ID30B: Current status and future developments

Andrew McCarthy (EMBL) and
Christoph Mueller-Dieckmann (ESRF)

EMBL

ID30B - Timeline

Beamline commissioning

Jan-June 2015

June 26th 2015

Inauguration

Nov 5/6

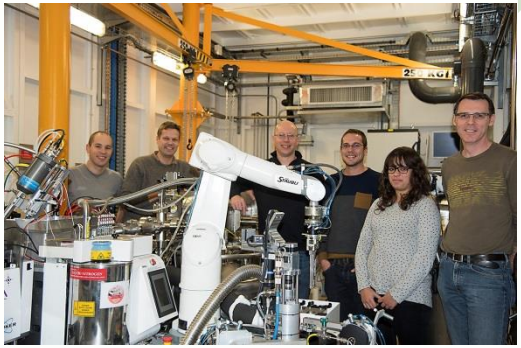
First FlexHCD users

4Q 2015

Feb 2015

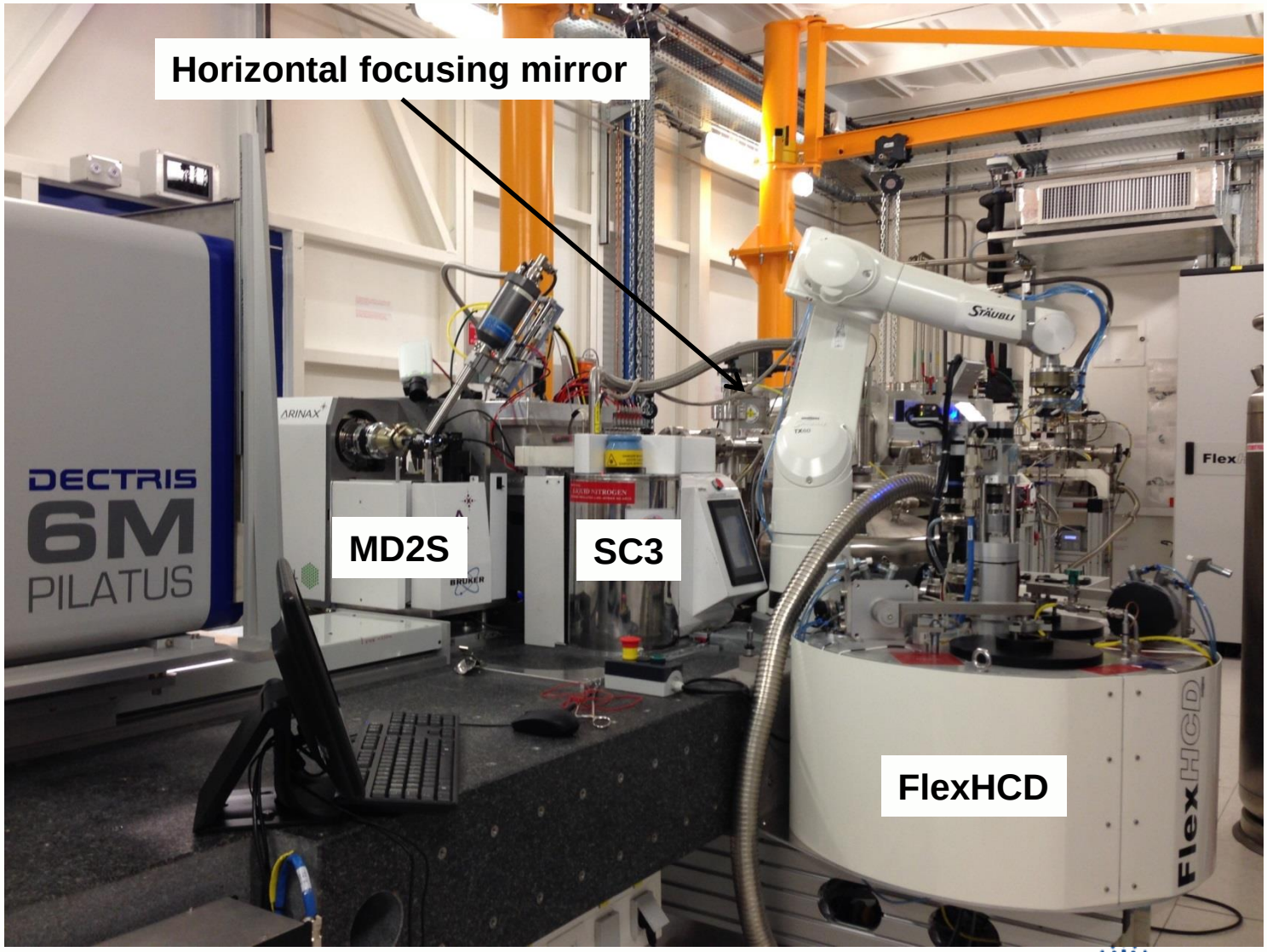
ID30B opens with SC3

June 2015



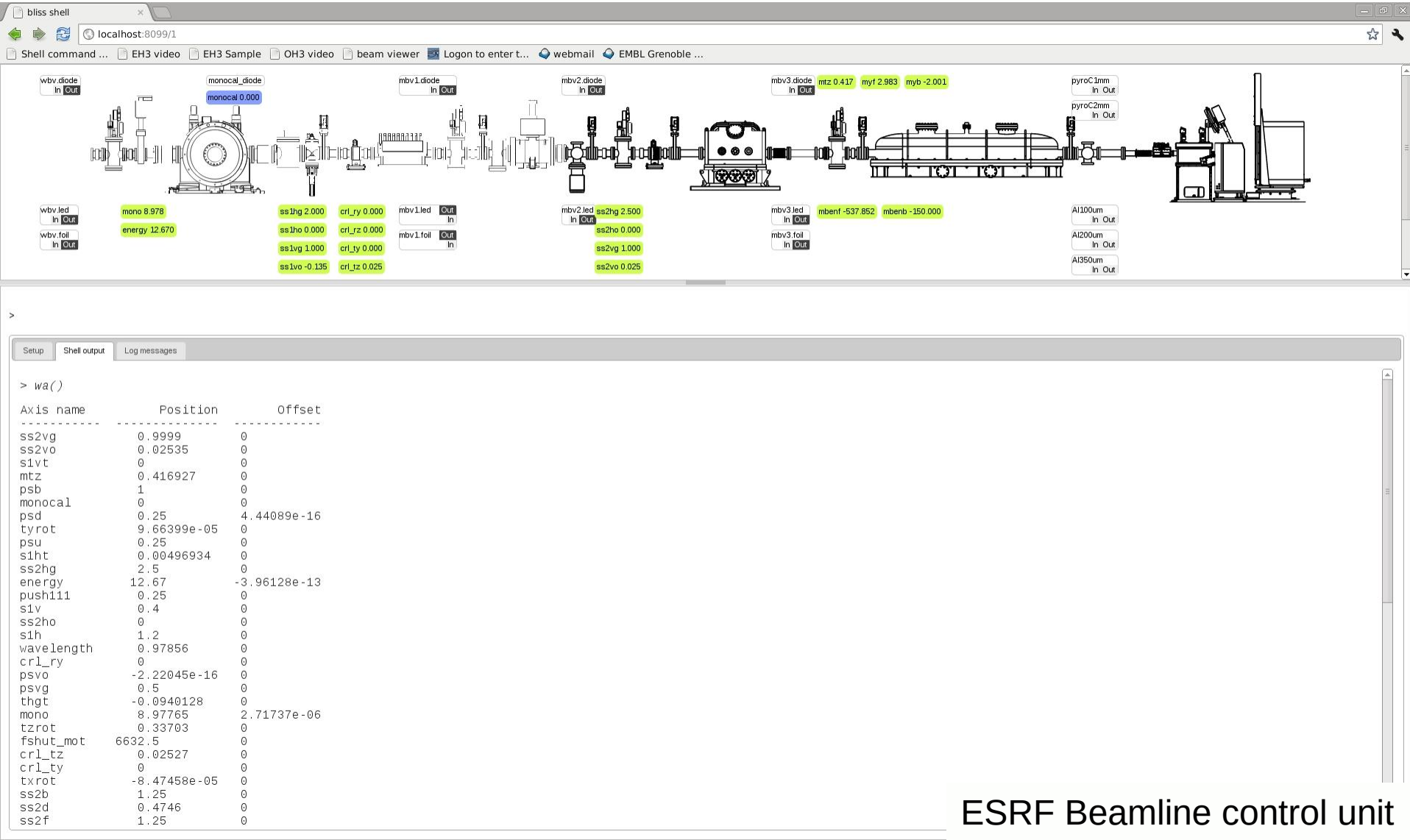
ESRF EMBL

ID30B – Experimental hutch



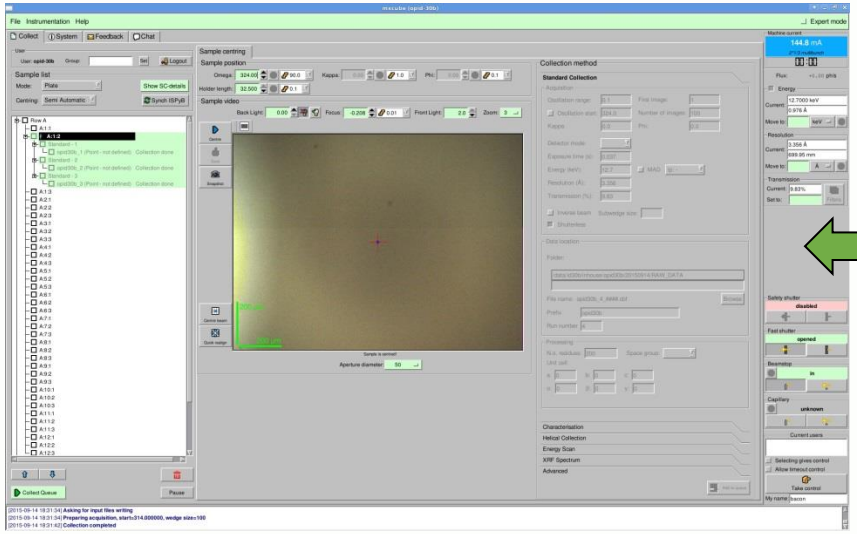
ESRF EMBL

ID30B – BLISS control software



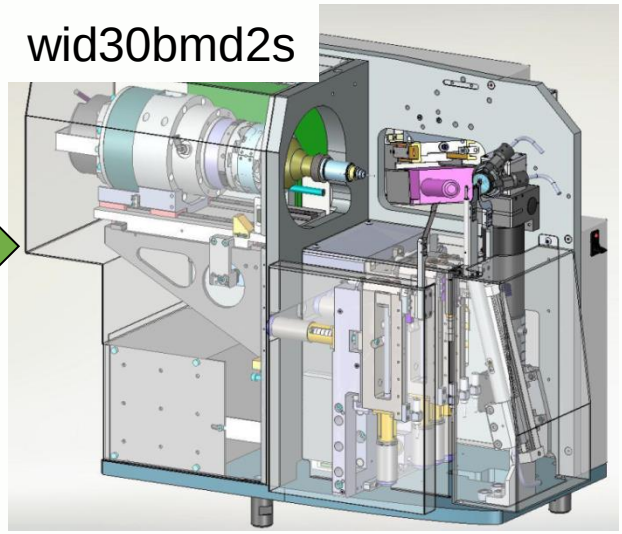
ESRF Beamline control unit

ID30B – ‘Event management’ communication

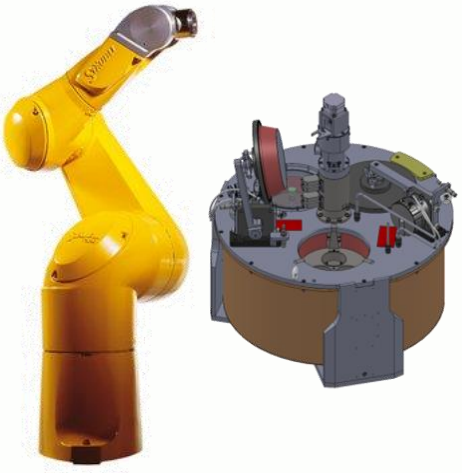


Event manager

wid30bmd2s



