



| The European Synchrotron



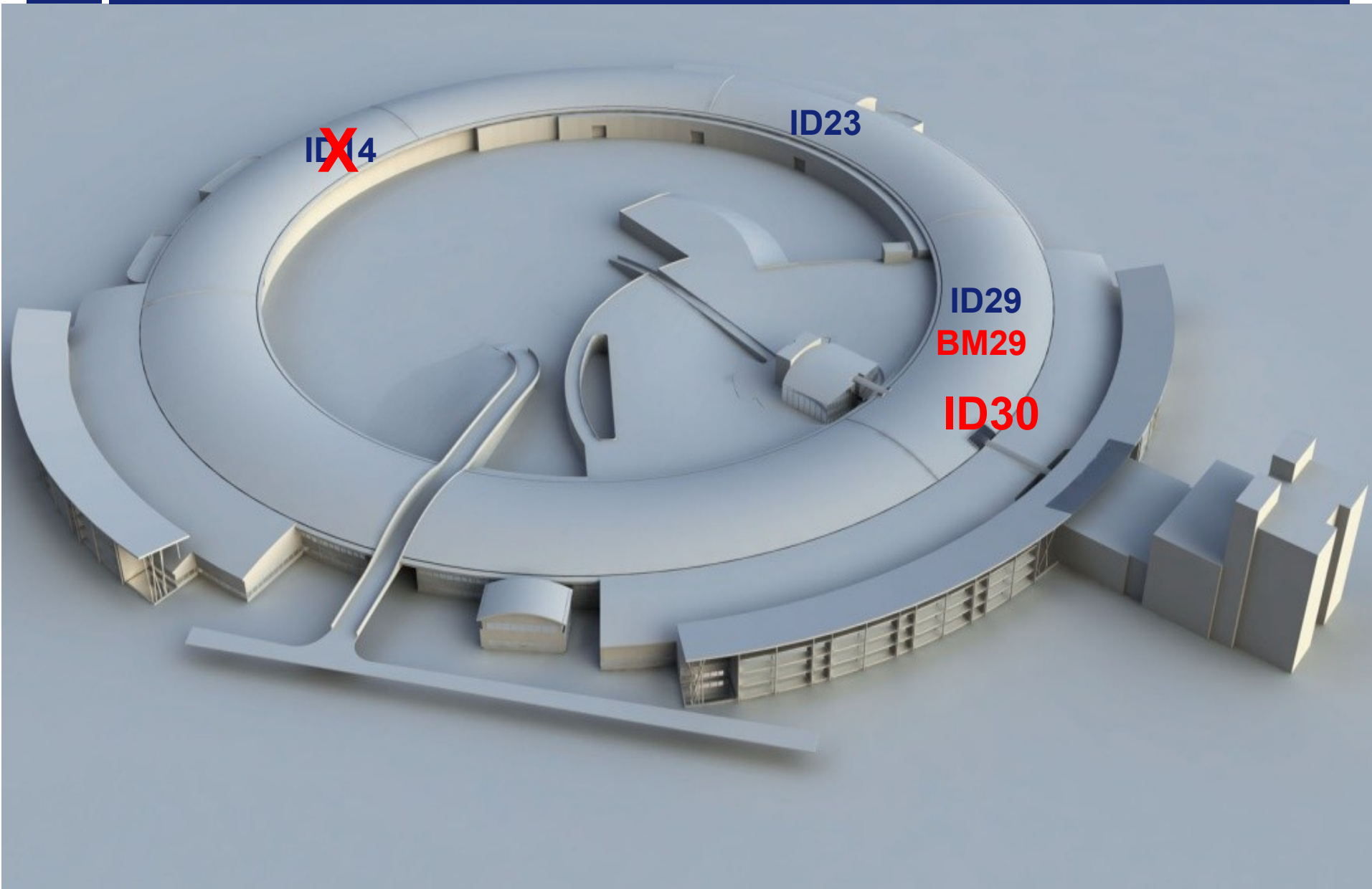
UPBL10

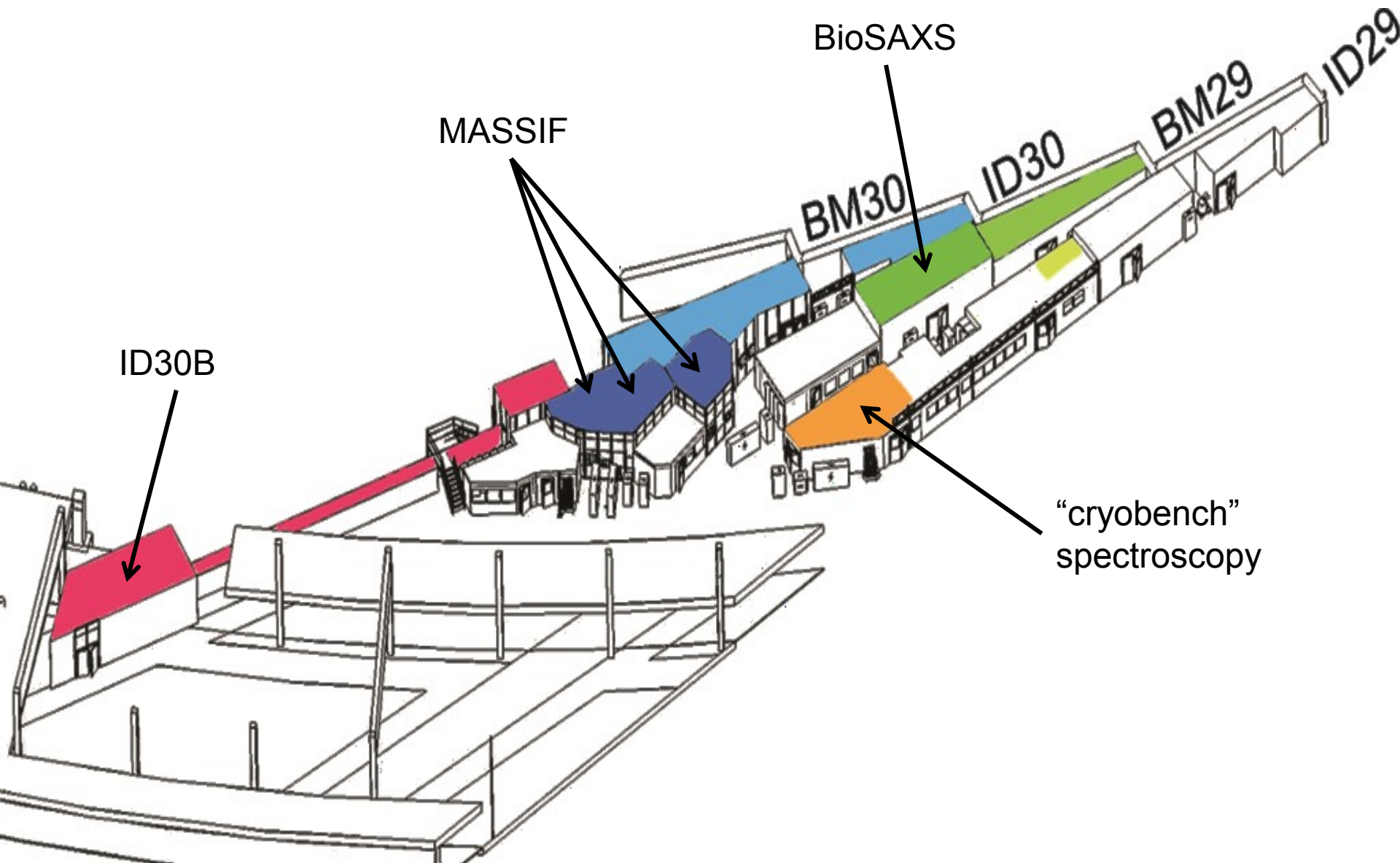
**the upgrade programme
for Structural Biology
at the ESRF**

