ESRF | The European Synchrotron

MxCuBE2

WHY A NEW MXCUBE?

- Evaluate and collect of MASSIF samples
- Fully exploit µbeam 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

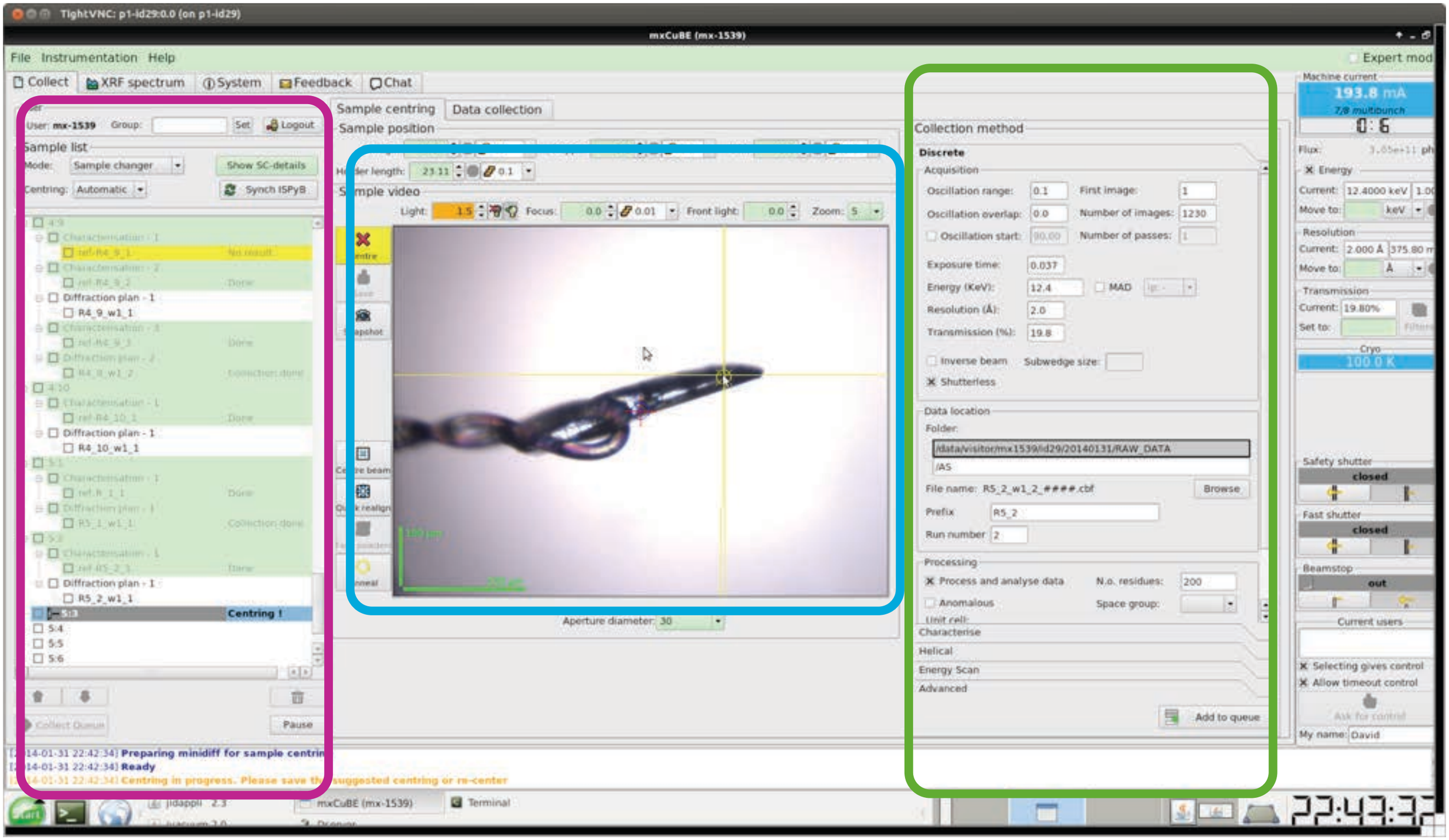
TIME

- 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

THE LOGIC

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

GUI



SC - Queue **Sample - Position** **Tasks - Data Collection**

WHAT CAN YOU DO?

Which? Where? What?

