

MXCuBE @ ESRF

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ESRF Structural Biology Group



MXCuBE is used by ~3000 people every year at the ESRF alone

- 1 full time programmer (Marcus Oskarsson)
- 2 part time support (Matias and Antonia)

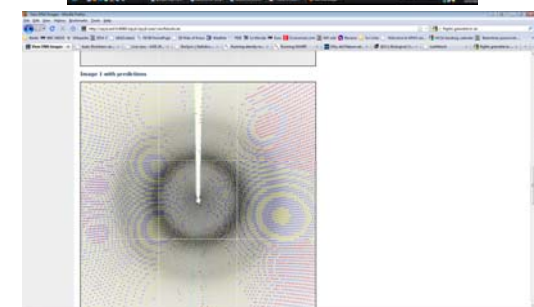
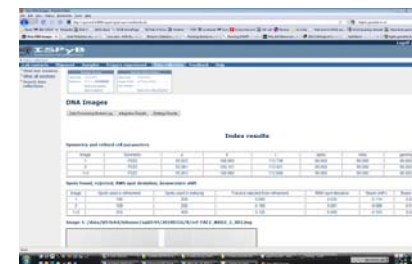
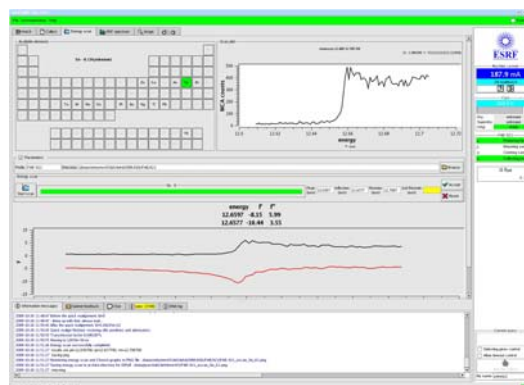
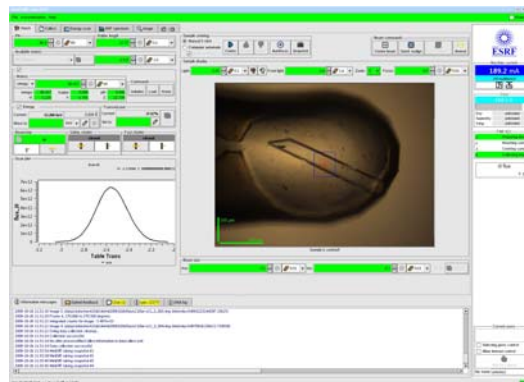


MXCuBE

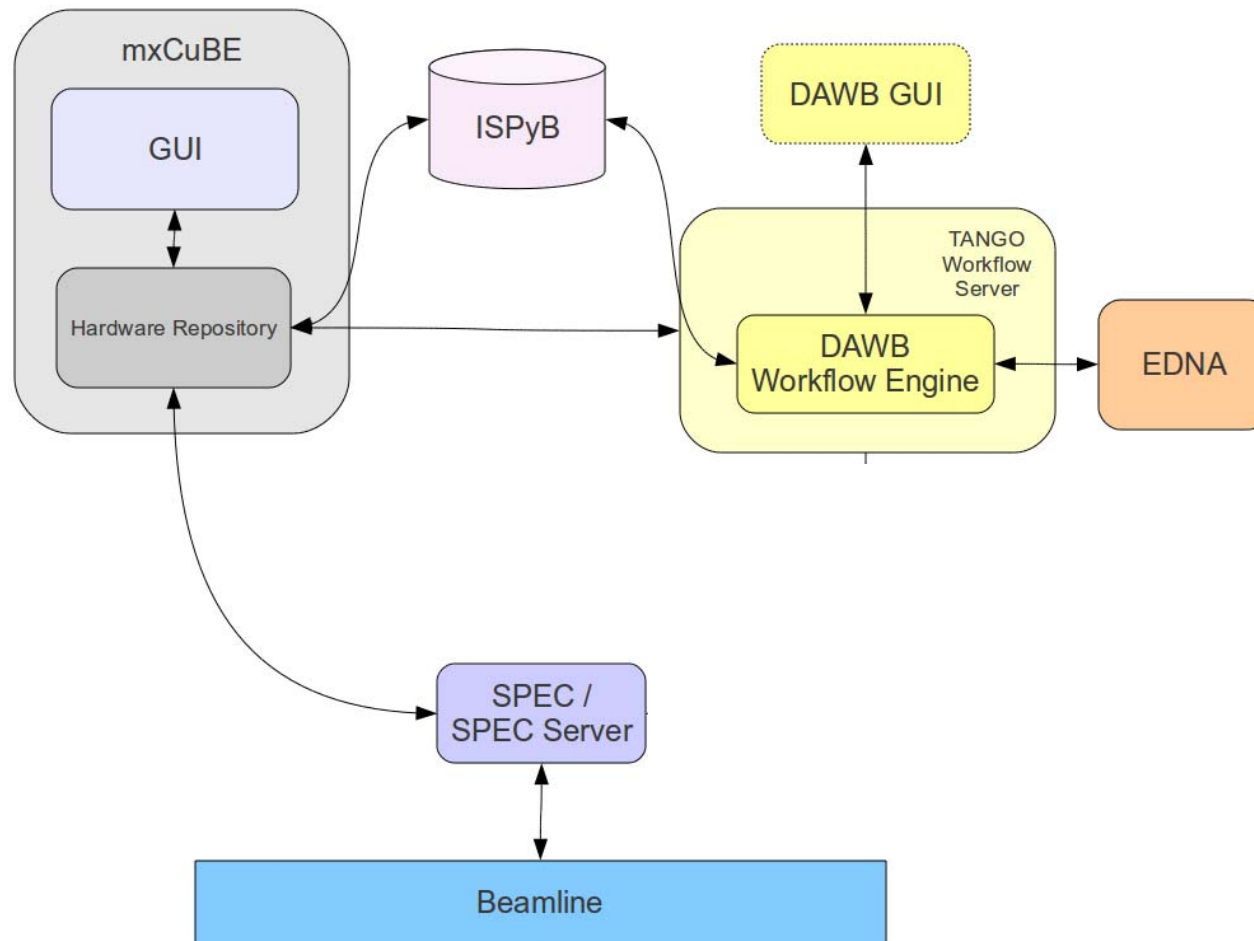
DNA / EDNA

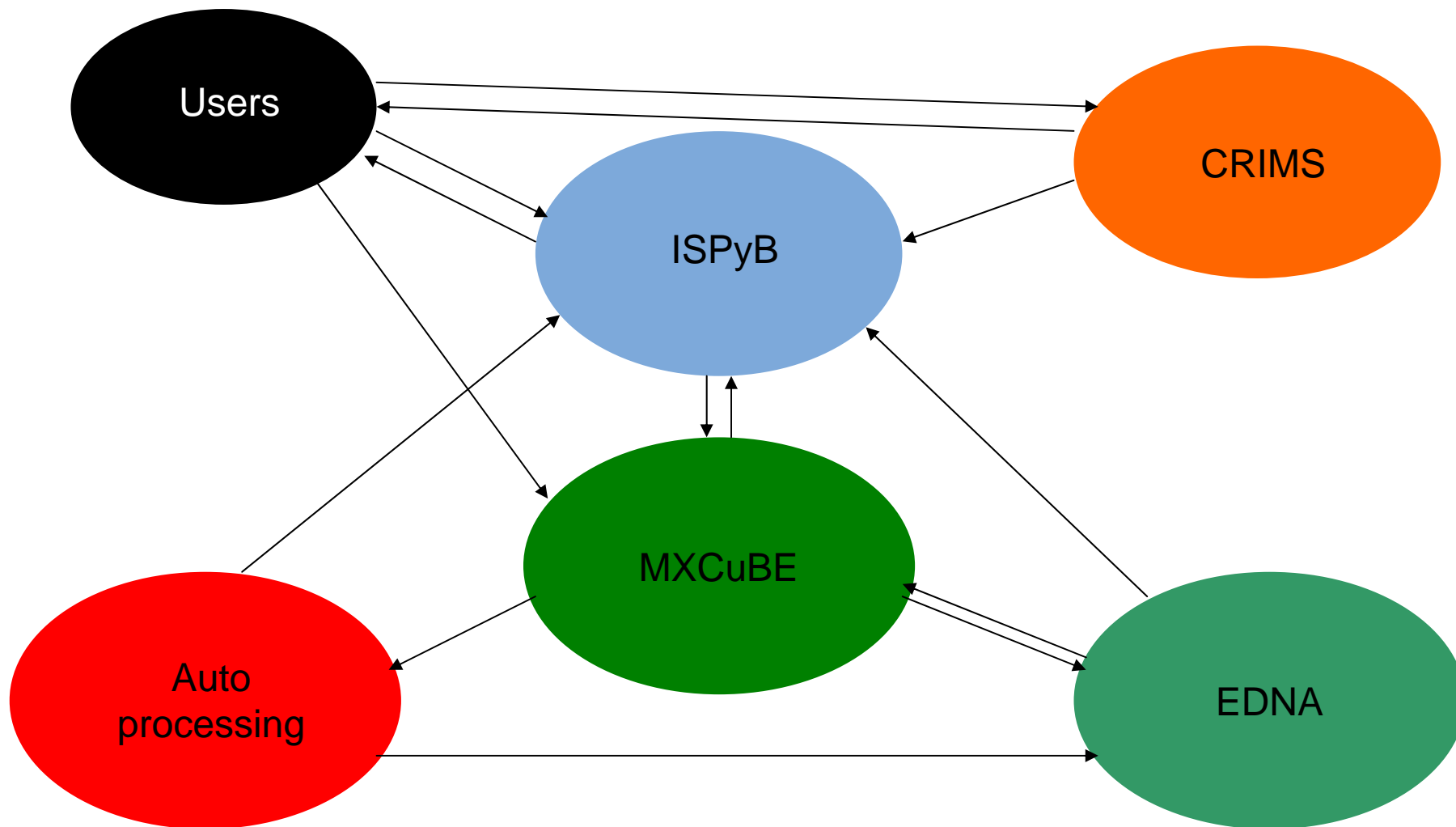


Sample Changer



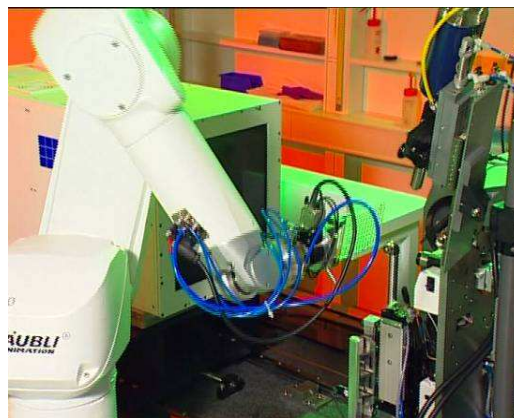
ISPyB







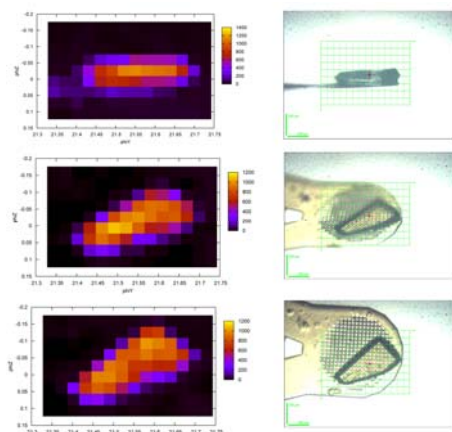
Direct Data collection for ultra HT screening