UPBL10 = BM29 + *MASSIF* + ID30B

- where?
- what?
- why?
- when?





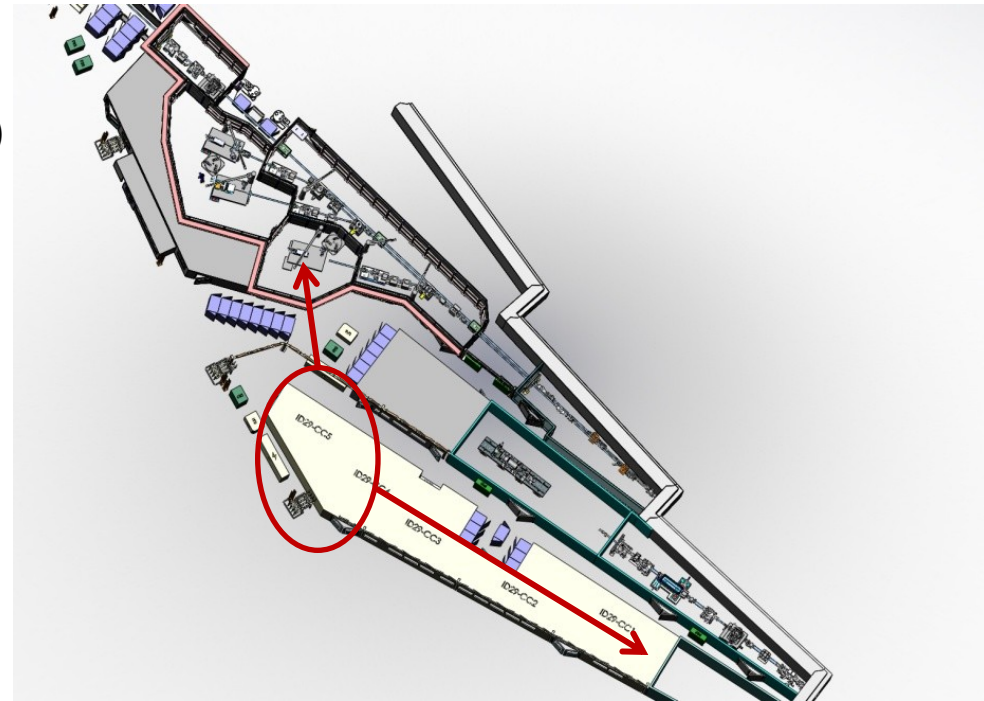


- where?
- what?
- why?
- when?

“Cryobench”

online and offline spectroscopy
(UV-VIS, fluorescence, Raman)

operational sine 12.2009



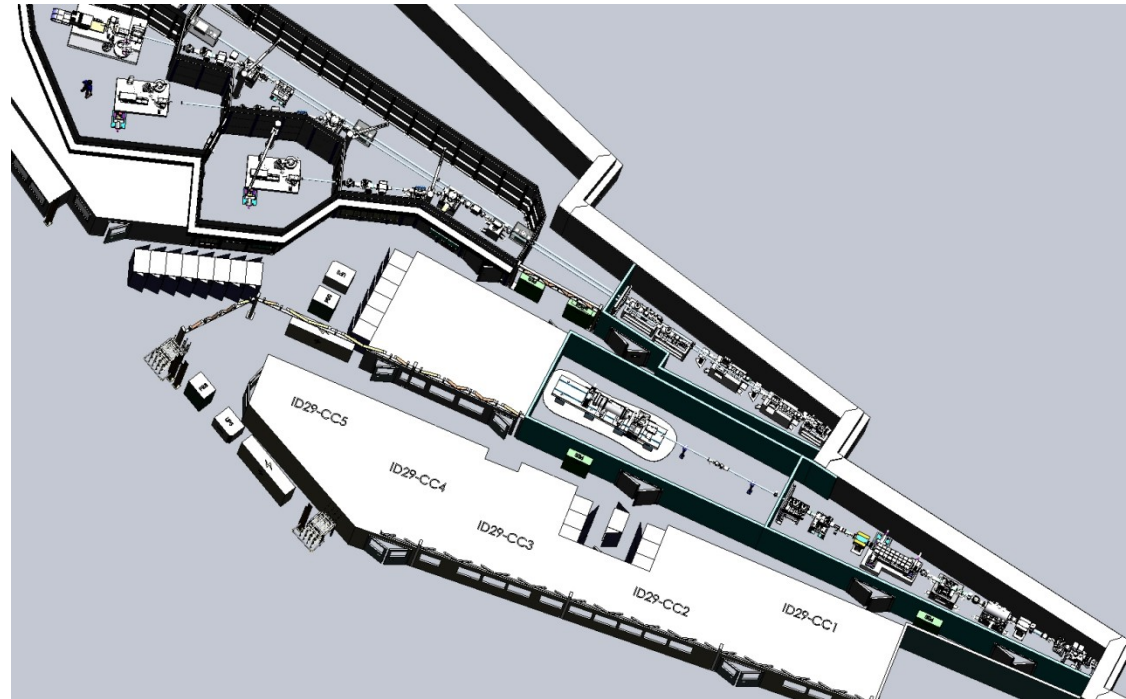
→ extraction of supplementary useful information

