

ID30B: Current status and future developments

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Christoph Mueller-Dieckmann (ESRF)

EMBL



ID30B - Timeline

June 26th 2015

Inauguration

Nov 5/6

First FlexHCD
users

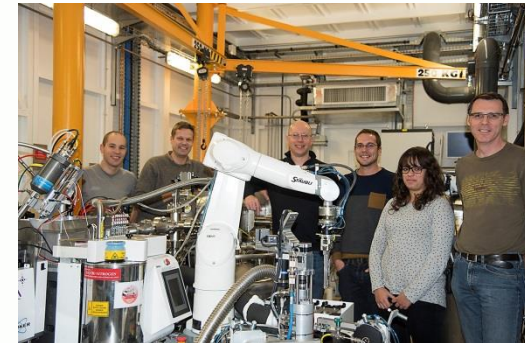
4Q 2015

Beamline
commissioning
Jan-June 2015

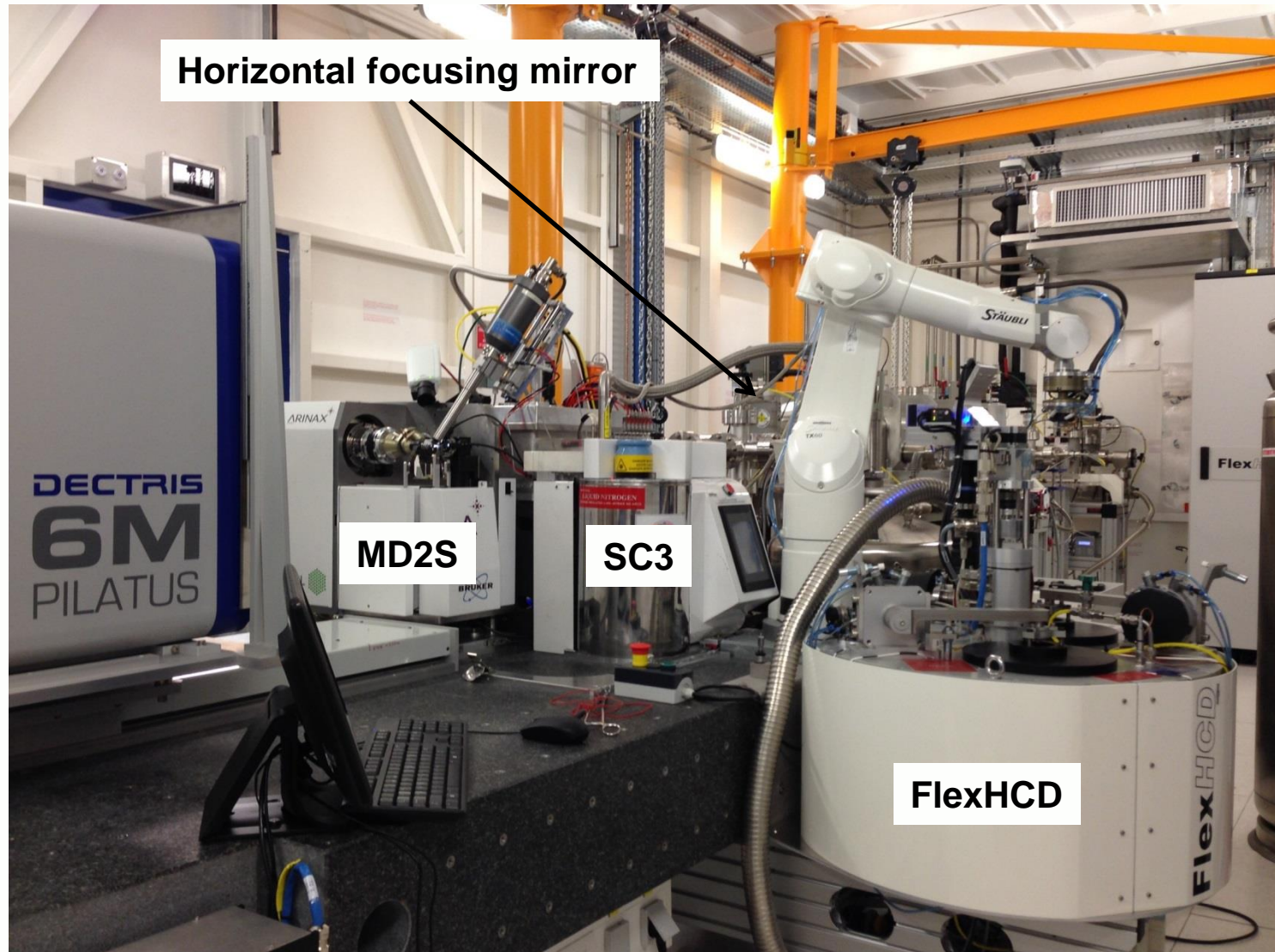


Feb 2015

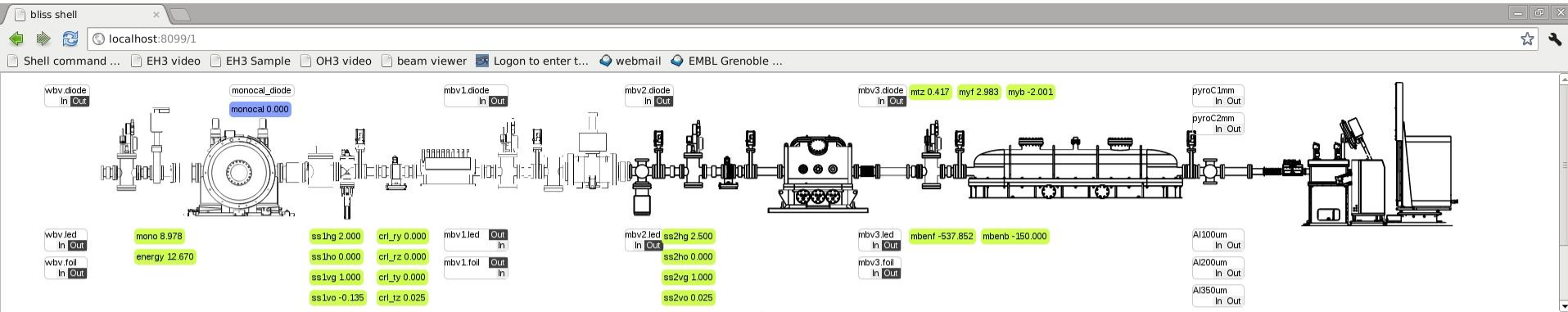
ID30B opens
with SC3
June 2015



ID30B – Experimental hutch



ID30B – BLISS control software



```

Setup  Shell output  Log messages

> wa()

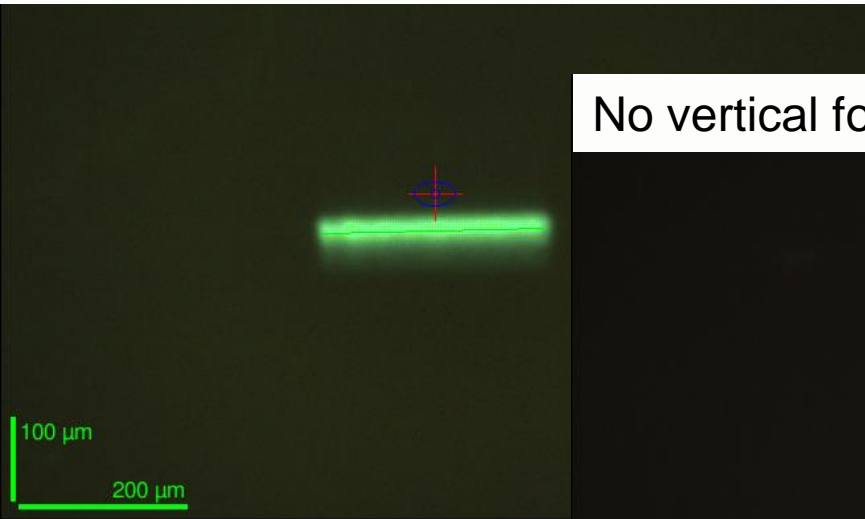
Axis name      Position      Offset
-----
ss2vg          0.9999        0
ss2vo          0.02535      0
s1vt          0             0
mtz           0.416927     0
psb           1             0
monocal       0             0
psd           0.25         4.44089e-16
tyrot        9.66399e-05  0
psu          0.25         0
s1ht         0.00496934   0
ss2hg        2.5          0
energy       12.67        -3.96128e-13
push111      0.25         0
s1v          0.4          0
ss2ho        0             0
s1h          1.2          0
wavelength   0.97856      0
cr1_ry       0             0
psvo         -2.22045e-16 0
psvg         0.5          0
thgt         -0.0940128   0
mono         8.97765      2.71737e-06
tzrot        0.33703      0
fshut_mot    6632.5       0
cr1_tz       0.02527      0
cr1_ty       0             0