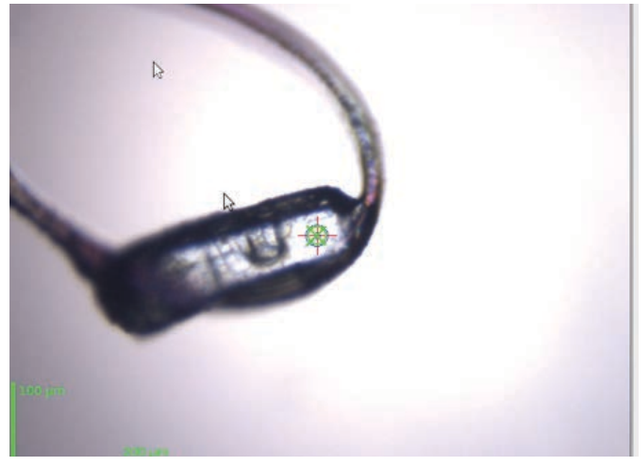
Combinations are infinite. For example:

- 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
- .....

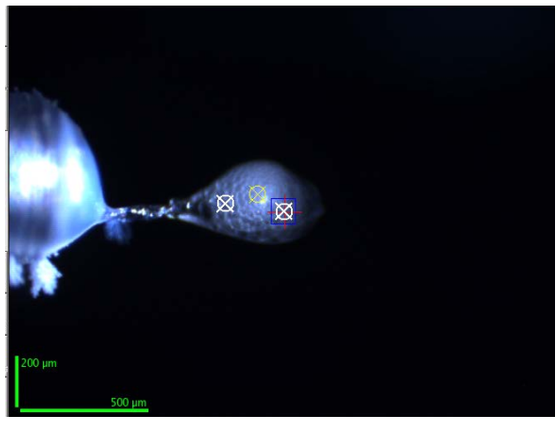
Characterization no strategy

Successful Characterization