<http://www.esrf.fr/UsersAndScience/Experiments/MX/Cryobench>

bioSAXS

high-throughput solution
scattering for SB

operational since 07.2012



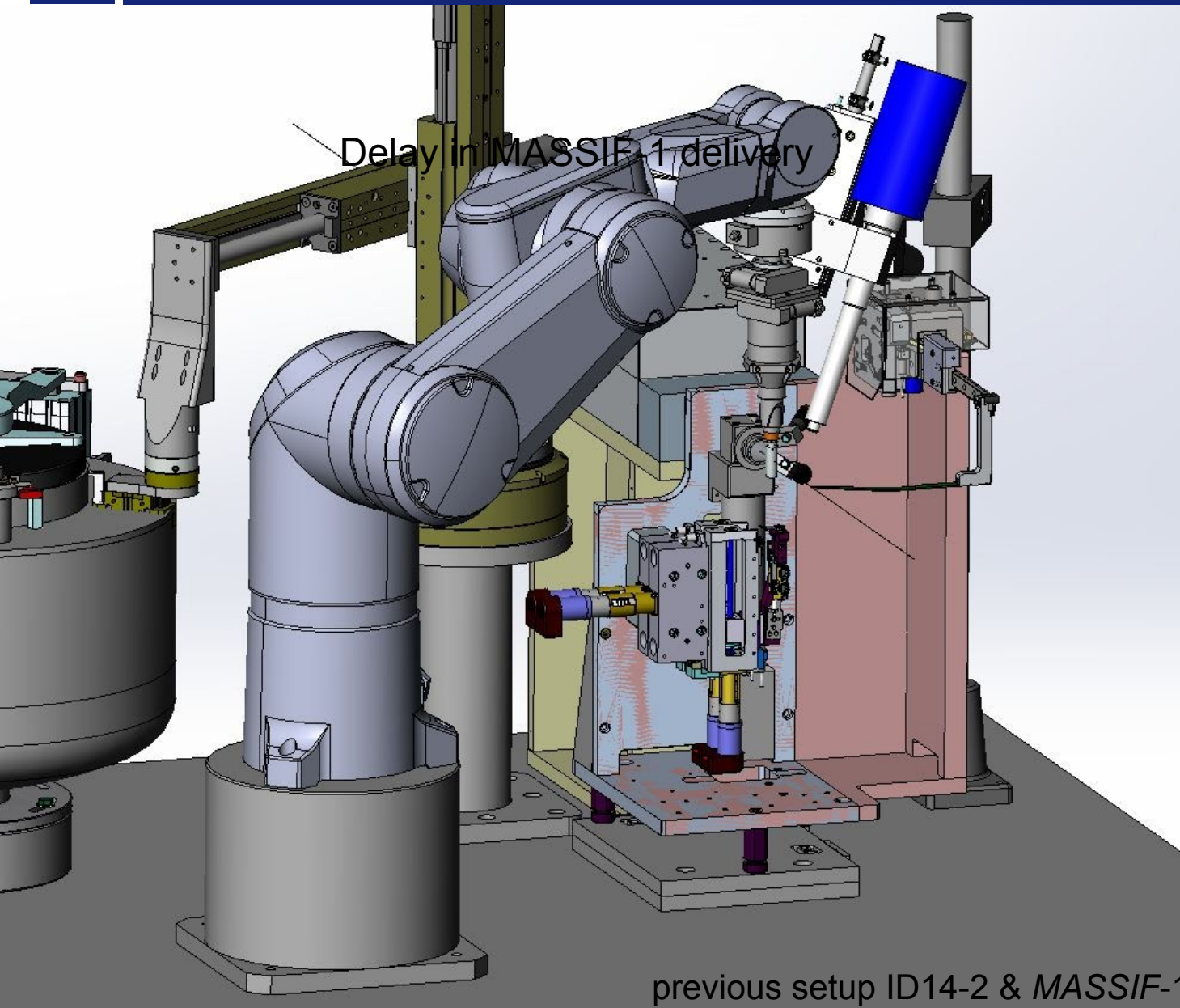
→ independent beam line: energy tunable, highly automated

http://www.esrf.fr/UsersAndScience/Experiments/MX/About_our_beamlines/BM29

Massively Automated Sample Evaluation and Screening Integrated Facility

Aim:

- evaluation of many samples in a reasonable time frame
- enables to quickly perform “standard” experiments
- extraction of useful information



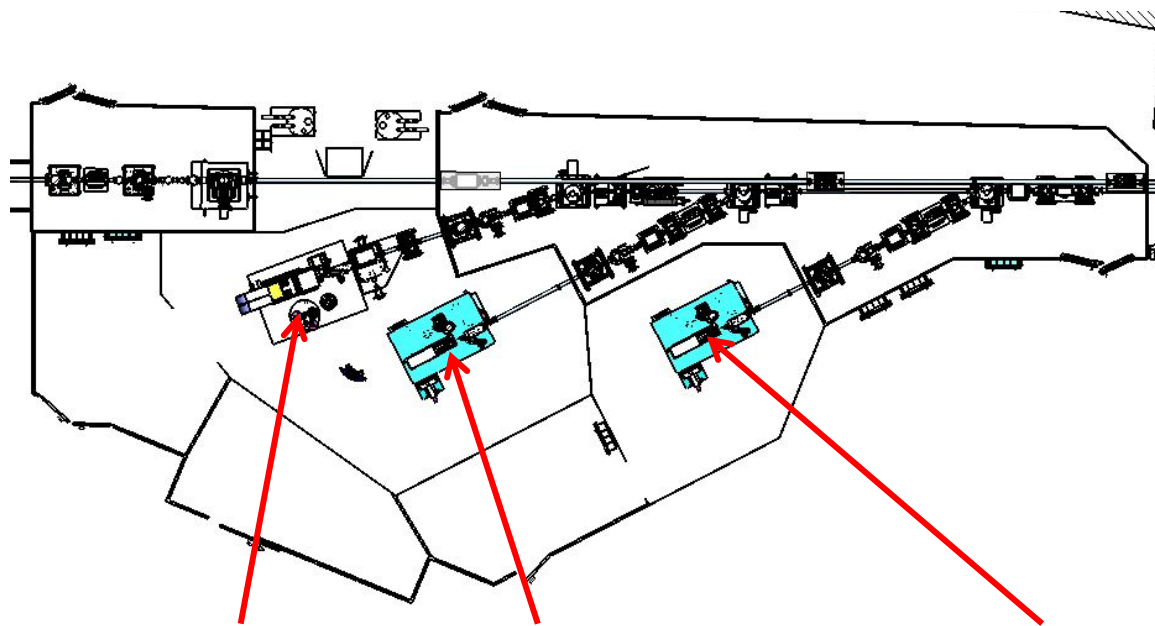
limitations

- high SOC
- no “shutterless” DC
- limited Ω -rotation
- limited diagnostics
- data transfer issues

→ replacement
RoboDiff

MASSIF

high-throughput
sample evaluation



MASSIF-3

MASSIF-2

MASSIF-1

beam size

$> 10 \mu\text{m}^2$

$100 - 50 \mu\text{m}^2$

$200 - 50 \mu\text{m}^2$

flux

$\sim 10^{13}$ ph/s

$\sim 10^{13}$ ph/s

$\sim 5 \times 10^{13}$ ph/s

detector

Eiger 4M
750 Hz

?