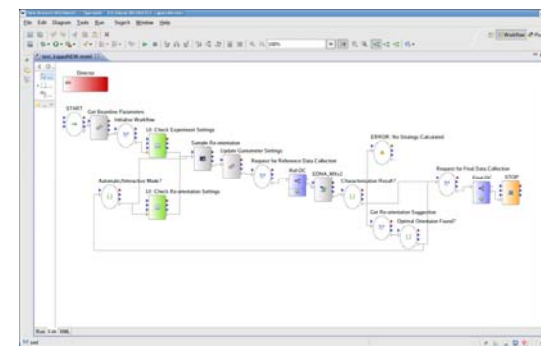
In situ screening



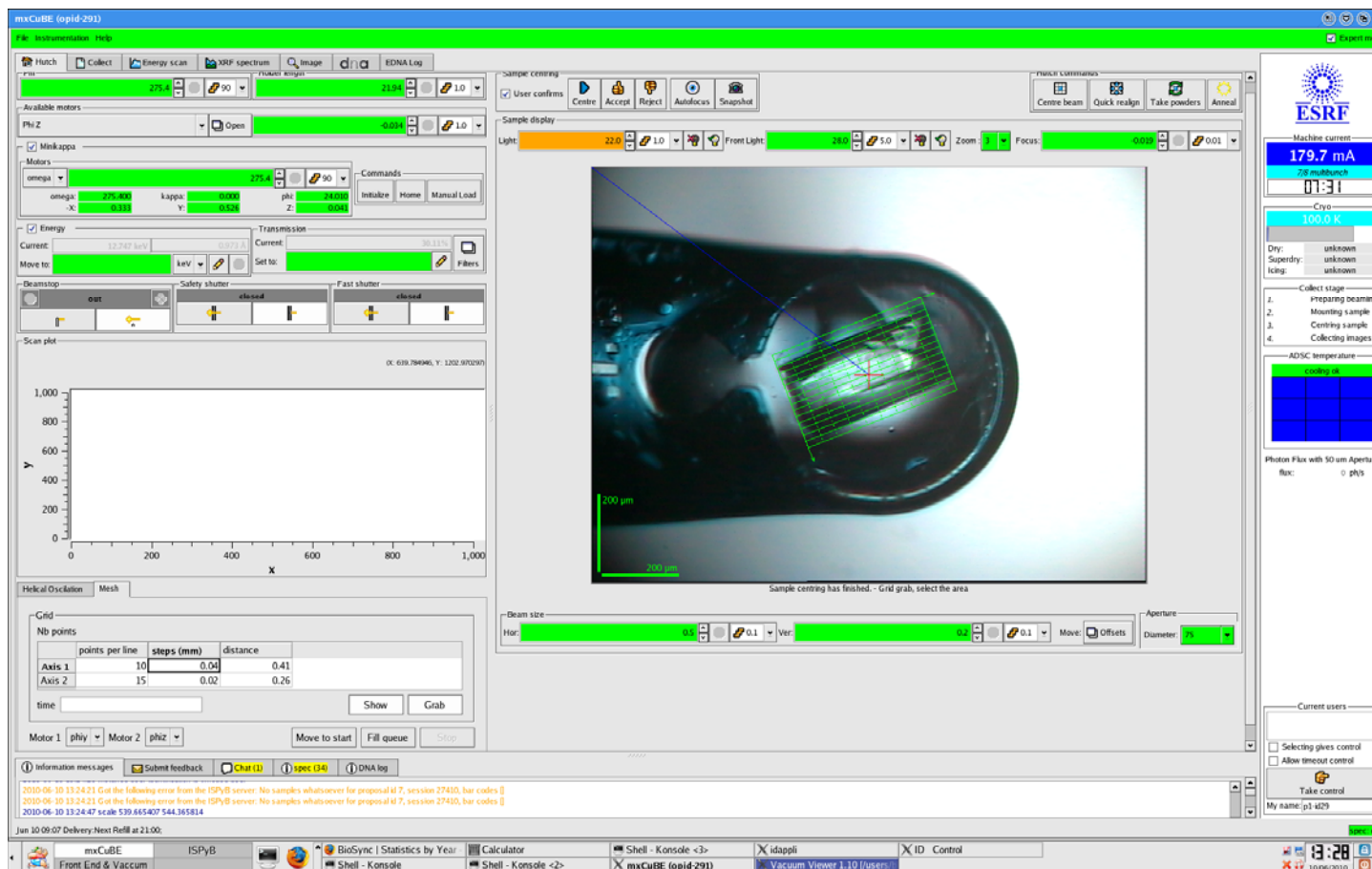
Dehydration screening



Complete characterisation of crystals



Workflow control of sample movement, screening, distribution and data collection



mxCuBE (opid-291)

Machine current: 179.7 mA

Cryo: 100.0 K

Photon Flux with 50 µm Aperture flux: 0 ph/s

Axis	points per line	steps (mm)	distance
Axis 1	10	0.04	0.41
Axis 2	15	0.02	0.26

Sample centring has finished. - Grid grab, select the area

Current users: [] Selecting gives control [] Allow timeout control [] Take control [] My name [j] 429

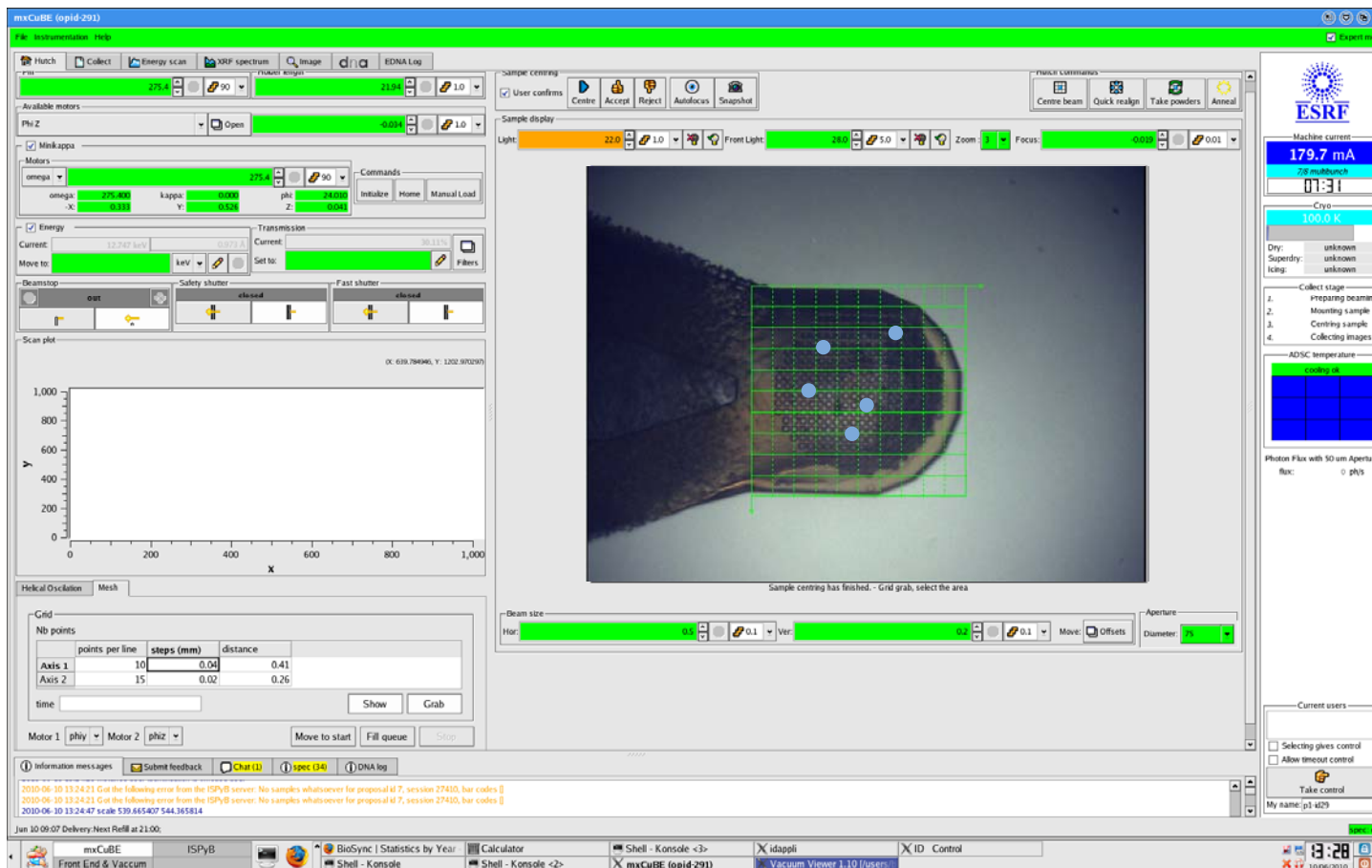
System messages:

- 2010-06-10 13:24:21 Got the following error from the ISPyB server: No samples whatsoever for proposal id 7, session 27410, bar codes []
- 2010-06-10 13:24:21 Got the following error from the ISPyB server: No samples whatsoever for proposal id 7, session 27410, bar codes []
- 2010-06-10 13:24:47 scale 539.665407 544.365814

Jun 10 09:07 Delivery: Next Refill at 21:00.

Taskbar: mxCuBE, Front End & Vaccum, ISPyB, BioSync, Statistics by Year, Calculator, Shell - Konsole <3>, idappli, ID Control, Shell - Konsole, Shell - Konsole <2>, mxCuBE (opid-291), Vacuum Viewer 1.10 [users...]