Proposed Diffraction plan



Collected Diffraction plan



Mounted sample and status

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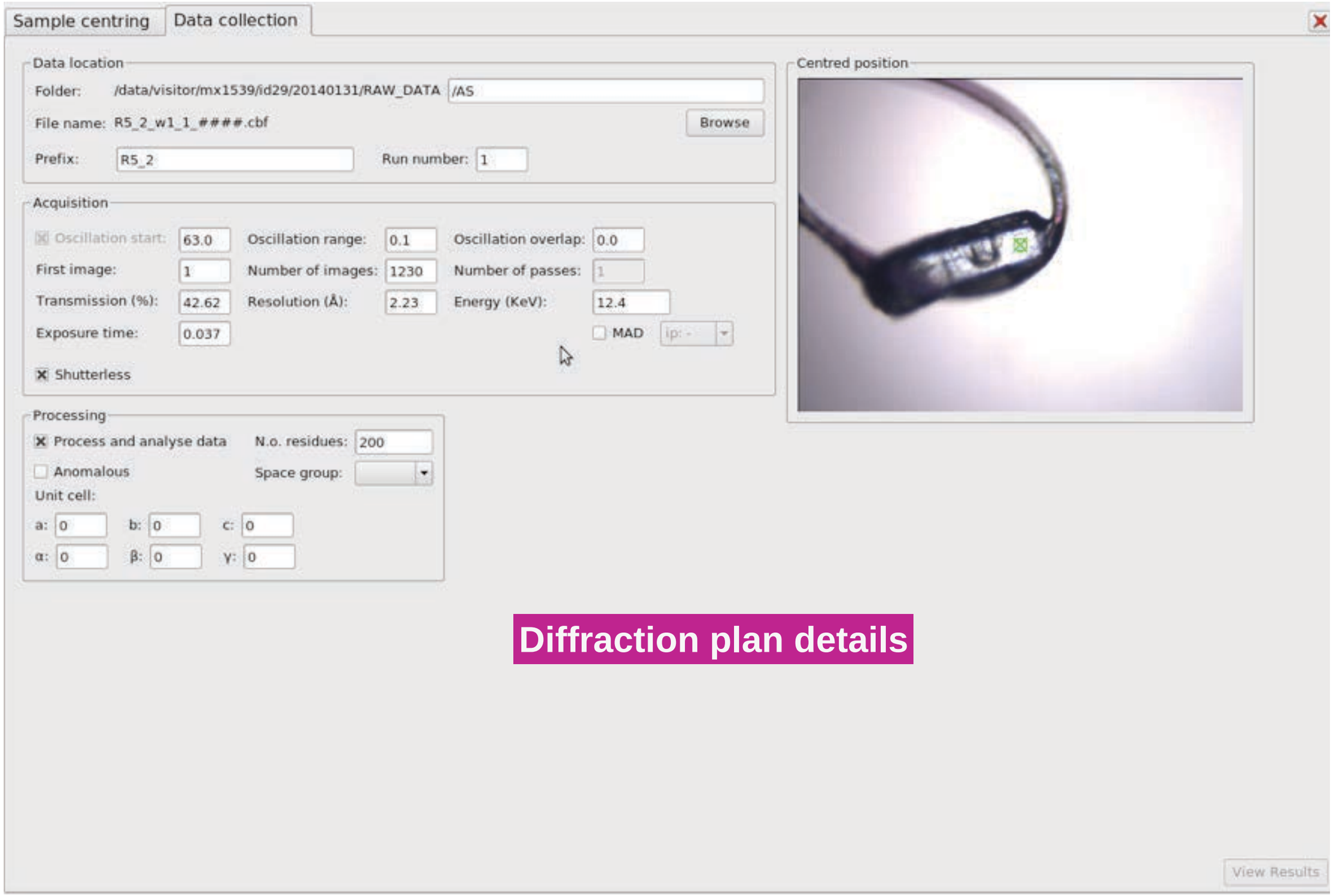
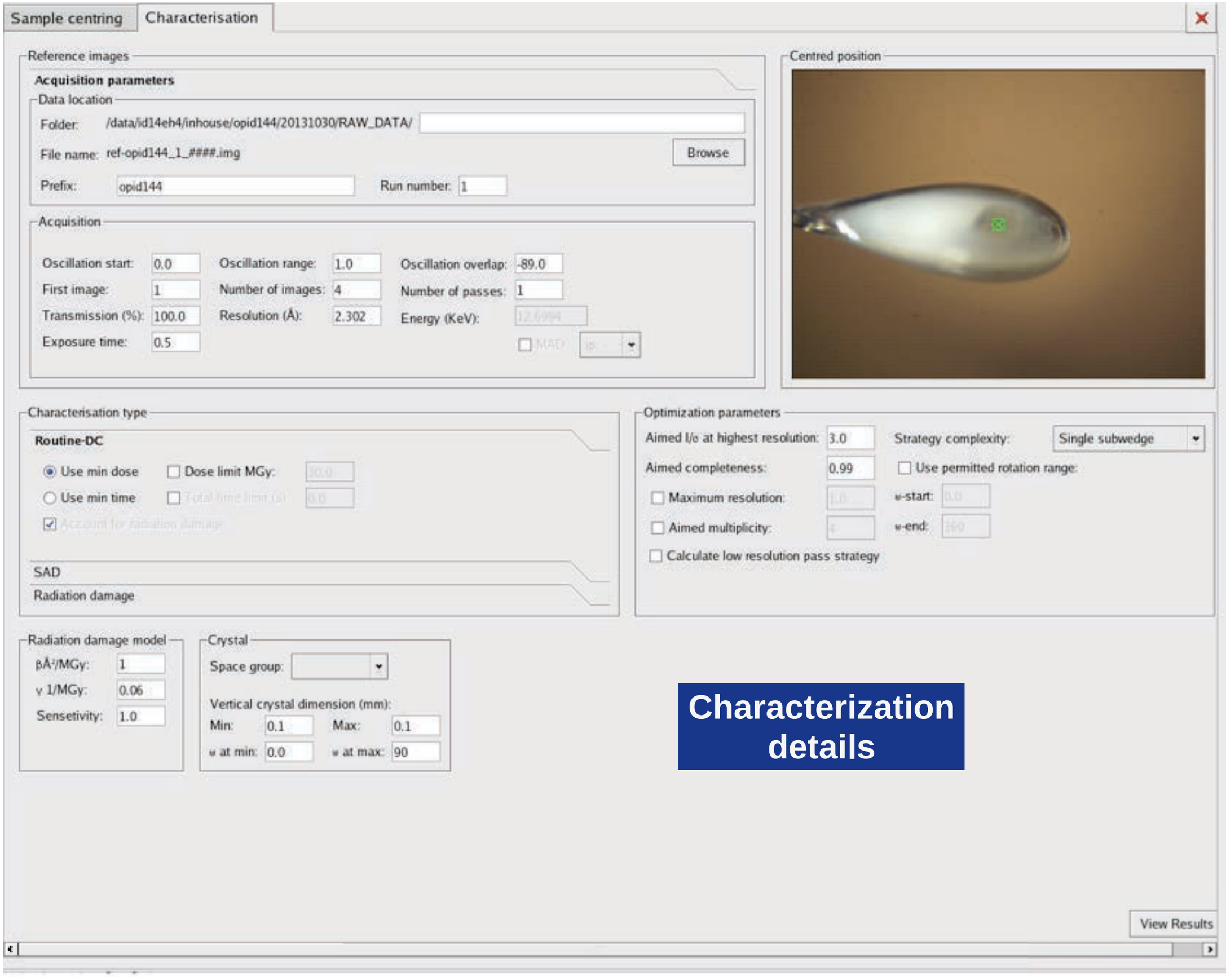
DETAILS - DATA COLLECTION