wid30bpcflex1

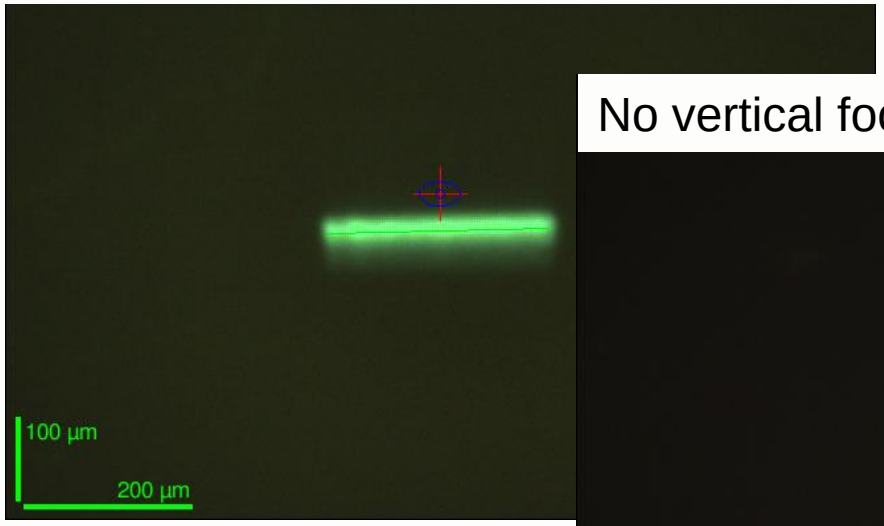


ESRF EMBL

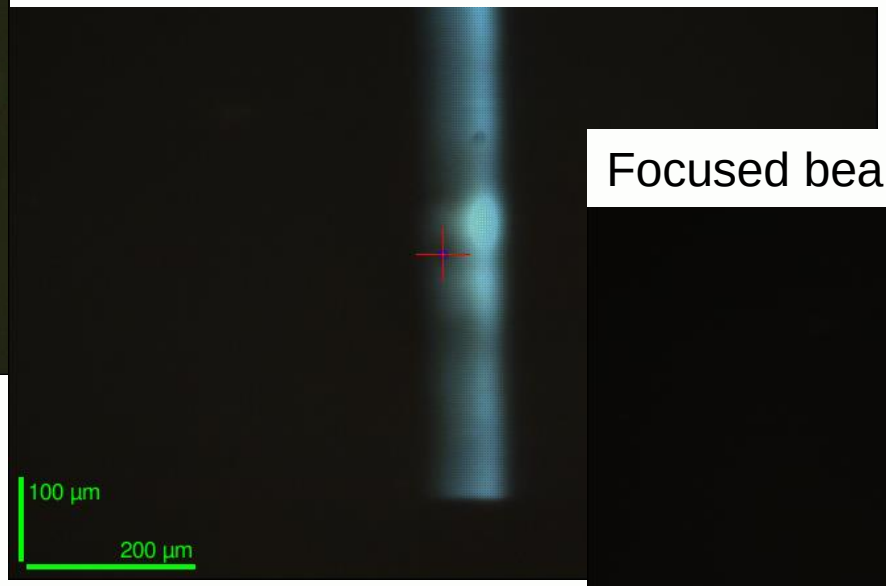
ID30B – Variable focusing capabilities

Flux ~ 6x10^{12} phs/sec/mm^2 at 12.7 keV
Beam size: <40μm^2

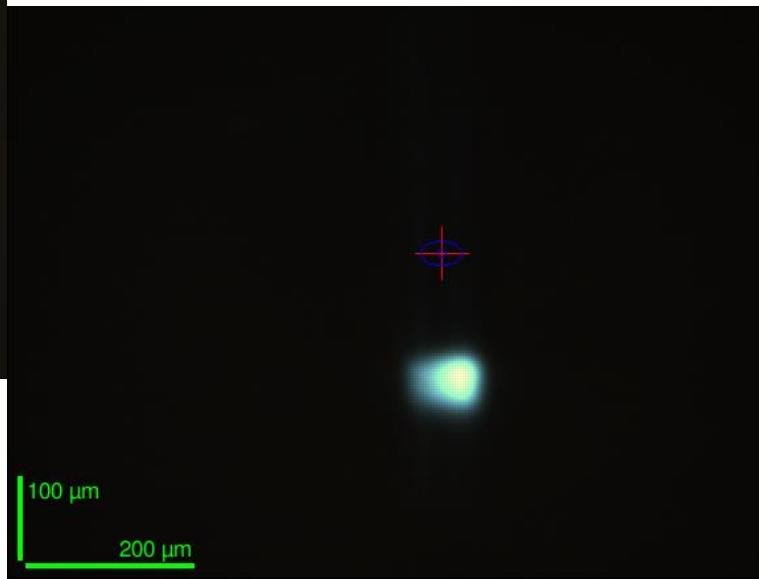
Vertical focusing, no horizontal focusing
(mirror unbent)



No vertical focusing – mirror bent



Focused beam



ID30B – Apertures (75, 50, 30, 20, 10μm²)

ESRF EMBL

ID30B – Good data quality

andrewmc@pc386: ~

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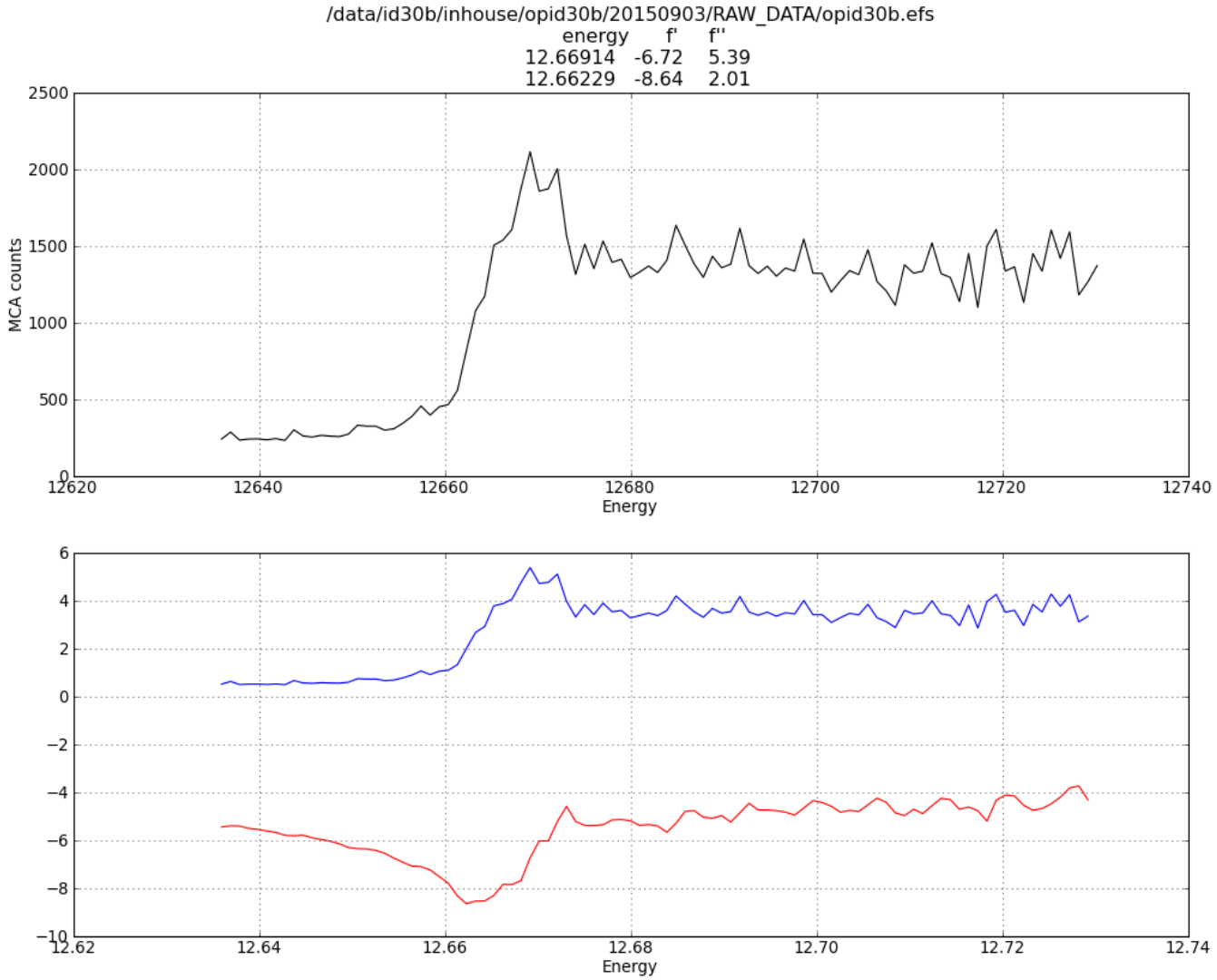
```
R-meas   = redundancy independent R-factor (intensities)
           Diederichs & Karplus (1997), Nature Struct. Biol. 4, 269-275.

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   = percentage of correlation between random half-sets
 Corr      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(-)|/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     NUMBER OF REFLECTIONS    COMPLETENESS R-FACTOR  R-FACTOR COMPARED I/SIGMA   R-meas  CC(1/2)  Anomal  SigAno   Nano
  LIMIT     OBSERVED  UNIQUE  POSSIBLE     OF DATA   observed  expected                                      Corr

   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
```

ESRF EMBL

ID30B – Fast energy scans



ID30B – Automatic structure solution

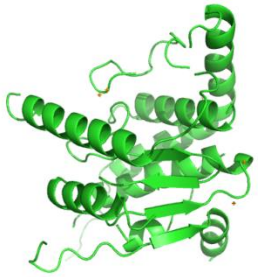
opid30b (1.4 Å)

FAE Se at Br edge

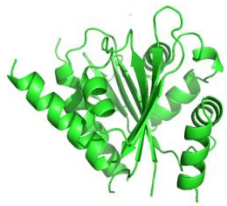
MX-ihr4 (2.4 Å)