Pilatus3 2M
250 Hz

from beg. 2015

from 07.2014

How can *MASSIF* support **your** science?

- characterise your crystal / sample beforehand
- evaluate your crystals automatically, before your 'real' experiment
- screen (many) crystals for e.g. ligand / fragment binding
- or simply collect good diffraction data

You make the decisions

Sample evaluation:

- is it my sample?
- where is my sample?
- where is the best part of my sample?
- does my sample contain what I expect/wish ?
- how to increase resolution / data quality?
- where to best collect diffraction data?
- how to avoid too much radiation damage?
- has my ligand/inhibitor/activator/fragment bound?

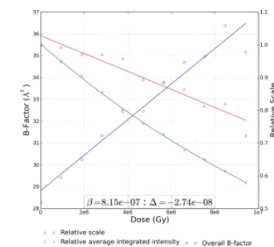
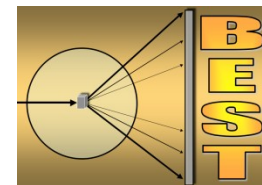
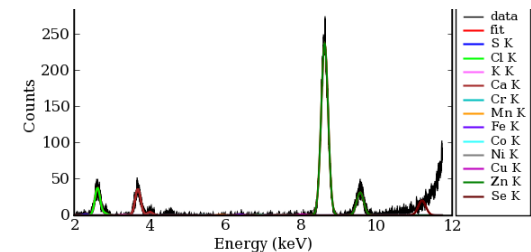
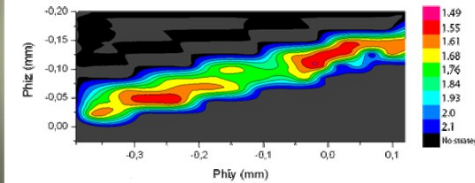
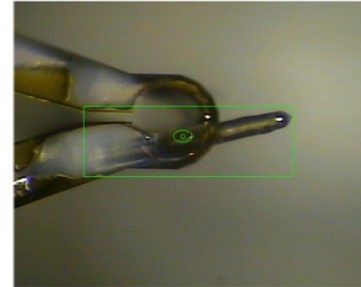
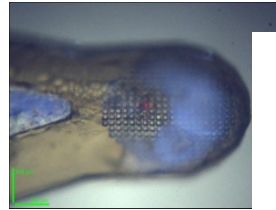


Image Prefix	Run No	Experiment Type	Protein Acronym	Start Time	# images	Experiment Parameters (Expand)	Status	Space Group	Completeness	Resolution	Rsymm Inner Outer Overall	Unit_cell a, b, c alpha, beta, gamma	Sample Ranking	Skip	Comments
		All	All										Rank	<input checked="" type="checkbox"/>	Save
killme2	1	SAD		12-03-2013 08:24:00	587			I 4 3 2		100.0 - 3.27 1.57 - 1.52 100.0 - 1.52	6.4 73.5 9.4	78.5, 78.5, 78.5 90.0, 90.0, 90.0	EDNA	<input type="checkbox"/>	
ref-killme2	1	SAD		12-03-2013 08:21:10	2			I 4		1.49		78.378, 78.378, 78.18 90.0, 90.0, 90.0	<input checked="" type="checkbox"/>	<input type="checkbox"/>	
killme	1	SAD		12-03-2013 08:08:49	1								<input type="checkbox"/>	<input type="checkbox"/>	
		All	All										Rank	<input type="checkbox"/>	Save