System tray: 13:28, 10/06/2010

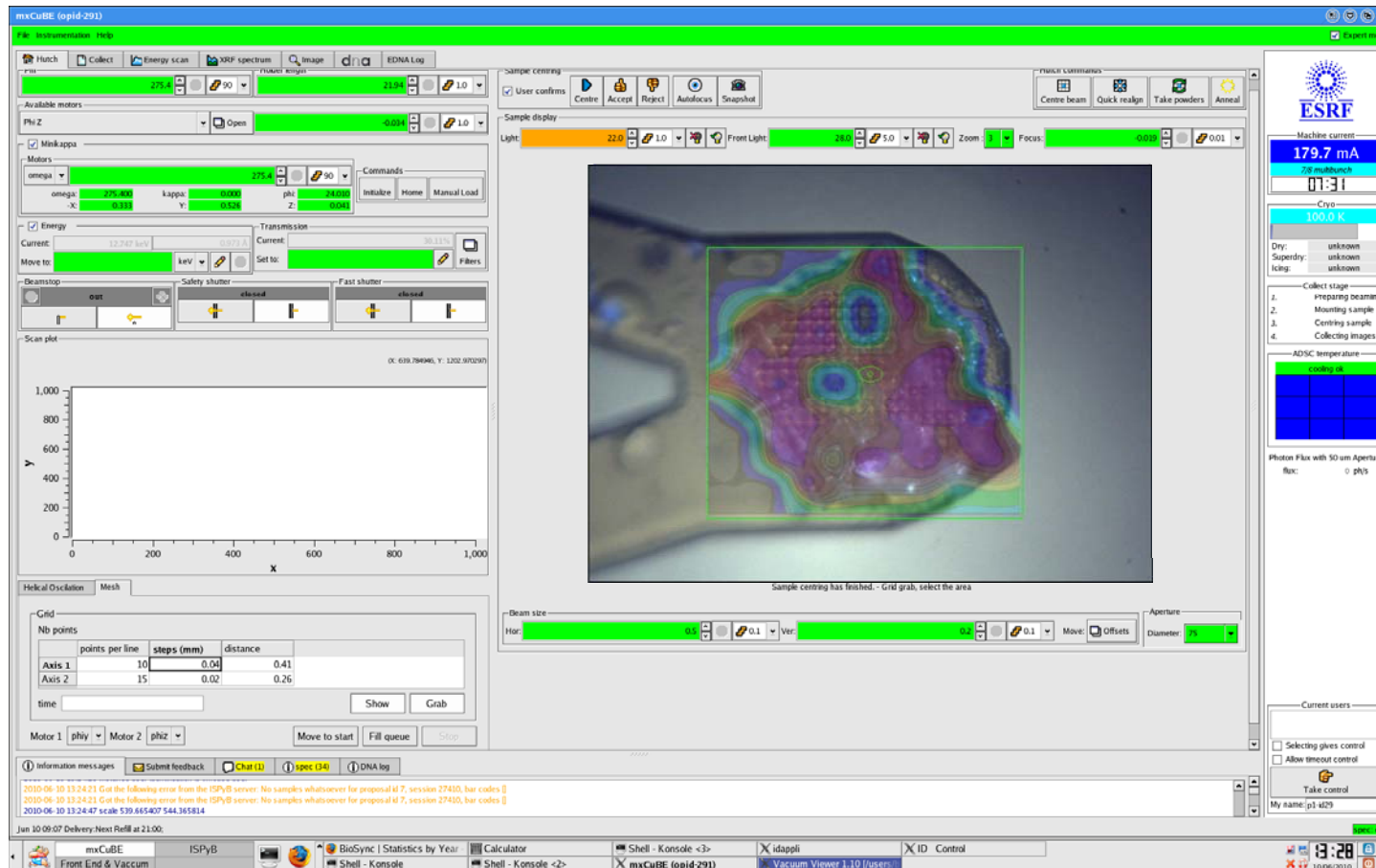


The screenshot displays the mxCuBE control interface for proposal ID 291. The main window shows a sample image with a green grid overlay, indicating that sample centering is complete. The interface includes several control panels:

- Available motors:** Includes controls for Phi Z, Minkappa, and Motors (omega, kappa, phi, -X, Y, Z).
- Energy:** Shows current energy (13.747 keV) and transmission (30.11%).
- Beamstop:** Controls for out, safety shutter, and fast shutter.
- Scan plot:** A graph showing the scan area with X and Y axes ranging from 0 to 1,000.
- Grid:** A table for defining the grid parameters:

Axis	points per line	steps (mm)	distance
Axis 1	10	0.04	0.41
Axis 2	15	0.02	0.26

The interface also features a status bar at the bottom with information messages, a taskbar with open applications (mxCuBE, ISPyB, BioSync, etc.), and a system tray showing the date and time (13:28 on 10/06/2010).



The screenshot displays the mxCuBE control software interface. The main window is titled "mxCuBE (opid-291)". It features a top menu bar with options like "Hutch", "Collect", "Energy scan", "XRF spectrum", "Image", and "EDNA Log". Below the menu is a toolbar with buttons for "Centre", "Accept", "Reject", "Autofocus", and "Snapshot".

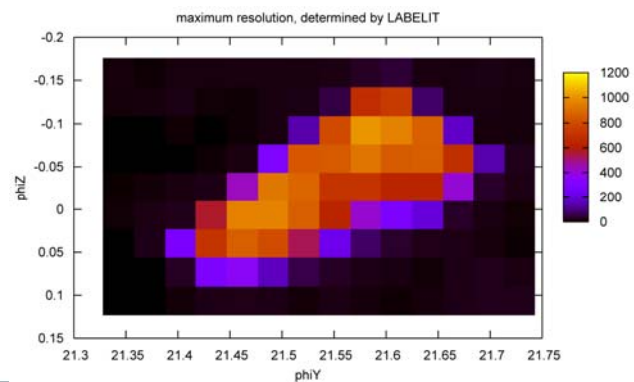
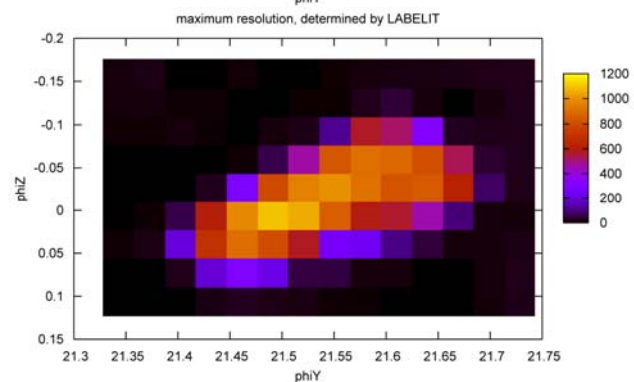
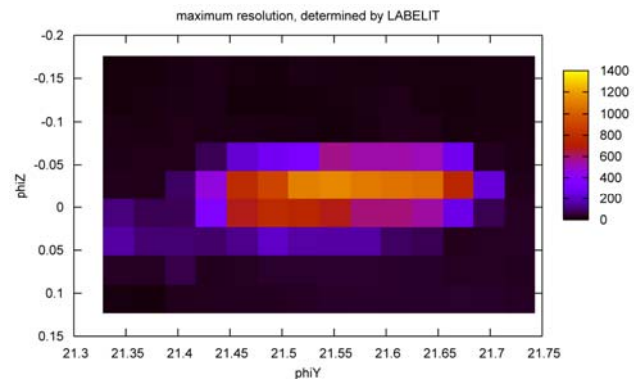
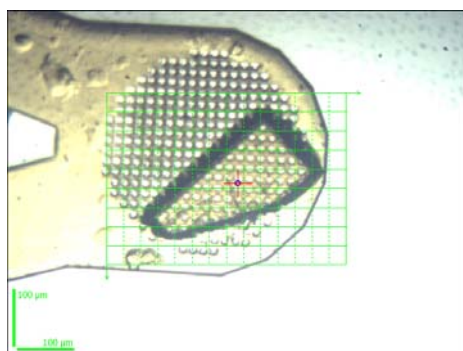
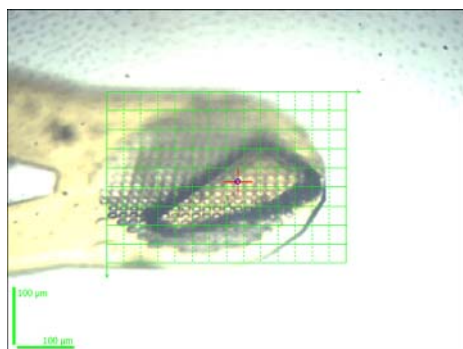
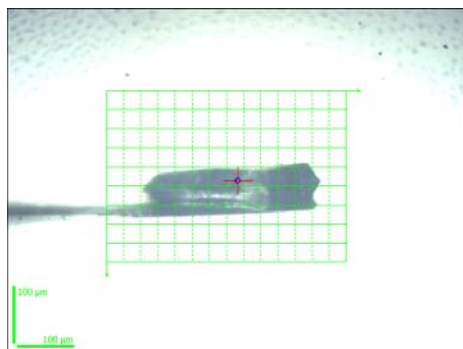
The interface is divided into several panels:

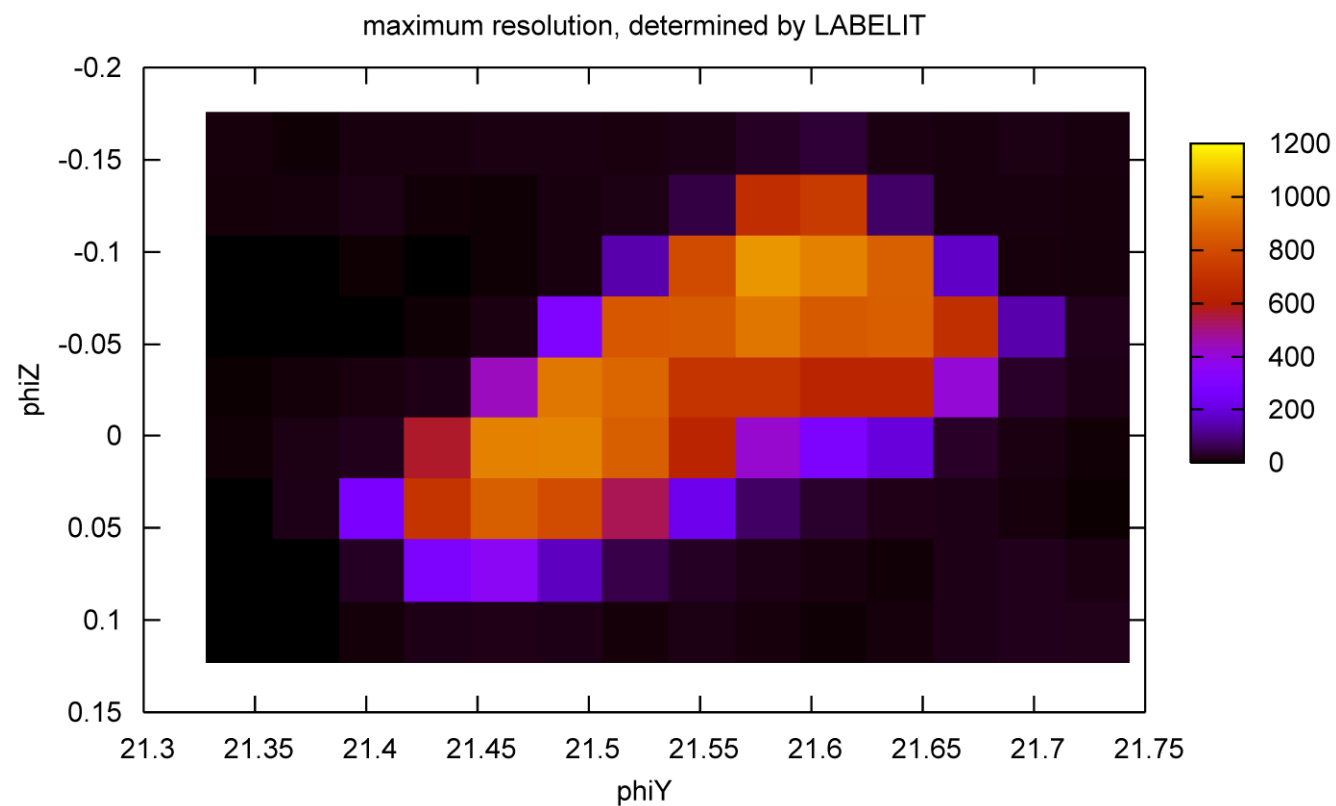
- Available motors:** Includes "Phi Z" and "Minkappa" sections with various motor controls and status indicators.
- Energy:** Shows "Current" and "Transmission" settings.
- Beamstop:** Contains "Safety shutter" and "Fast shutter" controls.
- Scan plot:** A graph showing the scan area with X and Y axes ranging from 0 to 1,000.
- Grid:** A section for defining the grid parameters, including "Nb points", "points per line", "steps (mm)", and "distance".
- Sample display:** A central image showing a diffraction pattern with a grid overlay. Below the image, it says "Sample centring has finished - Grid grab, select the area".
- Beam size:** Controls for "Hor" and "Ver" beam dimensions.
- Aperture:** A control for the aperture diameter.