Thaumatin (Gd)

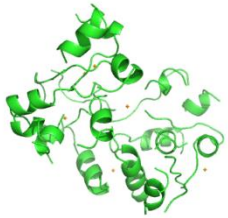
MX-1695 (2.3 Å)



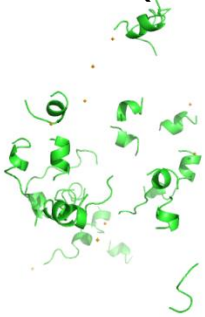
MX-1737 (1.4 Å)



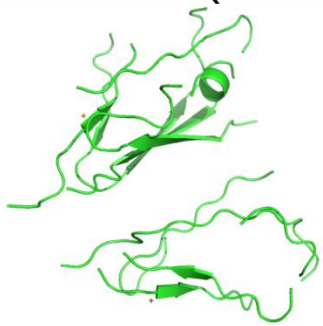
MX-1749 (2.9 Å)



MX-1743 (3.9 Å)



MX-1696 (2.1 Å)

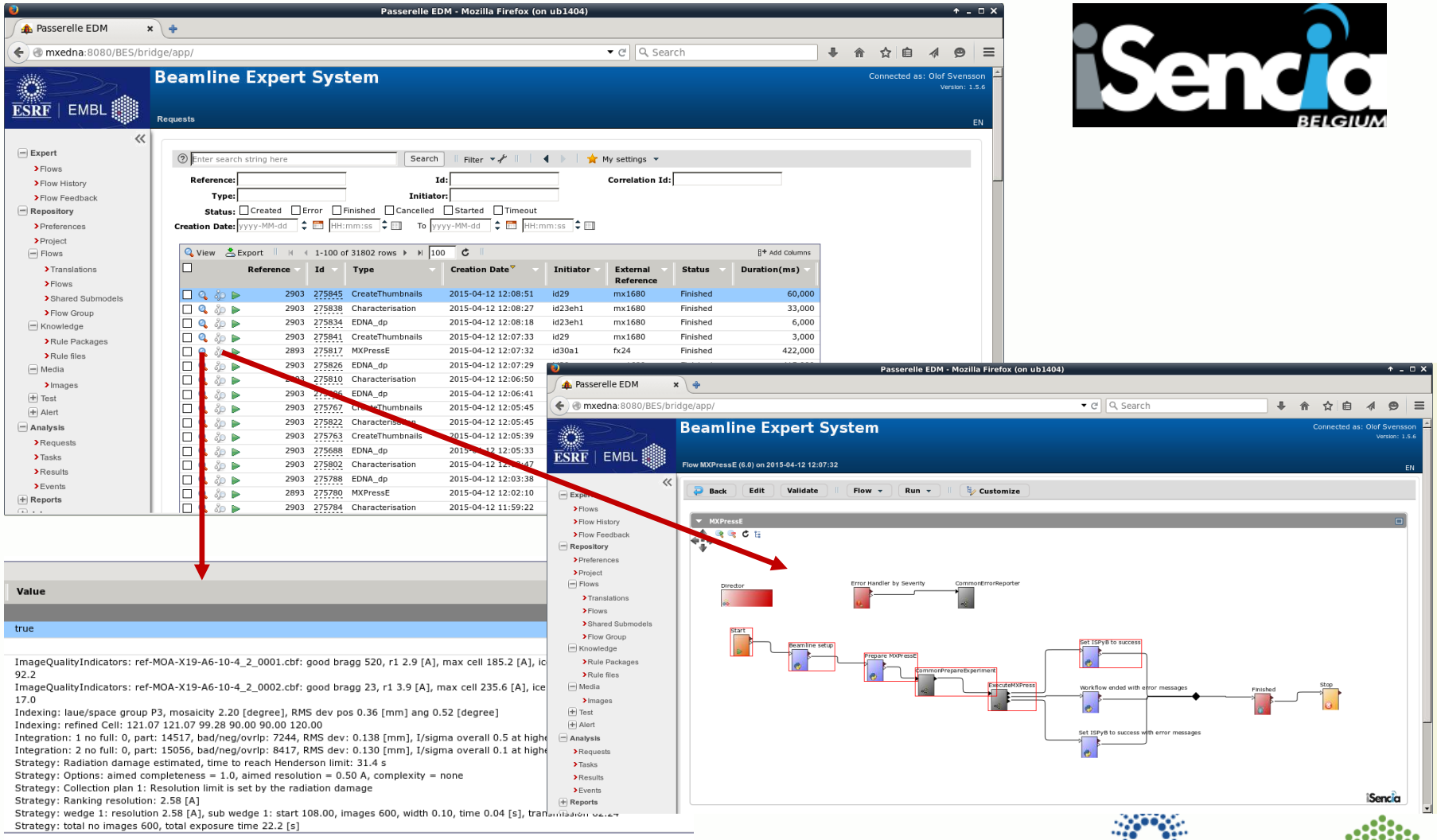


MX-1737 (4.2 Å)