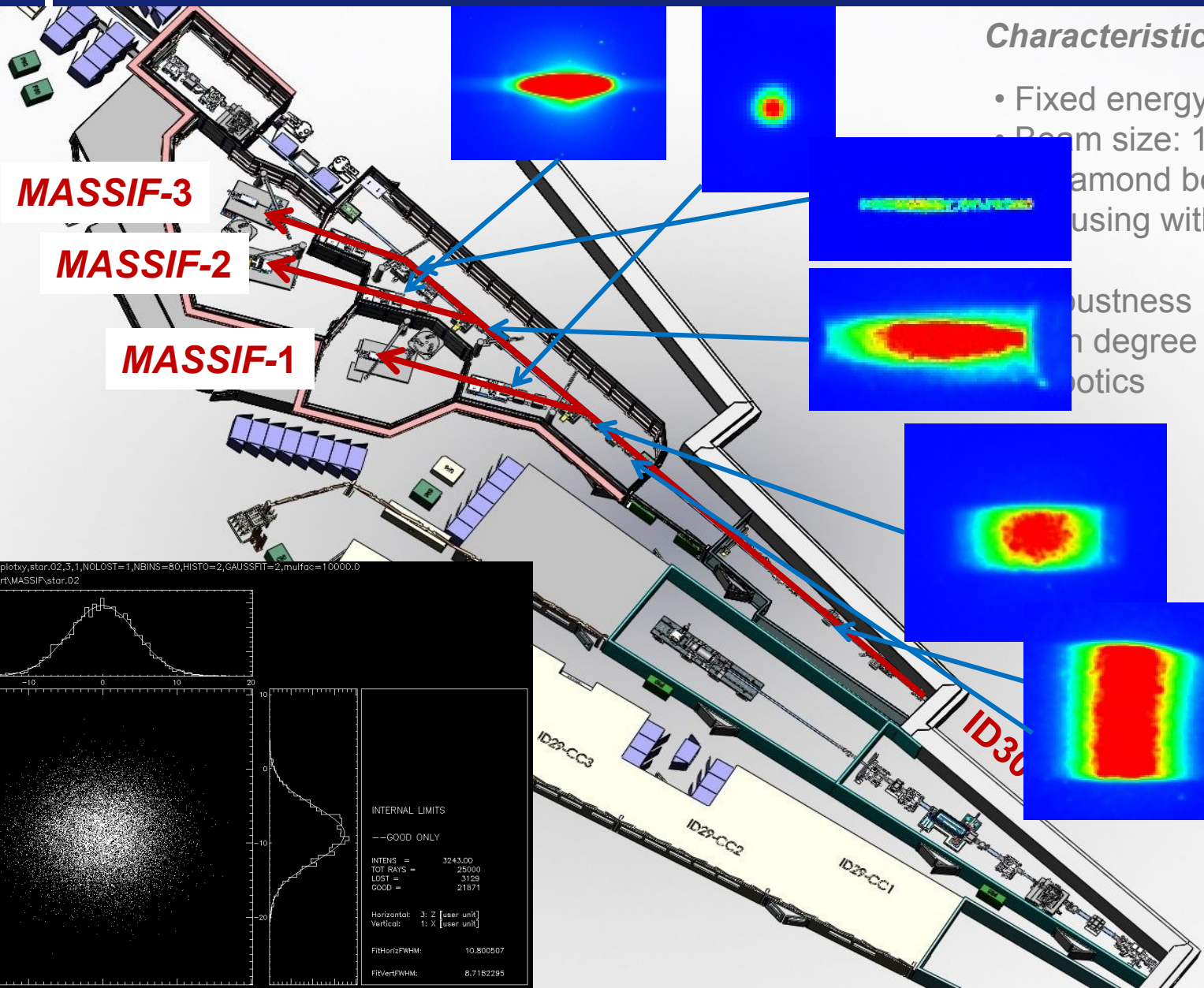
DataCollectionGroups

EnergyScans

XRF Spectra

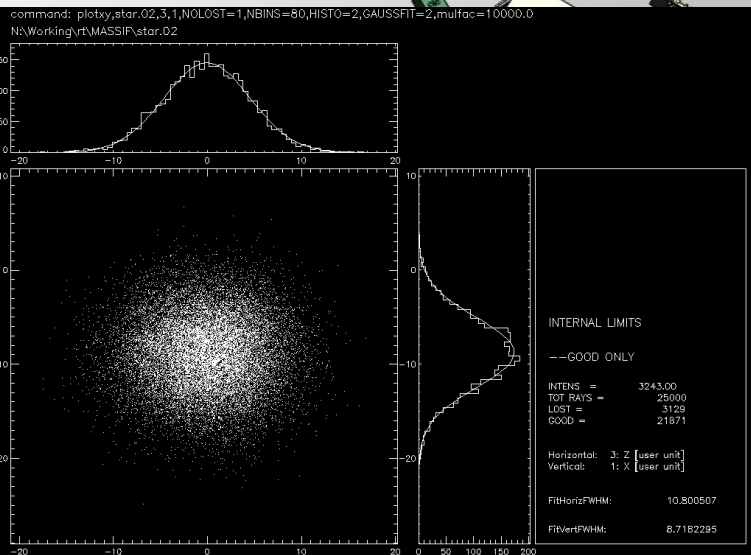
Energy (keV)	Exposure Time (s)	Start Time	End Time	Beam size Hor. (μm)	Beam size Ver. (μm)	Transm. Factor (%)	Spectrum	Html Report	Comments
									Save
12.743	1	27-02-2013 09:01:59	27-02-2013 09:01:59	0	0	2.259		u1-1-2_27_Feb_2013_01.html u1-1-2_27_Feb_2013_01.html	
									Save

MASSIF



Characteristics:

- Fixed energy (~12.8 keV)
- Beam size: 100 μm + 10 μm
- Diamond beam splitters
- Using with CRLs
- ML mirror
- Robustness
- High degree of automation
- Optics



- Beam delivery and positional stability
- Sample preparation and delivery
- Sample changing
- Data collection
- Data treatment and mining
- Data deposition