txrot        -8.47458e-05 0
ss2b         1.25         0
ss2d         0.4746       0
ss2f         1.25         0
  
```


ID30B – Variable focusing capabilities

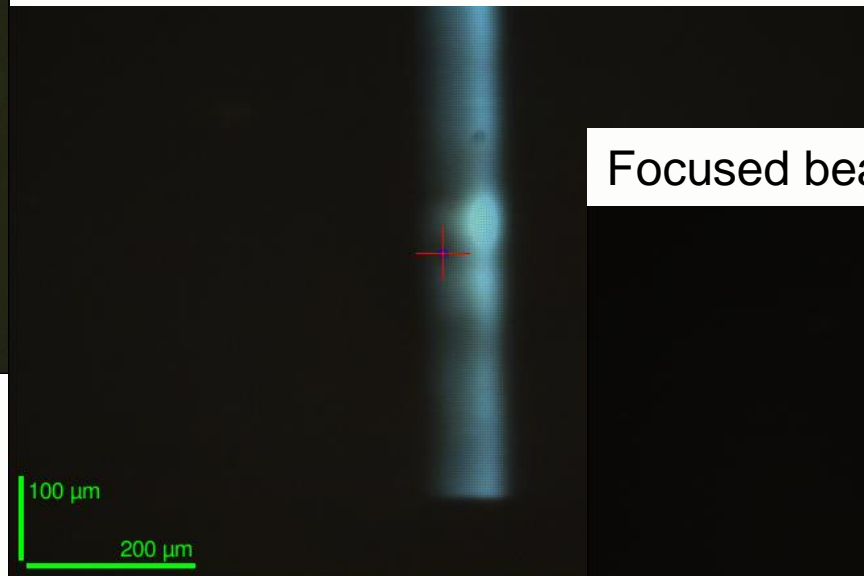
Flux $\sim 6 \times 10^{12}$ phs/sec/mm² at 12.7 keV

Beam size: $< 40 \mu\text{m}^2$

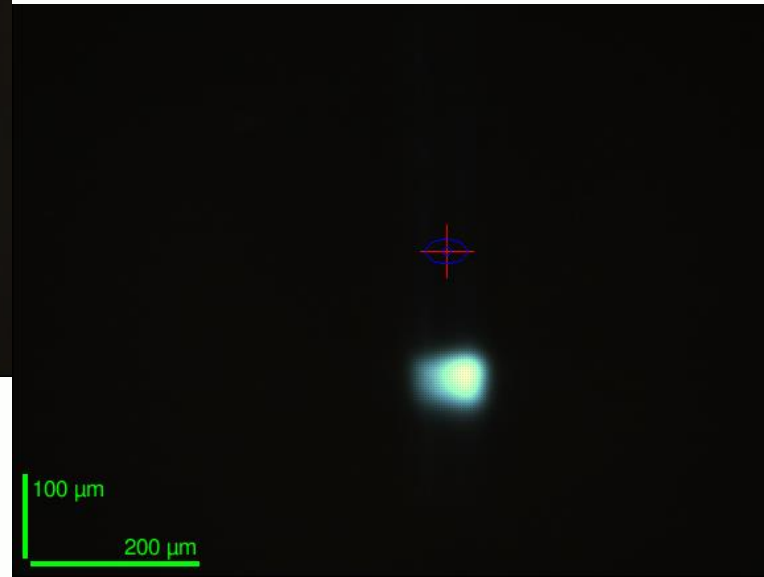
Vertical focusing, no horizontal focusing
(mirror unbent)



No vertical focusing – mirror bent



Focused beam



ID30B – Apertures (75, 50, 30, 20, 10 μm^2)



ID30B – Good data quality

andrewmc@pc386: ~

File Edit View Search Terminal Help

R-meas = redundancy independent R-factor (intensities)
Diederichs & Karplus (1997), Nature Struct. Biol. 4, 269-275.

CC(1/2) = percentage of correlation between intensities from
random half-datasets. Correlation significant at
the 0.1% level is marked by an asterisk.
Karplus & Diederichs (2012), Science 336, 1030-33

Anomal
Corr = percentage of correlation between random half-sets
of anomalous intensity differences. Correlation
significant at the 0.1% level is marked.

SigAno = mean anomalous difference in units of its estimated
standard deviation ($|F(+)-F(-)|/\text{Sigma}$). F(+), F(-)
are structure factor estimates obtained from the
merged intensity observations in each parity class.

Nano = Number of unique reflections used to calculate
Anomal_Corr & SigAno. At least two observations
for each (+ and -) parity are required.

SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE ≥ -3.0 AS FUNCTION OF RESOLUTION

RESOLUTION LIMIT	NUMBER OF REFLECTIONS			COMPLETENESS OF DATA	R-FACTOR observed	R-FACTOR COMPARED expected	I/SIGMA	R-meas	CC(1/2)	Anomal Corr	SigAno	Nano	
	OBSERVED	UNIQUE	POSSIBLE										
15.00	149	53	66	80.3%	3.1%	2.8%	140	31.53	3.8%	99.7*	34	1.074	10
10.00	447	122	128	95.3%	3.1%	3.0%	445	38.99	3.6%	99.9*	-11	0.762	43
6.00	2381	599	601	99.7%	3.1%	3.1%	2352	38.96	3.6%	99.8*	-2	0.846	273
4.00	6626	1684	1701	99.0%	3.1%	3.1%	6534	38.72	3.5%	99.8*	0	0.808	743
3.50	5061	1172	1179	99.4%	2.9%	3.2%	4999	39.83	3.3%	99.9*	2	0.803	576
3.00	8922	2059	2068	99.6%	3.1%	3.3%	8845	37.02	3.4%	99.9*	-3	0.787	1043
2.60	12119	2945	2955	99.7%	3.6%	3.8%	11999	29.67	4.2%	99.8*	0	0.828	1310
2.20	23647	5445	5463	99.7%	4.4%	4.5%	23486	25.91	5.0%	99.8*	-3	0.846	2729
2.00	19126	4538	4555	99.6%	5.2%	5.3%	19013	20.99	6.0%	99.7*	3	0.868	2327
1.80	27749	6775	6799	99.6%	7.4%	7.2%	27567	14.85	8.5%	99.5*	1	0.869	3201
1.60	44243	10527	10553	99.8%	12.5%	12.1%	44025	9.12	14.2%	98.7*	2	0.870	5573
1.40	72325	17375	17410	99.8%	23.4%	23.1%	71972	4.83	26.7%	95.4*	-2	0.817	9361
1.20	119668	30341	30889	98.2%	54.5%	55.8%	118696	1.89	62.8%	77.1*	-1	0.757	16359
total	342463	83635	84367	99.1%	5.4%	5.5%	340073	10.52	6.2%	99.9*	0	0.809	43548



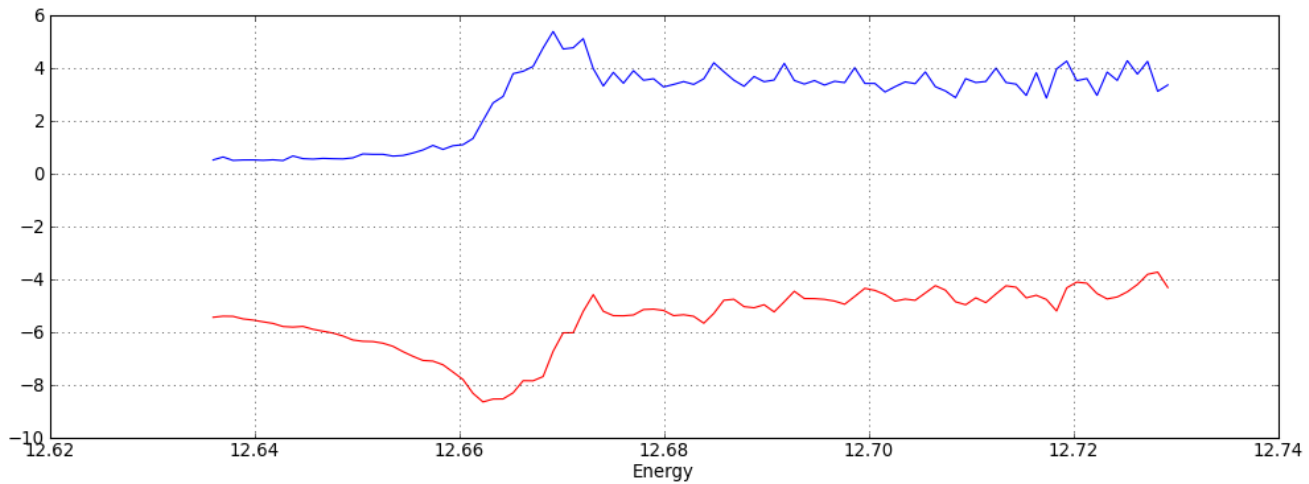
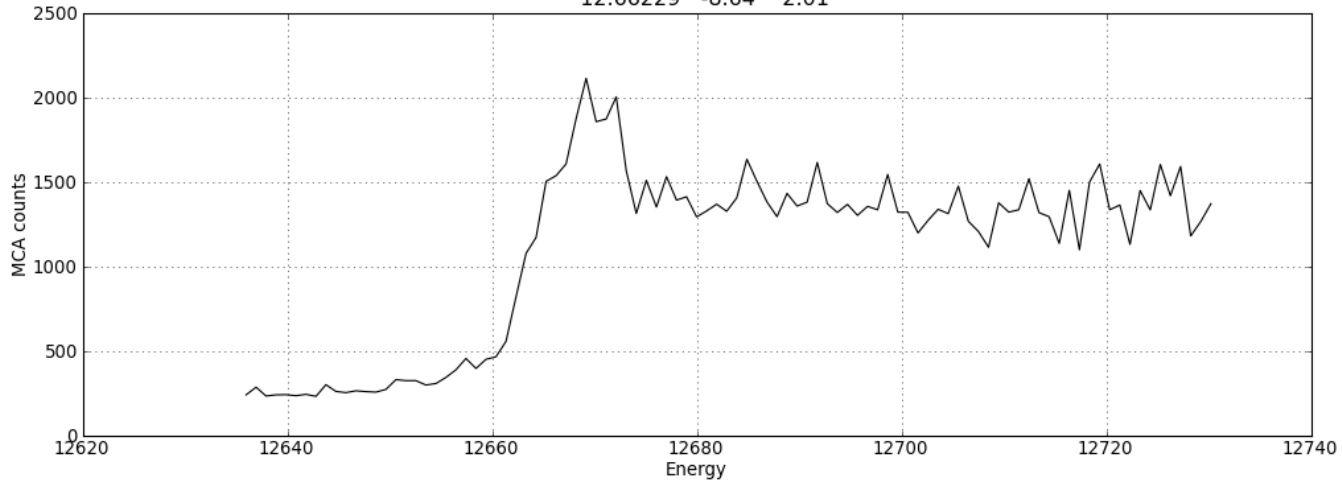
EMBL



ID30B – Fast energy scans

/data/id30b/inhouse/opid30b/20150903/RAW_DATA/opid30b.efs

energy	f'	f''
12.66914	-6.72	5.39
12.66229	-8.64	2.01

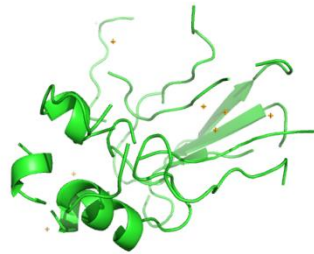


ID30B – Automatic structure solution

opid30b (1.4 Å)



MX-ih4 (2.4 Å)



MX-1695 (2.3 Å)



MX-1737 (1.4 Å)



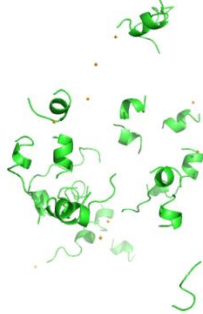
FAE Se at Br edge

Thaumatin (Gd)

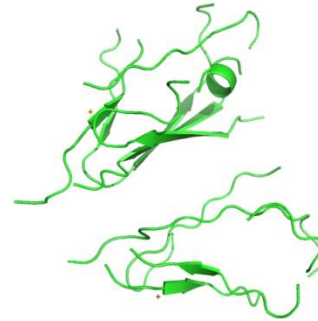
MX-1749 (2.9 Å)



MX-1743 (3.9 Å)



MX-1696 (2.1 Å)



MX-1737 (4.2 Å)