ESRF EMBL

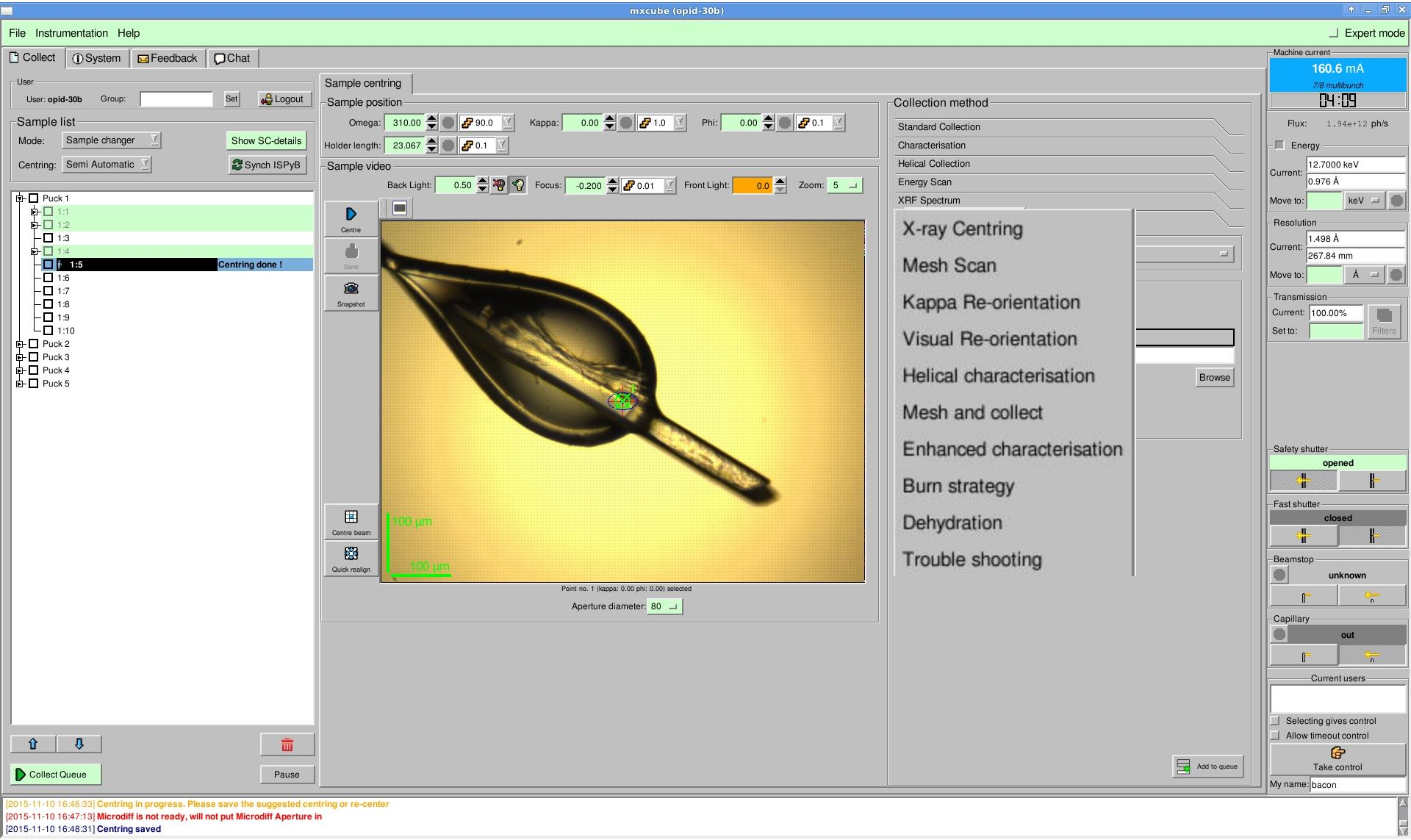
EMBL-ESRF Beamline Expert System

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



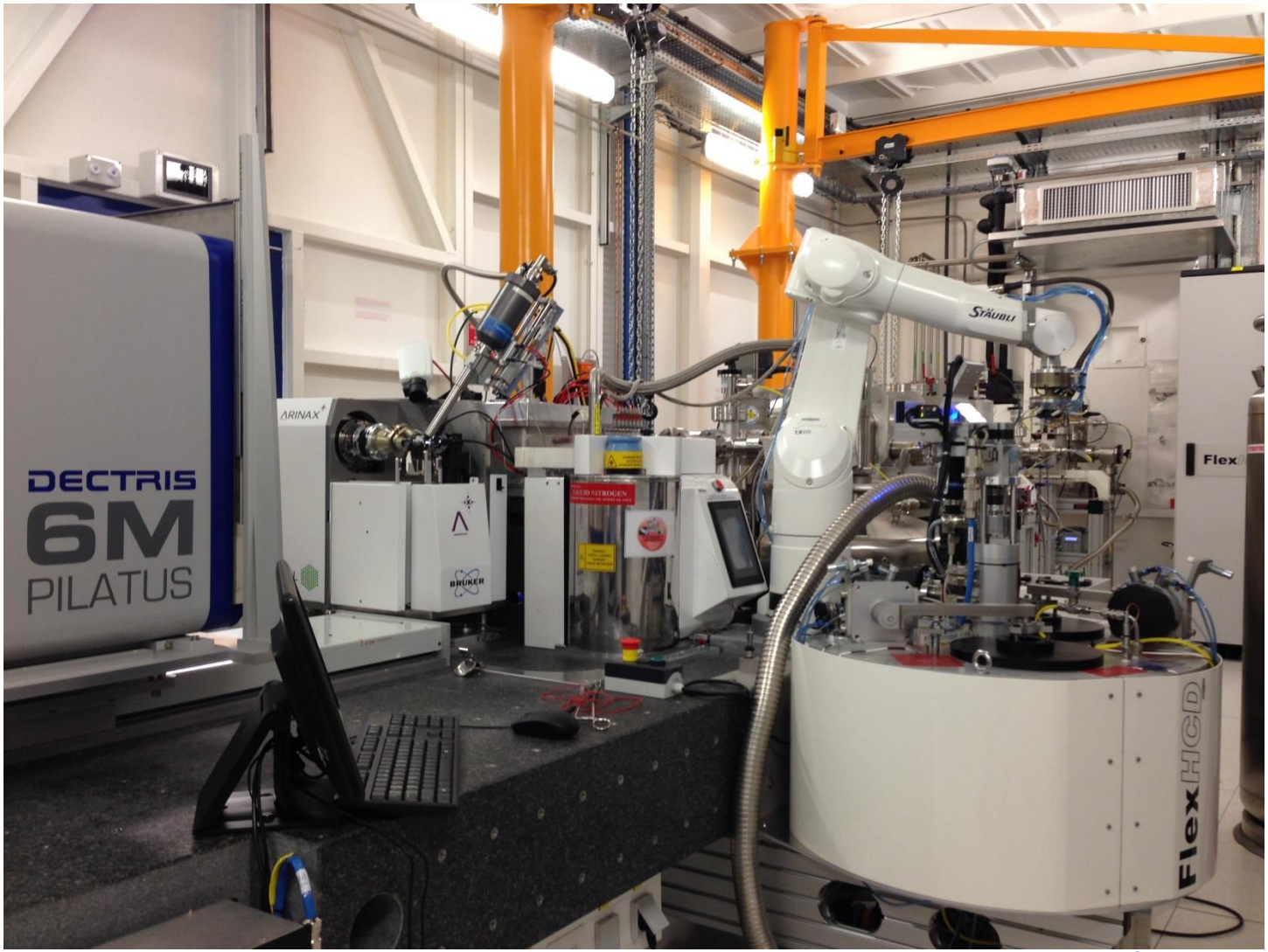
Brockhauser *et al*. *Acta Crystallogr*. *D Biol*. *Crystallogr*. (2012) **68**, 975-984.