CRLs, beam splitter, feedback

SPINE, NewPin, CrystalDirect

Hardware development

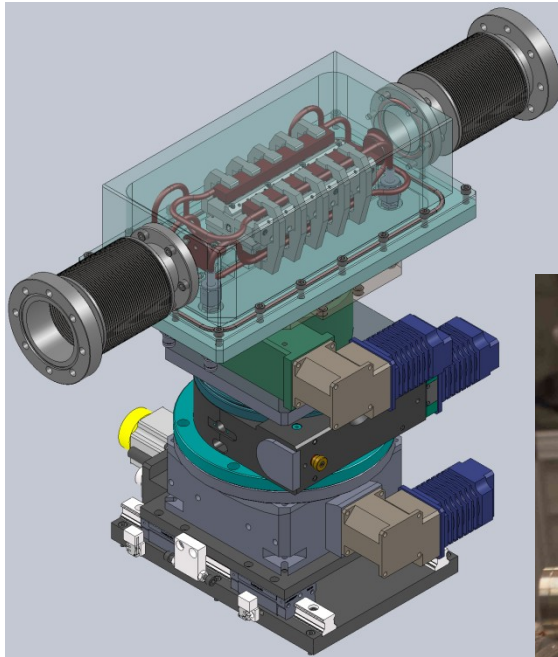
newDewar + newRobot

DDC, MxCuBE, EDNA, BEST

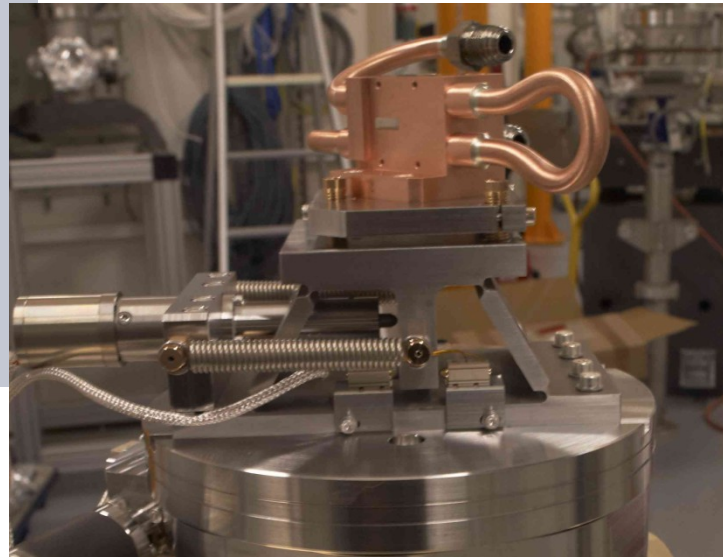
autoproc, ISPYB

Software development

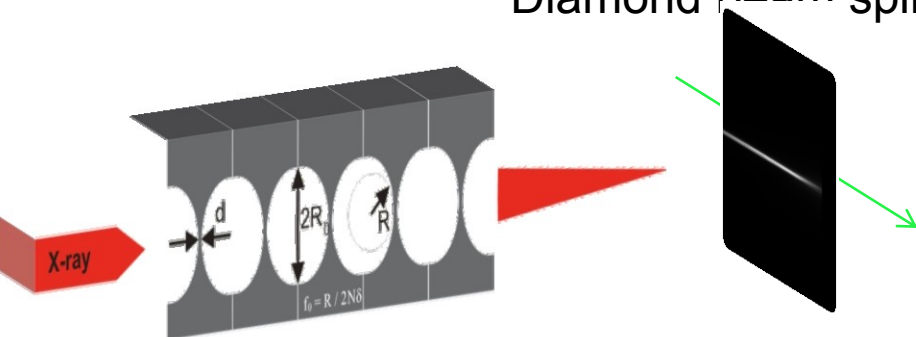
MASSIF – HARDWARE



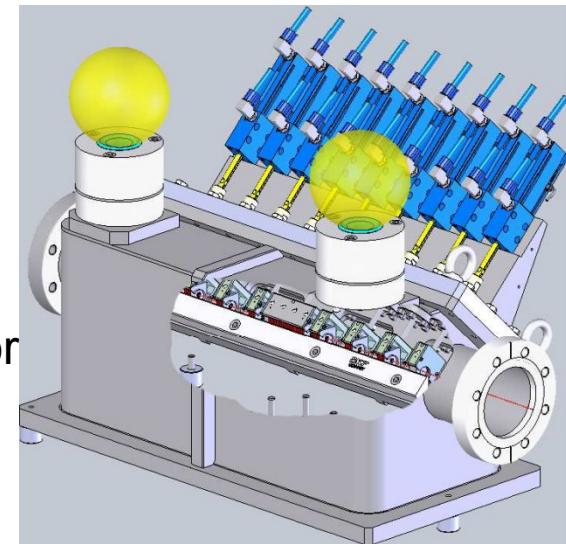
white beam CRL



Diamond beam splitting monochromator



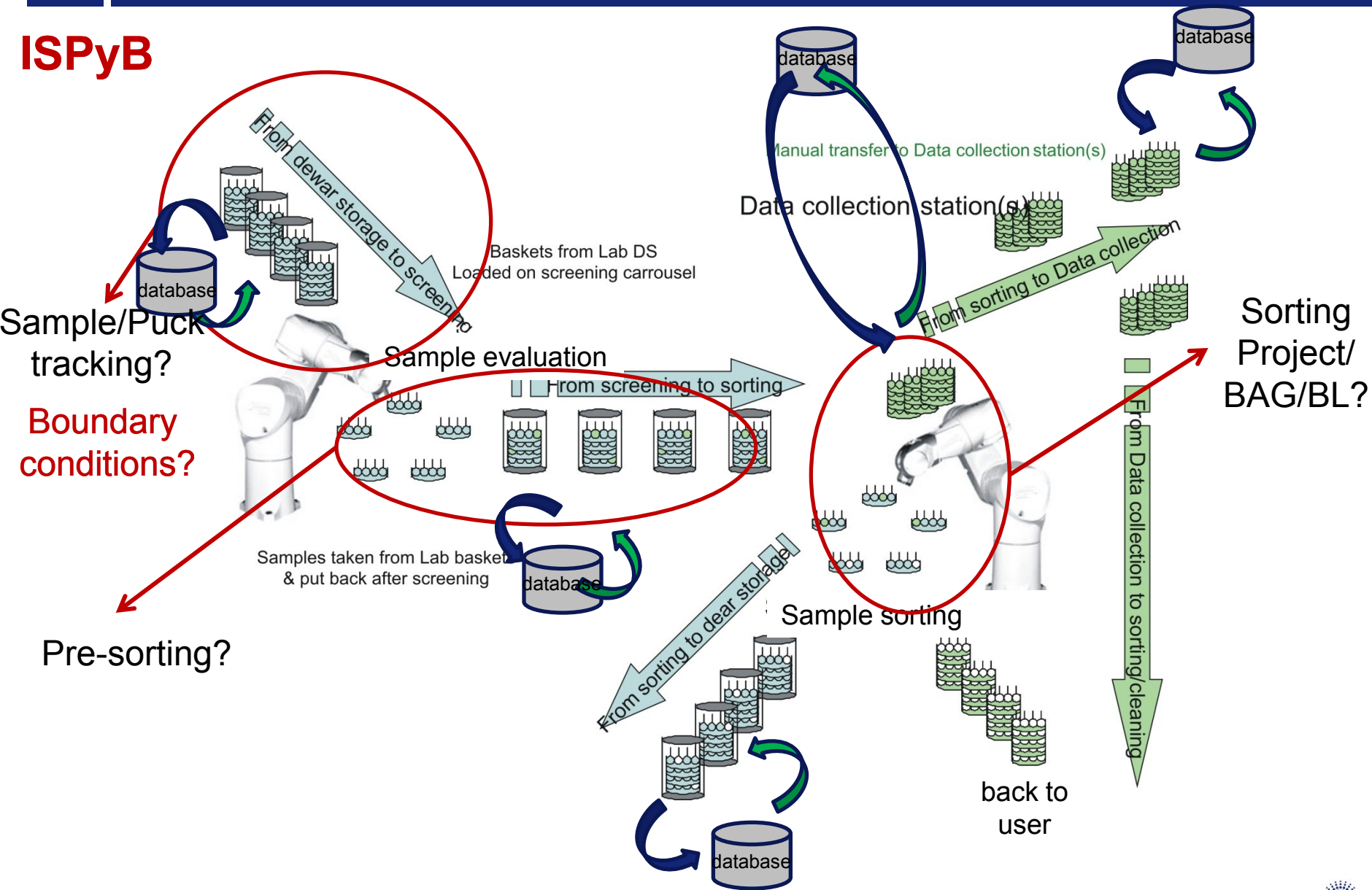
robotics and
high capacity dewar



translocator

MASSIF – SAMPLE FLOW

ISPyB

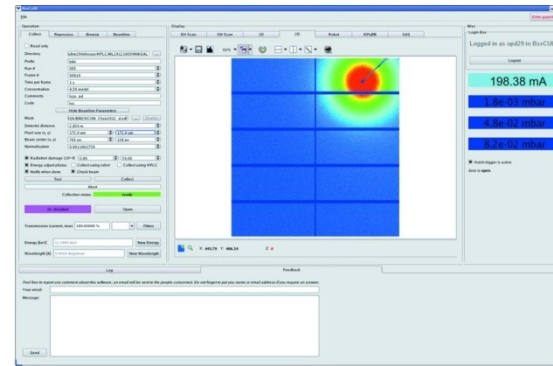
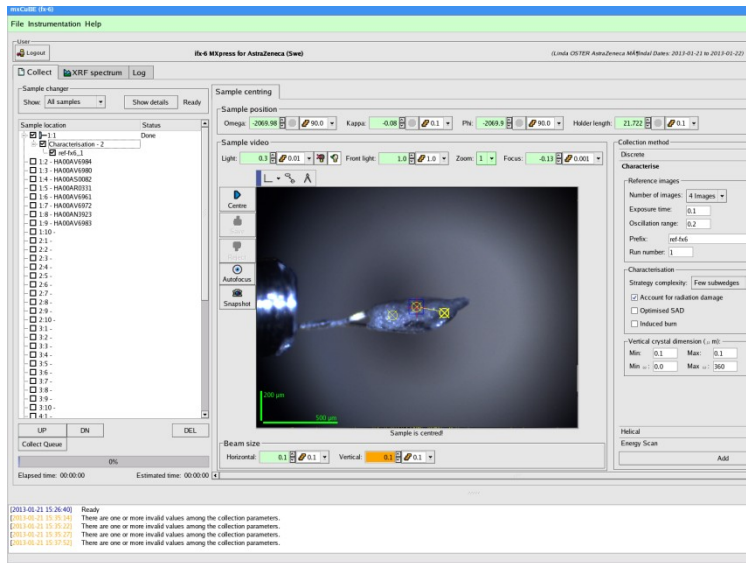