EMBL-ESRF Beamline Expert System

- Passerelle-EDM – A Web interface for workflow execution that logs all metadata stored in database



Passerelle EDM - Mozilla Firefox (on ub1404)

Passerelle EDM

Beamline Expert System

Connected as: Olof Svensson
Version: 1.5.6

Reference: Id: Correlation Id:

Type: Initiator:

Status: Created Error Finished Cancelled Started Timeout

Creation Date: To

Reference	Id	Type	Creation Date	Initiator	External Reference	Status	Duration(ms)
2903	275845	CreateThumbnails	2015-04-12 12:08:51	id29	mx1680	Finished	60,000
2903	275838	Characterisation	2015-04-12 12:08:27	id23eh1	mx1680	Finished	33,000
2903	275834	EDNA_dp	2015-04-12 12:08:18	id23eh1	mx1680	Finished	6,000
2903	275841	CreateThumbnails	2015-04-12 12:07:33	id29	mx1680	Finished	3,000
2893	275817	MXPressE	2015-04-12 12:07:32	id30a1	fx24	Finished	422,000
2903	275826	EDNA_dp	2015-04-12 12:07:29				
2903	275810	Characterisation	2015-04-12 12:06:50				
2903	275796	EDNA_dp	2015-04-12 12:06:41				
2903	275767	CreateThumbnails	2015-04-12 12:05:45				
2903	275822	Characterisation	2015-04-12 12:05:45				
2903	275763	CreateThumbnails	2015-04-12 12:05:39				
2903	275688	EDNA_dp	2015-04-12 12:05:33				
2903	275802	Characterisation	2015-04-12 12:04:47				
2903	275788	EDNA_dp	2015-04-12 12:03:38				
2893	275780	MXPressE	2015-04-12 12:02:10				
2903	275784	Characterisation	2015-04-12 11:59:22				

Value

true

ImageQualityIndicators: ref-MOA-X19-A6-10-4_2_0001.cbf: good bragg 520, r1 2.9 [A], max cell 185.2 [A], ic 92.2
ImageQualityIndicators: ref-MOA-X19-A6-10-4_2_0002.cbf: good bragg 23, r1 3.9 [A], max cell 235.6 [A], ic 17.0
Indexing: laue/space group P3, mosaicity 2.20 [degree], RMS dev pos 0.36 [mm] ang 0.52 [degree]
Indexing: refined Cell: 121.07 121.07 99.28 90.00 90.00 120.00
Integration: 1 no full: 0, part: 14517, bad/neg/ovrlp: 7244, RMS dev: 0.138 [mm], I/sigma overall 0.5 at high
Integration: 2 no full: 0, part: 15056, bad/neg/ovrlp: 8417, RMS dev: 0.130 [mm], I/sigma overall 0.1 at high
Strategy: Radiation damage estimated, time to reach Henderson limit: 31.4 s
Strategy: Options: aimed completeness = 1.0, aimed resolution = 0.50 A, complexity = none
Strategy: Collection plan 1: Resolution limit is set by the radiation damage
Strategy: Ranking resolution: 2.58 [A]
Strategy: wedge 1: resolution 2.58 [A], sub wedge 1: start 108.00, images 600, width 0.10, time 0.04 [s], transmission 0.27
Strategy: total no images 600, total exposure time 22.2 [s]

Passerelle EDM - Mozilla Firefox (on ub1404)

Passerelle EDM

Beamline Expert System

Connected as: Olof Svensson
Version: 1.5.6

Flow MXPressE (6.0) on 2015-04-12 12:07:32

Back Edit Validate Flow Run Customize

Director

Error Handler by Severity

CommonErrorReporter

Set 1595b to success

Workflow ends with error messages

Finished

Stop

Set 1595b to success with error messages

Workflows implemented in MxCuBE

mxcube (opid-30b) Expert mode

File Instrumentation Help

Collect System Feedback Chat

User: opid-30b Group: [] Set Logout

Sample list
Mode: Sample changer Show SC-details
Centring: Semi Automatic Synch ISPyB

Sample centring
Sample position
Omega: 310.00 90.0 Kappa: 0.00 1.0 Phi: 0.00 0.1
Holder length: 23.067 0.1

Sample video
Back Light: 0.50 Focus: -0.200 0.01 Front Light: 0.0 Zoom: 5

Collection method
Standard Collection
Characterisation
Helical Collection
Energy Scan
XRF Spectrum

X-ray Centring
Mesh Scan
Kappa Re-orientation
Visual Re-orientation
Helical characterisation
Mesh and collect
Enhanced characterisation
Burn strategy
Dehydration
Trouble shooting

Machine current
160.6 mA
7/8 multibunch
04:09
Flux: 1.94e+12 ph/s
Energy
Current: 12.7000 keV
0.976 A
Move to: keV
Resolution
Current: 1.498 A
267.84 mm
Move to: A
Transmission
Current: 100.00%
Set to: Filters

Safety shutter: opened
Fast shutter: closed
Beamstop: unknown
Capillary: out
Current users
Selecting gives control
Allow timeout control
Take control
My name: bacon

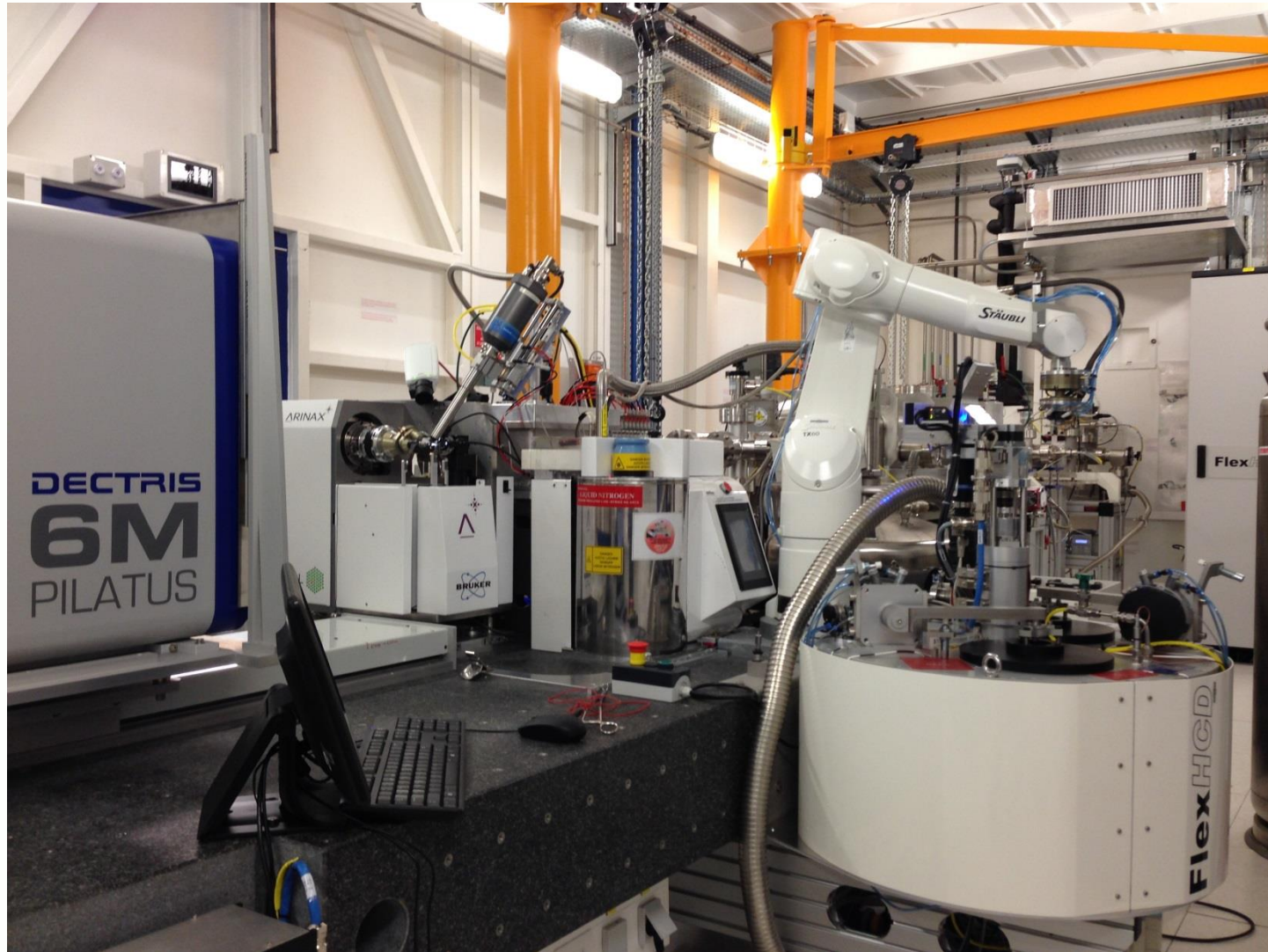
Centring done!