Workflows implemented in MxCuBE



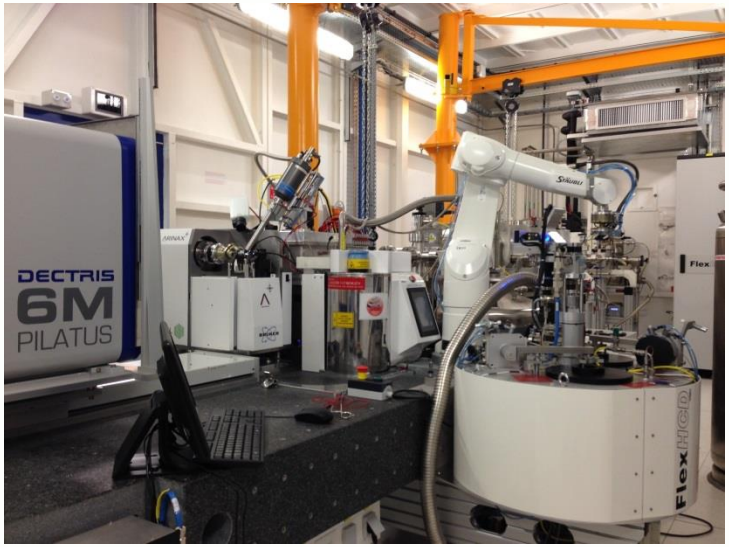
ESRF EMBL

FlexHCD robot



ESRF EMBL

FlexHCD – A versatile sample changer



SPINE baskets (x12) = 120 samples

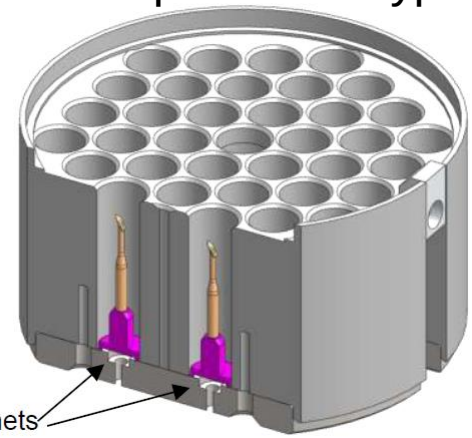
ESRF
SLS
BESSY
PETRAIII
ALBA

Unipucks (x12) = 192 samples

Most US sites

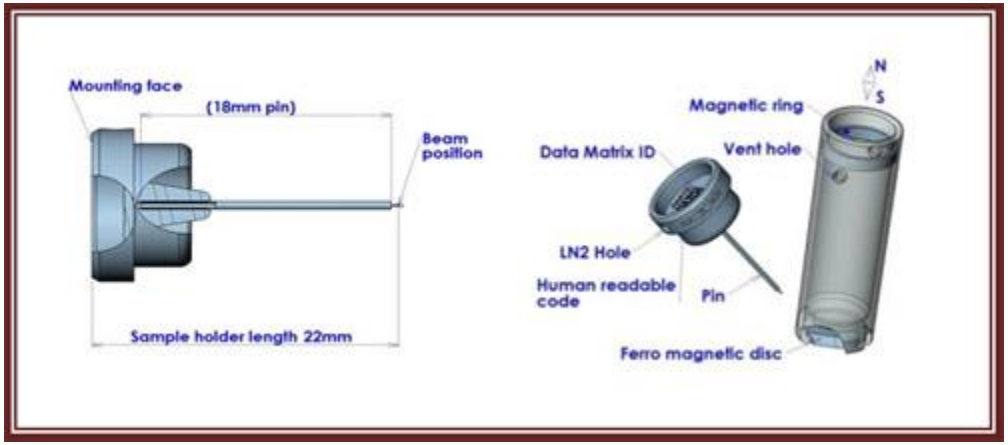
Europe:
DLS
SOLEIL

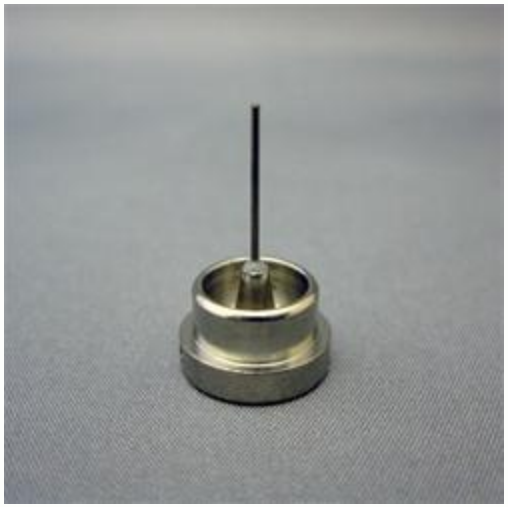
New sample holder types (36 samples)



ESRF EMBL

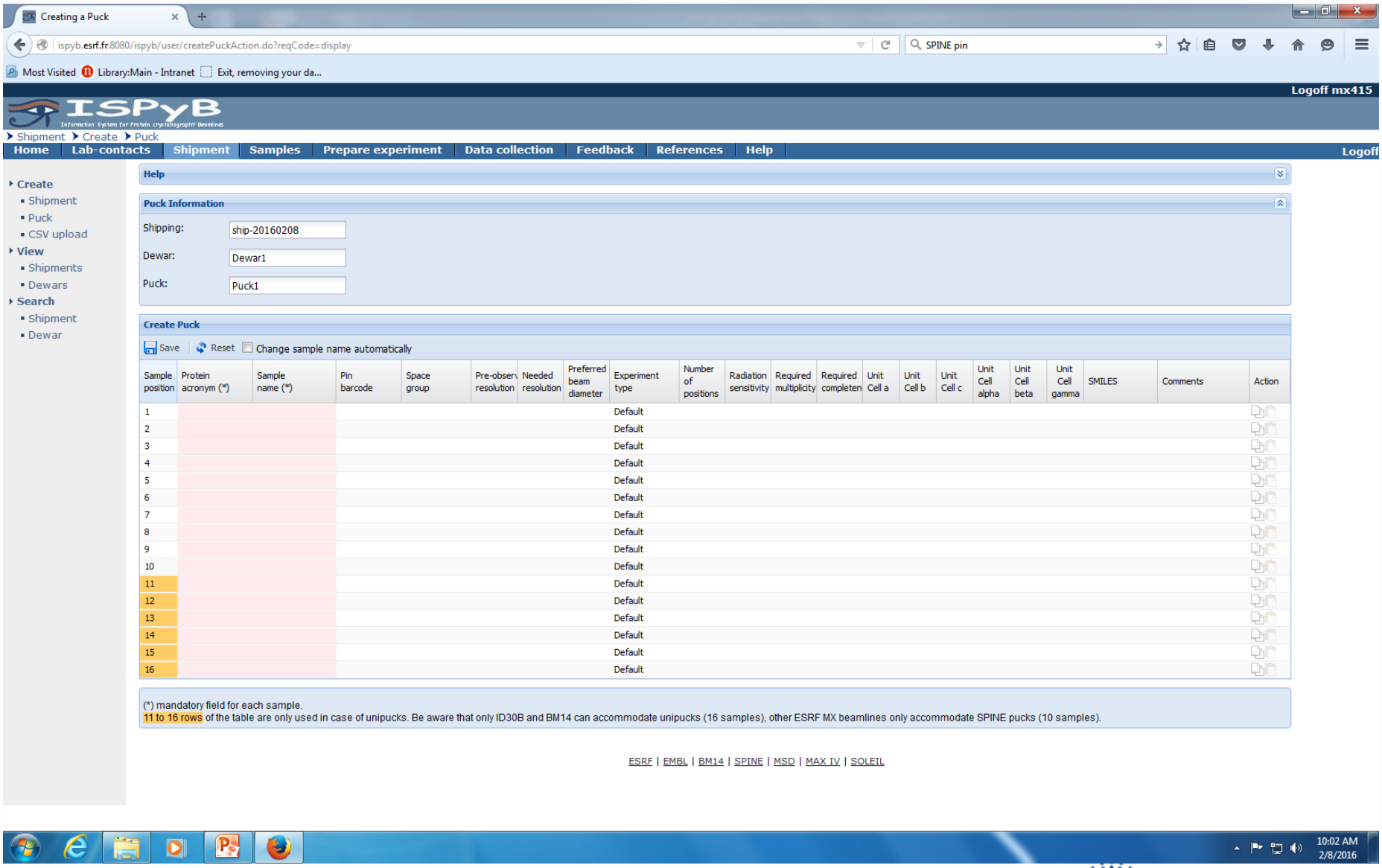
FlexHCD – Only SPINE pins allowed





ESRF EMBL

FlexHCD – Unipuck integration in ISPyB



Creating a Puck

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

SPINE pin

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

Logoff mx415

ISPyB
Information System for Protein crystallography Beamlines

Shipment > Create > Puck

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

- Create
  - Shipment
  - Puck
  - CSV upload
- View
  - Shipments
  - Dewars
- Search
  - Shipment
  - Dewar

Help

Puck Information

Shipping: ship-20160208

Dewar: Dewar1

Puck: Puck1

Create Puck

Save | Reset | 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 completen	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).