Workflows

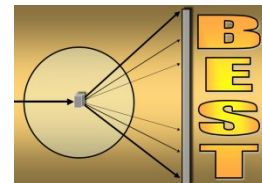
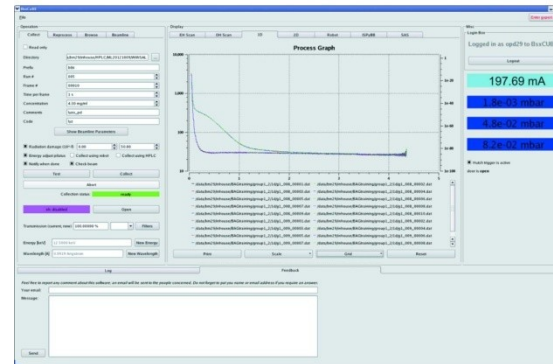
- burn strategy
- Xray centering
- helical
- mesh
- HCA

autoproc

MxCuBE 2.0

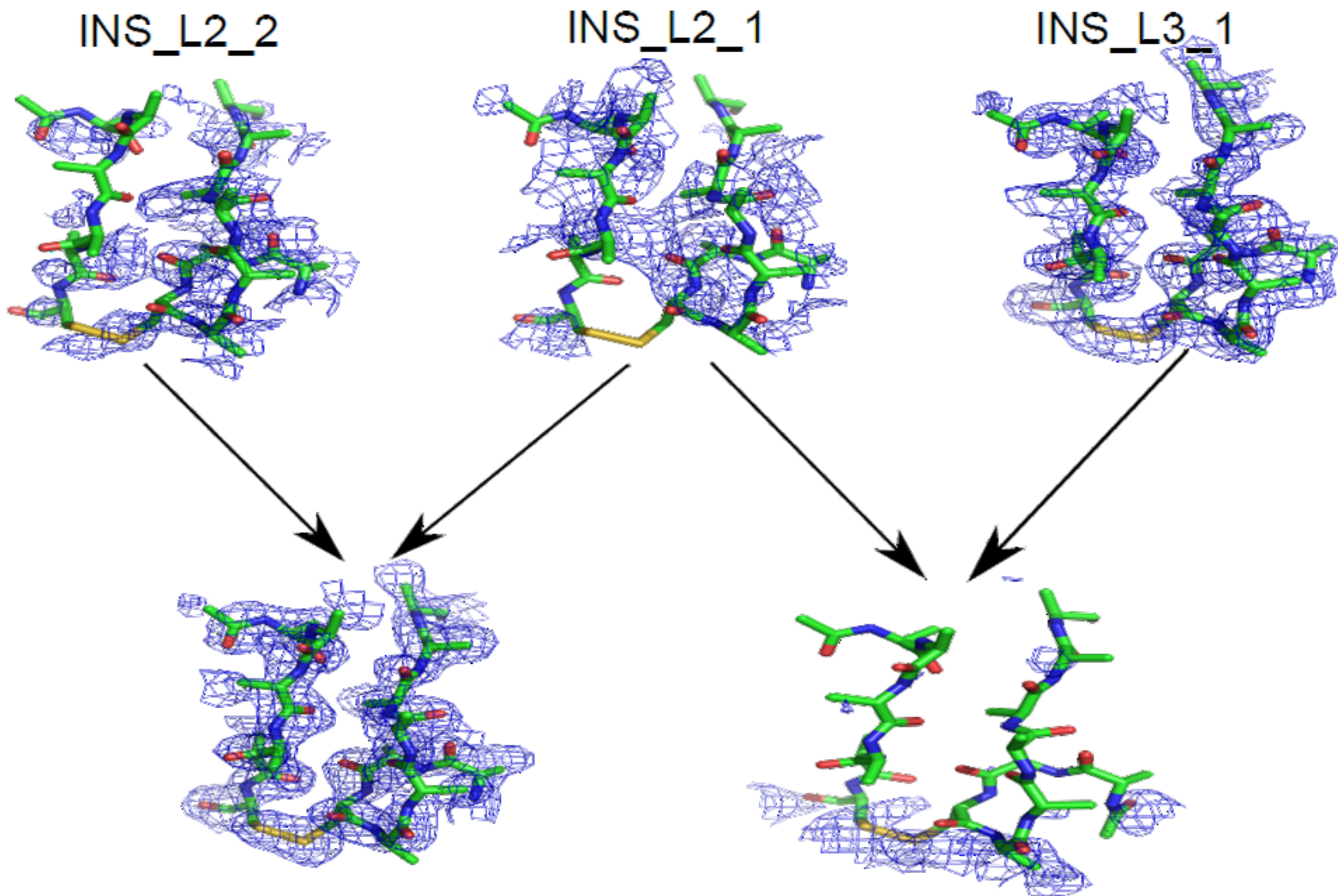


EDNA



... and many others

Hierarchical cluster analysis (hca)



MASSIF – SOFTWARE

login

define BL/date HDD

start backup

ESRF MX Data Backup

Please log in:

Username: opid30 Password: ***** Login

Source Directory (opid30)

Update

/usr/share

Get Size 2.3 GB Browse

Target Directory

Update Unmount

FAT: /media/DaveDisk (free: 24 GB of 466 GB)

/media/DaveDisk/ESRF_opid30/

Get Size 161 MB Browse

```
Running "du -hs --apparent-size /media/DaveDisk/ESRF_opid30/" ...
Figured out du PID: 5198
Running "du -hs --apparent-size /usr/share" ...
Figured out du PID: 5210

Running this rsync command:
rsync -rtx --modify-window=1 --progress /usr/share /media/DaveDisk/ESRF_opid30/
Figured out rsync PID: 5222
```

share/anthy/dic/udict
share/anthy/dic/utf8.t
share/anthy/dic/zipcode.t
share/app-install/
share/app-install/desktop/2ds1andemo.desktop
share/app-install/desktop/3dchess.desktop
share/app-install/desktop/AClock.desktop
share/app-install/desktop/AcetoneISO.desktop
share/app-install/desktop/Balder2D.desktop