100 µm
100 µm
Point no. 1 (kappa: 0.00 phi: 0.00) selected
Aperture diameter: 80

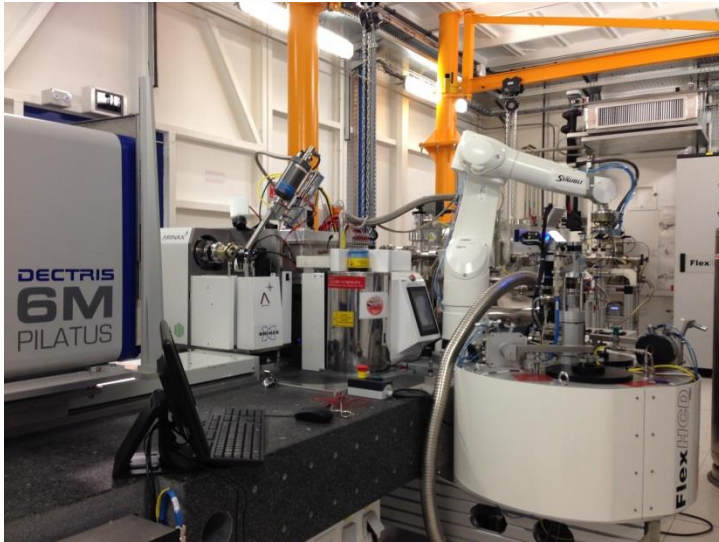
Collect Queue Pause

[2015-11-10 16:46:33] Centring in progress. Please save the suggested centring or re-center
[2015-11-10 16:47:13] Microdiff is not ready, will not put Microdiff Aperture in
[2015-11-10 16:48:31] Centring saved

