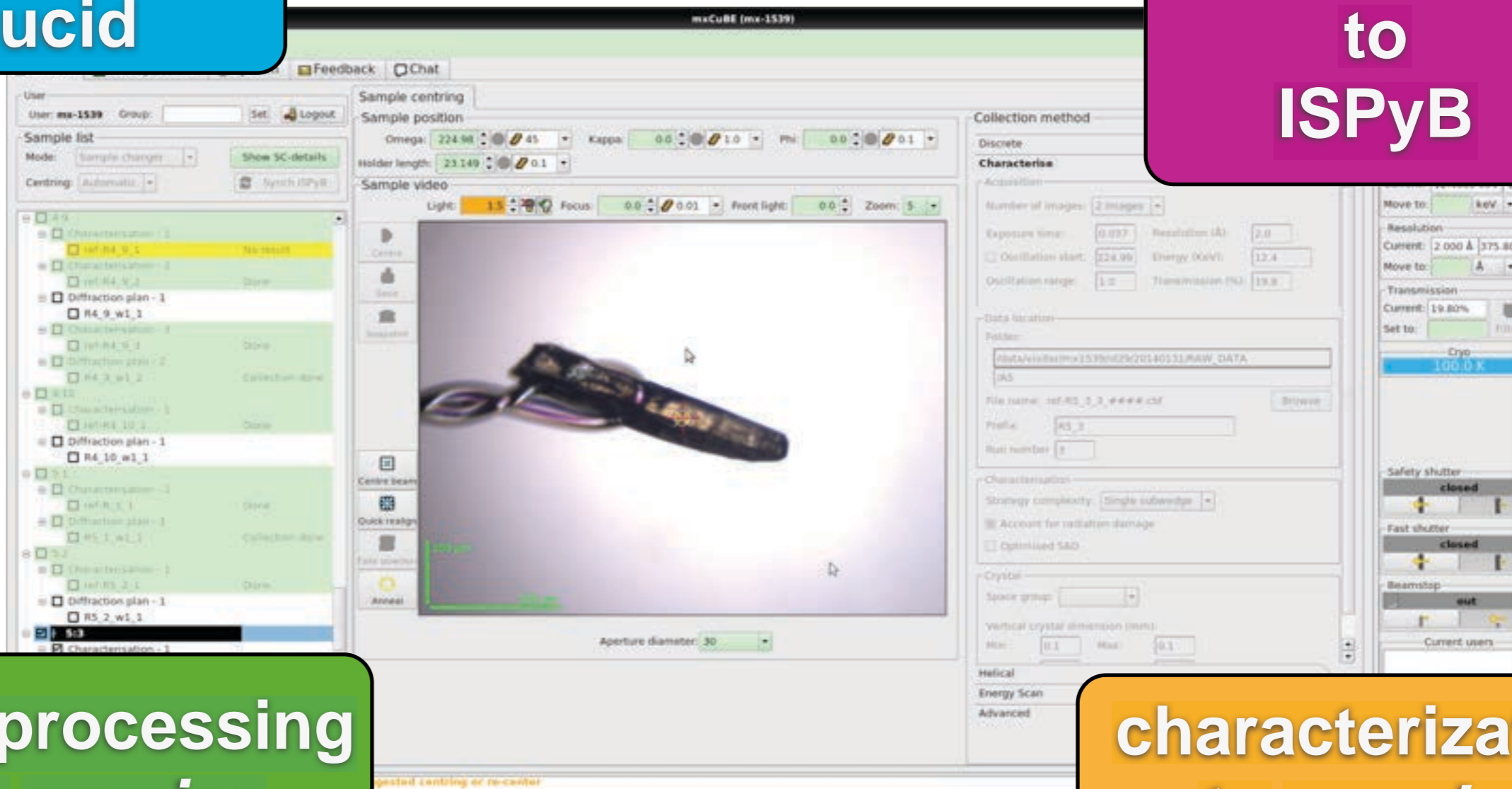
DNA server

SIMPLER AND ROBUST

MxCuBE2

lucid

webservices
to
ISPyB

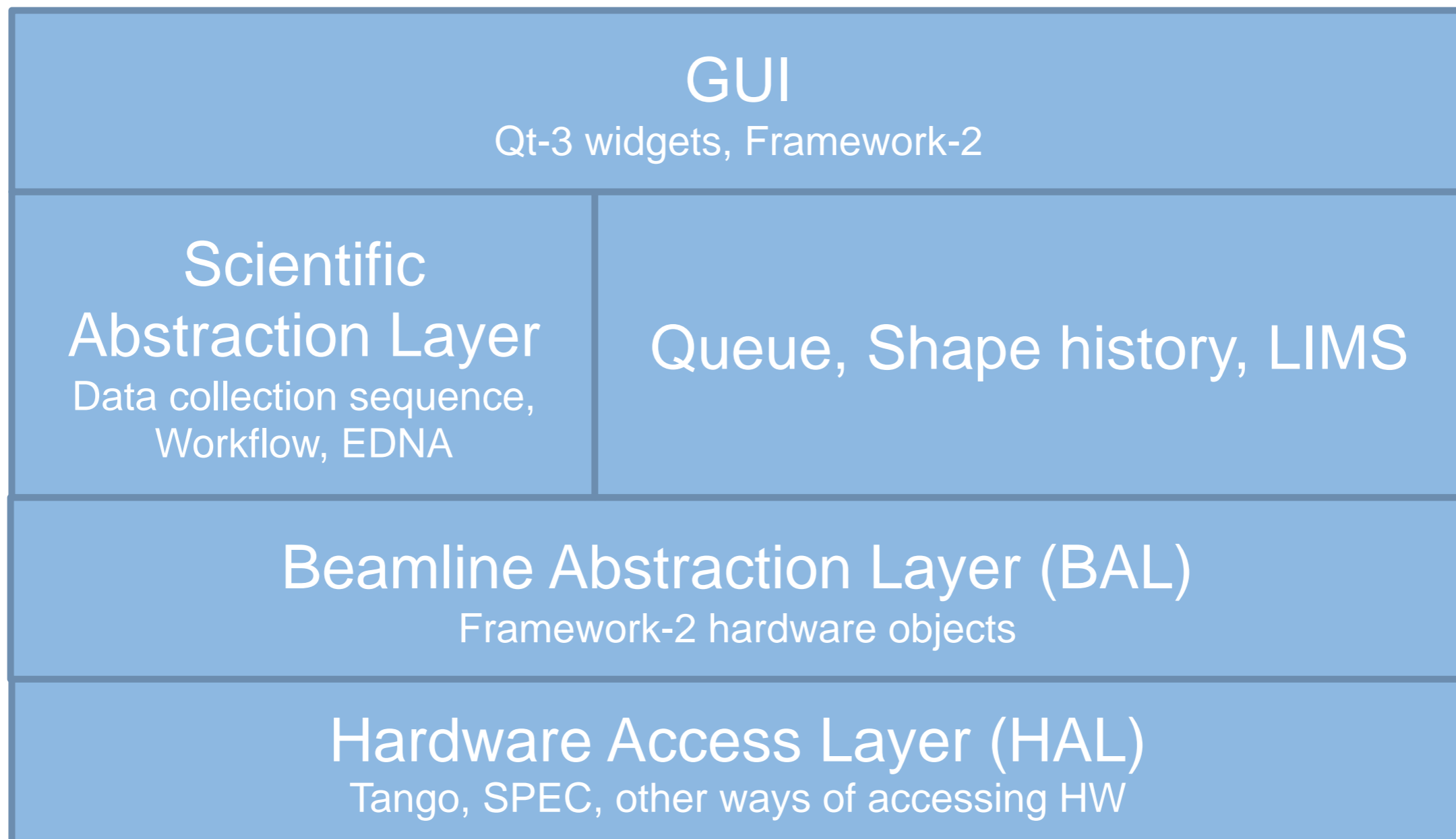


autoprocessing
to *mxnice*

characterization
to *mxedna*

SPEC

MXCUBE2 STRUCTURE



BETTER AND EASIER INTEGRATION WITH ISPYB

- Sample location
- 1:1 - TRYP-sample1
 - 1:2 - TRYP-sample2
 - 1:3 - TRYP-sample3
 - 1:4 - TRYP-sample4
 - 1:5 - FAE-sample5
 - 1:6 - FAE-sample6
 - 1:7 - FAE-sample7