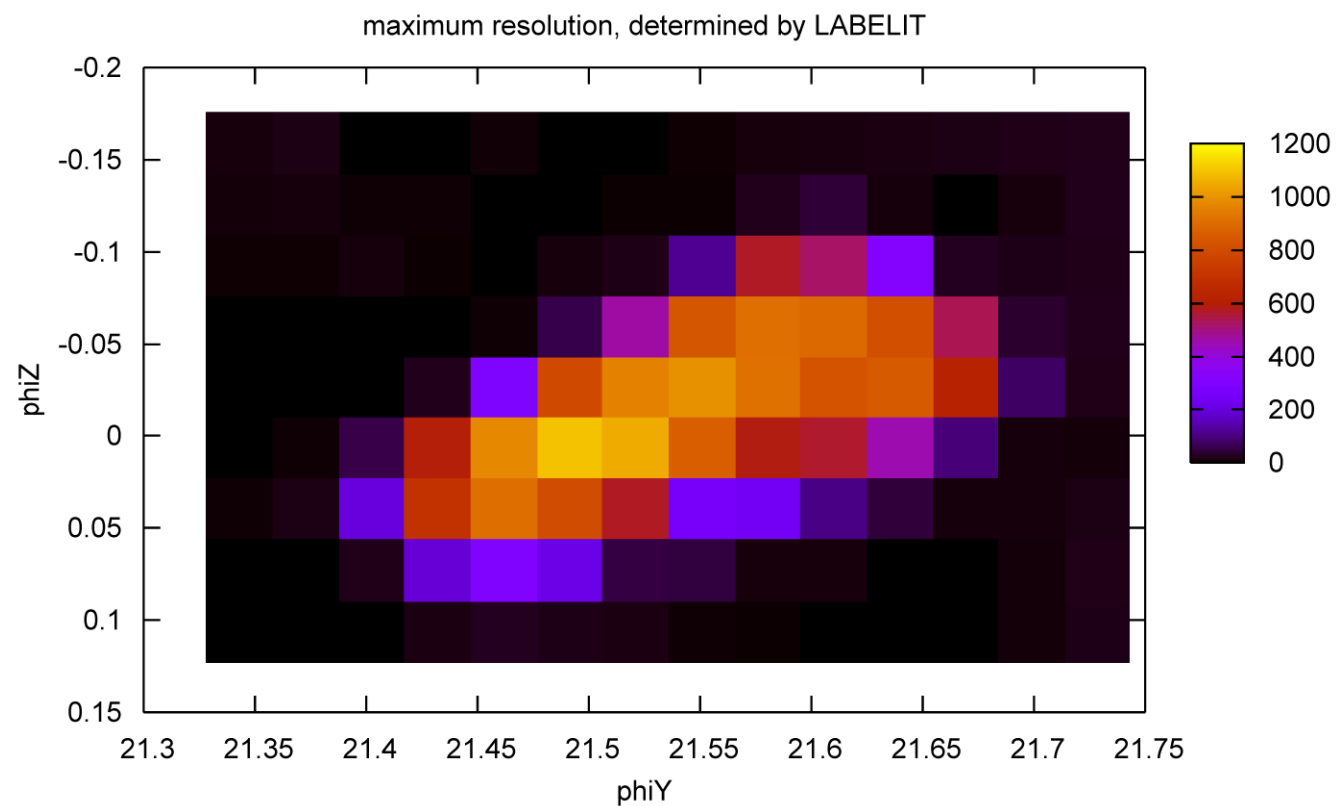
On the right side, there is a sidebar with various status indicators and controls:

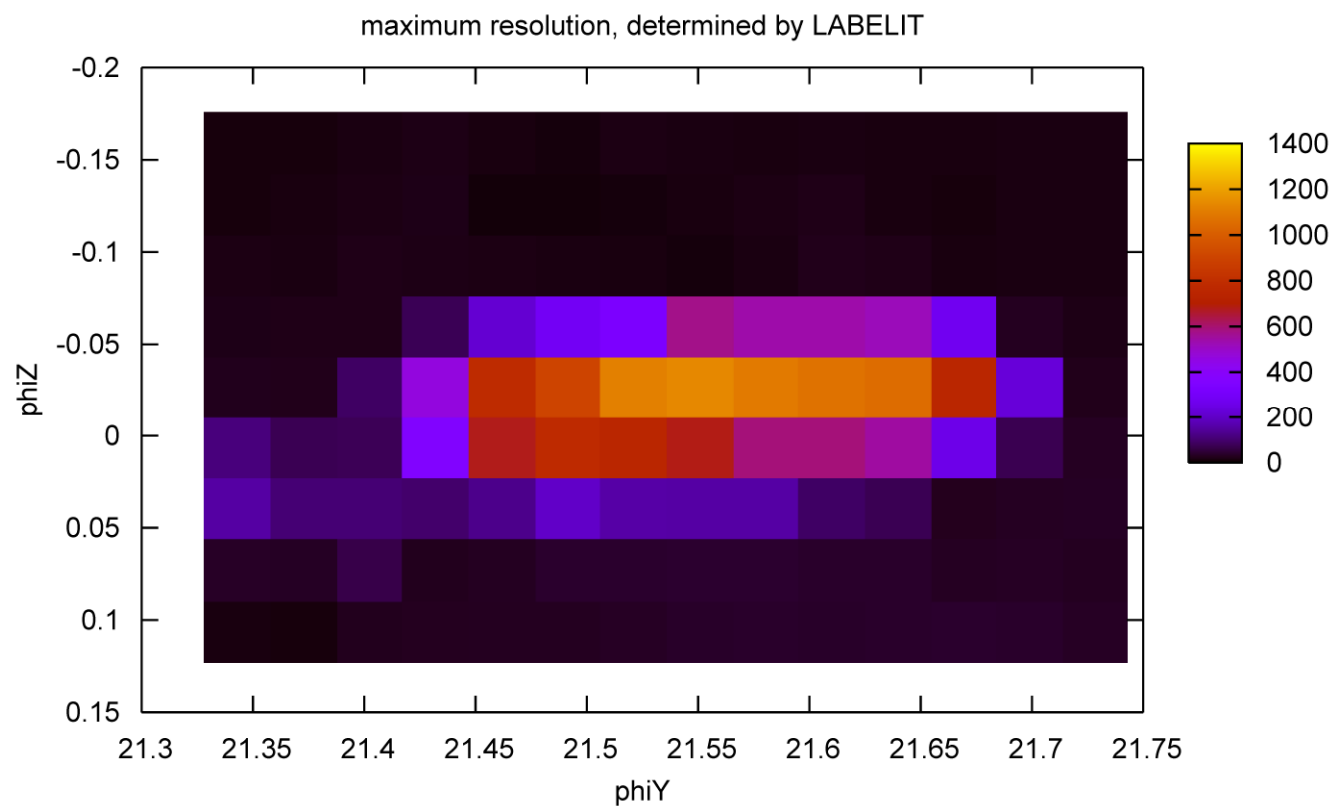
- Machine current:** 179.7 mA.
- Cryo:** 100.0 K.
- ADC temperature:** Cooling OK.
- Photon Flux with 50 um Aperture flux:** 0 p/s.
- Current users:** My name: pl 429.

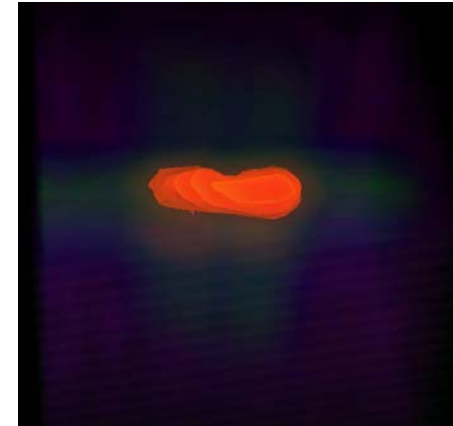
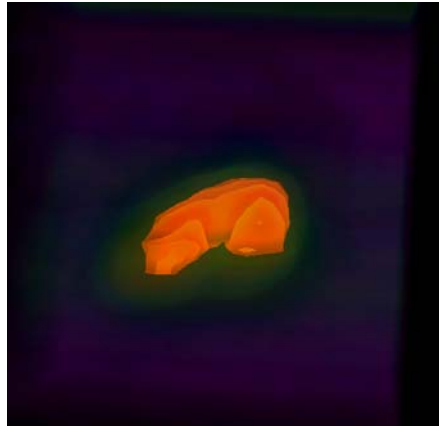
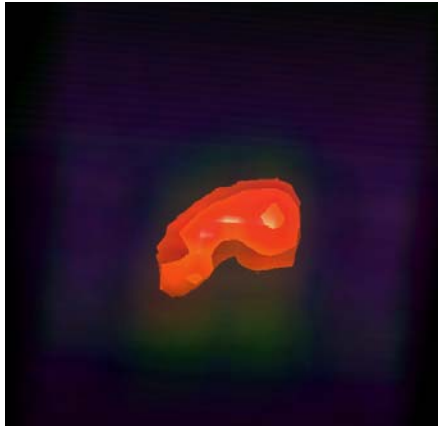
At the bottom, there is a taskbar with several open windows, including "mxCuBE", "ISPyB", "BioSync | Statistics by Year", "Calculator", "Shell - Konsole", "idappli", and "Vacuum Viewer 1.10 /users...". The system tray shows the date and time as 13:28 on 15/06/2010.

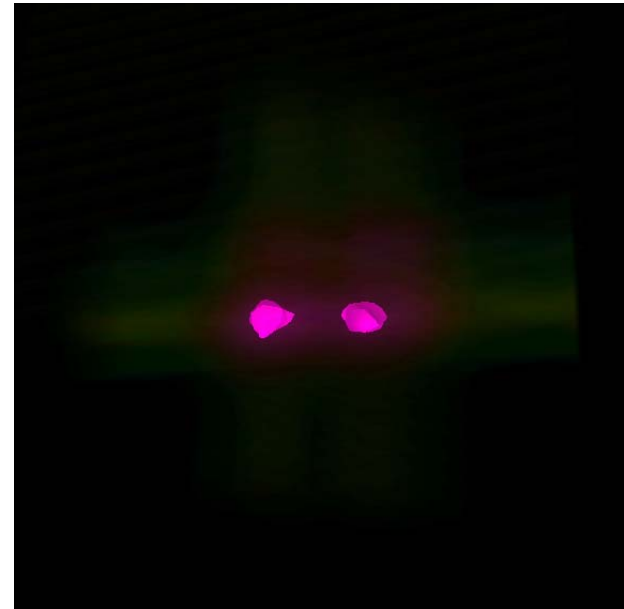
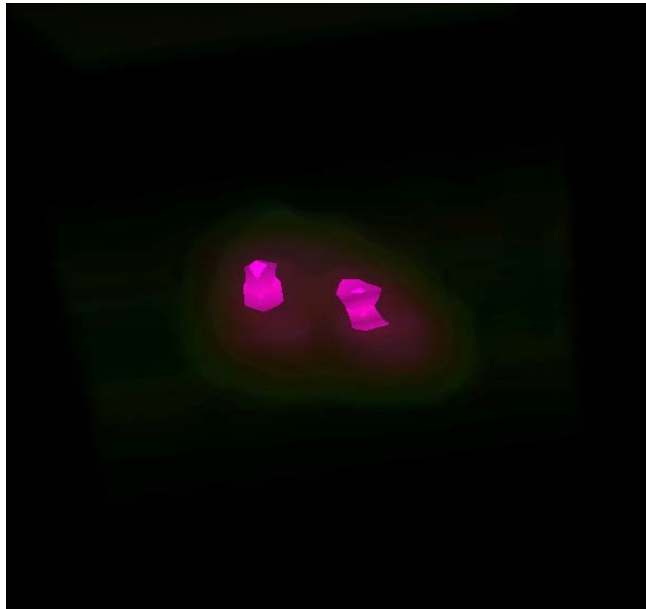