FlexHCD robot



FlexHCD – A versatile sample changer



SPINE baskets (x12) = 120 samples



ESRF
SLS
BESSY
PETRAIII
ALBA

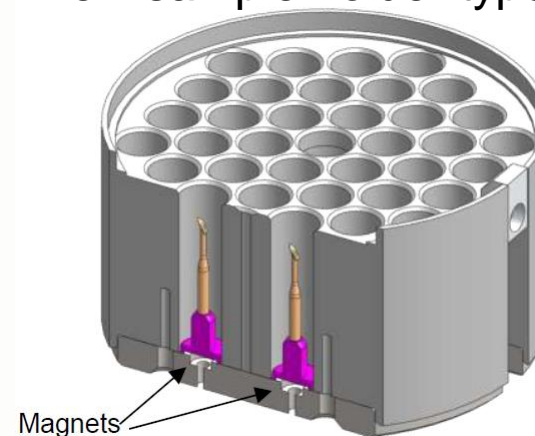
Unipucks (x12) = 192 samples



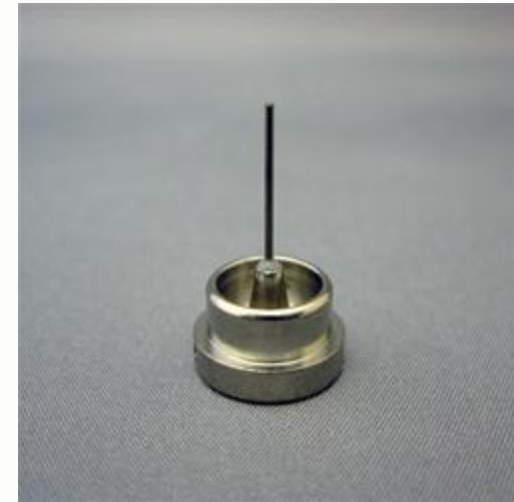
Most US sites

Europe:
DLS
SOLEIL

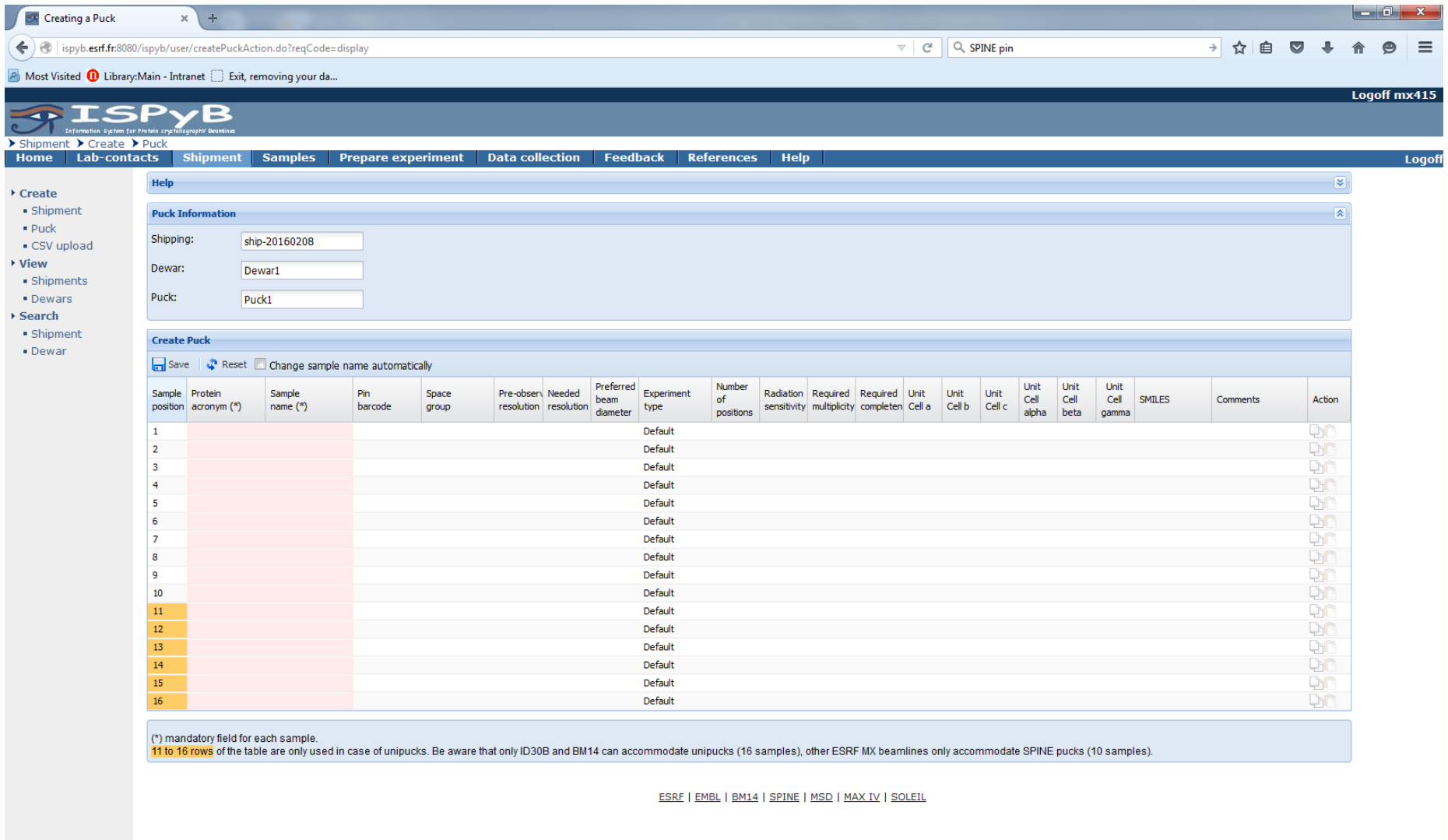
New sample holder types (36 samples)



FlexHCD – Only SPINE pins allowed



FlexHCD – Unipuck integration in ISPyB



Creating a Puck

ispyb.esrf.fr:8080/ispyb/user/createPuckAction.do?reqCode=display

Most Visited Library:Main - Intranet Exit, removing your da...

ISPyB
Information System for Protein crystallography beamlines

Shipment Create Puck

Home Lab-contacts Shipment Samples Prepare experiment Data collection Feedback References Help

Logoff mx415

Help

Puck Information

Shipping:

Dewar:

Puck:

Create Puck

Change sample name automatically

Sample position	Protein acronym (*)	Sample name (*)	Pin barcode	Space group	Pre-observ resolution	Needed resolution	Preferred beam diameter	Experiment type	Number of positions	Radiation sensitivity	Required multiplicity	Required completeness	Unit Cell a	Unit Cell b	Unit Cell c	Unit Cell alpha	Unit Cell beta	Unit Cell gamma	SMILES	Comments	Action	
1								Default														
2								Default														
3								Default														
4								Default														
5								Default														
6								Default														
7								Default														
8								Default														
9								Default														
10								Default														
11								Default														
12								Default														
13								Default														
14								Default														
15								Default														
16								Default														

(*) mandatory field for each sample.
11 to 16 rows of the table are only used in case of unipucks. Be aware that only ID30B and BM14 can accommodate unipucks (16 samples), other ESRF MX beamlines only accommodate SPINE pucks (10 samples).

[ESRF](#) | [EMBL](#) | [BM14](#) | [SPINE](#) | [MSD](#) | [MAX IV](#) | [SOLEIL](#)



10:02 AM
2/8/2016



FlexHCD MxCuBE integration

The screenshot displays the mxcube (opid-30b) control interface. The main window is titled "mxcube (opid-30b)" and includes a menu bar with "File", "Instrumentation", and "Help". Below the menu bar are buttons for "Collect", "System", "Feedback", and "Chat".

The interface is divided into several sections:

- User Information:** Shows "User: opid-30b" and "Group:" with a "Set" button and a "Logout" button.
- Sample list:** A tree view on the left shows a hierarchy of samples. The selected sample is "3:3", which is highlighted in blue and has a "Centring done!" status. Below it, "Standard - 1" and "Test_1 (Point - 1)" are listed.
- Sample centring:** A central panel titled "Sample centring" shows "Flex" mode. It includes a "Mount/unmount samples by right-clicking on the data collection tree on the left" instruction. Below this are "Flex Actions" (Scan, Park, Init) and "Contents" (Reset sample changer contents, Flex Contents). The "Flex Contents" section shows a grid of baskets (Basket 1 to Basket 23) with numbered slots (1-10 or 1-16) for each.
- Machine current:** A panel on the right shows "Machine current" at 158.8 mA, "Flux: +0.00 ph/s", "Energy" at 12.3000 keV, "Current: 1.008 Å", "Resolution" at 3.488 Å, and "Transmission" at 100.00%.
- Safety and Shutter:** A section at the bottom right shows "Safety shutter" (closed), "Fast shutter" (closed), "Beamstop" (out), and "Capillary" (out).
- Current users:** A section at the bottom right shows "Current users" with a "Selecting gives control" checkbox, "Allow timeout control" checkbox, and a "Take control" button. The user name "My name: bacon" is displayed.

At the bottom of the interface, there are three status messages:

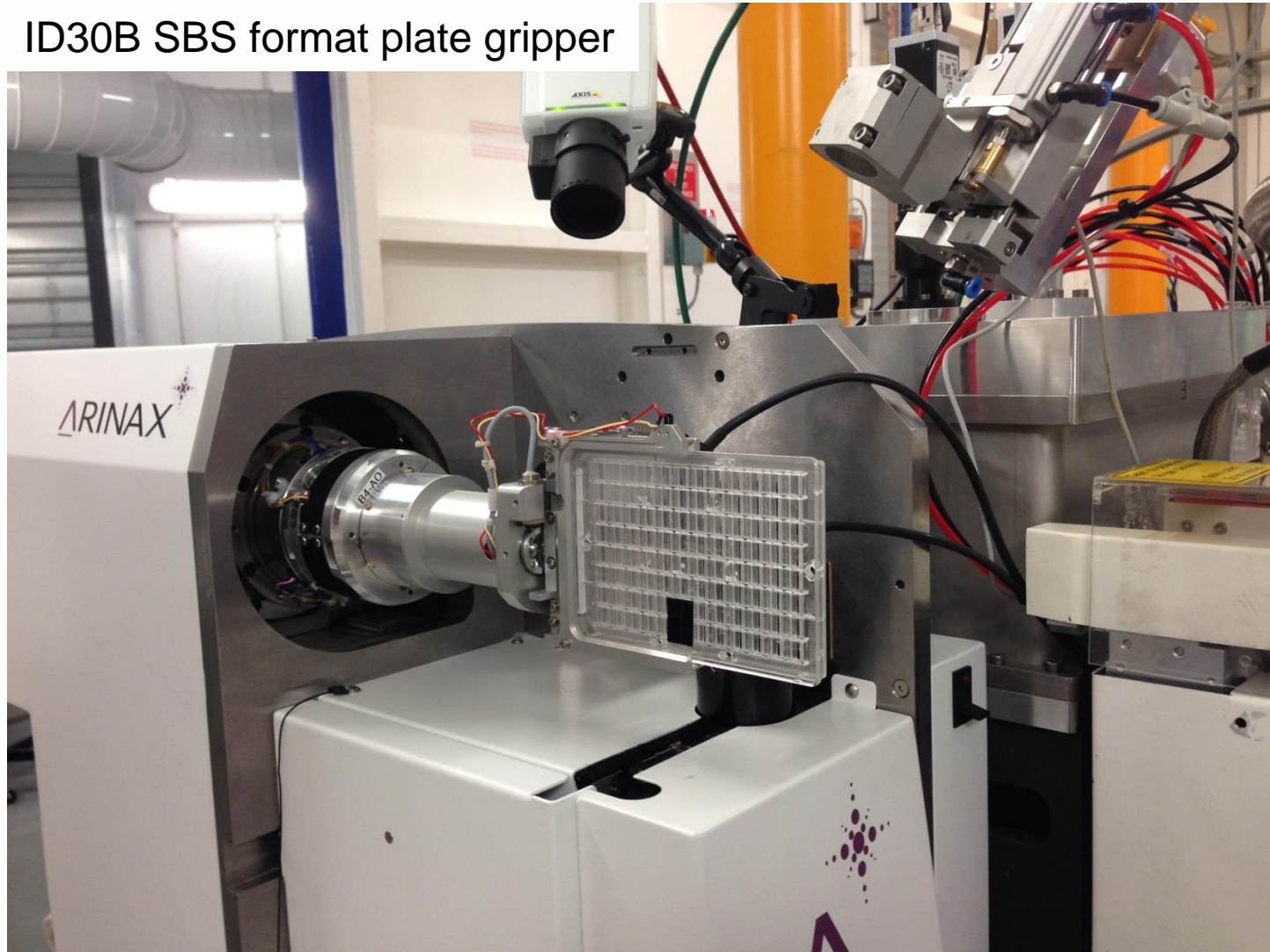
- [2015-11-27 18:15:36] All centred positions associated with this sample will be lost.
- [2015-11-27 18:17:44] Centring in progress. Please save the suggested centring or re-center
- [2015-11-27 18:18:02] Centring saved

A. Khadrouche and G. Papp (EMBL) and A. Beteva (ESRF)



ID30B – MD2S allows plate screening capability

ID30B SBS format plate gripper



In situ plate data collection in MxCuBE

The screenshot displays the MxCuBE software interface for in situ plate data collection. The main window is titled "mxcube (mx-1743)" and includes a menu bar with "File", "Instrumentation", and "Help".

Sample centring: The "Sample position" section shows Omega at 316.36, Kappa at 0.00, and Phi at 0.00. The "Sample video" section shows Back Light at 0.60, Focus at -0.729, and Front Light at 0.0. A central video window displays a sample image with a 100 µm scale bar and a "Point no. 2 selected" label. The "Aperture diameter" is set to 50.

Collection method: The "Standard Collection" section includes "Acquisition" parameters: Oscillation range (0.1), First image (1), Oscillation start (316.36), Number of images (10), Kappa (0.0), and Phi (0.0). Other parameters include Detector mode, Exposure time (0.037 s), Energy (12.7 keV), Resolution (1.997 Å), and Transmission (100.0%).

Data location: The "Folder:" field is set to "/data/visitor/mx1743/id30b/20151104/RAW_DATA". The "File name:" is "xyla_23_###.cbf" and the "Run number" is 23.

Processing: The "Processing" section shows "N.o. residues" set to 200 and "Space group" set to "unknown".

Machine current: The top right corner shows a machine current of 185.4 mA and a flux of +0.00 ph/s.

Sample list: A tree view on the left shows a list of samples, including "Standard - 7" through "Standard - 15" and "xyla_13 (Point - 1)" through "xyla_22 (Point - not defined)".

Right sidebar: The sidebar contains controls for "Energy" (12.7000 keV), "Resolution" (1.997 Å), "Transmission" (100.00%), "Safety shutter" (closed), "Fast shutter" (closed), "Beamstop" (in), "Capillary" (unknown), and "Current users" (My name: bacon).

[2015-11-04 11:49:00] Asking for input files writing
[2015-11-04 11:49:00] Preparing acquisition, start=314.730000, wedge size=10
[2015-11-04 11:49:04] Collection completed

ID30B - Plate screening capability (2016)