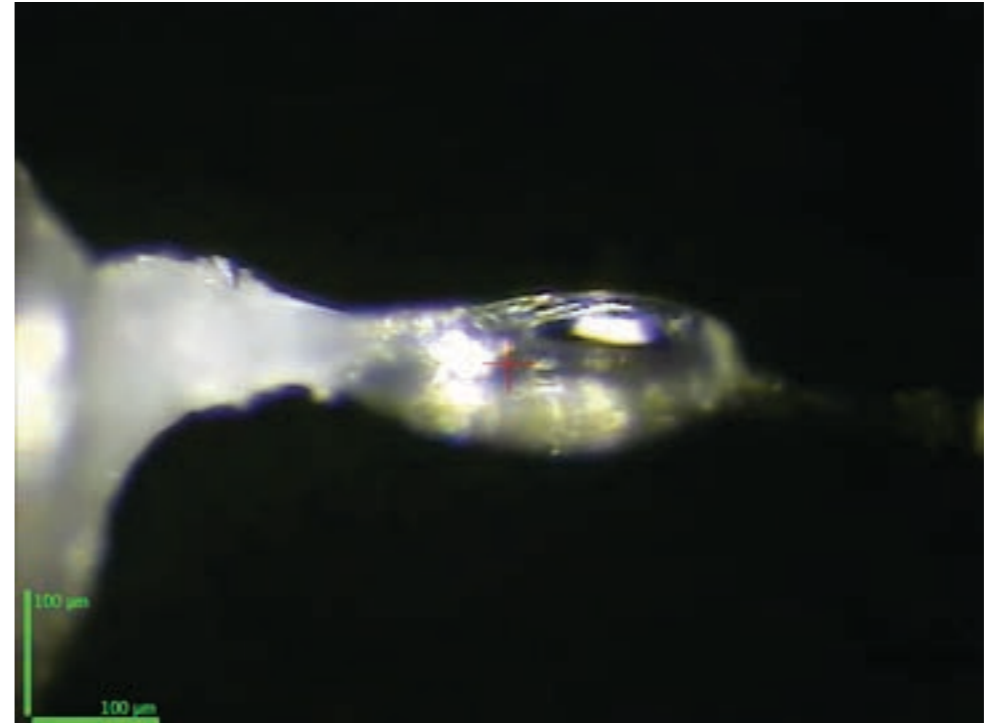
Sample list

Image Prefix	Run No	Experiment Type	Protein Acronym	Start Time	# images	Experiment Parameters (Expand)	Status	Space Group	Completeness	Reso
4_w1	1	OSC		03-02-2014 12:08:50	2000	(i)	●●●●	P 1 21 1	100.0 2.23 100.0	
ref-4	1	Characterization		03-02-2014 12:05:55	2	(i)	●●●●	P2		2
3_w1	1	OSC		03-02-2014 12:00:05	2000	(i)	●●●●			
ref-3	1	Characterization		03-02-2014 11:58:58	2	(i)	●●●●	P2		1
1_w1	2	OSC		03-02-2014 11:50:36	2350	(i)	●●●●	P 1 21 1	47.85 1.83 47.85	
ref-1	2	Characterization		03-02-2014 11:47:42	2	(i)	●●●●	P2		1
		OSC		03-02-2014 11:39:04	2000	(i)	●●●●	P 1 21 1	100.0 2.32 100.0	
		Characterization		03-02-2014 11:35:25	2	(i)	●●●●	P2		1
		Characterization		03-02-2014 11:30:27	2	(i)	●●●●			
ref-3400	1	Characterization		03-02-2014 11:25:01	2	(i)	●●●●	P3		1
ref-0648	1	Characterization		03-02-2014 11:20:36	2	(i)	●●●●			