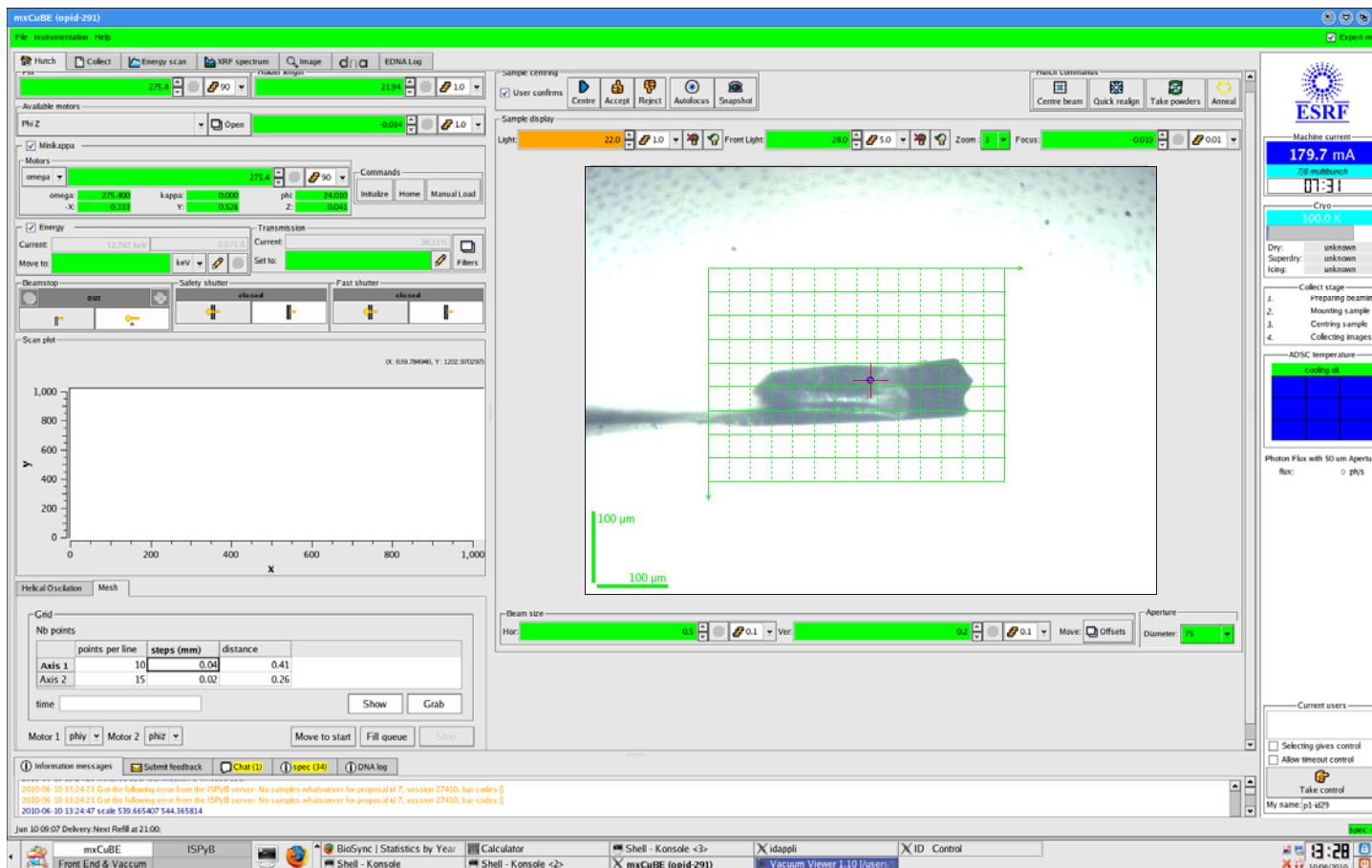








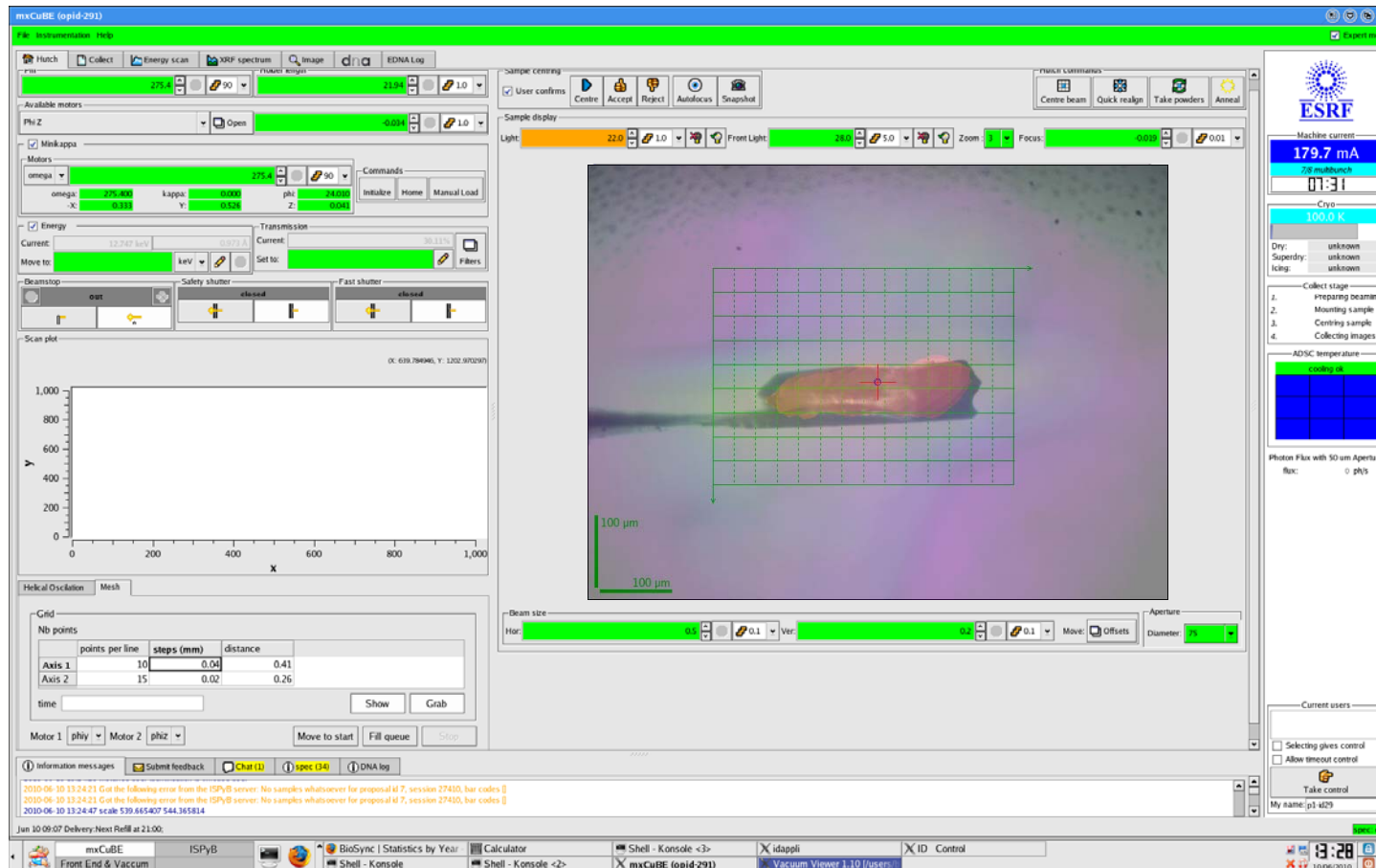




The screenshot displays the mxCuBE control software interface. The main window is titled "mxCuBE (opid-291)".

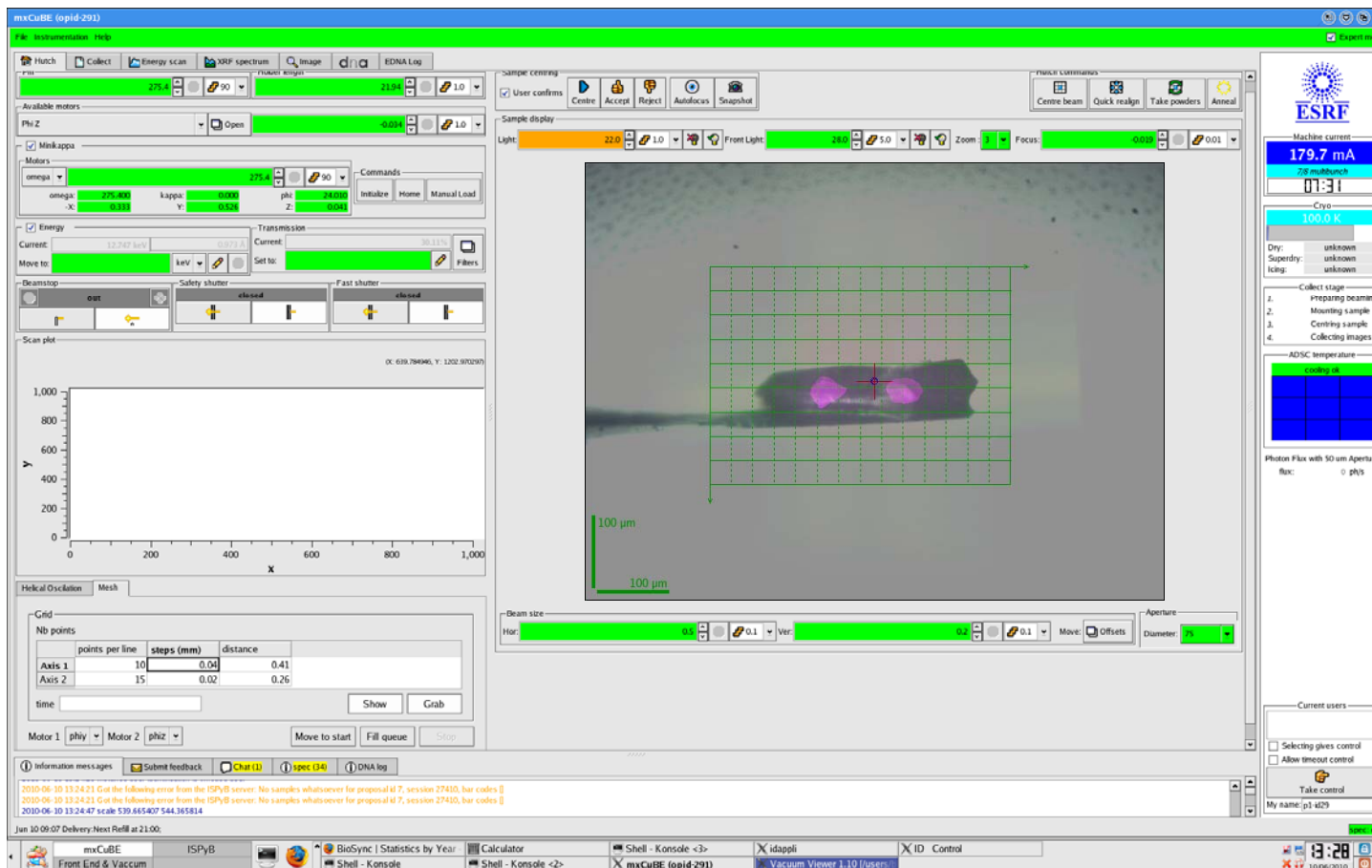
- Top Panel:** Includes menu items (Hutch, Collect, Energy scan, XRF spectrum, Image, EDNA Log) and a "Sample centering" section with buttons for "User confirms", "Centre", "Accept", "Reject", "Autofocus", and "Snapshot".
- Left Panel:** Contains "Available motors" (Phi Z, Minkappa), "Motors" (omega, kappa, phi, X, Y, Z), "Energy" (Current, Move to, Transmission), "Beamstop" (out, safety shutter, Fast shutter), and "Scan plot" (a graph with X and Y axes from 0 to 1,000).
- Bottom Left Panel:** "Helical Oscillation" section with a "Grid" table:

Nb points	points per line	steps (mm)	distance
Axis 1	10	0.04	0.41
Axis 2	15	0.02	0.26
- Center Panel:** "Sample display" showing a diffraction image with a green grid overlay. A scale bar indicates 100 μm. Below the image are "Beam size" (Hor, Ver) and "Aperture" (Diameter) controls.
- Right Panel:** "Status" sidebar with ESRF logo, "Machine current" (179.7 mA), "Cryo" (100.0 K), "Dry/Superdry/Icing" status, "Collect stage" (preparing decamane, Mounting sample, Centring sample, Collecting images), "ADC: temperature" (cooling ok), "Photon Flux with 50 μm Aperture flux", and "Current users" (My name: pl429).
- Bottom Panel:** "Information messages" showing error logs from the ISPyB server. The taskbar at the very bottom shows open applications like mxCuBE, ISPyB, BioSync, Calculator, Shell - Konsole, idappli, and Vacuum Viewer 1.10.



The screenshot displays the mxCuBE control software interface. The main window is titled 'mxCuBE (opid-291)'. It features several control panels:

- Top Panel:** Includes 'Hutch' (Collect, Energy scan, XRF spectrum, Image, EDNA Log) and 'Sample centering' (User confirms, Centre, Accept, Reject, Autofocus, Snapshot).
- Left Panel:** 'Available motors' (Phi Z, Minkappa) and 'Motors' (omega, kappa, phi, -X, Y, Z) with numerical values and control buttons.
- Energy Section:** 'Energy' (13.747 keV) and 'Transmission' (30.11%) with 'Current' and 'Move to' controls.
- Beamstop Section:** 'Beamstop' (out) and 'Fast shutter' (closed) controls.
- Scan Plot:** A graph showing 'Scan plot' with X and Y axes ranging from 0 to 1,000.
- Grid Section:** 'Grid' settings for 'Nb points' (points per line, steps (mm), distance) for Axis 1 and Axis 2.
- Motor Section:** 'Motor 1' (phiy) and 'Motor 2' (phiz) with 'Move to start', 'Fill queue', and 'Stop' buttons.
- Central Display:** 'Sample display' showing a diffraction image with a grid overlay and a scale bar of 100 μm.
- Right Sidebar:** 'ESRF' logo, 'Machine current' (179.7 mA), 'Cryo' (100.0 K), 'Dry', 'Superdry', 'Icing', 'Collect stage' (preparing octamene, mounting sample, centering sample, collecting images), 'ADC: temperature' (cooling ok), 'Photon Flux with 50 μm Aperture flux', and 'Current users' (My name: pl429).
- Bottom Panel:** 'Information messages' (Submit feedback, Char (1), spec (34), DNA log) and a taskbar with various application windows.

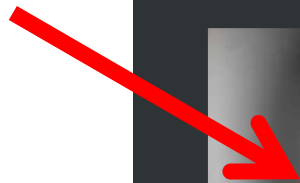


The screenshot displays the mxCuBE control interface for a synchrotron beamline. The main window is titled 'mxCuBE (opid-291)'. It features several control panels:

- Top Panel:** Includes buttons for 'Hutch', 'Collect', 'Energy scan', 'XRF spectrum', 'Image', and 'EDNA Log'. Below this are 'Available motors' and 'Phi Z' controls.
- Motors Panel:** Shows motor positions for omega (275.4), kappa (0.000), phi (24.010), -X (0.133), and Y (0.524). It also includes 'Commands' like 'Initialize', 'Home', and 'Manual Load'.
- Energy Panel:** Displays 'Energy' (13.747 keV) and 'Transmission' (30.11%). It has 'Move to' and 'Set to' fields.
- Beamstop Panel:** Contains 'out', 'Safety shutter', and 'Fast shutter' controls.
- Scan Plot:** A graph showing the scan path with X and Y axes ranging from 0 to 1,000.
- Grid Panel:** A table for defining the grid parameters:

Axis	points per line	steps (mm)	distance
Axis 1	10	0.04	0.41
Axis 2	15	0.02	0.26
- Sample Display:** A central window showing a diffraction pattern on a grid. The pattern consists of two bright spots. Scale bars indicate 100 μm.
- Right Sidebar:** Contains status information:
 - Machine current: 179.7 mA
 - Temperature: 100.0 K
 - Collect stage: preparing oxamine
 - ADSC temperature: cooling ok
 - Photon Flux with 50 μm Aperture flux: 0 p/s
- Bottom Panel:** Includes 'Information messages', 'Submit feedback', and 'Char (1)'. It also shows a list of current users and control options like 'Selecting gives control' and 'Allow timeout control'.

Crystal position
Recording tool

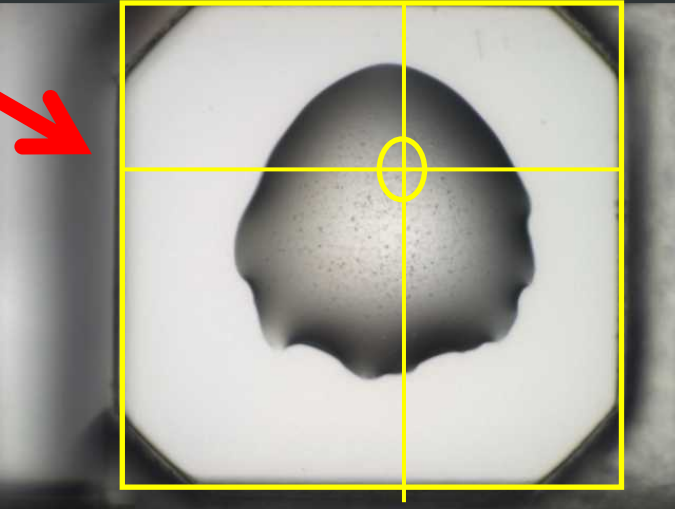


Mount Crystal



Trial : PYL5-2637-27/02/2009 [Send to ISPyB](#)

PYL5 - 0.8 mg/ml	S = 90 % T = 97	T < 50	T < 50
PYL5 - 1.6 mg/ml	S = 70 % T = 97	T < 50	T < 50 T < 50
PYL5 - 3.2 mg/ml	S = 70 % T = 97	T < 50	T < 50 T < 50



Add/Modify comment lines: [[Show Form](#)]

FZ018150

[Drop History](#)
[High Quality](#)
[High Tracking](#)
[Mount Crystal](#)

Experimentation conditions

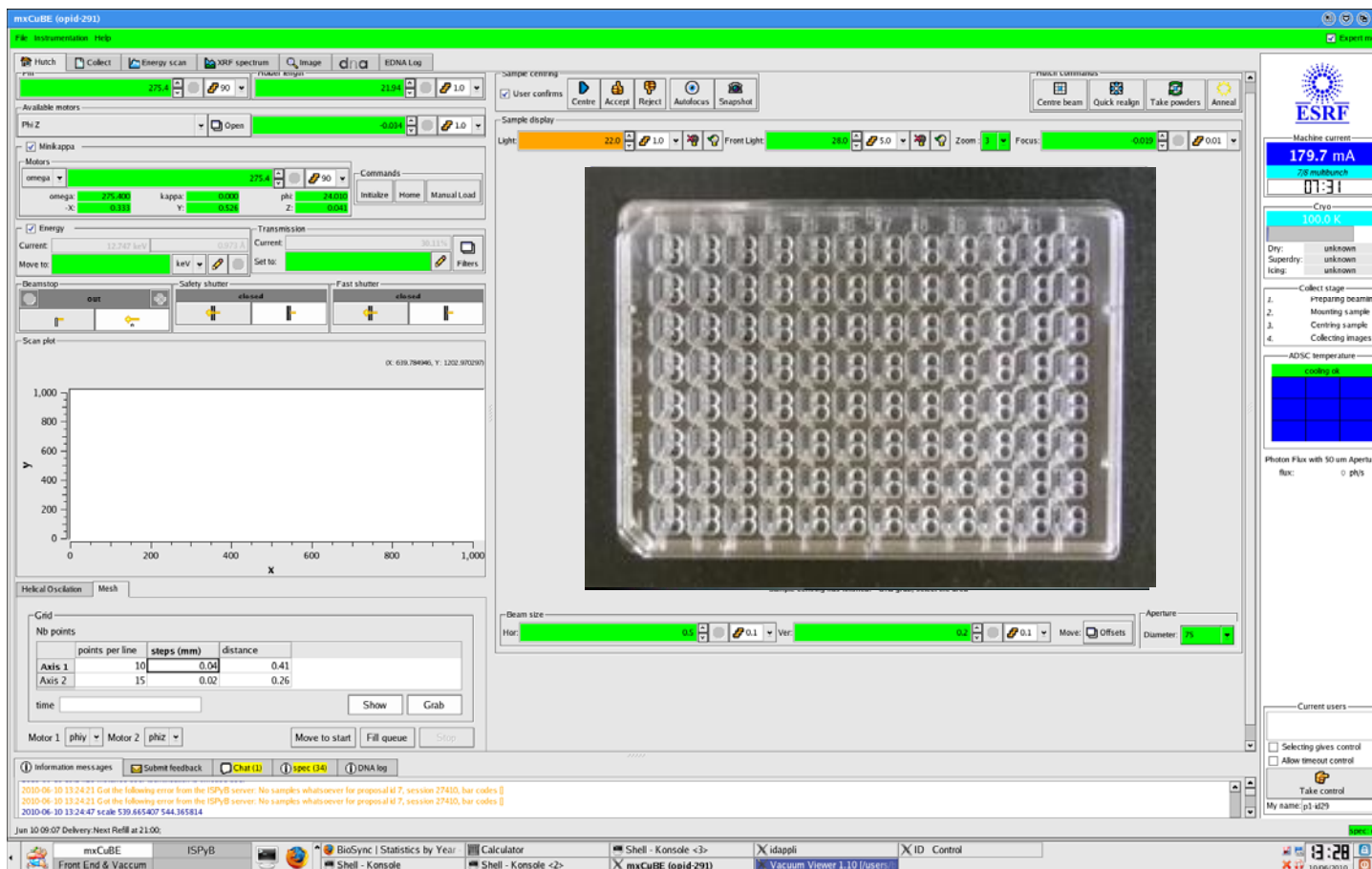
Type = Sitting Drops
Screentype = plate_2_hampton

Well	Reagent number	Plate name	Screen name	Sup
D09	20	plate_2_hampton	Crystal Screen PBG-Ion	Ham

Left Shelf :