DETAILS - CHARACTERIZATION



Characterization details

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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

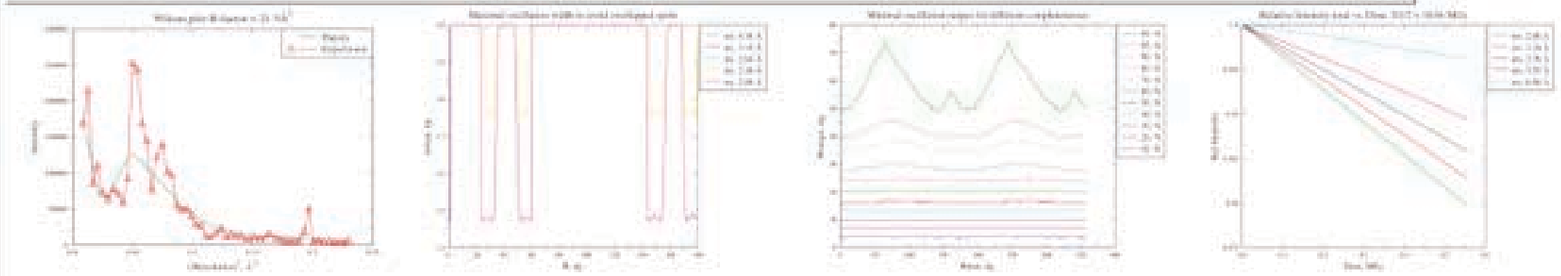
Characterization details (results)

Collection plan strategy (RADDOSE 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.

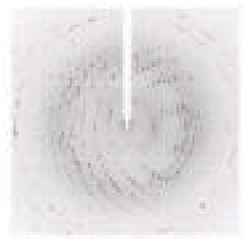
Resolution limit is set by the initial image resolution								
Wedge	Subwedge	Start (°)	Width (°)	No images	Exp time (s)	Max res (Å)	Rel trans (%)	Distance (mm)
1	1	48.00	1.45	86	0.10	2.06	49.63	302.23

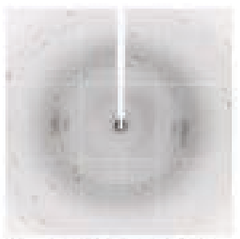


Indexing summary: Selected spacegroup: P3, forced space group:

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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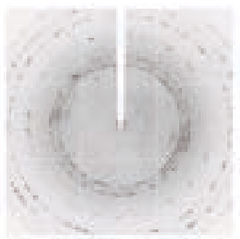
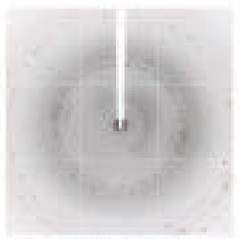

ref-opid144_1_0002.img


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

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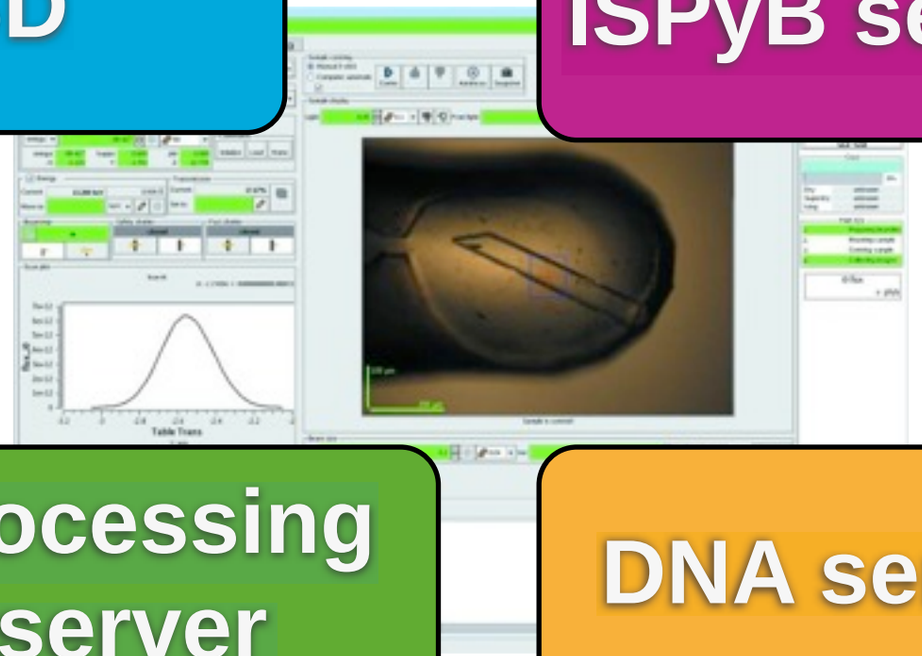
SIMPLER AND ROBUST