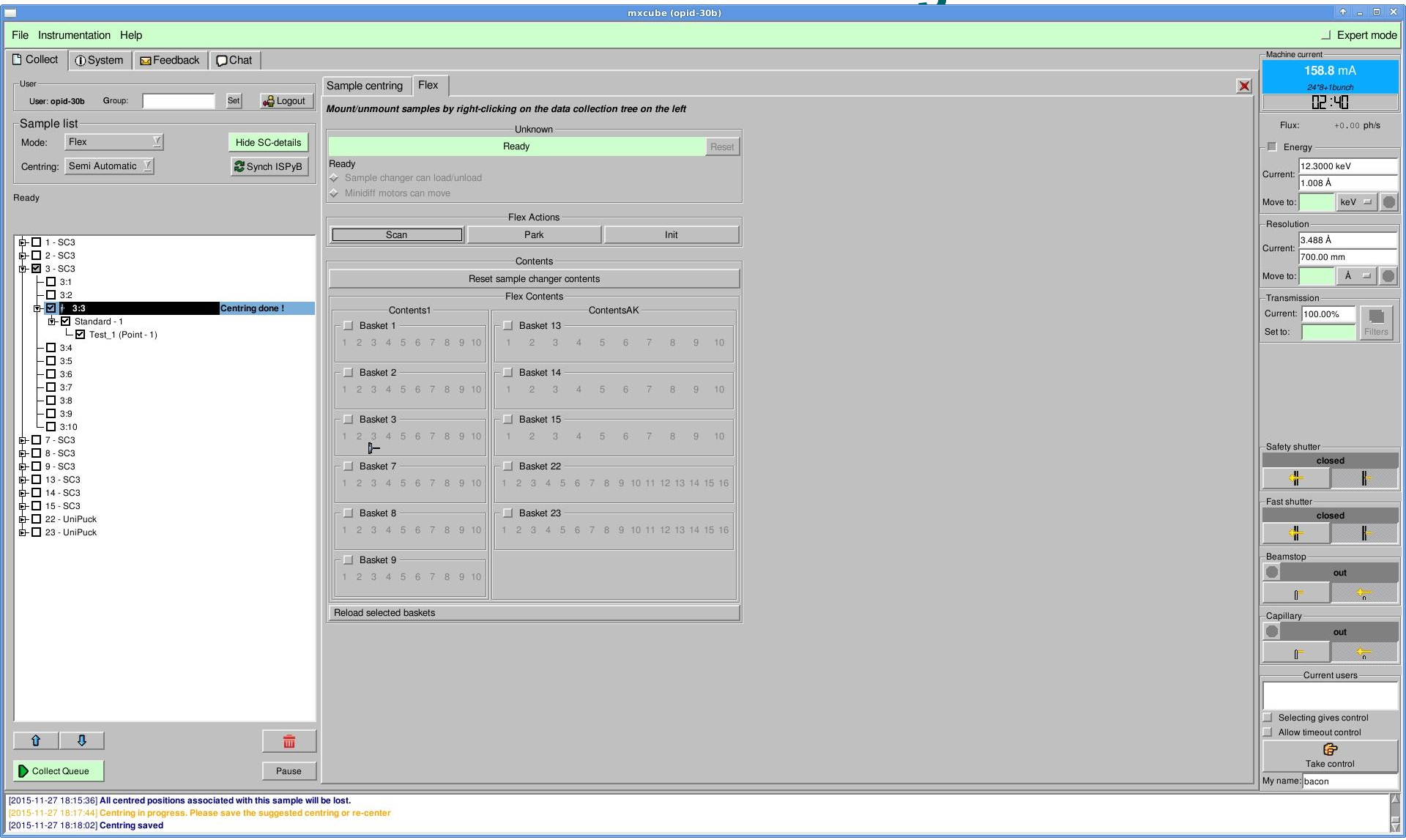
ESRF | EMBL | BM14 | SPINE | MSD | MAX IV | SOLEIL