Plate manipulator
nozzle

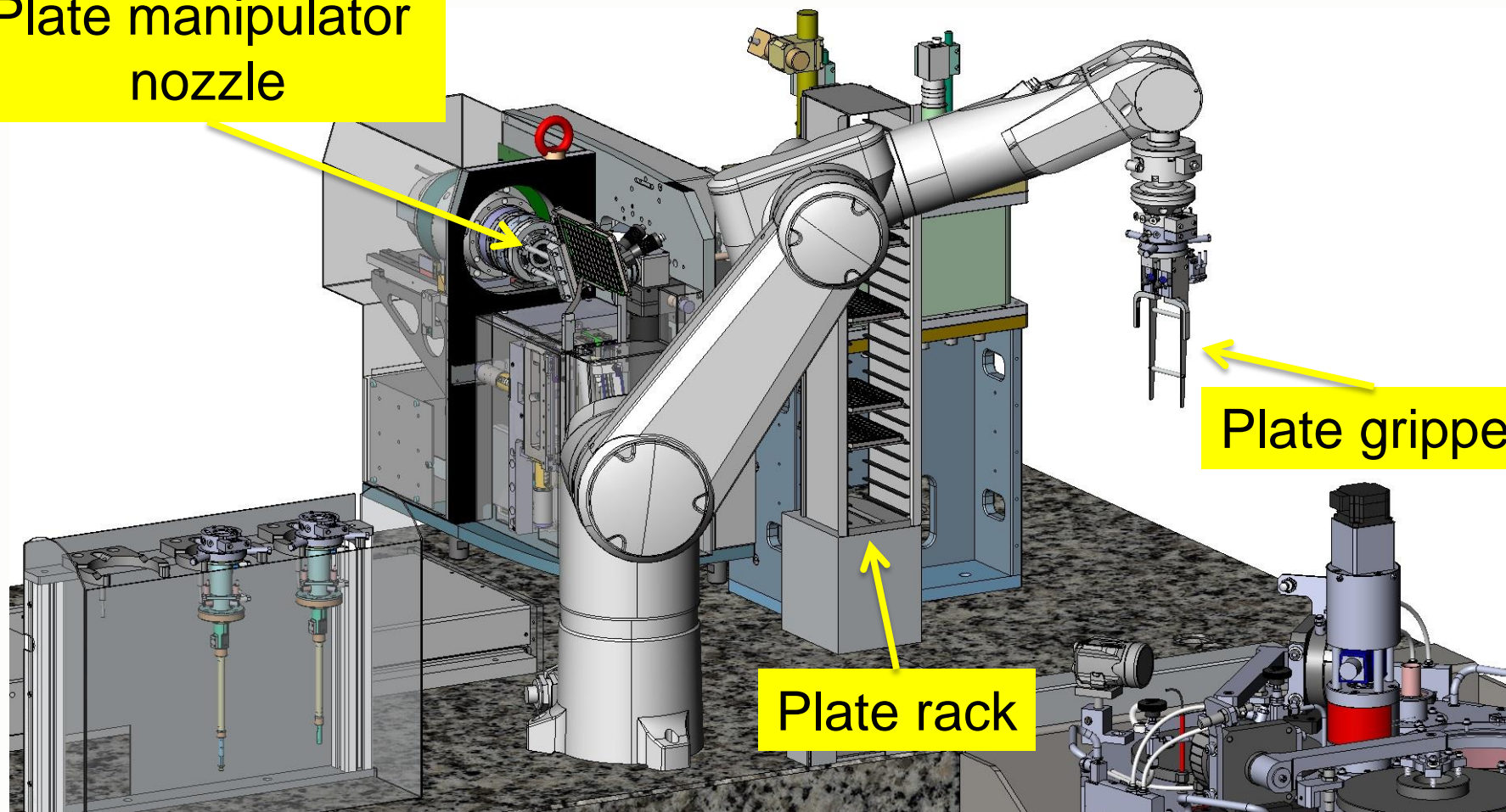


Plate gripper

Plate rack

ID30B – To do

Immediate future (February 2016)

- Finalise FlexHCD integration
- Integrate *in situ* plate screening
- Software improvements

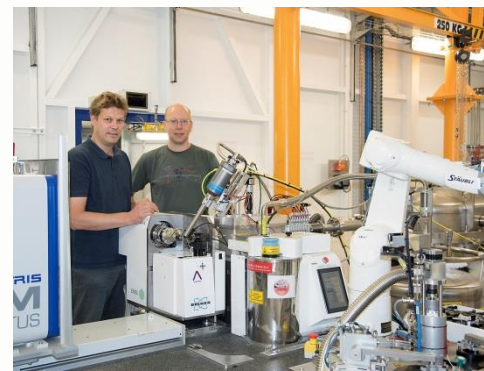
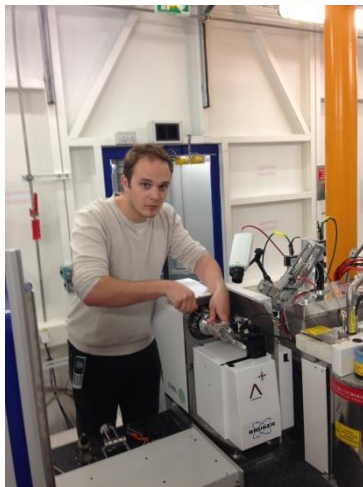
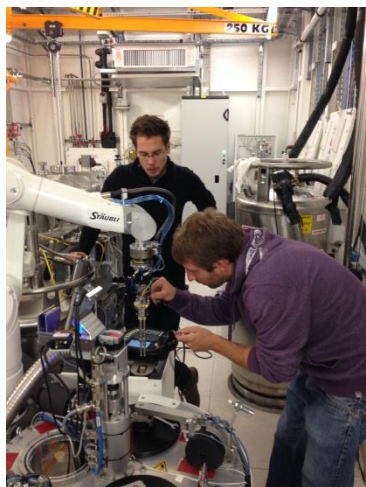
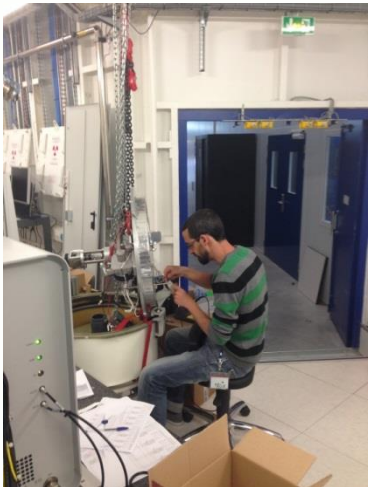
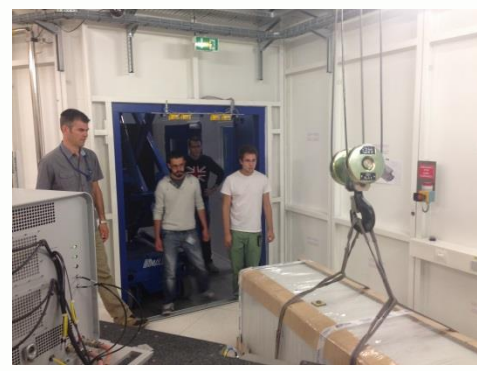
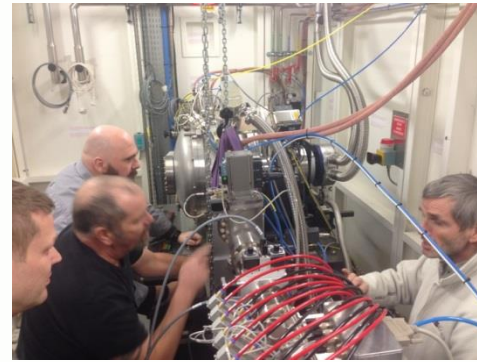
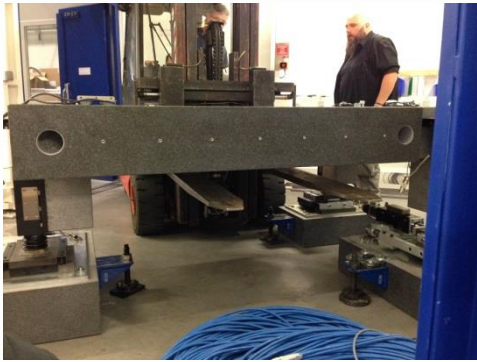
Near future

- Find a solution to (or minimise) the beam drift
- Further investigate the vertical focusing problem
- Work on variable focusing routines (coordinated bender movement)
- Introduce Unipuck mounting and test miniSpine mounting capabilities

Future plans

- Test microfluidic chip data collection possibilities
- Automate data collection (MASSIF workflows)
- Commission phase plate (Daniele)

Many thanks to all involved



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Franck Felisaz
Robert Janocha
Marcos Lopez-Marrero
Gergely Papp
Christopher Rossi
Jeremy Sinoir
Clement Sorez

Josan Marquez
Guillaume Hoffmann
Zuzanna Kaczmarska

ESRF

Jean Susini
Harald Reichert

Gordon Leonard
Sean McSweeney (NSLS II)
Christoph Müller-Dieckmann
Philippe Carpentier
Daniele de Sanctis
David Flot
Didier Nurizzo
David von Stetten
Pascal Theveneau
Hugo Caserotto
Fabien Dobias
Thierry Giraud
Mario Lentini
Werner Schmid
John Surr
Antonia Beteva
Matias Guijarro
Olof Svensson

Ray Barrett
Carole Clavel
Thierry Martin
Jean-Michel Georgoux
Renata Witch

UVHCI/IBS

Eva Pebay-Peyroula
Winfried Weissenhorn

Sandrine Vignon

Sylvie Costa
Corinne Iodice