C3D

mxCu

ISPyB server



Processing server

DNA server

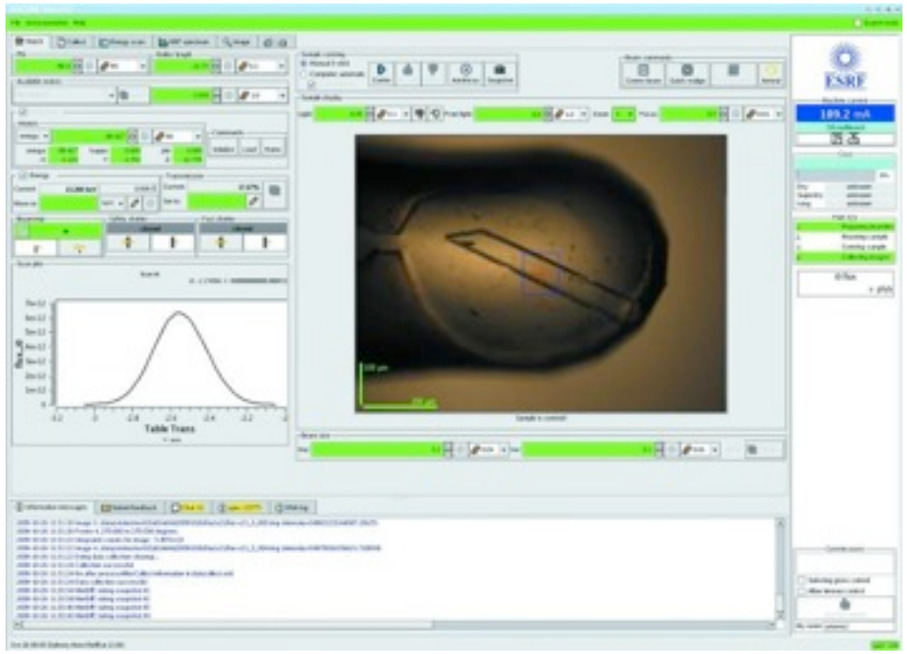
SPEC

SIMPLER AND ROBUST

C3D

ISPyB server

mxCuBE



Processing server

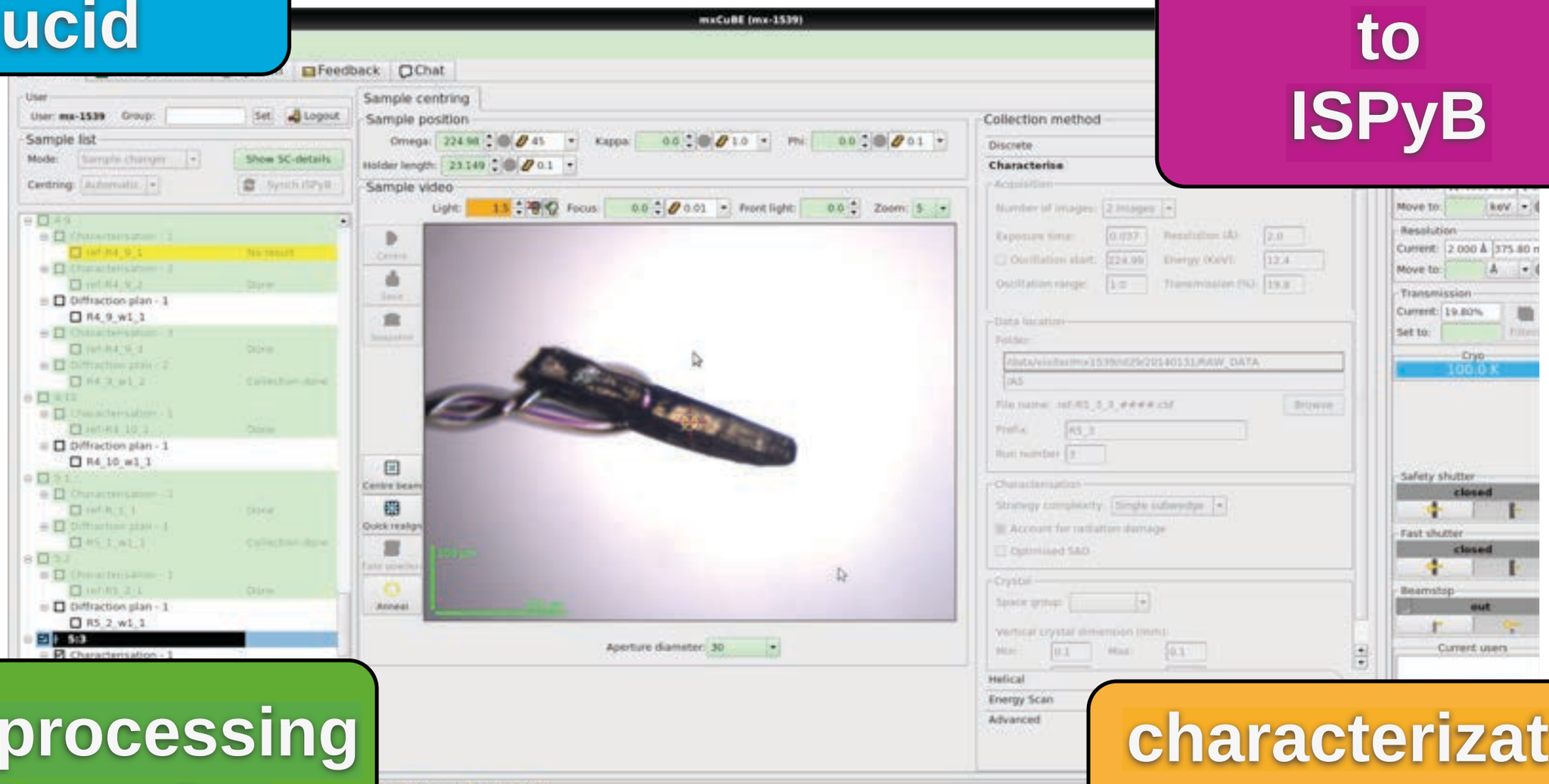
SPEC

DNA server

SIMPLER AND ROBUST

lucid

MxCuBE2



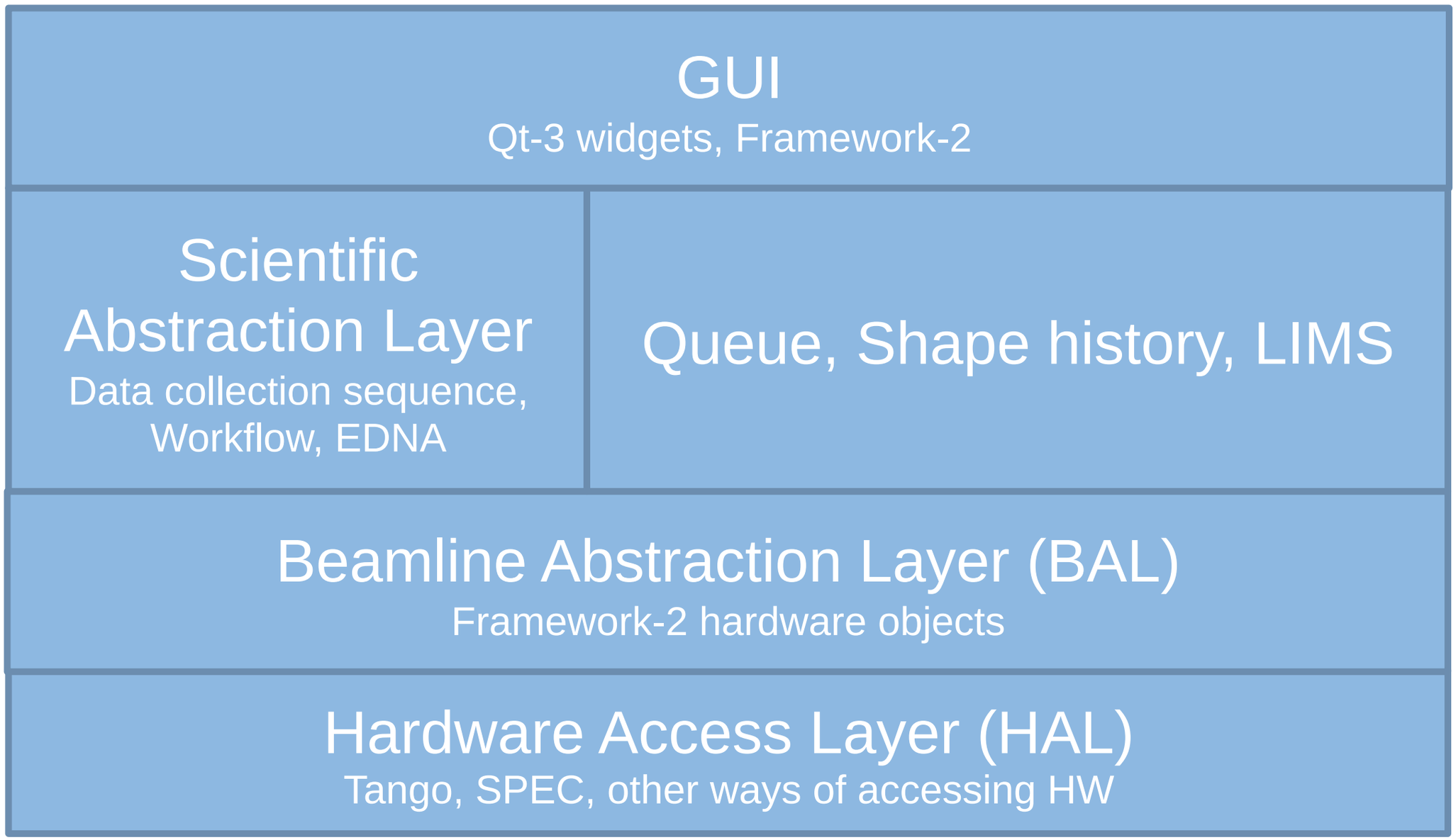
webservices to ISPyB

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

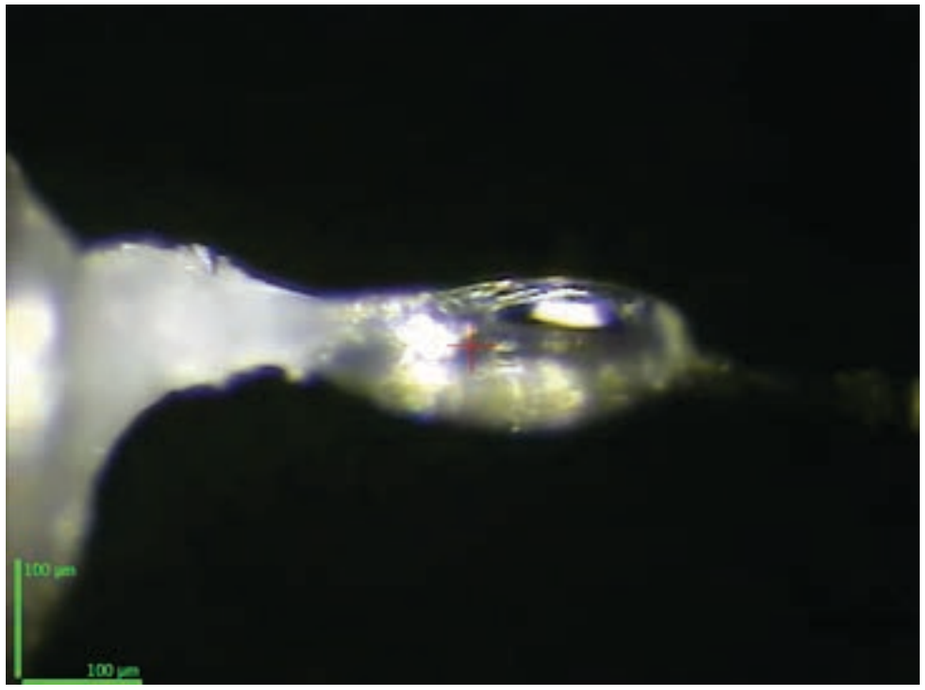