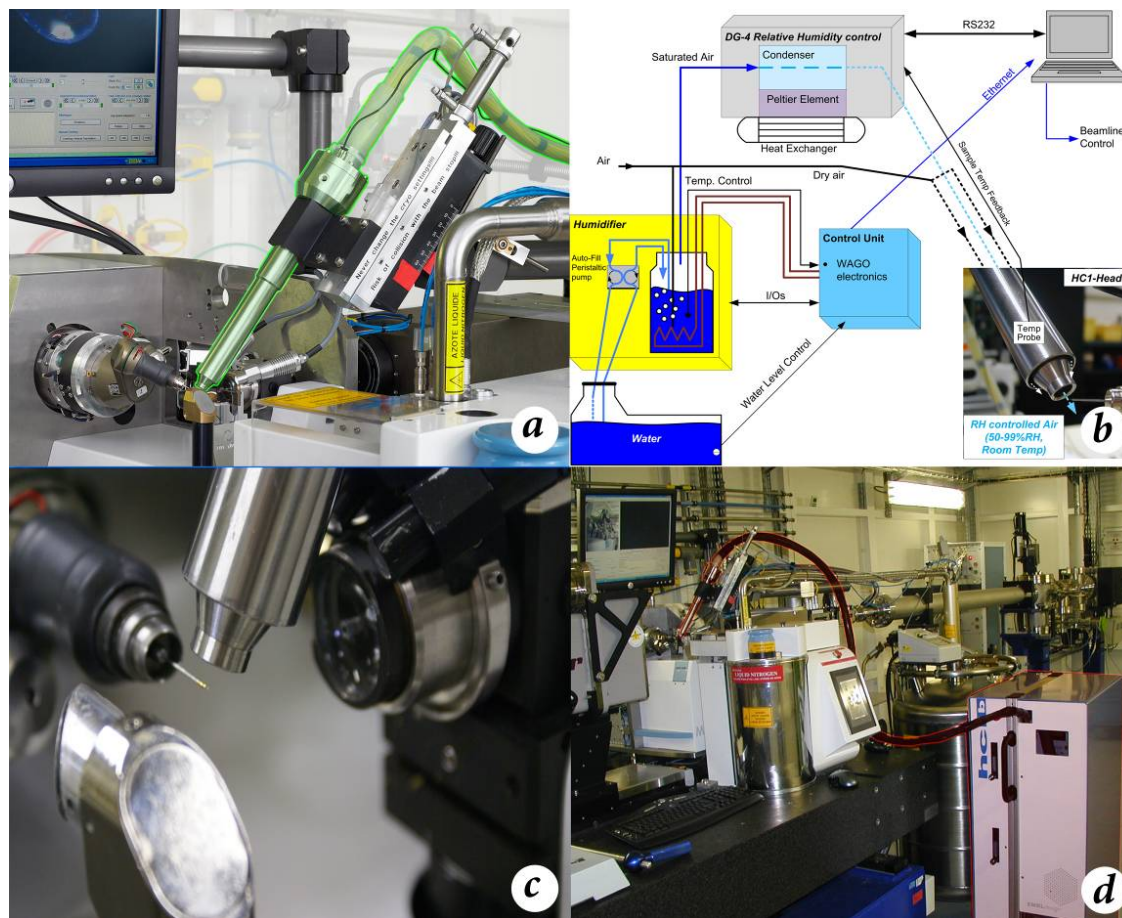
Mounted Crystal	Sent to ISPyB	Collected Images
Details	No	180
Details	No	2

Score = 4 - Inspection 1 - 02 Mar 2009 - [See full plate](#)
 Score = 4 - Inspection 1 - 02 Mar 2009 - [See full plate](#)

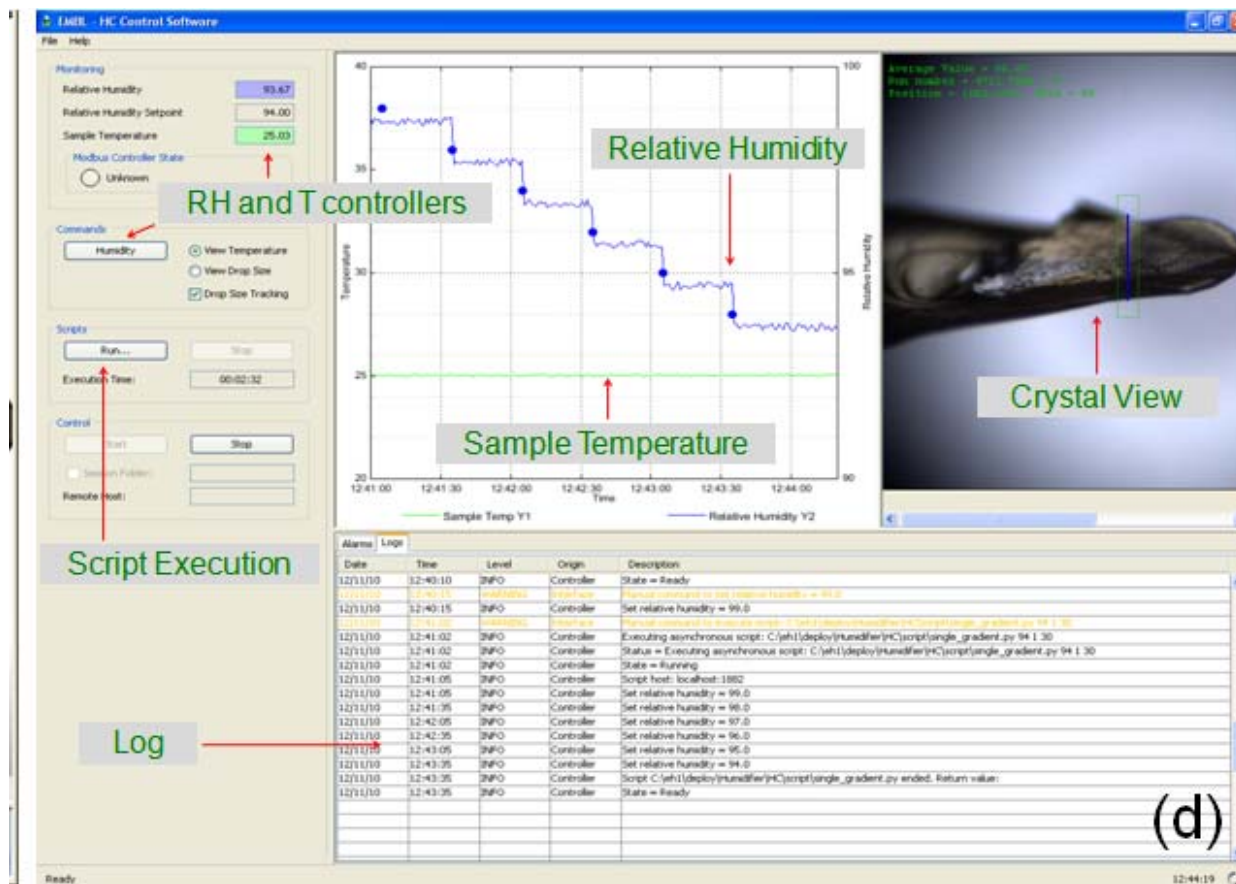


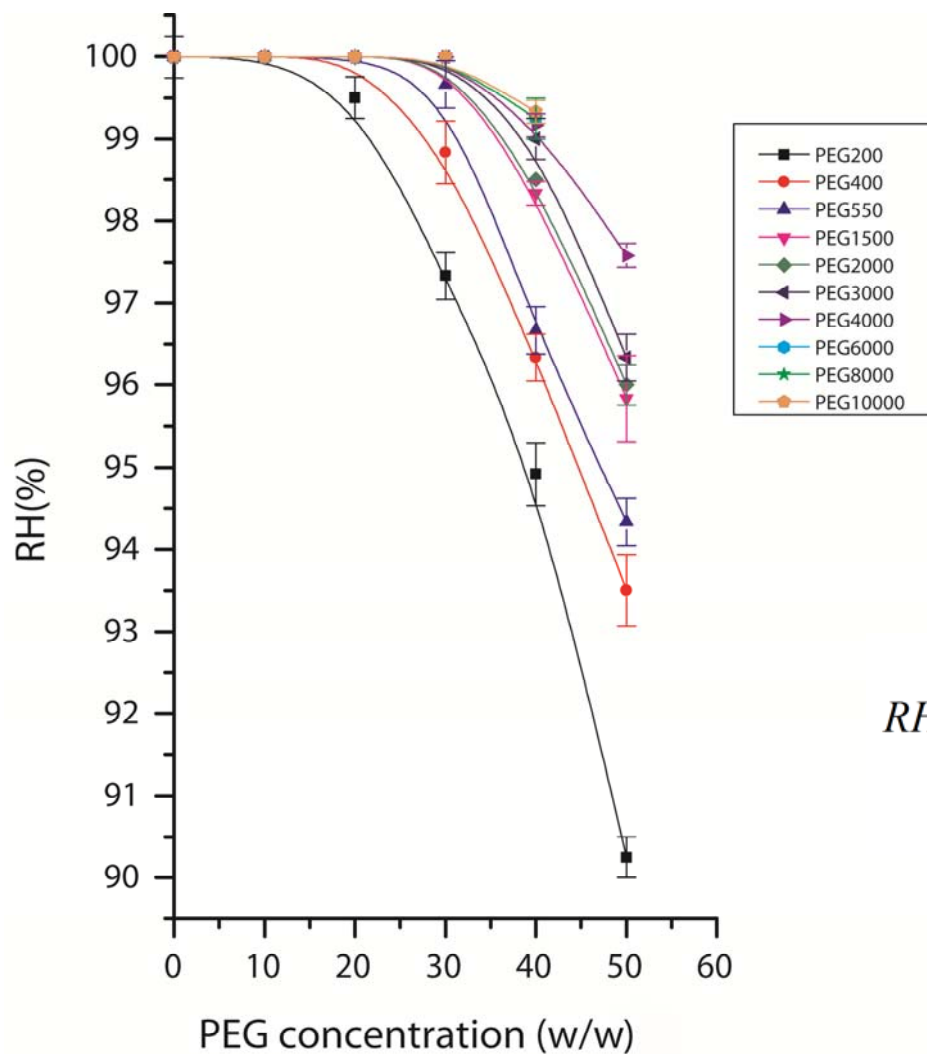
The screenshot displays the mxCuBE (opid-291) control interface. The main window features a central 'Sample display' showing a grid of 10x10 sample positions. The interface includes several control panels: a top menu bar with 'Hutch', 'Collect', 'Energy scan', 'XRF spectrum', 'Image', and 'EDNA Log'; a left sidebar with motor controls (Phi Z, Minkappa, Motors) and energy/transmission settings; a bottom-left 'Scan plot' area with a graph; and a right sidebar with status indicators (Machine current: 179.7 mA, Cryo: 100.0 K) and a 'Collect stage' checklist. The bottom of the window shows a Windows taskbar with various open applications like 'mxCuBE', 'ISPvB', and 'BioSync'.