31%

Automatically restart synchronisation

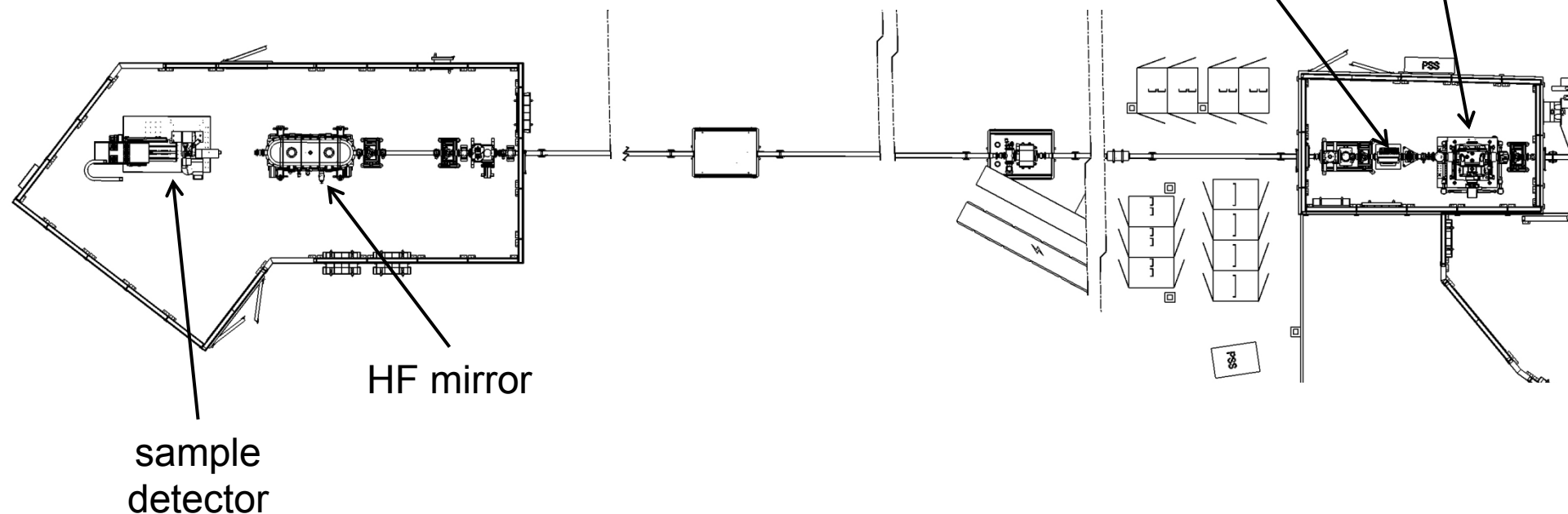
Run Rsync Stop Rsync Clear Log About Exit

ID30B

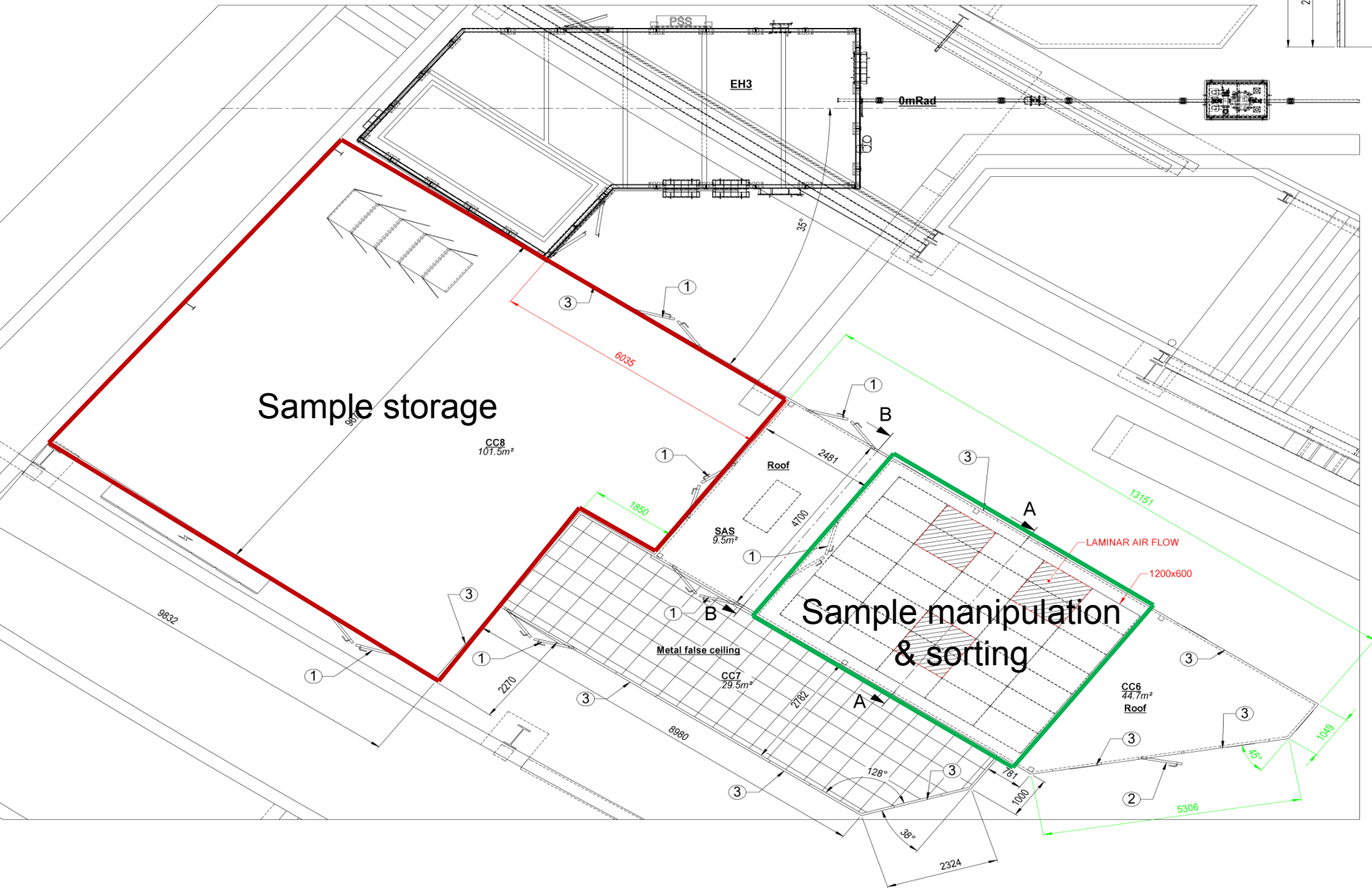
MAD
 variable beam size
 Pilatus3 6M detector
 cryogenic & RT
 in-plate measurements

Si(111)
 monochromator

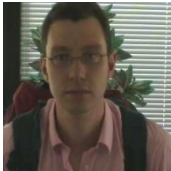
CRLs
 vertical



from beg. 2015



THANKS



+ software developers

+ support groups

+ users

The European Synchrotron