Data are labeled by type OSC, Characterization, Helical, Mesh etc, and corresponding results and parameters are filled

see Stephanie's talk

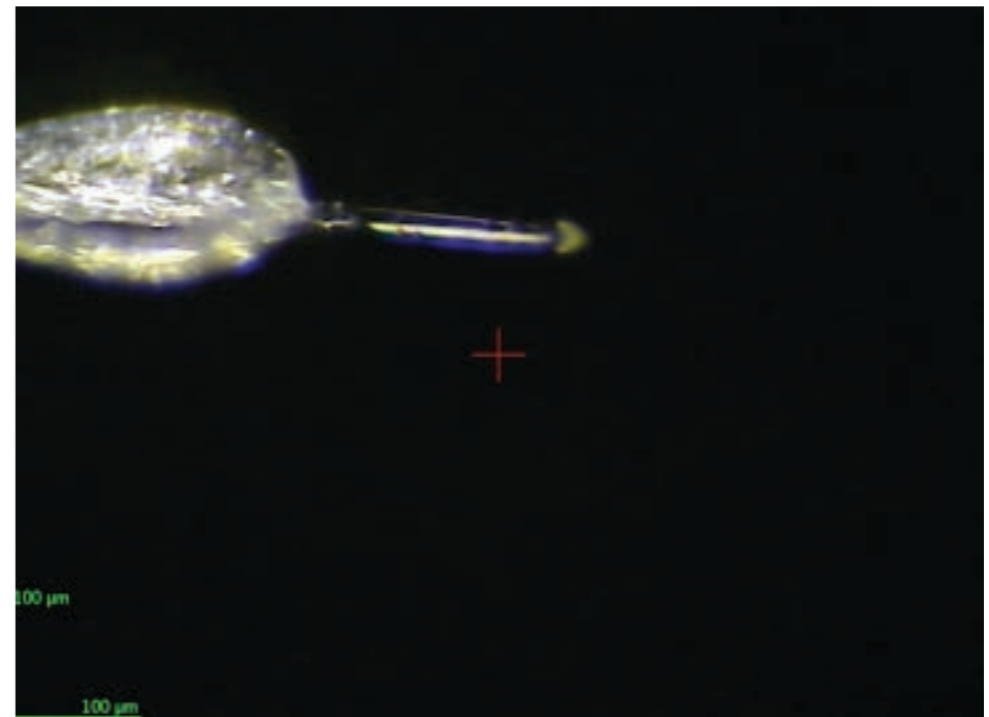
SCIENTIFIC ABSTRACTION LAYER



Open to external descriptors:
build more complex data
collection

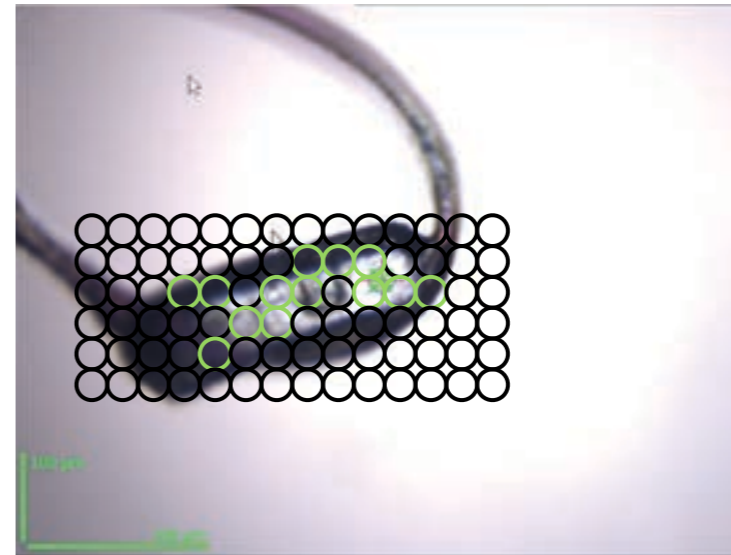
Possible to interactively fill the
queue with different tasks,
analyse results and expand,
without limit to imagination

see Olof's talk



WHERE WE ARE GOING?

New tools for meshes and sample interaction
Use beamsize as mesh unit
Overlay results of mesh



Abstract diffractometer descriptor

Expand Data Collection Model
Other axes DC (κ ...)
Beamsize descriptor

.....

Adapt interface to *RoboDiff* and *NewDewar*
Generic SC
Plate screening

Redesign Data collection group concept
Tag data collections???

WHERE DO YOU WANT US TO GO?



MxCuBE is a big project that runs with small resources

It is shared among different institutions, BESSY, EMBL, GLOBAL PHASING, MAXLAB, SOLEIL

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Automation Task Force

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