10:02 AM
2/8/2016

ESRF

EMBL

FlexHCD MxCuBE integration



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

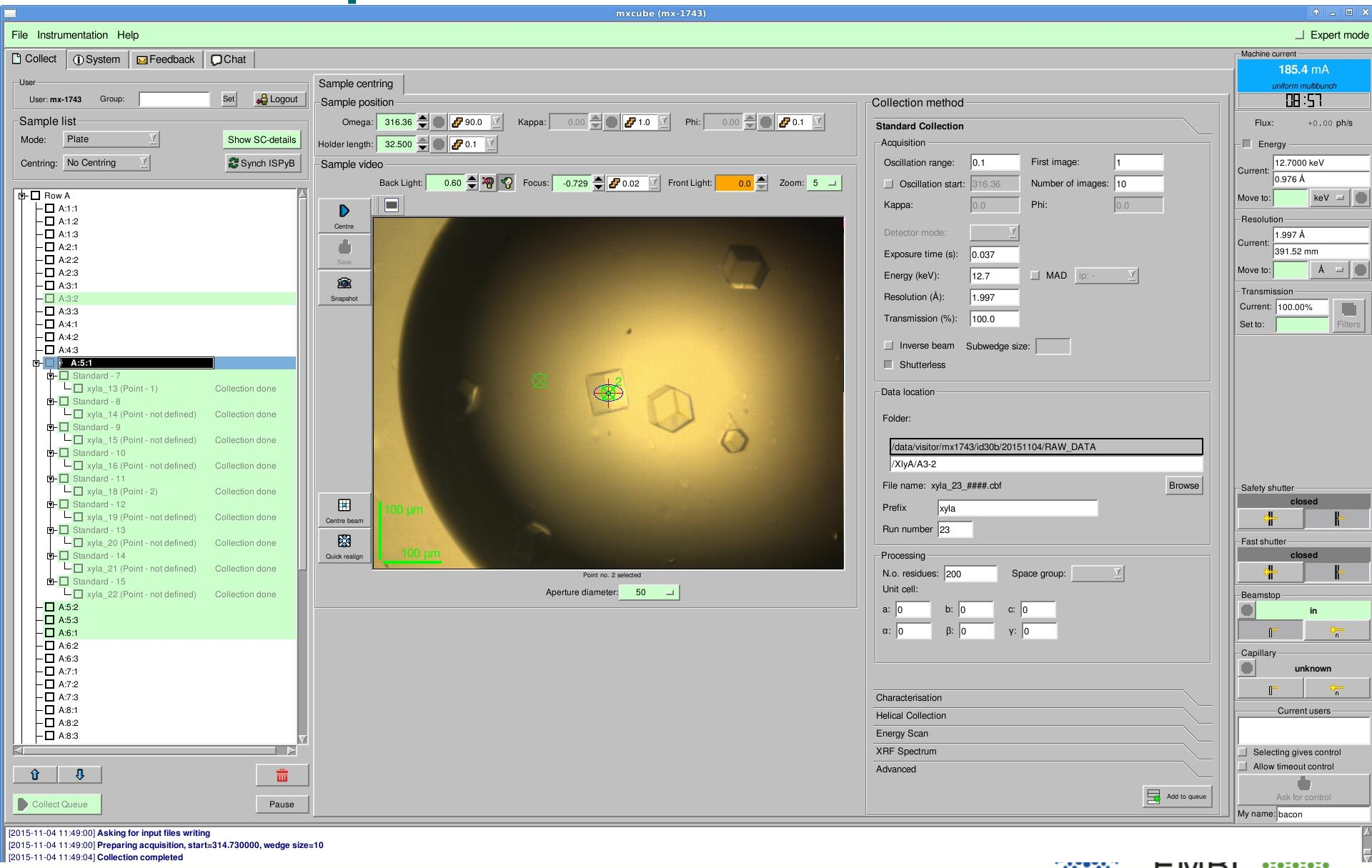
ESRF EMBL

ID30B – MD2S allows plate screening capability

ID30B SBS format plate gripper

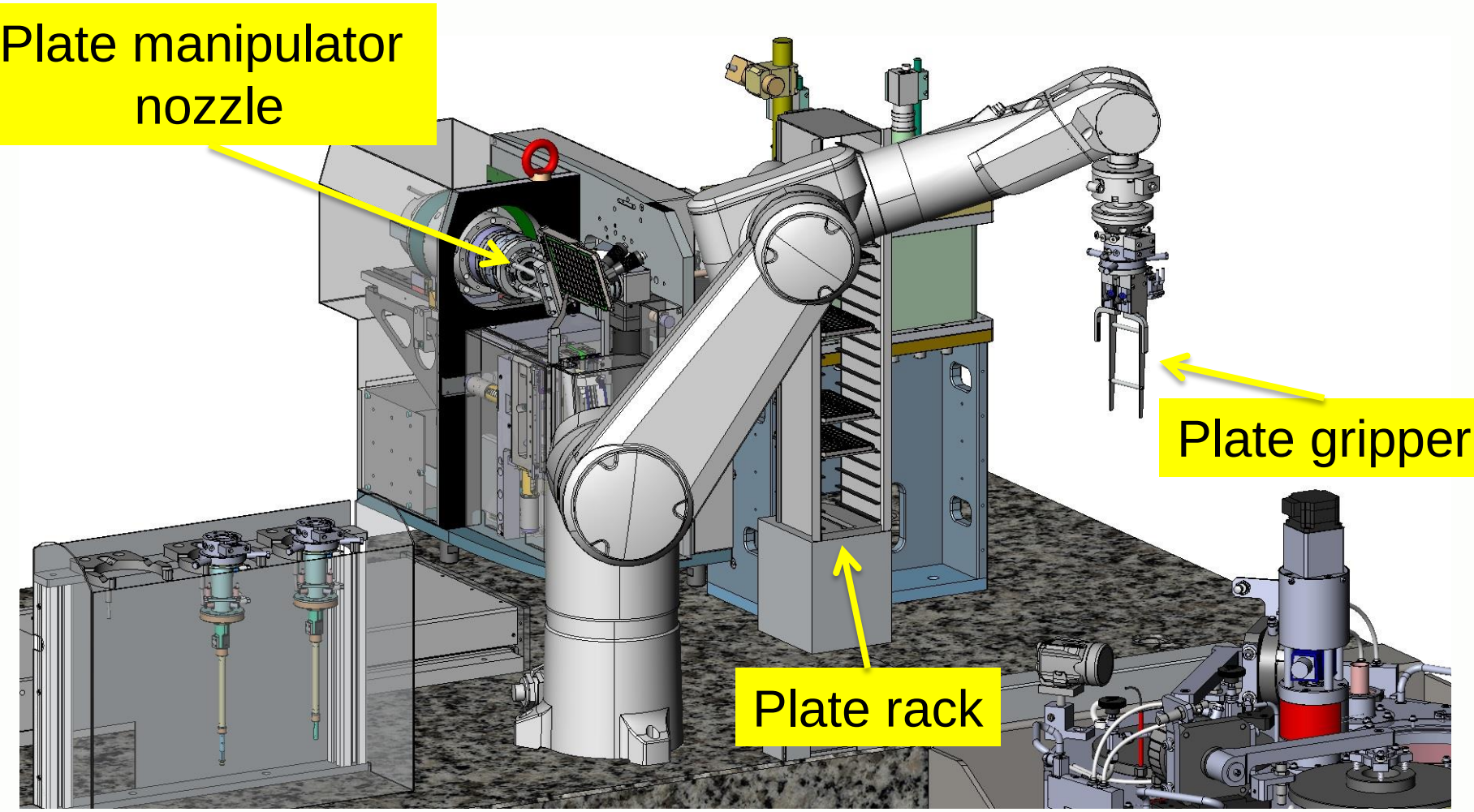
ESRF EMBL

In situ plate data collection in MxCuBE



J. Sinoir *(EMBL-GR)*, I. Karpics (EMBL-HH) and A. Beteva *(ESRF)*

ID30B - Plate screening capability (2016)



ESRF EMBL

ID30B – To do

Immediate future (February 2016)

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

Near future

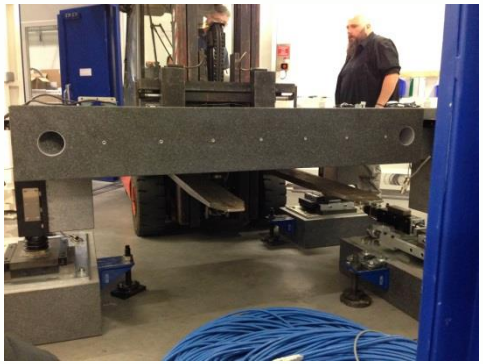
- Find a solution to (or minimise) the beam drift
- Further investigate the vertical focusing problem
- Work on variable focusing routines (coordinated bender movement)
- Introduce Unipuck mounting and test miniSpine mounting capabilities

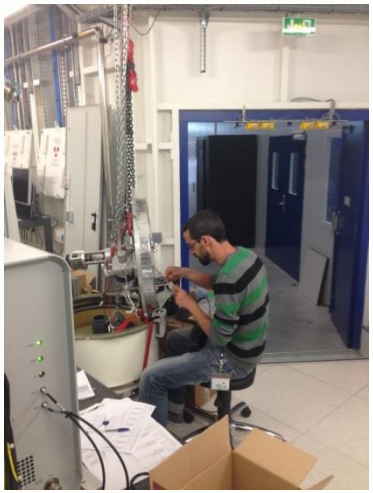
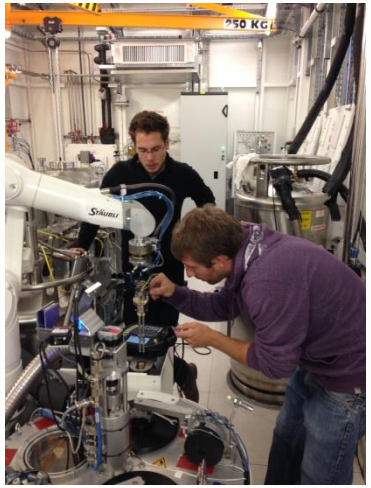
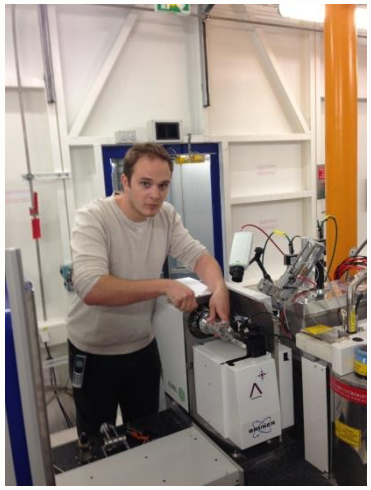
Future plans

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

ESRF EMBL

Many thanks to all involved



ESRF EMBL

Acknowledgements

EMBL Grenoble

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Gergely Papp
Christopher Rossi
Jeremy Sinoir
Clement Sorez

Josan Marquez
Guillaume Hoffmann
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Harald Reichert

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Christoph Müller-Dieckmann
Philippe Carpentier
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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

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Corinne Iodice