<http://go.esrf.eu/HC1b>



Sanchez-Weatherby *et al.* 2010 *Acta Cryst.* **D65**, 1237-1246





$$RH = 1 - \frac{xM}{xM + \frac{1000}{18}(1 - yM)}$$

$$RH = \frac{1}{1 + \frac{x}{1-x} \frac{18}{n}}$$

$$RH = \frac{1}{1 + \frac{18x}{(1-x)m}} \exp\left\{ \frac{(1-m/n)}{1 + \frac{(1-x)m}{18x}} \right\}$$

<http://go.esrf.eu/RH>

The screenshot displays the MXCuBE control interface with the following components:

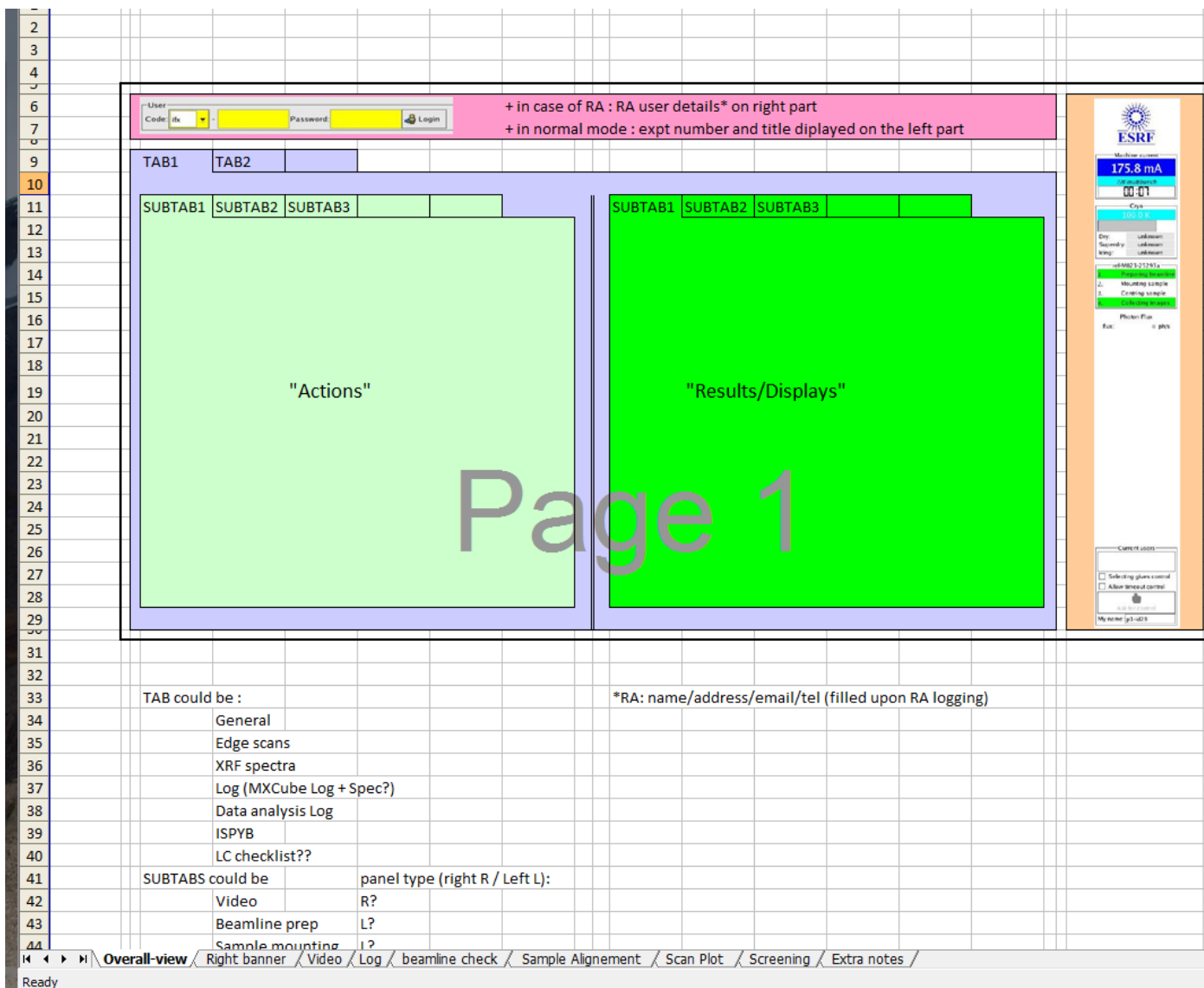
- Top Panel:** File, Instrumentation, Help menus and a toolbar with buttons for Hutch, Collect, Energy scan, XRF spectrum, Image, and dna.
- Motor Controls:**
 - Phi: 89.4, Holder length: 22.75
 - Omega: 89.427, Kappa: 0.000, Phi: 0.000
 - Energy: 13.200 keV, 0.939 Å, 17.67% transmission
- Sample Display:** A central image of a sample with a red crosshair and a blue box. Text below reads "Sample is centred!".
- Scan Plot:** A graph titled "Scan 61" showing flux_{i0} vs Table Trans. The y-axis ranges from 0 to 7e+12, and the x-axis ranges from -3.2 to -2.2. A single peak is visible at approximately -2.6.
- Right Panel:**
 - Machine current: 189.2 mA
 - Cryo: 100.1 K
 - Beam commands: Centre beam, Quick realign, Take pattern, Anneal
 - Sample display: Light, Front light, Zoom, Focus
 - Beam size: Hor, Ver
 - Current users: Selecting gives control, Allow timeout control, Ask for control, My name: artemis2
- Bottom Panel:** Information messages, Submit feedback, Chat (1), spec (2377), and DNA log.

A

The screenshot shows the MXCuBE control interface. At the top, it displays the user 'mx-415 TEST' and the facility name 'MCCARTHY E.S.R.F. Dates: 2009-10-26 to 2009-10-27'. A table lists available samples with columns for Name, Acronym, Barcode, Location, Space group, a, b, c, α , β , γ , Mir.res., and Basket. Below the table, transmission parameters are shown: Current 13.899 keV, 0.939 Å, 17.67%, and Resolution 1.790 Å. The interface also includes a 'Sample changer' section with 'Ready' status, 'Current basket (AAA04A)', and 'Current sample (CA00AE0350)'. A 'Parameters' section shows directory and file information for 'FAE-X21'. A log window at the bottom displays system messages.

B

This panel provides detailed control for the sample changer. It shows the status as 'Ready' and 'Standby'. Key information includes 'Machine current: 189.4 mA', 'Current basket (AAA04A): 3', and 'Current sample (CA00AE0350): 100.1 K'. The 'Sample is mounted' status is highlighted in green. The 'Position' is set to 1 and 'Holder length' is 22 mm. The panel includes buttons for 'Unmount CA00AE0350', 'Reset sample changer contents', and 'Scan selected baskets'. A 'Current users' section at the bottom shows 'Artemis2' with 'Add for control' and 'My name' fields.



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User Code: [dropdown] Password: [input] Login

+ in case of RA : RA user details* on right part
+ in normal mode : expt number and title displayed on the left part

TAB1 TAB2

SUBTAB1 SUBTAB2 SUBTAB3

SUBTAB1 SUBTAB2 SUBTAB3

"Actions"

"Results/Displays"

Page 1

TAB could be :

- General
- Edge scans
- XRF spectra
- Log (MXCube Log + Spec?)
- Data analysis Log
- ISPYB
- LC checklist??



*RA: name/address/email/tel (filled upon RA logging)

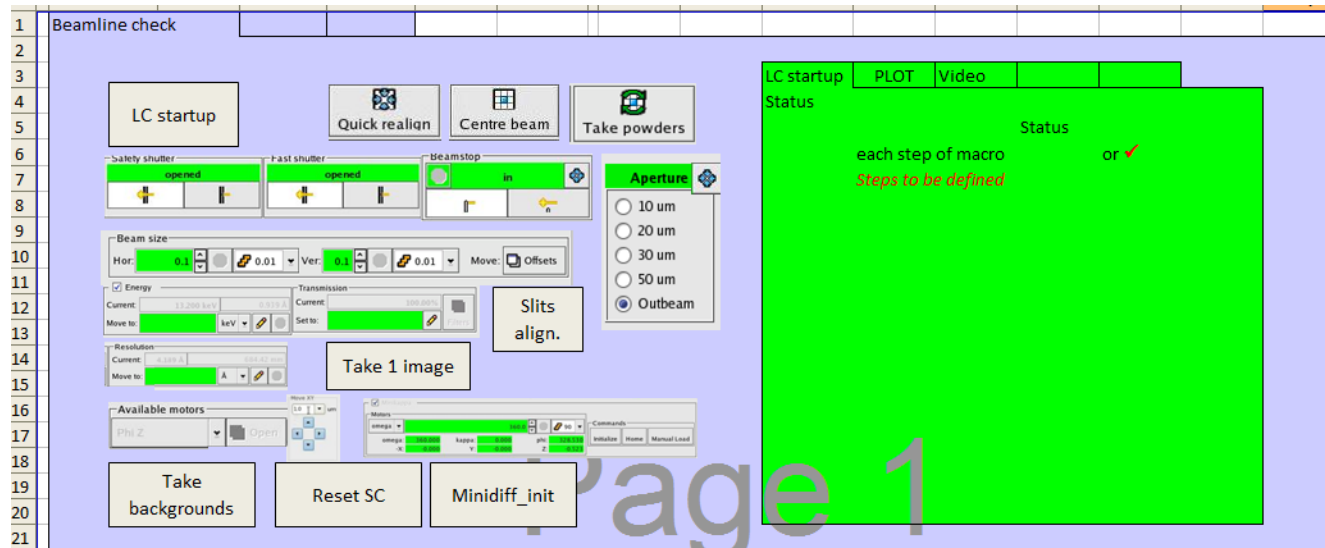
SUBTABS could be panel type (right R / Left L):

- Video R?
- Beamline prep L?
- Sample mounting L?

Overall-view / Right banner / Video / Log / beamline check / Sample Alignment / Scan Plot / Screening / Extra notes


Ready

	<p>Logo</p>
<p>Machine current 175.8 mA 7/8 multibunch 00:07</p>	<p>Machine current Machine message Cryo : just temp value (=get rid of rest) - <i>should follow same color code as rest = 100K green /+-5K orange /away >+-5K red?</i></p>
<p>Machine status: message</p> <p>Cryo 100K</p> <p>ADSC temperature cooling ok</p>	<p>ADSC: temp control of quadrants for beamlines concerned Photon flux RA interface (names, selecting give control...) Status of sample: name - steps with green(done successfully) /yellow (in progress)/ red(failed) - clicking on red message brings to Mxcube information message TAB or SC TAB</p>
<p>Beamline</p> <ol style="list-style-type: none"> Beam center Quick Realign <p>Photon Flux flux: 0 ph/s</p>	<p><i>Chat message : Once Chat "new message" clicked -brings the chat TAB to the eye & this info disappears from main banner</i> <i>Matthew to provide snapshot coming from Facebook</i></p> <p><i>UV oscillation???</i></p> 
<p>ref-M023-25293a</p> <ol style="list-style-type: none"> Mounting sample Centring sample Collecting images Un Mounting sample 	
<p>Chat New message waiting</p>	
<p>Current users</p> <p><input type="checkbox"/> Selecting gives control</p>	



"Take 1 image" could be by default 0.5sec/0.5deg or beamline dependent to align beamstop/check diffraction on detector is ok

Plot & Video subtabs as in general subtabs

Click on  will open tuning non-modal pop-up of this kind:



If apertures are tuned: title should be name of aperture

Acknowledgments:

Sean McSweeney
Gordon Leonard
Christoph Mueller-Dieckmann
ID13 – mesh scans
Olof Svenson – EDNA
Sasha Popov
Didier Nurizzo
Matt Gerring
Philippe Carpentier
David Flot
Matias Gujjarro
Antonia Beteva
Elspeth Gordon
Stephanie Monaco
Daniele De Sanctis
Patrice Brechereau
Pascal Theveneau
Isabel Baker
Max Nanao
Sandor Brockhauser
Andrew McCarthy
Florent Cipriani

Structural Biology Group
EMBL Instrumentation/Synchrotron Science