Sample list

Image Prefix	Run No	Experiment Type	Protein Acronym	Start Time	# images	Experiment Parameters (Expand)	Status	Space Group	Completeness	Resc
		All	All							
4_w1	1	OSC		03-02-2014 12:08:50	2000			P 1 21 1		
ref-4	1	Characterization		03-02-2014 12:05:55	2			P2		
3_w1	1	OSC		03-02-2014 12:00:05	2000					
ref-3	1	Characterization		03-02-2014 11:56:56	2			P2		
1_w1	2	OSC		03-02-2014 11:50:36	2350			P 1 21 1		
ref-1	2	Characterization		03-02-2014 11:47:42	2			P2		
		OSC		03-02-2014 11:39:04	2000			P 1 21 1		
		Characterization		03-02-2014 11:35:25	2			P2		
		Characterization		03-02-2014 11:30:27	2					
ref-3400	1	Characterization		03-02-2014 11:25:01	2			P3		
ref-0648	1	Characterization		03-02-2014 11:20:36	2					

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

see Stephanie's talk

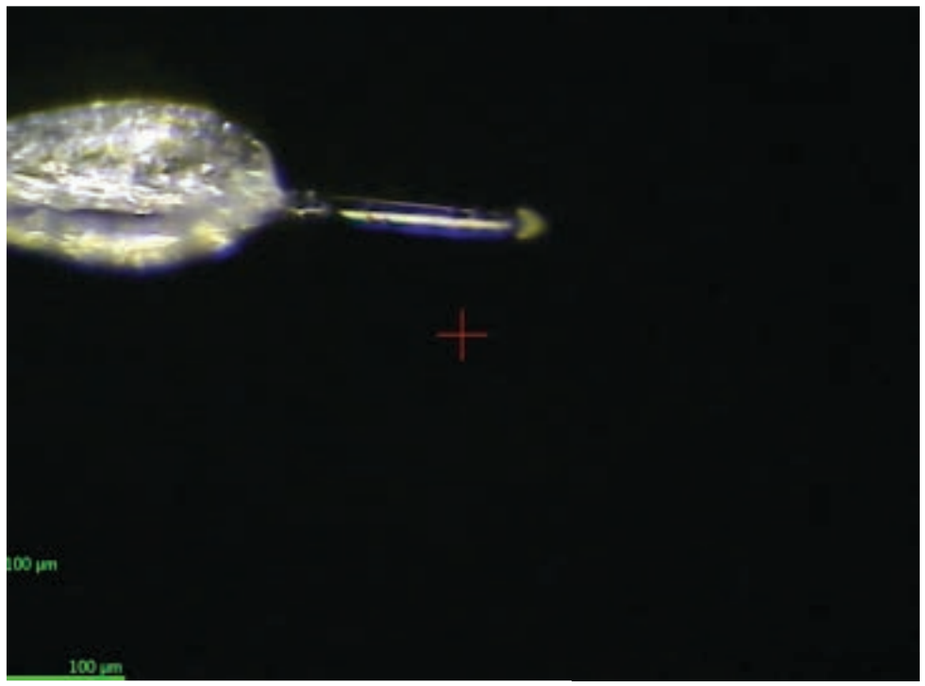
SCIENTIFIC ABSTRACTION LAYER



Open to external descriptors: build more complex data collection

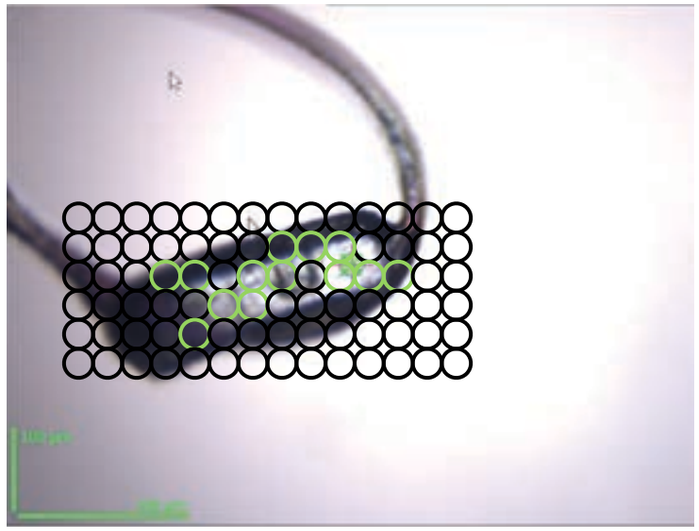
Possible to interactively fill the queue with different tasks, analyse results and expand, without limit to imagination

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 (kappa...)
- 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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